

*Proceedings of the
Conference on Numerical
Methods in High Temperature Physics*

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CONTENTS

Numerical Methods in High Temperature Physics	vii
Forward	
R. Dautray	viii
Abstract	1
The Generalized Riemann's Problem	
A. Bourgade	2
A Fast High Precision Rezoning Algorithm	
B. Meltz	13
T. V. D. Schemes for Lagrangian Hydrodynamics	
J. C. Desgraz	24
A Fast Smooth Particle Hydrodynamics Code	
W. Benz	37
A Smoothed Particle Code for 2D Compressible Multifluid Flows	
F. Bailly and J. Ovardia	50
Multigroup Direct Methods for Solving Radiative Transfer Equations	
R. Sentis	62
Sodium Vapor Lamp: Diffusion Plus Transport	
G. H. Nickel and R. W. Whitaker	73
Boltzman-Folker-Planck Calculations Using Standard Discrete-Ordinates Codes	
J. E. Morel	96
Physico-Numerical Treatment of Large Angle Scattering During Alpha Particle Slowing Down	
J. P. Morreeuw	112
Numerical Treatment of the Transport of Fast Charged Particles in a Spherical Plasma	
G. Malinie, D. Verwaerde, M. Cardot, and J. Serviere	123
Vector and Parallel Computation in Production Codes	
G. Meurant and M. Patron	134
A Deterministic Method for Convection Diffusion Equation	
F. Hermeline and D. Besnard	142
A Molecular Dynamics Simulation of the Two-Dimensional Ion-Electron Plasma in the Strong Coupling Regime	
J. Clerouin and J. P. Hansen	153

Relativistic Hydrodynamics and Heavy Ion Reactions	
D. Strottman	165
Matter Ejection and Gas Interaction Physical and Computational Models	
G. Guri and V. Frachet	173
A Personal View on Homogenization	
L. Tartar	185
Turbulence Theory for Material Mixtures	
D. C. Besnard	196
Second Order Scheme for Reacting Flows: Application to Detonation	
A. Bourgeade	212
GAIA: A 2-D Curvilinear Moving Grid Hydrodynamic Code	
H. Jourden	224
Front Tracking for a Two-Dimensional Detonation Front	
A. Bourgeade	238
New Modellings of Material Behavior in the Eulerian Hydrodynamics Code CEE	
E. Bottet and D. Pirotais	251
Adaptive Mesh Experiments in 1D Hydrodynamics	
B. Meltz	263
A Quadratic Analysis of Linear Transport Equations	
D. Verwaerde	279
Use of the Chebyshev-Legendre Quadrature Set in Discrete-Ordinate Codes	
W. F. Walters	292
Long Distance Propagation with DFE: A Discontinuous Finite Element Scheme	
P. Daronian	302
Comparison of Two Models of Rayleigh-Taylor Induced Turbulent Mixing	
D. Besnard et. al.	308
An Alternative Solution to the Numerical Modeling of Mixing by Rayleigh-Taylor Instability	
C. Bianchi, S. Paul., and C. Fauquembergue	319

Numerical Methods in High Temperature Physics

A conference was held at Los Alamos National Laboratory, February 2-6, 1987 which dealt with techniques in modeling and numerically solving problems in the high temperature regime. This meeting brought together researchers from the Commissariat a L'Energie Atomique (CEA) and Los Alamos National Laboratory to present mathematical and numerical methods that have been recently developed to treat these problems. The focus of the papers presented is on the two- and three-dimensional hydrodynamics treatment of flow in the high temperature regime (>1 ev). The papers present the hydrodynamics numerical methods that have been successful for an accurate treatment along with methods for treating such effects as turbulence and other hydrodynamic instabilities. When the temperature becomes high enough, thermal radiation in the fluids and charged particle effects become important. General methods for treating radiation and charged particle transport are included in this compendium as well as some detailed considerations associated with transport problems in general.

As a whole, this collection of papers gives a good summary on the approaches used in treating problems in the high temperature regime. This meeting also provided researchers an excellent opportunity to interact on the problems of interest and gain new perspectives on the usefulness and applicability of their various methods and approaches.

The editors would like to thank the authors of the papers for their time and effort in presenting their work. We also acknowledge the efforts of the organizers of the conference from the CEA: B. Mercier, P. Boue, and D. Verwaerde. And finally we gratefully acknowledge the support, contributions, and encouragement of the Scientific Advisor for the CEA, R. Dautray, and of R. Thorn and R. Selden from Los Alamos.

05,27,1988

LANL/CEA MEETING ON "COMPUTATIONAL METHODS IN
HIGH TEMPERATURE PHYSICS" (February 1987)

FOREWORD by Robert DAUTRAY

The study of hydrodynamic flows at high temperature reaches now a level of great fruitfulness. It is a vast field covering not only the regular flows of only one fluid phase, but also the flows of several phases, and specially diphasic ones. The kind of distribution of the matter in each of these phases is still not well known, and the same for his evolution and influence on the phenomena occuring inside the matter.

We are just starting to understand the instability of these flows, their evolution towards turbulence and the description of this turbulence. For this purpose, we need a 3D modelization : this task is opening to us.

In these flows of matter described by non linear equations, discontinuity of speed and pression (shocks), appear and evolve in a way just empirically explored in the plain 3D world as it is the rule in such non linear phenomena.

All along these processes, the numerical tools and the experiments are on their way each separated, with their own constraints, the confrontation between them beeing often difficult. All this prescribe to the scientists to get out of their habits and to face other ways of thinking and exploring. I consider this book as a good contribution in this direction.

Proceedings of the Conference on Numerical Methods in High Temperature Physics

**Held at the Los Alamos National Laboratory
Feb 2-6, 1987**

Abstract

These proceedings contain full papers presented at the Los Alamos Conference on High Temperature Physics. This conference discussed many aspects of high temperature physics including hydrodynamics, radiation and particle transport and some computational issues important for efficient calculations. The meeting was held between researchers from Los Alamos and the French Commissariat a L'Energy Atomique (CEA).

THE GENERALIZED RIEMANN'S PROBLEM.

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RESUME : Cet article montre comment le problème de Riemann généralisé peut être résolu dans le cas des écoulements réactifs.

ABSTRACT

We study the flow resulting from a discontinuity line between two fluids. Those two fluids are, at the initial time, in two different and non necessarily constant states. The first two terms of an asymptotic expansion for this flow are derived as solutions of ordinary differential equations.

Those terms are obtained not only in planar, cylindrical or spherical symmetry, but also for inert or reacting fluids. The expansion is introduced in a second order Godunov type scheme that gives very nice results.

I - INTRODUCTION

In the last paper of the series "Towards the Ultimate Conservative Scheme" [1] Bram Van Leer introduced characteristic equations for discontinuous flow and used them in order to compute the evolution in time of a discontinuity line between two non constant states. Such a flow will be called in the following "generalized Riemann's problem" (G.R.P) in order to differentiate it from the classical Riemann's problem where the states on each side of the discontinuity line are constant.

Those equations were given without any proof or explanation. Since, M. Ben Artzi and J. Falcovitz have shown in their papers [2, 3 and 4] how to get other equations, which in certain cases give back those of B. Van Leer. In a recent report [5] I obtained also these new equations with the use of another method.

Although the system of equations governing reacting flows is no longer strictly hyperbolic, the preceding method can still be used. And this paper will show how to solve the GRP in the case of reacting fluids.

The resulting scheme as well as further details will appear in my next paper [7].

II - EQUATIONS

1. Problem to solve

At the initial time two fluids are in contact. The surface which separates them is, a plane, a cylinder, a sphere or a section of duct. If at that time the two fluids were at constant states, we would have to solve classical Riemann's problem [6]. Actually we want to consider fluids whose state varies in fonction of the position of the considered point, and we want to know how the resulting flow around the contact discontinuity will differ from the solution of the R.P.

The equation verified by the flow are, of course, the Euler's equations combined with the reaction rate equation :

$$\begin{aligned} (1) \quad & \frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial r} + \rho \frac{\partial v}{\partial r} + \chi \rho v = 0, \\ (2) \quad & \frac{\partial v}{\partial t} + v \frac{\partial v}{\partial r} + \frac{1}{\rho} \frac{\partial P}{\partial r} = 0, \\ (3) \quad & \frac{\partial E}{\partial t} + v \frac{\partial E}{\partial r} + \frac{1}{\rho} \frac{\partial (Pv)}{\partial r} + \chi \frac{P}{\rho} v = 0, \\ (4) \quad & \frac{\partial \omega}{\partial t} + v \frac{\partial \omega}{\partial r} = f(P, \rho, \omega); \end{aligned}$$

with ρ : density
 v : velocity
 e : specific internal energy
 P : pressure
 E : specific total energy
 ω : concentration of reaction products
 χ : function of r depending on the geometry $(0, \frac{1}{r}, \frac{2}{r}, \frac{A'(r)}{A(r)})$

The equation of state is given by :

$$e = \frac{P - c^0 (\rho - \rho^0)}{(\gamma - 1) \rho} + (1 - \omega)q$$

where γ, c^0, ρ^0 are functions of ω . We can notice that if c^0 is zero we get the equation of state of a polytropic gas. In the following P^0 will denote $\rho^0 \frac{c^0}{\gamma}$

In each domain where the flow is smooth equation (3) can be replaced by

$$(3 \text{ bis}) \quad \frac{\partial s}{\partial t} + v \frac{\partial s}{\partial r} = f\left(\frac{\partial s}{\partial \omega}\right)_{e, \rho} = k,$$

where s is given by : $s = \frac{P + P^0}{\rho^\gamma}$

For ω fixed s is an increasing function of the entropy.

The system of equations 1, 2, 3bis and 4 can be written.

$$(5) \quad \frac{\partial U}{\partial t} + B(U) \frac{\partial U}{\partial r} + G(U) = 0 ;$$

$$\text{with } U = \begin{pmatrix} \rho \\ v \\ s \\ \omega \end{pmatrix}, \quad B(U) = \begin{pmatrix} v & \rho & 0 & 0 \\ \gamma \frac{P+P^0}{\rho^2} & v & \rho^{\gamma-1} & \frac{1}{\rho} \left(\frac{\partial P}{\partial \omega} \right) \\ 0 & 0 & v & 0 \\ 0 & 0 & 0 & v \end{pmatrix} \text{ and } G(U) = \begin{pmatrix} \chi \rho v \\ 0 \\ -k \\ -f \end{pmatrix}.$$

$B(U)$ is diagonalizable with the eigenvalues

$$\lambda_1 = v - c, \quad \lambda_2 = \lambda_3 = v, \quad \lambda_4 = v + c ; \text{ where } c^2 = \gamma \frac{P + P^0}{\rho}$$

The eigenvectors are :

$$R_1 = \begin{pmatrix} \rho \\ -c \\ 0 \\ 0 \end{pmatrix}, \quad R_2 = \begin{pmatrix} -\eta \rho \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad R_3 = \begin{pmatrix} -\theta \rho \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad R_4 = \begin{pmatrix} \rho \\ c \\ 0 \\ 0 \end{pmatrix}$$

$$\text{with } \eta = \frac{1}{\gamma s} \text{ and } \theta = \frac{\left(\frac{\partial P}{\partial \omega} \right)_{s, \rho}}{\rho c^2}.$$

Whith our equation of state

$$\theta = \frac{\dot{\gamma}}{\gamma} \log \rho - \frac{\dot{p}}{\rho c^2} \frac{0}{}, \text{ where } \dot{\psi} = \frac{\partial \psi}{\partial \omega}.$$

On each side of the contact discontinuity, the initial state is given by U_+ , state on the right, and U_- , state on the left, as well as by the space derivatives $\frac{\partial U_+}{\partial r}$ and $\frac{\partial U_-}{\partial r}$.

Let U_0 be the solution of the Riemann's problem with U_- and U_+ as initial data (here $f = \chi = 0$). If r_0 denotes the position of the discontinuity at the initial time, U_0 is a function of $\frac{x}{t} = \frac{r - r_0}{t}$ [6]. By analogy we are looking for a solution

$$U(x, t) = U_0 \left(\frac{x}{t} \right) + t U_1 \left(\frac{x}{t} \right) + O(t^2),$$

for t small.

Moreover, in each domain where the flow is smooth, in order to take the characteristic directions into account, $\alpha_1, \alpha_2, \alpha_3$ and α_4 are defined by :

$$U_1 \left(\frac{x}{t} \right) = \alpha_1 \left(\frac{x}{t} \right) R_1 \left(\frac{x}{t} \right) + \alpha_2 \left(\frac{x}{t} \right) R_2 \left(\frac{x}{t} \right) + \alpha_3 \left(\frac{x}{t} \right) + \alpha_4 \left(\frac{x}{t} \right) R_4 \left(\frac{x}{t} \right).$$

Here and in the following $R_1(\frac{x}{t})$, $R_2(\frac{x}{t})$, $R_3(\frac{x}{t})$ and $R_4(\frac{x}{t})$ denote the eigenvectors of $B(U_0)$.

2. The equations for $(\alpha_1, \alpha_2, \alpha_3, \alpha_4)$

In the half plane $(x, t; t \geq 0)$ the solution U_0 determines two kinds of domains : domains where U_0 is constant and domains where U_0 is a rarefaction wave [6].

a) U_0 is constant

In such a domain R_1, R_2, R_3, R_4 are constant too, such that if $\xi = \frac{x}{t}$, and since

$$U = U_0 + t \sum_i \alpha_i(\xi) R_i + O(t^2)$$

$$\text{we get : } \frac{\partial U}{\partial t} = \sum_i (\alpha_i(\xi) - \xi \alpha'_i(\xi)) R_i + O(t)$$

$$\text{and } \frac{\partial U}{\partial x} = \sum_i \alpha'_i(\xi) R_i + O(t)$$

Moreover

$$B(U) = B(U_0) + O(t) \quad \text{and} \quad G(U) = G(U_0) + O(t)$$

and the system (5) can be written :

$$\sum_{i=1}^4 (\alpha_i(\xi) - \xi \alpha'_i(\xi)) R_i + B(U_0) \left(\sum_{i=1}^4 \alpha'_i(\xi) R_i \right) + G(U_0) + O(t) = 0.$$

Thus, since the R_i 's are the eigenvectors of $B(U_0)$ the α_i 's verify

$$(A) \quad (\lambda_i - \xi) \alpha'_i + \alpha_i + g_i = 0 \quad i = 1, 4.$$

$$\text{with } g_2 = -k, \quad g_3 = -f, \quad g_1 = g_4 = \frac{1}{2} (\chi v_0 + \eta g_2 + \theta g_3).$$

Notice that here $k = k(P_0, \rho_0, \omega_0)$

b) U_0 is a 1-rarefaction wave

In such a domain we have [6]

$$U_0(\xi) = \frac{\rho_-}{\gamma+1} \left(\frac{\gamma-1}{\gamma+1} \frac{v_-}{c_-} + \frac{2}{\gamma+1} - \frac{\gamma-1}{\gamma+1} \frac{\xi_-}{c_-} \right) \frac{2}{\gamma-1}$$

$$U_0(\xi) = \frac{2}{\gamma+1} \xi + \frac{\gamma-1}{\gamma+1} \left(v_- + \frac{2 c_-}{\gamma-1} \right)$$

s_-
 ω_-

such that $U_0'(\xi) = -\frac{2}{(\gamma+1)c} R_1$ with $c = \frac{\gamma-1}{\gamma+1} (v_- + \frac{2 c_-}{\gamma-1} - \xi)$ and

$\frac{\partial U_0}{\partial R} = \frac{1}{r} U_0'(\xi)$ is non zero such that in order to get the terms of order -1 and 0 in t for $B(U)$ $\frac{\partial U}{\partial R}$ we need the term of order 1 in t for $B(U)$:

$$B(U) = B_0(\xi) + t B_1(\xi) + O(t^2).$$

We have

$$B_0 = B(U_0)$$

$$\text{and } B_1 = \begin{pmatrix} \frac{c^2}{\rho} \left(\frac{2c_1}{c} - \frac{\rho_1}{\rho} \right) \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} \rho_1 & 0 & 0 \\ v_1 & - & - \\ 0 & v_1 & 0 \\ 0 & 0 & v_1 \end{pmatrix}$$

with, by definition of the α_i 's,

$$\rho_1 = \rho (\alpha_1 - \eta \alpha_2 - \theta \alpha_3 + \alpha_4)$$

$$v_1 = -c (\alpha_1 - \alpha_4)$$

$$c_1 = \frac{c}{2} ((\gamma-1) \alpha_1 + \eta \alpha_2 + (v + \theta) \alpha_3 + (\gamma-1) \alpha_4)$$

$$\text{where } v = \frac{\dot{\gamma}}{\gamma} + \frac{\dot{p}^0}{p + p^0} = -\frac{(\gamma+1)c}{2} \theta'.$$

Moreover the R_i 's are non constant functions of ξ which verify

$$R_1' = -\frac{1}{2c} R_1 + \frac{\gamma-3}{2(\gamma+1)c} R_4,$$

$$R_2' = \frac{\eta}{(\gamma+1)c} (R_1 + R_4),$$

$$R_3' = \frac{\theta + v}{(\gamma+1)c} (R_1 + R_4),$$

$$R_4' = \frac{\gamma-3}{2(\gamma+1)c} R_1 - \frac{1}{2c} R_4,$$

Since U_0 and U_1 are functions of ξ , we have the relations

$$\frac{\partial U_0}{\partial t} = -\frac{\xi}{t} U_0, \quad \frac{\partial U_0}{\partial t} = \frac{1}{t} U_0, \quad \frac{\partial U_1}{\partial t} = \frac{\xi}{t} U_1' \quad \text{and} \quad \frac{\partial U_1}{\partial t} = \frac{1}{t} U_1'$$

Thus the equations (5) becomes :

$$-\frac{\xi}{t} U_0 + U_1 - \xi U_1' + \frac{1}{t} B_0 U_0 + B_0 U_1' + B_1 U_0 + G(U_0) + O(\tau) = 0.$$

Considering only the terms in $\frac{1}{t}$ we get : $-\xi U_0 + B_0 U_1' = 0$,
which is verified by definition of U_0 .

For the terms of order 0 in t we get the equation :

$$U_1 - \xi U_1' + B_0 U_1' + B_1 U_0 + G(U_0) = 0.$$

But we have also

$$U_1 = \sum_i \alpha_i R_i, \quad U_1' = \sum_i \alpha_i' R_i + \sum_i \alpha_i R_i' \quad \text{and}$$

$$B_1 U_0 = (\alpha_1 + \frac{\eta}{\gamma+1} \alpha_2 + \frac{\theta + \nu}{\gamma+1} \alpha_3 + \frac{\gamma-3}{\gamma+1} \alpha_4) R_1 + (\frac{3-\gamma}{\gamma+1} \alpha_1 - \frac{3\eta}{\gamma+1} \alpha_2 - \frac{\nu+3\theta}{\gamma+1} \alpha_3 + \frac{3-\gamma}{\gamma+1} \alpha_4) R_4$$

Thus if we project the equation above for U_1 on each R_i , we get the system

$$2\alpha_1 + \frac{\eta}{\gamma+1} \alpha_2 + \frac{\nu+\theta}{\gamma+1} \alpha_3 + \frac{\gamma-3}{\gamma+1} \alpha_4 + g_1 = 0$$

$$(B) \quad c\alpha_2' + \alpha_2 + g_2 = 0$$

$$c\alpha_3' + \alpha_3 + g_3 = 0$$

$$2c\alpha_4' + \frac{3-\gamma}{\gamma+1} \alpha_4 - \frac{\eta}{\gamma+1} \alpha_2 + \frac{\nu-\theta}{\gamma+1} \alpha_3 + g_4 = 0$$

In the case of 4- rarefaction wave, we just have to exchange α_1 and α_4 and to replace c by $-c$ such that the α_i 's are solution of

$$-2c\alpha_1' + \frac{3-\gamma}{\gamma+1} \alpha_1 - \frac{\eta}{\gamma+1} \alpha_2 - (\frac{\nu+\theta}{\gamma+1} - c\theta') \alpha_3 + g_1 = 0$$

$$-c\alpha_2' + \alpha_2 + g_2 = 0$$

$$-c\alpha_3' + \alpha_3 + g_3 = 0$$

$$2\alpha_4 + \frac{\eta}{\gamma+1} \alpha_2 + \frac{\nu+\theta}{\gamma+1} \alpha_3 + \frac{\gamma-3}{\gamma+1} \alpha_1 + g_4 = 0$$

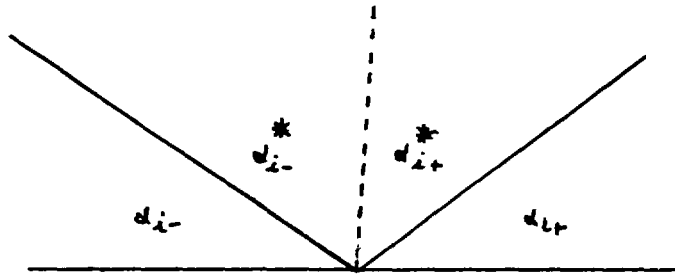
$$\text{with } g_1 = g_4 = \frac{1}{2} \left(\chi \left(\frac{2}{\gamma+1} \xi + \frac{\gamma-1}{\gamma+1} (\nu - \frac{2}{\gamma-1} c_+) \right) + \eta g_2 + \theta g_3 \right)$$

$$g_2 = -k(P_0(\xi), \rho_0(\xi), \omega_0)$$

$$g_3 = -f(P_0(\xi), \rho_0(\xi), \omega_0)$$

III - SOLUTION

In order to find the solution, we need to solve the systems above in each of the domains defined by U_0 . The boundary conditions defined on each discontinuity line by the jump conditions, allow then to compute the α_i 's in all the half plane $(x, t ; t > 0)$



a) Solution for the systems

The system A is easy to integrate since here the λ_i 's are constants as well as the g_i 's. The solution is given by

$$\alpha_i = K_i (\xi - \lambda_i) - g_i, \quad i = 1, 4$$

The K_i 's are four constants determined by the boundary conditions.

The system B is more complex but still integrable by noticing that c is an affine function of ξ and taking c as new variable. We get then, in addition to the relation between α_1 and α_2 , α_3 and α_4 ,

$$\alpha_1 = \frac{-\eta}{2(\gamma+1)} \alpha_2 - \frac{\nu+\theta}{2(\gamma+1)} \alpha_3 - \frac{\gamma-3}{2(\gamma+1)} \alpha_4 - \frac{1}{2} g_1 ;$$

$$\alpha_2 = L_2 c^{\frac{\gamma+1}{\gamma-1}} + G_2^2 ,$$

$$\alpha_3 = L_3 c^{\frac{\gamma+1}{\gamma-1}} + G_3^3 ,$$

$$\alpha_4 = L_4 c^{\frac{3-\gamma}{2(\gamma-1)}} - \frac{L_2 \eta}{3 \gamma - 1} c^{\frac{\gamma+1}{\gamma-1}} - \frac{L_3 c^{\frac{\gamma+1}{\gamma-1}}}{3 \gamma - 1} \left(\frac{\dot{\gamma}}{\gamma} (\log \rho - \frac{3(\gamma+1)}{(3\gamma-1)}) - (3 \gamma - 1) \frac{\dot{p}^0}{\rho c^2} \right) ;$$

$$+ G_2^4 + G_3^4 + G_4^4$$

where G_2^2 is a special solution of $c \alpha_2' + \alpha_2 + g_2 = 0$

G_3^3 is a special solution of $c \alpha_3' + \alpha_3 + g_3 = 0$

G_2^4 is a special solution of $2c \alpha_4' + \frac{3-\gamma}{\gamma+1} \alpha_4 - \frac{\eta}{\gamma+1} G_2^2 = 0$

G_3^4 is a special solution of $2c \alpha_4' + \frac{3-\gamma}{\gamma+1} \alpha_4 - (\frac{\theta}{\gamma+1} + \frac{c\theta'}{2}) G_3^3 = 0$

G_4^4 is a special solution of $2c \alpha_4' + \frac{3-\gamma}{\gamma+1} \alpha_4 + g_4 = 0$

The last equation has been integrated using the solution of the two other equations. The constants L_i are determined by the boundary conditions.

The case of system (C) is identical.

b) Boundary condition

There are four kinds of boundary conditions :

- Initial data
- Characteristic lines between rarefaction zone and constant zone
- Contact discontinuity
- Shocks

Let us consider first the initial data on the half line ($k = 0 ; x < 0$). It is one boundary of the domain where U_0 is constant and equal to U_- . In this domain

$$\alpha_i = K_{i-} (\xi - \lambda_{i-}) - g_i ; \quad i = 1, 4.$$

If we let t go to zero in the equation

$$U = U_0 + t (\alpha_1 (\xi) R_{1-} + \alpha_2 (\xi) R_{2-} + \alpha_3 (\xi) R_{3-} + \alpha_4 (\xi) R_{4-}) + O(t^2)$$

we get, since $\xi = \frac{x}{t} = \frac{r - r_0}{t}$,

$$U = U_- + x \sum K_{i-} R_i = U_- + x \left(\frac{\partial U}{\partial r} \right)_- \text{ for } r = 0 \text{ and } x < 0.$$

Thus, by definition of the R_1 's.

$$\left(\frac{\partial \rho}{\partial r}\right)_- = K_{1-} - \eta_- K_{2-} - \theta_- K_{3-} + K_{4-}$$

$$\left(\frac{\partial v}{\partial r}\right)_- = c_- (-K_{1-} + K_{4-})$$

$$\left(\frac{\partial s}{\partial r}\right)_- = K_{2-}$$

$$\text{or } K_{1-} = \frac{1}{2c_-^2} \left(\left(\frac{\partial P}{\partial r}\right)_- - \rho_- c_- \left(\frac{\partial v}{\partial r}\right)_- \right)$$

$$K_{2-} = \left(\frac{\partial s}{\partial r}\right)_- = \frac{+1}{\rho_- \eta_-} \left(\frac{1}{c_-^2} \left(\frac{\partial P}{\partial r}\right)_- - \left(\frac{\partial \rho}{\partial r}\right)_- - \rho_- \theta_- \left(\frac{\partial \omega}{\partial r}\right)_- \right)$$

$$K_{3-} = \left(\frac{\partial \omega}{\partial r}\right)_-$$

$$K_{4-} = \frac{1}{2c_-^2} \left(\left(\frac{\partial P}{\partial r}\right)_- + \rho_- c_- \left(\frac{\partial v}{\partial r}\right)_- \right)$$

The results are the same for the right initial data ; we get then

$$\alpha_{1+} = K_{1+} (\xi - \lambda_{1+}) - g_{1+} \text{ with :}$$

$$K_{1+} = \frac{1}{2c_+^2} \left(\left(\frac{\partial P}{\partial r}\right)_+ + \rho_+ c_+ \left(\frac{\partial v}{\partial r}\right)_+ \right),$$

$$K_{2+} = \left(\frac{\partial s}{\partial r}\right)_+ = \frac{1}{\rho_+ \eta_+} \left(\frac{1}{c_+^2} \left(\frac{\partial P}{\partial r}\right)_+ - \left(\frac{\partial \rho}{\partial r}\right)_+ - \rho_+ \theta_+ \left(\frac{\partial \omega}{\partial r}\right)_+ \right),$$

$$K_{3+} = \left(\frac{\partial \omega}{\partial r}\right)_+,$$

$$K_{4+} = \frac{1}{2c_+^2} \left(\left(\frac{\partial P}{\partial r}\right)_+ + \rho_+ c_+ \left(\frac{\partial v}{\partial r}\right)_+ \right).$$

On the boundaries between a constant domain and 1- rarefaction wave, α_2 , α_3 and α_4 are continuous ; while for 4- rarefaction wave α_1 , α_2 and α_3 are continuous.

On the contact discontinuity, the continuity of P and v implies the continuity of P_1 and v_1 with

$$v_1 = c (\alpha_4 - \alpha_1) \text{ and } P_1 = \rho c^2 (\alpha_1 + \alpha_4)$$

For a shock the conditions are not so easy to get and in order to simplify it is useful to start with the right shock relations. Indeed most relations make use of the speed of the shock

$$\sigma = \sigma_0 + t \sigma_1 + O(t^2)$$

while σ_1 is useful not for computing $\alpha_1, \alpha_2, \alpha_3$ or α_4 but for getting the right position of the shock. We thus have to consider only relations without σ . Let $(P^*, v^*, \rho_\epsilon^*, \omega^*)$ be the state behind the shock and $(P_\epsilon, v_\epsilon, \rho_\epsilon, \omega_\epsilon)$ be the state ahead. We consider thus a 4- shock for $\epsilon = 1$ and a 1- shock for $\epsilon = -1$.

The relations we want are the Hugoniot relation :

$$\rho_\epsilon^* (P_\epsilon + \mu^2 P^* + (1 + \mu^2) P^0) = \rho_\epsilon (P^* + \mu^2 P_\epsilon + (1 + \mu^2) P^0)$$

the relation giving v^* :

$$v^* = v_\epsilon + \epsilon (P^* - P_\epsilon) \sqrt{\frac{1 - \mu^2}{\rho_\epsilon (P^* + \mu^2 P_\epsilon + (1 + \mu^2) P^0)}}$$

and $\omega_\epsilon^* = \omega_\epsilon$.

The first two can be found in [6] the last is simply the Hugoniot condition for ω in lagrangian coordinates.

On the shock the $\alpha_{1\epsilon}$'s are known since the initial data give the $K_{1\epsilon}$'s. Then the equality of terms of order 1 in the relations above leads to three relations for the $\alpha_{1\epsilon}^*$'s. The last one, in order to determine the $\alpha_{1\epsilon}^*$'s is given by the boundary conditions on the contact discontinuity.

if we put

$$v_1 = -c (\alpha_1 - \alpha_4), P_1 = \rho c^2 (\alpha_1 + \alpha_4), \rho_1 = \rho (\alpha_1 - \eta \alpha_2 - \theta \alpha_3 + \alpha_4), \omega_1 = \alpha_3$$

the three relations are ($\dot{\psi} = \frac{\partial \psi}{\partial \omega}$)

$$\rho_{1\epsilon}^* (P_\epsilon + \mu^2 P^* + (1 + \mu^2) P^0) + P_{1\epsilon}^* (\mu^2 \rho_\epsilon^* - \rho_\epsilon^*) + \rho_\epsilon^* (2\mu \dot{\psi} (P^* + P^0) + (1 + \mu^2) \dot{P}^0) \omega_{1\epsilon} = \rho_{1\epsilon} (P^* + \mu^2 P_\epsilon + (1 + \mu^2) P^0) + P_{1\epsilon} (\mu^2 \rho_\epsilon - \rho_\epsilon^*) + \rho_\epsilon (2\mu \dot{\psi} (P^* + P^0) + (1 + \mu^2) \dot{P}^0) \omega_{1\epsilon},$$

$$v_1^* - \epsilon P_{1\epsilon}^* \left(\frac{1}{W_\epsilon} - \epsilon \frac{v^* - v_\epsilon}{2(P^* + \mu^2 P_\epsilon + (1 + \mu^2) P^0)} \right) = v_{1\epsilon} - \epsilon P_{1\epsilon} \left(\frac{1}{W_\epsilon} + \epsilon \mu^2 \frac{v^* - v_\epsilon}{2(P^* + \mu^2 P_\epsilon + (1 + \mu^2) P^0)} \right)$$

$$- \frac{v^* - v_\epsilon}{2 \rho_\epsilon} \rho_{1\epsilon} + \dot{W}_\epsilon \omega_{1\epsilon},$$

$$\omega_{1\epsilon}^* = \omega_{1\epsilon};$$

$$\text{with } W_\epsilon = \sqrt{\frac{\rho_\epsilon (P^* + \mu^2 P_\epsilon + (1 + \mu^2) P^0)}{1 - \mu^2}}$$

IV - CONCLUSION

The results above allow, as will be shown later [7], to extend Van Leer's scheme to reacting flows with very encouraging results.

Moreover they are a step towards a better understanding of the interaction of chemical reaction on hydrodynamics.

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A FAST HIGH PRECISION REZONING ALGORITHM

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ABSTRACT

In an adaptive mesh algorithm, as well as to maintain a proper mesh in a standard quadrilateral hydro code, it is necessary to have a rezoning algorithm. It should be as accurate as possible, in order to introduce the less possible diffusion, and fast, to be performed as often as needed.

The one we present, which makes use of the "lagrangian alternate direction" method, but not flux or operator splitting, reduces drastically the number of geometrical calculations (intersections of lines and areas of polygons), and transfers the rezoning work itself to a 1D algorithm, which can be made as fast and precise as needed.

The "lagrangian alternate direction" method consists in intersecting only the I-lines of the old mesh with the J-lines of the new one. This requires that both meshes be quadrilateral, logically similar with the same corners and, at last approximately, the same boundaries. It requires, further, that the lines, whose intersection is looked for, intersect only once. This is why, in lagrangian calculations, the rezoning should be performed before the mesh has become a complete mess. In contrast, the algorithm needs not both meshes to have the same number of cells in corresponding directions.

We present the method, with special emphasis on the treatment of node centered velocities, and a variety of examples : pure advection, static rezoning, hydro-calculations with automatic rezoning.

It is well known that a fluid dynamics calculation generally needs remapping to go to its end with a lagrangian hydrocode. Remapping, which is also an essential part of an adaptive mesh algorithm, is composed of 2 parts:

- define a new mesh, that we call remeshing,
- transfer physical quantities, as well as any other information, from the old mesh to the new one, that is generally called rezoning.

While the first part has been satisfactorily solved long time ago, the rezoning was, until recently, a cure worse than the disease : highly diffusive with 1st order method, non conservative with other types of interpolation.

Besides, with the leap-frog scheme, which is still commonly used, the node-centered velocities require a special treatment to approach conservation of both momentum and kinetic energy. Furthermore, the great number of geometrical calculations made the price nearly prohibitive. All these difficulties led to a very restricted use of remapping : as late as possible, and on the smallest possible region. This is contrary to the "proper" way to remap, which is : as soon as needed, and on the largest possible domain, to avoid possible difficulties when connecting remapped and non-remapped regions.

In the recent years, many authors ([D], [S], [Z]) successfully applied the advection feature of new hydro-schemes to the 2D rezoning problem of centred quantities, but the complexity question is still present.

The geometrical part of the rezone is very complex for at least 3 reasons :

- There are a great number of intersecting cells to compute.
- There are an even greater number of useless calculations to perform, to determine those intersections. The number of these extra calculations can be reduced, by a sweeping process along the grid-lines, as shown in [R], but this algorithm does not fit well with modern computers.
- The number of sides of the intersecting cells is arbitrary (ranging from 3 to 8), making almost impossible a fast computing of their volumes.

Requirements.

Generally speaking, lagrangian hydro-codes deal with quadrilateral cells, logically structured in rectangular domains containing one single material. Essentially 2 sorts of calculations need remapping :

- distortions of the mesh, arising from high deformations, shear flow, or from numerical instabilities.
- need to adapt the mesh to some particular feature (adaptive mesh technique).

In both cases, one single remap is not enough to drive the calculation to its end, emphasizing the constraints of cost and precision. In the case of adaptive mesh algorithm, because the feature tracked has no reason to be stationary. And in the distorted case, the instabilities will develop again as soon as the mesh is rearranged.

A new rezoning algorithm.

This algorithm rezones a physical domain onto it self. We suppose that both meshes are logically rectangular meshes, with the same corners and at least approximately the same boundaries, but possibly not the same number of cells in each direction.

Then we can represent both meshes overlapping on the same domain, and coinciding on the boundaries (fig 1).

Consider now the third mesh, that we call intermediate, with nodes at the intersection of the I -lines of one mesh with the J -lines of the other.

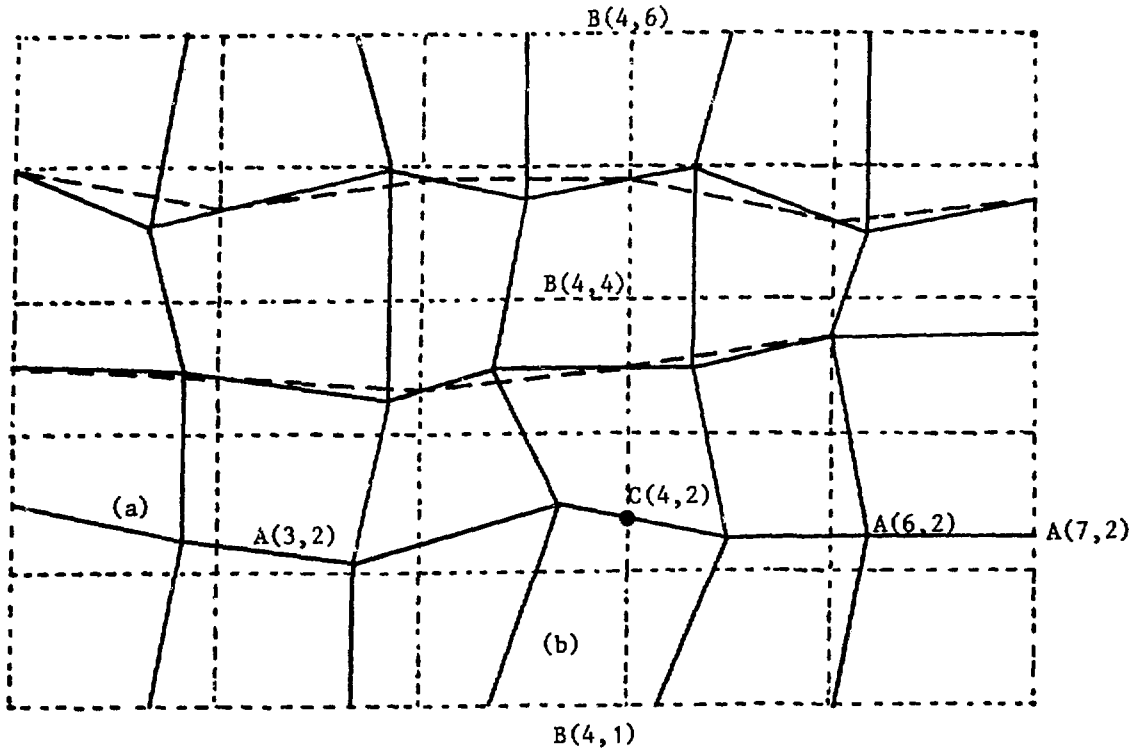


Fig. 1 .

The point $C(4,2)$ is at the intersection of the $(.,2)$ line of mesh A (a) and the $(4,.)$ line of mesh B (b). A row of cells of mesh A (full lines) is rezoned on a row of cells of mesh C (dashed lines). Then cells of mesh C are rezoned on mesh B (dotted lines).

We can see that this mesh has its rows of cells approximately coincident with the rows of the old mesh, and its columns approximately coincident with the columns of the new mesh. So we can remap the physical quantities from the old mesh to the intermediary, by rows, through a 1D algorithm, and then from the intermediary to the new mesh, by columns.

We can say that it is an alternate-direction approximate remapper.

This method has several decisive advantages :

- A drastic reduction of the number of calculations. Not all the intersections are calculated (12 out of 32 in fig.1), with few sweeping work.

- The volumes of the intersected cells are not calculated : only are those of the intermediate mesh, which makes about 4 times less. Furthermore, they all are quadrilateral, and properly set, computerwise speaking.

- The rezoning work itself is imparted to a 1-D algorithm, which can easily be constructed with all the desirable properties : high order of precision, conservativeness, capability to handle an arbitrary number of cells, and speed (ours is fully vectorised).

- The use of 1-D rezoning algorithms makes it possible to give to the node velocities a satisfactory treatment.

On the other hand, the method has 2 main drawbacks :

- The rezoning is performed on domains (rows of quadrilateral cells) which are not exactly equal, making corrections necessary, for conservativeness.

- For the same reason, positivity and monotony cannot be guaranteed.

About the "approximateness" of the method, it must be said that :

- Conservativity is not an incantation, some magic word that assures you are doing a good job. After all, the 1st order rezone is the only linear, conservative, monotonic scheme, and it is one of the worst.

- There are several ways to correct the 1-D rezoning to provide conservativity, while maintaining monotony, as far as possible.

- Effects of the failure of monotony have not yet been observed ; and, if any, they will certainly not be worse than the disturbance due to distorted mesh or to a poor precision rezone.

The benefits of the method are spectacular, in precision as well as in C.P.U. time : it runs at least 15 times faster than our previous 1st order algorithm.

The 1-D rezone algorithm used is a variant of PPM scheme of Colella and Woodward [C-W], which is 3rd order and able to handle arbitrary meshes staying monotonic. The difference with original scheme is that the interpolating function in each cell consists of 2 straight lines instead of a parabola (fig.2), providing a better approximation to shocks without being discontinuous.

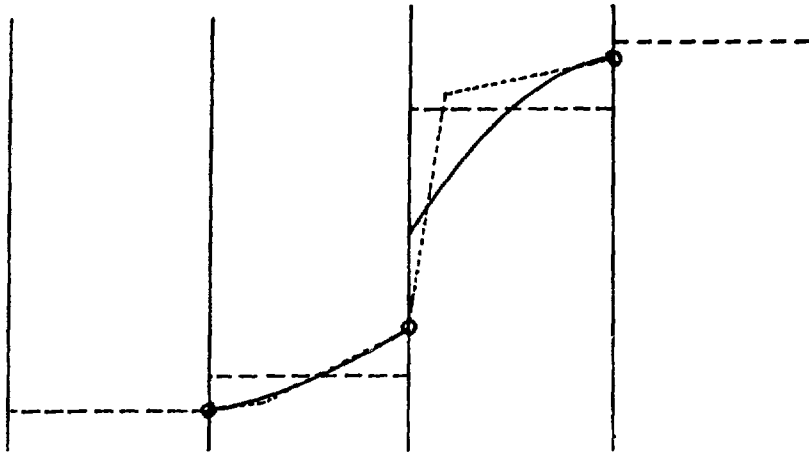


Fig.2

The use of 2 straight lines (dotted) in each cell gives steeper gradients than the original PPM parabola (full), while maintaining continuity with the interpolated values (cercles) at the zone edges.

Test problems.

First test case (fig.3), known as the 'key problem' was proposed by D.S.Bailey for the Asilomar Rezoning Workshop [W]. It consists of a key of density 1 moving in a density 0.01 background. The movement is such that every point describes a circle of radius equal to five cells. The initial and final density distribution are shown after one revolution, 157 iterations with Courant number 0.2 and rezoning after every time step, with the 1st, 2nd and 3rd version of the 1-D rezone algorithm. Also is shown a run with Courant number 1. (36 iterations) and 3rd order rezoning (fig.5).

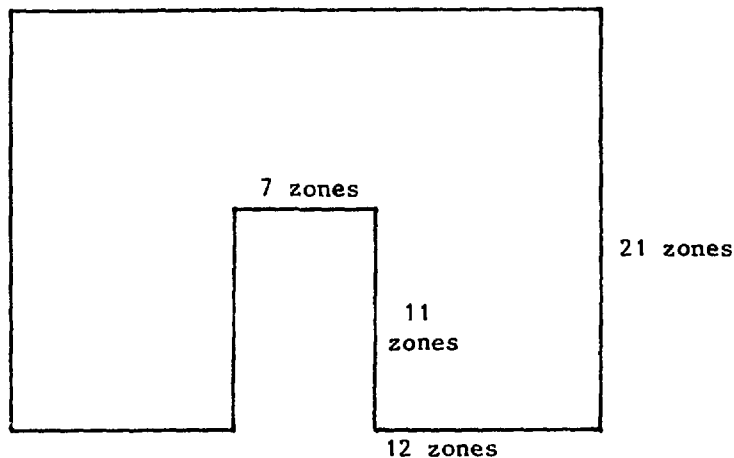


Fig.3

The "key problem". The movement is a "translation" along a circle of radius equal to five zones.

In order to show that the method has no spurious grid effect, we constructed an other advection test, where the phenomenon is not connected with the direction of the grid lines. It consists of a thick sphere of density .1 which is collapsed towards the center, each node having a centripete velocity with modulus equal to its radius (fig.4). 136 time steps, with Courant number .4 and rezoning after every time step, are needed to reach the final position. The final density profiles are shown (fig.6) with 1nd, 2nd and 3rd order rezoning. The results are summarized in the table below, showing that the gain between 2nd and 3rd order is greater in anisotropy (difference between biggest and smallest peak value) than in the peak value itself.

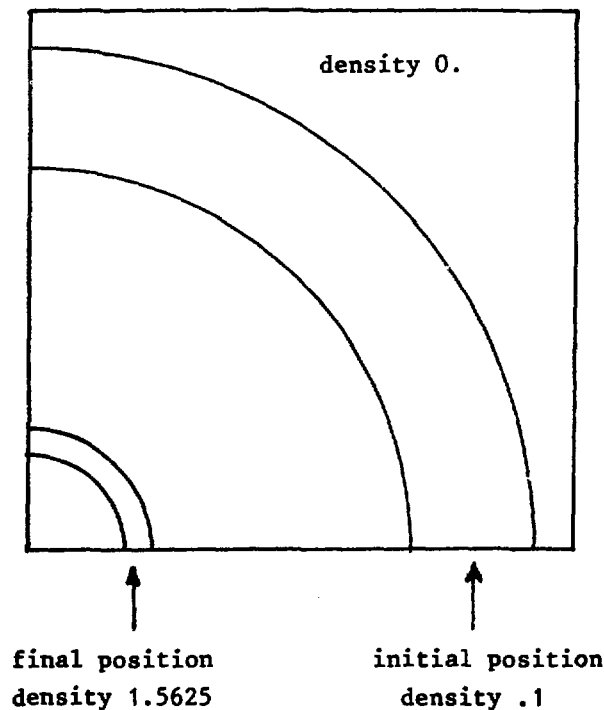


fig.4

Spherical advection on a rectangular 60 x 60 grid

order	1	2	3
peak value	.796 (51%)	1.371 (88%)	1.501 (96%)
anisotropy	9.9%	8.9%	2.6%

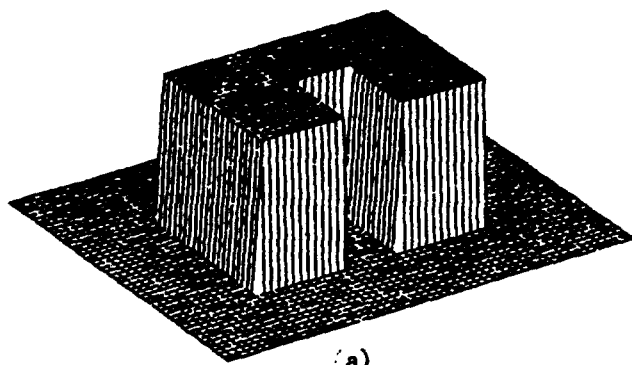
When remapping is used for cosmetics, as in standard lagrangian calculations, the way it is used is not irrelevant. Failure of hydro calculations with great deformations appears when transient phenomena, such as shocks, meet regions where the grid has previously been distorted by instabilities. So the proper way to remap is to do it as soon as instabilities develop, and to do it in the largest possible zone. Our remapping is governed by a set of criteria that detect the growing of classical instabilities, such as hourglasses and chevrons, together with distortions of the mesh due to the flow itself.

This is demonstrated in a 2D hydrodynamic test, consisting of a rectangular domain filled with perfect gas, of which 2 sides move at a prescribed velocity, inducing two shocks that have a complex interaction.

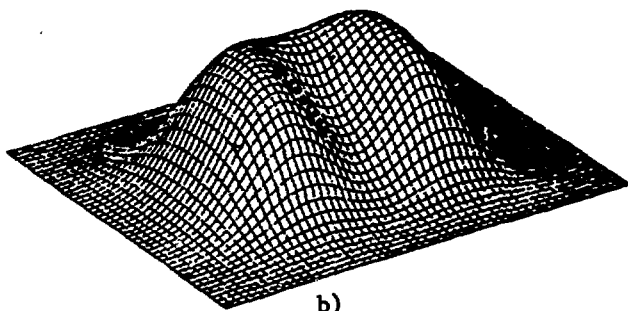
The non remapped run (fig.7) reaches the time of $8.E-4$ after 3859 time steps. The grid then is very distorted, making the continuation insignificant. On the other hand, the remapped run (fig.8) took 844 time steps, with 16 remappings. The density contours show that the remapping stabilize the flow without introducing any spurious effect.

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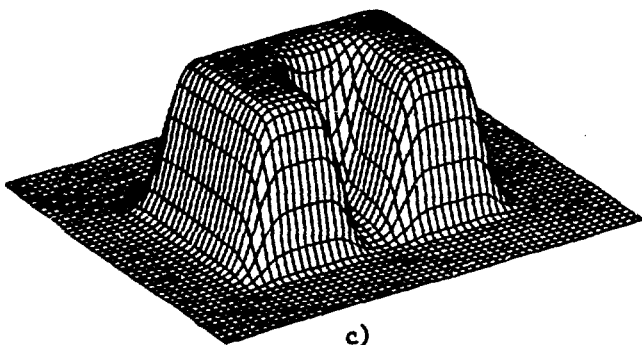
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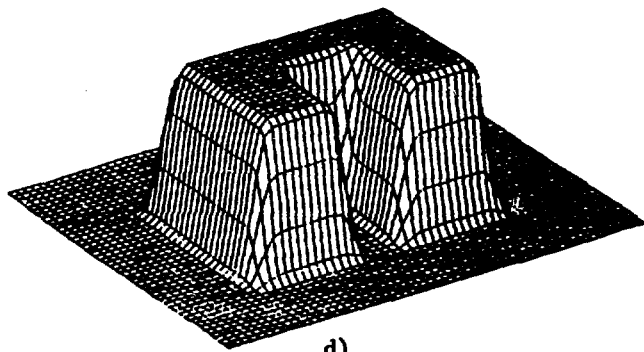
a)



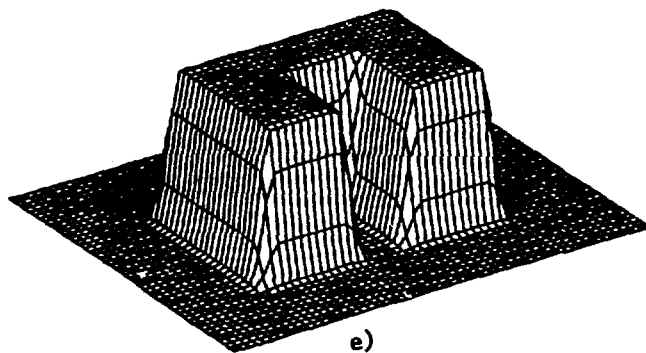
b)



c)



d)



e)

Fig. 5

a) Initial density distribution

b),c),d) Final density distribution after one revolution, 157 iterations and Courant number .2, with 1st (b), 2nd (c) and 3rd (c) order algorithm.

e) Same problem with Courant number 1. and 3rd order algorithm.

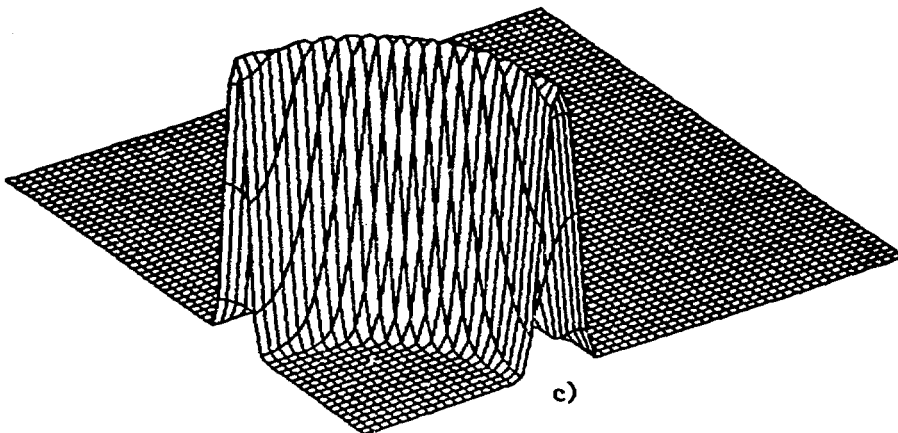
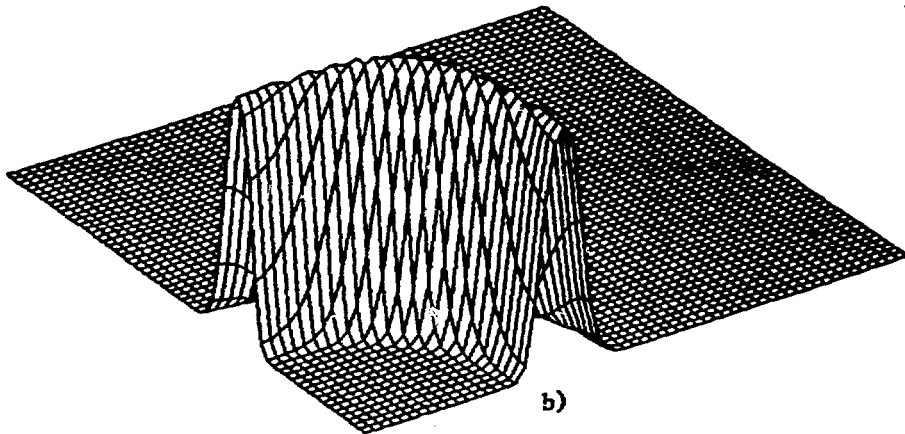
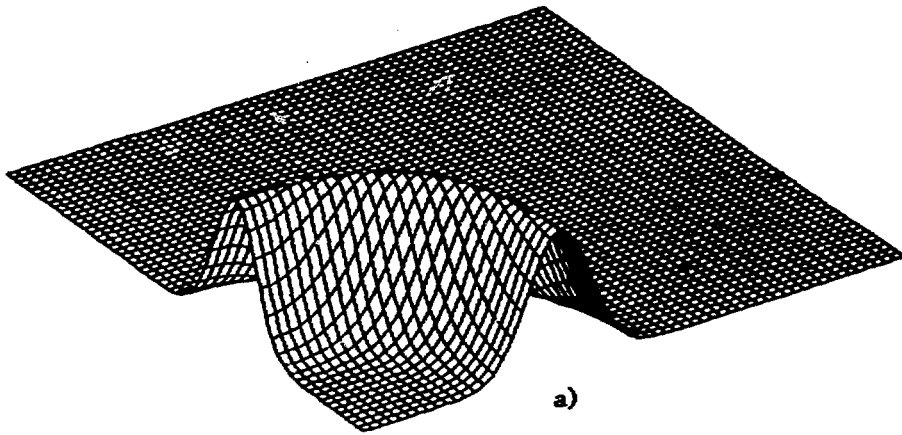


Fig. 6

Spherical advection test

Final density distribution with 1st (a), 2nd (b) and 3rd (c) order rezoning.

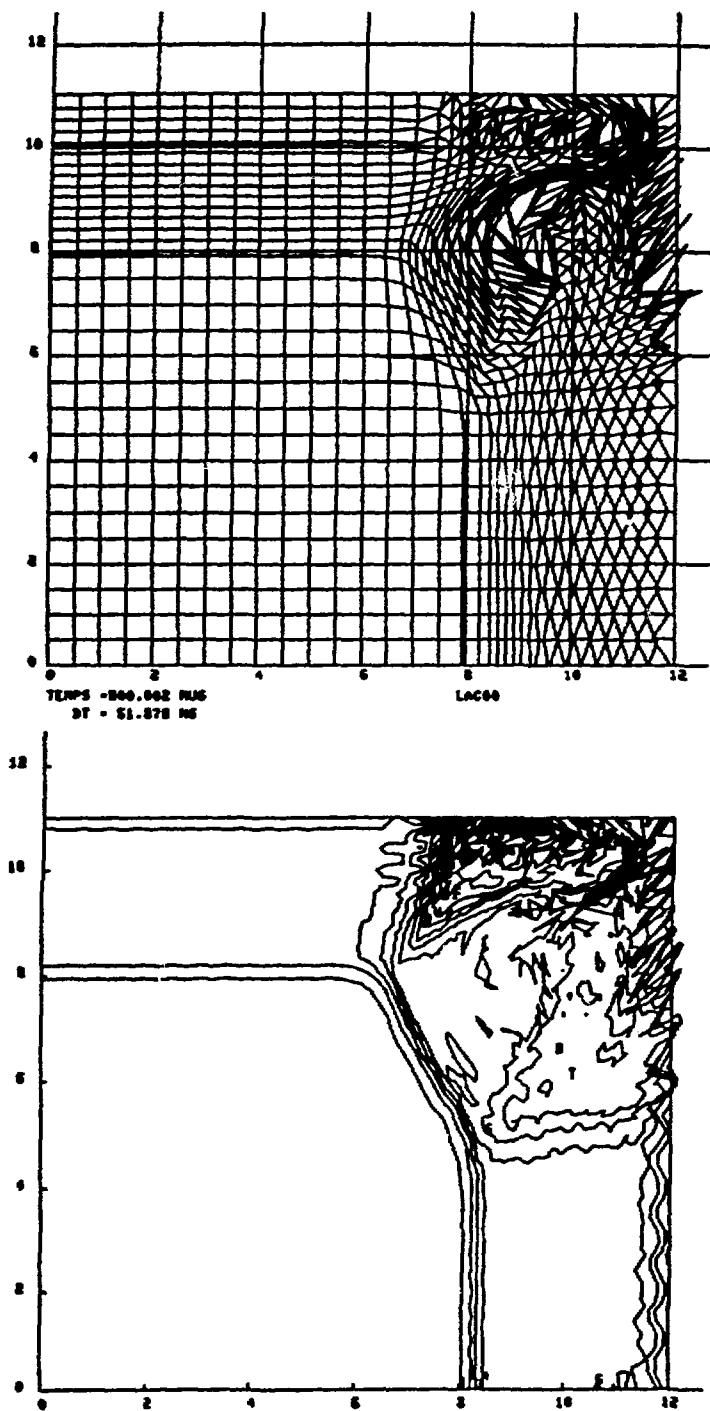


Fig. 7

2D hydro-test -Non remapped run- 3859. time steps.
 Grid (top) and density contours (bottom).

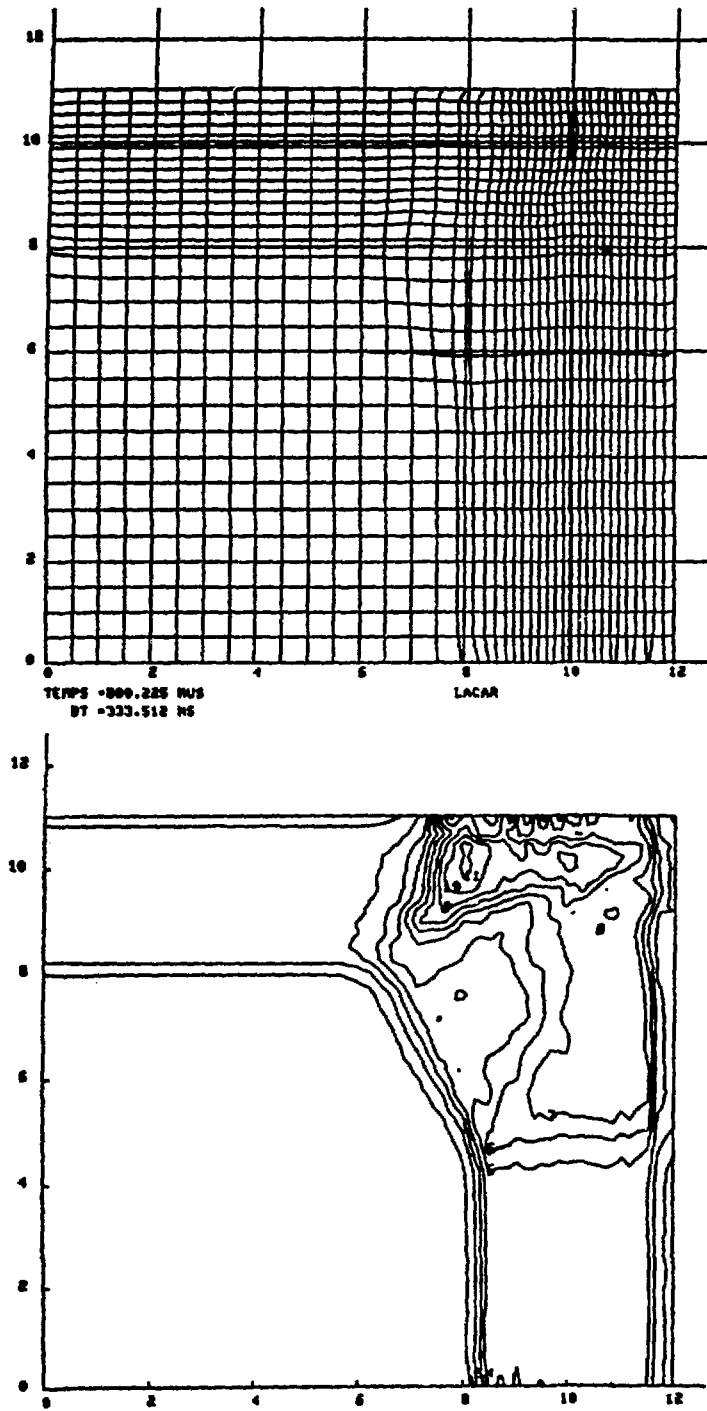


Fig. 8

2D hydro-test -Remapped run- 844 time steps + 16 rezonings.
Grid (top) and density contours (bottom)

T.V.D. SCHEMES FOR LAGRANGIAN HYDRODYNAMICS

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ABSTRACT

We present here two extensions of T.V.D schemes for solving the equations of hydrodynamics in one space dimension. The first is the preprocessing method. The second is the limited antidiffusion method.

I - INTRODUCTION

The aim of this study is to construct numerical schemes for solving hydrodynamics equations in one space dimension. We shall consider only the lagrangian coordinates. The schemes must satisfy :

- high accuracy
- T.V.D
- solutions of Riemann problem are used (Godunov type schemes)

These properties can be achieved by two ways :

The first one is the preprocessing method : high accuracy and T.V.D properties are obtained by handling data for Riemann problems. MUSCL scheme by Van Leer [6] and PPM scheme [2] are examples.

The second way is the postprocessing method : the Riemann problems are first resolved. High accuracy is obtained by adding antidiffusion terms which are limited in order to satisfy T.V.D properties. Example of such schemes : P.K Sweby [4], S. Chakravarthy and S. Osher [1].

T.V.D schemes were first introduced by A. Harten [3]. They are constructed from two schemes (the underlying schemes) : a monotone first order accurate scheme and a high resolution scheme. The monotone scheme that we shall use will be the Godunov scheme. We consider first the scalar linear case. Following B. Van Leer [5]

we construct a scheme which is accurate to the third order in space and time. This scheme is non monotonic. We modify it by using slope limiters. We demonstrate the T.V.D properties under some conditions on limiters. Next we shall consider the scalar non linear case. We shall show how to write the previous scheme in terms of antidiffusion method. We shall demonstrate the T.V.D properties. Finally we shall show how to extend previous schemes to lagrangian hydrodynamics in one space dimension. Numerical results will be presented and comparisons made.

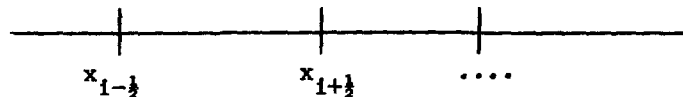
II - LINEAR CASE - PREPROCESSING METHOD

II.1 - Construction of the scheme

Let us consider the initial value problem, where a is constant :

$$(1) \quad \begin{aligned} u_t + au_x &= 0, \quad x \in \mathbb{R}, \quad t > 0 \\ u(x, 0) &= u_0(x) \end{aligned}$$

For numerical approximation let $(x_{i+\frac{1}{2}})$ be a set of points :



so we define a mesh : $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ is the cell i

$$\Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}, \quad x_i = \frac{1}{2} (x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}})$$

Δt is the time step. u_i^n is the approximation of $u(x_i, n \Delta t)$. We consider numerical schemes written in conservation form :

$$(2) \quad u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x_i} (f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}})$$

where $f_{i+\frac{1}{2}}$ is the numerical flux at $x_{i+\frac{1}{2}}$.

Godounov method applied to (1,1) gives the well known upwind scheme :

$$(3) \quad f_{i+\frac{1}{2}} = \begin{cases} a u_i & \text{if } a > 0 \\ a u_{i+1} & \text{if } a < 0 \end{cases}$$

This scheme is obtained by solving Riemann problems at each $x_{i+\frac{1}{2}}$ with the following data :

$$(4) \quad u_0(x) = \begin{cases} u_i & \text{for } x < x_{i+\frac{1}{2}} \\ u_{i+1} & \text{for } x > x_{i+\frac{1}{2}} \end{cases}$$

In order to improve accuracy we use another definition for these data.

B. Van Leer [5] showed that we could define a parabolic representation of the approximate solution in each cell i . One of his schemes can be interpreted as follows :

for $x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$, we define a function u_h :

$$u_h(x, t) = u_1^n + \frac{\delta_{i+\frac{1}{2}}}{2} [(x - x_i) + P(x)] + \frac{\delta_{i-\frac{1}{2}}}{2} [x - x_i - P(x)]$$

$\delta_{i+\frac{1}{2}}$ and $\delta_{i-\frac{1}{2}}$ are approximations of the first derivatives at $x_{i+\frac{1}{2}}$ and $x_{i-\frac{1}{2}}$:

$$\delta_{i+\frac{1}{2}} = \frac{u_{i+1} - u_i}{x_{i+1} - x_i}, \quad \delta_{i-\frac{1}{2}} = \frac{u_i - u_{i-1}}{x_i - x_{i-1}}$$

$P(x) = \frac{3\eta}{\Delta x_i} [(x - x_i)^2]$, where η is a parameter $\in [-1, +1]$. $\eta = 1/3$ corresponds to third order in space. $\eta = 0$ corresponds to piecewise linear representation. Third order accuracy in time is achieved as follows :

Exact solution of (1) is given by :

$$u(x, t) = u_0(x - at) \quad \text{or at a given } t :$$

$$(6) \quad u(x, t + \tau) = u(x - a\tau, t), \quad \tau > 0$$

we suppose that u_h verifies (6) too. An averaged value of u_h over the whole time step is calculated. For $a > 0$, and using $\xi = x_{i+\frac{1}{2}} - a\tau$

$$(7) \quad (u_{i+\frac{1}{2}}^-)^{n+\frac{1}{2}} = \frac{1}{\Delta t} \int_0^{\Delta t} u_h(x_{i+\frac{1}{2}}, t + \tau) d\tau = \frac{1}{a\Delta t} \int_{x_{i+\frac{1}{2}} - a\Delta t}^{x_{i+\frac{1}{2}}} u_h(\xi, t) d\xi,$$

Finally the numerical flux that we use is $a(u_{i+\frac{1}{2}}^-)^{n+\frac{1}{2}}$

In the case of a regular mesh this numerical flux can be rewritten :

$$(8) \quad f_{i+\frac{1}{2}} = a \left[(u_i + \frac{1-v}{6} ((2-v)(u_{i+1} - u_i) + (1+v)(u_i - u_{i-1}))) \right]$$

where v is the Courant number $a \frac{\Delta t}{\Delta x}$.

A Taylor expansion shows that the corresponding scheme is accurate to third order in space and time.

II.2 - Monotonicity

It is well known that the previous scheme is non monotonic and yields numerical results with spurious oscillations. To overcome this difficulty, B. Van Leer proposed the following method : let $\bar{u}(x) = u_i^n$ in the cell i . The monotonicity condition says that if $\bar{u}(x)$ is monotonic, then $u_h(x)$ must be monotonic again. In practice we try to satisfy the sufficient requirements : if u_i^n lies between u_{i-1}^n and u_{i+1}^n then $u_h(x)$, $x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ lies between u_{i-1}^n and u_{i+1}^n :

$$(9) \quad \min(u_{i-1}^n, u_{i+1}^n) \leq u_h(x) \leq \max(u_{i-1}^n, u_{i+1}^n)$$

If $u_h(x)$ has an extremum in the cell i , the slopes are set equal to zero, hence $u_h(x) = u_i^n$. The inequalities (9) rewritten give :

$$\delta_{i-\frac{1}{2}} \leq (1 + \frac{2 \Delta x_{i+1}}{(1-\eta)\Delta x_i}) \delta_{i+\frac{1}{2}} \quad \text{and} \quad \delta_{i+\frac{1}{2}} \leq (1 + \frac{2 \Delta x_{i-1}}{(1-\eta)\Delta x_i}) \delta_{i-\frac{1}{2}}$$

to satisfy these conditions we multiply the slopes by a limiter. A limiter is a uncton of consecutive slopes, via ratios r^+ and r^- which are defined by :

$$(10) \quad r_{i+\frac{1}{2}}^+ = \frac{\delta_{i-\frac{1}{2}}}{\delta_{i+\frac{1}{2}}}, \quad r_{i+\frac{1}{2}}^- = \frac{1}{r_{i+\frac{1}{2}}^+}$$

Therefore we find that a possible choice for the limiter ψ is

$$(11) \quad \psi(r^\pm) = \max(0, \min(1, b^\pm r^\pm)) \quad \text{where} \quad b^\pm = 1 + \frac{2 \Delta x_{i+1}}{(1-\eta)\Delta x_i}$$

For regular mesh $b^\pm = \frac{3-\eta}{1-\eta}$

II.3 - T.V.D properties

We assume that $v < 1$. We consider a regular mesh. Let us write :

$$\Delta u_{i+\frac{1}{2}} = u_{i+1} - u_i$$

$$\psi_{i+\frac{1}{2}}^+ = \psi(r_{i+\frac{1}{2}}^+), \quad r_{i+\frac{1}{2}}^+ = \frac{\Delta u_{i-\frac{1}{2}}}{\Delta u_{i+\frac{1}{2}}}$$

$$\psi_{i+\frac{1}{2}}^- = \psi(r_{i+\frac{1}{2}}^-), \quad r_{i+\frac{1}{2}}^- = 1/r_{i+\frac{1}{2}}^+$$

We have the following result :

Lemma 1. Let $\phi(r)$ be a limiter such as :

$$\phi(r) = 0 \quad \text{for } r < 0$$

$$\phi(r) = \min(1, br) \quad \text{for } r > 0, \quad b \text{ is a parameter } > 1.$$

Then, the scheme defined by the numerical flux

$$f_{i+\frac{1}{2}} = a u_1^n + \frac{1-\eta}{4} [(1+\eta) \phi_{i+\frac{1}{2}}^+ \Delta u_{i+\frac{1}{2}} + (1-\eta) \phi_{i+\frac{1}{2}}^- \Delta u_{i-\frac{1}{2}}]$$

where η is a parameter such as $|\eta| < 1$ is T.V.D under the conditions :

$$\text{if } r < 1 \quad b < \frac{3+\eta}{1+\eta} \quad \text{and} \quad \text{if } r > 1 \quad b < \frac{3-\eta}{1-\eta}$$

Proof : We first rewrite the scheme in the form :

$$(12) \quad u_i^{n+1} = u_i^n - C_{i-\frac{1}{2}} (u_i^n - u_{i-1}^n) + D_{i+\frac{1}{2}} (u_{i+1}^n - u_i^n)$$

It is shown by A. Harten [3] that sufficient conditions for the scheme to be T.V.D are :

$$C_{i+\frac{1}{2}} > 0, \quad D_{i+\frac{1}{2}} > 0, \quad C_{i+\frac{1}{2}} + D_{i+\frac{1}{2}} < 1 \quad \forall i+\frac{1}{2}$$

In order to write the scheme in the form (12) we use :

$$\Delta u_{i-\frac{1}{2}} = r_{i+\frac{1}{2}}^+ \Delta u_{i+\frac{1}{2}}, \quad \Delta u_{i-3/2} = r_{i-\frac{1}{2}}^+ \Delta u_{i-\frac{1}{2}}$$

substituting into the terms which are multiplied by $(1-\eta)$ and then using $\Delta u_{i+\frac{1}{2}} =$

$\frac{\Delta u_{i-\frac{1}{2}}}{r_{i+\frac{1}{2}}^+}$ we get the required form with

$$C_{i+\frac{1}{2}} = 0, \quad D_{i-\frac{1}{2}} = v \left(1 + \frac{1-v}{2} \right) \left[\frac{\phi(r_{i+\frac{1}{2}}^+)}{r_{i+\frac{1}{2}}^+} - \phi(r_{i-\frac{1}{2}}^+) \right]$$

where $\phi(r) = \frac{1}{2} [(1+\eta) \phi(r) + (1-\eta)r \phi(\frac{1}{r})]$

The first two conditions are satisfied. It remains to satisfy $D_{i-\frac{1}{2}} < 1 \quad \forall i$

Since $v < 1$, this inequality becomes : $\left[\frac{\phi(r)}{r} - \phi(s) \right] < 2 \quad r \text{ and } s$

The properties of $\phi(r)$ imply : $\phi(r) = 0$ for $r < 0$ and $\phi(r) > 0$ for $r > 0$. It follows :

$$(14) \quad \phi(r) < \max(2, 2r)$$

here $\phi(r) = \frac{1}{2} [(1 + \eta) \min(1, br) + (1 - \eta) \min(r, b)]$ and we have to consider different cases depending on the value of r :

small values of r : $r < 1/b$

$$(14) \text{ leads to } b < \frac{3 + \eta}{1 + \eta}$$

great values of r : $r > b$ we obtain $b < \frac{3 - \eta}{1 - \eta}$

intermediate values of r : $1/b < r < b$

$\phi(r)$ does not depend on b and (14) is always satisfied since $\frac{1 - \eta}{2} < 2$.

Remarks :

- 1 - If a is < 0 we get a similar result by replacing r by $1/r$
- 2 - The numerical flux (8) corresponds to $\eta = \frac{1 - 2v}{3}$
- 3 - Many other forms of limiters can lead to a T.V.D scheme : See P.K Sweby [4]
- 4 - Whatever we do, third order is lost.

III - NON LINEAR CASE (POSTPROCESSING OR ANTIDIFFUSION)

The numerical flux (8) is interpreted as the numerical flux of the upwind scheme plus antidiffusion terms. Let us consider now the initial value problem :

$$(15) \quad \begin{aligned} u_t + [f(u)]_x &= 0 \\ u(x, 0) &= u_0(x), \quad x \in \mathbb{R}, \quad t > 0 \end{aligned}$$

Following P.K Sweby [4], S. Chakravarthy and S. Osher [1], we find that a possible extension of (8) is :

$$(16) \quad f_{i+\frac{1}{2}} = \frac{f_{i+1} + f_i}{2} - \frac{a_{i+\frac{1}{2}} \lambda}{2} (f_{i+1} - f_i) - \sigma_{i+\frac{1}{2}} (f_{i+\frac{1}{2}}^g - 2f_{i+\frac{1}{2}}^g + f_{i-\frac{1}{2}}^g)$$

where $f_i = f(u_i)$, $\lambda = \frac{\Delta t}{\Delta x}$, $a_{i+\frac{1}{2}} = \frac{f_{i+1} - f_i}{u_{i+1} - u_i}$ and $f_{i+\frac{1}{2}}^g$ is the numerical flux of Godunov scheme at $x_{i+\frac{1}{2}}$. $\sigma_{i+\frac{1}{2}}$ is a coefficient which will be defined later. We now want to write (16) in form of Godunov flux plus antidiffusion terms. Let us use the flux-splitting method :

$$(17) \quad \Delta f_{i+\frac{1}{2}}^+ = f_{i+1} - f_{i+\frac{1}{2}}^g, \quad \Delta f_{i+\frac{1}{2}}^- = f_{i+\frac{1}{2}}^g - f_i$$

If we suppose that $a = \frac{\partial f}{\partial u}$ does not vanish between x_i and x_{i+1} we can write

$$a = a^+ a^- \text{ with } a^\pm = \frac{\Delta f_{i+\frac{1}{2}}^\pm}{u_{i+1} - u_i} \quad (18). \text{ There are only two possibilities :}$$

$$a^+ = 0 \quad \text{or} \quad a^- = 0 \quad \text{so} \quad a^+ a^- = 0 \quad \text{and} \quad a^+ \Delta f^- = a^- \Delta f^+ = 0$$

$$\text{let } \alpha^\pm = \frac{1 \mp a_{i+\frac{1}{2}}^\pm \lambda}{2}, \text{ the flux becomes}$$

$$(19) \quad f_{i+\frac{1}{2}} = f_{i+\frac{1}{2}}^g + (\alpha^+ - \sigma) \Delta f_{i+\frac{1}{2}}^+ - (\alpha^- - \sigma) \Delta f_{i+\frac{1}{2}}^- - \sigma (\Delta f_{i+3/2}^- - \Delta f_{i-1/2}^+)$$

The antidiffusion terms are limited, as seen in the previous section. Let $\phi(r)$ be a limiter. The ratios $r^\pm$ are now defined by :

$$(20) \quad r_{i+\frac{1}{2}}^+ = \frac{\Delta f_{i-\frac{1}{2}}^+}{\Delta f_{i+\frac{1}{2}}^+}, \quad r_{i+\frac{1}{2}}^- = \frac{\Delta f_{i+3/2}^-}{\Delta f_{i+\frac{1}{2}}^-}$$

the limited flux is :

$$(21) \quad f_{i+\frac{1}{2}}^g + (\alpha^+ - \sigma) \phi(r_{i+\frac{1}{2}}^+) \Delta f_{i+\frac{1}{2}}^+ - (\alpha^- - \sigma) \phi(r_{i+\frac{1}{2}}^-) \Delta f_{i+\frac{1}{2}}^- \\ - \sigma \left(\phi\left(\frac{1}{r_{i+\frac{1}{2}}^-}\right) \Delta f_{i+3/2}^- - \phi\left(\frac{1}{r_{i+\frac{1}{2}}^+}\right) \Delta f_{i-1/2}^+ \right)$$

If $\sigma = 0$ we get, except some details, the scheme proposed by Sweby [4]. Let $v_{i+\frac{1}{2}}$ be the Courant number :

$$v_{i+\frac{1}{2}} = \lambda \left| \frac{f_{i+1} - f_i}{u_{i+1} - u_i} \right|. \text{ We have the following result :}$$

Lemma 2

Let $\psi(r)$ be a limiter such as

$$\psi(r) = 0 \quad \text{for } r < 0$$

$$\psi(r) = \min(1, br) \quad \text{for } r > 0$$

b a parameter such as $1/2 < b < 1$

The scheme whose numerical flux is given by (21) is T.V.D under the conditions :

$$0 < \sigma < \alpha, \quad v < \frac{1}{1+b}$$

$$\text{and if } r < 1 \quad b < \frac{q - \sigma}{\alpha - \sigma}$$

$$\text{if } r > 1 \quad b < \frac{q - \alpha + \sigma}{\sigma}, \quad \forall i$$

Proof - We put the scheme in the form (12) using the definition of $r^\pm$:

$$\Delta f_{i+3/2}^- = r_{i+\frac{1}{2}}^- \Delta f_{i+\frac{1}{2}}^-, \quad \Delta f_{i-\frac{1}{2}}^+ = r_{i+\frac{1}{2}}^+ \Delta f_{i+\frac{1}{2}}^+$$

$$\text{let } \phi^\pm(r) = (\alpha^\pm - \sigma) \psi(r) + \sigma r \psi\left(\frac{1}{r}\right)$$

the flux becomes :

$$f_{i+\frac{1}{2}} = f_{i+\frac{1}{2}}^G + \phi^+(r_{i+\frac{1}{2}}^+) \Delta f_{i+\frac{1}{2}}^+ - \phi^-(r_{i+\frac{1}{2}}^-) \Delta f_{i+\frac{1}{2}}^-$$

we use again the definition of $r^\pm$:

$$\Delta f_{i+\frac{1}{2}}^+ = \frac{\Delta f_{i-\frac{1}{2}}^+}{r_{i+\frac{1}{2}}^+} \quad \text{and} \quad \Delta f_{i-\frac{1}{2}}^- = \frac{\Delta f_{i+\frac{1}{2}}^-}{r_{i-\frac{1}{2}}^-}$$

The scheme can be written as follows :

$$u_1^{n+1} = u_1 - \lambda (\Delta f_{1+\frac{1}{2}}^- + \Delta f_{1+\frac{1}{2}}^+) - \lambda \left[\frac{\phi^+(r_{1+\frac{1}{2}}^+)}{r_{1+\frac{1}{2}}^+} - \phi^+(r_{1-\frac{1}{2}}^+) \right] \Delta f_{1-\frac{1}{2}}^+ \\ + \lambda \left[\phi^-(r_{1+\frac{1}{2}}^-) - \frac{\phi^-(r_{1-\frac{1}{2}}^-)}{r_{1-\frac{1}{2}}^-} \right] \Delta f_{1+\frac{1}{2}}^-$$

using (18) : $\lambda \Delta f_{1-\frac{1}{2}}^+ = v_{1-\frac{1}{2}}^+ \Delta u_{1-\frac{1}{2}}$, with $v_{1+\frac{1}{2}}^\pm = \lambda a_{1+\frac{1}{2}}^\pm$

It follows that the scheme is in the required form with

$$C_{1+\frac{1}{2}} = -v_{1+\frac{1}{2}}^- (1 + Q^-) , \quad D_{1-\frac{1}{2}} = v_{1-\frac{1}{2}}^+ (1 + Q^+)$$

where
$$Q^\mp = \frac{\phi^\mp(r_{1\mp\frac{1}{2}}^\mp)}{r_{1\mp\frac{1}{2}}^\mp} - \phi^\mp(r_{1\pm\frac{1}{2}}^\mp)$$

A property of Godunov scheme is that $v^- < 0$, $v^+ > 0$. Let us suppose that

$|Q^\pm| < q \forall r^-$ and r^+ then the inequalities $C_{1+\frac{1}{2}} > 0$ and $D_{1+\frac{1}{2}} > 0$ are satisfied when

$$q \geq 1 : C_{1+\frac{1}{2}} + D_{1+\frac{1}{2}} = v_{1+\frac{1}{2}}^+ (1 + Q^+) - v_{1+\frac{1}{2}}^- (1 + Q^-) < 1$$

leads to
$$v_{1+\frac{1}{2}}^+ - v_{1+\frac{1}{2}}^- = v_{1+\frac{1}{2}} < \frac{1}{1+q}$$

It remains to find when the conditions $|Q^\pm| < q$ are satisfied.

Similarly (lemme 1) we get : $0 < \sigma < \alpha^\pm$ and

$$\text{if } r^\pm < 1 \quad b^\pm < \frac{q - \sigma}{\alpha^\pm - \sigma}$$

$$\text{if } r^\pm > 1 \quad b^\pm < \frac{q - \alpha^\pm + \sigma}{\sigma}$$

Remark : we can use a symmetric $(\psi(r) = r \psi(\frac{1}{r}))$ limiter. Thus $\phi^\pm = \phi$. The terms depending on σ vanish.

IV - EXTENSION TO SYSTEMS OF CONSERVATION LAWS

Although T.V.D properties have no meaning for non linear systems, the extension of such schemes gives excellent results. The system of equations in langrangian coordinates can be written in the form

$$(21) \quad v_t + (F(v))_m = 0$$

Where v is the vector $\begin{pmatrix} V \\ u \\ E \end{pmatrix}$ and $F(v) = \begin{pmatrix} -u \\ p \\ pu \end{pmatrix}$

ρ is the density, $V = 1/\rho$; u is the velocity, p the pressure, E the total energy $E = \epsilon + 1/2 u^2$ where ϵ is the specific internal energy. The equation of state is $p = p(\rho, \epsilon)$, m the mass coordinate is related to the spatial coordinate x :

$$m(x) = \int_{x_0}^x \rho(\xi) d\xi$$

A, the jacobian matrix of F has three real eigenvalues : $-C$, 0 , C where C is the lagrangian sound speed. There exist several methods for extending previous numerical schemes to systems. Many of them need to know jacobian matrix and eigenvectors. In our extension we want to avoid the calculus of such quantities. We prefer as in the P.P.M method to work directly with the quantities needed by the resolution of Riemann problems. This quantities are density, velocity and pressure. In preprocessing method we apply the method described in section II to each quantity. In the postprocessing (antidiffusion) method we must first rewrite the approximate system making some simplifications. The numerical flux of the Godunov scheme may be written as :

$$F_{i+\frac{1}{2}}^G = \begin{pmatrix} -u_{i+\frac{1}{2}}^* \\ p_{i+\frac{1}{2}}^* \\ p_{i+\frac{1}{2}}^* \quad u_{i+\frac{1}{2}}^* \end{pmatrix}$$

where u^* and p^* are given by a resolution of a Riemann problem. Let us define the vector ΔF^- and ΔF^+ :

$$\Delta F_{i+\frac{1}{2}}^- = F_{i+\frac{1}{2}}^G - F_i, \quad \Delta F_{i+\frac{1}{2}}^+ = F_{i+1} - F_{i+\frac{1}{2}}^G$$

$$\text{where } F_1 = \begin{pmatrix} -u_1 \\ p_1 \\ p_1 u_1 \end{pmatrix}$$

Now we split the jacobian matrix : $A = A^+ + A^-$ such $A^- A^+ = 0$

A^- (resp. A^+) has only negative (resp. positive) eigenvalues .

The extension of the terms depending on a^+ and a^- in (19) is ($\lambda = \Delta t / \Delta m$)

$$\frac{1}{2} [(I - \lambda A_{i+\frac{1}{2}}^+) \Delta F_{i+\frac{1}{2}}^+ - (I + \lambda A_{i+\frac{1}{2}}^-) \Delta F_{i+\frac{1}{2}}^-]$$

we approximate $A_{i+\frac{1}{2}}^+$ by $C_{i+\frac{1}{2}} I$ and $A_{i+\frac{1}{2}}^-$ by $-C_{i+\frac{1}{2}} I$

thus the corresponding term becomes :

$$\frac{1 - C_{i+\frac{1}{2}} \lambda}{2} (\Delta F_{i+\frac{1}{2}}^+ - \Delta F_{i+\frac{1}{2}}^-)$$

the limiter is a diagonal matrix defined by

$$\phi(R) = \begin{pmatrix} \phi(r) & \\ & \phi(s) \end{pmatrix} \begin{pmatrix} \phi(r) & \phi(s) \end{pmatrix}$$

where r (resp. s) is the ratio of consecutive gradient of velocity (resp. pressure)

$$r_{i+\frac{1}{2}}^+ = \frac{u_1^* - u_{i-\frac{1}{2}}^*}{u_{i+1} - u_{i+\frac{1}{2}}^*} \quad s_{i+\frac{1}{2}}^+ = \frac{p_1^* - p_{i-\frac{1}{2}}^*}{p_{i+1} - p_{i+\frac{1}{2}}^*}$$

$$r_{i+\frac{1}{2}}^- = \frac{u_{i+3/2}^* - u_{i+1}}{u_{i+\frac{1}{2}}^* - u_1} \quad s_{i+\frac{1}{2}}^- = \frac{p_{i+3/2}^* - p_{i+1}}{p_{i+\frac{1}{2}}^* - p_1}$$

the entire extension of (21) is given by :

$$F_{i+\frac{1}{2}}^G + \left(\frac{1 - C_{i+\frac{1}{2}} \lambda}{2} - \sigma_{i+\frac{1}{2}} \right) [\phi(R_{i+\frac{1}{2}}^+) \Delta F_{i+\frac{1}{2}}^+ - \phi(R_{i+\frac{1}{2}}^-) \Delta F_{i+\frac{1}{2}}^-]$$

$$- \sigma_{i+\frac{1}{2}} \left[\phi\left(\frac{1}{R_{i+\frac{1}{2}}}\right) \Delta F_{i+3/2}^- - \phi\left(\frac{1}{R_{i+\frac{1}{2}}^+}\right) \Delta F_{i-\frac{1}{2}}^+ \right]$$

where $\sigma_{i+\frac{1}{2}}$ is a scalar which depends on the Courant number $C_{i+\frac{1}{2}}\lambda$. The elements of $\phi(\frac{1}{R})$ are $\phi(\frac{1}{R})$, $\psi(\frac{1}{S})$ and $\psi(\frac{1}{R})\psi(\frac{1}{S})$.

V - NUMERICAL RESULTS

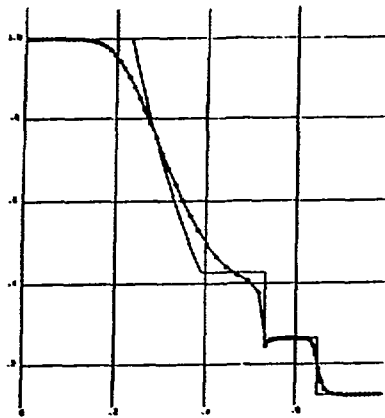
Two problems : the shock tube problem used by Sod and the shock tube problem used by P. Colella and P. Woodward. We show the results obtained by Godunov scheme, preprocessing method and antidiffusion method. In both cases we use 100 cells. In the preprocessing method η has no effect : $\eta = 0$ and $\eta = (1-2\epsilon)/3$ yield indistinguishable results.

In the antidiffusion method σ has negligible effect. We can use a symmetric limiter.

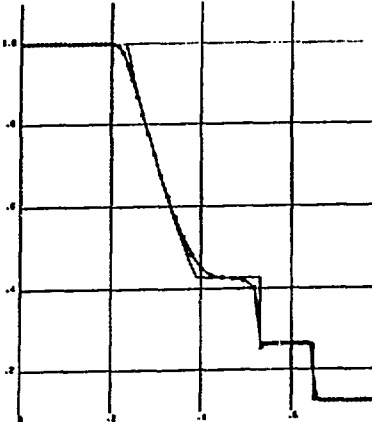
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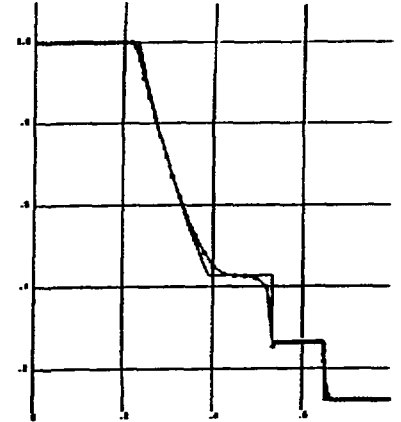
Godunov



Preprocessing

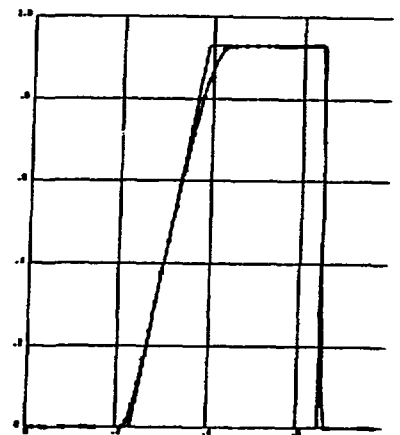
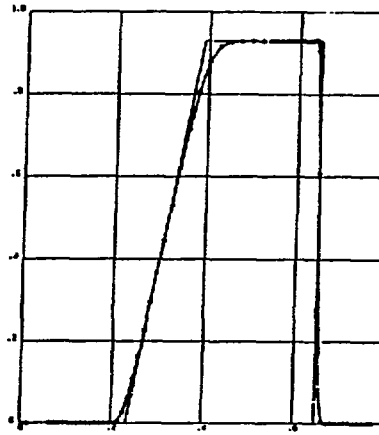
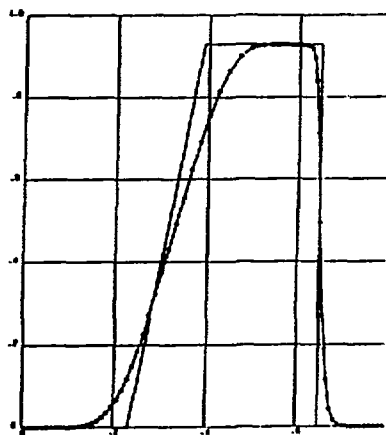


antidiffusion



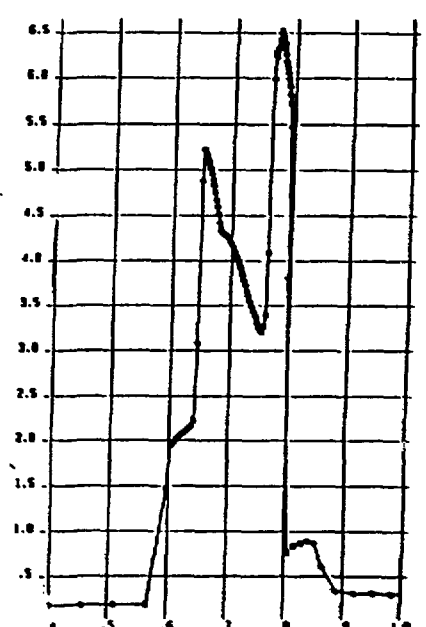
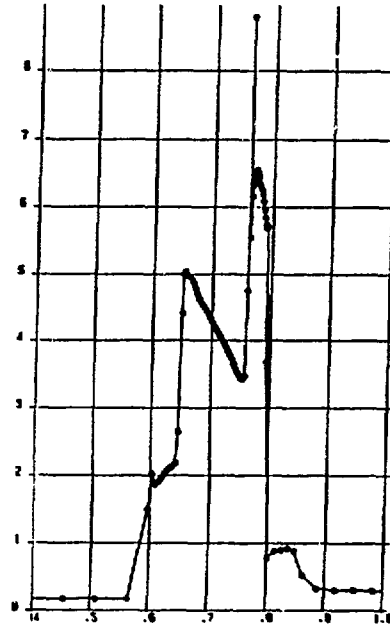
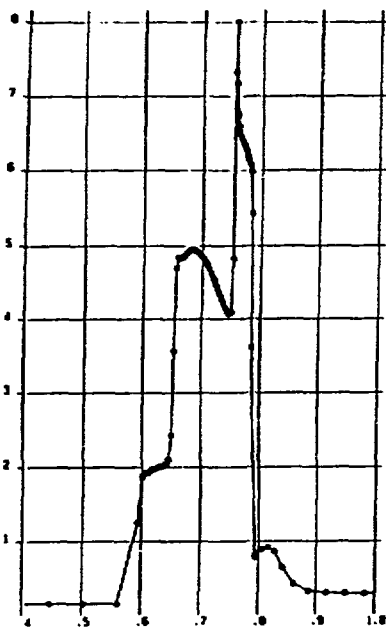
density

Sod's problem



Velocity

Sod's problem



density

Woodward's problem

A FAST SMOOTH PARTICLE HYDRODYNAMICS CODE

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Abstract

We present a procedure that allows for the vectorization of the linked list algorithm. We apply it to the calculation of the density and short-range forces in an SPH code. The procedure however, is more general and can be applied to all similar problems. When long range forces are absent the overall speed of the code is increased by a factor 3.6 for a completely 3-dimensional problem. In the presence of symmetry planes higher speedup can easily be obtained. As an example we show results from the simulation of the impact of a 10 km diameter asteroid hitting the Earth at 20 km/s. The problem was run using nearly 10^5 particles in less than one hour cpu time.

1. Introduction

The Smooth Particle Hydrodynamics (SPH) method was first proposed by Lucy in 1977 [1]. In the following years Gingold and Monaghan [2,3,4,5,6] gave the method a more rigorous mathematical aspect. By applying it to numerous astrophysical situations they showed that complicated, three-dimensional hydrodynamic problems can actually be solved using this method (for a complete review of astrophysical application of SPH see [7]). Surprisingly, this powerful method did not spread and only a very few people, essentially astronomers, continue to use it. We suspect that this situation stems from the fact that almost all of the papers describing the method have been published in the astronomical literature instead of in conventional computer method journals where new methods are usually published.

Although most readers may not be very familiar with SPH, it is not the purpose of this paper to give a complete description of the method. As we indicated above,

sufficient literature already exists that more than adequately covers the subject. We shall restrict ourselves to recalling the fundamentals of the method.

We are interested in presenting an algorithm that allows the vectorization of the most time consuming part of the SPH code. In the absence of long range forces, the most expensive part of SPH deals with finding all the neighbors within the short range force distance of any given particle. The problem of finding all neighbors within a fixed distance of any given object is obviously a general problem that potentially has wider application than just to a specific aspect of SPH. After presenting the algorithm in some detail, we will give various timing results that show the substantial speed-up achieved.

We then present, as an example, a simulation of the impact of a 10 km radius asteroid hitting the Earth surface at 20 km/s. This problem was modeled using 98256 particles and it took less than one hour cpu time using our new algorithm.

2. Smooth Particle Hydrodynamics

As mentioned in the introduction we will not review in detail the SPH method. We only recall here that SPH is a free Lagrangian (variable connectivity) approach for solving the conservation equations of hydrodynamics. A finite set of spatially extended Lagrangian particles replaces the continuum of hydrodynamical variables. The usual mesh is not needed; this technique therefore does not suffer from mesh tangling or inaccuracies associated with a severe distortion of the mesh. This method is therefore particularly suited for the simulation of highly distorted flows such as those occurring during impacts.

The simulation evolves in time by computing the trajectories of all particles given the various forces acting between them. These forces are derived from the interactions between the particles and the interactions are derived from the relative particle positions and velocities. The derivation of the forces makes use of the actual "shape" (or spatial distribution of the mass) of an individual particle. Several shapes have been proposed in the past ranging from polynomes [1], Gaussian [8], and exponential [9] to splines [5] defined on compact support. The latter shape was shown not only to interpolate better, but also only a limited number of particles contribute to the local density and pressure gradients, since the short-range forces are limited by the size of the compact support.

If not only the “shape” of the particles but also their actual size are the same, interactions can be computed fast and easily. This is achieved by using the so-called linked-list algorithm.

3. The Linked List Algorithm

In the absence of long-range forces such as self-gravity and coulomb interactions, the local properties of a fluid (density, pressure, viscosity etc.) are determined by the interaction of the fluid element with its immediate surroundings. Translated into the SPH jargon we say that the total force acting on a particle is determined only by the neighboring particles.

The exact number of contributing particles is found by determining how many of these particles are within a given distance of the particle on which we want to compute the force. An obvious way to do this would be to compute the distances to all the particles. This in the end would require the evaluation of at least $\frac{N^2}{2}$ distances. If N becomes large enough (a few thousand) this clearly becomes prohibitive. A simple way to reduce the cost of finding the neighbors is to use the so-called linked list algorithm, a process requiring roughly only $N \times N_{\text{neigh}}$ distance evaluations (N_{neigh} is the average number of contributing neighbors per particle). This well known algorithm has been advocated by Hockney and Eastwood [10] in their P³M code.

In the linked list algorithm, coordinate addresses rather than coordinates themselves are sorted. Address sorting is made possible by introducing the linked-list array $ll(i)$. If we let $hoc(q)$ be the head-of-chain table entry for chaining cell q , and let $ll(i)$ be the link coordinate for particle i , then the procedure for sorting coordinates into a list for each chaining cell by means of address sorting is :

1. set $hoc(q)$ to zero for all q .
2. locate cell containing particle i : $q = \text{int}(x_1/l_1, y_1/l_2, z_1/l_3)$
3. add particle i to head of list for cell q : $ll(i)=hoc(q)$, $hoc(q)=i$
4. repeat 2 and 3 for all particles.

Here l_1, l_2, l_3 are the cell dimensions in the x, y, z directions. In order to be effective for finding contributing neighbors we set $l_1 = l_2 = l_3 = 2h$ where $2h$ is now

the size of the compact support on which the actual shape of a particle is defined. The quantity h is called the smoothing length. Now for any given particle, the contributing neighbors can only be in the self or the neighboring cells. Therefore to compute local properties, it is sufficient to look up the particles inside these cells only.

However, Hockney and Eastwood cautioned that this may not be the fastest way for a vector machine since this algorithm involves a lot of indirect addressing. Indeed, on a Cray computer, the linked-list used to find the nearest neighbors does not vectorize forthrightly. Nevertheless, by a very large margin, it is still the fastest way to find these neighbors (much faster than a hierarchical tree based algorithm). Of course, running the most time consuming part of a large program on a vector machine in essentially a scalar mode leaves a lot to be desired.

The rest of the code (except for the equation of state) mostly contains easy to vectorize parts and in fact, effective vectorization of those parts is done automatically by the compiler. In the following sections and especially in the timing part, when we refer to the "vectorized code" we mean the code that contains the vectorized linked list algorithm explained below. Similarly, when we mention "scalar code", we mean the original code which does not contain this special algorithm, and in which the only vectorization is that produced automatically by the compiler.

3.1 Vectorization of the Linked List Algorithm

We now present our algorithm for vectorizing the calculation of the short range forces. In a smooth particle hydrodynamics code the short range forces are due to particles that are within a distance of $2h$ of the particle on which we want to compute the force. One can note that the same particles also determine the local density, so the algorithm can also be used to compute the local density.

As before, we partition the 3-dimensional problem space, containing N particles, into $M \times M \times M$ cells, each cell a cube of dimension $2h$. In this way, for each particle, all interacting particles will be found in the self cell and the 26 surrounding cells, thus reducing an N -squared calculational effort to a much smaller effort. Following the algorithm above, each particle is examined to determine which cell it occupies and a linked list is constructed for each cell which connects all the particles in that cell.

In our scheme, we choose to vectorize on the total number of particles in the problem. Previous attempts to vectorize on the number of particles that could interact with a given particle met with limited success because, in typical problems, the vectors ended up being rather short, thus limiting the speedup. We first describe our scheme in a very general way, then follow with a more detailed description.

Consider the N particles in our problem space. We wish to calculate the interaction contributions from all particles j ($j=1,N$) (of course, only a subset will in fact contribute) to particle i and to do that for all i ($i=1,N$). We can vectorize on the receiving particles (the i particles) by the following scheme. We maintain throughout our algorithm an i -vector which is simply a list of the particle numbers of the i particles. We also maintain a j -vector of equal length which contains, in a position corresponding to that of particle i in the i -vector, a single contributing particle number. We can then, in one vectorized operation, calculate the contribution of each particle in the j -vector on its corresponding particle in the i -vector. In other words, each vectorized operation calculates a contribution to every receiving particle. As a hypothetical example, the first part of our total calculation might be to calculate the contribution of each particle to itself. For this, the i -vector will contain all N particles, the j -vector will be identical to the i -vector, and the result of one vectorized operation will be the calculation of all the self contributions. Our next step would be to reload the j -vector with the next particle that interacts with the respective particle in the i -vector. We use the linked list for the i particle self-cell to find the next contributing j particle. We then calculate the contribution from these particles in the j -vector to the respective particles in the i -vector, reload the j -vector with the next particles from the linked lists, and continue until the linked lists are all exhausted. We have now calculated, for each particle in the i -vector, the contributions from all the particles within the same cell as the i particle. Then, for each of the i particles, we proceed to one of the surrounding twenty six cells (e.g. the one to the right) and reload the j -vector with the head-of-chain particle of its linked list. We continue with this process until we have calculated the contributions from all the surrounding cells, at which point our calculation is complete.

The detailed steps of the algorithm are shown in the sequence below. A discussion follows which clarifies some of the details and mentions other aspects of the algorithm.

1. Number all the particles.
2. Build the linked lists for all cells.
3. Let the contributing cell be the self cell.
4. Load the i-vector with the numbers of all of the particles.
5. For the k-th particle in the i-vector, determine the actual number of its contributing cell, then load the k-th position in the j-vector with the first particle in the linked list for that cell.
6. Calculate the i-to-j distances for all ij couples represented in the vectors.
7. Construct a subset i-vector and a subset j-vector containing only those ij couples for which the i-to-j distance is less than $2h$.
8. Calculate the j-to-i contributions of the couples in the subset vectors.
9. Reload the j-vector with the next particle in the contributing cell, that is, the next particle in its linked list.
10. When a particle in the i-vector has reached the end of the linked list for the contributing cell (there are no more particles in the contributing cell to interact with it), remove its number from the i-vector and remove the corresponding position from the j-vector.
11. Go back to step 6 and continue until every particle in the i-vector has exhausted its contributing linked list.
12. Let the contributing cell be the next surrounding cell.
13. Go back to step 4 and continue until all the surrounding cells are processed.
14. Calculation completed.

In step 3, we are starting a process of working our way through the self cells and their surrounding 26 cells. For each of these cells, we will calculate the contributions from particles in that cell to the appropriate particle in the i-vector. Note that self cell is a relative designation; it simply means the cell that the specific particle in the i-vector occupies. Different particles in the i-vector may have different self cells.

Throughout the whole calculational process described above, the physical data pertaining to particle i , such as mass, position, or velocity are unchanged. They retain their ordinal positions. For example, the mass for particle i is always in the i -th member of the mass array. We can then use the particle numbers that we carry

in the i-vector or j-vector as an indirect address into these physical data arrays. It is important that the FORTRAN compiler be able to generate code that uses indirect addressing in a vector way.

In steps 7 and 10, we are producing a smaller vector based on a specified condition so that in step 8 (contributions calculation), we will do no unnecessary calculations. This is our way of getting around testing within the innermost loop for the end of the linked list or for inter-particle distances greater than $2h$. Tests within the loop either inhibit the vectorization or cause calculation of unneeded results. This vector compression, of course, takes some calculational effort and, in fact, is a significant portion of the total calculational effort. However, in order to minimize the time spent in compression, we have coded vectorized compression routines in machine language that take advantage of the hardware gather/scatter options available on the CRAY-XMP.

Note that every step in the algorithm which deals in any way with particles is vectorized. Steps 3, 11, 12, and 13 do not deal with particles and are inherently trivial scalar operations.

The vectorized version of SPH incurs a storage penalty relative to the scalar version. In the algorithm described above, the penalty is $9N$ words of storage. Obviously $2N$ are needed for the i-vector and the j-vector and $2N$ more for the subset vectors. Not so obviously, 5 other scratch arrays are needed to allow the calculation to proceed in vector mode. We have not as yet attempted to minimize this storage penalty.

Note that for each i,j couple, we only calculate the interaction of j on i and rely on the fact that when this same couple occurs in reverse order somewhere else in the vectors, as it must, the reverse interaction will be calculated. This means that we do some duplicate calculation, such as the distance between i and j . Most scalar algorithms also calculate the interaction of i on j while the distance is known, and thus save the extra calculation of distance. However, our attempts to introduce this savings into the vectorized algorithm met with very limited success due largely to the following fact. A given particle can occur only once in the i-vector, but can occur in many positions of the j-vector. Thus, cumulative stores into the arrays indexed by the i-vector can be properly handled in vector mode, but cumulative stores into arrays indexed by the j-vector are, in general, unvectorizable operations.

The fact that a given particle can occur more than once in a j-vector also causes another problem. When accessing arrays indexed by the j-vector, memory conflicts can arise which slow the vector loading. In particular, note in step 5 that all particles in the same cell will have the same particle in the j-vector and we will thus suffer memory conflicts when accessing one of the physical arrays, for instance, the mass. The severity of this slowdown depends on the particle distribution and hence, on the case being run or on the time during the evolution of the problem. In a very dispersed distribution where, for arguments sake, only a single particle occupies each cell, there would be no repetition in the j-vector, we would not have the conflict detailed above, and the calculation would not be slowed because of this effect. On the other hand, at the beginning of the evolution, we are more likely to have numerous particles in a given cell and furthermore, they are likely to be numbered sequentially which exacerbates the problem. We have constructed a variant of the above algorithm that seems to help. We choose to "scramble" the contributing cells. In step 3, rather than always choosing the contributing cell to be the self cell, we make the contributing cell particle dependent. As an example, if particles numbered 1 through 5 were in the same cell, the variant would choose the contributing cell for particle 1 to be the self cell, but for particle 2, it would pick a different contributing cell, perhaps the adjacent cell to the right. For particle 3, it would pick still a different adjacent cell, say, the cell above, and so on. In subsequent steps, particles 1 through 5 thus interact, not with the same particle, but with particles in different cells and at least some of the memory conflicts are eliminated. Note that since there are only 27 self and adjacent cells, particle 28 would again be assigned the self cell and the pattern would repeat.

Our scheme is well suited to taking advantage of symmetry in the problem. To achieve this savings, we simply choose only the one half or the one quarter of the particles to one side of the symmetry planes(s) when loading receiving particles into the i-vector in step 4. The number of j particles considered will be slightly more than one half or one quarter, respectively, for in our algorithm, particles in the cell just outside the plane of symmetry (but within $2h$) need to be considered as contributing particles. We have variants for symmetry in the x direction and for concurrent symmetry in both x and y.

3.2 Timing

Absolute timing of the algorithm was found to be difficult. The amount of time spent by the SPH code to compute one time step depends on several factors like the average number of particles contributing to the local properties and the thermodynamical phase of the particles. The first factor is easy to understand; in a compressed material, any given particle has, by definition, a higher number of close neighbors and this results in a net increase of the number of interactions that have to be computed. The second one has to do with the properties of the equation of state. Depending on local temperature and density a particle will be in a vapor, liquid, solid or even mixed phase. Each phase is described by a different equation of state resulting in a different amount of computing requirements. If the equation of state is sufficiently complex it turns out that this part becomes the most expensive part of the computation.

To get a timing estimation that would take into account all these factors we decided to measure the time needed to run a specific problem from the beginning to a fixed evolution time. We give below the computing time needed to complete the simulation using the initial scalar code, different intermediate stages during speed-up and the final optimized version of the code. Since all other parts of the code have not been changed, the speed increase is really due to speed increase in the force calculation alone.

The typical problem we chose to run while working on the code was that of the perpendicular impact of a 20 g, 6.6 km/s spherical lead bullet on a 1/4 inch thick lead plate [11]. Several codes at Los Alamos have been run on this problem and experimental data were also available, so direct comparison could be made between the SPH calculations, the experiment, and the calculations made using the other codes. In the timing reported below we modeled the bullet using 672 particles and the target using 14112 particles. We used a simple Tillotson [12] equation of state for modeling the material properties. The simulation was stopped at 30 microseconds after the bullet hit the target (this corresponds to the time for which x-ray pictures of the experiment were obtained). Since the collision is head-on this is, in fact, a two-dimensional problem. However, we were interested in the development

of a fully three-dimensional code, so we did the computation in three dimensions. Nevertheless we did make use of symmetry planes to speed up the calculation.

In the table below we report some of the timing results that show the effects of various speed-up efforts. The times given are the sum of cpu, i/o and memory time.

	<u>Code Status</u>	<u>Time (min)</u>
1.	Original "scalar" code	113.0
2.	Vectorized code	37.5
3.	Vectorized, fast compression	32.0
4.	Vectorized, fast compression, scramble	31.0
5.	Vectorized, fast compression, scramble, x-reflection	18.0
6.	Vectorized, fast compression, scramble, x-y-reflections	11.4
7.	Vectorized, fast compression, scramble, x-y-eos-reflections	9.4

Clearly, vectorization alone is worth about a factor of 3, and by using our own compression subroutines we get another factor of 1.17. The scramble algorithm does not make much of a difference for this problem; the time gets shorter by only a factor of 1.03. Introducing a symmetry plane brings in a factor of 1.8. The reason that this factor is not exactly two comes from the situation that particles less than $2h$ from a symmetry plane see contributions from particles on the other side of the plane. We are therefore left with slightly more than one half of the interactions to compute. Finally, when only one quarter of the particles are used in the force calculation and also in the equation of state we get to our shortest time of 9.4 minutes. The overall speed increase compared to the original code is slightly more than a factor of 12. Notice however, that in case of a completely 3D problem without any planes of symmetry the corresponding speedup would only be about 3.6.

4. An Asteroid Hitting the Earth at 20 km/s

As a concrete example of the SPH code using our fast algorithm, we describe a simulation of an asteroid hitting the Earth at 20 km/s. This type of collision is now believed to be the cause of at least one massive extinction of species (including

the dinosaurs) at the end of the Cretaceous period. A review of this subject was recently written by Alvarez [13].

In this example we used 672 particles to model a 10 km diameter asteroid and 97584 particles to model a cylindrical piece of Earth about 100 km diameter and 60 km deep. The reason for the large difference in particle numbers between the asteroid and the piece of Earth comes from the fact that we are interested in the amount of material ejected up into the atmosphere (the atmosphere itself was not modeled). The material properties were again modeled using the Tillotson equation of state. In order to get the ejected fraction the simulation has to evolve to relatively late times. To avoid boundary effects the mass ratio between target and impactor has to be large. Since we found that the mass of individual particles can not differ by a large amount (no more than a factor 3 to 5) for a fixed smoothing length scale, the mass ratio had to be augmented with the large difference in the particle numbers.

As far as timing is concerned, running this problem on a Cray XMP-48 took 51.4 raw cpu minutes for 318 time steps. That works out to about 42 microseconds per particle per force-calculation. Total charge time (cpu + i/o + mem) runs about 1.5 to 2.0 times raw cpu.

Figure 1 shows a snapshot taken at 6.4 seconds after the asteroid hit the Earth. We have plotted the velocity vectors associated with all the particles contained in a thin vertical slab (about 2h thick). The smoothing length scale is of the order of the inter-particle spacing in the undisturbed Earth. Figure 2 displays at the same time the density contours in arbitrary units. Note that, although all variables are known only at particle locations, continuous quantities can be obtained by using the same particle based interpolation scheme found in the SPH code itself.

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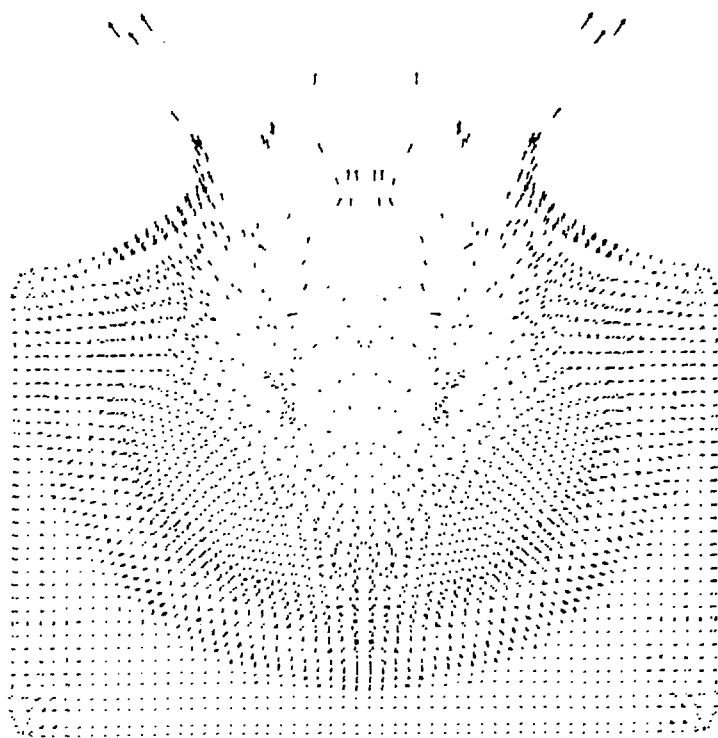


Figure 1

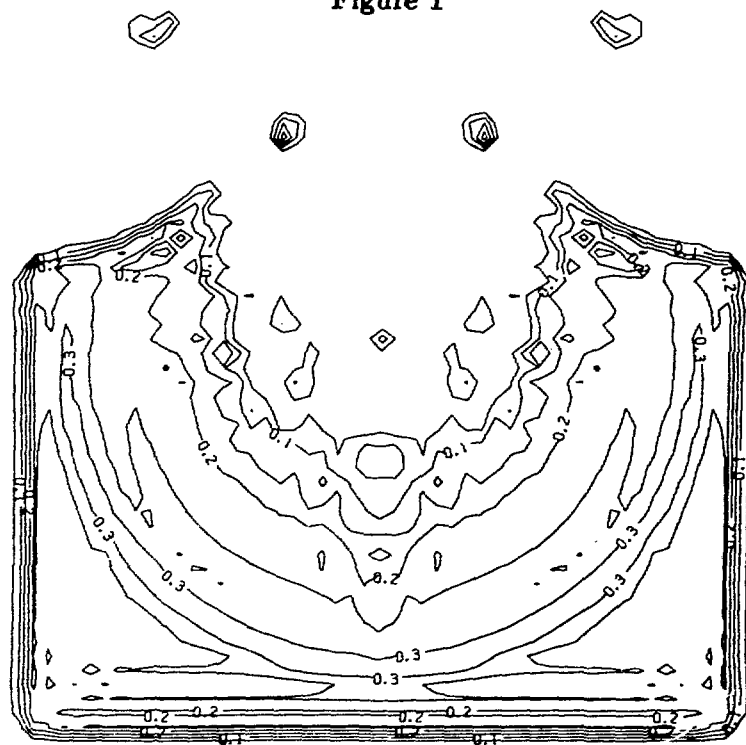


Figure 2

5. References

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A SMOOTHED PARTICLE CODE FOR 2D COMPRESSIBLE MULTIFLUID FLOWS

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ABSTRACT

The algorithm is based on an extension of Monaghan's smoothed particle method.

The code is able to compute multifluid unsteady flows involving strong shocks and great deformations. Each particle moves in the physical space with its mass, momentum, energy and material nature. The particles are Lagrangian and keep constant mass, but they exchange momentum and energy, by one to one interaction.

The interaction depends on the position of the particles, the amount of their quantities and the cut off. So the algorithm needn't any mesh.

In the present paper, first we describe the scheme, last we present a computed solution of a physical problem to show some possibilities of the method.

1/ INTRODUCTION

Classical numerical methods for flow computations used always fixed or moving mesh. In the case of 2D or 3D unsteady flows involving great deformations with material interfaces, it is very difficult to define a grid giving simultaneously good accuracy and robustness.

Models based on Eulerian hydrodynamics can handle deformations such as jet, eddies, but they have a poor resolution in regions of high compression.

The Lagrangian models are unable to compute great deformations without expensive rezoning, but they have a better resolution. Free lagrangian or adaptive mesh

methods have the both advantages, but generally the mesh computation is complicated.

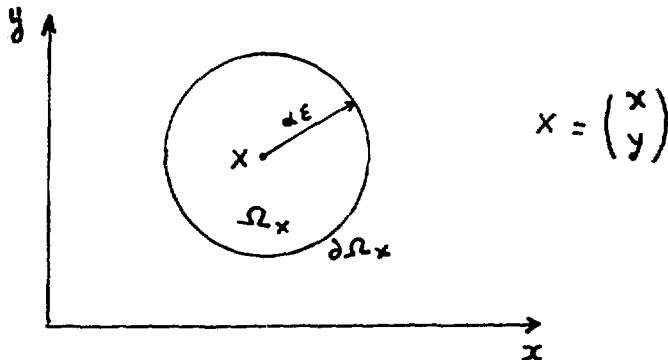
Therefore we have developed a smoothed particle multifluid 2D code, using no mesh. The particles move with the flow velocity. They conserve their mass and exchange their momentum and energy, by one to one interaction, so the algorithm is completely conservative.

2/ REGULARIZATION OF A FUNCTION.

2.1. Definition

Let a regularization function $\xi_\epsilon(x,y)$, such that :

$$(2.1) \quad \begin{aligned} \xi_\epsilon(X,Y) &= \xi_\epsilon(|X-Y|), \quad |X-Y| < \alpha\epsilon \\ \xi_\epsilon(X,Y) &= 0 \quad |X-Y| > \alpha\epsilon, \quad \alpha \in \mathbb{R}^+ \\ &\quad X \text{ and } Y \in \mathbb{R}^2 \end{aligned}$$



One deduces :

- For a given X , $\xi_\epsilon(X,Y)$ is constant on a circle of center X

$$(2.2) \quad \xi_\epsilon(X,Y) = 0 \text{ on the boundary } \partial \Omega_X$$

- $$(2.3) \quad \nabla_Y \xi_\epsilon(X,Y) = -\nabla_X \xi_\epsilon(X,Y)$$

by definition, the regularized function of $F(X)$ by $\xi_\epsilon(X,Y)$ is :

$$(2.4) \quad \overline{\overline{F(X)}} = \int_{\mathbb{R}^2} F(Y) \xi_\epsilon(X,Y) dY = \int_{\Omega_X} F(Y) \xi_\epsilon(X,Y) dY$$

then $F(Y)$ have to be defined on Ω_X .

2.2. Regularization of the gradient operator.

By definition, we have :

$$(2.5) \quad \overline{\nabla F(X)} = \int_{\Omega_X} \nabla F(Y) \xi_\epsilon(X, Y) dY$$

from (2.5) we obtain :

$$(2.6) \quad \overline{\nabla F(X)} = \int_{\partial\Omega_X} F(Y) \xi_\epsilon(X, Y) \vec{n} dY - \int_{\Omega_X} F(Y) \nabla_Y \xi_\epsilon(X, Y) dY$$

where $\vec{n}$ is the unit normal vector.

Taking (2.2) and (2.3) into account, we have :

$$(2.7) \quad \overline{\nabla F(X)} = \int_{\Omega_X} F(Y) \nabla_X \xi(X, Y) dY$$

It follows from (2.7) that :

$$\overline{\nabla F(X)} = \nabla \overline{F(X)}$$

Remark :

$$\int_{\Omega_X} F(X) \nabla_X \xi_\epsilon(X, Y) dY = \int_{\Omega_X} F(X) \xi(X, Y) \vec{n} dY$$

Taking (2.2) into account, it yields :

$$\int_{\Omega_X} F(X) \nabla_X \xi_\epsilon(X, Y) dY = 0$$

then we get :

$$(2.8) \quad \overline{\nabla F(X)} = \overline{\nabla F(X)} = \int_{\Omega_X} (F(X) + F(Y)) \nabla_X \xi_\epsilon(X, Y) dY$$

2.3. Regularization of divergence

$$\nabla \cdot \vec{U}(X) = \int_{\Omega_X} \nabla \cdot \vec{U}(Y) \xi_\epsilon(X, Y) dY$$

$$\nabla \cdot \vec{U}(X) = \int_{\partial\Omega_X} \vec{U}(Y) \xi_\epsilon(X, Y) \vec{n} dY - \int_{\Omega_X} \vec{U}(Y) \cdot \nabla_Y \xi_\epsilon(X, Y) dY$$

$$\nabla \cdot \vec{U}(X) = \int_{\Omega_X} \vec{U}(Y) \cdot \nabla_X \xi_\epsilon(X, Y) dY$$

$$(2.9) \quad \nabla \cdot \vec{U}(X) = \int_{\Omega_X} [\vec{U}(Y) - \vec{U}(X)] \cdot \nabla_X \xi(X, Y) dY$$

2.4. Conservation

We assume that :

$$(2.10) \quad \int_{R^2} \xi_\epsilon(X, Y) dY = 1$$

by definition we have : $\int_{R^2} \overline{\overline{F(X)}} dX = \int_{R^2} \left[\int_{R^2} F(Y) \xi_\epsilon(X, Y) dY \right] dX$

$$\int_{R^2} \overline{\overline{F(X)}} dX = \int_{R^2} F(Y) \left[\int_{R^2} \xi_\epsilon(X, Y) dX \right] dY$$

$$\int_{R^2} \overline{\overline{F(X)}} dX = \int_{R^2} F(Y) dY$$

3/ APPROXIMATION OF A FUNCTION BY MEANS OF PARTICLES :

3.1. Definition

Let a function $F(X)$ defined in Ω , $\Omega \subset R^2$. We consider a set of n points $\{X_i\}$ $X_i \in \Omega$, then we can approximate $F(X)$ by :

$$(3.1) \quad F(X) \approx \sum_{i=1}^{i=n} W(X_i) F(X_i) \delta(X - X_i)$$

$W(X_i)$ is a volume assigned to the point X_i .

$$\sum_i W(X_i) = \text{volume}(\Omega)$$

From (3.1), it follows that :

$$(3.2) \quad \int_{\Omega} F(X) dX \approx \sum_{i=1}^{i=n} W(X_i) F(X_i)$$

3.1 Approximation of the regularization of gradient and divergence

For the gradient we have : $\overline{\overline{\nabla F(X)}} = \int_{\Omega_X} (F(X) + F(Y)) \nabla_X \xi_\epsilon(X, Y) dY$

taking (3.2) into account, it yields :

$$\overline{\overline{\nabla F(X)}} \approx \sum_{j=1}^{j=n} W(X_j) (F(X) + F(X_j)) \nabla_X \xi_\epsilon(X, X_j)$$

from (3.1), it follows that :

$$\overline{\nabla F(X)} = \sum_{i=1}^{i=n} \sum_{j=1}^{j=n} W(X_i) W(X_j) (F(X_i) + F(X_j)) \delta(X - X_i) \nabla_{X_i} \xi_\varepsilon(X_i, X_j)$$

let X be equal to X_1 , we get :

$$(3.3) \quad \overline{\nabla F(X_1)} \approx \sum_j W(X_1) W(X_j) [F(X_1) + F(X_j)] \nabla_{X_1} \xi_\varepsilon(X_1, X_j)$$

By the same way, we find for the divergence :

$$(3.4) \quad \nabla \cdot \overline{\vec{U}(X_1)} \approx \sum_j W(X_1) W(X_j) [\vec{U}(X_j) - \vec{U}(X_1)] \nabla_{X_1} \xi_\varepsilon(X_1, X_j)$$

Remark :

If we have to approximate $\nabla \cdot \vec{G}(x)$, where $\vec{G}(X) = F(X) \cdot \vec{U}(X)$ we can write :
 $F(X) \nabla \cdot \vec{U}(X) + \vec{U}(X) \cdot \nabla F(X)$

Therefore :

$$\begin{aligned} \nabla \cdot \vec{G}(X_1) &\approx F(X_1) \sum_j W(X_1) W(X_j) [\vec{U}(X_j) - \vec{U}(X_1)] \cdot \nabla_{X_1} \xi_\varepsilon(X_1, X_j) \\ &\quad + \vec{U}(X_1) \sum_j W(X_1) W(X_j) [F(X_1) + F(X_j)] \nabla_{X_1} \xi_\varepsilon(X_1, X_j) \end{aligned}$$

we get :

$$(3.5) \quad \nabla \cdot \vec{G}(X_1) \approx \sum_j W(X_1) W(X_j) [\vec{U}(X_j) F(X_1) + \vec{U}(X_1) F(X_j)] \nabla_{X_1} \xi_\varepsilon(X_1, X_j)$$

4/ APPLICATION TO THE LAGRANGIAN HYDRODYNAMICS

4.1 Equation in lagrangian form

Consider a point $X = \begin{pmatrix} x \\ y \end{pmatrix}$, moving with the fluid velocity.

$$X = X(X^0, t), \quad X(X^0, 0) = X^0$$

$$\frac{dX}{dt} = \vec{V}$$

We denote by $J(X^0, t)$, the Jacobian $\begin{vmatrix} \frac{\partial x}{\partial x^0} & \frac{\partial x}{\partial y^0} \\ \frac{\partial y}{\partial x^0} & \frac{\partial y}{\partial y^0} \end{vmatrix}$

Therefore the lagrangian hydrodynamics equations, can be written :

$$(4.1) \quad \frac{1}{J(X^0, t)} \frac{\partial}{\partial t} [J(X^0, t) \rho(X^0, t)] = 0$$

$$(4.2) \quad \frac{1}{J(X^0, t)} \frac{\partial}{\partial t} [J(X^0, t) \rho(X^0, t) \vec{V}(X^0, t)] = -\nabla_X p(x, t)$$

$$(4.3) \quad \frac{1}{J(X^0, t)} \frac{\partial}{\partial t} [J(X^0, t) \rho(X^0, t) E(X^0, t)] = -\vec{V} \cdot \nabla_X p - p \nabla_X \cdot \vec{V}$$

(ρ = densite, $\vec{V}$ = velocity, E = total energy, p = pressure) with the state equation
 $p = p(\rho, e)$, $e = E - \frac{1}{2} \vec{V}^2$

4.2. Space discretization

Taking into account (3.1), (3.3), (3.5), we obtain :

$$(4.4) \quad \frac{W(X_1^0, t)}{J(X_1^0, t)} \frac{\partial}{\partial t} [J(X_1^0, t) \rho(X_1^0, t)] = 0$$

$$(4.5) \quad \frac{W(X_1^0, t)}{J(X_1^0, t)} \frac{\partial}{\partial t} [J(X_1^0, t) \rho(X_1^0, t) \vec{V}(X_1^0, t)] = \\ - \sum_j W(X_1^0, t) W(X_j^0, t) [p(X_1^0, t) + p(X_j^0, t)] \nabla_{X_1} \xi_e(X_1, X_j)$$

$$(4.6) \quad \frac{W(X_1^0, t)}{J(X_1^0, t)} \frac{\partial}{\partial t} [J(X_1^0, t) \rho(X_1^0, t) E(X_1^0, t)] = \\ - \sum_j W(X_1^0, t) W(X_j^0, t) [p(X_1^0, t) \vec{V}(X_j^0, t) + p(X_j^0, t) \vec{V}(X_1^0, t)] \nabla_{X_1} \xi_e(X_1, X_j)$$

Actually, we put :

$$(4.7) \quad W(X_1^0, t) = J(X_1^0, t) W(X_1^0, 0)$$

Therefore (4.4), can be written as :

$$(4.8) \quad \frac{\partial}{\partial t} [W(X_1^0, 0) J(X_1^0, t) \rho(X_1^0, t)] = 0$$

consequently, we get :

$$(4.9) \quad W(X_1^0, 0) J(X_1^0, t) \rho(X_1^0, t) = m_1$$

m_1 may be considered as the constant mass of a particle, located at $X(X_1^0, t)$.

From (4.7) and (4.9), we deduce the following form for the equations of conservation :

$$(4.10) \quad m_1 = ct$$

$$(4.11) \quad m_1 \frac{d\vec{V}}{dt} = - \sum_j \frac{m_1}{\rho(X_1^0, t)} \frac{m_j}{\rho_j(X_j^0, t)} [p(X_1^0, t) + p(X_j^0, t)] \nabla_{X_1} \xi_\varepsilon(X_1, X_j)$$

$$(4.12) \quad m_1 \frac{dE_1}{dt} = - \sum_j \frac{m_1}{\rho(X_1^0, t)} \frac{m_j}{\rho_j(X_j^0, t)} [p(X_1^0, t) \vec{V}(X_j^0, t) + p(X_j^0, t) \vec{V}(X_1^0, t)] \nabla_{X_1} \xi_\varepsilon(X_1, X_j)$$

The mass of each particle remains constant, but the momentum and the total energy change by interaction with other particles.

Consider equation (4.11), we see that the momentum interaction of the "j" particle on the "i" particle is :

$$\left(m_1 \frac{d\vec{V}_1}{dt} \right)_j = \frac{m_1}{\rho_1} \frac{m_j}{\rho_j} (p_1 + p_j) \nabla_{X_1} \xi_\varepsilon(X_1, X_j)$$

Conversely the interaction of "i" on "j" is :

$$\left(m_j \frac{d\vec{V}_j}{dt} \right)_i = \frac{m_1}{\rho_1} \frac{m_j}{\rho_j} (p_1 + p_j) \nabla_{X_j} \xi_\varepsilon(X_1, X_j)$$

We deduce that :

$$(4.13) \quad \left(m_1 \frac{d\vec{V}_1}{dt} \right)_j = - \left(m_j \frac{d\vec{V}_j}{dt} \right)_i$$

It follows from (4.13) that (4.11) meet the condition of conservation.

On the same way, we prove the conservation of total energy.

It is possible to replace equation of total energy by equation of internal energy.

$$m_1 \frac{de_1}{dt} = m_1 \frac{dE_1}{dt} - m_1 \vec{V}_1 \frac{d\vec{V}_1}{dt}$$

from (4.11) and (4.12), it follows :

$$(4.14) \quad m_i \frac{de_i}{dt} = - p_i \sum_j \frac{m_i}{\rho_i} \frac{m_j}{\rho_j} (\vec{v}_i - \vec{v}_j) \cdot \nabla_{X_j} \xi_\varepsilon(X_i, X_j)$$

4.3. Time discretization

$$(4.15) \quad m_i \vec{v}_i^{n+1} = m_i \vec{v}_i^n + m_i \left(\frac{d\vec{v}}{dt} \right)_i^n \Delta t$$

$$(4.16) \quad X_i^{n+1} = X_i^n + \vec{v}_i^{n+1} \Delta t$$

$$(4.17) \quad m_i e_i^{n+1} = m_i e_i^n + m_i \left(\frac{de}{dt} \right)_i^{n+\frac{1}{2}} \Delta t$$

$$(4.18) \quad p_i^{n+1} = p(\rho_i^{n+1}, e_i^{n+1})$$

with :

$$(4.19) \quad m_i \left(\frac{d\vec{v}}{dt} \right)_i^n = - \sum_j \frac{m_i}{\rho_i} \frac{m_j}{\rho_j} (p_i^n + p_j^n) \nabla_{X_j} \xi_\varepsilon(X_i^n, X_j^n)$$

$$(4.20) \quad m_i \left(\frac{de}{dt} \right)_i^{n+\frac{1}{2}} = - \frac{1}{2} (p_i^n + p_i^{n+1}) \sum_j \frac{m_i}{\rho_i^{n+\frac{1}{2}}} \frac{m_j}{\rho_j^{n+\frac{1}{2}}} (\vec{v}_j^{n+1} - \vec{v}_i^{n+1}) \cdot \nabla_{X_i} \xi_\varepsilon(X_i^{n+\frac{1}{2}}, X_j^{n+\frac{1}{2}})$$

$$(4.21) \quad \rho_i^{n+1} = \sum_j m_j \xi_\varepsilon(X_i^{n+1}, X_j^{n+1})$$

$$(4.22) \quad X_i^{n+\frac{1}{2}} = \frac{1}{2} (X_i^n + X_i^{n+1})$$

$$(4.23) \quad \rho_i^{n+\frac{1}{2}} = \frac{1}{2} (\rho_i^n + \rho_i^{n+1})$$

5/ ARTIFICIAL VISCOSITY

The introduction of an artificial viscosity is necessary to obtain the stability.

$$q(X, t) = -k \varepsilon \rho(X, t) C(X, t) a(X, t) \nabla \cdot \vec{v}(X, t)$$

where : k is an arbitrary coefficient
 ϵ is the parameter of the function $\xi_\epsilon(X,Y)$
 C is the speed of the sound
 a is a coefficient such that :

$$\begin{aligned} a &= 1 & \text{if } \nabla \cdot \vec{V} < 0 \\ a &= 0 & \text{if } \nabla \cdot \vec{V} > 0 \end{aligned}$$

Therefore (4.11), is changed in :

$$\begin{aligned} (4.11)' \quad m_1 \frac{d\vec{V}_1}{dt} &= - \sum_j \frac{m_1}{\rho_1} \frac{m_j}{\rho_j} (p_1 + p_j) \nabla_{X_1} \xi_\epsilon(X_1, X_j) \\ &- \frac{k\epsilon}{2} \sum_j \frac{m_1}{\rho_1} \frac{m_j}{\rho_j} (C_1 \rho_1 + C_j \rho_j) a_{1j} \frac{(\vec{V}_1 - \vec{V}_j) \cdot (X_1 - X_j)}{(X_1 - X_j)^2 + \beta^2 \epsilon^2} \nabla_{X_1} \xi_\epsilon(X_1, X_j) \end{aligned}$$

and (4.14) is changed in :

$$\begin{aligned} (4.14)' \quad m_1 \frac{de_1}{dt} &= - p_1 \sum_j \frac{m_1}{\rho_1} \frac{m_j}{\rho_j} (\vec{V}_j - \vec{V}_1) \cdot \nabla_{X_1} \xi_\epsilon(X_1, X_j) \\ &- \frac{k\epsilon}{2} \sum_j \frac{m_1}{\rho_1} \frac{m_j}{\rho_j} C_1 \rho_1 (V_j - V_1) a_{1j} \frac{(\vec{V}_1 - \vec{V}_j) \cdot (X_1 - X_j)}{(X_1 - X_j)^2 + \beta^2 \epsilon^2} \nabla_{X_1} \xi_\epsilon(X_1, X_j) \end{aligned}$$

$$\text{where : } a_{1j} = 1 \quad \text{if } (\vec{V}_1 - \vec{V}_j) \cdot (X_1 - X_j) \leq 0$$

$$a_{1j} = 0 \quad \text{if } (\vec{V}_1 - \vec{V}_j) \cdot (X_1 - X_j) > 0$$

6/ TIME STEP

$$(6.1) \quad \Delta t = \text{Max}_1 \left(\frac{\alpha \epsilon}{C_1} \right)$$

we recall that : $\xi_\epsilon(X_1, X_j) = 0$ if $|X_1 - X_j| > \alpha \epsilon$

(6.1) means that a perturbation moving at the speed sound, can interact with the neighbour particles.

7/ CHOICE OF THE REGULARIZATION FUNCTION $\xi_\epsilon(X,Y)$

We are seeking for a function such that :

$$\xi_\epsilon(X,Y) = \xi_\epsilon(r), \quad r = |X-Y|, \quad x, y \in \mathbb{R}^2$$

$$\int_0^{+\infty} \int_0^{2\pi} \xi_\epsilon(r) r \, dr \, d\theta = 1$$

$$\xi_\epsilon(r) = \frac{1}{\epsilon^2} \xi\left(\frac{r}{\epsilon}\right)$$

$$\xi_\epsilon(-r) = \xi_\epsilon(r)$$

The gaussian gives interpolation errors of $O(\epsilon^2)$

$$\xi_\epsilon(X, Y) = \frac{1}{\pi\epsilon^2} \exp\left(-\frac{(X-Y)^2}{\epsilon^2}\right)$$

If we take exactly the gaussian, each particle interact with all particles, so the summations are very expensive. In practice it is sufficient to take :

$$\xi_\epsilon(X, Y) = \frac{1}{\pi\epsilon^2} \exp\left(-\frac{(X-Y)^2}{\epsilon^2}\right), \quad |X-Y| < \alpha\epsilon$$

$$\xi_\epsilon(X, Y) = 0, \quad |X-Y| \geq \alpha\epsilon$$

Let $\alpha = 2.63$, then

$$1 - \int_0^{\alpha\epsilon} \int_0^{2\pi} \xi_\epsilon(r) r \, dr \, d\theta = 10^{-3}$$

$$\xi_\epsilon(\epsilon) = 3.15 \cdot 10^{-4}$$

The super gaussian gives interpolation errors of $O(\epsilon^4)$

$$\xi_\epsilon(X, Y) = \frac{1}{\pi\epsilon^2} \left(2 - \frac{(X-Y)^2}{\epsilon^2}\right) \exp\left(-\frac{(X-Y)^2}{\epsilon^2}\right)$$

The super gaussian is a function such that :

$$\int_0^{+\infty} \int_0^{2\pi} \xi_\epsilon(r) r \, dr \, d\theta = 1$$

and :

$$\int_0^{+\infty} \int_0^{2\pi} r^2 \xi_\epsilon(r) r \, dr \, d\theta = 0$$

In practice we take :

$$\xi_\epsilon(X, Y) = \frac{1}{\pi\epsilon^2} \left(2 - \frac{(X-Y)^2}{\epsilon^2} \right) \exp \left(- \frac{(X-Y)^2}{\epsilon^2} \right), |X-Y| \leq \alpha\epsilon$$

$$\xi_\epsilon(X, Y) = 0, |X-Y| > \alpha\epsilon$$

Let $\alpha = 3$, then :

$$1 - \int_0^{\alpha\epsilon} \int_0^{2\pi} \frac{1}{\pi\epsilon^2} \left(2 - \frac{r^2}{\epsilon^2} \right) \exp \left(- \frac{r^2}{\epsilon^2} \right) r \, dr \, d\theta = 10^{-3}$$

$$\xi(3\epsilon) \approx 2.74 \cdot 10^{-4}$$

8/ NUMERICAL RESULTS

To deal with the accuracy of the method we first present some results about the SOD's shock tube problem.

Initial conditions : $\rho_1 = 1$ $p_1 = 1$ $u_1 = 0$

$$\gamma = 1.4$$

$$\rho_2 = 0.125, p_2 = 0.1, u_2 = 0$$

The computation is first done with the following parameters :

regularization function parameter : $\epsilon = 0.01$

artificial viscosity coefficient : $k = 0.8$

number of particles for fluid 1 : $n_1 = 140$

mass of each particle for fluid 1 : $m_1 = 2.86 \cdot 10^{-3}$

number of particles for fluid 2 : $n_2 = 140$

mass of each particle for fluid 2 : $m_2 = 0.337 \cdot 10^{-3}$

The figure 1, shows the values of density, pressure and velocity. We can see that the shock is spread on 2ε . There are 6 particles in the shock zone.

IMPACT PROBLEM

When particle methods are used to simulate high speed collision, it may occur that particles penetrate the material interface.

The figure 2 shows the particles positions of the projectile and the target. Particles don't penetrate interface.

There are 1024 particles in the target, and 224 particles in the projectile.

The projectile velocity : $V = 100000$ cm/s.

The figure 3, shows the isovalues of pressure density and internal energy.

CONCLUSIONS

This method works without any mesh. The spatial resolution can be increased during the computation by reducing ε , without introducing any dissipation.

The numerical applications show that the code is able to compute shocks without numerical oscillations and collision without particles penetration.

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INTRODUCTION

The aim of this paper is the numerical treatment of the non linear terms of the radiative transfer equations. Of course we consider here only the simplest form of these equations, that is to say without taking into account hydrodynamic terms, Compton or Thomson scattering terms.

Provided the radiative transfer equations are transport equations, we consider here the diffusion form of these equations, so called "multigroup diffusion equations", (of course these equations are coupled with a non linear energy balance equation).

Indeed this form is more simpler than the original one. On the other hand we can see that the asymptotic solution of this system when the opacities go to infinity is the same as the asymptotic solution of the original system, that is to say solution given by the Rosseland approximation (see ref [1/]). Moreover it is possible to solve numerically a linear transport equation with the help of a diffusion one and a corrector which can be evaluated by a particular method, as it is shown in [2/].

After time and frequency discretisations we must solve the following system where the unknown functions are the radiative energy densities $\psi_n = \psi_n(x)$ in the frequency group n ($n = 1, 2, \dots, N$) and the temperature $T = T(x)$ (where the spatial variable x belongs to a bounded domaine D of R^3).

$$(1) \quad \frac{1}{\tau} (\psi_n - \psi_n^0) - \nabla \cdot \frac{1}{3 \sigma_n} \nabla \psi_n + k_n \psi_n = k_n B_n(T) \\ + \text{boundary conditions}$$

$$(1)^{bis} \quad e(T) - e(T^0) + \tau \sum_n [k_n B_n(T) - k_n \psi_n] = Q$$

where $\tau = c \cdot \Delta t$ (c is the light velocity and Δt the time interval).

$e(T)$ is the specific internal energy at the temperature T .

k_n and σ_n are the opacities in the group n [which depend on the spatial variable].

$B_n(T)$ is the integral of the Planck function in the group n .

T^0 and ϕ_n^0 are known at the beginning of the time interval.

Q is the external energy.

To solve this system we propose an iterative scheme called multigroup direct scheme, which has been introduced first in /3/ and which is based on the Newton method. After the first linearization of $B_n(T)$ and $e(T)$ by a very classical way, one must solve a large scale system which we handle with a synthetic acceleration method.

In the first part of this paper we describe the scheme ; afterwards we analyse this scheme in the case of the opaque limit. Then we compare this scheme with another one which is based (as in /4/) on a quite different linearization and we give numerical results.

1. Description of the multigroup Direct scheme

Let us denote :

$$\theta(T) = \sum_n B_n(T) \equiv a T^4 \quad \text{where } a \text{ is the radiative constant}$$

From now on, we will write $e(\theta)$ and $B_n(\theta)$ for $e(T)$ and $B_n(T)$ if $\theta = \theta(T)$, and we denote :

$$\begin{aligned} \theta^0 &= \theta(T^0) , & B_n^0 &= B_n(\theta^0) \\ \lambda &= \frac{\partial e}{\partial \theta}(\theta^0) \end{aligned}$$

$$\beta_n^0 = \frac{\partial B_n}{\partial \theta} (\theta^0)$$

If we first make the linearization of $B_n(\theta)$ and $e(\theta)$ by :

$$(2) \quad B_n^0 + \beta_n^0 (\theta - \theta^0) \quad \text{and} \quad e(\theta) + \lambda (\theta - \theta^0)$$

and we put that in equation (1) and (1)^{bis}, we obtain the following relationships for the temperature θ and the radiative intensity ϕ_n :

$$(3) \quad \tau^{-1} \lambda (\theta - \theta^0) + \sum_m [k_m^0 B_m^0 + k_m^0 \beta_m^0 (\theta - \theta^0) - k_m^0 \phi_m] = Q$$

$$(4) \quad \tau^{-1} (\phi_n - \phi_n^0) - \nabla \frac{1}{3\sigma_n} \nabla \phi_n + k_n^0 \phi_n = k_n^0 B_n^0 + k_n^0 \beta_n^0 (\theta - \theta^0)$$

That is to say we have to solve a set of n diffusion equations which are coupled altogether.

$$(5) \quad \tau^{-1} (\phi_n - \phi_n^0) - \nabla \frac{1}{3\sigma_n} \nabla \phi_n + k_n^0 \phi_n = k_n^0 B_n^0 + k_n^0 \beta_n^0 \frac{\eta^0}{L} \left[\sum_m (k_m^0 \phi_m - k_m^0 B_m^0) + Q \right]$$

$$\text{where } L = \sum_m k_m^0 \beta_m^0 \quad \text{and} \quad \eta^0 = L (\tau^{-1} \lambda + L)^{-1}$$

Of course it is not necessary to solve exactly this system. In fact we first solve a system where all the diffusion equations are decoupled ; afterwards we use a "synthetic diffusion" acceleration method in order to take into account the coupling between all the diffusion equations. And we go on with a new step of the Newton method, that is to say we linearize $B_n(\theta)$ and $e(\theta)$ around the temperature which has been evaluated after the first synthetic diffusion acceleration. We will emphasize the different steps of the scheme.

First we define $\phi_n^{\frac{1}{2}}$ as the solution of the following equation [which is the same as (5) but the coupling term] :

$$(6) \quad \tau^{-1}(\psi_n^{1/2} - \psi_n^0) - \nabla \frac{1}{3\sigma_n} \nabla \psi_n^{1/2} + k_n \psi_n^{1/2} = k_n B_n^0 + \\ + k_n \beta_n^0 \frac{\eta}{L} \left[\sum_m (k_m \psi_m^0 - k_m B_m^0) + Q \right]$$

Afterwards, we define w^1 (which does not depend on n) by putting $(\psi_n^{1/2} + \beta_n^0 w^1)$ in place of ψ_n in equation (5) and adding all the group-dependant equations. Thus it may be easily seen that w^1 satisfy the following equation :

$$(7) \quad \tau^{-1} w^1 - \nabla \left[\sum_m \frac{1}{3\sigma_m} \nabla \beta_m^0 w^1 \right] + (1-\eta^0) \left(\sum_m k_m \beta_m^0 \right) w^1 = \\ = \eta^0 \sum_m k_m (\psi_m^{1/2} - \psi_m^0)$$

Obviously we let :

$$(8) \quad \psi_n^1 = \psi_n^{1/2} + \beta_n^0 w^1$$

and we define $\theta^1 = \theta$, where θ is the solution of (3) with $\psi_m = \psi_m^1$. Now the first step of the scheme is achieved and we go on with a new step. If we linearize (1) and (2) around θ^1 we obtain [if we denote $\beta_n^1 = \frac{\partial B_n}{\partial \theta}(\theta^1)$; $\lambda^1 = \frac{\partial e}{\partial \theta}(\theta^1)$; $B_n^1 = B_n(\theta^1)$] :

$$(9) \quad \tau^1 \lambda^1 (\theta - \theta^1) + \frac{e(\theta^1) - e(\theta)}{\tau} + \sum_m [k_m B_m^1 + k_m \beta_m^1 (\theta - \theta^1) - k_m \psi_m^1] = Q$$

and :

$$(10) \quad \tau^{-1}(\psi_n - \psi_n^0) - \nabla \frac{1}{3\sigma_n} \nabla \psi_n + k_n \psi_n = k_n B_n^1 + k_n \beta_n^1 (\theta - \theta^1)$$

Then, by the same way as before we define $\psi_n^{3/2}$ as the solution of :

$$\begin{aligned}
 (11) \quad \tau^{-1}(\psi_n^{3/2} - \psi_n^0) - \nabla \frac{1}{3\sigma_n} \nabla \psi_n^{3/2} + k_n \psi_n^{3/2} = \\
 = k_n B_n^1 + k_n \beta_n^1 \frac{\eta^1}{L^1} \left[\sum_m (k_m \psi_m^1 - k_m B_m^1) + Q + \frac{e(\theta^1) - e(\theta^0)}{\tau} \right]
 \end{aligned}$$

(where $L^1 = \sum k_m \beta_m^1$, $\eta^1 = L^1(\tau^{-1} \lambda + L^1)^{-1}$).

and we define w^2 (independent on n) by putting $(\psi_n^{3/2} + \beta_n^1 w^2)$ in place of ψ_n in equation (9). Then let :

$$(12) \quad \psi_n^2 = \psi_n^{3/2} + \beta_n^1 w^2$$

and let θ^2 be the solution of (9) with $\psi_n = \psi_n^2$.

Afterwards we iterate upon convergence.

Remark : The choice of β_n^0 for the acceleration term $(\beta_n^0 w^1)$ in the first step corresponds to the principle of the synthetic acceleration. Indeed, if one define a coupling operator H by :

$$(13) \quad (H\Phi)_n = k_n \hat{\Phi}_n - k_n \beta_n^0 (\sum k_m \hat{\Phi}_m) / L \quad \forall \Phi = \{\hat{\Phi}_n\}$$

then the right hand side of (5) may be written in the following form :

$$\eta^0 k_n \psi_n^0 + (1 - \eta^0) k_n B_n^0 - \eta^0 (H(\psi - B^0))_n + \frac{k_n \beta_n^0}{L} \eta^0 Q$$

And when we make the calculus of $\psi^{1/2}$, the coupling operator is handled by an "explicit way", so in the acceleration step we have to add a term which is in the principal eigenspace of the coupling operator (here the eigenfunction is β_n^0).

2. Asymptotic analysis in the opaque limit

Assume that the whole spatial domain is an opaque medium that is to say that the mean free path k_n^{-1} , σ_n^{-1} are very small with respect to a typical size. Then we can make the following scaling :

$$(14) \quad \begin{aligned} \bar{k}_n &= \varepsilon k_n \\ \bar{\sigma}_n &= \varepsilon \sigma_n \\ \bar{x} &= x/\sqrt{\varepsilon} \quad \bar{v} = \frac{\partial}{\partial \bar{x}} \end{aligned}$$

where ε is a small parameter. The meaning of this scaling is the following : the typical size of the phenomena is small ($x \approx \bar{x} \sqrt{\varepsilon}$) but the typical mean free path is still smaller.

Then we see that :

$$(15) \quad L = \frac{1}{\varepsilon} \bar{L} \quad \text{where} \quad \bar{L} = \sum_n \beta_n^0 \bar{k}_n$$

$$1 - \eta^0 = \frac{\varepsilon}{\varepsilon + \tau \bar{L}/\lambda} \quad \frac{1 - \eta^0}{\varepsilon} = \frac{\lambda}{\tau \bar{L}} + O(\varepsilon)$$

If one introduces the operator $\bar{H}$ which is the same as H , but $\bar{k}_n$ and $\bar{L}$ are put in place of k_n and L , the system (3)(5) may be written in the following form :

$$(16) \quad \tau^{-1} (\psi_n - \psi_n^0) - v \frac{1}{3\sigma_n} \nabla \psi_n + \frac{1-\eta^0}{\varepsilon} \bar{k}_n (\psi_n - B_n^0) = -\frac{1}{\varepsilon} \eta^0 (\bar{H}(\psi - B^0))_n + \frac{\bar{k}_n \beta_n^0}{\bar{L}} \eta^0 Q$$

$$(17) \quad \tau^{-1} \lambda (\theta - \theta^0) = \frac{1-\eta^0}{\varepsilon} \sum_n \bar{k}_n (\psi_n - B_n^0) + (1-\eta^0) Q$$

Recall that (16) has to be considered with a boundary condition, for instance a non homogeneous Dirichlet boundary condition

$$\psi_n|_{\partial D} = B_n(\chi) \quad \forall n, \quad \text{for a given constant } \chi.$$

Let us write ψ_n^ε and θ^ε instead of ψ_n and θ . We will now study the limit of ψ_n^ε and θ^ε when ε goes to 0, in order to know if our time and frequency discretization

yield a "good solution" when we are in a very opaque case. Assume that the σ_n 's are bounded from below.

First we have to state a crucial lemma (which may be easily proved).

Lemma : The operator $\bar{H}$ has a simple principal eigenvalue which is 0. Moreover for any $y \in \mathbb{R}^N$ if we denote by $\bar{y}$ the projection of y onto the principal eigenspace (that is to say $\bar{y}_n = \beta_n^0 \sum y_\lambda$) there exists α positif such that :

$$\sum_n y_n (\bar{H}y)_n \geq \alpha \|y - \bar{y}\|^2$$

Now if we assume that θ^0 and ψ_n^0 are bounded and independant on ϵ , we see that θ^ϵ and ψ_n^ϵ are bounded. Let us denote :

$$y_n^\epsilon = \psi_n^\epsilon - B_n^0$$

Let us multiply (16) by y_n and integrate over x , then, adding all the obtained equations, we see that :

$$\begin{aligned} (18) \quad & \tau^{-1} \sum_n \int [\psi_n^\epsilon - \psi_n^0] + \left(\frac{1-\eta}{\epsilon}\right) k_n y_n^\epsilon y_n^\epsilon dx + \sum_n \int_D \frac{1}{3\sigma_n} \|\nabla y_n^\epsilon\|^2 + \\ & + \sum_n \int_D \frac{1}{3\sigma_n} B(\theta) \cdot \nabla y_n^\epsilon dx \\ & = \frac{-1}{\epsilon} \eta^0 \int_D \sum_n (\bar{H}y^\epsilon)_n y_n^\epsilon dx \leq 0 \end{aligned}$$

Then, since the family (y^ϵ) is bounded in $[L^2(D)]^N$, we see that :

$$\sum_n \left(\inf \frac{1}{3\sigma_n} \right) \|\nabla y_n^\epsilon\|_{L^2}^2 \leq c_2 \sum_n \|\nabla y_n^\epsilon\| + c_3 \quad (c_2, c_3 \text{ constant})$$

Thus the family (y^ϵ) is bounded in the Sobolev space $[H^1(D)]^N$ and there exists a sequence (still denoted (y^ϵ)) and a function y^* of $[H^1(D)]^N$ such that:

$$y_n^\epsilon \longrightarrow y_n^* \quad \text{in } L^2(D)$$

On the other hand, according to (18), and the previous lemma we see that :

$$\sum_n \|y_n^\varepsilon - \bar{y}_n^\varepsilon\|_{L^2(D)}^2 \leq \varepsilon \quad c^t$$

Thus we see that

$$\bar{y}_n^\varepsilon \longrightarrow y_n^*$$

That is to say that y_n^* is in the principal eigenspace of $\bar{H}$ and that there exists v^* (independent on n) such that $y_n^* = v^* \beta_n^0$. Thus :

$$(19) \quad \psi_n^\varepsilon \longrightarrow \psi_n^* = B_n^0 + v^* \beta_n^0 \quad \text{in } L^2(D)$$

Now if we consider the equation (17) we see with the help of (15) that :

$$(20) \quad \theta^\varepsilon - \theta^0 \longrightarrow v^* \quad \text{in } L^2(D)$$

Moreover if we assume that : $\psi_n^0 = B_n(\theta^0)$ and $\theta^0|_{\partial D} = \chi$, it may be easily checked that v^* satisfies :

$$(21) \quad \tau^{-1}(1+\lambda) v^* - \nabla \sum_n \frac{1}{3\sigma_n} \nabla (B_n^0 + v^* \beta_n^0) = 0, \quad v^*|_{\partial D} = 0$$

Since $B_n^0 + v^* \beta_n^0$ is very close to $B_n(\theta^0 + v^*)$, we see that v^* is very close to the solution v of the following equation :

$$\tau^{-1}(1+\lambda)v - \nabla \left[\sum_n \frac{1}{3\sigma_n} \frac{\partial B_n}{\partial \theta} (\theta^0 + v) \right] \nabla (\theta^0 + v) = 0, \quad v|_{\partial D} = 0$$

which is the first step for solving the Rosseland equation associated to the problem (1) (1)^{bis}.

3. Comparison with another linearization and numerical results

Let us now consider a scheme which is the same as the previous one, but with a quite different linearization of $B_n(\theta)$. This kind of scheme has been introduced in

/4/. The difference with the previous linearization is that $B_n(\theta)$ is linearized by :

$$(22) \quad B_n(\theta) \approx \frac{B_n^0}{\theta^0} \theta = B_n^0 + b_n^0 (\theta - \theta^0)$$

where $b_n^0 = \frac{B_n^0}{\theta^0}$

Let us remark that $\sum_n b_n^0 = 1$ and that $\sum_n \beta_n^0 = 1$. So rather than (5) we have to solve :

$$(23) \quad \tau^{-1}(\psi_n - \psi_n^0) - \nabla \frac{1}{3\sigma_n} \nabla \psi_n + k_n \psi_n = k_n b_n^0 \theta^0 + \frac{k_n b_n^0}{\tau^{-1}\lambda + \sum_m k_m b_m^0} [\sum_m k_m (\psi_m - b_m^0) + Q]$$

As it may be seen this equation is simpler than (5) because a simplification occurs in the right-hand side of (22). On the other hand, the same scheme as before may be developed with this linearization.

But if we perform the same asymptotic analysis as before, with the same scaling and the same assumptions, we can see that (19) and (20) hold, but w^* is put in place of v^* , and satisfies the following equation :

$$(24) \quad \tau^{-1}(1+\lambda) w^* - \nabla \sum_n \frac{1}{3\sigma_n} \nabla (B_n^0 + w^* b_n^0) = 0 \quad w^*|_{\partial D} = 0$$

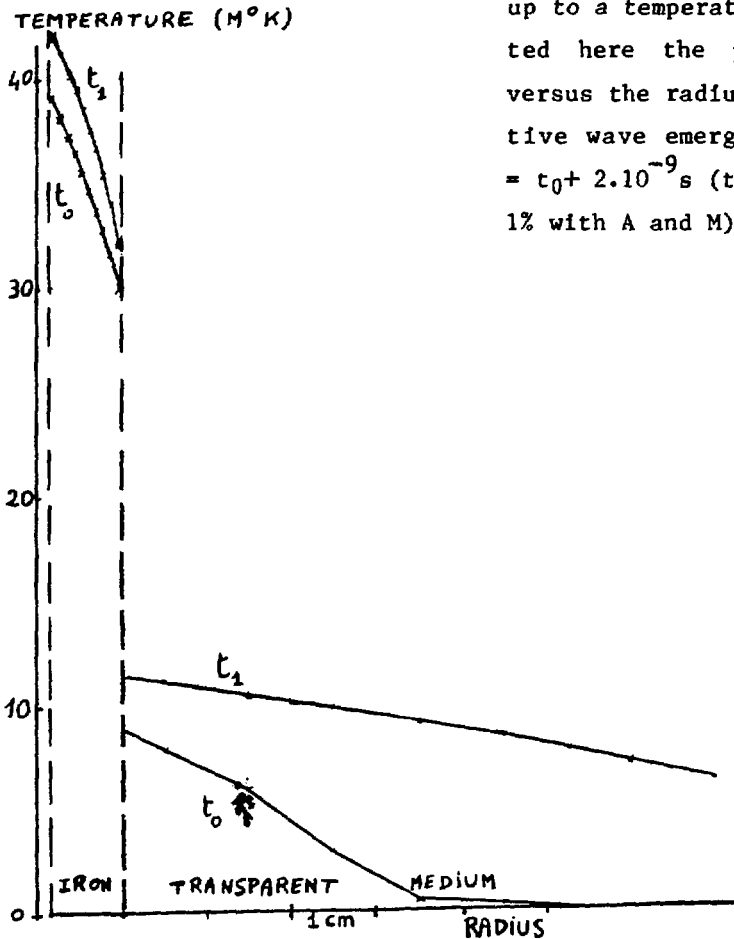
In the article [1], the solutions v^* and w^* of (23) and (24) are compared with solution u^* of the equation obtained after the first linearization of the Rosseland diffusion equation that is to say :

$$\tau^{-1}(1+\lambda) u^* - \nabla \left[\sum_n \frac{\beta_n^0}{3\sigma_n} \right] \nabla (\theta^0 + u^*) = Q \quad u^*|_{\partial D} = 0$$

Now we compare numerical results obtained, in a 1 dimensional spherical geometry, by the schemes corresponding to the linearization (2) and (22) which we call scheme A and scheme M respectively.

Consider a portion of sphere from iron whose thickness is .85 cm (this material is opaque for the considered temperature) and which is surrounded by a transparent medium.

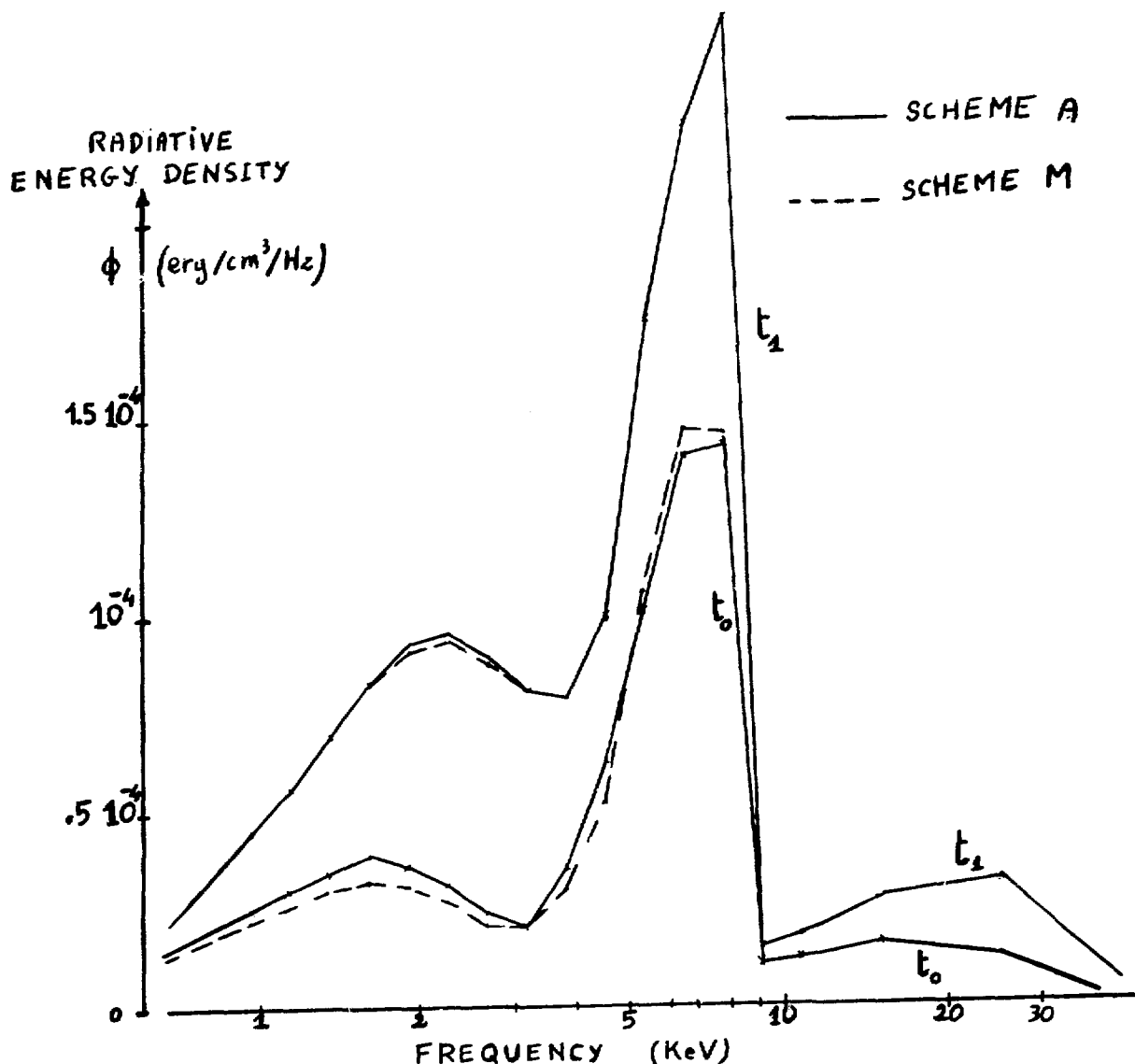
The initial temperature is $.1\text{M}^\circ\text{K}$ and the iron portion is heated from the interior up to a temperature of $42\text{ M}^\circ\text{K}$. We have plotted here the profile of the temperature versus the radius at time t_0 when the radiative wave emerge out of iron and at time $t_1 = t_0 + 2.10^{-9}\text{ s}$ (the profile is the same up to 1% with A and M).



Now we look at the spectrum of the radiative intensity in the first mesh of the transparent medium at times t_0 and t_1 . The radiative energy densities ϕ are plotted versus the frequency for both schemes, on the following page.

The stiff diminution at 9 KeV corresponds to a stiff growth of iron opacity for this frequency (known as the K-line of iron).

The two schemes yield quite the same results, except in the domain of low frequencies during the transient phase. It may be remarked that 2 iterations of the Newton's method are enough for each scheme. We can conclude that if a very high accuracy is not requested the scheme M is as good as the scheme A, which may be considered as a reference.



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SODIUM VAPOR LAMP: DIFFUSION PLUS TRANSPORT*

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ABSTRACT

The electrical and radiative properties of the sodium vapor lamp are modeled. Simple dimensional arguments lead to an understanding of the nonlinear interaction of the important processes, and a very detailed numerical model is described. It is shown that the total power and radiation efficiency depend sensitively on electrical conductivity, heat conduction, and especially on the nature of the radiative energy flux. Although heat transfer and electrical conduction can be described by diffusion theory, the radiative energy flux must be determined from transport theory with a scattering source function. Thus, the lamp can serve as a benchmark for numerical calculations of line transport in cylindrical plasmas whose optical thickness ranges from very large to very small.

I. INTRODUCTION

The high-pressure sodium vapor lamp is widely used around the world because it is relatively inexpensive, has an extremely long life, and can convert approximately 20% of the electrical power it consumes into visible photons with wavelengths near the peak of eye sensitivity [Jack and Koedam, 1974; Kaufman and Christensen, 1972]. The discharge is confined within a cylindrical tube of polycrystalline alumina, a few centimeters long and a few millimeters in radius. Tungsten electrodes, connected to the alumina niobium metal-to-ceramic seals, provide the electrical

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contact to a source of 60-Hz current, usually at the conventional 110-volt level. Typical lamps consume 100-400 watts of electrical power. The gas fill is nominally at about 1 atmosphere and consists mainly of mercury vapor, with about 30% sodium vapor and a small amount of inert gas to facilitate startup. When cold, the mercury and sodium are solid, and the discharge is initiated by a short high-voltage pulse. The joule heating in the inert gas (usually xenon) causes the mercury and sodium to vaporize as the lamp warms up. The operating temperature on the axis is nominally about 0.35 eV, and the wall temperature is about 0.1 eV. Experimental measurements indicate a quadratic dependence of temperature with radius [Ozaki, 1971]. At these temperatures and pressures, the ionization is confined to a region near the axis, only sodium atoms are ionized, and at most about 1% ionization occurs. Because the discharge is in a nearly neutral gas, the heat transport coefficient and electrical conductivity are determined by collisions with neutral species.

The purpose of this work was to use a well-understood radiating source to guide the creation of a numerical model for line dominated radiation transport in cylindrical plasmas. The engineering development of the sodium lamp into a commercial success was done by experiment and theory decades ago [Church, et al, 1966; deGroot and van Vliet, 1975; Jack and Koedam, 1974; Ten, et al, 1969; Kaufman and Christensen, 1972; Lowke, 1969; McVey, 1980; Ozaki, 1971 a, b, and c; van Trigt and Blom, 1975; Waszink, 1973; Wharby, 1980], and no essential new results are reported here. A possible exception is the role of photon scattering in the source function for numerical calculations.

LAMP MODEL

The description to follow uses MKS units, except that temperatures and photon energies are in electron volts. It is assumed that the discharge is one dimensional, in that finite length effects are not important and the electric field, E , between the electrodes is uniform. Furthermore, a constant current is assumed; because the characteristic response time of the discharge is much less than the time of variation of ordinary alternating current, a quasistatic model is almost certainly appropriate.

The discharge is understood completely once the variation of temperature T with radius r is determined. The equation for $T(r)$ involves a balance of terms:

$$\sigma E^2 + \text{div} [F_H + F_R] = 0 \quad (1)$$

The σE^2 term represents the volume rate of joule heating, where σ is the electrical conductivity. The heat conduction flux F_H depends on the heat conduction coefficient K_H , and the net radiative flux F_R depends on the radius. It will be seen that diffusion models for F_R are inadequate due to rapid variations of source function with radius and of optical depth with photon energy.

SIMPLE MODEL FOR A NONRADIATING DISCHARGE

A complete description of the lamp requires a detailed model of the electrical conductivity, heat conduction coefficient, photon cross section, and photon source function. Before getting enmeshed in each of these, it is interesting to consider a simplified model to clarify the general features and how they interact. For this purpose, the radiative flux will be ignored (or considered to have essentially the same radial dependence as the heat conduction flux). The electrical conductivity

$$\sigma = \frac{n_e e^2 t_e}{m} \quad (2)$$

where n_e is the electron density and t_e is the average electron collision time, will be modeled as

$$C_\sigma n_e T^{1/2} P^{-1} \quad (3)$$

In this expression, P is the (constant, uniform) gas discharge pressure and C_σ is a numerical constant. This assumes that the electron collision time t_e is given by λ_e/v_e , where the electron mean free path λ_e varies as the inverse of the neutral atom density $n_o \sim \frac{P}{T}$, and the electron velocity varies as $T^{1/2}$.

As is often assumed in simple models, the heat conduction coefficient is assumed to vary as a power n of the temperature, where n would be 0.5 for constant neutral-neutral collision cross section, and usually has a slightly higher value if velocity dependence of cross sections matters:

$$K_H = D_K T^n \quad (4)$$

The electron density is determined from the weak ionization limit of the Saha equation:

$$\frac{n_e n_t}{n_o} = (\text{degeneracy factor}) \left(\frac{2\pi m k T}{h^2} \right)^{3/2} e^{-\frac{I}{kT}} \quad (5)$$

Since n_t , the positive ion density, equates to n_e in this limit

$$n_e = C'_n n_o^{1/2} T^{3/4} e^{-\frac{I}{2kT}}$$

or

$$n_e = C_n P^{1/2} T^{1/4} e^{-\frac{I}{2kT}} \quad (6)$$

Inserting these expressions into Eq. (1) gives, after rearrangement

$$\tau^{3/4} e^{\frac{1}{2T_0}(1-\frac{1}{\tau})} + \frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d\tau^{1+n}}{d\rho} = 0 \quad (7)$$

where

$$\tau = \frac{T(\tau)}{T_0}$$

$$T_0 = T(o)$$

$$\rho = \frac{r}{\lambda} \quad (8)$$

$$\Lambda = \frac{R}{\lambda}$$

$$\lambda = \sqrt{\frac{C_K}{C_\sigma C_n(1+n)}} \frac{T_0^{3/8+\frac{n}{2}} P^{1/4} e^{\frac{1}{2T_0}}}{E}$$

Because of the extreme temperature dependence of the exponential in the source term for the divergence, this term is only appreciable in a region where $\rho < 1$; outside of this region, the divergence rapidly approaches zero. As $\rho \rightarrow 0$, where $\zeta \rightarrow 1$ and $\frac{dr}{d\rho} \rightarrow 0$, $\tau \simeq (1+\rho)^{\frac{1}{1+n}}$. Thus, this simple solution gives the temperature profile sketched in Fig. 1.

With the assumption that the current-carrying column has an area proportional to λ^2 , and knowing that the current density on the axis is given by $C_0 n_e(o) P^{1/2} T_0^{1/4} e^{-\frac{1}{2T_0}}$, the total current can be seen to vary as

$$I \sim \frac{C_K T_0^{1+n}}{E} \quad (9)$$

and

$$P = IEL \sim C_K L T_0^{1+n} \quad (10)$$

Thus, the enigmatic nature of glow discharges to have a decrease in current as the applied voltage increases is seen to be a result of the various nonlinear processes, leading to a smaller scale length λ as E is increased.

Another observation can be made from this simplified model: the difference between the observed quadratic dependence of T on r and the solution of the non-radiating discharge must be due to the radiative flux of energy. When the source for the thermal conduction flux is $\sigma E^2 + \text{div } F_R$, there will be a significant widening of this source. Radiation carries heat away from where it is created by joule dissipation, and deposits it in the outer radii of the discharge. This, in turn, causes a smoother function $T(r)$. An important effect of the radiative flux will therefore be a great increase in the current over a simple glow discharge, due to the great dependence of conductivity on temperature and the radial weight $2\pi r dr$.

In order to proceed with a more complete description, it is necessary to treat radiation transport and the atomic basis of opacity, radiative source function, and electrical and heat conductivity with some care. Brief overviews of each of these are given below, with details covered in the references.

RADIATION TRANSPORT [Aller, 1963; Griem 1969; Mihalas, 1978]:

To determine the transport of radiative energy within the discharge it is necessary to know how the opacity X_ν (in inverse meters) and the source function S_ν (in watts/m²/steradian/ev) depend on photon energy. The optical depth of the discharge, defined as $X_\nu R$, will be seen to vary from about 10^{-4} to 10^{+4} ; neither a diffusion model nor one of free streaming photons will suffice. Photons whose mean free path is very small can indeed be described by diffusion theory, but since the diffusion coefficient is proportional to mean free path, the flux of energy is very small. Conversely, free streaming photons with a very long mean free path are unlikely to be emitted because the emission density $X_\nu S_\nu$ varies directly with opacity. Most of the energy will therefore be transported by photons whose energy corresponds to optical depth near unity. It is necessary to solve the equation of transfer [Mihalas, 1978]

$$\frac{dI_\nu}{ds} = X_\nu(S_\nu - I_\nu) \quad (11)$$

numerically along numerous rays traversing the vapor. In Eq. (11), s is the coordinate along the ray and I_ν is the specific monochromatic intensity. Each ray is tangent to a radius included in the set of finite mesh radii $\{r_i\}$, which must include $r = 0$. For each ray with closest approach (or impact parameter) r_i there are m rays inclined to the cylinder axis by the angles of the gaussian quadrature set for $2m$ -degree integration. A set of photon energies chosen to represent both the steep line centers and the broad regions between lines is used to represent the photon energy dependences of opacity and source function. Precomputed geometry factors relate the integration along ray coordinate s to the opacity and source function, which are naturally defined as functions of radius. Rather than saving the angle dependent intensities at each radius, four angular moments of intensity are computed as the results of the calculation [Heasley, 1977]. The two moments most appropriate to

this problem are the mean intensity J_ν and the net radiated flux H_ν . J_ν is simply the integral of I_ν solid angle, whereas H_ν is the integral of I_ν weighted by the cosine of the angle between the ray and an outward normal to the cylinder. $H(r)$, the integral of H_ν over photon energy, represents the net flux of energy by photons, in watts/m².

OPACITY [Aller, 1963; Griem 1969; Mihalas 1978]:

The only atomic species interacting with photons in the sodium lamp is the sodium atom itself; the ionization potential and excitation energy of mercury and xenon are so much larger that they do not radiate or absorb photons at the temperatures found in the discharge region. Opacity is the product of number density of the sodium atoms and photon cross section per atom. The cross section, in turn, is the convolution of a Lorentz profile and Doppler broadening; the Lorentz width is composed of the natural width, resonance width, electron collisional width, the ion collisional width, and the van der Waals width [Aller, 1963; Griem, 1969; Kelch, 1975; Watanabe, 1941]. Although each of these processes is included in the model, the only important contributions here are from the natural width (due to spontaneous decay of individual atoms), the resonance width (due to collisions with other sodium atoms), and Doppler broadening. Atomic data for oscillator strengths (which determine the line magnitude) and natural widths are taken from astrophysical literature [Kelch, 1975], and the resonance broadening is taken from an experiment which is in very good agreement with theory [Watanabe, 1941].

RADIATIVE SOURCE FUNCTION [Mihalas, 1978]:

Often, the radiative source function S_ν is taken as the Planck function B_ν . This is of course only correct when the problem is in complete equilibrium, which implies uniform temperature over space scales of photon mean free path, among other constraints. When collisional and radiative processes leading to transitions between the atomic excitation states are not in equilibrium, the Planck function is no longer the proper source function. A reasonable approximation is to "correct" the equilibrium population of the upper state of a transition by multiplication with a "departure coefficient," usually denoted by b . In the outer radii of the discharge, the large photon flux streaming by from the bright core causes a radiative transition rate much higher than would normally occur at the local temperature. Unless this increased rate is overwhelmed by collisional processes, more sodium atoms will be in the upper state of a transition than the Boltzmann factor would predict (that is, $b > 1$). In the sodium lamp, b only differs from unity in the outermost layer of the vapor. A much more important deviation from local thermal equilibrium is due to photon scattering. For the Planck function to be the proper source function, it is necessary that photons absorbed by the atoms "deposit" their energy in the local pool of degrees of freedom, to be reemitted as photons according to the local statistical probabilities. If the photon flux J_ν is much higher than the local value of

B_ν and photon emission is much more probable than nonradiative transitions, the source function approaches J_ν . This can be represented by assuming that

$$S_\nu = (1 - \epsilon)J_\nu + \epsilon B_\nu \quad (12)$$

In this equation, the "source coefficient" ϵ is the ratio of nonradiative (or collisional) deexcitation rate to the total deexcitation rate (photon emission plus collisional deexcitation). In the sodium lamp, ϵ is near unity at the center because of the rapid transition rates due to electron collisions, but it drops to small values in the outer layers. Although this process is in large part responsible for the high illumination efficiency of the lamp, it introduces an extreme numerical difficulty. This is because the problem becomes an integro-differential equation, in which the initially unknown intensity J_ν is a major contributor to the source function. Iteration procedures appropriate for the optically thin case converge extremely slowly for photons whose energy is such that their mean free path is small. It is here that the previously unused angular moments of intensity could be useful: they make it possible to generate a closed set of differential equations (called the moment equations) which approximate the nonlocal transport problem and can guide iteration procedures in optically thick problems. In the calculation reported here, this complication has been neglected. As a consequence, the radiative intensity in the core of the main transition line is underestimated, and the actual lamp behavior is correspondingly different than computed by this model. Some other possible complications which have been considered but found to be of little consequence are: radiative processes due to molecular formation and dissociation [Konowalow and Julienne, 1980; Woerdman and de Groot, 1981]; anisotropic scattering in the source function; frequency redistribution within the emission profile during scattering; negative ions and electron detachment [John, 1975]; multiple photon excitation and ionization; reradiation into the plasma by the alumina walls; impurities in the sodium and mercury; excess concentration of sodium atoms in the hotter core ("Knudsen effect"); heat transport by convection; and continuum lowering of excitation energies due to the free electron density.

ELECTRICAL CONDUCTIVITY [Frost, 1961]:

The usual expression for electrical conductivity (Eq. (2)) is correct for plasmas, solids, nearly neutral gases, etc.—as long as the average electron collision time is correctly defined! In the case of a gas where electron collisions are principally with neutral atoms, the proper averaging procedure is considered to be the one given by the Sommerfeld model, in which the collision integral in the Boltzmann equation is approximated by a velocity dependent relaxation from the perturbed electron distribution function to the equilibrium value. This leads to an averaging of $\tau_e(v) = \lambda_c/v_e$ weighted by v^2 times the Maxwellian distribution of electron velocities:

$$\tau_e = \frac{2}{3} \frac{1}{v_m^2} \int_0^\infty v^2 \tau(v) F_o(v) dv \quad (13)$$

where

$$v_m^2 = \frac{2kT}{m}$$

$$F_o(v) = \frac{\sqrt{\pi}}{2v_m} e^{-\frac{v^2}{v_m^2}}$$

The collision time as a function of velocity is found by computing the mean free path for electron collisions with all species present, including positive ions. Collision cross sections for momentum transfer with the atoms are taken from the extensive compilation of Kieffer [Kieffer, 1973], and the Coulomb cross section is used for ion collisions. As a check on the model, numerical integration of Eq. (13) for collisions with ions alone reproduces the Spitzer expression for plasma conductivity very nearly if the numerical coefficient for the Coulomb cross section is chosen properly. This is a slightly different prescription than the one often used, which averages the separate conductivities for neutral and ionized gases.

HEAT CONDUCTION COEFFICIENT [Flynn and Peavy, 1968; Hirshfelder, et al., 1954; Minges and Denman, 1966; Shkarofsky, et al., 1966]:

The calculation of heat conduction coefficients for gaseous mixtures can become exceedingly involved if treated in full generality. The product of free path and velocity should be averaged over all pairs of interacting particles as well as the distribution functions. This should be computed using the actual interaction potentials for each pair of atoms (or ions, electrons, molecules, etc.) $V_{ij}(r)$. This has the consequence that mixtures have heat conduction coefficients that may differ from the averages of values for pure gases. Additionally, the migration of charged species should be constrained by the condition of electrostatic balance (usually referred to as ambipolar diffusion). For this calculation, a simpler model using hard sphere collisions was used, with a power law temperature dependence to account for the velocity dependence of cross sections. The contribution to heat conduction by charged species was only crudely approximated; in spite of their great velocity, electrons are always a minor constituent, and in the central region where free electrons are present, the temperature gradient is small. Also, the flux of energy in the lamp core is dominated by radiative terms. Even though it would certainly be possible to model the heat conduction with much more care, the overall effect would probably be minor. This prescription, when applied to pure gases of sodium, xenon, and mercury gives good agreement with experiments [Minges and Denman, 1966].

Representative photon cross sections, electrical conductivity, and heat conduction coefficients are shown in Figs. 2-3, with units chosen for comparison with the data used in Ref. 9. The gas used here and in subsequent calculations consists of 30% sodium, 8% xenon, and 62% mercury by atom density. The cross sections correspond to a temperature of 0.35 electron volts, a total gas density of $2 \times 10^{24} \text{ m}^{-3}$ and an electron density of 10^{22} m^{-3} . The 100 watt version of this lamp is presumed to have a radius of 2 mm and a length of 3.5 cm, with a static applied potential of 100 volts.

CALCULATIONAL MODEL:

The computer program solves Eq. (1) iteratively for $T(r)$, using the constitutive coefficients and cross sections described above. First, radiation is ignored and the temperature profile is computed for joule heating and thermal conduction alone. Knowing this temperature profile, a source function (initially Planck) is calculated, and the photon transport problem is solved. The boundary condition at the lamp center is $\frac{dT}{dr} = 0$. At the alumina wall, the temperature is determined by the condition that the total radiative flux $H(r)$ plus blackbody emission from the wall at temperature $T(R)$, integrated over the outside surface, equals the total electrical power absorbed in the discharge. As an illustration of the importance of scattering in the source function, the results of the calculation to this point are reviewed.

The Planck source function is shown in Fig. (4). The temperature profile and first two radiation moments are shown in Figs. 5 to 7. In the radiation plots, the photon energy (or wavelength) dependence is given for various radii, the larger values generally being at smaller radius. Note the development of line core reversal in J_ν for increasing radius, and the small net flux in H_ν at line center for all radii. Because the source function does not include scattering at this point, the net radiative flux and temperature profile are seriously in error; although this lamp should consume roughly 100 watts of electrical power, the model without scattering predicts only about 11 watts. The radiated flux from this source function is so small the simple nonradiating model applies very well; the dotted line in Fig. 5 shows the solution of Eq. (7), and the solid lines are the successive iterations to converge on the desired outer boundary condition.

Figure 8, an overlay of the Planck function B_ν and the moment J_ν , both for various radii, shows the origin of the difficulty. At all radii, there is equality of B_ν and J_ν at the line center. This is to be expected in the optically thick case. Note, however, that whereas J_ν in the wings of the main line is many orders of magnitude smaller than B_ν near the lamp center, the situation is reversed near the outer wall. This shows why scattering is so important; J_ν is much greater than B_ν precisely where ϵ is small. Performing one more iteration with scattering included gives the results in Figs. 9 to 11. The temperature profile is now much broader, which has a large effect on the total current. The electrical power consumption has increased to about 150 watts, and the photon spectrum and efficiency are close to reported values. Because the objectives of the original program, to develop and validate a

computer model for line transport in cylindrical plasmas, appear to have been met, further refinements of this calculation have not been attempted.

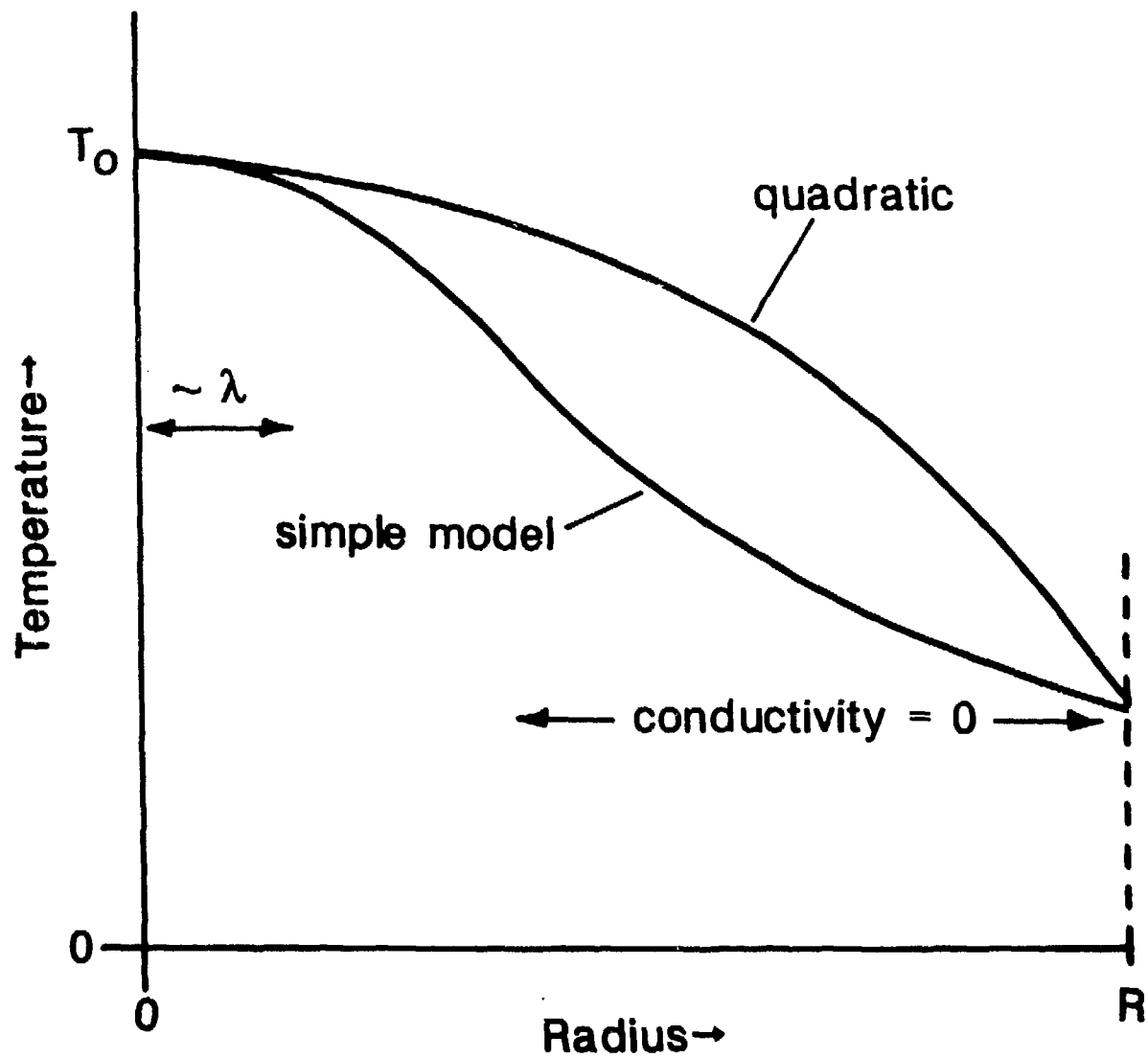
CONCLUSIONS

Comparison of a simple nonradiating glow discharge model and a radiating model with both a Planck source function and a scattering source function shows that the correct prediction of the sodium lamp electrical input and photon efficiency requires a detailed model for the radiation transport. Many atomic lines must be included and a full transport treatment (rather than a diffusion model) is necessary, as is a source function which includes photon scattering. Although not described in this note, the moment equations for radiative fluxes can provide an iterative scheme for proper convergence of scattering source function and the resulting radiant intensities. The very reasonable agreement of lamp operating parameters and output spectrum with model predictions would seem to indicate that this numerical scheme provides an accurate description of radiation in line-dominated cylindrical plasmas.

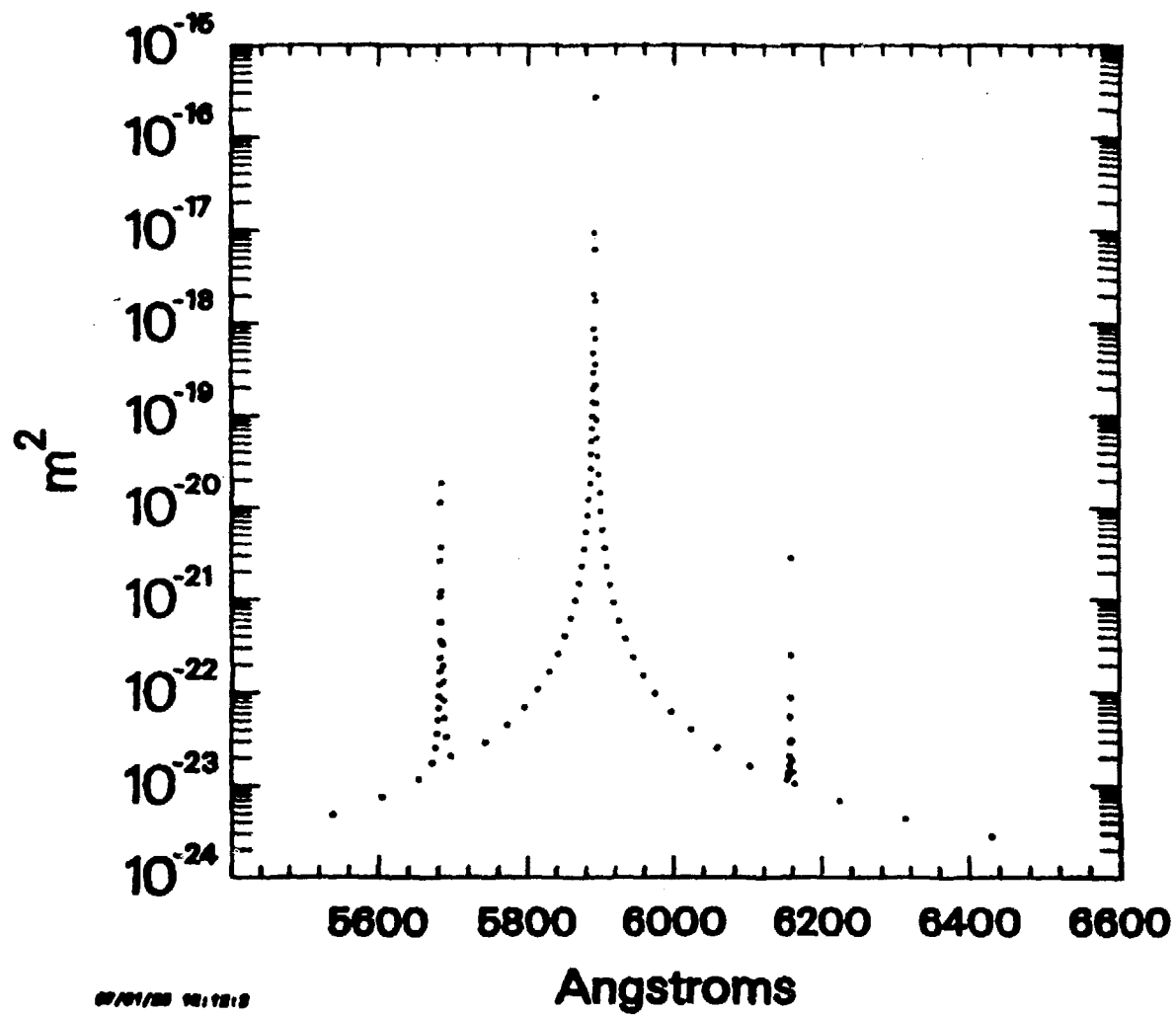
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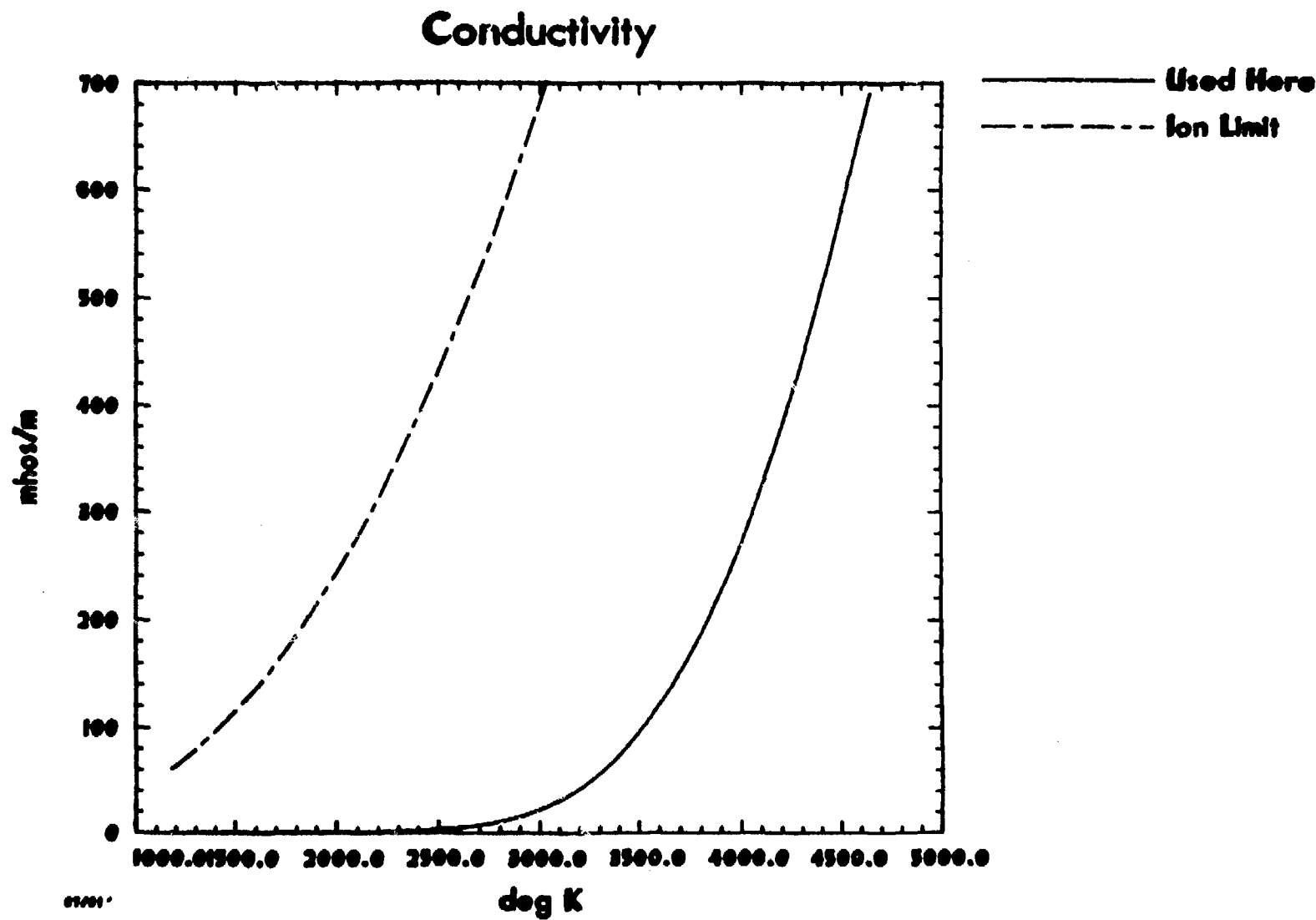
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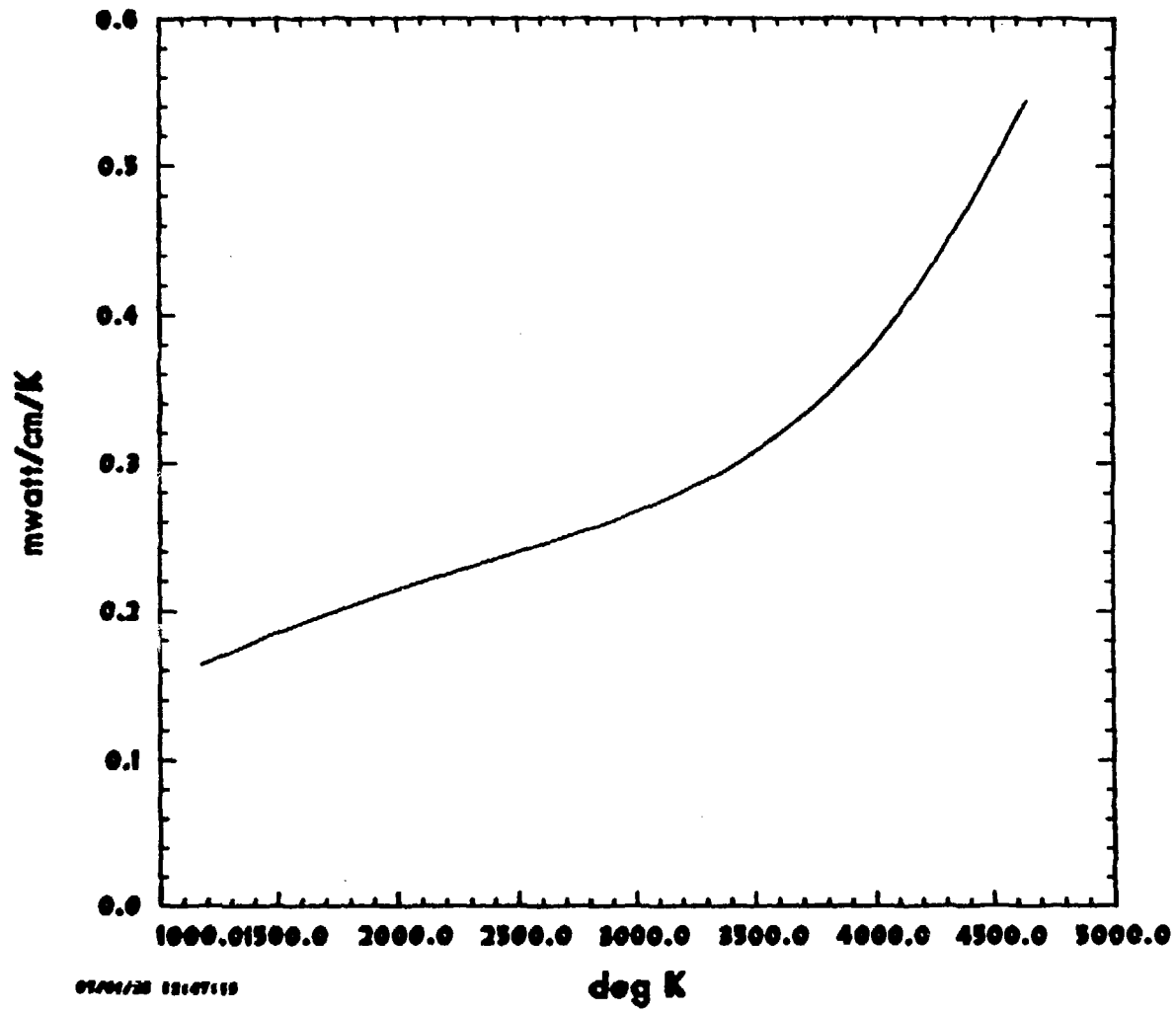


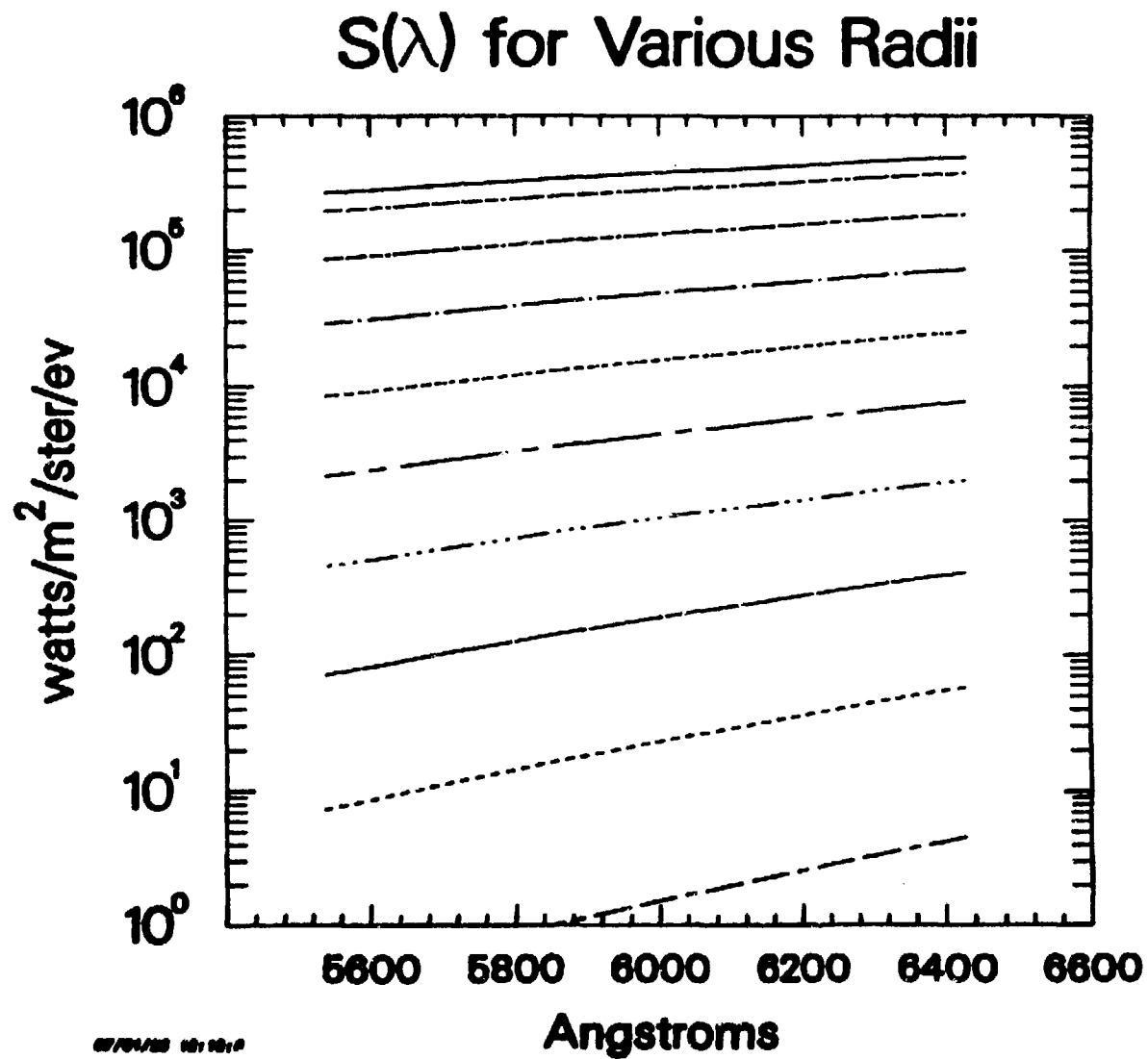
Photon Cross Section

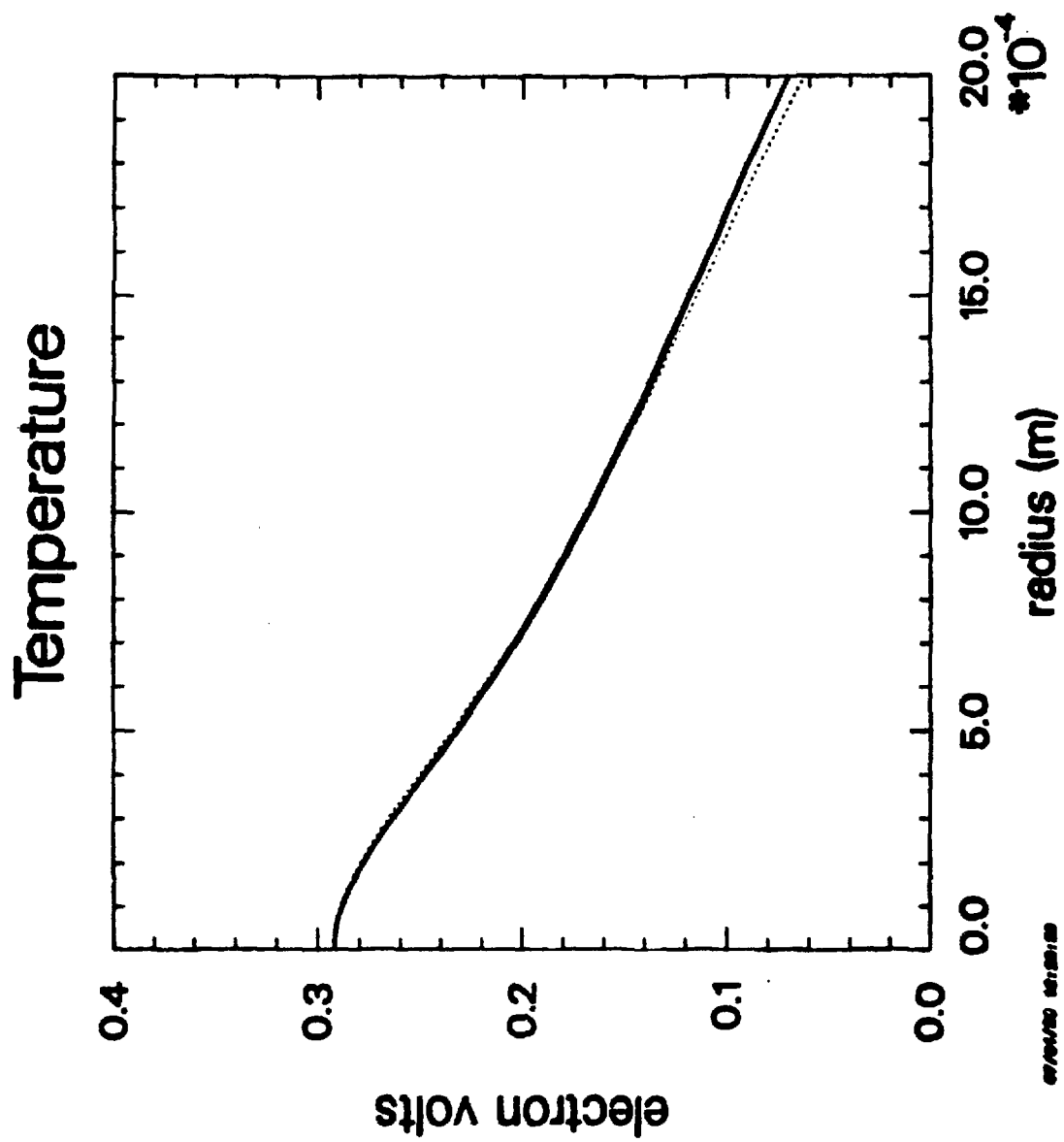


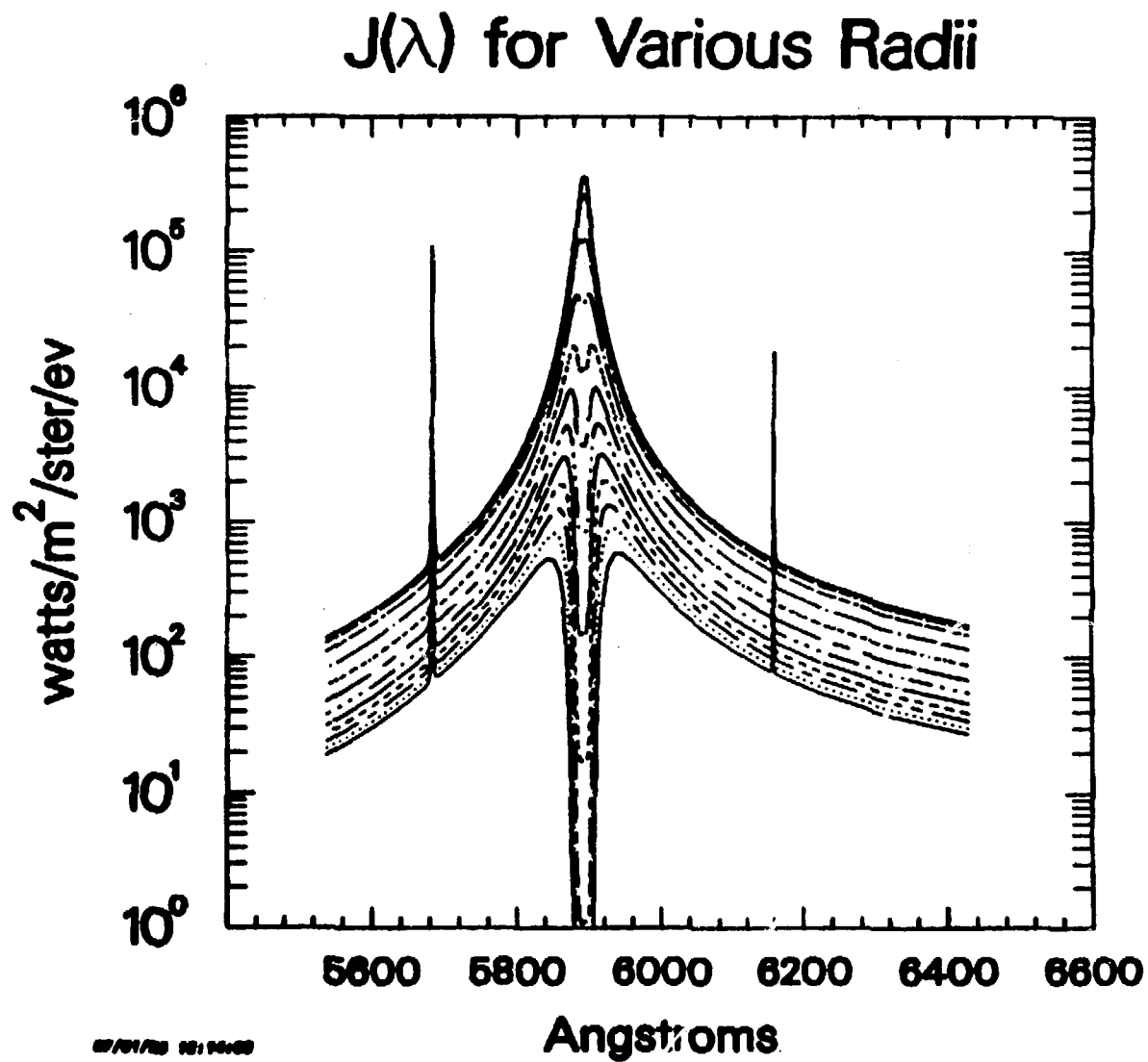


Heat Conduction

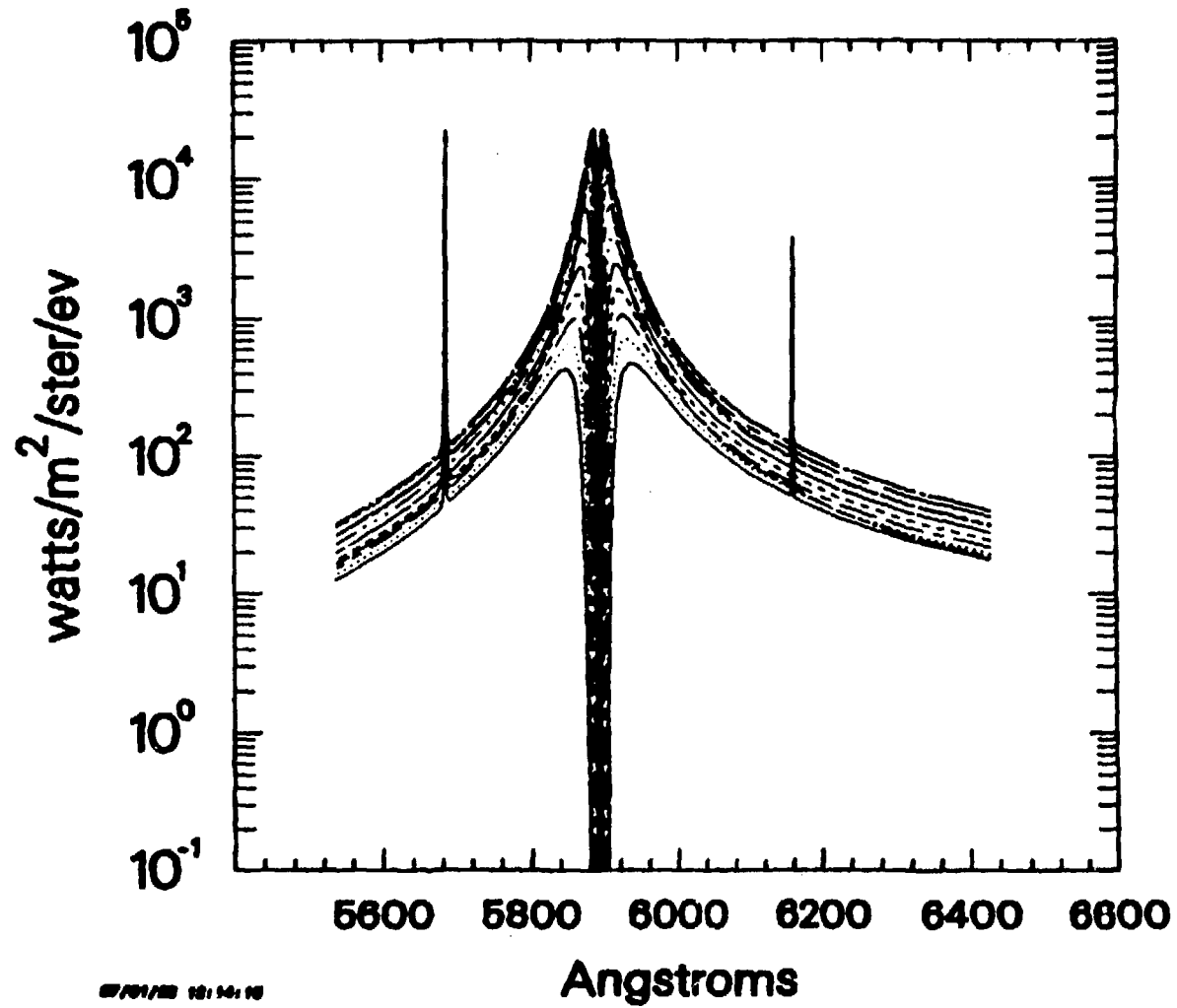


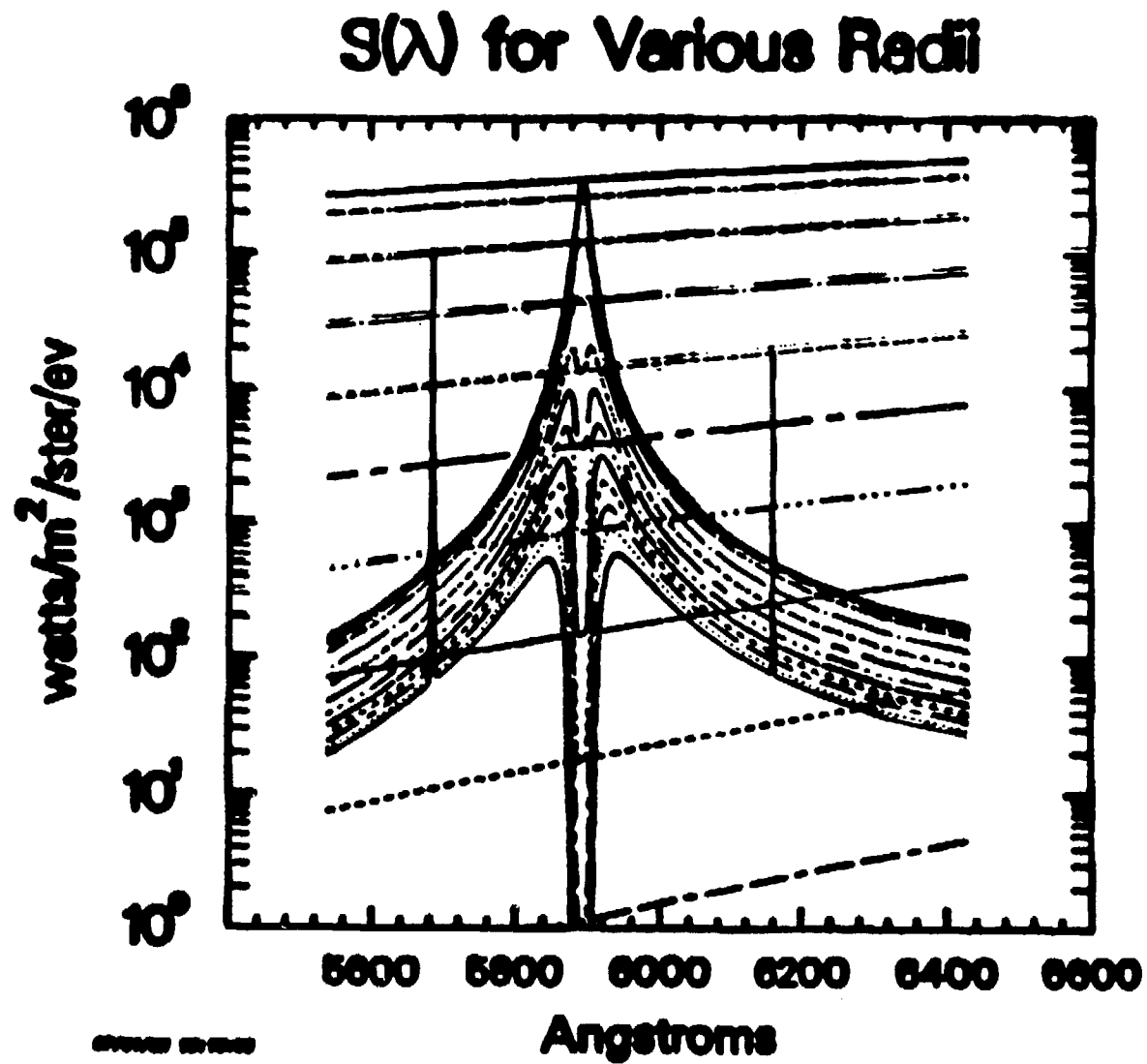


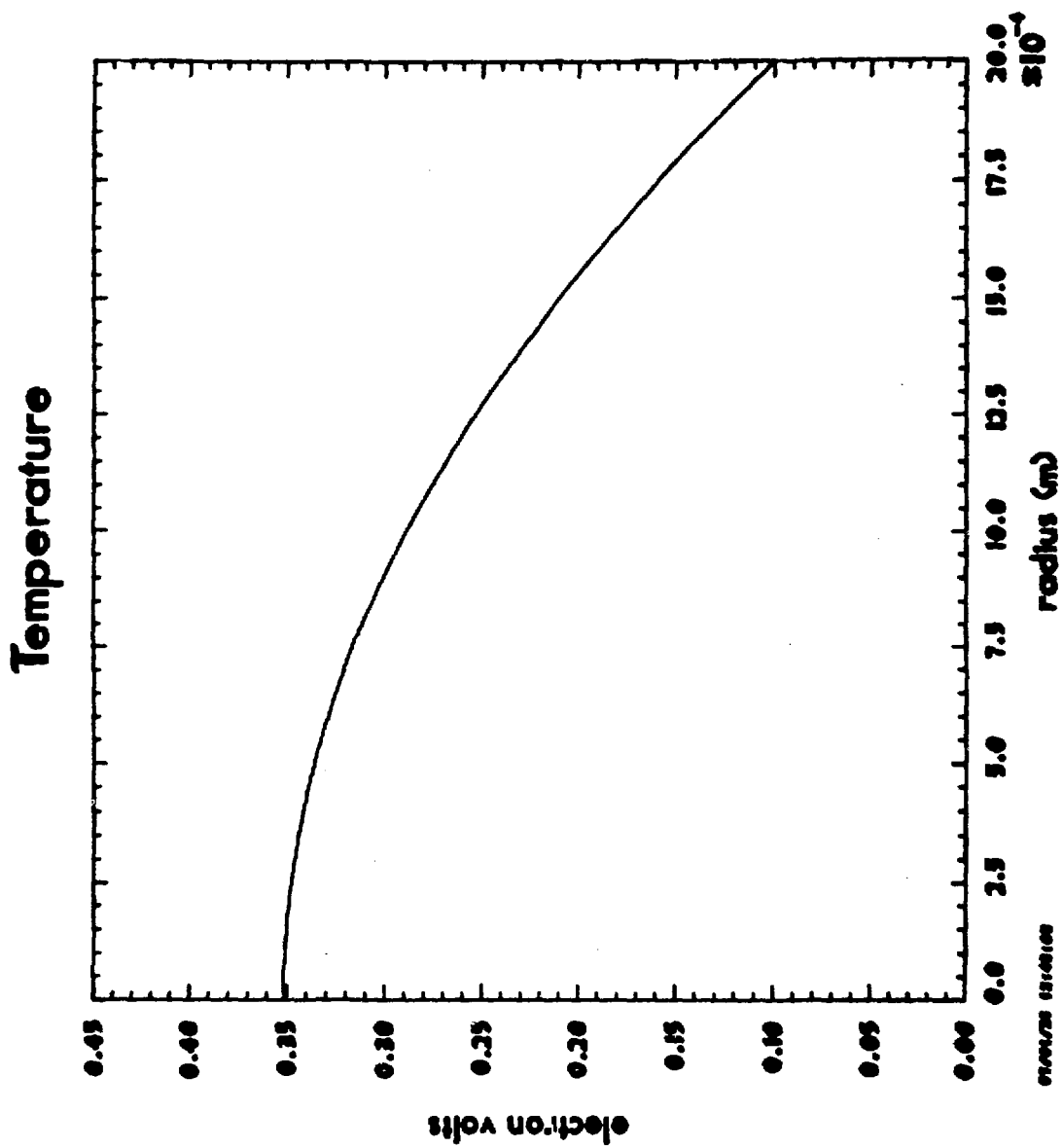




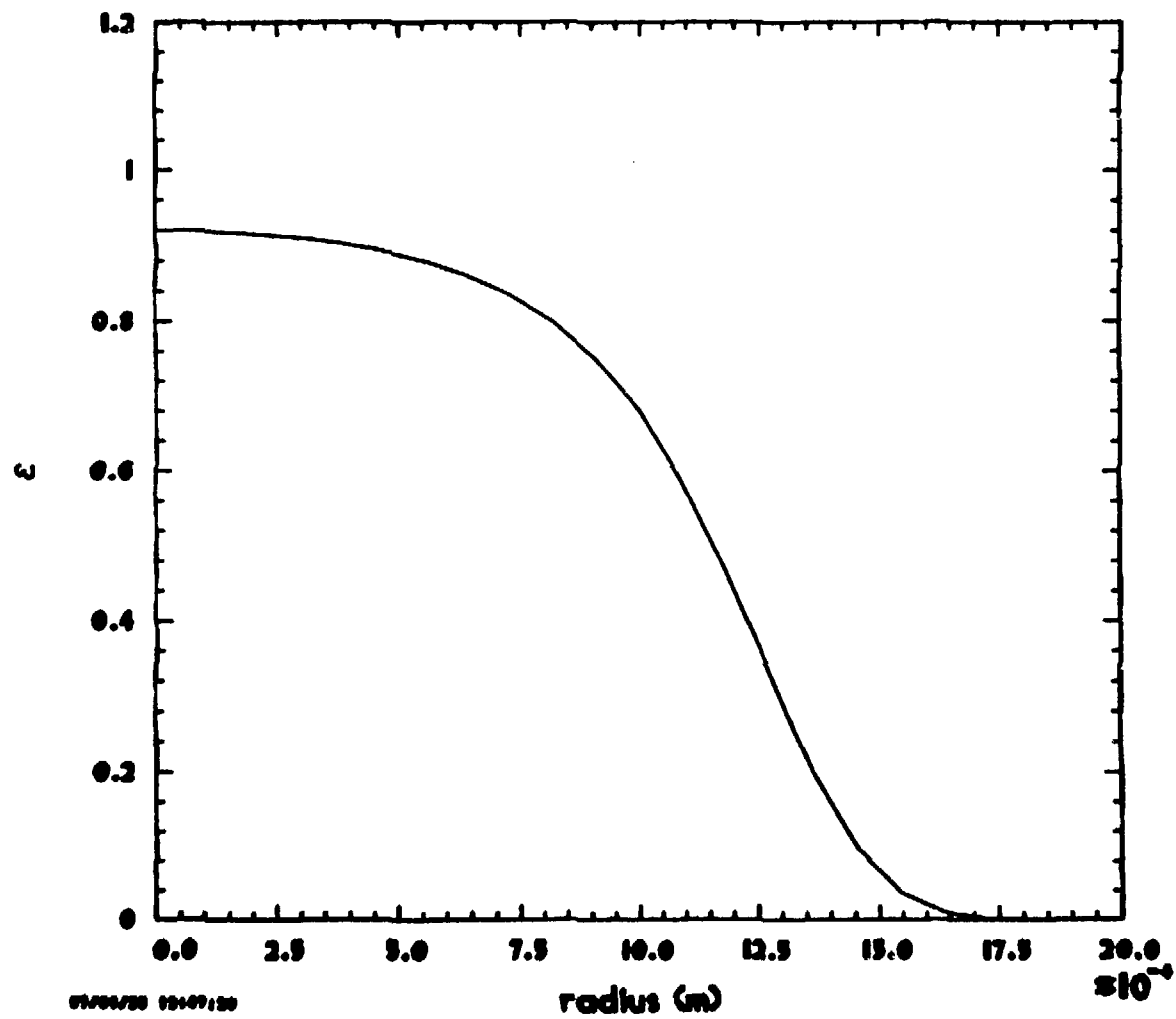
$H(\lambda)$ for Various Radii



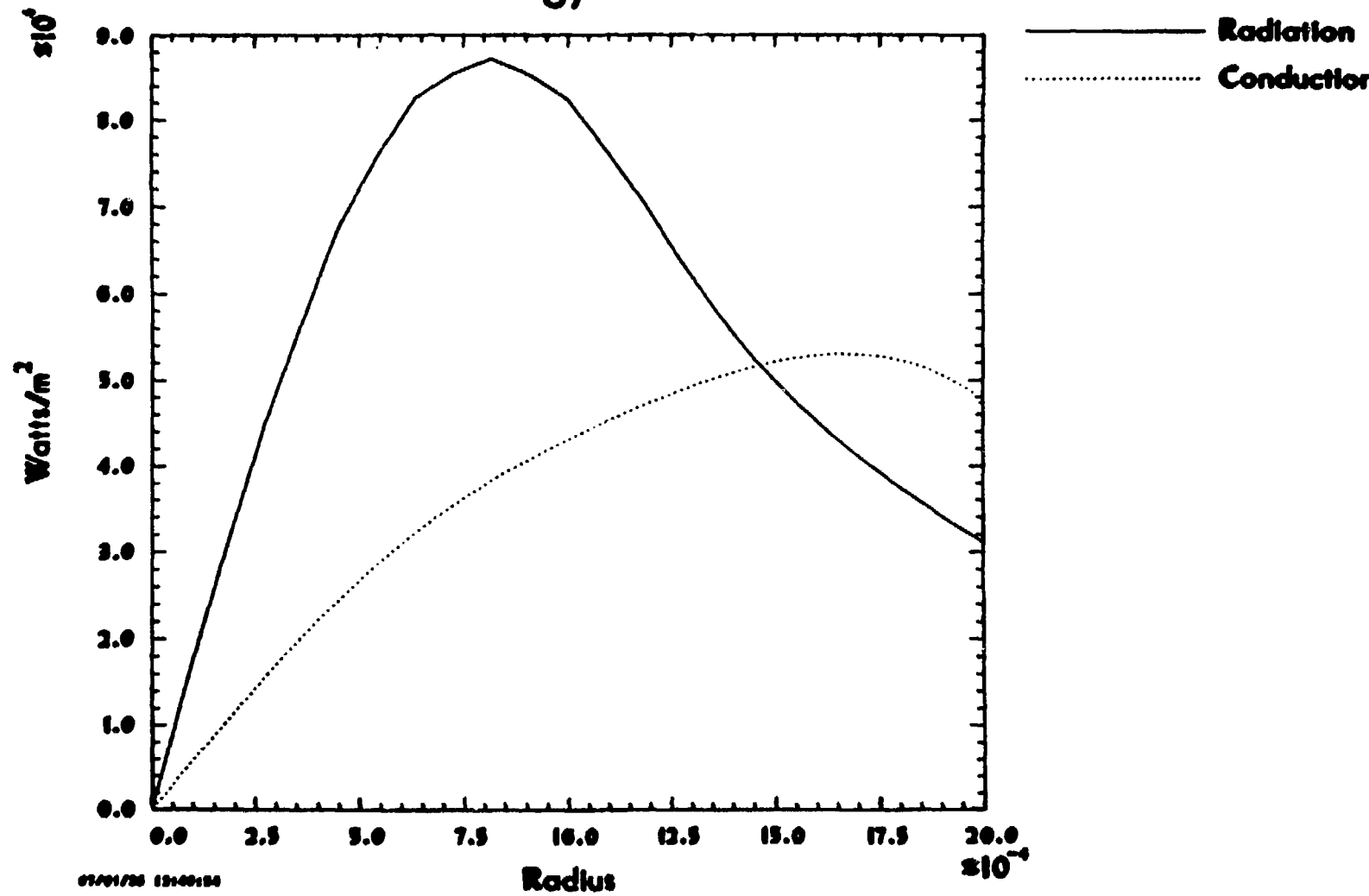




Source Coefficient ε



Energy Flux



BOLTZMANN-FOKKER-PLANCK CALCULATIONS USING STANDARD DISCRETE-ORDINATES CODES

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ABSTRACT

The Boltzmann-Fokker-Planck (BFP) equation can be used to describe both neutral and charged-particle transport. Over the past several years, the author and several collaborators have developed methods for representing Fokker-Planck operators with standard multigroup-Legendre cross-section data. When these data are input to a standard S_n code such as ONETRAN, the code actually solves the Boltzmann-Fokker-Planck equation rather than the Boltzmann equation. This is achieved without any modification to the S_n codes. Because BFP calculations can be more demanding from a numerical viewpoint than standard neutronics calculations, we have found it useful to implement new quadrature methods and convergence acceleration methods in the standard discrete-ordinates code, ONETRAN. We discuss our BFP cross-section representation techniques, our improved quadrature and acceleration techniques, and present results from BFP coupled electron-photon transport calculations performed with ONETRAN.

I. INTRODUCTION

Fokker-Planck operators are asymptotic approximations to the Boltzmann scattering operator that apply in the forward-peaked elastic scattering limit.¹ Highly forward-peaked scattering kernels are often quite difficult to numerically approximate, whereas Fokker-Planck operators, which are differential operators, can often be approximated using straightforward differencing techniques. Hence charged-particle transport, which is dominated by highly forward-peaked elastic coulomb scattering, is often described with a transport equation that has Boltzmann operators describing the "large-angle" scattering and Fokker-Planck operators describing the "small-angle" scattering. Such an equation is known as a Boltzmann-Fokker-Planck (BFP) equation. Much attention has been given to BFP equations over the last several years.^{1,2,3} These equations have been used for both charged-particle and neutral-particle transport calculations. Several years ago, we demonstrated that the Fokker-Planck equation for charged-particles transporting in fully-ionized plasmas can be solved in 1-D slab and spherical geometries using standard discrete-ordinates codes.¹ No code modifications are necessary. The Fokker-Planck operators are represented in terms of multigroup-Legendre cross-section coefficients. Thus, one need simply input appropriate cross-section data to perform a Fokker-Planck calculation. Over the last several years, we have been investigating the generalization of existing discrete-ordinates codes to allow both Fokker-Planck and Boltzmann-Fokker-Planck calculations in all geometries. In addition, we have sought to improve our multigroup cross-section representations for the Fokker-Planck operators. The purpose of this paper is to briefly review our Fokker-Planck operator representations and the new S_n methods that we have developed, and to demonstrate the effectiveness of our approach when applied to coupled electron-photon transport calculations.

II. MULTIGROUP REPRESENTATIONS FOR FOKKER-PLANCK OPERATORS

In this section we derive simple representations for two Fokker-Planck operators. Our primary purpose is to convey the basic approach used in deriving such representations. A Fokker-Planck equation that can be used to describe the transport of charged-particles in plasmas is given by:¹

$$\mu \frac{\partial}{\partial z} \psi = \frac{\alpha}{2} \frac{\partial}{\partial \mu} \left[(1 - \mu^2) \frac{\partial}{\partial \mu} \psi \right] + \frac{\partial}{\partial E} (S\psi) + Q \quad , \quad (1)$$

where z is the space coordinate, μ is the direction cosine of the transport particle relative to the z -axis, ψ is the angular flux, α is the momentum transfer, S is the stopping power, and Q is the source function. We refer to the Fokker-Planck angular and energy operators in Eq. (1) as the angular diffusion (AD) operator and the continuous-slowing-down (CSD) operator, respectively. The AD operator approximates the Boltzmann scattering operator in the limit as the scattering cross section goes to infinity, and the average cosine of the scattering angle goes to unity in such a way that the average change in the particle direction per unit pathlength is constant and is given by the momentum transfer (steradians/pathlength). The

momentum transfer is commonly referred to as the transport-corrected cross section in the neutron transport literature. The AD operator causes a particle to continuously diffuse in direction space rather than discretely scatter. The CSD operator approximates the Boltzmann scattering operator in the limit as the scattering cross section goes to infinity and the average energy loss per unit pathlength goes to zero in such a way that the average energy loss per unit pathlength remains constant and is given by the stopping power (energy/pathlength). The CSD operator causes a particle to continuously lose energy rather than lose it in discrete-scattering events.

The multigroup Boltzmann equation solved by standard discrete-ordinates codes is:⁴

$$\mu_m \frac{\partial}{\partial z} \psi_{m,g} + \sigma_{t,g} \psi_{m,g} = \left[\sum_{k=1}^G \sum_{\ell=0}^L (2\ell + 1) \sigma_{k \rightarrow g, \ell} \Phi_{k, \ell} P_{\ell}(\mu_m) \right] + Q_{g,m} \quad , \quad m = 1, N \quad , \quad g = 1, G \quad , \quad (2)$$

where m is the direction index, g is the group index, N is the total number of directions, G is the total number of groups, L is the degree of the Legendre cross-section expansion, $\sigma_{t,g}$ is the total cross section for group g , $\sigma_{k \rightarrow g, \ell}$ is the ℓ 'th Legendre moment of the cross section for scattering from group k to group g , $\Phi_{k, \ell}$ is the ℓ 'th Legendre moment of the angular flux for group k , and $P_{\ell}(x)$ is the Legendre polynomial of degree ℓ . To solve Eq. (1) using Eq. (2), we must appropriately define the cross-section coefficients. We first consider the AD operator. Note that this operator changes the particle direction, but not the particle energy. Thus, the cross-section coefficients corresponding to this operator must be within-group scattering coefficients. The key to approximating the AD operator with the Boltzmann scattering operator is found because both of these operators have the same eigenfunctions, namely, the Legendre polynomials:

$$\frac{\alpha}{2} \frac{\partial}{\partial \mu} \left[(1 - \mu^2) \frac{\partial}{\partial \mu} P_{\ell}(\mu) \right] = -\frac{\alpha}{2} \ell(\ell + 1) P_{\ell}(\mu) \quad , \quad (3)$$

$$\int_{-1}^{+1} \sigma_s(\mu_0) P_{\ell}(\mu') d\mu' - \sigma_s P_{\ell}(\mu) = -(\sigma_0 - \sigma_{\ell}) P_{\ell}(\mu) \quad . \quad (4)$$

Legendre expansion coefficients for the AD operator are obtained by equating the eigenvalues in Eqs. (3) and (4):

$$\sigma_0 - \sigma_{\ell} = \frac{\alpha}{2} \ell(\ell + 1) \quad , \quad \ell = 0, L \quad . \quad (5)$$

The difference between the zero'th and ℓ 'th moments is defined by Eq. (5); but to obtain a specific definition for each moment, we must define σ_0 . The value of σ_0 can be arbitrarily chosen; but to ensure stability in the source iteration process, it is required that

$$|\sigma_{\ell}| \leq \sigma_0 \quad , \quad \ell = 0, L \quad . \quad (6)$$

A simple definition that satisfies Eq. (6) can be obtained by requiring that σ_L be zero. Specifically, this requirement gives:

$$\sigma_0 = \frac{\alpha}{2} L(L + 1) \quad . \quad (7)$$

From Eqs. (5) and (7) we obtain the desired definition for each moment:

$$\sigma_\ell = \frac{\alpha}{2} [L(L+1) - \ell(\ell+1)] \quad , \quad \ell = 0, L \quad . \quad (8)$$

It can be shown that if one uses the moments defined by Eq. (8) and a Legendre expansion of degree $N-1$ in conjunction with Gauss quadrature of order N in 1-D slab geometry calculations, the resulting S_N solutions will be equivalent to P_{N-1} solutions (spherical-harmonic solutions of degree $N-1$) to the Fokker-Planck equation.¹

Next, we consider the CSD operator. The first step in obtaining coefficients for this operator is to difference this operator using a first-order forward difference. Neglecting the angular discretization and the AD operator in Eq. (1) and assuming a uniform group structure for simplicity, we obtain:

$$\mu \frac{\partial}{\partial z} \psi(E_g) = \frac{[S(E_{g-1})\psi(E_{g-1}) - S(E_g)\psi(E_g)]}{\Delta E} \quad , \quad (9)$$

where g is the energy group index, $g=1$ corresponds to the highest energy group, E_g denotes the midpoint energy for group g , and ΔE denotes the group width. Next we relate the multigroup and discrete fluxes as follows:

$$\psi_g = \psi(E_g) \Delta E \quad . \quad (10)$$

Using Eq. (10), we transform Eq. (9) from the differential to the multigroup basis:

$$\mu \frac{\partial}{\partial z} \psi_g = \frac{[S_{g-1}\psi_{g-1} - S_g\psi_g]}{\Delta E} \quad . \quad (11)$$

Finally, we re-write Eq. (11) in the following way:

$$\mu \frac{\partial}{\partial z} \psi_g + \left(\frac{S_g}{\Delta E} \right) \psi_g = \int_{-1}^{+1} \left(\frac{S_{g-1}}{\Delta E} \right) \delta(\mu_0 - 1) \psi_{g-1}(\mu') d\mu' \quad . \quad (12)$$

Equation (12) is analogous in form to Eq. (2). Thus, the coefficients for the CSD operator can be obtained by direct comparison of Eqs. (2) and (12). Recalling that the Legendre moments of the delta-function are all unity, we obtain:

$$\sigma_{r,g} = \frac{S_g}{\Delta E} \quad , \quad (13a)$$

$$\begin{aligned} \sigma_{k-g,\ell} &= \frac{S_{g-1}}{\Delta E} \quad , \quad \ell = 0, L \quad , \quad \text{for } k = g-1 \quad , \\ &= 0 \quad , \quad \text{otherwise} \quad , \end{aligned} \quad (13b)$$

where $\sigma_{r,g}$ denotes the effective removal cross section for group g . This approximation is completely equivalent to the forward-difference approximation as long as the truncated Legendre expansion for the delta-function is "exact." That is to say that the scattering kernel constructed from the truncated delta-function expansion must act as the identity:

$$\sum_{\ell=0}^L (2\ell+1) \Phi_{k,\ell} P_\ell(\mu_m) = \psi_{k,g} \quad . \quad (14)$$

It can be shown that if Legendre expansions of degree $N-1$ are used in conjunction with an N -point Gauss quadrature in either 1-D slab or spherical geometries, Eq. (14) will be satisfied.

III. LIMITATIONS OF MULTIGROUP FOKKER-PLANCK REPRESENTATIONS

The derivations of the preceeding section demonstrate the basic approach that is taken to derive multigroup approximations to Fokker-Planck operators. These approaches are useful, but limited. For instance, the CSD operator representation requires that Gauss quadrature be used. Since Gauss quadrature only exists for 1-D slab and spherical geometries, this representation can only be used in these geometries. Although it is not obvious, the AD operator representation cannot be expected to be accurate under all circumstances unless Gauss quadrature is used. Thus, further extensions of this approach clearly require an improved quadrature treatment. We have developed such a treatment and it is called the Galerkin quadrature method.^{5,6} We shall not describe this method in detail here. Instead, we simply note that it offers many advantages relative to the standard quadrature method. Most importantly, it can be applied in both one-dimensional and multi-dimensional problems, and all "Galerkin quadratures" give an exact treatment for straight-ahead delta-function scattering when they are used in conjunction with Legendre expansions of appropriate degree. Thus, the Galerkin quadrature method allows us to use our multigroup BFP approach in all geometries. Finally, we note that it can be important to use Galerkin quadrature whenever highly forward-peaked scattering is present in a problem because it has been found that standard quadrature techniques can lead to unstable scattering matrices under such conditions.⁶

We have derived a first-order approximation to the CSD operator, but higher-order approximations can be used. In particular, the second-order diamond-difference scheme can be applied to the CSD operator and represented in multigroup form.⁷ When this is done, certain of the effective group-to-group transfer coefficients are negative. These coefficients appear in such a way that they do not interfere with the convergence of the standard source iteration method, but they can cause problems with the negative flux fixup schemes that are implemented in many discrete-ordinates codes. Thus it is best to perform Fokker-Planck calculations with higher-order spatial difference schemes such as the linear-discontinuous scheme employed in the ONETRAN⁸ code, that can be used without negative flux fixup. The linear-discontinuous differencing scheme can also be applied to the CSD operator and represented in multigroup form. However, this approximation not only leads to negative coefficients but to upscatter as well.⁹ Unfortunately, the infinite-medium spectral radius of the outer iteration operator is unity with this type of upscatter, and the convergence rate in most practical problems is unacceptably slow. A synthetic acceleration scheme has been developed which reduces the spectral radius to 0.1,⁹ but this acceleration scheme applies only to the upscatter resulting from the LD-CSD operator. Since it cannot be applied to general types of upscatter, it is not suitable for a general-purpose S_n code. Thus, the best approximation to the CSD operator that one can obtain with standard S_n codes is the diamond difference approximation. If one is willing to explicitly include the CSD operator in an S_n code and modify the basic algorithm, the LD-CSD operator

can be efficiently solved by treating it like an extra spatial derivative and explicitly sweeping the space-angle-energy mesh.¹⁰

If the stopping power in Eq. (1) is small and the system is optically thick, the spectral radius of the inner iteration process approaches unity. Thus, acceleration is required under these circumstances. In the limit as the scattering becomes increasingly forward-peaked, standard diffusion-synthetic acceleration becomes ineffective.¹¹ Improved performance can be obtained by using the P_1 equations as the low-order equations in the synthetic scheme rather than the diffusion equation. This approach represents a straightforward modification of the standard DSA scheme and is referred to as two-moment DSA. This nomenclature arises from the fact that only the zero'th moment of the scattering source is accelerated in standard DSA, but both the zero'th and first moments are accelerated in the two-moment scheme. Like standard one-moment DSA, two-moment DSA becomes ineffective in limit as the scattering becomes increasingly forward-peaked, but two-moment DSA is always significantly more effective than one-moment DSA in the forward-peaked limit.¹¹ Thus, while two-moment DSA does represent a significant improvement relative to standard DSA, it does not represent a complete solution to the problem of accelerating the S_n equations with highly anisotropic scattering. Testing of the two-moment DSA scheme has shown that negative flux fixup schemes are much more likely to destabilize the DSA algorithm if the scattering is very forward-peaked rather than isotropic.¹¹ This difficulty can be avoided by using higher-order difference schemes that do not require negative flux fixup. However, DSA with higher-order spatial difference schemes presents a problem in itself because the derivation of the spatially-differenced diffusion equation from the spatially-differenced S_n equations (required to ensure unconditional stability of the DSA method) can be quite difficult even in 1-D slab geometry.¹² To avoid this difficulty, an S_2 -synthetic acceleration method for the 1-D S_n equations has been developed.^{13,14} The central idea of this method is straightforward. Rather than use the P_1 equations directly as the low-order equations in the synthetic scheme, use a similarity transformation to put the P_1 equations in an S_2 form and difference the resulting S_2 equations the same way that the S_n equations are differenced. Consistency between the spatial differencing of the S_n equations and the low-order equations is thus trivially achieved. Although it is considerably more expensive to directly solve the S_2 equations than the diffusion equation, the 1-D S_2 equations are relatively inexpensive to directly solve. For instance, the diffusion equation derived from the S_n equations with linear-discontinuous spatial differencing gives a three-diagonal matrix equation with one unknown per spatial cell edge, whereas the S_2 equations with linear-discontinuous spatial differencing give a seven-diagonal matrix equation with four unknowns per spatial cell.

The moment representation for the AD operator can yield negative angular flux solutions under certain circumstances. These negative angular fluxes are usually sufficiently small that they do not affect the accuracy of the scalar flux solution. But if accurate angular fluxes in all directions are required, these negative angular fluxes can present a problem. One-dimensional slab and spherical geometry finite-difference schemes for the AD operator have been developed which are exact in the diffusion limit and give unconditionally positive angular flux solutions.¹⁵ However,

finite-difference AD operators cannot be represented with a diagonal matrix in the Legendre basis, thus they cannot be represented in terms of effective cross-section moments. These, then, can only be implemented in S_n codes through modification of the codes. Furthermore, the development of AD differencing schemes for standard multidimensional triangular quadrature sets is not straightforward. Conversely, the moment representation for the AD operator is very versatile in that it can be applied (in conjunction with Galerkin quadrature) in multiple dimensions.

IV. MODIFICATIONS TO ONETRAN

We have implemented the Galerkin quadrature method and the S_2 -synthetic acceleration method in the discrete ordinates code, ONETRAN.⁸ We stress that although these methods were developed for BFP calculations, they represent general S_n methods that can be applied to standard neutronic and photonic calculations as well. We have also implemented a new angular differencing scheme for the streaming operator in ONETRAN that eliminates the classic "flux-dip" problem.¹⁶ However, this improvement is of much greater significance for neutronics calculations than for charged-particle calculations.

V. COMPUTATIONAL EXAMPLES

In this section we present coupled electron-photon transport calculations performed with the new version of ONETRAN. The multigroup BFP data used in the calculations was generated with the CEPXS code.¹⁷ This code was developed in collaboration with Dr. Leonard J. Lorence, Jr. of Sandia National Laboratories. All calculations presented in this section were performed by Dr. Lorence in support of experimental projects. Thus, realistic rather than ideal calculations are presented.

The first problem considered consists of "fission-spectrum" electrons isotropically incident from the left upon a 2-cm-thick aluminum slab. The "fission spectrum" is that characteristic of beta particles emitted by fission products and contains electrons with energies from about 8 MeV to 50 keV. The ONETRAN calculation for this problem was carried out with 50 spatial cells, S_8 Gauss quadrature, P_7 cross-section expansions, 50 electron groups linearly spaced from 8 MeV to 10 keV, and 30 similarly spaced photon groups. For comparison, a Monte Carlo calculation was performed with the ITS-TIGER code.¹⁸ A sufficient number of Monte Carlo histories was run to obtain a one-sigma relative deviation of no more than 20 percent in the energy deposited in each spatial cell. The energy deposition profiles calculated with the discrete ordinates and Monte Carlo codes are compared in Fig. 1. The agreement is excellent. However, the ONETRAN calculation required approximately 37 minutes of CPU time on a VAX 11/780 computer whereas the TIGER calculation required approximately 1230 minutes of CPU time on the same computer. Thus, ONETRAN/CEPXS gives the same accuracy as the Monte Carlo code, but is approximately 35 times faster for this problem.

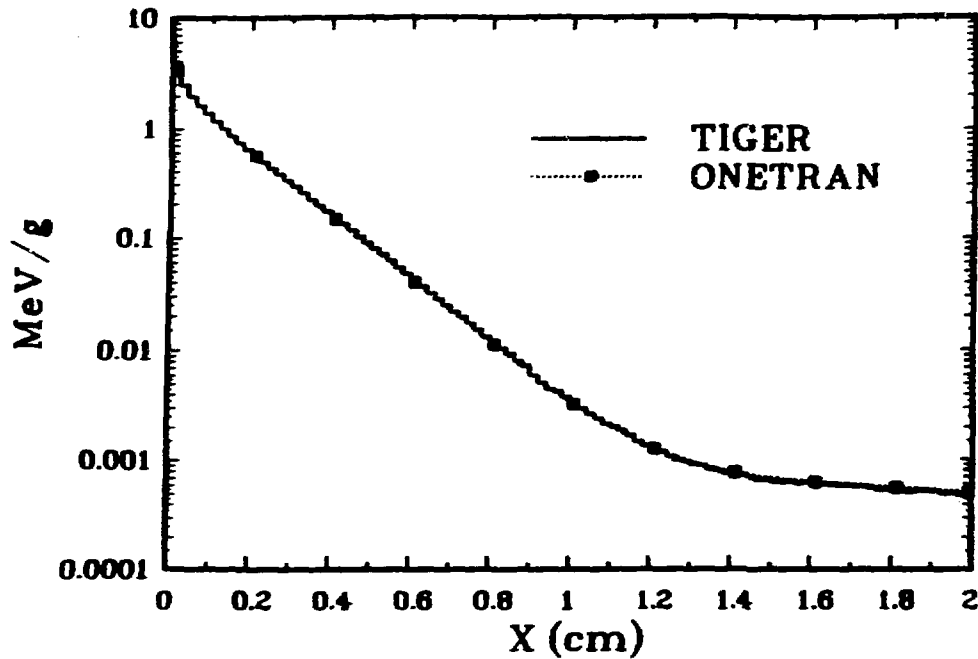


Fig. 1. Energy Deposition Profile for Fission Electrons Isotropically Incident Upon a Slab of Aluminum.

The second problem consists of the same spectrum of electrons isotropically incident from the left upon a 1-D slab model of a shielded integrated circuit chip. This model is referred to as the RADPAK model.¹⁹ The RADPAK geometry is shown in Fig. 2. The energy deposited in the silicon region per electron entering the slab was calculated with both ONETRAN and ITS-TIGER. The ONETRAN calculation gave 5.92×10^{-5} MeV and ITS-TIGER gave $5.7 \pm 0.3 \times 10^{-5}$ MeV. Note that the calculations agree to within the one-sigma deviation quoted for the Monte Carlo calculation. The ONETRAN calculation required approximately 62 minutes of CPU time on a VAX 11/780 computer and the TIGER calculation required approximately 1835 minutes. Thus, ONETRAN/CEPXS gives the same accuracy as TIGER for this problem, but is about 30 times faster.

Al	W	Al	Si	Al ₂ O ₃	W	Al
40	40	3	6	20	40	40
mm1	mm1	mm1	mm1	mm1	mm1	mm1

Fig. 2. RADPAK 1-D Geometry.

The third problem is identical to the second except that we performed an adjoint calculation with ONETRAN to calculate the energy deposition in the silicon as a function of energy for both electrons and photons isotropically incident from the left. The group-dependent response values are plotted in Fig. 3. Each histogram corresponds to a group. Let R_g^e and R_k^p denote the electron and photon responses associated with electron group g and photon group k , respectively. The energy deposited in the silicon per electron in group g entering the slab is given by $4R_g^e$. Similarly, the energy deposited in the silicon per photon in group k entering the slab is given by $4R_k^p$. Thus, the response curves obtained with a single ONETRAN adjoint calculation allow one to obtain the energy deposited in the silicon for an arbitrary electron or photon source spectrum. This adjoint calculation required about 90 minutes of CPU on a VAX 11/780 computer. Standard coupled electron-photon Monte Carlo codes such as ITS-TIGER do not offer an adjoint capability.

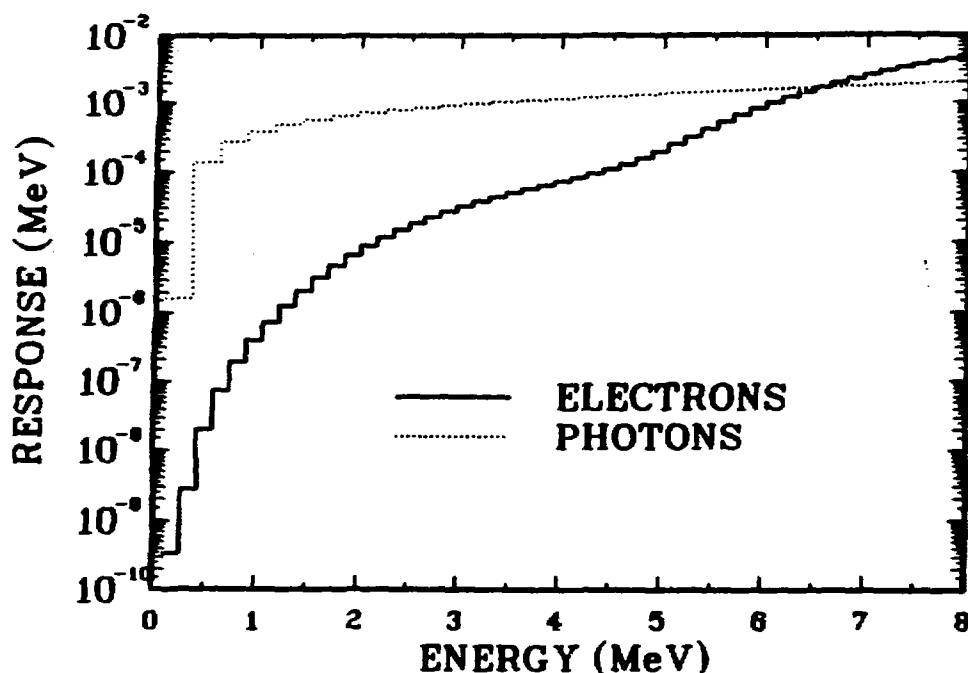


Fig. 3. Adjoint Solutions for Electrons and Photons Isotropically Incident Upon the RADPAK Configuration from the Left. The dose to the silicon chip in the RADPAK configuration can be calculated for any source spectrum of electrons and/or photons with these curves.

The fourth problem consists of a plane wave of 100-keV photons incident from the left upon a slab of graphite. We have calculated the photoemission efficiency (electrons emitted per photon entering the slab) at the right face of the slab with both ONETRAN and ITS-TIGER as a function of slab thickness. The efficiencies are plotted in Fig. 4. The agreement between the calculations is excellent. The CPU times required by each code as a function of slab thickness are plotted in Fig. 5. The calculations were performed on a CRAY XMP. Note that the ONETRAN CPU

times are constant at about 60 seconds whereas the ITS-TIGER CPU times steadily increase from about 100 seconds to about 10000 seconds. Thus, ONETRAN gives the same accuracy as ITS-TIGER but is over 100 times faster. A constant CPU time was achieved with ONETRAN by using the same total number of spatial cells in each calculation and varying the spacing such that the right edge of the slab was always well resolved. The ITS-TIGER calculations were carried out with a special version of TIGER called IFS-TIGER, which was developed specifically for this type of problem.

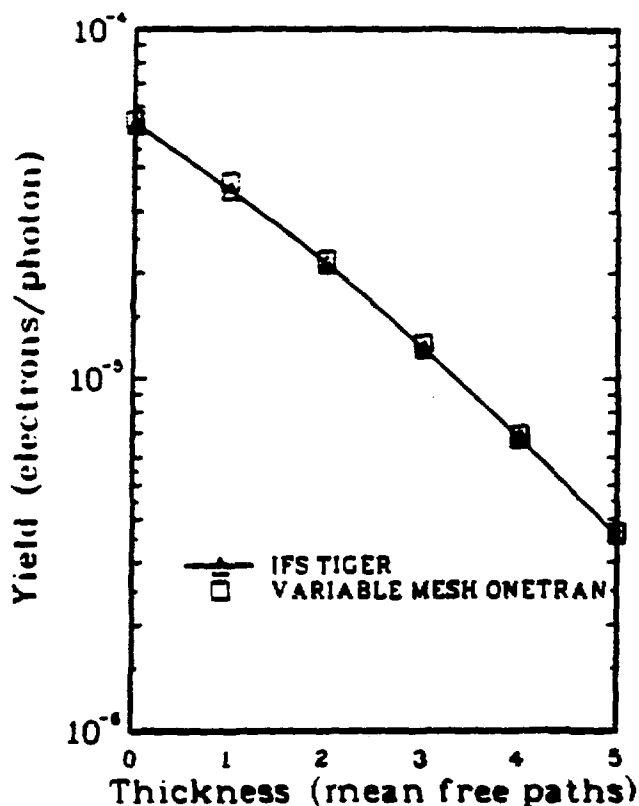


Fig. 4. Transmitted Electron Photoemission Yield as a Function of Slab Thickness for 100 keV Electrons Normally Incident Upon a Slab of Graphite. The slab thickness is given in photon mean-free-paths.

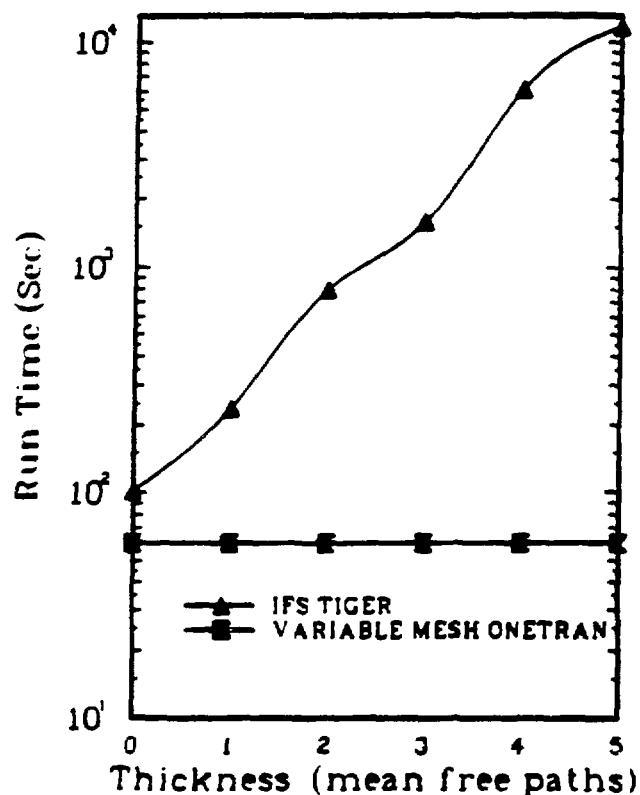


Fig. 5. CPU Times for Monte Carlo and S_n Methods for Photoemission Calculations as a Function of Graphite Slab Thickness.

The fifth problem consists of a plane-wave of Co-60 gamma-rays incident upon a two-layer slab of lithium-fluoride and lead. We have calculated the energy deposition profile for this problem using both ONETRAN and ITS-TIGER. The corresponding curves are plotted in Fig. 6. The agreement between the calculations is quite good. The ONETRAN calculation required about 2 minutes of CPU time on a CRAY-XMP and ITS-TIGER required about 20 minutes of CPU time. This calculation was performed with a version of ITS-TIGER that was modified specifically for this problem to achieve the highest efficiency possible. The charge deposition was also calculated for this problem with ONETRAN and ITS-TIGER. However, we were unable to obtain reasonable statistical accuracy with ITS-TIGER after an hour of CPU time on a CRAY-XMP. All charge deposition values were estimated to have one-sigma relative deviations of over 100 percent. It was estimated that at least 10 hours of CPU time would be required to obtain reasonable statistical accuracy. Thus, even though the Monte Carlo method is reasonably efficient for calculating the energy deposition in this problem, it is prohibitively expensive for calculating charge deposition. Conversely, ONETRAN provides both the energy and charge deposition profiles with equal efficiency. Considering the results which

LiF - Pb Detector Problem

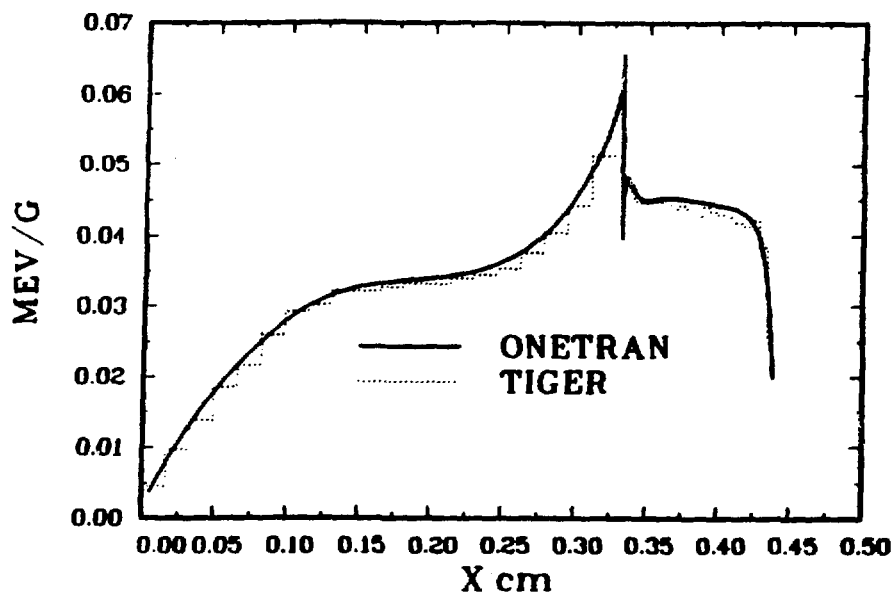


Fig. 6. Dose Profile for Co-60 Gamma Rays Normally Incident from the Left Upon a Sandwich of LiF and Pb. The left and right portions of the slab are LiF and Pb, respectively.

LiF - Pb Detector Problem

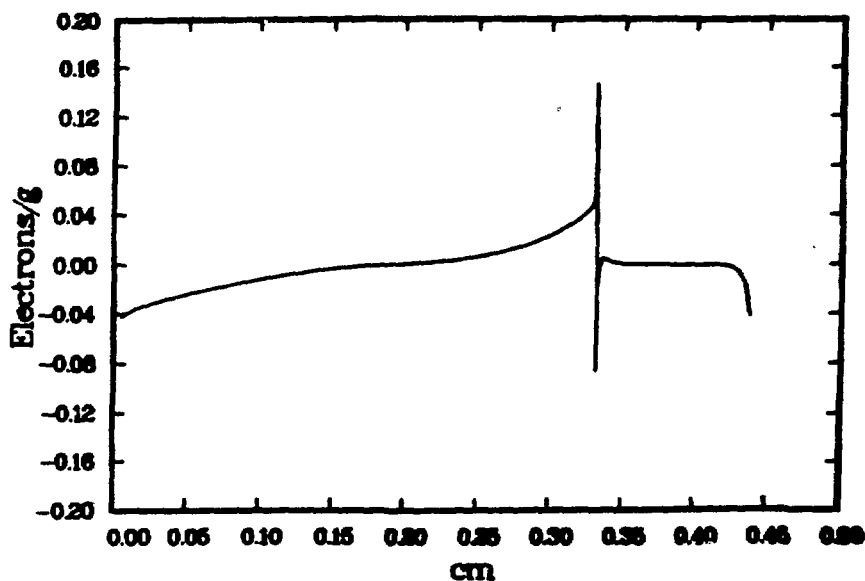


Fig. 7. Charge Profile for Co-60 Gamma Rays Normally Incident from the Left Upon a Sandwich of LiF and Pb. The left and right portions of the slab are LiF and Pb, respectively.

we have obtained, it seems quite fair to expect that ONETRAN would run on the order of 1000 times faster than ITS-TIGER on this charge deposition calculation, however, we cannot confirm this because of the expense of performing the Monte Carlo calculations. The charge deposition profile calculated with ONETRAN is plotted in Fig. 7. Note the rapid variation of the solution in the boundary layers near the material interface and the outer faces. A very non-uniform spatial mesh was used to resolve this behavior.

VI. CONCLUSIONS

Our results clearly demonstrate that coupled electron-photon BFP calculations can be efficiently and accurately performed with standard discrete-ordinates codes designed only to solve the Boltzmann equation. For a large class of realistic problems, the discrete-ordinates method is very much more efficient than the Monte Carlo method. In the near future, we hope to apply our BFP method to other types of transport calculations. In particular, we intend to compare the discrete ordinates method with standard Monte Carlo methods for ion transport problems of interest to materials scientists.

The accuracy of the approximations for Fokker-Planck operators that can be used with standard discrete ordinates codes is limited by the restriction that these approximations be representable in multigroup-Legendre form. These approximations appear to be adequate for a wide range of coupled electron-photon transport problems, but greater accuracy is desirable for other types of calculations. This can only be achieved by explicitly writing discrete ordinates codes to solve the Boltzmann-Fokker-Planck equation rather than just the Boltzmann equation. We believe that the results that we have obtained for coupled electron-photon BFP calculations justifies the development of such codes. In the near future, we hope to develop such a code for 1-D slab geometry calculations and use it to test the accuracy of our BFP methods for ion transport calculations of interest to the materials science community.

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TRAITEMENT PHYSICO NUMERIQUE DU TERME DE DIFFUSION
A GRAND ANGLE LORS DU RALENTISSEMENT DES PARTICULES ALPHA

J.P. MORREEUW

Résumé

Le traitement du ralentissement des particules alpha conduit à un membre de droite, $(\frac{\partial n}{\partial t})_c \equiv \frac{\partial}{\partial E} (F_e + F_i)$, où E est l'énergie de la particule, et où $F_e = K_e (\frac{n}{v} + kT_e \frac{\partial}{\partial E} \frac{n}{v})$.

Sous l'hypothèse des ions au repos, la contribution ionique peut être décrite en terme de noyau de Green :

$$F_i = \int G(E, E') n(E') dE'$$

Nous utiliserons dans ce travail la forme du noyau $G(., E)$ pour approcher F_i sous la forme $An + Y$, où Y est solution d'une équation différentielle $BY + C \frac{\partial Y}{\partial E} = n$.

Le problème mathématique est alors bien posé, il peut être discrétisé de manière stable par un schéma décentré. Ce schéma peut être implanté très aisément dans toute méthode de moments classique .

PHYSICO-NUMERICAL TREATMENT OF LARGE ANGLE SCATTERING DURING
ALPHA PARTICLE SLOWING DOWN

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ABSTRACT

In the theoretical treatment of alpha particle slowing down the right-hand side of the energy equation is of the form

$$\left(\frac{\partial n}{\partial t}\right)_c \equiv \frac{\partial}{\partial E} (\mathcal{F}_e + \mathcal{F}_i)$$

where E is energy of the particle.

The electronic contribution $\mathcal{F}_e$ is

$$\mathcal{F}_e = K_e \left\{ \frac{n}{v} + kT_e \frac{\partial}{\partial E} \frac{n}{v} \right\}$$

If we assume the ions to be at rest, the ionic contribution is described with the help of a Green kernel :

$$\mathcal{F}_i(E) = \int \mathcal{G}(E, E') n(E') dE'$$

The aim of our work is to use the shape of the $\mathcal{G}(., E)$ function to approximate $\mathcal{F}_i$ under the form :

$$\mathcal{F}_i \approx An + Y$$

$$B Y + C \frac{\partial Y}{\partial E} = n$$

where A, B and C are functions of E.

The mathematical problem is then well posed, and the discretization by one-sided difference scheme is stable.

The implementation of this treatment is very easy in any deterministic standard moment method.

1 - INTRODUCTION

The slowing down of a suprathermal test particle (alpha particle) by a continuous background of weakly coupled plasma is described by the equation

$$(1) \quad \left(\frac{dn}{dt}\right)_{\text{coll}} = \int k(\underline{x}, \underline{p}' \rightarrow \underline{p}) n(\underline{x}, \underline{p}') d\underline{p}' - n(\underline{p}) \int k(\underline{x}, \underline{p} \rightarrow \underline{p}') d\underline{p}' ,$$

where $n d\underline{p} d\underline{x}$ is the particle density in the phase space,
 $\underline{p}$ is the particle momentum,
 and $k(\underline{x}, \underline{p}' \rightarrow \underline{p})$ is a collision kernel.

Assuming background isotropy, we average (1) over the direction, and we get the equation for the particle density per unit energy N , written in relativistic notation

$$(2) \quad \left(\frac{dN}{dt}\right)_{\text{coll}} = \int K_0(W', W) \frac{N(W')}{p' W'} dW' - \frac{N(W)}{pW} \int K_0(W, W') dW' ,$$

where W is the relativistic energy of the particle, and using the first order moment, we get the equation for the energy flux per unit energy F :

$$(3) \quad \left(\frac{dF}{dt}\right)_{\text{coll}} = \int K_1(W', W) \frac{F(W')}{p'^3 W'} dW' - \frac{F(W)}{pW} \int K_0(W, W') dW' .$$

Assuming that the plasma is in equilibrium at temperature T , we use the principle of detailed balancing and get the symmetry relations

$$(4) \quad e^{-\frac{W'}{kT}} k(\underline{p}' \rightarrow \underline{p}) = e^{-\frac{W}{kT}} k(\underline{p} \rightarrow \underline{p}') ,$$

and

$$(5) \quad e^{-\frac{W'}{kT}} K_1(W', W) = e^{-\frac{W}{kT}} K_1(W, W') .$$

Under this last assumption, one can also derive for any function U the following fundamental relation:

$$(6) \quad \int K_1(W', W) U(W') dW' - U(W) \int K_1(W, W') dW' \\ = \frac{\partial}{\partial W} \int e^{-\frac{W'}{kT}} G_1(W', W) \left\{ kT \frac{\partial}{\partial W'} \left[e^{\frac{W'}{kT}} U(W') \right] \right\} dW' ,$$

where G_1 is defined as follows :

$$(7) \quad kT e^{-\frac{W'}{kT}} G_1(W', W) = \iint_{\substack{W_1 > W > W_2 \\ W_1 > W' > W_2}} e^{-\frac{W_1}{kT}} K_1(W_1, W_2) dW_1 dW_2 .$$

The kernel G_1 has the same symmetry property as K_1 , and therefore one can iterate the procedure and obtain the expressions :

$$(8) \quad \left(\frac{dN}{dt}\right)_{\text{coll}} = \frac{\partial}{\partial W} A_1^0 E kT e^{-\frac{W}{kT}} \frac{\partial}{\partial W} \left(e^{\frac{W}{kT}} \frac{N}{pW} \right) + \frac{\partial^2}{\partial W^2} \mathcal{L}^0 \left\{ kT^2 \frac{\partial^2}{\partial W^2} \left(e^{\frac{W}{kT}} \frac{N}{pW} \right) \right\} ,$$

$$(9) \quad \left(\frac{dF}{dt}\right)_{\text{coll}} = \frac{A_0 F}{p^3 W} + \frac{\partial}{\partial W} A_1^1 E kT e^{-\frac{W}{kT}} \frac{\partial}{\partial W} \left(e^{\frac{W}{kT}} \frac{F}{p^3 W} \right) + \frac{\partial^2}{\partial W^2} \mathcal{L}^1 \left\{ kT^2 \frac{\partial^2}{\partial W^2} \left(e^{\frac{W}{kT}} \frac{F}{p^3 W} \right) \right\} ,$$

where E is the kinetic energy ($W - mc^2$),
and $\mathcal{L}^0$ and $\mathcal{L}^1$ are self-adjoint linear operators.

We can reiterate and get the formal expansions

$$(10) \quad \left(\frac{dN}{dt}\right)_{\text{coll}} = \sum_{i=1}^{\infty} \frac{\partial^i}{\partial W^i} A_1^0 E^i kT^i e^{-\frac{W}{kT}} \frac{\partial^i}{\partial W^i} \left(e^{\frac{W}{kT}} \frac{N}{pW} \right) ,$$

$$(11) \quad \left(\frac{dF}{dt}\right)_{\text{coll}} = -A_0 \frac{F}{p^3 W} + \sum_{i=1}^{\infty} \frac{\partial^i}{\partial W^i} A_1^1 E^i kT^i e^{-\frac{W}{kT}} \frac{\partial^i}{\partial W^i} \left(e^{\frac{W}{kT}} \frac{F}{p^3 W} \right) .$$

In order to compute these collision terms, we will assume that the large energy exchange interactions are well described by the binary (nuclear and Coulomb) shock theory, with no use of any screening potential. Then the contribution of collective effects is included in the A_0 , A_1^0 and A_1^1 terms alone, and the $\mathcal{L}^0$ and $\mathcal{L}^1$ operators (and the $A_1^1 - p^2 A_1^0$ coefficient) can be computed using the classical binary theory.

So we get the contribution to large energy exchange interactions of each of the different species of the background plasma, and thus the generalization to the case of several species of field particles at different temperature. In fact only particles of almost the same mass as the test particle have large energy exchange effects ; so, one can consider only one field particle temperature.

The terms in the formal expansion (10) can be easily obtained, and each of them satisfy the detailed balance property. But it can be seen that the A_1^0 coefficients are positive, so that each even order truncation leads us to an ill-conditioned problem. Then, even if the first order truncation gives the classical second order Fokker-Planck expansion, higher order truncations are uncertain, and too difficult to use.

Our aim will now be to get a well-posed approximation that gives an accurate description of large energy exchange interactions.

2 - APPROXIMATION OF THE DENSITY EQUATION

The density equation (10) :

$$\left(\frac{dN}{dt}\right)_{\text{coll}} = \sum_{i=1}^{\infty} \frac{\partial^i}{\partial W^i} A_1^0 E^i kT^i e^{-\frac{W}{kT}} \frac{\partial^i}{\partial W^i} \left(e^{\frac{W}{kT}} \frac{N}{pW} \right) ,$$

can be written

$$(12) \quad \left(\frac{dN}{dt}\right)_{\text{coll}} = \frac{\partial}{\partial W} \int e^{-\frac{W'}{kT}} G_0(W', W) \left\{ kT \frac{\partial}{\partial W'} \left(e^{\frac{W'}{kT}} \frac{N(W')}{p'W'} \right) \right\} dW' ,$$

where $G_0(W', W)$ is described by the classical binary shock theory, at least out of a neighbourhood of $W = W'$.

If we assume the field particle to be at rest, the G_0 kernel is very easy to obtain in the cases of non relativistic Coulomb scattering and of isotropic scattering (which is a good approximation of nuclear scattering). We get :

$$(13) \quad G_0(W, W') = a(W) g_0\left(\frac{E'}{E}\right) ,$$

and the shape of the g_0 function can be seen on Figure 1 (as well as g_1 corresponding to the flux equation).

We see that the kernel G_0 is composed of a small energy loss part, close to a Dirac function, including the collective effects, and a large energy loss part, which can be approximated by the resolvent of a first order differential equation.

Mathematically speaking, this means that we can choose a function ϕ such that

$$(14) \quad \int e^{-\frac{W'}{kT}} G_0(W', W) U(W') dW' = E(A^0 - \phi) e^{-\frac{W}{kT}} U + S(U)$$

defines an inversive symmetrical operator

$$\mathcal{S} : U \rightarrow Y = \mathcal{S}(U) ,$$

whose inverse

$$\mathcal{M} : Y \rightarrow U = \mathcal{M}(Y)$$

is close to a symmetrical second order differential operator.

By identification with the first two terms of expansion (10), this operator must be written :

$$(15) \quad U = \frac{e}{\phi E} \frac{W}{kT} \left\{ Y - \frac{\partial}{\partial W}(BEY) - kT \frac{\partial}{\partial W} \left(B \phi E^2 \frac{\partial}{\partial W} \left(\frac{Y}{\phi E} \right) \right) \right\} ,$$

where B is defined by the relation :

$$(16) \quad A_2^0 = B \phi \left\{ 1 + \frac{\partial}{\partial W} \left(\frac{e}{\phi E} \frac{W}{kT} kT \frac{\partial}{\partial W} (A_2^0 E^2 e^{-\frac{W}{kT}}) \right) \right\} .$$

The ϕ function will be chosen such that the problem is well-posed, and the approximation accurate.

A necessary condition for this is :

$$(17) \quad \phi < A_1^0 .$$

A sufficient condition is then $B > 0$ and $\phi > 0$, but we believe that a weaker condition can be used to get an a priori estimate uniformly in the temperature T.

Roughly speaking we will choose ϕ in order both to recover the 3rd term of expansion (10), and to satisfy (17). If this is not possible, and although A_1^0 describes mainly small angle scattering, we take :

$$\phi = A_1^0 .$$

Figure 2 shows the approximation for Coulomb and isotropic scattering on a field particle at rest. The accuracy is very good for the isotropic case, and qualitatively correct for the Coulomb case. In all these cases conditions $B > 0$ and $\phi > 0$ are satisfied.

An alternative choice to approximate the $\mathcal{M}$ operator is :

$$(15bis) \quad U = \frac{e}{\phi E} \left\{ Y - \frac{\partial}{\partial W} EBY \right\} ,$$

where B is defined by the relation

$$(16bis) \quad A_2^0 - \frac{kT}{E^2} \frac{\partial}{\partial W} A_2^0 E^2 = B \phi \left\{ 1 + \frac{\partial}{\partial W} \left(\frac{e}{\phi E} kT \frac{\partial}{\partial W} (A_2^0 E^2 e^{-\frac{W}{kT}}) \right) \right\} .$$

We thus get a simpler expression which leads us to a well-posed problem and satisfies the detailed balance property, although we loose the symmetry property of the operator $\mathcal{M}$.

The explicit determination of the physical coefficient B and ϕ from the Coulomb and nuclear cross sections is not difficult if either Coulomb or nuclear scattering is dominant over the other in the large angle effects. This is generally true ; if not, large angle effects are negligible as compared with the electronic small angle scattering.

As far as the flux equation is concerned, we will just mention that the same kind of approximation can be used, although the A_1^1 coefficients are not positive. We show in figure 3 the value of the normalized expansion coefficients :

$$\Sigma_0 = \frac{A_1^1}{A_0} ; \quad \Sigma_1 = \frac{A_2^1}{A_0} ; \quad \Sigma_2 = 2 \frac{A_3^1}{A_0} ,$$

for various field particle mass. We can see that all the coefficients are positive as is the case for the density equation ; if not the first term of expansion (11) is dominant ; In this last case it is possible to correct the A_2^1 coefficients, and then use the same procedure as that used to obtain expression (15) and (16) for the density equation.

3 - NUMERICAL DISCRETIZATION

Before choosing the discretization we have to remember that :

- The straight line slowing down is the dominant phenomenon.
- Our main purpose is to describe the energy exchange.
- We want to be able to use a very low number of energy groups (or a grey method).

Physical considerations show that the quantity $E A_1^0 \frac{N}{pW}$ has to be described by a piece-wise constant function, and the particle sources located at the upper bound of the energy interval.

For the above reasons we split the particle density into energy groups, taking the mean value at the center of the group, and we use a one-sided difference scheme :

$$(18) \quad (\delta^+ u)_i = \frac{1}{\Delta_i} (u_{i+1} - u_i) \quad \text{as "upwind difference"} ,$$

$$(\delta^- u)_i = \frac{1}{\Delta_i} (u_i - u_{i-1}) \quad \text{as "downstream difference"} ,$$

where Δ_i is the width of the energy group i .

For the density equation in each group we get :

$$(19) \quad \left(\frac{dN}{dt} \right)_i = (\delta^+ \left(\frac{E(A_1^0 - \phi)}{pW} \right) (N + kT pW \delta^- \left(\frac{N}{pW} \right)) + Y)_i ,$$

where Y_i is defined by :

$$(20) \quad \left\{ \frac{\phi E}{pW} \right\}_i (N + kT pW \delta^- \left(\frac{N}{pW} \right))_i = Y_i - (\delta^+ (\{EB\} (Y + kT \phi E \delta^- \left(\frac{Y}{\phi E} \right)))) ,$$

with

$$\left\{ \frac{E A_1^0}{pW} \right\}_i = \frac{\Delta_i E_{i+\frac{1}{2}}}{\int_{E_{i-\frac{1}{2}} A_1^0}^{E_{i+\frac{1}{2}} pW} dW} ; \quad \left\{ \frac{E \phi}{pW} \right\}_i = \left(\frac{\phi}{A_1^0} \right)_i \left\{ \frac{E A_1^0}{pW} \right\}_i .$$

As regards time discretization of these equations, it can be shown, assuming constant coefficients, that the fully implicit as well as the centered semi-implicit schemes are stable as soon as :

$$(21) \quad \left\{ \frac{E(A_1^0 - \phi)}{pW} \right\} > 0 ; \quad \left\{ \frac{E \phi}{pW} \right\} > 0 ; \quad \{EB\} > 0 .$$

We believe that the last two conditions are not necessary, even if they are generally satisfied.

If we use the simplified formulation (15bis), instead of (20) we get

$$(20bis) \quad \left\{ \frac{\phi E}{pW} \right\}_i (N + kT p W \delta^-(\frac{N}{pW}))_i = Y_i - (\delta^+(\{EB\} Y))_i .$$

It can be shown that time resolution of this equation by a direct method is stable.

This resolution is like a Jacobi Method, with all values being taken at the end of the time step, except the $(\frac{N}{pW})_{i-1}$ value used in the $\delta^-(\frac{N}{pW})$ term, which is taken at the beginning of the time step, the energy groups being described in decreasing energy order. This property avoids any splitting in the space-time resolution.

4 - CONCLUSION

In this study we give a description of the large angle scattering operator for moment equations, with no use of any arbitrary cut-off angle, and we show that this operator can be computed by a pure binary collision theory.

We give an approximation of this operator by an inverse method, which is very accurate for a more or less important phenomenon, the dominant phenomenon being the straight line slowing down.

This approximation could also work for a treatment of thermalization, not considered in the present analysis.

It can be easily used for semi-analytical model, or numerically under a stable discretisation.

The numerical treatment, at least under its simplified form, can be implemented as a minor modification in a classical moment method, and gives an efficient tool to compute the large angle scattering effects.

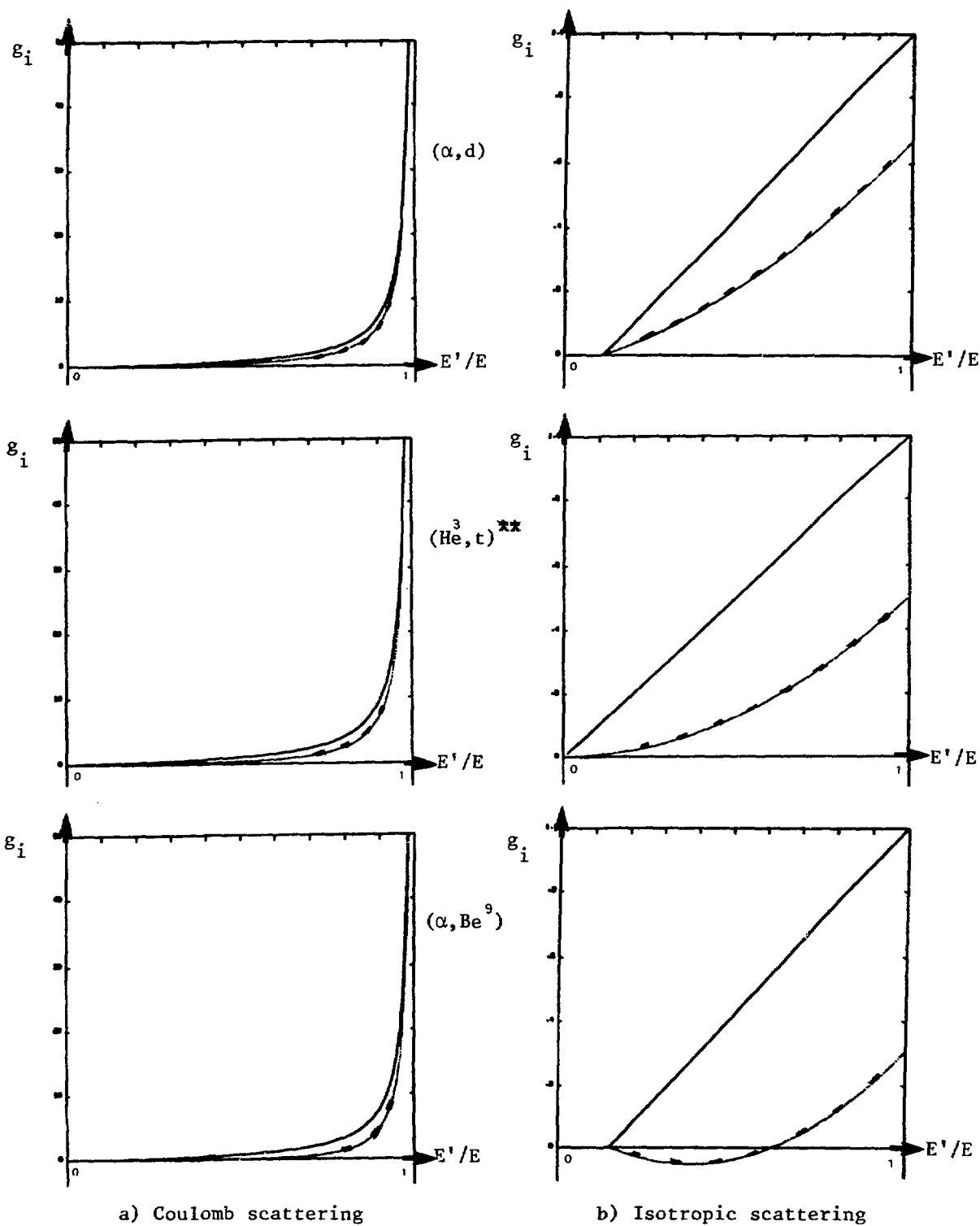


Figure 1 : Shape of the kernel $G_i(W, W')$
for density and energy flux equation

* The dashed line corresponds to energy flux equation

120 ** Or (α, He^4) supposed to be unlike particles

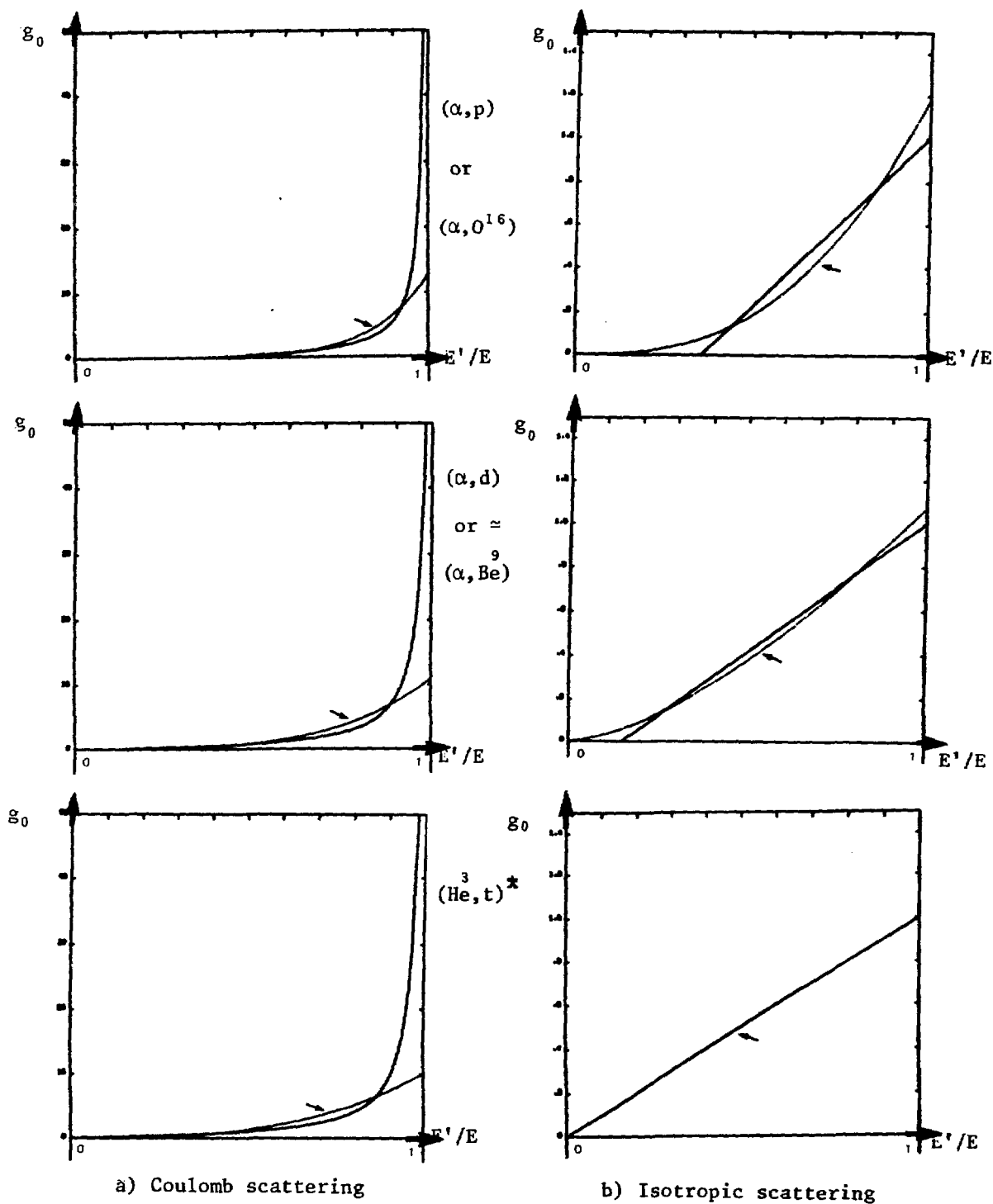
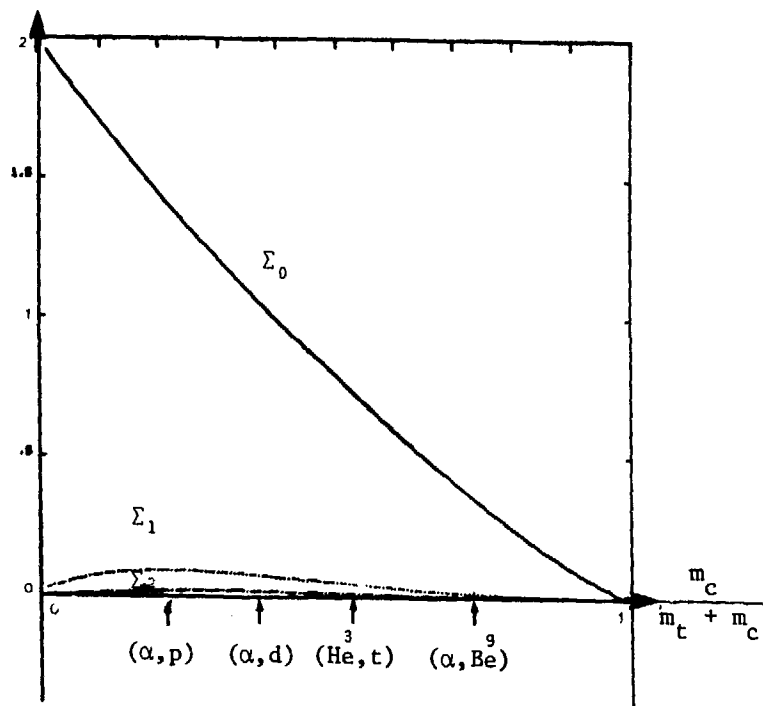
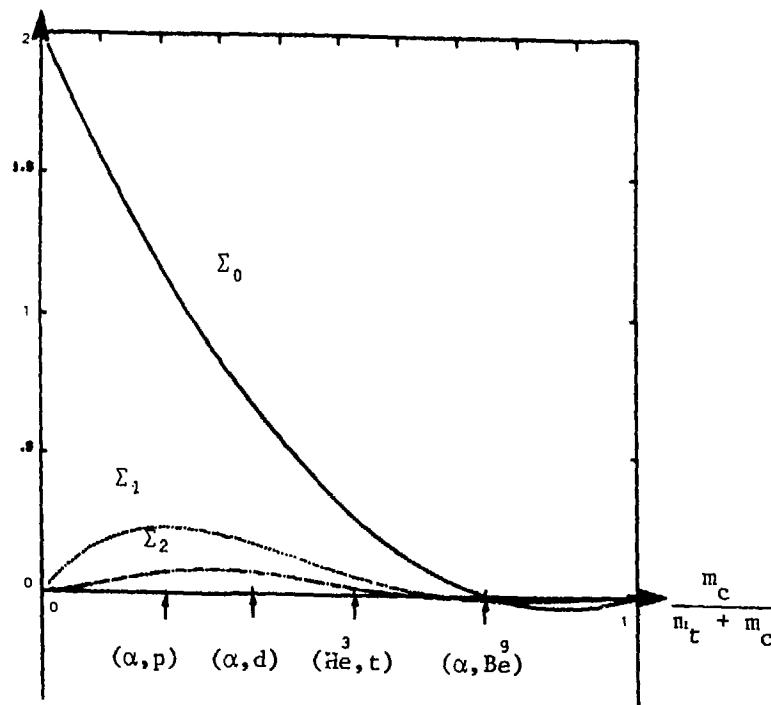


Figure 2 : Approximation of the kernel $G_0(W, W')$
for density equation

* Or (α, He⁴) supposed to be unlike particles



a) Coulomb scattering



b) Isotropic scattering

Figure 3 : Normalized value of expansion coefficients

of the energy flux equation

$$\Sigma_0 = A_1^1/A_0 \quad , \quad \Sigma_1 = A_2^1/A_0 \quad , \quad \Sigma_2 = 2 A_3^1/A_0$$

NUMERICAL TREATMENT OF THE TRANSPORT OF FAST CHARGED PARTICLES IN A SPHERICAL PLASMA

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Abstract: *We propose a numerical scheme for solving the time-dependent linear Boltzmann -Fokker-Planck (BFP) equation governing the transport of fast charged particles in a spherical plasma. The spatial and angular variables are treated altogether by a finite difference Diamond scheme, and a discontinuous finite element multigroup method is used to deal with the energy variable. This method assumes that the flux is a linear function of the energy within each group, with a possible discontinuity at the upper energy boundary of each group. Numerical results for the solution of several benchmark problems are presented.*

1. INTRODUCTION

As it is well known, the energy deposition of fast ions in plasmas is an important problem for thermonuclear fusion. If the plasma is in thermal equilibrium, the distribution function of the suprathermal component is governed by a linear transport equation. Since the scattering of charged particles is highly forward-peaked, the classical Boltzmann equation is usually approximated by the Fokker-Planck equation, which is valid in the assumption of small angle collisions. Recently a new transport equation (Boltzmann-Fokker-Planck equation) has been proposed by Ligou¹ in order to combine the advantages of the Boltzmann equation (accurate treatment of the large angle collisions) with those of the Fokker-Planck formalism.

This paper describes a numerical code which has been developed to solve the BFP equation in a spherical plasma. When the spherical symmetry is assumed, the angular fluxes of charged particles depend on only four variables: the distance from the center, the cosine of the angle between the radial outward direction and the direction of the propagation, the energy and the time. In the code presented here, the spatial and angular variables are treated altogether by a Diamond scheme, and the energy variable is solved by a discontinuous finite element method. A description of the numerical method for the BFP equation without angular diffusion is given in Section 2, and numerical results on some benchmark problems are presented in Section 3. Section 4 describes an iterative treatment of the Fokker-Planck angular diffusion operator, and Section 5 is our conclusion.

2. NUMERICAL METHOD

The BFP equation can be derived from the classical Boltzmann equation used in neutron transport theory (see e.g. Przybylski and Ligou²). In one-dimensional spherical

geometry it can be written as follows:

$$\begin{aligned} & \frac{1}{v} \frac{\partial \varphi}{\partial t} + \mu \frac{\partial \varphi}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial \varphi}{\partial \mu} + (\Sigma_s + \Sigma_a) \varphi \\ &= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_{\ell}(\mu) \int_0^{\infty} \Sigma_{s,\ell}(E' \rightarrow E) \Phi_{\ell}(E') dE' + \frac{\partial}{\partial E} (S\varphi) + T \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial \varphi}{\partial \mu} + Q \quad (1) \end{aligned}$$

where $\varphi(r, \mu, E, t)$ and $Q(r, \mu, E, t)$ are the angular fluxes and external sources of charged particles, S is the stopping power of the plasma, T is the angular diffusion coefficient (in most cases the differential angular diffusion term is small compared to the slowing down term), Φ_{ℓ} is the ℓ -th Legendre moment of φ , and the other notations have their usual meaning.

Eq. 1 has to be solved for $0 < r < R$, $-1 < \mu < +1$ and $E_{th} < E < E_{max}$, where R is the plasma outer radius, E_{th} is the mean energy of thermal ions and E_{max} is the maximum energy of the fast ions. The boundary conditions are given by:

$$\begin{cases} \varphi(R, \mu, E, t) = 0 & \text{for } \mu \leq 0 \\ \varphi(r, \mu, E_{max}, t) = 0 \\ \varphi(r, \mu, E, 0) = \varphi_0(r, \mu, E) \end{cases}$$

2.1 Spatial and angular discretization

We will first consider the stationnary BFP equation, leaving aside all angular diffusion terms (the integral Boltzmann scattering operator can be dealt with by the standard iterative method used in neutron transport calculations, and an iterative treatment for the Fokker-Planck diffusion operator will be described in Section 4). Eq. 1 is thus reduced to a purely hyperbolic form:

$$\mu \frac{\partial \varphi}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial \varphi}{\partial \mu} + \Sigma \varphi - \frac{\partial (S\varphi)}{\partial E} = Q \quad (2)$$

The three first terms of Eq. 2 are similar to the left hand terms of the spherical neutron transport equation. We thus have chosen to deal with them by the classical Diamond approximation. The spatial mesh $\{r_0 = 0, r_1, \dots, r_i, r_{i+1}, \dots, r_N = R\}$ usually comes from a coupled hydrodynamics code, and the angular mesh $\{\mu_{1/2} = -1, \mu_{3/2}, \dots, \mu_{m-1/2}, \mu_{m+1/2}, \dots, \mu_{M+1/2} = +1\}$ is chosen symmetric about $\mu = 0$. If we use the notation of Reed and Lathrop³, we obtain on each cell $\{r_i, r_{i+1}\} \times \{\mu_{m-1/2}, \mu_{m+1/2}\}$ a differential relation in energy which is as follows:

$$\mu_m \left\{ \frac{A_{i+1} \varphi_{i+1} - A_i \varphi_i}{V_{i+1/2}} \right\} + \left\{ \frac{\alpha'_{m+1/2} \varphi_{m+1/2} - \alpha'_{m-1/2} \varphi_{m-1/2}}{V_{i+1/2} w_m} \right\} + \Sigma \varphi - \frac{\partial}{\partial E} (S\varphi) = Q \quad (3)$$

φ is the flux value at the "center" of the cell $\{r_{i+1/2}, \mu_m\}$ defined by

$$\begin{cases} r_{i+1/2} = a_{i+1/2} r_{i+1} + (1 - a_{i+1/2}) r_i & 0 < a_{i+1/2} < 1 \\ \mu_m = r_m \mu_{m+1/2} + (1 - r_m) \mu_{m-1/2} & 0 < r_m < 1 \end{cases}$$

$\varphi_i, \varphi_{i+1}, \varphi_{m-1/2}$ and $\varphi_{m+1/2}$ are the flux values at the center of each cell's face, and the other coefficients are:

$$\begin{cases} A_i = 4\pi r_i^2 \\ V_{i+1/2} = \frac{4\pi}{3}(r_{i+1}^3 - r_i^3) \\ \alpha' = (A_{i+1} - A_i)\alpha \\ \alpha_{m+1/2} - \alpha_{m-1/2} = -\mu_m w_m \quad (\text{and } \alpha_{1/2} = 0) \\ w_m = \mu_{m+1/2} - \mu_{m-1/2} \end{cases}$$

It is assumed that the variation of φ over each cell is linear in r and μ :

$$\begin{cases} \varphi = a_{i+1/2}\varphi_{i+1} + (1 - a_{i-1/2})\varphi_i & (4a) \\ \varphi = \tau_m\varphi_{m+1/2} + (1 - \tau_m)\varphi_{m-1/2} & (4b) \end{cases}$$

Substituting (4a) and (4b) into (3) and taking into account that we already know two of the fluxes φ_i, φ_{i+1} and $\varphi_{m-1/2}$ (either from boundary conditions or by prior calculation in adjoining cell) we get a first order differential equation involving only the unknown function $\varphi(E)$:

$$\begin{aligned} & \left[\Sigma - \frac{\mu_m A_i}{(1 - a_{i-1/2})V_{i+1/2}} + \frac{\alpha'_{m+1/2}}{\tau_m w_m V_{i+1/2}} \right] \varphi - \frac{\partial}{\partial E}(S\varphi) \\ & = Q - \left(A_{i+1} + \frac{a_{i+1/2}}{1 - a_{i+1/2}} A_i \right) \frac{\mu_m \varphi_{i+1}}{V_{i+1/2}} + \left(\alpha'_{m-1/2} + \frac{1 - \tau_m}{\tau_m} \alpha'_{m+1/2} \right) \frac{\varphi_{m-1/2}}{w_m V_{i+1/2}} \end{aligned} \quad (5)$$

(Here we have supposed that the two known fluxes were φ_{i+1} and $\varphi_{m-1/2}$). It has been shown by Reed and Lathrop³ that with a suitable choice of the parameters $\alpha_{i+1/2}$ and τ_m the resulting scheme is second order accurate with respect to r and μ .

2.2 Discontinuous finite element method for the energy variable

After Diamond approximation of the spatial and directional derivatives, we have to solve on each $r \times \mu$ cell a differential equation which in any case can be put in the form:

$$A\varphi - \frac{\partial}{\partial E}(S\varphi) = B \quad \text{for } E_{th} < E < E_{max} \quad (6)$$

We will assume that φ is a linear function of the energy within each group $\{E_1, E_2\}$ with a possible discontinuity at the upper energy limit E_2 . Therefore φ is determined by the knowledge of $\varphi_1 = \varphi(E_1)$, $\varphi_2 = \varphi(E_2)$ and φ_{ext} the limit of $\varphi(E)$ as $E \rightarrow E_2^+$:

$$\varphi(E) = \varphi_1 \psi_1(E) + \varphi_2 \psi_2(E) + (\varphi_{ext} - \varphi_2)H(E - E_2) \quad (7)$$

where $\psi_1(E) = (E_2 - E)/\Delta E$, $\psi_2(E) = (E - E_1)/\Delta E$, and H is the Heaviside function. The behavior of $\varphi(E)$ is shown in Fig. 1. Eq. 6 can be replaced by the following variational problem:

$$\int_{E_1}^{E_2} \left(A\varphi - \frac{\partial}{\partial E}(S\varphi) - B \right) f(E) dE = 0 \quad (8) \quad \forall f \text{ linear on } \{E_1, E_2\}$$

It is obviously sufficient to satisfy (8) for $f = \psi_1$ and $f = \psi_2$, since every linear function on $\{E_1, E_2\}$ is a linear combination of ψ_1 and ψ_2 . Substituting Eq. 7 into Eq. 8, we obtain after a few straightforward calculations:

$$\begin{cases} \varphi_1 \left[\int A \psi_1^2 dE - \int \frac{S \psi_1}{\Delta E} dE + S(E_1) \right] + \varphi_2 \left[\int A \psi_1 \psi_2 dE - \int \frac{S \psi_2}{\Delta E} dE \right] = \int B \psi_1 dE \\ \varphi_1 \left[\int A \psi_1 \psi_2 dE + \int \frac{S \psi_1}{\Delta E} dE \right] + \varphi_2 \left[\int A \psi_2^2 dE + \int \frac{S \psi_2}{\Delta E} dE \right] = S(E_2) \varphi_{ext} + \int B \psi_2 dE \end{cases}$$

(all integrals taken from E_1 to E_2)

We can thus get φ_1 and φ_2 by solving these two simultaneous equations, provided that φ_{ext} has already been obtained from the solution of the neighboring group (for the highest energy group we have $\varphi_{ext} = 0$). It should be pointed out that this method does not assume any linear dependence of the physical quantities $S(E)$, $Q(E)$ and $\Sigma(E)$ within each group.

The computation flow along the space-direction-energy mesh is shown in Fig. 2. We begin with the straight inward direction $\mu = -1$ and the outside of the sphere where the boundary condition is known. This provides input for the treatment of the first inward direction $\mu = \mu_1$. Then we deal with all inward directions, proceeding from the outside to the center. In each $r \times \mu$ cell, Eq. 5 is solved from $E = E_{max}$ to $E = E_{min}$. For the outward directions, the calculation proceeds from the center to the outside, and the center-boundary values are obtained from the central values of the flux in the reflected directions.

2.3 Time discretization

Let us consider a time step $\{t, t + \Delta t\}$ and an intermediate value of the time $\theta = t + h \Delta t$ (with $0 < h < 1$). A finite difference time approximation of Eq. 1 is:

$$\frac{\varphi(t + \Delta t) - \varphi(t)}{v \Delta t} + \Omega \nabla \varphi(\theta) + \Sigma \varphi(\theta) - \frac{\partial}{\partial E} [S \varphi(\theta)] = Q(\theta) \quad (9)$$

(once again we have supposed that all the angular diffusion terms are included in $Q(\theta)$.)

Assuming that $\varphi(\theta)$ is a linear function of time over $\{t, t + \Delta t\}$, we see that Eq. 10 is reduced to a stationary equation at the time θ :

$$\Omega \nabla \varphi(\theta) + \left(\Sigma + \frac{1}{h v \Delta t} \right) \varphi(\theta) - \frac{\partial}{\partial E} [S \varphi(\theta)] = Q(\theta) + \frac{\varphi(t)}{h v \Delta t} \quad (10)$$

Solving Eq. 10 by the procedure described above we get $\varphi(\theta)$, and $\varphi(t + \Delta t)$ is given by:

$$\varphi(t + \Delta t) = \frac{\varphi(\theta) - (1 - h) \varphi(t)}{h}$$

As it is well known, this scheme is unconditionally stable for $0.5 \leq h \leq 1$. The influence of the choice of h will be described on a practical example in the next Section.

3. NUMERICAL RESULTS

3.1 Homogeneous sphere with a constant source of particles

Let us consider Eq. 1 with $\Sigma_a = 1$, $\Sigma_s = 0$, $S = 1$, $T = 0$ and $Q = 1$:

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \Omega \nabla \varphi + \varphi - \frac{\partial \varphi}{\partial E} = 1 \quad (11)$$

An analytical solution of this equation can easily be obtained through the method of characteristics. Fig. 3 shows a comparison between the numerical and analytical solutions of Eq. 11 for a sphere with radius $R = 1$ and within an energy domain defined by $E_{max} = 1$ and $E_{th} = 0.1$. We consider particles having a mass equal to unity so we have $v = \sqrt{2E}$. The quantity displayed as a function of time for each energy group is:

$$F(E, t) = \int_0^1 \varphi(R, \mu, E, t) \mu d\mu$$

(F is equal to the leakage of particles out of the sphere per unit energy divided by 4π)

The analytical solution (displayed on Fig. 3a) show a steady rise of $F(E, t)$ from zero to a stationary value depending on E . This value is reached at a time given by:

$$t(E) = \int_E^{E_{max}} \frac{dE}{vS(E)} = \sqrt{2} - \sqrt{2E}$$

($t(E)$ is the time spent by a particle of initial energy E_{max} to slow down to energy E). After a time $t = \sqrt{2} - \sqrt{0.2} \simeq 0.967$, F is stationary at all energies, as it can be noticed on Fig. 3a.

The numerical calculations have been performed with 20 shells, 12 directions, 12 groups and a time step $\Delta t = 0.03$. Figs. 3b,c,d show the results for $h = 0.5$ (time-centered scheme), $h = 1$ (fully implicit scheme) and $h = 0.45$ (conditionally stable scheme). Good results are obtained with the two first schemes (the time centered scheme being slightly more accurate). As it can be expected, the third scheme is unstable since the time step used is too large.

3.2 Transport of 3.5 Mev alpha particles in a deuterium-tritium plasma

A classical benchmark is the problem of the energy deposition of 3.5 MeV alpha particles in a DT plasma. Fig. 4 shows the results obtained with our code in the following case:

- plasma radius: $R=0.02$ cm
- plasma density: $\rho=1000$ g cm⁻³
- plasma temperature: $T_i=T_e=50$ keV
- source uniformly distributed from $r=0$ to $r=R/10$

The calculations have been performed with 50 shells, 12 directions and 35 groups. The quantities displayed are the time rate of energy deposition to ions and electrons, integrated over each shell and normalized to the total energy source. One can notice on Figs. 4 a,b,c

the progressive widening of the deposition profiles from the center to the outside of the plasma sphere. When the time becomes greater than $t_1 = 2.2 \cdot 10^{-12} s$ (slowing down time of an alpha particle for $\rho = 1000$ and $T=50$ keV) the deposition profiles remain constant, as in the previous example.

4. ITERATIVE TREATMENT OF THE ANGULAR DIFFUSION TERM

The effect of the differential angular diffusion term is to redistribute the particles in direction without affecting their energy. It is therefore possible to study the treatment of this term on a simplified, monoenergetic and time-independent equation:

$$\mu \frac{\partial \varphi}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial \varphi}{\partial \mu} + \Sigma \varphi = Q + T \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial \varphi}{\partial \mu} \quad (12)$$

As pointed out by Morel⁴, the zero-th and first moment of the angular diffusion operator satisfy the two following properties:

$$\begin{cases} T \int_{-1}^{+1} \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial \varphi}{\partial \mu} d\mu = 0 \\ T \int_{-1}^{+1} \mu \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial \varphi}{\partial \mu} d\mu = -2T\Phi_1 \end{cases}$$

The only discrete approximation preserving these two properties is (see Ref. 4 for proof):

$$T \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial \varphi}{\partial \mu} \Big|_{\mu=\mu_m} = 2T \frac{\alpha_{m+1/2} \dot{\varphi}_{m+1/2} - \alpha_{m-1/2} \dot{\varphi}_{m-1/2}}{w_m} \quad (13)$$

where $\{\alpha_{m+1/2}, m = 0, \dots, M\}$ are identical to the curvature coefficients defined in Section 2.1 and $\dot{\varphi}_{m+1/2} = (\varphi_{m+1} - \varphi_m) / (\mu_{m+1} - \mu_m)$. Since the angular diffusion term is usually quite small, it can be considered as a small perturbation and solved by an iterative method. However it is not possible to perform iterations directly on the right side of Eq. 12, since the presence of angular derivatives would produce strong numerical instabilities. A better procedure is to iterate on the right side of the following approximation for Eq. 12, which results from Eqs. 3 and 13:

$$\begin{aligned} \mu_m \left\{ \frac{A_{i+1} \varphi_{i+1} - A_i \varphi_i}{V_{i+1/2}} \right\} + \left\{ \frac{\alpha'_{m+1/2} \varphi_{m+1/2} - \alpha'_{m-1/2} \varphi_{m-1/2}}{V_{i+1/2} w_m} \right\} + \Sigma' \varphi_m & \quad (14) \\ = Q + \frac{2T}{w_m} \left\{ \frac{\alpha_{m-1/2} \varphi_{m-1}}{\mu_m - \mu_{m-1}} + \frac{\alpha_{m+1/2} \varphi_{m+1}}{\mu_{m+1} - \mu_m} \right\} \end{aligned}$$

The "pseudo-capture" Σ' is given by:

$$\Sigma' = \Sigma + \frac{2T}{w_m} \left\{ \frac{\alpha_{m-1/2}}{\mu_m - \mu_{m-1}} + \frac{\alpha_{m+1/2}}{\mu_{m+1} - \mu_m} \right\}$$

This method, which is more implicit than the preceding one, has a far better stability. The number of iterations required turns out to be approximately proportional to T/w_m^2 ,

so this scheme is not well suited if w_m becomes small (however this is not a problem for practical calculations, which are performed with 8 or 16 directions only).

Fig. 5 presents numerical solutions of Eq. 12 obtained with this scheme, for a sphere with radius $R = 1$ and an isotropic source Q equal to 1 for $0 \leq r \leq R/2$ and having a zero value elsewhere. Σ is equal to 0, and the values of T are: 0 (Fig. 5a), 0.2 (Fig. 5b) and 0.4 (Fig 5c). The mesh consists in 40 shells and 32 directions. The quantity displayed is φ as a function of r and μ . When $T = 0$ we notice that φ is very anisotropic at the outer edge of the sphere. As expected, the effect of the introduction of T is to redistribute the flux in direction and to reduce sharply the anisotropy.

5. CONCLUSION

The numerical method we have developed for the slowing down and transport of fast ions in a spherical plasma is based on a classical Diamond scheme for the treatment of the space and angular variables, and deals with the energy variable by a finite element method. This treatment gives more accurate results than a multigroup diffusion, and is less time-consuming than a Monte-Carlo method. The code based on the formalism described in this paper has been tested on a Cray-1 computer and can be used for reaction rate or energy deposition calculations. When a single iteration per time step is needed (*i.e.* when no angular scattering is taken into account), typical run times are $\leq 1s$ per time step with a standard mesh ($\simeq 50$ shells, 12 directions and 42 groups). The energy deposition results are in good agreement with other methods designed for this kind of problems⁵. The use of a discontinuous finite element scheme provides a very good accuracy in energy, which is required for the calculation of reaction rates.

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Fig. 1: Discontinuous linear approximation for $\varphi(E)$

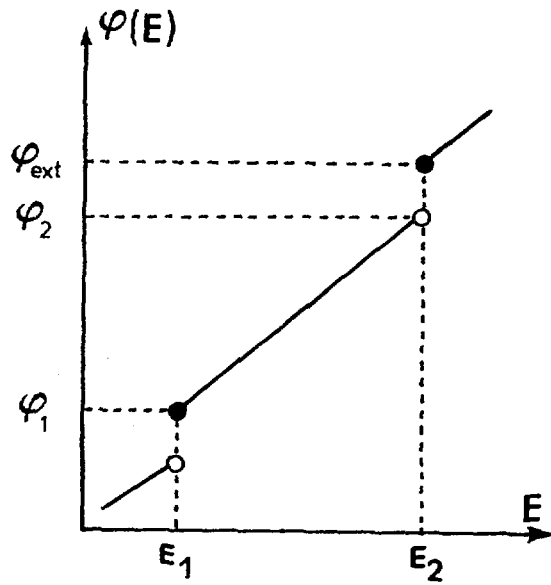


Fig. 2: Computation flow along the space-energy-direction mesh

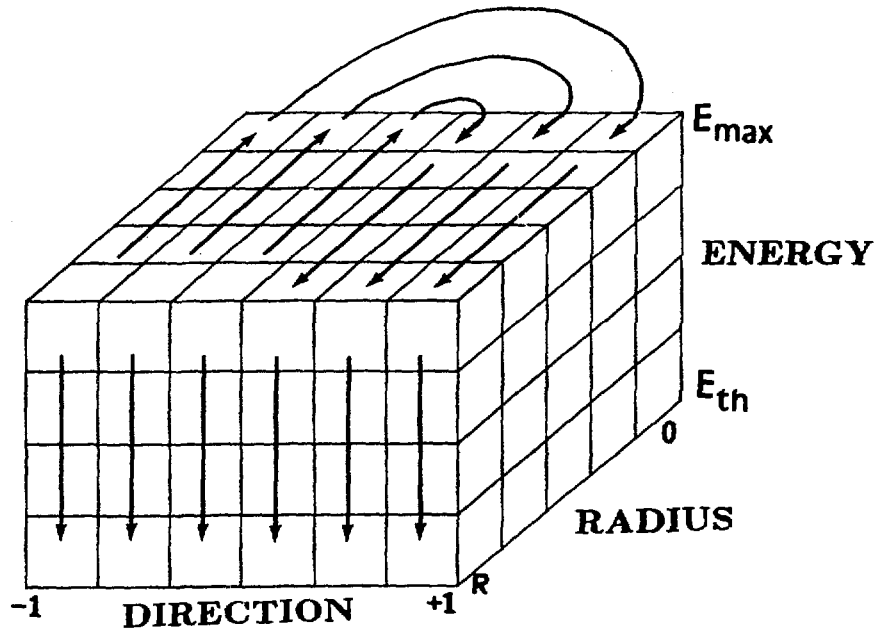


Fig. 3: Homogeneous sphere with a constant source of particles

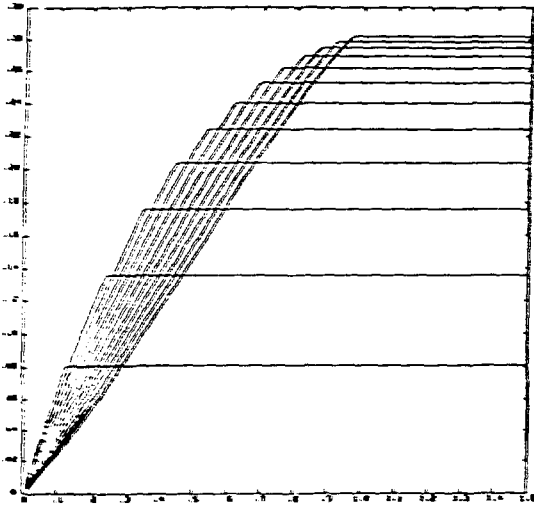


Fig. 3a: Analytical solution

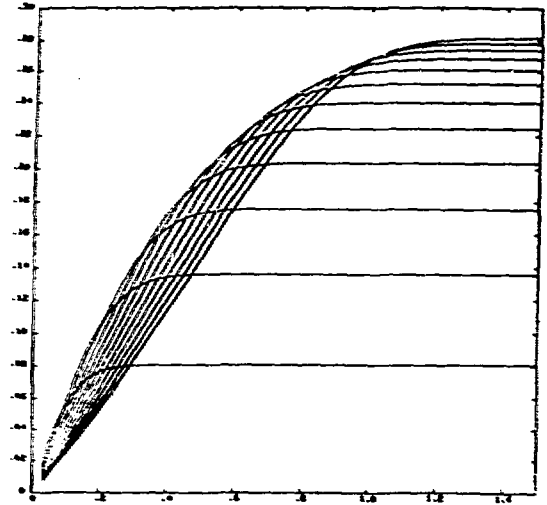


Fig. 3b: Numerical solution ($h = 1$)

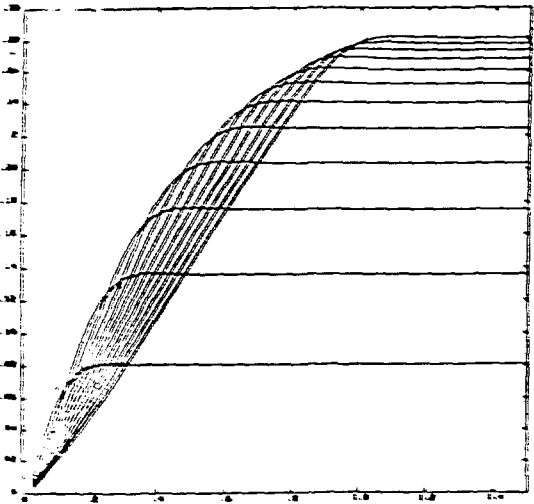


Fig. 3c: Numerical solution ($h = 0.5$)

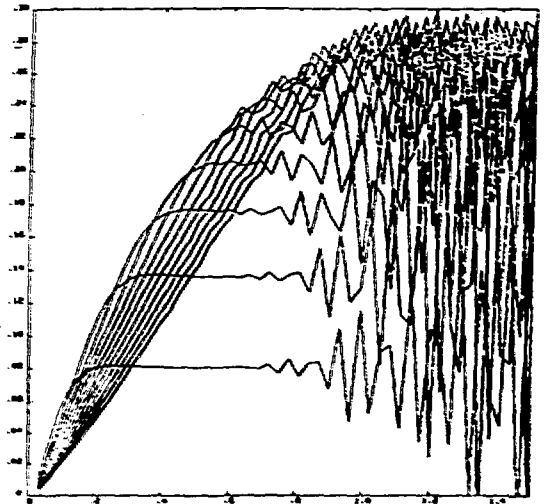


Fig. 3d: Numerical solution ($h = 0.45$)

Fig. 4: Transport of 3.5 MeV alpha particles in a DT plasma
Time rate of energy deposition to ions and electrons integrated over each shell and normalized to the total energy source

Fig. 4a:
time=0.71 10⁻¹²

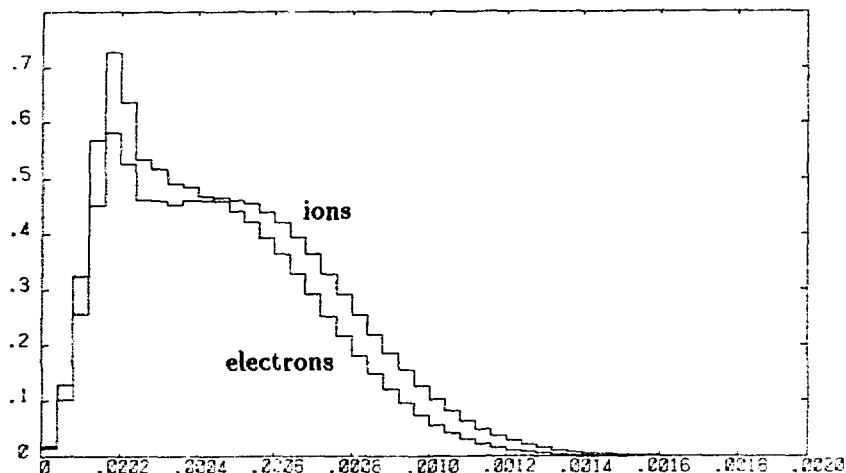


Fig. 4b:
time=1.46 10⁻¹²

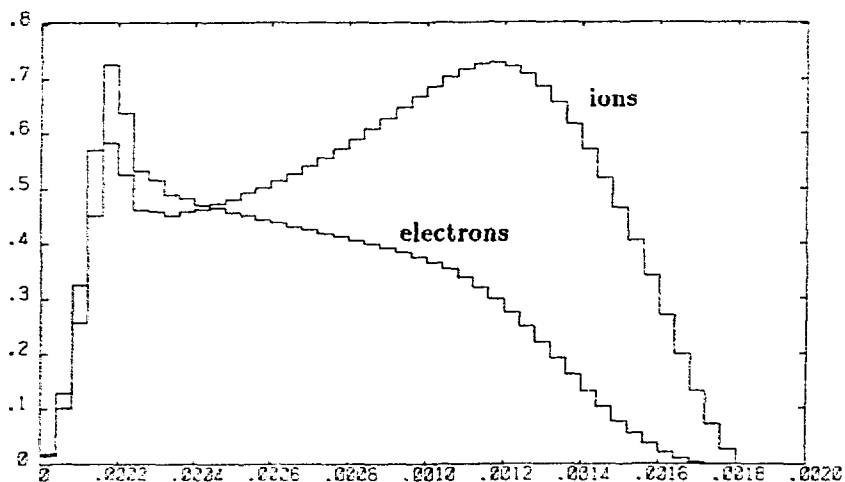


Fig. 4c:

time=2.21 10⁻¹²

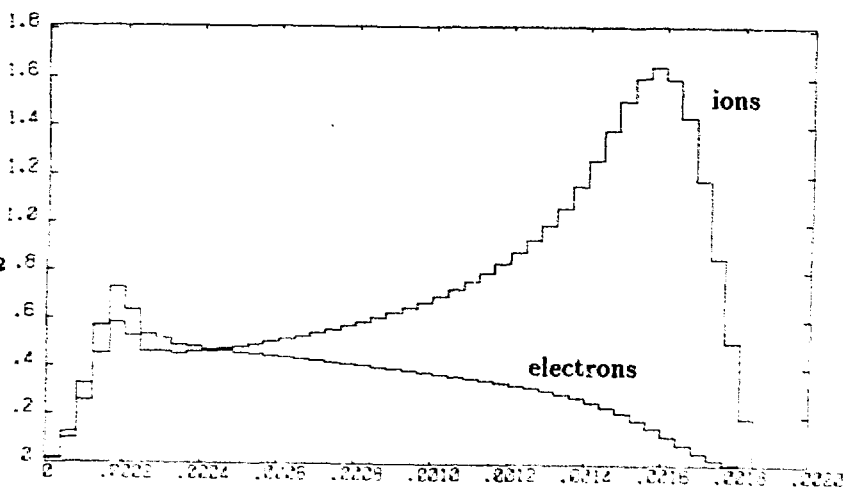


Fig. 5: Effect of the angular diffusion term

Fig. 5a: $T=0$

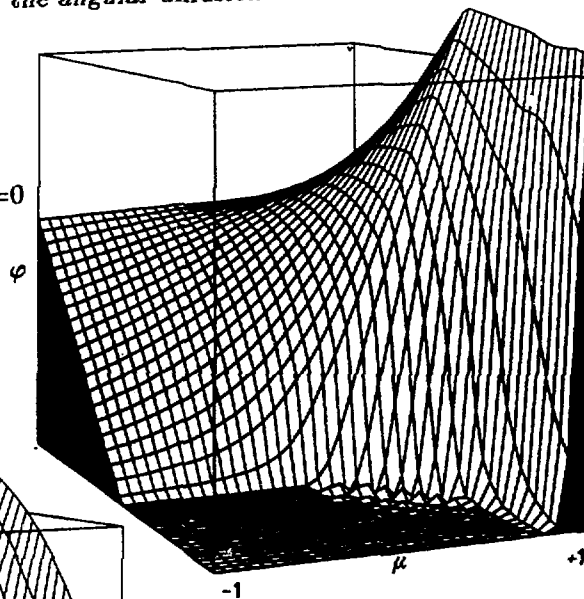


Fig. 5b: $T=0.2$

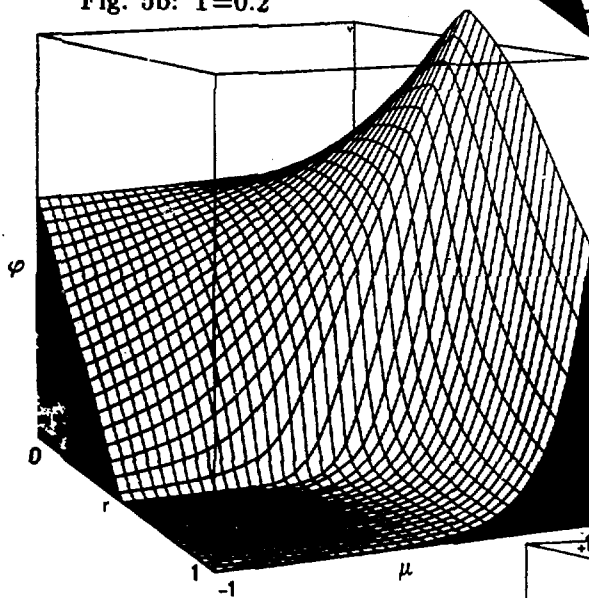
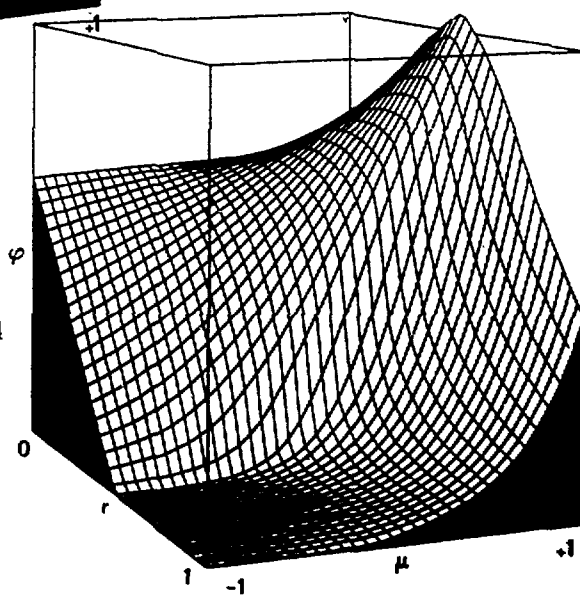


Fig. 5c: $T=0.4$



VECTOR AND PARALLEL COMPUTATION IN PRODUCTION CODES

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1/ INTRODUCTION

The aim of this paper is to discuss some issues about introducing vector and parallel computation in production codes. As an example, we will consider a large 2D Lagrangian hydrocode with diffusion approximation of radiation.

During the last years there has been an ongoing effort at our laboratory towards the use of vector machines and there will be one for the use of parallel computers. This paper is a summary of our goals.

In section 1, we describe the benchmark set we use to evaluate computers. In the past years, we get results from a lot of different computers including Japanese supercomputers, CRAY X-MP, CRAY 2, SCS-40 and others, cf /2/. This benchmark helped us to motivate our interest for the CRAY X-MP/4 as our production machine.

Section 2 shows the vectorization level we reach for the code on CRAY 1S and address the problem of equation of state (EOS) computation.

Section 3 explains our hopes regarding the use of this code on the CRAY X-MP/4, introducing parallel computation.

Finally section 4 indicates some perspectives for large production codes, like this one, on the next generation of computers.

2/ THE CEA BENCHMARK

Although it is very difficult to devise benchmarks which can really represent a given workload, we choose and adapted some of our codes to try to get comparisons between different supercomputers and to see if they are suited to our workload. It

must be said, of course, that one cannot get too general conclusions from our results because, for instance, as we solve only problems of medium size, we are more interested in the speed of computers than in large memory sizes and consequently there is no code testing intensive I/O in our benchmark. For our laboratory, computing speed and throughput are the premium needs.

The CEA benchmark is composed of roughly 20 different codes, ranging from small kernels to unclassified excerpts of large production codes. Some of these codes are completely scalar and some are completely or partially vectorized. Special codes have been written to test the multitasking (and microtasking) facility on the CRAY X-MP.

A description of some of these codes is following:

- BKERN contains about 30 kernels ranging from SAXPY-like ones to indirect addressing, tests and more complex operations designed to test chaining. It is used to assess the speed of supercomputers on basic operations and also the ability of compilers to automatically vectorize these operations.

As an example, for the multiplication of a five diagonal matrix by a vector, done diagonal by diagonal, we get 59 Mflops on CRAY 1-S (CFT 1.13), 128 Mflops on CRAY X-MP (CFT 1.14), 88 Mflops on CRAY 2 (CFT 2.70) and 27.5 Mflops on SCS-40.

The second layer is made of algorithms which are heavily used in production codes.

- BVCG

This is different vectorized conjugate gradient methods (cf./3/ /4/), to solve a sparse linear system arising from five point finite difference scheme discretization of elliptic partial differential equation. This algorithm is the heart in some of our production codes.

Below are Mflops results for CG with different preconditioners, in decreasing order of vectorization ratio, the second figure is the speed ratio relative to CRAY 1-S.

CRAY 1-S	CRAY X-MP	CRAY 2
53	127/2.39	67/1.26
50	127/2.54	60/1.2
44	97/2.20	53/1.2
35	78/2.22	45/1.28
20	27/1.35	21/1.05
13	19/1.46	10/0.77

We must add that the least computing time is not given by the fastest speed

because all these preconditioners, of course, do not give the same number of iterations. Results using multitasking have been given in /1/, /6/.

- BTEQF

Interpolation code for EOS computations. As we will see in next section, this is a very important part of our production code and it is uneasy to vectorize.

Then there is a final layer made up with large excerpts from production codes.

- BSLS ~ BSLV

One dimensional lagrangian hydrocode for slab geometry using Richtmyer scheme and perfect gas law.

The S version is almost completely scalar and the V one is vectorized (for CRAY machines).

We measure the performances (Mflops) on three different parts of the code HYD : velocities and pseudo viscosities computation, DT : computation of the next time step, BIL : energy balance computation.

Results for vector code are :

	CRAY 1-S	CRAY X-MP	CRAY 2
HYD	34.3	57.8	45.6
DT	3.9	5.	1.
BIL	20.7	39.7	19.8

- BPIC ~ BPAI

There are two versions of our large 2D hydrocode, one using constant strides on a simple geometry, the other one using indirect adresssing.

- BMCVEC

Vectorized Monte-Carlo method to solve the neutron transport equation. cf. /1/

- BSAMB

A vectorized finite element method to solve the transport equation. This method requires I/O on the CRAY 1-S.

This benchmark set is useful in two ways :

~ giving results to compare computers on our specific workload.

- giving examples to show what vectorization techniques we can use and what maximum performances we can reach with the algorithms which are the most important ones for our laboratory.

The results of this benchmark study showed us that the CRAY X-MP is very well suited to our needs.

2/ VECTORIZATION OF THE PRODUCTION CODE

In this section we are interested in vectorizing the solving of the energy balance equation, that is to say : solving a non linear diffusion equation. The algorithm we used is a damped Newton-like method with a sophisticated algorithm for time stepping control. Every Newton iteration, we have a sparse linear system to solve. This is done with a preconditioned conjugate gradient method. So, we have an inner-outer iteration. Interaction with matter is given by EOS and opacities computations.

Before vectorization, excluding EOS and opacities, there were 7 % of vector floating point operations and consequently 93 % of scalar floating point operations giving a 2.14 Mflops speed on the CRAY 1-S; this can be regarded as a very low performance.

To vectorize we had to completely rewrite the code, taking out of the loops the many tests that were trying to save floating point operations on a scalar machine. We needed also to change the way to handle boundary conditions. Before vectorization, we had to make a test to know if a given node is a boundary node, now, we are managing lists of nodes for a given boundary condition.

Even though the discretization is done with finite differences, the numbering of the nodes is done in a finite element way, that is to say we are able to use any numbering scheme. This implies that we heavily rely on indirect addressing.

After the vectorization process, the EOS computations represents 8.3 % of the total, opacities 11.1 %, computation of the linear system matrix is 24.3 %, conjugate gradient algorithm to solve this system 26.5 %, computation of the next time step is 1.1 %, and there are 17 % of mainly unvectorized tallies operations to check energy balance in the system.

This effort gives us the reward of a factor of 10 increase in performance for solving the non linear energy equation.

The main problem we found during this study was vectorizing equation of state (and opacities) computations .

The problem can be summarized as follows : given three vectors ρ , T and MAT of densities, temperatures and material indices, compute two vectors ϵ and $\frac{\partial \epsilon}{\partial T}$ which are the energy per unit of mass and its derivative with respect to temperature.

In the scalar version, EOS computations were done using different models for each type of EOS. To vectorize we chose to interpolate in grids of points for all physical medium and EOS types we use.

Interpolation points were chosen in such a way that interpolation error is less than 1 % in all usually interesting ranges of ρ and T .

In order to simplify vectorization, we choose linear interpolations and $\frac{\partial \epsilon}{\partial T}$ is the derivative of the interpolate which means that the derivative is discontinuous at boundaries. The main difficulty is that different EOS types can occur randomly in MAT . The naive approach of constructing vectors with consecutive elements of the same type cannot work well, because vector lengths will be too short. Constructing one vector of ρ and T for each type with gather and scatter operations will be too costly.

The first step in interpolating, is to locate the elements ρ_i , T_i of vectors ρ and T in the grids for the right type of equation given by MAT_i . We tried two different solutions to this problem. The first one assume that all EOS types have the same T -grid. A bias b is added to the density such that :

$$\bar{\rho}_i = \rho_i + b (MAT_i - 1)$$

This idea comes from the fact that during Newton iterations density ρ is constant, hence the biasing has to be done only once for each time step. We then find the locations of ρ and T in the grids using special CRAY functions.

With this biasing trick we have only to interpolate (and to locate ρ and T) in only one large grid.

The other idea we tried, is to have a unique grid in ρ and T for every type of EOS. Let X be this grid, we define a much finer regular grid Z (a so called "hair comb"), $Z(i+1) - Z(i) = p$, $\forall i$. Then we locate the teeth of the comb in X , defining JZ such that $JZ(i) = k$ if :

$$X(k) < Z(i) < X(k+1)$$

The indices $J(i)$ of vector Y are then simply given by division and indirect adresssing, if :

$$JY(1) = \left\lceil \frac{Y(1) - Z(1)}{P} \right\rceil + 1$$

then :

$$J(1) = JZ (JY (1))$$

Knowing the distribution of vectors ρ and T in the grids, we can then interpolate. Special CAL routines have been coded on the CRAY 1-S to do the required gathers and interpolations.

The execution times (in seconds) for the three approaches : scalar, bias and hair comb, are given by the following figures with respect to vector length.

VL	scalar	bias	hair comb
10	$0.86 \cdot 10^{-3}$	$0.65 \cdot 10^{-4}$	$0.59 \cdot 10^{-4}$
500	0.040	$0.173 \cdot 10^{-2}$	$0.116 \cdot 10^{-2}$
5000	0.406	$0.171 \cdot 10^{-1}$	$0.114 \cdot 10^{-1}$

This shows that on this problem great savings can be achieved with a little effort through vectorization.

4/ PARALLEL COMPUTATION

During the last years, we made several experiments to develop parallel methods for the algorithms we used in our code. Obviously a lot of the methods we use are inherently parallel; for instance, the construction of the Jacobian matrix in the Newton method, or the EOS computations. The most difficult part to parallelize is the conjugate gradient solver. There are a lot of data dependancies in the conjugate gradient algorithm due to the scalar products we have to compute every iteration. Some methods to alleviate these problems have been given in /6/. But the main question is to devise vector or parallel preconditionners. New proposals in this direction have been defined in /4/,/6/,/7/, using domain decomposition techniques.

With the methods in /6/, we obtain speed up of 3.2 with 4 processors, the speed up being only bounded by memory contention between the processors.

So there are great hopes that, with introduction of these parallel methods in our production code, we can get a very good speed-up on a CRAY X-MP/4, at least between two and three with multitasking.

Microtasking is even more promising for small size problems.

Another method which is heavily used in our laboratory, the Monte-Carlo method, is very well suited for parallel computation with a few powerful processors. Speed-up up to 3.5 have been reached, cf. /1/

5/ PERSPECTIVES AND CONCLUSION

It is likely that during next years, computers will get more and more processors (at least up to 64) with, still, a shared memory. So it is really important to develop basic algorithms for these machines and to train the numerical analysts and programmers to the use of these sophisticated tools. The studies we made in the last years are aimed to reach this goal.

As we would like to be able to use our codes on different machines, we will try to emphasize the portability issue. There is always a struggle between portability and efficiency. For instance, at the beginning of CRAY machines, it was necessary to code in a very special way to get (a part) of the maximum performance. Do we have to agree doing such things ?

Our philosophy is that it is wise to do only this weird coding in very well specified areas and that it has to be done through the use of functions or macros which can be easily replaced by more straight coding.

This is because compilers are improving a great deal and they can now vectorize loops that needed special treatment a while ago.

This portability issue is also very important for parallel computation and preprocessors (like microtasking), describing parallelism through directives which are ignored by other computers, seem very interesting.

In our laboratory we want to promote an effort to get portability and efficiency.

This is mandatory to prepare the coming of the french supercomputer ISIS which is supposed to be delivered by Bull at the end of 1987.

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A DETERMINISTIC PARTICLE METHOD FOR CONVECTION DIFFUSION EQUATION

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ABSTRACT

Particle methods are well suited for solving transport equations. We generalize this technique to transport-diffusion equations. The treatment of the diffusion term is based upon its reinterpretation as a nonlinear convection term. The numerical solution of the Heat Diffusion Equation is compared with the corresponding exact solution. Its stability as a function of particle size and time step is studied. This method is then applied to the Fokker Planck Equation specialized to fast-ions transport.

I - INTRODUCTION

Particle methods have been widely used in plasma physics, due to their flexibility, therefore their ability to solve complicated transport problems. Quite recently, some interest has been raised in using such techniques to solve Transport-Diffusion Equations such as Fokker-Planck Equation. Besides Monte Carlo methods [1], two deterministic methods have been developed for solving the diffusion part of FPE. They are both based upon an approximation of the particle distribution function as a sum of weighted functions [2]. This approximation is smoothed by convolution and inserted in the equation. One then obtains a set of ordinary differential equations for the weight of each particle, its velocity and its position. They differ by the interpretation that is done in the second method. The diffusion equation is reevaluated as a nonlinear convection equation, following an idea suggested by Fronteau [3,4], and Degond [5]. This new approach is presented in Section II, and its stability is studied numerically.

In Section III, this technique is applied to charged particle transport simulation, solving a specialized Fokker-Planck Equation.

II - A PARTICLE METHOD FOR DIFFUSION EQUATION

We consider the following equation :

$$\begin{cases} \frac{\partial f}{\partial t} - \sigma \frac{\partial^2 f}{\partial x^2} = 0, \\ (x, t) \in \mathbb{R} \times [0, T] \\ f(x, 0) = f^0(x) \end{cases} \quad (1)$$

Let us suppose that : $f > 0$

Equation (1) can be rewritten as a non-linear transport equation

$$\begin{cases} \frac{\partial f}{\partial t} + \frac{\partial}{\partial x} [A(f) f] = 0 \\ (x, t) \in \mathbb{R} \times [0, T] \end{cases} \quad (2)$$

$$\text{with } A(f) = -\sigma \frac{1}{f} \frac{\partial f}{\partial x}$$

For a smooth enough ψ function, we can write

$$\int f^0 \psi dx \approx \sum_{j=1}^N \omega_j^0 f^0(x_j^0) \psi(x_j^0)$$

Therefore a approximation of f^0 is given by

$$\tilde{f}^0(x) = \sum_{j=1}^N \omega_j^0 f_j^0 \delta(x - x_j^0) \quad (3)$$

$$\text{with } f_j^0 = f^0(x_j^0)$$

A "weak" solution of Eq. (2) is then written :

$$f(x, t) = \sum_{j=1}^N \omega_j(t) f_j(t) \delta[x - x_j(t)]$$

where, for every j , $\omega_j(t)$, $f_j(t)$ and $x_j(t)$ are solutions of the equations :

$$\begin{cases} \frac{d}{dt} (\omega_j(t)) = \omega_j(t) \frac{\partial}{\partial x} [A(f(x_j(t)), t)], \\ \omega_j(0) = \omega_j^0, \\ \frac{d}{dt} (\omega_j(t) f_j(t)) = 0, \\ \omega_j(0) f_j(0) = \omega_j^0 f_j^0, \\ \frac{d}{dt} (x_j(t)) = A(f(x_j(t)), t) \\ x_j(0) = x_j^0. \end{cases} \quad (4)$$

Then,

$$f(x, t) = \sum_{j=1}^N \omega_j^0 f_j^0 \delta(x - x_j(t))$$

A smooth approximation for the solution of Eq. [1] is obtained by a convolution of f with a "shape" function $\zeta_\epsilon(x)$, and we obtain

$$\tilde{f}(x, t) = \sum_{j=1}^N \omega_j^0 f_j^0 \zeta_\epsilon(x - x_j(t)). \quad (5)$$

Convergence properties of such a method have been studied elsewhere [6]. Replacing f with $\tilde{f}$ in $A(f)$, we obtain

$$A(f(x_j(t))) = \sigma \left[\sum_{k=1}^N \omega_j^0 f_j^0 \zeta'_\epsilon(x_j(t) - x_k(t)) \right] / \left[\sum_{k=1}^N \omega_j^0 f_j^0 \zeta_\epsilon(x_j(t) - x_k(t)) \right] \quad (6)$$

The last equation of system (4) is discretized with an explicit scheme. This scheme being given, the main point of interest is its stability. This can be estimated empirically in the following way; In the case of an explicit finite-difference scheme for Eq. (1), the stability criterion is the CFL condition, i.e.,

$$\max_{1 \leq j \leq N} \left(\max_{j \leq n \leq M} |A(f(j\Delta x, n\Delta t))| \right) < \frac{\Delta x}{\Delta t} \quad (7)$$

The analogous criterion in our case is :

$$\max_{1 \leq j \leq N} (\max_{1 \leq n \leq M} (|A(f(x_j^n, n \Delta t))|)) < \frac{\epsilon}{\Delta t}$$

If two particles are at the same location at time t , this equation means that they cannot be farther than 2ϵ apart at the end of the time step. From Eq. (8), we deduce the stability criterion

$$\sigma \max_{1 \leq j \leq N} (\max_{1 \leq n \leq M} (\left| \frac{\sum_{k=1}^N \omega_k f_k \zeta_\epsilon(x_j^n - x_k^n)}{\sum_{k=1}^N \omega_k f_k \zeta_\epsilon(x_j^n - x_k^n)} \right|)) < \frac{\epsilon}{\Delta t} \quad (9)$$

For the sake of simplicity, we choose ζ_ϵ to be

$$\begin{aligned} \zeta_\epsilon(x) &= 0, \quad |x| > \epsilon, \\ \zeta_\epsilon(x) &= \frac{1}{2\epsilon}, \quad |x| < \epsilon, \end{aligned} \quad (10)$$

and an approximation of the δ function derivative to be the hat function derivative

If N_j^n is the number of particles at time step n , located in the interval $[x_j^n - \epsilon, x_j^n + \epsilon]$, we have :

$$\sum_{k=1}^N \omega_k^0 f_k^0 \zeta'_\epsilon(x_j^n - x_k^n) = \frac{1}{2\epsilon} \sum_{k \in \mathcal{J}_j^n} \omega_k^0 f_k^0, \quad (11)$$

$$\text{and} \quad \sum_{k=1}^N \omega_k^0 f_k^0 \zeta'_\epsilon(x_j^n - x_k^n) < \frac{N_j^n}{\epsilon} \max_{k \in \mathcal{J}_j^n} \left| \omega_k^0 f_k^0 \right|$$

where $\mathcal{J}_j^n$ is the set of particles described above.

A sufficient condition such that Eq. (9) is satisfied is

$$\sigma \max_{1 \leq j \leq N} (\max_{1 \leq n \leq M} (\frac{\max_{k \in \mathcal{J}_j^n} (\omega_k^0 f_k^0)}{\sum_{k \in \mathcal{J}_j^n} \omega_k^0 f_k^0}) \frac{\Delta t}{\epsilon}) < \frac{1}{2} \quad (12)$$

A comment can be done about Eq. (12) ; this criterion can be optimized with a careful choice of the initial approximation for f . If we choose $\tilde{f}^0$ such that

$$\omega_k^0 f_k^0 = \frac{1}{N}, \forall k,$$

Eq. (12) becomes :

$$\sigma \frac{\Delta t}{\varepsilon^2} < \frac{1}{2} \quad (13)$$

Having assumed that ε is the analogous of the mesh size Δx in a finite-difference scheme, we recognize that Eq.(13) is the same criterion than for a standard explicit finite-difference scheme [7]. Numerical experiments shows that Eq. (13) is a good criterion of stability for this particle method. On Figure (1) are displayed numerical and exact solutions of the heat diffusion equation for various ratios of $(\Delta t/\varepsilon^2)$, with the same number of particles per length ε . Figure (2) shows the convergence of the method with the number of particles. This method can be used for more general equations such as transport-difusion equations. This is the subject of Section III.

III - A PARTICLE METHOD FOR FOKKER-PLANCK EQUATION

We consider here the Fokker-Planck Equation specialized to charged particle transport. In the case of a 1.D planar spatial dependency of the particles distribution function, we have :

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial x} (\mu v g) + \frac{\partial}{\partial v} (A(x, v)g) + \frac{\partial}{\partial v} (B(x, v) \frac{\partial g}{\partial v}) + \frac{\partial}{\partial \mu} ((1-\mu^2)C(x, v) \frac{\partial g}{\partial \mu}) = 0 \quad (14)$$

where $g = v^2 f$

For our calculations, we choose here

$$B \equiv 0,$$

$$A(v) = -\alpha_e v - \alpha_i v^{-2}$$

$$\text{and} \quad C(v) = -\gamma_e v^{-2} - \gamma_i v^{-3},$$

where α_e , α_i , γ_e and γ_i are some numbers depending upon the masses of electrons, background ions and fast ions. The approximated function $\tilde{g}$ that is solution of Eq.(14) is :

$$\tilde{g}(x, v, \mu, t) = \sum_{j=1}^N \omega_j^0 g_j^0 \delta(x - x_j(t)) \delta(v - v_j(t)) \delta(\mu - \mu_j(t)) \quad (16)$$

where x_j , v_j and μ_j are solutions of the following O.D.E's

$$\begin{aligned} \dot{x}_j(t) &= \mu_j(t) v_j(t), \\ x_j(0) &= x_j^0, \\ \dot{v}_j(t) &= A(v_j(t)) \\ v_j(0) &= v_j^0 \\ \dot{\mu}_j(t) &= B(v_j(t), \mu_j(t), g(x_j(t), v_j(t), \mu_j(t))), \\ \mu_j(0) &= \mu_j^0, \\ B(v, \mu, g) &= (1 - \mu^2) C(v) \frac{1}{g} \frac{\partial g}{\partial \mu} \end{aligned} \quad (17)$$

From this solution, we can calculate the energy deposition to the ions and the electrons of the background plasma

$$\begin{aligned} \dot{E}(x, t) &= \int_0^v \int_{-1}^1 v^2 \frac{\partial}{\partial v} (A(v)g) dv d\mu, \\ \text{or} \quad \dot{E}(x, t) &= 2 \sum_{j=1}^N \omega_j^0 g_j^0 \left(\alpha_e v_j^2(t) + \alpha_i \frac{1}{v_j(t)} \right) \zeta_e(x - x_j(t)) \end{aligned} \quad (18)$$

A time integration gives the total deposition between times 0 and t.

Figure (3) shows the results obtained in the case a planar isotropic source of 1 Mev protons in a 50 Kev BDT plasma ($\approx 2.31 \text{ g cm}^{-3}$), with and without diffusion. The difference between the two cases is small regarding energy deposition, but Figure (4), displaying phase space plots at different times, exhibits the diffusional effect of collisions.

IV - CONCLUSION

These results show that particle methods can be generalized to solve Transport-Diffusion equations. This increases even more their well known flexibility. The actual scheme can be used only for cases when the diffusion terms are not dominant. However, implicitness should guarantee better results for strongly collisional media.

This technique has been applied to plasma physics problems such α -particles and protons transport, but also to solid state physics. Future directions are the study of implicit schemes, and also the implementation of Dirichlet boundary conditions, which is more delicate than reflective boundaries.

Acknowledgement :

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FIGURE 1

HEAT DIFFUSION EQUATION - EFFECT OF Δt and ϵ

$N = 50$ particles per ϵ , $t = 0.5$

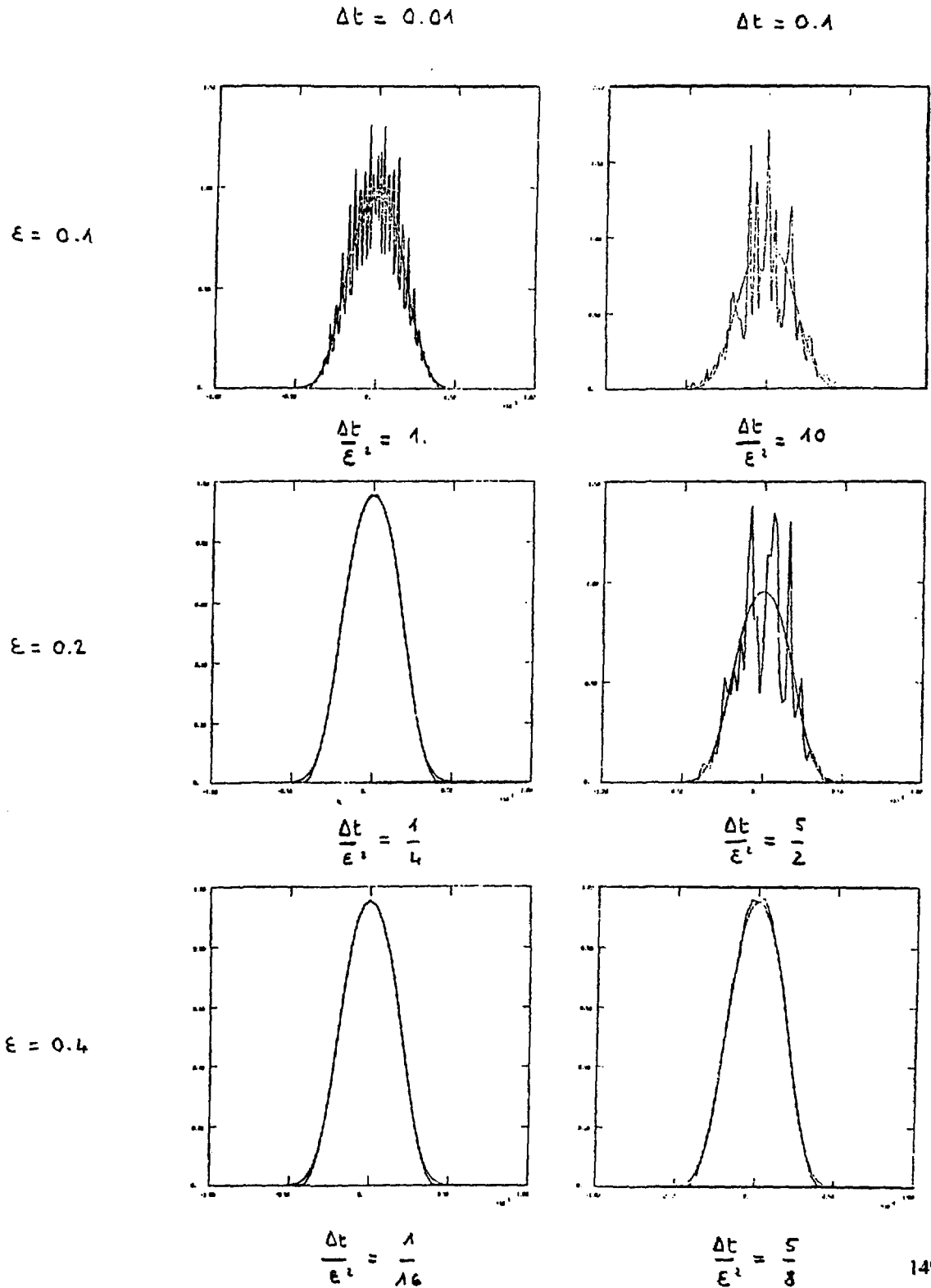
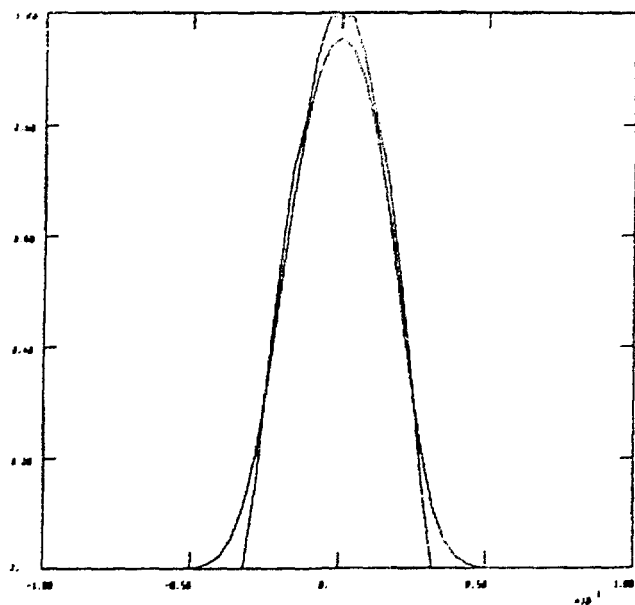
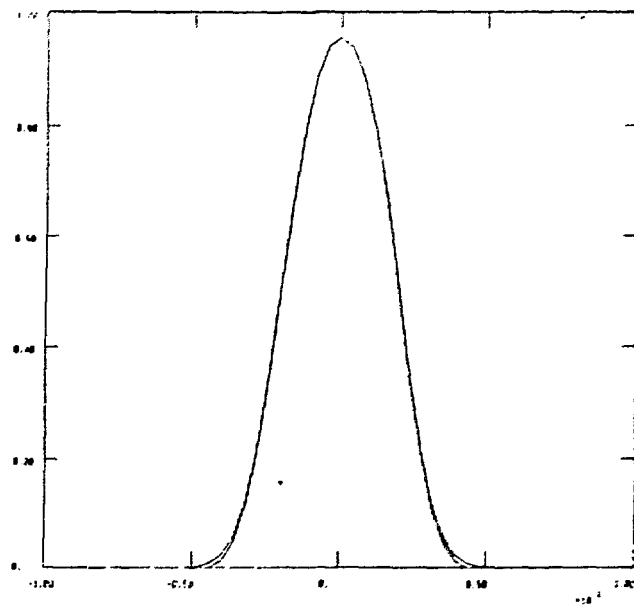


FIGURE 2
HEAT DIFFUSION EQUATION - EFFECT OF N

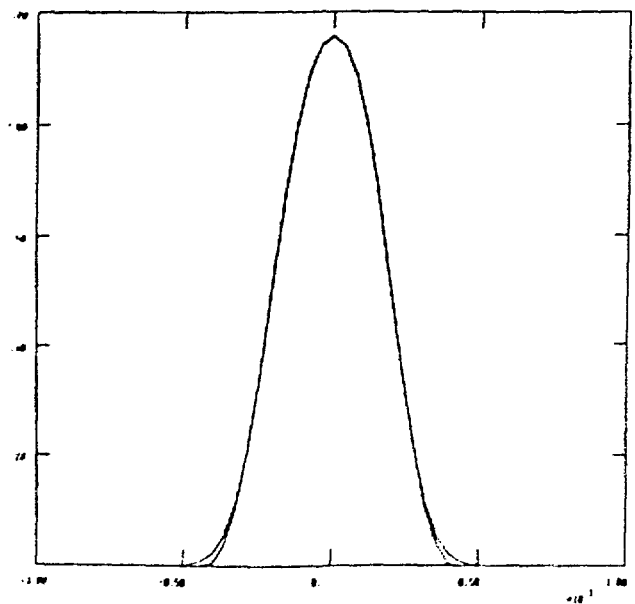
$\varepsilon = 0.4, \Delta t = 0.01, \tau = 0.5$



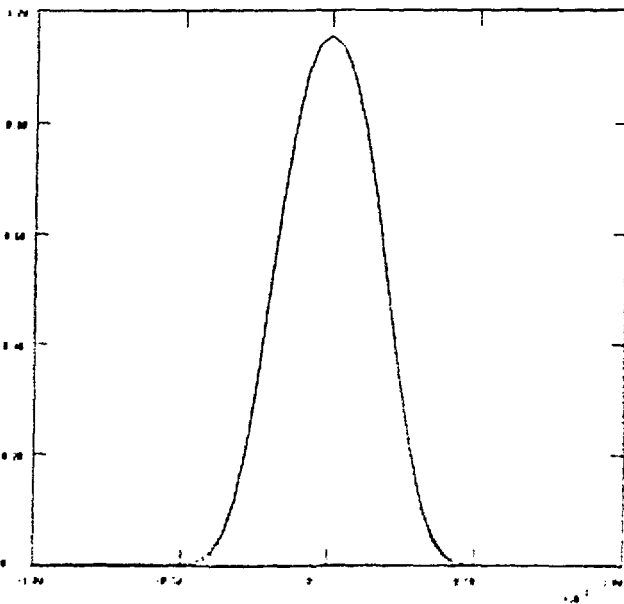
$N = 50$



$N = 1000$



$N = 500$



$N = 3000$

FIGURE 3

Energy deposition to the plasma : left, without diffusion ; right, with diffusion.

(e) : deposition to the electrons

(i) : deposition to the ions

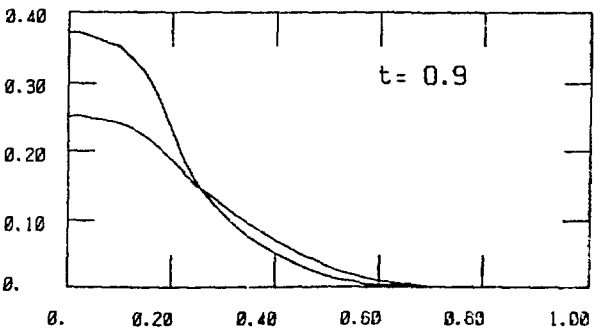
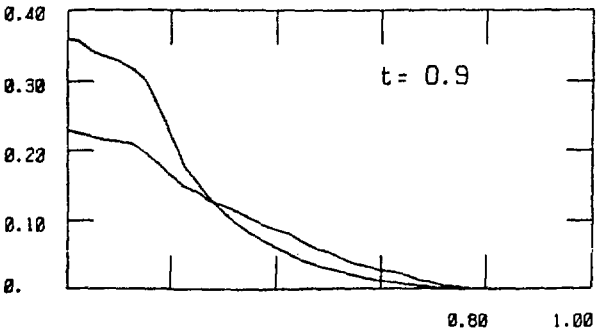
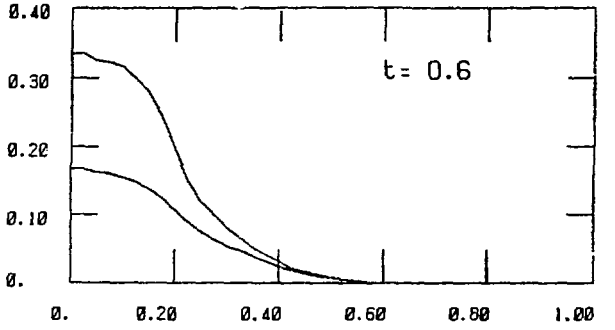
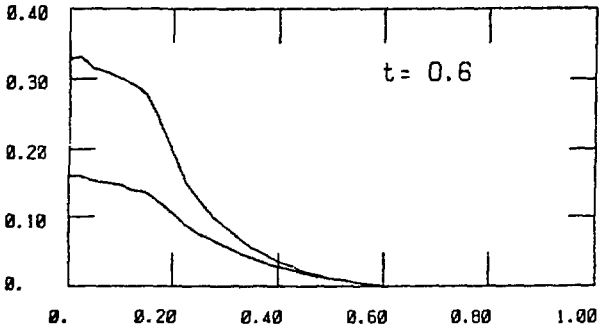
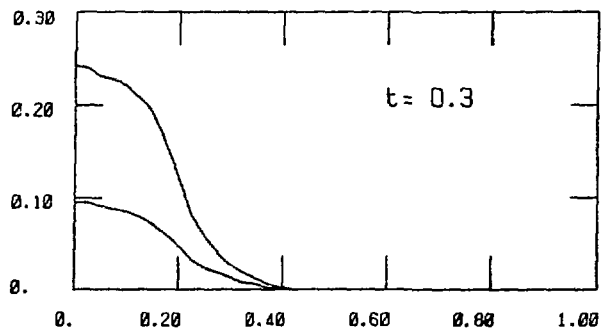
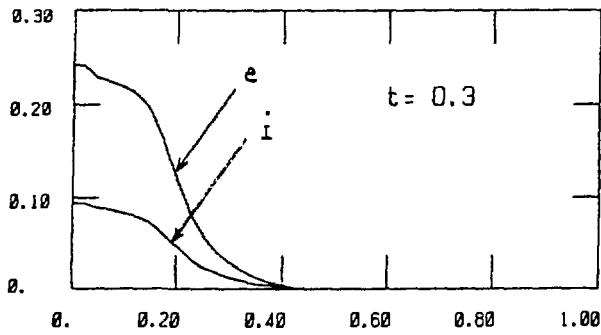
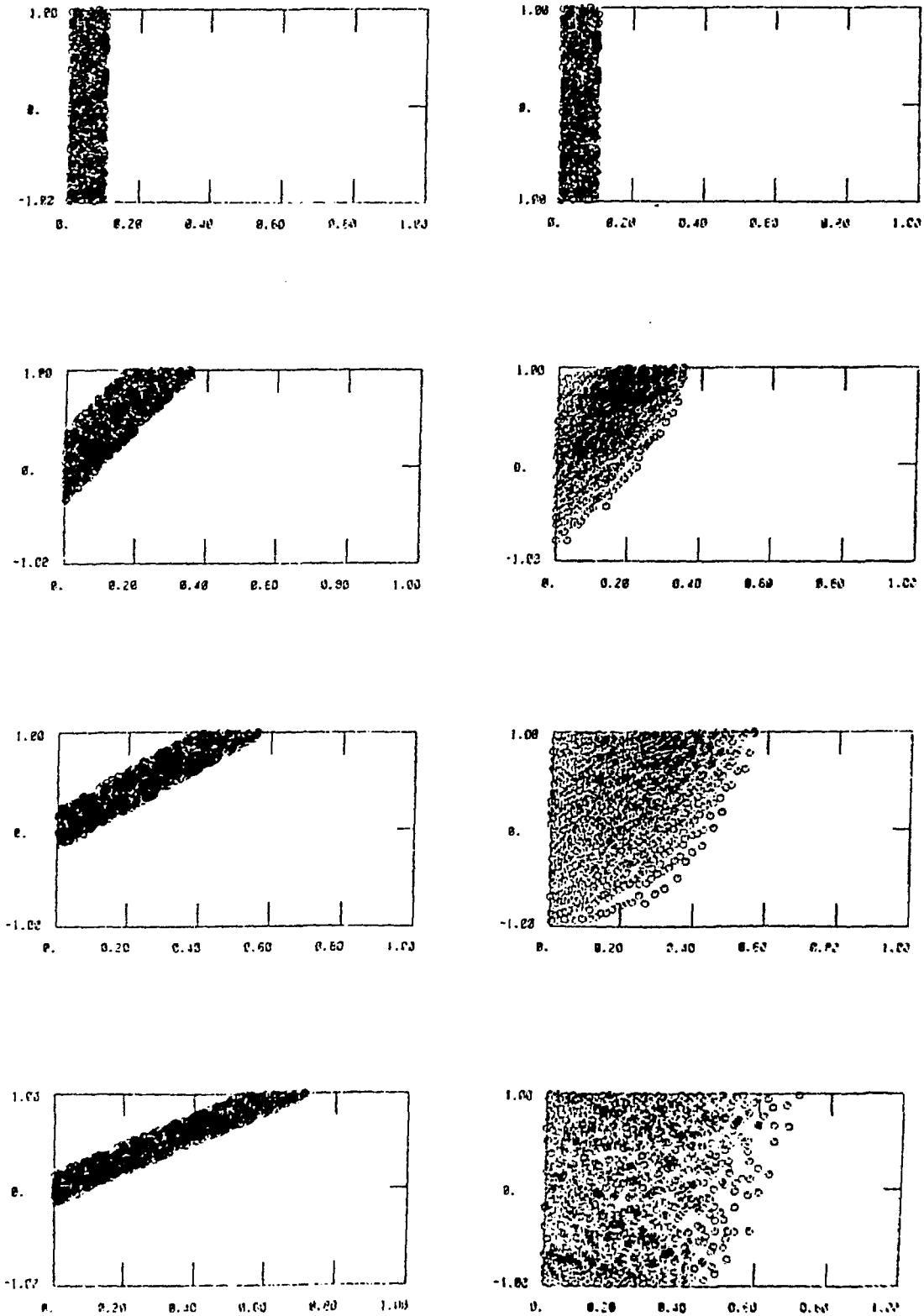


FIGURE 4

(x, μ) phase space at time 0, 0.3, 0.6, 0.9 ; left without diffusion ; right with diffusion.



A MOLECULAR DYNAMICS SIMULATION OF THE TWO-DIMENSIONAL ION-ELECTRON
PLASMA IN THE STRONG COUPLING REGIME

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ABSTRACT

We have carried out Molecular Dynamics simulations on a two-dimensional plasma made up of ions of charge $+e$ and size d held fixed (infinite mass) on the sites of a hexagonal lattice, and of classical electrons of charge $-e$ moving in the periodic field of the ions. This fixed-ion model maps the dielectric-plasma transition of the two-dimensional Coulomb gas onto a delocalization transition of the electrons. The main "diagnostics" in our simulations are the electron self-diffusion constant D and the d.c conductivity σ , which vanish below a density dependent threshold temperature T_1 . The simulations amount to integrating the coupled classical equations of motion on the CRAY-1 over times spanning up to 10^3 plasma oscillations, and allow a detailed study of ion-electron recombinations and the single-particle and collective motions of the electrons.

Some of the salient results are the following :

- a) The screening length diverges as the temperature is lowered toward the transition temperature T_1 :
- b) The specific heat exhibits a peak at a temperature T_2 slightly above T_1 , which is more pronounced at lower densities :
- c) an additional damping mechanism of the plasma waves arises due to the recombinations (i.e. electron localization). The Langmuir waves are over-damped below a temperature well above T_1 , and their frequency lies below the electron-plasma frequency in the long wavelength ($k \rightarrow 0$) limit. Their dispersion function $\omega(k)$ turns out to be an oscillating function of k .

1/ THE ION-ELECTRON PLASMA : WHY TWO DIMENSIONS ?

The aim of this work is to reproduce some properties of non-ideal plasmas, like ICF plasmas in the ablation region or shock-compressed high-Z materials. For us a non-ideal plasma is a strongly coupled and partially ionized plasma . Ionization is a very complex mechanism and we need a simple model to reproduce macroscopic results of this process. Two-dimensional plasmas provide us such a model . If we consider the classical electron gas, made up of oppositely charged particles, it is obvious that electrons and ions tend to collapse. But the dielectric behaviour crucially depends on dimensionality. In one dimension, where the potential $V(r)$ is proportional to r ($V(r) \sim r$), the Coulomb gas is dielectric at all temperatures : opposite charges are always bound in pairs /1/. In three dimensions ($V(r) \sim \frac{1}{r}$) the Coulomb gas is believed to be a conductor as long as it remains in a disordered phase. The two-dimensional case ($V(r) \sim \ln(r)$) is the most interesting since the corresponding Coulomb gas is a dielectric (as in 1 D) below some density-dependent critical temperature T_c , while it is a conductor (as in 3 D) above that temperature. The existence of the low temperature phase, where pairs of opposite charges form dipolar "molecules" can be ultimately traced back to the weakly binding character of the 2-D logarithmic potential at large r . This dielectric-plasma transition has been studied theoretically by Kosterlitz and Thouless /2/, and provides us a simple classical model of ionization/recombination processes.

On the other hand, the strong coupling of non-ideal plasmas suggests the use of the well-known Molecular Dynamics method (MD), which is very simple, easy to vectorize and very powerful for diagnostics, especially for dynamic diagnostics.

Hence the Two Dimensional Coulomb Gas (TDCG) is a good candidate to be our model of non-ideal plasma .

In the next section, we are giving some details on the model and on computational tools. We will then show the delocalization transition and its consequences on static properties, like the screening length. At last we will study dynamic diagnostics such as the velocity autocorrelation function $Z(t)$ and the charge fluctuation spectrum $S(k, \omega)$.

2/ MODEL AND COMPUTATIONAL TOOLS :

The singularity of the 2D Coulomb potential $V(r) = e^2 \ln(r/L)$ may be regularized at short distances by adding a repulsive core of radius σ between ions and electrons (L is an arbitrary scaling length, and e is the electron charge). The total potential is :

$$V(r) = -e^2 \ln(r/L) \quad \text{for ion-ion or electron-electron (Z=1) interactions} \quad 1.a$$

$$V(r) = e^2 \left[\left(\frac{\sigma}{r} \right)^{10} + \ln\left(\frac{r}{L}\right) \right] \quad \text{for ion-electron interactions} \quad 1.b$$

An equilibrium state of the system is characterized by a reduced density $\eta = n \sigma^3$, where n is the density, and by a coupling parameter $\gamma = e^2 / k_B T$, where k_B is the Boltzman constant and T the absolute temperature. We define a reduced temperature by $T^* = 1/\gamma = k_B T / e^2$. Here γ is the electron-electron coupling parameter. For electrons and ions with a charge Z the coupling is Z times greater and Z^2 times greater for ion-ion interactions. In real plasmas of high Z , the coupling between ions can be very large ($\gamma_{ii} \sim 100$ for gold at $n=100 \text{ g/cm}^3$ and $T=10^{-1} \text{ keV}$). Previous calculations with the "One Component Plasma" model (OCP) have shown that ions form a nearly periodic lattice for such coupling /3/. In order to simulate this ion-ion high coupling with $Z=1$ ions, we have fixed them on the sites of a regular lattice. Then the N interacting electrons of mass m move in the periodic field of the ions. In this way we transform the original Two-Component Coulomb Gas into an inhomogeneous One-Component Plasma of classical electrons in a periodic (rather than uniform) neutralizing ionic background. The plasma-dielectric transition is now transformed into a classical delocalization transition revealed by the onset of electron self-diffusion D .

Given the potential $V(r)$ between two particles we can compute the total force F_i acting on a particle i located at $R_i(t)$ with a velocity $V_i(t)$. The equations of motion have been integrated with the "leap-frog" version of the familiar Verlet algorithm /4/ :

$$V_i(t + \Delta t/2) = V_i(t - \Delta t/2) + F_i(t) \cdot \Delta t / m \quad 2.a$$

$$R_i(t + \Delta t) = R_i(t) + V_i(t + \Delta t/2) \cdot \Delta t \quad 2.b$$

$$V_i(t) = \frac{1}{2} [V_i(t + \Delta t/2) - V_i(t - \Delta t/2)] \quad 2.c$$

We have performed constant energy simulations or constant temperature simulations by adding a friction term in eq (2a) /5/.

The time step Δt must be adjusted on the highest frequency. In the high temperature plasma phase we expect the dynamics to be dominated by the plasma frequency $\omega_p = 2\pi \frac{ne^2}{m}$ while in the low-temperature phase the characteristic frequencies are those of the individual motion of each electron in the field of the ion with which it is paired. A simple independent pair model /5/ leads to an estimation of the frequencies corresponding to the rotational motion of the electron around its own ion, and radial vibrational motion. Typically these frequencies are an order of magnitude

larger than ω_p . For this reason a sufficiently short time-step, typically $\omega_p \cdot \Delta t \approx 0.005$, must be used to ensure a good conservation of total energy.

During the simulation, positions and velocities of each electron are stored on a magnetic tape. By running a post-processor after the simulation we can compute a lot of diagnostics very economically.

The static diagnostics are: thermodynamic properties as compressibility or specific heat, static structure factor $S(k)$ and pair correlation function $g(r)$. The dynamic diagnostics are: trajectories, self-diffusion constant D and electrical conductivity σ , velocity autocorrelation function $Z(t)$ and charge fluctuation spectrum $S(k, \omega)$. Each quantity is averaged over the N particles and over the recorded time trajectories.

3/ DELOCALIZATION TRANSITION :

The easiest way to gain some information from a MD simulation is to plot out the trajectories of all particles over some chosen time interval τ . A typical example for $\eta = 0.01$, $T^* = 0.232$ and $\tau = 247 \omega_p^{-1}$ is shown in fig. 1. At these temperature "bound" and "free" (diffusing) electrons are seen to coexist in an "ionization equilibrium". Of course if the simulation were carried out over longer times, the bound electrons would eventually become delocalized, while the diffusing ones would be momentarily trapped. Below a threshold temperature $T_1^* = 0.175$ all electrons are tightly bound with their ionic partner and we do not observe delocalizations (at last for times as long as $10^3 \omega_p^{-1}$). As we rise the temperature more and more electrons are delocalized and can take part to the onset of electrical conductivity. For $T_2^* = 0.25$ the collective break-up of electron-ion pairs induces a maximum in the specific heat C_s . The two temperatures: T_1^* (delocalization threshold) and T_2^* (maximum in the specific heat) are different but tend together to the same limit $T^* = 1/2$ when η goes to zero. This limit is the "collapse" temperature for point particles without repulsive core /6/. For $T^* = 0.50$ the plasma is "fully ionized" and trajectories are filling the whole box (apart from small hard ionic disks). The system now behaves nearly as the OCP.

Spatial correlations are characterized by the static structure factor $S(k)$ which is the density-density correlation function (fig 2):

$$S(k) = \frac{1}{N} \langle \rho_k \cdot \rho_{-k} \rangle \quad 3 a.$$

$$\rho_k = \sum_{i=1}^N e^{ik \cdot R_i} \quad 3 \text{ b.}$$

In the plasma phase ($T^* = 0.56$, $\gamma = 1.8$) $S(k)$ is very close to the one computed by Jancovici /7/ in the OCP model at $T^* = 0.50$. In the long wavelength limit, $k \rightarrow 0$, we can approximate $S(k)$ by /8/ :

$$S(k)_{k \rightarrow 0} = \frac{k_D^2 / k_s^2}{1 + k^2 / k_s^2} \quad 4.$$

where $k_D = 1/\lambda_D$ is the inverse Debye length and $k_s = 1/\lambda_s$ the inverse screening length. We have used this approximation to compute λ_s as the temperature decreases from the plasma phase. The screening length appears to diverge at the transition in agreement with intuition (the number of "free" electrons, acting on collective screening, vanishes).

Note that in the localized phase. $S(k)$ is not the Fourier transform of $g(r)$, the pair distribution function, computed directly from the coordinates of each particle. This fact is due to the complete loss of correlations between electrons, each one paired with its own ion (and consequently fully screened). The structure of $g(r)$ exhibits the localization effect, while $S(k)$ exhibits correlations.

IV/INDIVIDUAL AND COLLECTIVE MOTION:

The delocalization transition may be most conveniently characterized by individual versus collective modes . The individual motion is revealed by the self diffusion constant which can be estimated by the Einstein relation :

$$D = \lim_{t \rightarrow \infty} \frac{1}{4t} \langle [R_1(t) - R_1(0)]^2 \rangle \quad 5$$

or equivalently by the time integral of the correlation function $Z(t)$

$$D = -\frac{k_B T}{m} \int_0^\infty Z(t) dt \quad 6.a$$

$$Z(t) = \frac{\langle v_1(t) \cdot v_1(0) \rangle}{\langle [v]^2 \rangle} \quad 6.b$$

where $V_i(t)$ is the velocity of particle i at time t . Replacing $V_i(t)$ by $\Sigma V_i(t)$ we obtain the current autocorrelation function $J(t)$ of which the time integral gives the electrical conductivity σ .

Two examples of $Z(t)$ and of its Fourier transform (spectrum) $\tilde{Z}(\omega)$ are shown in Fig. 3. The contrast between high and low temperature phase is striking.

In the plasma phase $Z(t)$ decays monotonically and $D \sim \tilde{Z}(\omega = 0)$ is large. In the dielectric phase $Z(t)$ exhibits marked oscillations and the spectral analysis reveals a sharp resonance which can be associated with the rotational motion of individual electrons, and a broad high frequency vibrational band; D is now strictly zero.

$J(t)$, which is a collective quantity, turns out to be indistinguishable from $Z(t)$ in the dielectric phase, showing that dynamics is dominated by individual particle motion (no cross correlations) and hence $\sigma \approx 0$. On the other hand, in the plasma phase collective behaviour becomes increasingly important as T increases and $J(t)$ differs more and more significantly from $Z(t)$, decaying much more slowly. This feature can be attributed to the fact that electron-electron collisions conserve momentum, and hence the electric current, but decorrelate individual velocities.

The collective behaviour of the plasma may be also characterized by the charge fluctuation spectrum $S(k, \omega)$, or dynamic structure factor. $S(k, \omega)$ is the Fourier transform of the charge autocorrelation function :

$$S(k, \omega) = \frac{1}{2\pi} \int_0^\infty e^{i\omega t} \frac{1}{N} \langle \rho_k(t) \cdot \rho_{-k}(0) \rangle dt \quad 7.$$

We have computed $S(k, \omega)$ for wavenumbers k compatible with periodic boundary conditions.

As long as the wavelength $\lambda = 2\pi/k$ is significantly larger the screening length λ_s , $S(k, \omega)$ exhibits a sharp resonance at a frequency close to ω_p . This is a manifestation of plasma oscillations (plasmon mode). A hydrodynamic calculation /9/ gives the long-wavelength limit of $S(k, \omega)$ related to the complex a.c. conductivity

$$\sigma(\omega) = \sigma'(\omega) + i \sigma''(\omega) = \int_0^\infty e^{i\omega t} J(t) dt \quad 8.a$$

$$s(\omega) = \lim_{k \rightarrow 0} \frac{S(k, \omega)}{S(k)} = \frac{\sigma'(\omega)}{[\omega - 2\pi\sigma''(\omega)] + 2\pi\sigma'(\omega)} \quad 8.b$$

In the long wavelength limit we can observe in fig. 4 a peak shifted below the plasma frequency and broadened. This damping increases as the temperature is lowered and hence must be associated with the electron/ion recombination (no Landau damping

at $k=0$). The plasmon peak at $k \neq 0$ fully disappears at $T^* = 0.312$ when only 10% of the electrons are localized. If we plot the frequency of this plasmon peak versus wave-number k we can observe a very unusual oscillating dispersion relation $\omega(k)$ (fig. 4b). This pattern is presumably due to the coupling between plasmons and periodic ionic background. Finally note that each time the relation $\omega = \omega(k)$ exhibits a maximum, the group velocity $\delta\omega/\delta k$ goes to zero. Consequently it seems that for peculiar wavenumbers k , the plasmons are not able to carry energy. We suggest that inhibition of heat transport in laser plasma experiments could be partly explained by a coupling mechanism between plasma waves and strongly coupled ionic structure .

Simulations with other boundary conditions and with a more efficient regularization are in progress in order to confirm this coupling .Simultaneously Mean Field Theory is used to explain the shift and the broadening of the dynamic structure factor /10/.

FIGURE CAPTIONS

Fig.1: Trajectories of 108 electrons in a hexagonal Lattice of fixed ions at $\eta = 0.01$ over $247 \omega_p^{-1}$.

Fig.2: Static structure factor $S(k)$ in the plasma phase versus $q = ka$. The M.D. results are for $T^* = 0.56$ (circles), $T^* = 0.312$ (triangles) and $T^* = 0.238$ (squares) the full curves obtained by least squares fits of the small k limit /4/ to be MD data up to $q \sim 2$. The data for $T^* = 0.56$ are surprisingly close to the exact structure factor of the 2D OCP at $T^* = 0.5$ (dashed curve).

insert: Reduced screening length $\lambda_s^{*2} = (\lambda_s / \lambda_D)^2$ versus $\gamma = 1 / T^*$.

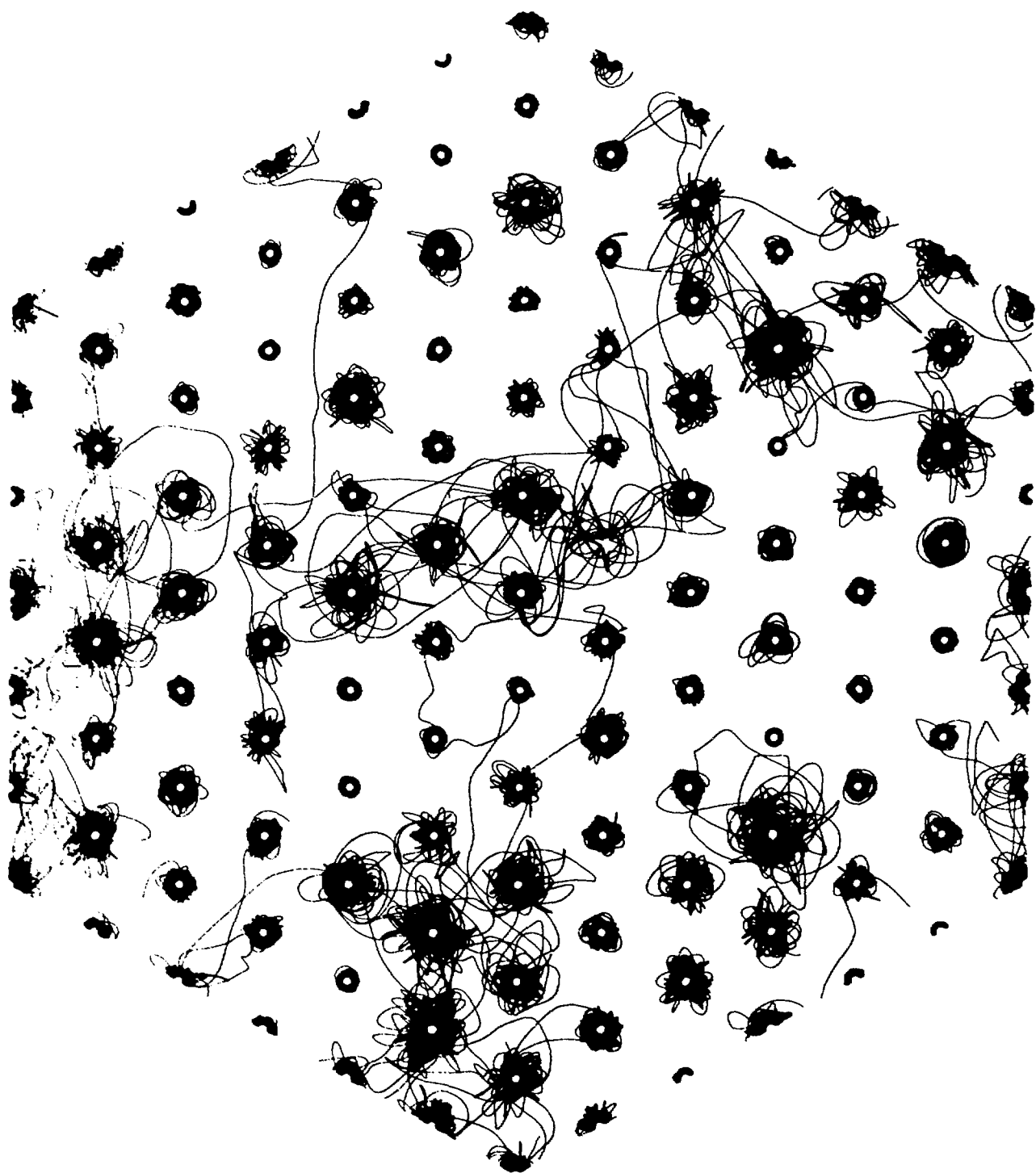
Fig.3: Normalized velocity and current autocorrelation function: $Z(t)$ (full curves) versus reduced time for $T^* = 0.175$ or $v = 5.7$ and $T^* = 0.56$ or $\gamma = 1.8$. Normalized spectra $\tilde{Z}(\omega)$ versus reduced frequency.

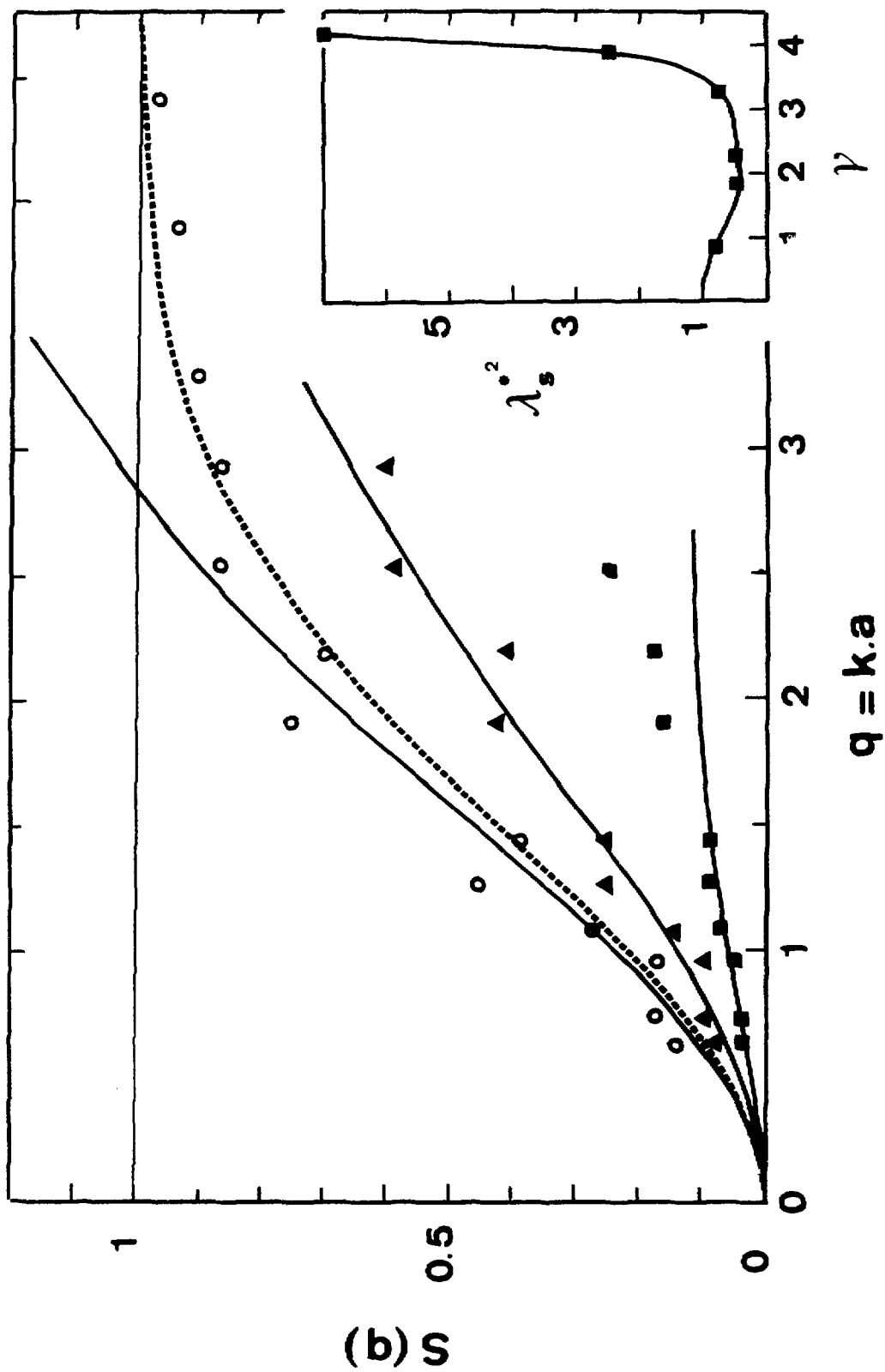
Fig.4: Long wavelength limit $s(\omega)$ of the charge fluctuation spectrum at $T^* = 0.56$.

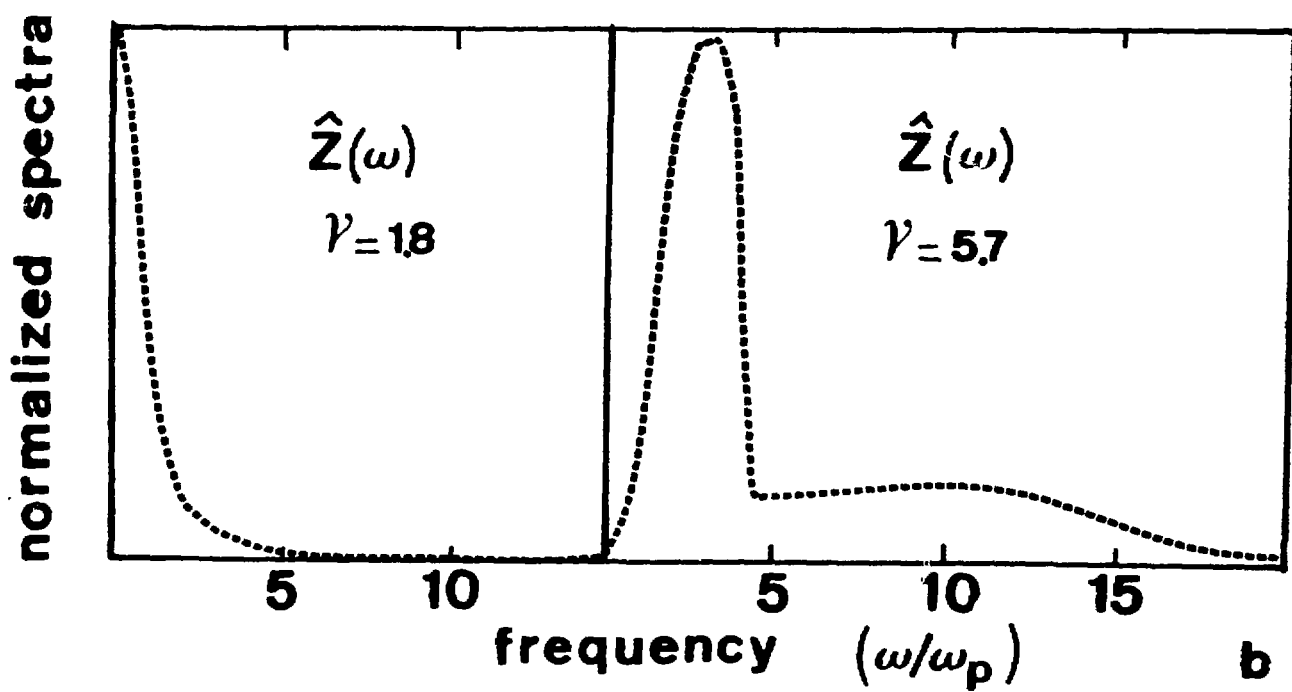
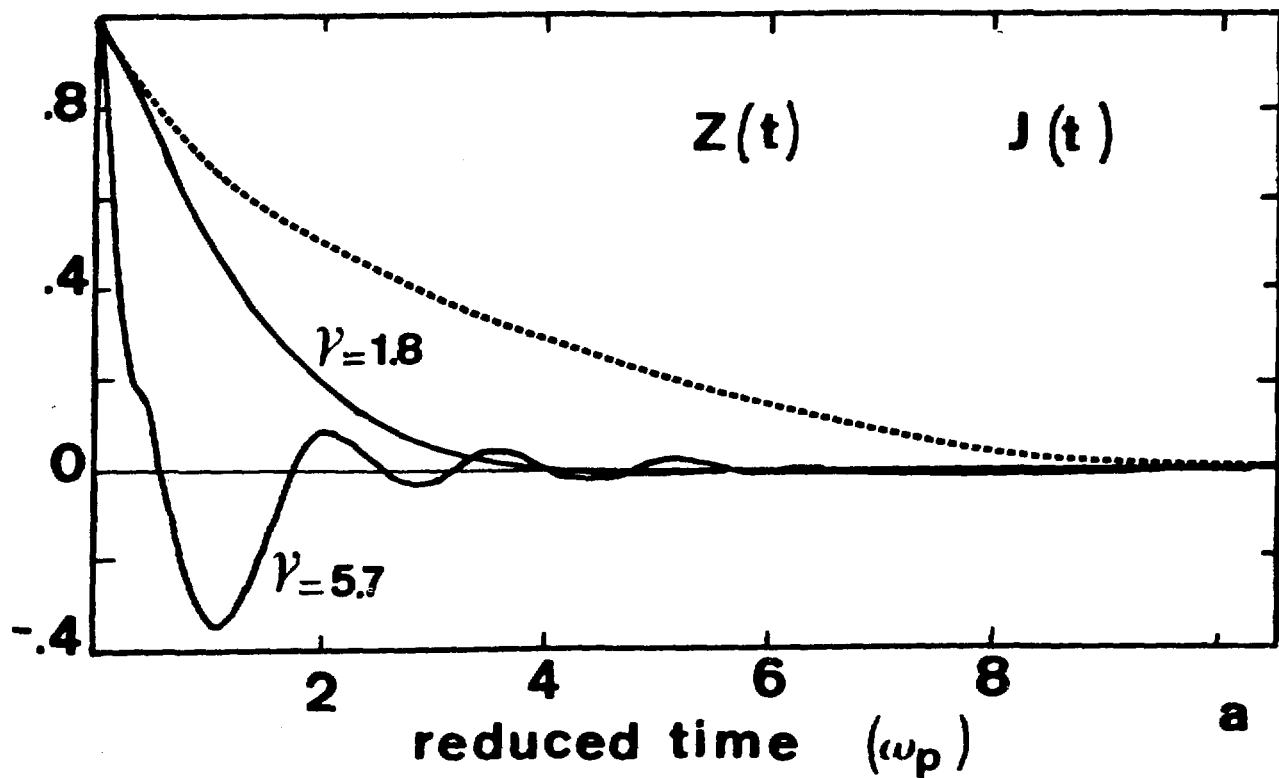
Insert : dispersion curve $\omega = \omega(k)$. Each point is given with its own full width at half maximum. The continuous line is the Vlasov curve and the dotted line is a tentative dispersion relation.

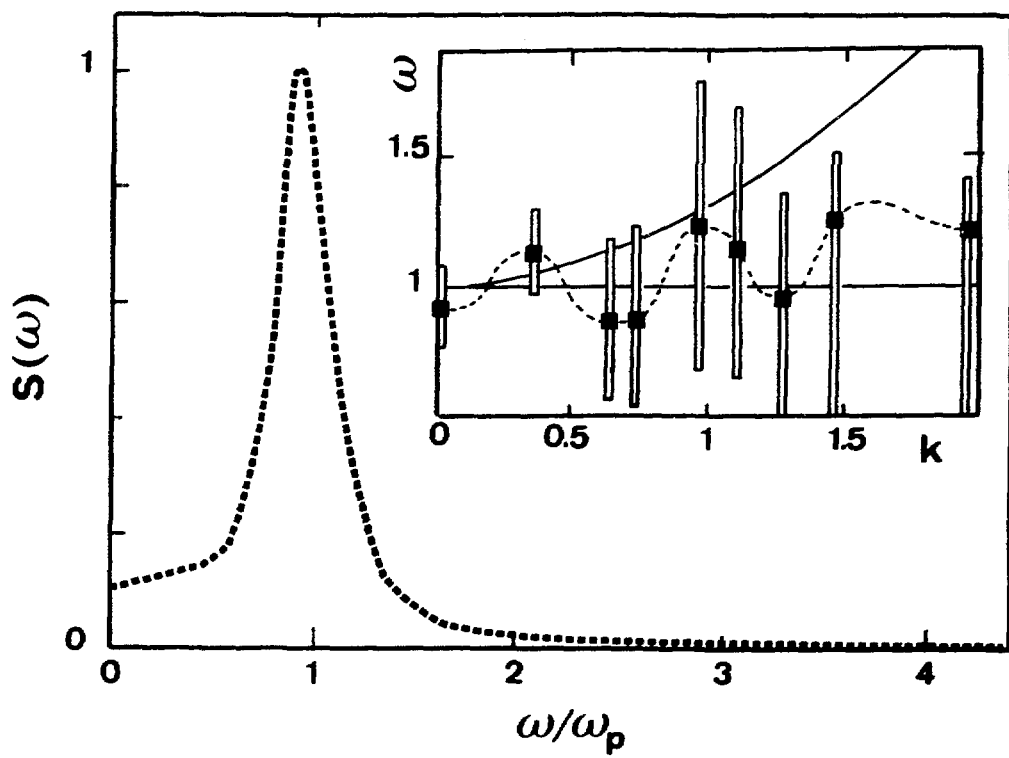
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RELATIVISTIC HYDRODYNAMICS AND HEAVY ION REACTIONS

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Abstract

The possibility of forming a new state of nuclear matter - the quark-gluon plasma - in relativistic heavy ion collisions is currently the subject of intense theoretical and experimental investigation. The possible formation and evolution of the plasma is investigated using relativistic hydrodynamics. Nuclei are nearly transparent at the high bombarding energies involved and it is necessary to use a two-fluid model to describe the initial stages of the reaction. The current status of the numerical techniques and the relevant physics is reviewed.

It is generally conceded that nucleons are composed of quarks and gluons, although these basic constituents of matter have not been directly observed. The quarks are (massless) point-like objects carrying charge, baryon number and other quantum numbers such as strangeness, color and flavor. The gluons are the massless agents which mediate the strong interaction. The quark-quark interaction increases with their relative distance and thus are normally confined to individual nucleons: they can only exist in multiples of three. However, from the current theory of the strong interaction - quantum chromodynamics - arises the possibility that a phase transition may occur. If nuclear matter is sufficiently compressed that the nucleons begin to overlap - or the matter is heated sufficiently - a phase transition will occur. The quarks will become deconfined and a new state of matter will be formed: *the quark-gluon plasma*. There are three places wherein the quark-gluon plasma might be found:

- 1) in the milliseconds of the universe after the big bang;
- 2) the interior of neutron stars;
- 3) in the heated volume of dense nuclear matter formed during the collision of relativistic heavy ions.

Clearly the first two of these are not readily accessible to laboratory experiments. However, the third is currently the subject of intense and exciting experimental and theoretical efforts. The principal theoretical tool used to describe the time evolution of the reactions is relativistic hydrodynamics.

The use of hydrodynamics to describe the collision of hadronic matter has a long history which dates from work of Fermi [1], Pomeranchuk [2] and Landau [3] in the early fifties. They attempted to describe proton-proton scattering and the concomitant production of pions using statistical and hydrodynamical concepts. Their success encouraged other, later applications to different reactions, both at higher energies as well as for heavier, composite particles. Since this early work, the models have been refined and

fresh concepts have been advanced utilizing new ideas from particle physics, quantum chromodynamics and other fields such as astrophysics. This article will very briefly review a few of the varied applications relativistic hydrodynamics has in the area of heavy ion reactions. A two-fluid model which overcomes certain of the limitations of the usual relativistic hydrodynamics in describing the physical processes and which also avoids the problems with causality associated with the introduction of dissipation into the hydrodynamic equations will be described. We refer the reader to the literature for more detailed descriptions of the application of hydrodynamics to heavy ion reactions [4,5] and hadron-hadron collisions [6,7].

At the relativistic velocities employed in the experiments, it is normal to measure mass, temperature and energy in units of energy as follows from the famous Einstein mass-energy equivalence relation $E = m c^2$. The standard unit of energy the electron volt or multiples of this such as a million electron volts which is abbreviated MeV and one thousand MeV or a GeV. The rest mass of a proton is approximately 939 MeV or 0.939 GeV. Protons accelerated at CERN in Geneva have a kinetic energy of 200 GeV. Objects having a non-zero velocity relative to an observer's rest-frame are contracted by an amount $\gamma = [1 - \beta^2]^{-1/2}$ where $\beta = v/c$ and c is the velocity of light. From simple relativistic expressions one has

$$E = m c^2 = T + m_0 c^2 = \gamma m_0 c^2$$

where T is the kinetic energy and m_0 is the rest mass. Hence,

$$\gamma = 1 + T/m_0 c^2.$$

At these energies the Lorentz contraction factor γ is 213 and the velocity is 0.999989 c . That is, the objects are 213 times larger in the transverse direction than in the longitudinal direction. Such severe distortions are difficult to model. However, because of Lorentz invariance the reaction can equally well be described in the center-of-mass frame in which each of the objects have an equal and opposite momentum. In this frame the two nucleons move towards each other with a velocity of 0.9953 c or a γ of 10.4.

It is not *a priori* apparent that hydrodynamics will be valid for the description of heavy ion reactions. An examination of the conditions necessary for the validity of hydrodynamics indicates that the requirements are only marginally fulfilled. For example, the number of particles which are involved in a heavy ion collision ranges from perhaps only a hundred to a thousand. Hence, the number of degrees of freedom is large compared to one, but relatively small compared to a usual fluid. If one creates a quark-gluon plasma during the collision, then the number of degrees of freedom will increase by at least a factor of three.

There is also the condition that there be sufficient time for the establishment of local, thermal equilibrium; this also is marginally satisfied. A lower limit on the collision time for two heavy ions may be roughly estimated as the nuclear diameter divided by the velocity of light, or about 5×10^{-23} s. Nucleons interact by exchanging pions and it requires about 5×10^{-24} s for two adjacent nucleons to exchange a pion. Since this interaction time is about one-tenth of the total collision time, some degree of local equilibrium will be established. This will be particularly true for central collisions of large nuclei for which the matter in the interior will be confined for longer periods than the above estimate. Further, for moderate bombarding energies, the actual

reaction time is around 20×10^{-23} s which is appreciably larger than the simple above argument suggested.

The question of whether there is local equilibrium has been investigated by many authors using a variety of numerical methods. Although there is time for only a very few collisions, because of the very strong nucleon-nucleon interaction, near-equilibrium conditions seem to prevail. A detailed computer simulation for the case of molecular collisions has been made by Bird [8] who concluded that only 2 - 3 collisions are needed to achieve thermal equilibrium. Bondorf and Zimányi [9] have investigated the approach to equilibrium using a time-dependent Boltzmann equation. They concluded that the pion and proton spectra suggest that the momentum distributions are very near their equilibrium values. During sufficiently energetic reactions, new particles such as pions or deltas may be created; such particles are short lived, either being rapidly absorbed in the case of pions, or decaying into a nucleon and a pion. Montvay and Zimányi [10] have investigated whether chemical equilibrium is reached; they conclude that it is not reached although the system is not very far from it.

Finally, it is not unrealistic to treat the nucleons as classical particles for the energy regimes in which we shall be interested. For relativistic nucleons their momenta is greater than 1 GeV/c and their corresponding de Broglie wavelength is 0.4 fm (one fermi, fm, is 10^{-13} cm) which is less than the radius of a nucleon and much less than that of a nucleus.

The applications of relativistic fluid dynamics to heavy ion reactions have assumed there to be no dissipation. (There is some early work on hadron-hadron reactions by the Russian school which attempted to include the effects of viscosity. This work assumed the validity of the Landau equations and is reviewed by Feinberg [6].) In the Los Alamos effort the three dimensional relativistic Euler equations are solved numerically using the particle-in-cell method developed by Harlow [11,12]. Since the PIC method is well-known and the differences required for the relativistic equations are treated in ref. 12, the method of numerical solution will not be discussed here. The particle-in-cell method allows calculations in cases of extreme distortion and shear including cases where cavities appear in the fluid. It also allows beautiful graphical representations of the fluid (cf., ref. 5). However, it consumes vast amounts of computer memory.

The equation of state for nuclear matter is unknown; indeed, one of the goals of heavy ion reactions is to investigate the equation of state. Since theoretical calculations of the energy and pressure of nuclear matter as a function of density and temperature are quite uncertain, one usually is forced to make assumptions regarding the equation of state. It is normal in nuclear physics to call the energy per nucleon, $E(n)$, the equation of state rather than expressing the pressure as a function of temperature and density. The two are of course equivalent since one may obtain the pressure from the usual thermodynamic relation

$$P = \left(\frac{\partial E}{\partial V} \right)_S ,$$

where S is the entropy. Examples of some zero-temperature equations of states which have been used are shown in fig. 1. One further usually assumes that

the matter obeys a Fermi gas equation of state for non-zero temperature. For densities greater than five times normal nuclear matter density, a number of possible scenarios have been proposed. Currently, the most plausible one is that at sufficiently high densities or temperatures, the nucleons 'melt' and a quark-gluon plasma is formed in which the identities of the individual nucleons is lost and the constituent quarks and gluons are free to briefly roam about the relatively large collision volume.

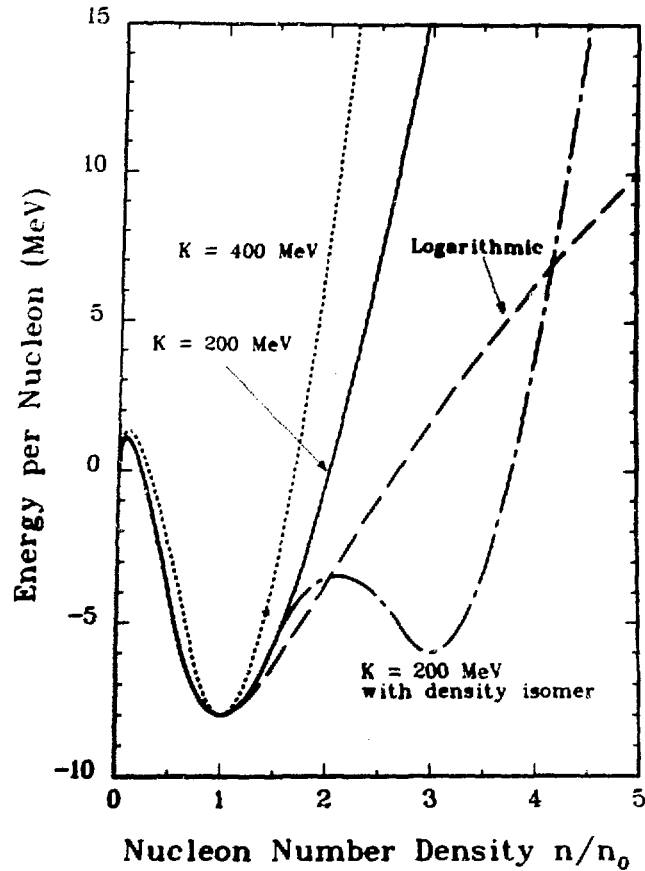


Fig. 1. A plot of the ground state energy per nucleon $E(n)$ as a function of density for four different phenomenological expressions. The quantity K is the compression modulus of nuclear matter, the canonical value of which is 200 MeV.

An example of the time development of a heavy ion reaction is shown in fig. 2 which shows the collision of two equal mass nuclei at 850 MeV/nucleon. From a knowledge of the velocity vectors of the fluid in each cell at the end of the calculation, one may calculate the double differential cross section $d^2\sigma/dE d\Omega$ which may be compared with experiment. In general the agreement is satisfactory. In fact hydrodynamic calculations predicted that in certain reactions, the relative incompressibility of nuclear matter would cause the projectile to glance off the target and produce a distinctive signal in the angular distribution. This "sideways" flow was subsequently experimentally observed. For details see ref. 4.

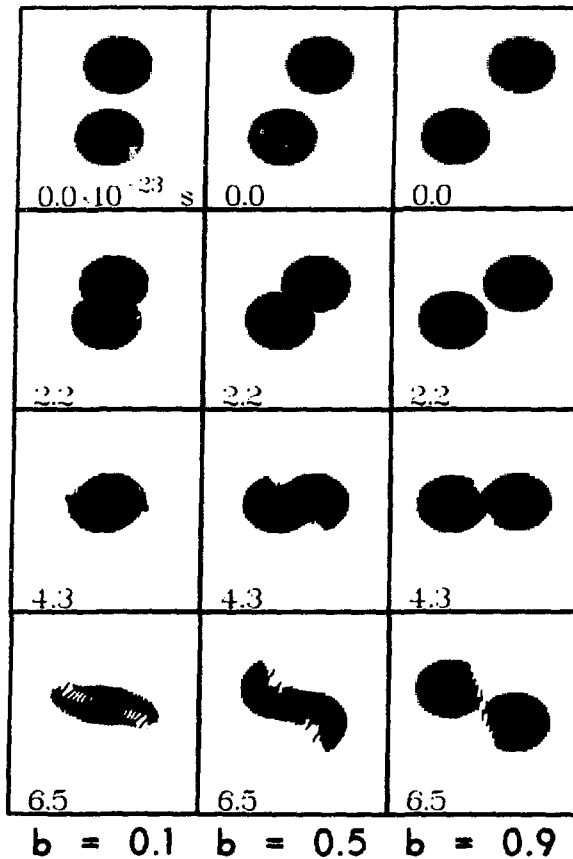


Fig. 2. Matter distributions for two equal-mass nuclei at 162 MeV/nucleon in the center-of-mass (equivalent laboratory energy is 800 MeV/nucleon). Three impact parameters are shown in units of the sum of the radii of the two nuclei. Since the Euler equations are scale invariant, the figure applies to arbitrary mass nuclei, although the time scale is appropriate only for ^{238}U on ^{238}U .

A close examination of fig. 2 will demonstrate that the calculation reproduces the result that for a one-fluid system with no viscosity, the mean-free-path of the matter is zero. (This is more easily seen when the matter from each nucleus is plotted in color as in ref. 5.) This is not a serious problem at low bombarding energies of less than a GeV per nucleon for which the mean free path of a nucleon in the nucleus is much shorter than the nuclear diameter. However, as the energy of the projectile increases, the nucleus becomes more transparent and the assumption of a zero mean-free-path becomes untenable. The effect of non-zero mean-free-paths has been known for some time from high energy proton-nucleus experiments at Fermi Lab and CERN; in these experiments the so-called leading particles punch through the target and carry away a significant amount of the energy of the incident proton. One could simulate to a small extent the effects of a non-zero mean-free-path by introducing viscosity. However, this would introduce all the

problems associated with the acausal behaviour as demonstrated by Hiscock and Lindblom [13,14]. In any event, this would be inadequate when the mean-free-paths become so long that some of the nucleons can traverse the entire target and emerge on the far side. Further, as the energies increase it becomes less likely that local thermal equilibrium is instantaneously established at the interface of the two nuclei.

To describe the situation in which large mean-free-paths are involved, a two-fluid model was introduced [15]. To obtain the equations which describe the two-fluid model, each nucleus is assumed to be a fluid which has the identical properties of the fluid representing the other nucleus. When the two fluids collide they are allowed to exchange energy and momentum at a finite rate proportional to the relative velocity of the two nuclei and to the nucleon-nucleon cross section σ_{NN} . Thus, the rate of momentum loss is finite and the two fluids will interpenetrate. The amount of interpenetration is small at low energies for which σ_{NN} is large and increases as σ_{NN} decreases. The Euler equations which ensure particle number conservation remain unchanged, but the equations ensuring energy and momentum conservation must be modified to allow an interchange of these quantities. The changes are in the form of additional terms, the magnitude of which can be estimated from kinetic theory: if one knows the collision rate and the amount of energy and momentum lost in each collision, then the total amount of loss may be found.

The expression for the collision rate is

$$R_{\text{coll}} = N_1 N_2 \sigma_{NN} v_{\text{rel}}$$

where N_1 and N_2 are the densities of the two fluids and v_{rel} is the relativistic generalization of the relative velocity. The generalized Euler equations for fluid one are

$$\partial_t \mathbf{M}_1 + \nabla(\mathbf{v}_1 \cdot \mathbf{M}_1) = -\nabla P - R_{\text{coll}} K (\gamma_1 \mathbf{v}_1 - \gamma_2 \mathbf{v}_2)/Y$$

$$\partial_t E_1 + \nabla(\mathbf{v}_1 E_1) = -\nabla P - R_{\text{coll}} K (\gamma_1 - \gamma_2)/Y$$

where M_1 and E_1 are the momentum and energy densities of fluid one and Y is the scalar product of the two four-velocities

$$Y = (u_1 u_2).$$

The quantity K determines the amount of energy-momentum loss and is fixed by comparing with high energy nucleon-nucleus reactions. The equations for fluid two are obtained by interchanging the indices 1 and 2.

Unlike the Euler equations, eqs (2) and (3) are not scale invariant; the calculated results will depend the masses of the nuclei involved which is entirely reasonable. A similar consequence occurs if one uses the Navier-Stokes equations. However, unlike the case of the Navier-Stokes equations which introduces dissipation through higher order derivatives of the velocity, the two-fluid model partially achieves the same result by eliminating derivatives in the additional terms.

The additional coupling terms in eqs. (2) and (3) describe the friction between the two nuclei entirely in terms of two-body collisions of the constituent nucleons. It is assumed that the nucleon-nucleon cross section is the free NN cross section σ_{NN} and is independent of density and temperature; this assumption is surely poor at high temperatures and densities. It is further

assumed that the Fermi velocities of the nucleons may be ignored. For large relative velocities this is a good approximation (the Fermi velocity at normal nuclear density is approximately $0.27\ c$); for lower bombarding energies, one must worry about the effects due to the Fermi velocity. For methods which partially take into account the effects of the Fermi velocity, the reader is referred to refs. 5 and 15. In addition both the one-fluid and two-fluid models necessarily omit binding energy effects.

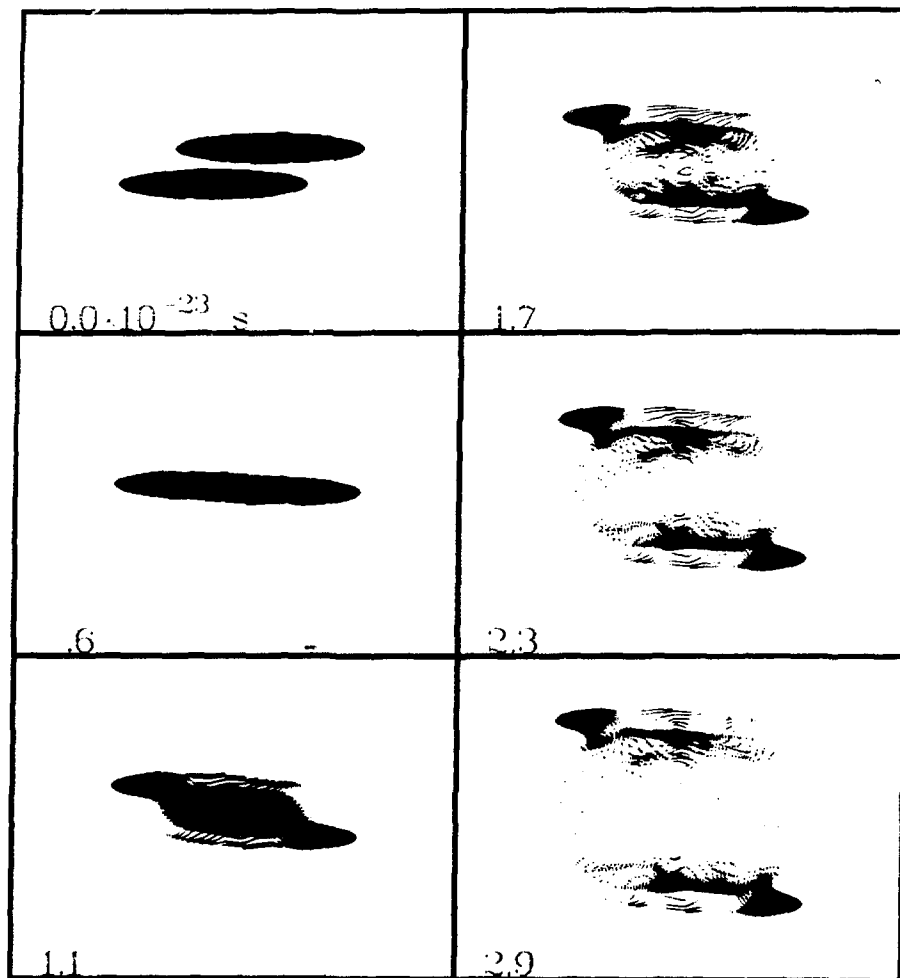


Fig. 3. Matter distributions for ^{238}U on ^{238}U calculated in the center-of-mass system with the two-fluid model. The center-of-mass kinetic energy is $5\ \text{GeV/nucleon}$ (equivalent laboratory energy is $73.7\ \text{GeV/nucleon}$) and the impact parameter is 0.3 .

In figure 3 results are shown for a collision between two equal mass nuclei, each having an energy of $5\ \text{GeV}$ per nucleon in the center of mass frame. (This energy corresponds to a velocity of $0.987c$ in the center of mass or a velocity of $0.99992c$ in the laboratory frame.) The effects of a non-zero mean-free-path are immediately evident. The two nuclei essentially pass

through each other, although each nucleus exerts a drag upon the other. In the one-fluid model the matter at the interface of the two nuclei would have come to a halt. All the kinetic energy must be converted into thermal energy. Hence, the one-fluid model can expect to exhibit a larger thermal pressure than does the two-fluid model. This will result in the nuclear matter blowing up and disintegrating sooner.

Experiments have recently begun at CERN which collide 200 GeV/nucleon ^{16}O ions on nuclear targets in a search for signals of a quark-gluon plasma. Similar experiments will soon begin at lower energies at Brookhaven National Laboratory. In all these experiments relativistic hydrodynamics will play an essential role in the interpretation of results.

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MATTER EJECTION AND GAS INTERACTION

PHYSICAL AND COMPUTATIONAL MODELS

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ABSTRACT

The present study is essentially intended to build up a physical model concerned with matter ejection. The so called phenomenon, i.e., an emission of microjets, can be observed in a strong shock wave, while emerging from the surface of the metallic samples. The presence of geometrical defects on the surface particularly induce the existence of those microjets, whose dynamic characteristics are conditioned by parameters such shock pressure, surface aspect, nature and structure of the tested material.

The different phases of microjet formation process are described as initiation, formation and feeding with respect to the real geometrical defects. The interaction with an adjacent gaseous medium is also taken into account.

The previous part of the described process is shown in a brief survey before a more thorough study of the gas-particles interaction.

Due to the presence of the gas, the ejected particles may be very strongly slowed down. The deceleration process description can present complex aspects : more or less elongated jets shapes, fragmentation, supersonic flow, ablation effects... The model we have done will take these patterns into account with the purpose of interpreting experimental results. The computational code based on this model allows us to determine the evolutive parameters of the microjets and particles, and therefore essentially to estimate the stopping distances, all the characteristic times and the ablation specific parameters.

I - INTRODUCTION

In the context of our experimental studies about ejected matter generated by strong shock wave emerging from the free surface of a sample, we have worked out a theoretical hydrodynamic model which describes the space-time evolution of jets coming from calibrated geometrical defects. (ref.1).

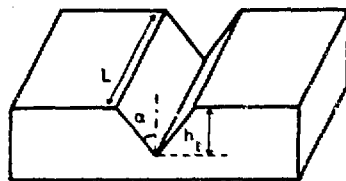
This model takes into account sample composition, geometrical defects shapes, shock wave characteristics, free surface velocity. The different phases of jets are quantitatively described. (ref.2).

This model is an essential tool to apprehend ejected matter physics.

II - ASSUMPTIONS

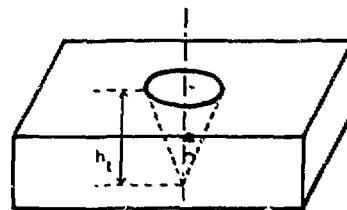
We assume :

- sample free surface geometrical defects are :
 - . a single groove or hole (localized defect) (fig.1 and 2).
 - . wedge-shaped grooves (distributed defects) (fig.3).



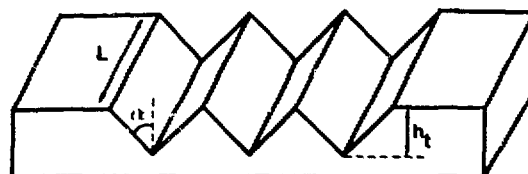
single groove

Fig.1



conical cavity

Fig.2



wedge-shaped grooves

Fig.3

- The self similar adiabatic flow is described by the conservation equations :

$$\frac{\partial \rho}{\partial t} + \text{div } \rho \vec{v} = 0$$

$$\rho \frac{d\vec{v}}{dt} = - \text{grad } p$$

$$\frac{d\varepsilon}{dt} + p \frac{d(1/\rho)}{dt} = Q$$

- We consider two different patterns of density :

- . homogeneous density:

The jet has a Gaussian shape. Its density is constant at one given time. The figure 4 shows ejecta contours for a wedge-shaped groove and a conical cavity.

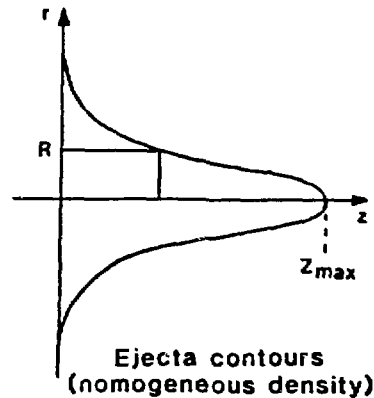
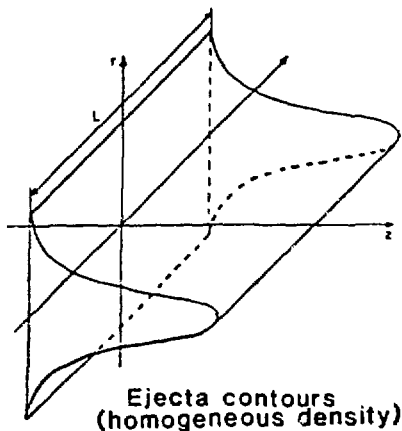


Fig.4

- . inhomogeneous density:

We assume a (r,z) Gaussian density distribution. Contour doesn't exist anymore since the density tends to zero as r and z approach infinity. So in this case, jet shape is given by isodensity curves (fig.5).

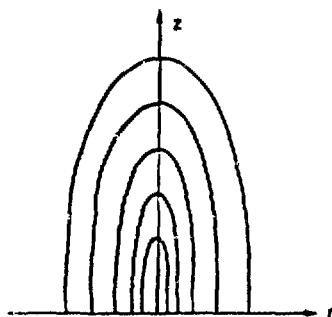


Fig.5

III - RESULTS

The theoretical model gives (fig.6) :

- 1 - the microjet feeding
- 2 - the total ejected matter mass with the particles velocity
- 3 - the jet space-time behavior (homogeneous density)
- 4 - the jet space-time behavior (inhomogeneous density).

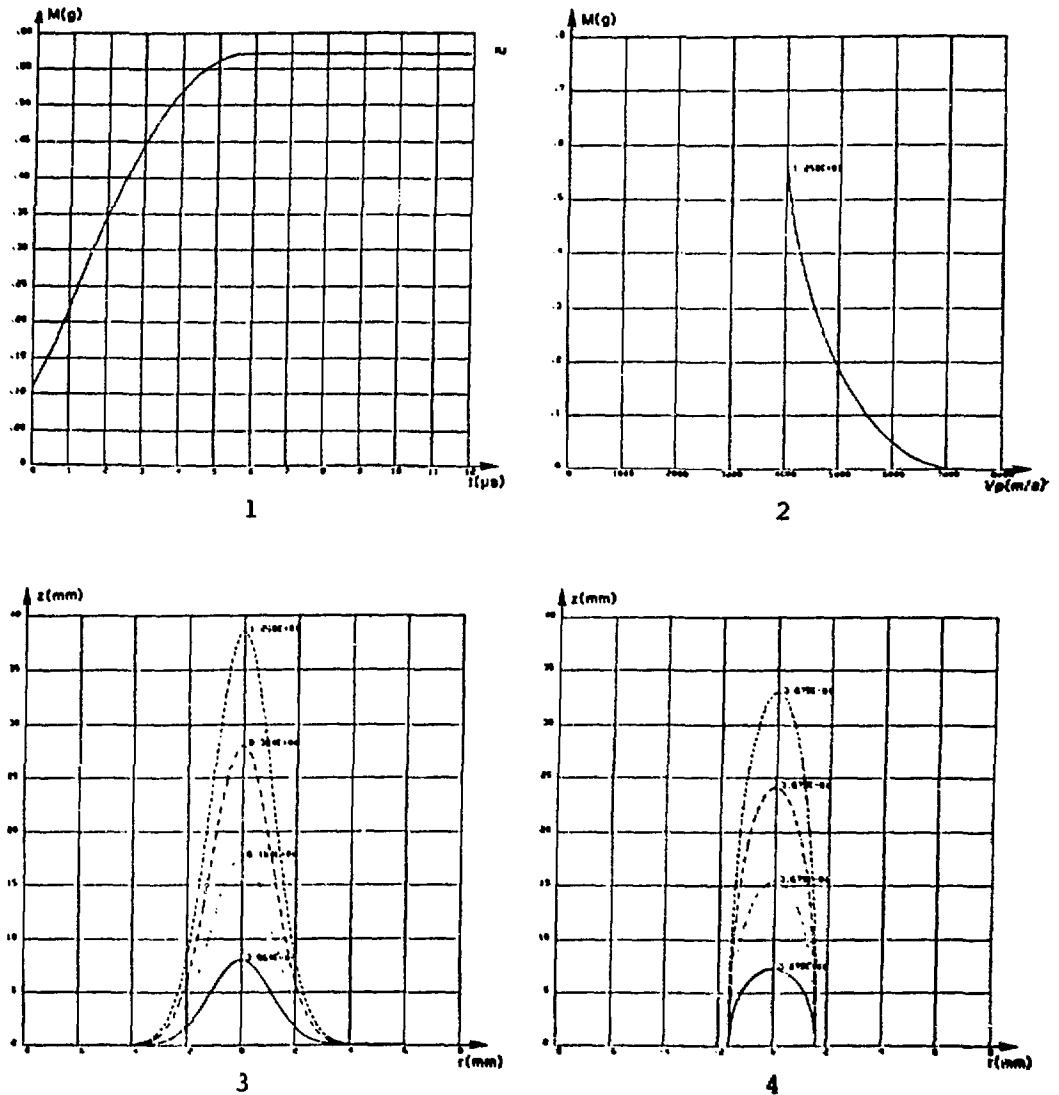
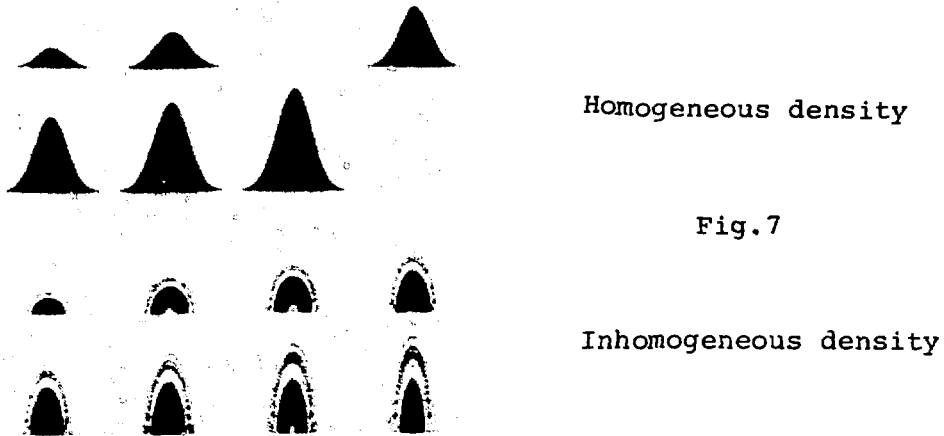


Fig.6

Theoretical results and X-ray images are then efficiently compared with a specific image processing system leading to appropriate shape extraction and density map reconstruction.

A specific software has been developed to compare the model theoretical results and experimental data issued from radiographs. These comparisons are performed on an image processing display in term of microjet shape, surface mass values and density maps (fig.7).



We also compare these theoretical results to those given by Doppler Laser Interferometry (DLI) and shadowgraphy. (ref.3).

The figure 8 shows the evolution jet contour observed by shadowgraphy.

DIAGNOSTIC : Shadowgraphy BETWEEN TWO PICTURES : 227 ns
 DEFECT : groove 90° in angle (copper sample)
 SHOCK : explosive plane wave generator (560 kbar)

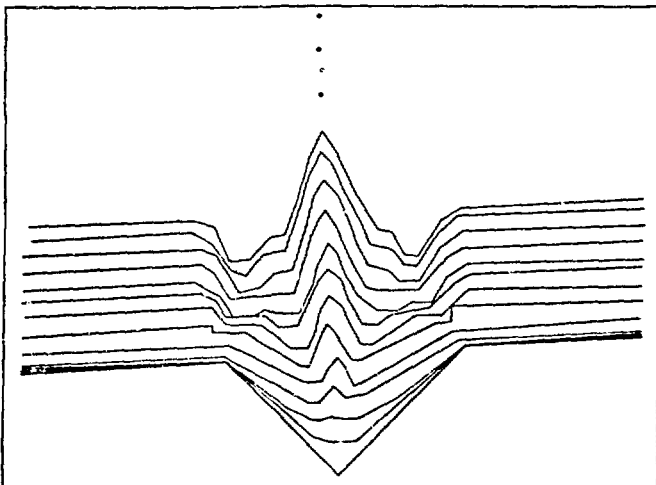
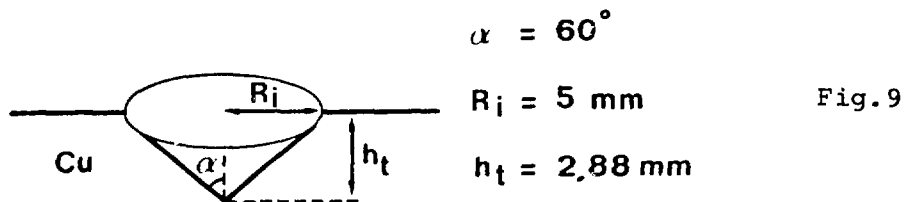


Fig.8

IV - MODEL USE - EXAMPLE

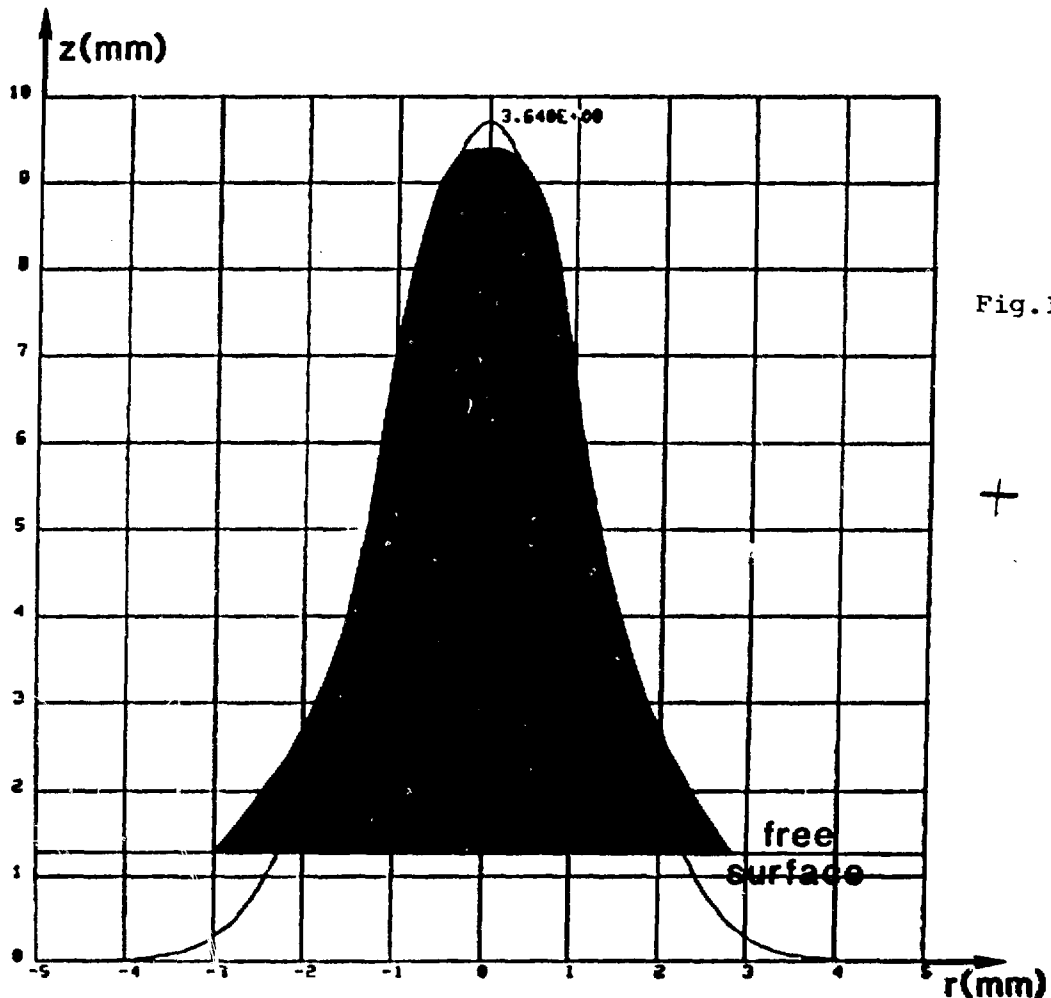
For a specific diagnostic, we compare theoretical and experimental results (average density and shape of a jet coming from a localized defect).

The shock ($P = 1250$ kbar) is generated by a two stage light gas gun (CAGL at C.E.Vaujours). The target is a copper disk with a conical cavity drilled into its surface (fig.9).



- The shock velocity is measured by Mylar gauges.
- We reconstruct the jet density map from the experimental X-ray image and calibration steps.

The figure 10 shows, we obtain a good fit between experimental and calculated shape and average densities.(ref.4).



Let's notice that we can't measure the density inside theoretical defect by radiography: it explains the lack of accuracy nearby the free surface.

This hydrodynamic model describes jet feeding and evolution of a non-fragmented microjet. In a short while, fragmentation occurs and resultant particles interact with surrounding gas.

It is the so-called gas-particles interaction.

V - MATTER EJECTION AND GAS INTERACTION

Due to the presence of the gas, the ejected particles may be very strongly slowed down. This process is complex : more or less elongated microjets, fragmentations, supersonic flow, ionization, ablation and accretion phenomena. Depending on experimental conditions, the induced shock is located in front or at the back of the head of ejecta.

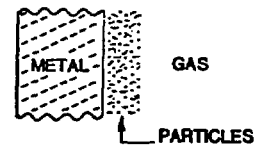


Fig.11

We observe these previous phenomena using X-ray radiography or shadowgraphy diagnostics and we explain the corresponding experimental results by the means a theoretical model. Here, we will emphasize the head of ejecta space-time behaviour. It can be described, taking into account the following simple assumptions : considering contiguous dihedral (i.e. wedge-shaped) grooves made of tin - 300 μm width, 100 μm depth - the head of ejecta motion is likened to a sphere motion ; the initial diameter of the sphere is equal to one groove width and its center is coinciding with the head of ejecta. The sphere moves at the same velocity as does the head of ejecta and it is ablated as soon as it moves. If no ablation occurs, the sphere diameter will be constant.

VI - HYDRODYNAMIC MODEL : SPHERE ABLATION AND VELOCITY DECREASE.

Depending on the Reynolds number Re , the sphere motion is driven by a 2 or 4 equations system ; from it, we calculate the $U(t)$ velocity and $X(t)$ location.

To simplify, let us define the drag coefficient C_x of the sphere as follows (subsonic flow) :

$$53.33 \leq Re \leq 250000 \Rightarrow C_x = 0.45 : \text{Newtonian regime} \\ \text{(first wakes regime)}$$

$$0 < Re \leq 53.33 \Rightarrow C_x = 24/Re : \text{Stokes regime.}$$

$$\text{and } Re = \frac{|U| d \rho_1}{\mu} \quad (d : \text{sphere diameter, } \rho_1 : \text{density of gas, } \mu : \text{absolute viscosity of gas}).$$

A) Newtonian regime (first wakes regime)

$$53.33 \leq \frac{|U| d \rho_1}{\mu} \leq 250000$$

1) The velocity $U(t)$ is solution to the simplified B.B.O. (BASSET, BOUSSINESQ, OSEEN) equation (Ref.5)

$$\frac{\pi}{6} d^3 \rho_2 \frac{dU}{dt} = - C_x \frac{\pi d^2 \rho_1}{4} \frac{U|U|}{2} - \frac{1}{2} \frac{\pi}{6} d^3 \rho_1 \frac{dU}{dt} - \frac{3}{2} d^2 \sqrt{\pi \rho_1 \mu} \int_0^t \left[\frac{dU}{d\tau} / \sqrt{t-\tau} \right] d\tau$$

(ρ_1 : sphere density, t and τ are times).

$$\text{The Basset term } - \frac{3}{2} d^2 \sqrt{\pi \rho_1 \mu} \int_0^t \left[\frac{dU}{d\tau} / \sqrt{t-\tau} \right] d\tau$$

is a "memory" function or "hereditary" term. Its expression has been rigorously validated only for $Re < 1$. With a Newtonian regime of flow about the sphere, it will be an upper bounds value.

The Basset term is negligible if $\sqrt{\rho_1/\rho_2} \ll 1$ or if $Re \gg 1000$. When the initial Reynolds number $Re_* = \frac{|U_0| d \rho_1}{\mu}$ is large enough

($Re_* > 10000$), the hereditary term of Basset also can be neglected, because in this case, the sphere decelerates mostly with a Newtonian regime of flow about it, even if, at the end of the sphere run the Stokes regime is realized, provided that $\rho_1 / \rho_2 < 1$ (ref. 6).

In the B.B.O. equation, the drag value is :

$$C_x = 0.45 f_M \quad \text{assuming that}$$

$$M = \frac{U}{c} \left\{ \begin{array}{ll} M < 0.5 & \Rightarrow f_M = 1 \\ 0.5 \leq M \leq 1 & \Rightarrow f_M = 2.444 \frac{U}{c} - 0.222 \\ & \text{(linear approximation)} \\ 1 \leq M & \Rightarrow f_M = 2.222 \end{array} \right.$$

(M : Mach number, c : sound speed)

The f_M dimensionless parameter takes into account the supersonic flow motion, if any.

Finally, we get the sphere position by integration :

$$X(t) = \int_0^t U(\tau) d\tau$$

2) Figure 12 is a sketch of our proposed model of the sphere ablation (ref. 7). Very accurate results stem from this model.

In the sphere frame (gas velocity : $-U$), we have :

$$2\pi\rho_2 \left(\frac{d}{2} - \frac{\epsilon}{2}\right) \epsilon U dt = -\pi d^2 dr$$

with $d = 2r \geq 2\epsilon \geq 0$

(worn away mass equals sphere mass decrease)

$$\text{Therefore : } \frac{dr}{dt} = - \frac{(d-\epsilon)\epsilon U}{d^2} \text{ if } 2\epsilon < d$$

$$\text{and } \frac{dr}{dt} = 0 \quad \text{if } 2\epsilon \geq d$$

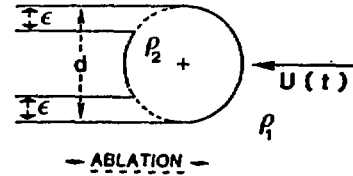


Fig.12

The sketch in the figure 12 has been chosen because the diameter of the wake behind the sphere is close to the sphere diameter. This occurs when a Newtonian regime of flow (first wakes regime) is realized about the sphere.

3) In order to calculate $\epsilon(t)$, we use the following relation :

$$\textcircled{1} \quad \left(\frac{\epsilon\rho_2}{d\rho_1}\right)^2 \text{Re} = \frac{\eta^2}{4}, \quad \eta \approx 63.497 \quad (\text{Re} = \frac{Ud\rho_1}{\mu})$$

The expression given in the relation $\textcircled{1}$ is a similarity factor for the hydrodynamic ablation flow. The ablation process stops when some geometrical conditions occur ($d \leq 2\epsilon$ for the Newtonian regime) or when the Stokes regime of flow about the sphere is realized, whatever the diameter value.

B) Stokes regime

$$\frac{|U| d \rho_1}{\mu} \leq 53.33$$

1) In this case, the $U(t)$ function also is solution to the simplified B.B.O. equation (ref.5), in the same way as in the Newtonian regime :

$$\frac{\pi}{6} d^3 \rho_2 \frac{dU}{dt} = -C_x \frac{\pi}{4} d^2 \rho_1 \frac{|U|U}{2} - \frac{1}{2} \frac{\pi}{6} d^3 \rho_1 \frac{dU}{dt} - \frac{3}{2} d^2 \sqrt{\pi \rho_1 \mu} \int_0^t \left[\frac{dU}{d\tau} / \sqrt{t-\tau} \right] d\tau$$

But, here, the value of the drag can be written

$$C_x = 24 \frac{\mu}{|U| d \rho_1}$$

and the hereditary Basset term can be neglected only if

$$\sqrt{\rho_1/\rho_2} \ll 1 \text{ (ref. 6).}$$

2) Assuming no ablation process in this case :

$$\frac{dr}{dt} = 0 \quad \text{or} \quad d = 2r \geq 2\epsilon = 0$$

The sphere diameter becomes therefore constant if the Stokes regime of flow is realized. In this Stokes regime there is no ablation process, because the wake behind the sphere is very small and ablation products are confined by the gas surrounding the sphere.

VII - COMPARISON WITH EXPERIMENTAL DATA

To obtain a good agreement between the physical model and the experimental data, three experiments were carried out. A 400 kbar shock wave moving in the tin sample (slab symmetry) will emerge, depending on the experiment,

- a) into argon at 8 bar initial pressure,
- b) into argon at 4 bar initial pressure,
- c) into air at 1 bar initial pressure.

The initial velocity of head ejecta was 1740 m/s. Into the argon, the shock front wave was in front of the head ejecta whereas in the air the shock front was at the back of the head of ejecta. One feature stands out : the value $\eta = 63.497$ fits well the experimental results.

GAS-PARTICLES INTERACTION STUDIES : Results with shadowgraphy

SUPERPOSITION OF EJECTA HEADS FOR THE DIFFERENT EXPERIMENTS

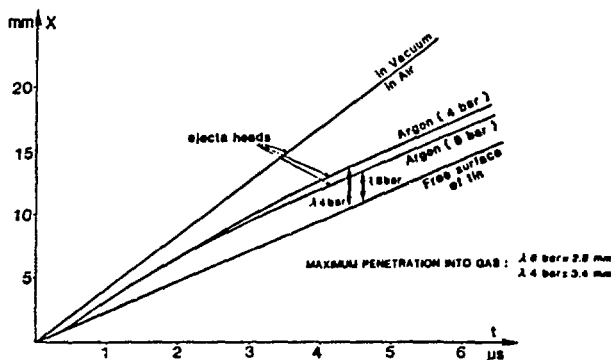
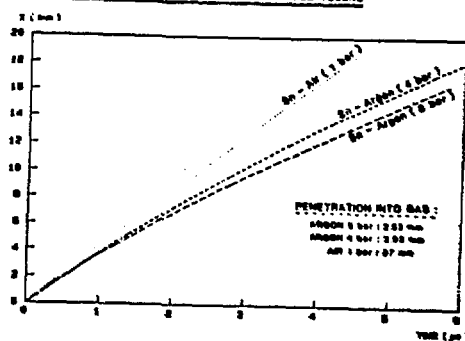


Fig.13

Fig.14

EJECTA HEADS POSITION : Theoretical results



All the numerical results were computed by the means of a Fortran program based on our physical model (finite differences method to equations integration).

The next figure points out how the diameters of the spheres are varying, due to the ablation.

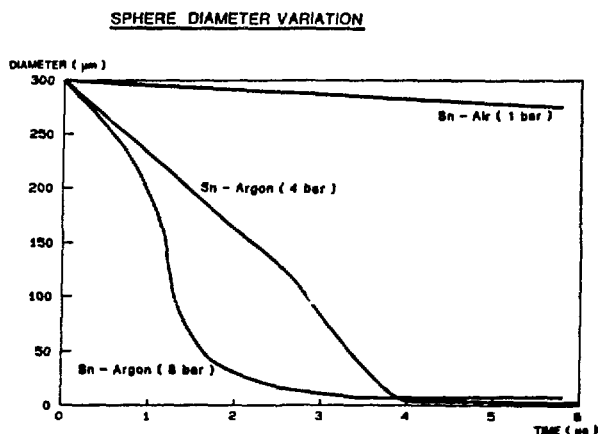


Fig.15

VIII - CONCLUSION

More experiments are scheduled in order to get our model valid in the largest domain. To reach this goal we will also modify some assumptions in a more sophisticated way to obtain numerical results closer to the experimental ones.

The authors wish to thank P. CHAPRON, M. DULON, P. ELIAS, J.P. GEX, J.L. ROUHCICCIOLI and T. TIFFEAU for their suggestions, comments and technical support concerning this study.

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A PERSONAL VIEW ON HOMOGENIZATION

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It has become quite difficult to give a complete view of a field which, almost unknown in most mathematical circles 15 years ago, has grown to such an extent that one begins to feel the need for good books of exposition summarizing all the preceding work. A fair description of all the aspects of homogenization would be impossible to consider in such a reduced space, but the field can certainly be well attacked with the basic set of references [1] to [6] : two books specialized in the periodic case, one by A. BENSOUSSAN, J.L. LIONS and G. PAPANICOLAOU [2] and one by E. SANCHEZ-PALENCIA [3], one summer school on homogenization [5] and three conferences dedicated to the questions of inhomogeneous or disordered media and homogenization from either a physicist or a mathematician point of view [1], [4] and [6].

I want to describe here the evolution of some ideas which I have encountered or introduced in the field. Although some technical results may be described in an impersonal way if they can be derived from basic methods by anyone who is asked to perform them, ideas should be tied to persons : the field has developed mostly through the interactive work of a small group of specialists, and I prefer a personal point of view on these questions (that many will find biased) to the kind of impersonal compilation of articles that library oriented people prefer, who often forget to quote the author of ideas that they have heard, sometimes directly, with the fallacious pretext that they have not been printed yet.

Evolution of some ideas

Under the name homogenization are collected all the mathematical results who help understanding the relations between the microstructure of a material and its macroscopic properties. Although such a goal has been the concern of physicists for a long time, it is only recently that mathematicians have found different ways to attack this kind of questions : indeed, if the notion of effective coefficients has been discussed at length by physicists, it is difficult to find a precise mathematical definition of what is meant by this term. There were some mathematicians, like J.B. KELLER, who did understand what it was and attacked the question using probabilistic ideas, but the earlier mathematical result in a non probabilistic setting

seems to be due to S. SPAGNOLO (1967). His work was not motivated by any application and was concerned by an abstract problem of convergence of Green's functions for second order elliptic equations : it was then called G-convergence. An Italian school grew then, under the scientific influence of E. DeGIORGI, more concerned with convergence questions than with application of these ideas to continuum mechanics and physics; an account of this different point of view and of the related notion of Γ -convergence can be found in the book of H. ATTOUCH [7].

In France the first mathematical results in that direction were made by F. MURAT (1970); he was looking at an academic question of optimization where one controls the coefficient of a second order elliptic equation and he also found strange phenomena concerning the convergence of minimizing sequences. Interested by his results, I started collaborating with him on that question, and after solving a more general problem we became aware of the Italian school and of the interpretation of relating microscopic and macroscopic quantities in some articles of E. SANCHEZ-PALENCIA, who was using the approach of multiscale expansions. We did not write much of our results but, although we had no knowledge of specific problems, we were motivated mostly by optimal design questions. After these early results I tried to understand applications to physics because I could describe the question of the relation between microscopic and macroscopic levels with the mathematical tool of weak convergence. I thought at that time that physicists had not understood this question of homogenization because we had found that they were concerned with giving an effective conductivity coefficient for a mixture of two isotropic materials in term of the proportions used and this was in contradiction with our results : a mixture could be anisotropic and (except in one dimension) the effective conductivity tensor could not be determined from the knowledge of the proportions alone. We had obtained very simple bounds on the effective coefficients at the time but we were not yet able to characterize the materials that could be obtained by mixing two different isotropic materials. During a stay in Madison (1974-75), I simplified the proofs, mostly by a repeated use of the div-curl lemma that I had just found with F. MURAT, and found references about other approaches by G. PAPANICOLAOU, who used a probabilistic framework, and by J.B. KELLER who had worked in that field for some time then. I was also told about the work of I. BABUSKA who was concerned with some applications in engineering, and when I came back to France I found that J.L. LIONS was working with A. BENSOUSSAN and G. PAPANICOLAOU in situations with periodic microstructure. The book that they wrote later ([2]) is a basic reference for the periodic setting, but from my point of view the assumption of periodicity was unnecessary; indeed, in order to prove the convergence of some of the formal expansions obtained by the multiscale approach, they often had to use the simplifying ideas that I had derived for the general case (they quoted my ideas as an energy method, which is inappropriate). In a series of lectures in Paris in 1977 I had

discussed of different improvements that I had made from the initial work with F. MURAT, but the corresponding notes of this "cours Peccot" were never written; one can sometime find references to it which show that some later improvements had their roots in this course which contained the basic tools for other cases, like domains with holes and some nonlinear problems. F. MURAT did write some part of the homogenization results in a similar course and coined the denomination H-convergence to describe my approach to these questions. My main idea was that homogenization problems were explained through the repeated use of a general argument that F. MURAT and myself had obtained as an improvement of our div-curl lemma : he had called it compensated compactness, but, as it became clear to me later, this was the first draft of what should become a general theory of oscillations in nonlinear partial differential equations [8]. Having still a lot of open questions to solve in our approach of optimal design, F. MURAT and myself were alone avoiding the periodicity assumptions used by most of the french school.

Obtaining better bounds on effective coefficients was one of my main concern, and I devised a method based on compensated compactness which required to guess quite technical quadratic quantities and it was only in 1980 that I found the way to apply it to bound the effective conductivity of isotropic mixtures; as I was visiting New-York, I immediately learned from G. PAPANICOLAOU and R. KOHN of earlier bounds obtained by Z. HASHIN & S. SHTRIKMAN (1962). I realized the extent of what physicists "knew" on the question ([1]) and heard for the first time about the ideas of D. BERGMAN. Indeed these bounds were the same than mine, but the first part of their argument could hardly be considered as a proof (their intuition was good, indeed, but it is only recently that R. KOHN & G. MILTON have been able to write a complete proof following the same lines); the second part of their paper showed that the bounds were optimal and they used a classical formula for a sphere imbedded in a uniform medium : this part was easy to transpose to my setting and this concluded my proof of the characterization of the isotropic materials that could be obtained by mixing two isotropic materials with given proportions (in any dimension). I tried then to generalize that characterization to anisotropic mixtures with F. MURAT, and the main technical difficulty was overcome by explicit formulas for ellipsoids, which appeared to be linked to ellipsoidal coordinates. I presented the result at a meeting in New-York ([4]), but wrote the details only much later ([9]). The characterization that I had found with F. MURAT was the conclusion of a research related to optimal design questions and, beginning to overcome difficulties in writing, we finally published our first joint paper in [5]; by that time we knew that another group had found that optimal design problems could often have no classical solution because of an homogenization effect and that some kind of mixture could be optimal : in Leningrad, LUR'IE and his coworkers had discovered some paradoxes in studying more realistic situations from an engineering point of view. This is an application

of homogenization techniques which is now receiving more attention ([4],[6]).

There were precise formulas expressing the effective coefficients in the periodic case (that were often quoted as explicit) which consisted in solving a few boundary problems on a period cell; the only situation known (for a diffusion equation) where everything could be written explicitly was related to our computation for confocal ellipsoids, which contained as particular limiting cases both concentric spheres and plane layers. However there were some situations where the effective coefficient could be computed, because of symmetries, without any knowledge of the internal field in the composite material : the earlier remark of this kind, due to J.B. KELLER (1964), shows that an infinite checkerboard made with two isotropic material is macroscopically isotropic and that its conductivity is the geometric mean of the two conductivities. Following the ideas of D. BERGMAN ([1], [5]) it was then classical, when discussing the effective properties of a mixture, to fix the geometry of the different interfaces and to consider the conductivities of the different components used as many parameters; D. BERGMAN was considering a global quantity, like the stored energy, and he noticed that his function could be extended to complex values of the parameters and was satisfying some special properties which enabled him to use some representation theorem (for one complex variable, the basic property is to map the upper half plane into itself, referred as Herglotz's property; it leads, by Cauchy's representation theorem, to Stieltjes functions and there is a close connection with questions of Padé approximants). In 1982, I discussed with many of the idea that functions "à la Bergman" could create a new mathematical tool that will enable to study completely both evolution of mixtures and instabilities of interfaces. The first step in this direction was to define a local matrix valued function in the spirit of the global scalar function used by D. BERGMAN and, although we did not write the details then, I discussed with F. MURAT about it : it was easy to do the abstract part from what we knew, but there were technical difficulties due to the matrix setting and we did not know any analogous representation theorem that could help us. Anyway our program of studying the materials that could be created by mixing precise quantities of given constituents, became concerned with characterizing the "generalized Bergman's functions" (in the scalar case G. MILTON had characterized the two-dimensional case corresponding to mixing two materials).

A formula for layers had been known for a long time : F. MURAT had obtained it in his early work and I had taught how to write it in a more intrinsic way when layering arbitrary materials in arbitrary directions. Although I thought that our construction of ellipsoids could hardly be avoided, I was quite surprised when P. BRAIDY and D. POUILLoux showed (1982) that the same materials could be obtained by iterated layers in orthogonal directions; unexpectedly, their material had the same Bergman's function than the one made with coated ellipsoids. A year later, I discovered a better way to look at the formula for layers. I first used the formula that I knew

to compute the differential variation of the conductivity tensor when one adds an infinitesimal layer of a material with general conductivity tensor A in an arbitrary direction e ; this argument gave me a differential equation (each choice of A and e defining a vector field in the space of matrices) which, by integration gave me a formula for layers (equivalent to the one I knew, of course) which had the advantage of a better analytic form which made reiteration easy and this gave a generalization of the construction of P. BRAIDY and D. POUILLOUX (who had assumed a common basis of eigenvectors for the two materials that they were mixing, as did, independently, LUR'IE and his collaborators). After discussing it with R. KOHN, I realized that there was a quicker way to obtain the result and I wrote a few months later the details of this simplified approach [9]. Meanwhile I had discussed with G. MILTON who had, independently, used the same differential idea in his constructions related to the effective medium theory and I thought of using my approach (which was more general) to understand more on the construction of the "generalized Bergman's function" : I had noticed that the reiteration of the formula for layers could be done at the level of the differential equation that I had obtained and this was a classical relaxation process "à la Pontryaguin" when one understood the construction of new composite materials as traveling in the space of matrices (with a mathematically oriented mind, I did not assume that my conductivity tensors were symmetric, which I thought to be non physical until I found in a paper of D. BERGMAN that this happened in the Hall effect). For each choice of A and e , one had a vector field in the space of matrices and jumping from one vector field to another at high frequency made possible to go in an average direction, described at a mathematical level by a probability measure "à la L.C. Young" with support in the set of matrices A corresponding to the materials at our disposition and the set of unit vectors e . In his construction, G. MILTON gave the same weight to all vectors e (which is the case of the formula for concentric spheres) and, as he was interested in mixing two materials with proportion θ and $(1-\theta)$, the answer he had found appeared to be the stationary solution corresponding to my average vector field associated to a combination of Dirac masses. I could easily generalize with an arbitrary probability measure, but remarked that stationary solutions of my average (in A, e) differential equation could not span all the materials that could be constructed; I thought of using periodic solutions instead of only constant ones and I conjectured that they would give the characterization that I was looking for. As the differential equation that I had obtained was of Riccati type, for which some algebraic properties are known, I thought that this would end in very explicit formulas but I could not conclude. This was the extent of what I knew in May 1985 when I openly presented this last idea in discussing some question in nonlinear elasticity (I believe that understanding connections between different questions studied at the moment is the clue for developing a new mathematical tool that will unify these apparently unrelated questions.

The model problem

The mathematical models considered are systems of partial differential equations, supposed to describe some properties at a scale ϵ , and we want to understand what will happen to the solutions if ϵ tends to 0. More generally one considers oscillating solutions of some classical equation and try to describe the limits of different quantities. This leads first to prove some results that have been accepted for a long time and then to identify more delicate situations where the answer, when the mathematician finally obtains it, can differ from the rules that physicists have been using. It should not be forgotten that the more important open problems are related to hyperbolic equations, but for reasons of limited space, and because it is still necessary to simplify the mathematical results obtained, we will only consider a diffusion equation, where the temperature θ^ϵ satisfies

$$(1) \quad \left\{ \begin{array}{l} - \sum_{i,j} \frac{\partial}{\partial x_i} (K_{ij}^\epsilon(x) \frac{\partial \theta^\epsilon}{\partial x_j}) = 0 \text{ in } \Omega \\ \theta^\epsilon(x) = T(x) \text{ given on the boundary of } \Omega. \end{array} \right.$$

The tensor K is symmetric positive (κI for an isotropic material) and ϵ is a positive parameter which will tend to 0 : a typical problem of homogenization corresponds to rapid variations of K in x with a characteristic length ϵ , for example

$$(2) \quad K_{ij}^\epsilon(x) = c_{ij}(x, \frac{x}{\epsilon}) \text{ with } c(x, y) \text{ periodic in } y \text{ (period cell denoted by } Y).$$

As one expects, θ^ϵ converges, as ϵ tends to 0, to a fonction θ^0 , but its derivatives only converge weakly (the analog of taking the mean value in y in case (2)). θ^0 is the temperature in a material having a conductivity tensor K^0 which presents slow variations with respect to x , and the main difficulty is to understand what are the weak limits of terms like $K_{ij}^\epsilon \frac{\partial \theta^\epsilon}{\partial x_j}$. In case (2) there are formulas for "computing" $K^0(x)$, corresponding to the harmonic mean in dimension 1

$$(3) \quad \kappa^0(x) = \left(\frac{1}{Y} \int_0^Y c(x, y)^{-1} dy \right)^{-1},$$

but not as simple in dimension greater. If $K^\epsilon(x) = \kappa^\epsilon(x)I$, then $K^0(x)$ need not be of this form so one of the goal of the mathematical theory of homogenization is to identify types of equations which are stable for some convergences like weak convergence. K^0 is not obtained by averaging simple functions of K^ϵ , although one does find formulas in books giving properties of mixtures in term of proportions : in

dimension greater than 1 such formulas are wrong from a mathematical point of view, but they can be quite accurate from a practical point of view because they are approximations obtained under some kind of information upon the repartition of the constituents (which is rarely explicit or replaced by an invocation to randomness). In case (2) one obtains K^0 by solving a few partial differential equations on the period cell Y . For x fixed and a vector λ of R^N , one seeks a function w_λ satisfying

$$(4) \quad \left| \begin{array}{l} - \sum_{i,j} \frac{\partial}{\partial y_i} (c_{ij}(x,y) \frac{\partial w_\lambda}{\partial y_j}) = 0 \\ w_\lambda - \lambda \cdot y \text{ periodic on } Y, \end{array} \right.$$

and $K^0(x)\lambda$ is given by the formula

$$(5) \quad (K^0(x)\lambda)_i = \frac{1}{|Y|} \sum_j \int_Y c_{ij}(x,y) \frac{\partial w_\lambda}{\partial y_j} dy$$

where $|Y|$ is the volume of the period cell Y . For a given x , $K^0(x)$ is known from the solutions for N independent λ (symmetries often simplify these computations). Then

$$(6) \quad \left| \begin{array}{l} K_{ij}^\varepsilon(x) \frac{\partial \theta^\varepsilon}{\partial x_j} \rightarrow (\text{weakly}) \frac{1}{|Y|} \int_Y c_{ij}(x,y) \frac{\partial}{\partial y_j} w_{\lambda(x)} dy \\ \text{with } \lambda(x) = \text{grad} \theta^0(x), \end{array} \right.$$

so in general $K_{ij}^\varepsilon \frac{\partial \theta^\varepsilon}{\partial x_j}$ does not converge to $K_{ij}^0(x) \frac{\partial \theta^0}{\partial x_j}$ for each j , although

$$(7) \quad \sum_j K_{ij}^\varepsilon(x) \frac{\partial \theta^\varepsilon}{\partial x_j} \rightarrow (\text{weakly}) \sum_j K_{ij}^0(x) \frac{\partial \theta^0}{\partial x_j}$$

and

$$(8) \quad \sum_{i,j} K_{ij}^\varepsilon(x) \frac{\partial \theta^\varepsilon}{\partial x_j} \frac{\partial \theta^\varepsilon}{\partial x_i} \rightarrow (\text{weakly}) \sum_{i,j} K_{ij}^0(x) \frac{\partial \theta^\varepsilon}{\partial x_j} \frac{\partial \theta^\varepsilon}{\partial x_i}.$$

Without going into the details or the physical interpretation of these results, we want to notice that they rely on the fact that the vector fields $E^\varepsilon = -\text{grad} \theta^\varepsilon$ and $D^\varepsilon = K^\varepsilon E^\varepsilon$ are such that $\text{curl } E^\varepsilon$ and $\text{div } D^\varepsilon$ are (bounded) square integrable functions;

the definition of w_λ has analogies with experimental methods for "identifying" K^0 .

Layered media

If the coefficients only depend of one variable, say x_1 , the effective coefficients are obtained by simple weak limits (averages in y in case (2)) : here

$$(9) \quad \left\{ \begin{array}{l} (K_{11}^E)^{-1} \rightarrow (\text{weakly}) (K_{11}^0)^{-1} \\ K_{1j}^E (K_{11}^E)^{-1} \rightarrow (\text{weakly}) K_{1j}^0 (K_{11}^0)^{-1} \\ K_{i1}^E (K_{11}^E)^{-1} \rightarrow (\text{weakly}) K_{i1}^0 (K_{11}^0)^{-1} \\ K_{1j}^E - K_{i1}^E K_{1j}^E (K_{11}^E)^{-1} \rightarrow (\text{weakly}) K_{1j}^0 - K_{i1}^0 K_{1j}^0 (K_{11}^0)^{-1}. \end{array} \right.$$

and this is valid without symmetry assumptions on K . If the material used are isotropic, the effective material is anisotropic (with partial isotropy in $x_2, \dots, x_N$) : K_{11}^0 is the harmonic mean of the κ^E , K_{jj}^0 the arithmetic mean for $j \neq 1$ and all others coefficients are zero (notice that the geometric parameter of the direction of the layers cannot be deduced from the proportions used). Formula (9) consists in performing three successive operations : first a nonlinear mapping which transforms the tensor K into a list of quantities, here $(K_{11})^{-1}$, $K_{1j}(K_{11})^{-1}$, $K_{i1}(K_{11})^{-1}$, and $K_{1j} - K_{i1}K_{1j}(K_{11})^{-1}$; then a linear operation of weak limit (integrating in y in case (2)); finally the reciprocal transformation of the one used in the first step. This is an example of a general algorithm for layered media (for elliptic systems, not necessarily linear) which uses here only the information that curl E and div D are square integrable functions : it implies that the components of the vector $V_c = (D_1, E_2, \dots, E_N)$ cannot oscillate while those of the vector $V_d = (E_1, D_2, \dots, D_N)$ may; writing the constitutive law $D = KE$ in the equivalent form $V_d = MV_c$, defines a nonlinear mapping Φ which associates M to K and the formula for the layers says that $\Phi(K^E)$ converges weakly to $\Phi(K^0)$. Mixing two materials of conductivity tensors A and B with proportions θ and $(1-\theta)$ in layers perpendicular to an arbitrary vector e , produces an effective tensor $B(\theta)$ given by

$$(10) \quad B(\theta) = \theta A + (1-\theta)B - \theta(1-\theta)(B-A) \frac{e \otimes e}{\theta(Be \cdot e) + (1-\theta)(Ae \cdot e)} (B-A)$$

which can be written as

$$(11) \quad (B(\theta)-A)^{-1} = \frac{(B-A)^{-1}}{1-\theta} + \frac{\theta}{(1-\theta)} \frac{e \otimes e}{(Ae \cdot e)},$$

a formula more adequate for adding successive layers in different directions e , but with the same material A . An infinitesimal layer leads to the differential equation

$$(12) \quad \frac{dB}{d\theta} = A - B - (A-B) \frac{e \otimes e}{(Ae \cdot e)} (A-B),$$

which enables to add layers in any direction e with any material A . Each (e, A) defines a vector field in the space of matrices and, by a classical relaxation process (following ideas of L.C. Young and Pontryaguin) one can approach an averaged field

$$(13) \quad \frac{dB}{dt} = F(t, B) = (\mu^t, A - B - (A-B) \frac{e \otimes e}{(Ae \cdot e)} (A-B))$$

where μ^t is a probability measure in (e, A) . If μ^t is independent of t , the stationary points of (13), solutions of $F(B) = 0$, play an important role; in a similar way, if μ^t is periodic, one can consider the periodic solutions of (13) who take values B which can be constructed with the different materials A used by the measures μ^t , with proportions that can be easily computed from the μ^t .

Bounds on effective coefficients

In dimension greater than 1 the knowledge of proportions cannot characterize the effective conductivity tensor and it is important to know precise bounds. Let us denote by $K^-(x)$ and $K^+(x)$ the harmonic and arithmetic means

$$(14) \quad (K^E(x))^{-1} \rightarrow (\text{weakly}) (K^-(x))^{-1} ; K^E(x) \rightarrow (\text{weakly}) K^+(x)$$

which are average resistivity and conductivity tensors, and give bounds for K^0

$$(15) \quad K^-(x) \leq K^0(x) \leq K^+(x).$$

In the isotropic case, we have scalar functions $\kappa^-(x)$ and $\kappa^+(x)$ and the eigenvalues of $K^0(x)$ fall between $\kappa^-(x)$ and $\kappa^+(x)$ (in the case of layers one eigenvalue is $\kappa^-(x)$ and the others are $\kappa^+(x)$). The matrix $K^0(x)$ also satisfies some other inequalities, but the question of finding the optimal bounds for $K^0(x)$ is not understood in general. For two isotropic materials of conductivity α and β (with $\alpha < \beta$) we use the local proportion θ of the material of conductivity α so that

$$(16) \quad \kappa^-(x) = \frac{\alpha\beta}{(1-\theta(x))\beta + \theta(x)\alpha} ; \kappa^+(x) = (1-\theta(x))\alpha + \theta(x)\beta,$$

and the eigenvalues $\lambda_j^0(x)$ of the effective matrix $K^0(x)$ must satisfy

$$(17) \quad \left| \begin{array}{l} \kappa^-(x) \leq \lambda_j^0(x) \leq \kappa^+(x) \text{ for all } j \\ \sum_1 \frac{1}{\lambda_1(x) - \alpha} \leq \frac{1}{\kappa^-(x) - \alpha} + \frac{N-1}{\kappa^+(x) - \alpha} \\ \sum_1 \frac{1}{\beta - \lambda_1(x)} \leq \frac{1}{\beta - \kappa^-(x)} + \frac{N-1}{\beta - \kappa^+(x)} \end{array} \right.$$

These inequalities are optimal and, in order to express the result when the effective material is isotropic, we use the following quantity $E_N(\gamma, \delta; \eta)$, which is linked to the case of spherical inclusions of an isotropic material of conductivity γ imbedded, with proportion η , into a material of conductivity δ (in dimension N)

$$(18) \quad \frac{E_N(\gamma, \delta; \eta) - \delta}{E_N(\gamma, \delta; \eta) + (N-1)\delta} = \eta \frac{\gamma - \delta}{\gamma + (N-1)\delta}.$$

If all the $\lambda_j(x)$ are equal to $\kappa^0(x)$ one obtains

$$(19) \quad E_N(\beta, \alpha; 1-\theta(x)) \leq \kappa^0(x) \leq E_N(\alpha, \beta; \theta(x))$$

which are the classical bounds of Z. HASHIN and S. SHTRIKMAN, attained in the case of concentric spheres, while the anisotropic bounds (17) are attained by confocal ellipsoids; using different variational principles, which express the fact that the solution of (1) minimizes some functional, one can obtain other bounds on the effective conductivity which take into account more information than the proportions used. D. BERGMAN has developed the idea of changing the conductivities while keeping the same microgeometry (see [1],[4],[5],[6], where one will also find the related work of G. MILTON) : if one takes $\alpha = 1$, $\beta = z$, and assumes that the effective material is isotropic with tensor $B(z)I$ (it does not depend on x if the coefficients are periodic) the main remark is that B can be extended to the complex plane with a cut on the real negative axis into a holomorphic function mapping the upper half plane into itself, allowing a representation

$$(20) \quad B(z) = b_0 + b_\infty z + \int \frac{d\mu(t)}{t - z}$$

where b_0 and b_∞ are nonnegative and $d\mu(t)$ is a nonnegative measure with support in $(-\infty, 0]$. In dimension 2, B is also constrained by the identity $B(z)B(1/\bar{z}) = 1$. One

has $B(1) = 1$, $\frac{dB}{dz}(1)$ is the proportion of the material of conductivity z , and the Taylor expansion at 1 can be obtained from correlations (multiple integrals in case (2)). If one transforms all the information into constraints on B , it usually determines a convex set for the unknown $(b_0, b_\infty, d\mu)$; the best estimates for the value of $B(z_0)$ is obtained from an optimization problem whose solution is usually given by a rational fraction (with formulas similar to Padé approximants). Finally, we will notice that the differential equation (13) enables to compute a "generalized Bergman's function" but a lot remains to be done in that direction.

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TURBULENCE THEORY FOR MATERIAL MIXTURES

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ABSTRACT

Normal acceleration and/or tangential slippage at a deformable material interface can result in the unstable amplification of perturbations, the creation of turbulence, and considerable mixing of mass, momentum, and energy. When the mixing layer has grown to thicknesses large compared with the initial perturbation amplitude, the initial conditions become irrelevant and the development proceeds in a simple, self-similar fashion.

Analysis of these processes can be accomplished by a two-field (interpenetrational) approach or, more generally, by means of single-field turbulence transport theory for a material with large density variations. In the limit of ordered, well-defined interpenetration of distinctly separate entities, the turbulence equations must approach two-field theory as an idealization, thereby partially guiding closure derivations for the more general representation. Challenges to closure are also partially resolved through the derivation of transport equations for the most important of the difficult terms, for example, to describe mass flux and root-mean-square density fluctuations.

Much of the necessary theory for these and related analyses has been derived and tested by means of analytical and numerical solutions. Potential applications include the problem of mixing in ICF capsule implosions and investigation of impedance for shock-induced slippage at gas-metal interfaces.

INTRODUCTION

Fluid dynamic instabilities can occur whenever there is an excess of large-scale energy in the coordinate system of mean flow. If this excess energy is kinetic, then it may transform directly to heat, provided that viscous dissipation is sufficiently large; the creation of disordered energy is immediately manifested at the smallest possible scale, that of molecular fluctuations. More commonly this inevitable transition from order to disorder takes place through an intermediate set of length scales; turbulence eddies are formed and the energy cascades through a progression of smaller and smaller sizes on its way toward the purely molecular fluctuations.

When turbulence occurs, the mean-flow profiles of mass, momentum, and energy density can be profoundly altered. In particular, we investigate turbulence and its effects near an interface between two different mean-flow states. In Kelvin-Helmholtz (KH) circumstances, the interface separates materials with different tangential components of mean-flow velocity; in addition, the materials may have different properties such as density and/or compressibility. In the Rayleigh-Taylor (RT) case the two materials necessarily have different densities and the instability is driven by the component of pressure gradient normal to the interface. In neither case need the interface be sharp; the essential ingredient is the presence of large-scale energy (kinetic or potential, respectively) that can be transformed (through the amplifying forces of instability) to small-scale, less-ordered, motion.

Classic Rayleigh-Taylor instability is driven by higher pressure on the side with lower density. Generation of this driving force is usually initiated by the propagation of compression or expansion waves to the boundary from nearby walls. With walls at rest the application of a body force (e.g., gravity) is sufficient to initiate these waves, which for incompressible fluids reach the interface "instantaneously" and maintain a persistent pressure gradients. Shocks and large-jump rarefaction

waves (e.g. from rapidly moving walls) create, in contrast, one or many pressure-gradient impulses of relatively brief duration.

Linear stability analysis for a sharp interface between two incompressible fluids shows that when the larger pressure is on the side of the fluid with higher density, the interface stability is exactly neutral in the absence of dissipation; any surface waves merely slosh about without change in amplitude. If, however, the pressure gradient were abruptly removed at some particular phase of the sloshing, the velocity field existing at that moment would thereafter persist, and the amplitude would coast with that velocity field. If the amplitude were decreasing at that moment, it would coast through zero and thereafter grow with reversed phase, linearly in time, to arbitrarily large reversed amplitude (actually brought eventually to rest by dissipation). This is one subset of the Rayleigh-Taylor case called Richtmyer-Meshkov (RM) instability.

Richtmyer-Meshkov instability in its current meaning more typically refers to behavior following shock passage from the denser side to the lighter side. The brief but strong pressure gradient simply initiates coasting growth with a change of phase from the initial perturbation. The finite duration of a rarefaction wave passing from the lighter to heavier side accomplishes a similar behavior, but the phase and speed of the coasting growth depend on these properties at the instant of pressure gradient termination and not directly on the initial phase itself.

Low-amplitude behavior for these various circumstances is amenable to linear stability analysis in some interesting but idealized cases, showing that KH and RT instabilities grow exponentially in amplitude with a time scale that depends strongly on the wavelength of the perturbation. Nonlinear effects, however, alter the exponential growth rate as soon as the amplitude exceeds some fairly small fraction of the wavelength. Assuming a constant pressure gradient, a constant value for the dominant wavelength and no "disruptive" mechanism, RT instability would grow to

a "spike-and-bubble" stage, in which the heavier fluid penetrates the lighter with constant acceleration and the lighter penetrates the heavier in broad-nosed bubbles at a fixed terminal speed. In reality, however, the bubbles coalesce into successively larger structures, the spikes are broken and/or laterally deflected, and growth of the mixing layer takes place with constant acceleration in both directions. (A simple heuristic calculation shows how this accelerative bubble motion takes place. With form drag, it is easily shown that a spherical object whose radius grows in proportion to the distance it has traveled will forever accelerate with a constant fraction of the body-force acceleration.)

KH instability exhibits a similar late-stage nonlinear behavior. Perturbations at a given wavelength can draw energy from the mean flow only as long as the mixing-layer width does not greatly exceed that wavelength. Thus, a continuously expanding mixing layer preferentially feeds energy into a succession of larger and larger wavelengths with an effect similar to that of bubble coalescence in the RT case. In both circumstances, the late nonlinear growth phase proceeds in a self-similar manner that is completely independent of the initial perturbations.

The nature of this self-similarity can be expressed for the RT case as

$$W = g t^2 f_{RT} \left(\frac{x}{g t^2} \right),$$

and for the KH case as

$$W = U_o t f_{KH} \left(\frac{x}{U_o t} \right),$$

in which W is the width of the turbulent mixing zone, g is the body-force acceleration (e.g., the ratio of pressure gradient to density), U_o is the jump in mean-flow velocity

across the interface, x and t are space and time coordinates, and the f 's are "universal" functions of their arguments. The RM case is like that of the KH circumstance, with U_0 being the velocity carried by the perturbation at the end of the accelerative impulse.

The transition from exponential growth to self-similar behavior is of great interest. It determines the time required for initial conditions to become irrelevant, which can, indeed, be very short for such physical circumstances as capsule collapse in laser-driven inertial-confinement fusion (ICF). It also is of considerable significance in initiating the finite-difference representation of material interfaces for numerical calculations of material mixing.

THEORETICAL ANALYSIS

There are two very different approaches to the solution of interface turbulence problems. One uses the equations for multiphase interpenetration of two materials, supplemented by turbulence transport equations that represent the diffusive effects of disordered fluctuations. The other [1] is based on the turbulence transport equations for a single field, with the two-material properties represented by a concentration or "color" variable [2] (e.g.; salt, gaseous species, heat, or dust). Despite their very different appearance, these two approaches are, in principle, identical; however, in practice it is a formidable task to demonstrate this equivalence. Each approach requires some degree of empiricism and heuristic reasoning to be put into tractable form, and each relies to some extent on the other in development of the formulation. The multiphase representation is helpless to describe the disordered effects without the introduction of variables that represent the Reynolds stress and turbulence length scale, together with transport equations to describe their evolution [3]. One-field modeling likewise relies on the ordered-penetration of two-field theory to guide moment closures for that limiting part of the dynamics.

Considerable progress has been made from the multiphase viewpoint [3,4]. The emphasis for our current work, however, is on the single-field turbulence-transport approach. The foundation for this development lies in the theory of turbulence transport for a single incompressible fluid with density that is constant in both position and time [2]. To extend this work it has been sufficient to restrict our analysis to fluids with far subsonic fluctuations in velocity, not requiring, however, that the mean flow necessarily be subsonic. (For some problems this restriction will have to be removed, for example, in circumstances of strongly supersonic slip between two materials.) Thus, the microscopic density of an element of fluid along the path of its motion changes only as a result of mean-flow compression or expansion, and/or as a result of the molecular-scale exchange of concentration or color with adjacent elements.

In comparing multiphase theory with single-field turbulence transport theory, it is important to note that orderly bi-directional interpenetration of two materials is an idealization that occurs in nature only if the local Reynolds number based on entity size is sufficiently small ($Re \leq 1$ or so). For larger Reynolds numbers, the turbulent part of two-phase flow includes both fluctuations at the entity scale and larger-scale fluctuations resulting from the intrinsic instability that draws energy from the drag decay of interpenetrational energy [3]. It is crucial to the single-field turbulence representation of two-phase flow, however, that even the "orderly" bi-directional part of the interpenetration be included in that part of the overall energy that we attribute to the turbulence. Thus, the fluxes of mass, momentum, energy, and concentration calculated from our turbulence approach necessarily include both an "ordered" part and a "disordered" part to the closure of each transport moment. Only the latter bears close relationship to the diffusional closures of the other constant-density turbulence transport theories.

THE TURBULENCE TRANSPORT EQUATIONS

The starting point for the theory is the set of Euler equations for a single fluid with variations in density that are much too large for the Boussinesq approximation. The primary field variables are ρ , the mass density; m_i , the momentum density; p , the pressure; and c , the concentration. A derived variable that requires careful consideration is the velocity, $u_i \equiv m_i/\rho$. To proceed, the primary variables are split into their mean and fluctuating parts, in which mean denotes the average over an ensemble of realizations, and the fluctuations signify departure of the individual members of the ensemble.

$$\rho \equiv \bar{\rho} + \rho'$$

$$m_i \equiv \overline{m_i} + m_i'$$

$$p \equiv \bar{p} + p'$$

$$c \equiv \bar{c} + c'$$

Velocity can likewise be split in this manner, with

$$u_i \equiv \overline{u_i} + u_i'$$

but a more meaningful definition of mean velocity is that which carries the observable momentum, so that we often work with

$$\tilde{u}_i = \overline{m_i} / \bar{\rho} .$$

It is important to note that $\bar{u}$ and $\bar{u}_i$ are usually not equal, becoming the same only in the absence of turbulence or in the case of constant density in both space and time.

Insertion of this decomposition of field variables into the Euler equations results in mean-flow equations that are modified by an appropriately generalized Reynolds stress,

$$R_{ij} \equiv \overline{m_i m_j} / \bar{\rho} - \bar{m}_i \bar{m}_j / \bar{\rho} .$$

As in the classic theories of turbulence transport, the dynamics of R_{ij} itself can likewise be derived from the Euler equations, immediately introducing a variety of closure challenges. These in turn are met through the use of various additional modeling derivations, postulates, or transport equations. A version of this procedure has been described by Andronov, et al. [2]; for small-density variations, some similar procedures were presented by Chen and Nikitopolous [5], Lumley [6], and Mellor and Yamada [7].

In our current version of the theory, our primary transported variables are R_{ij} (the generalized Reynolds stress), D_{ij} (the loss rate from cascade to small-scale turbulence), $A_i \equiv \overline{\rho' u_i'}$, the mass flux relative to a coordinate system moving with a mean velocity u_i such that $\bar{\rho} u_i \equiv \bar{\rho} \bar{u}_i + A_i$, and $B \equiv \overline{\rho' \rho'}$ (a measure of the density fluctuation from one to another of the large-scale turbulence eddies). Often we introduce a length scale, s , for the largest eddies, and use this in an approximation from which D_{ij} can be estimated.

APPLICATION TO INTERFACIAL TURBULENCE

Consider the case of one-dimensional spatial variation in the mean-flow quantities, for example, along the interface normal in RT and KH circumstances. Let this

direction be x and the time, t . For the RT case, the significant variables are $\bar{\rho}$, $\bar{u}$, $\tilde{u}$, s , and

$$k_{\parallel} \equiv R_{xx} / \bar{\rho}$$

$$k_{\perp} \equiv (R_{yy} + R_{zz}) / \bar{\rho}$$

$$a_x \equiv A_x / \bar{\rho}$$

$$b \equiv B / \bar{\rho}$$

Thus the variables have dimensions of density, velocity, and (velocity)². For the KH case we also have $k_{xy} \equiv R_{xy} / \bar{\rho}$, in which it is assumed that the mean-flow velocity jump, U_0 , takes place in the y direction. If the two materials in the KH case have the same density, then $a_x \equiv 0$ and $b \equiv 0$.

The self-similar behavior is exhibited for the KH case with constant density by

$$length = U_0 t f\left(\frac{x}{U_0 t}\right)$$

$$velocity = U_0 f\left(\frac{x}{U_0 t}\right)$$

$$energy/mass = U_0^2 f\left(\frac{x}{U_0 t}\right)$$

and for the RT case by

$$density = \rho_{ref} f\left(\frac{x}{g t^2}\right)$$

$$length = (gt^2)f\left(\frac{x}{gt^2}\right)$$

$$velocity = (gt)f\left(\frac{x}{gt^2}\right)$$

$$energy/mass = (gt)^2f\left(\frac{x}{gt^2}\right)$$

in which the f 's are universal functions, one for each of the relevant variables.

Two types of analysis can be accomplished with these self-similar assumptions: local and global. Local analysis introduces the mixing width, W , with self-similar variations as described for length, and approximates the gradients of mean-flow quantities by the ratio of jump to width, for example

$$\frac{\partial \bar{\rho}}{\partial x} \rightarrow \frac{\Delta \bar{\rho}}{W}$$

Insertion of the assumed self-similar functions into the full turbulence transport equations with these gradient approximations demonstrates the validity of self similarity, but does not furnish enough conditions for determining the f functions, or even their values at $x = 0$.

Global self-similar analysis does not introduce W , but proceeds by substituting the functional forms into the full turbulence transport equations (without gradient approximations). The result is a coupled set of ordinary differential equations in the independent self-similarity variable, for which the boundary conditions far from the

interface are precisely sufficient for unique determination of all the f functions in terms of the modeling parameters occurring in the theory.

NUMERICAL SOLUTION OF THE SELF-SIMILAR EQUATIONS

The coupled sets of ordinary differential equations for the f functions in each case (RT or KH) are strongly nonlinear. The similarity variable,

$$\xi \equiv \frac{x}{U_o t} \quad (\text{KH case})$$

or

$$\xi \equiv \frac{x}{g t^2} \quad (\text{RT case})$$

varies from $-\infty$ to $+\infty$, with boundary conditions specified at both ends, so that a simple marching solution is not feasible. We use, instead, a false-time relaxation procedure, in which $\partial f / \partial t'$ is added to each equation, converting the set to partial differential equations that are solved from some prescribed initial profile to late enough for a steady state to be attained. The nonzero part of this solution lies in a relatively restricted domain, well within the limits $-1 < \xi < +1$ for both cases. Thus the finite-difference computational mesh can be restricted to that interval; indeed, for the KH case with no density jump, symmetry properties allow finite-difference resolution to be restricted to the interval $0 < \xi < 1$.

These same problems could also be solved numerically in the x - t coordinate system, but experience with this procedure shows that a large region of space must be resolved in order for the evolving solution to reach self similarity, and the calculations proved excessively expensive.

In general circumstances that are not self-similar, we expect that solutions for interesting problems will always require numerical analysis in one or several spatial coordinates and time. In that type of problem the transient evolution is significant and there is no necessity for the solution to expand to its fully self-similar phase. Shocks or rarefactions intersecting material interfaces are examples of relevant problems that we solve in this manner. If there is a tangential component to the pressure jump, then slippage is induced and the combined RT and KH dynamics result in turbulence enhancement to the shear impedance in addition to the mixing of materials. Fully two- or three-dimensional problems with large mean-flow contortions will certainly require elaborate computer codes for coupling the complex mean-flow dynamics with the evolution of the turbulence and mixing variables. Results of such calculations will be discussed elsewhere.

EXAMPLES OF SELF-SIMILAR SOLUTIONS

There is a large parameter space for which meaningful calculations can be performed, varying both the "universal" modeling coefficients in the turbulence equations to exhibit their effects and the physical parameters that describe a variety of possible combinations of velocity and/or density jumps and accelerative pressure differences. In this paper we describe two of our calculations, one for a pure KH case and one for a pure RT case. Details for these and many other examples are presented in a separate report. Our goal in this paper is to show qualitatively the nature of the results obtainable from the analysis.

Results are plotted in Figs. 1 and 2 for density and the dimensionless f 's for function of the dimensionless self-similarity variable, ξ . Each f is identified by its corresponding physical variable, for example f/a refers to the f function in $a = gt f(x/gt^2)$. The results in these figures are after sufficient false-time relaxation for the attainment of a steady state. These functions exhibit the "universal" behavior associated

with the chosen set of "universal" constants in the turbulence equations, for which it should be emphasized that there is relatively little freedom for adjustment. For the RT case these functions have not had the Atwood number, A_t (here equal to $2/3$) divided out of the plots.

One especially significant feature of these results is the width of the mixing layer for the RT case. Penetration into the heavier material at the left extends to $\xi = -0.035$; penetration into the lighter material at the right extends to $\xi = +0.08$. A variety of relevant experiments [8] show that these penetration depths in physical space extend to $x = -0.06 A_t g t^2$ and $x = +0.12 A_t g t^2$, respectively for $\rho_{\text{HEAVY}}/\rho_{\text{LIGHT}} = 5$. In this calculation, $A_t = 2/3$, so that agreement with the calculation is quite good.

DISCUSSION

Material mixing at an unstable interface can be represented by means of single-field turbulence transport equations. Two-field equations can also be used for this purpose, but other investigators have shown that they must be supplemented by equations describing the turbulence fluctuations for each field [8] and accordingly offer little advantage over the single-field turbulence approach. Moreover, the two-field equations are not relevant to such problems as fire plumes in which the large density differences are not associated with a pair of identifiable materials. The use of single-field turbulence transport equations for all these circumstances is not so restricted.

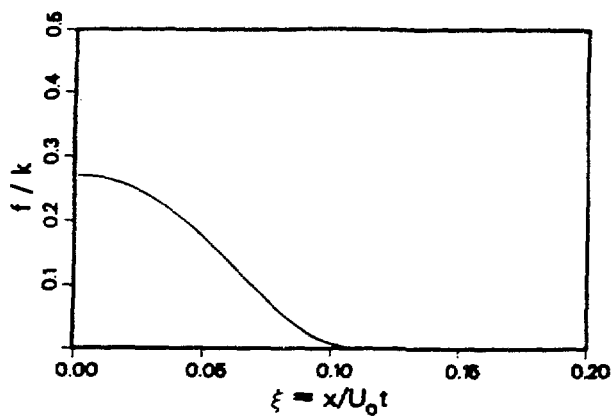
The presence of "universal" parameters in the turbulence modeling is of concern, whether we work with single-field transport or two-field transport with supplementary turbulence. Three considerations mitigate the distress associated with potential uncertainty for the values of these parameters. First, the derivations themselves indicate considerable restriction to the possible values they can take. Second,

comparisons with experiments further confine the ranges of possible values, in ways that are now appearing to be significantly independent of the particular problem being investigated. Third, recent work by Yakhot and Orszag [9] is resulting in fundamentally based predictions for the parameter values that equal those required for agreement with experiments.

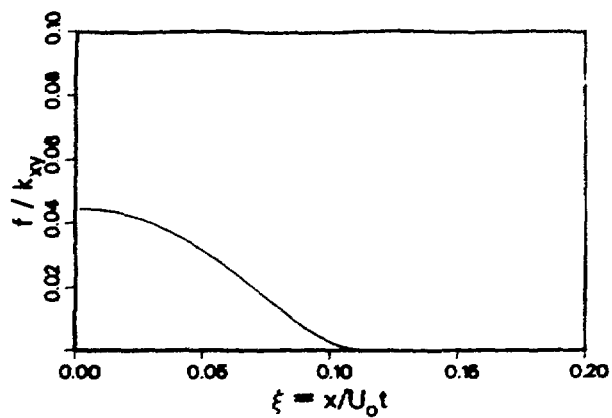
Concern for the complexity of turbulence transport modeling has been expressed by investigators working within severe budgetary constraints for their high-speed computer calculations. Thus, there is significant incentive to find a reasonable compromise between the most elaborate expressions of the theory and those that can be implemented with ease and efficiency. To explore the range of possibilities requires numerous calculations and comparisons with experiments, many of which are in progress at Limeil, Los Alamos, and elsewhere. Each investigator will have to choose the appropriate level of complexity on the basis of accuracy requirements and the constraints of applicability and available resources. It is likely that meaningful turbulence mixing studies will not be easy for any but the simplest circumstances.

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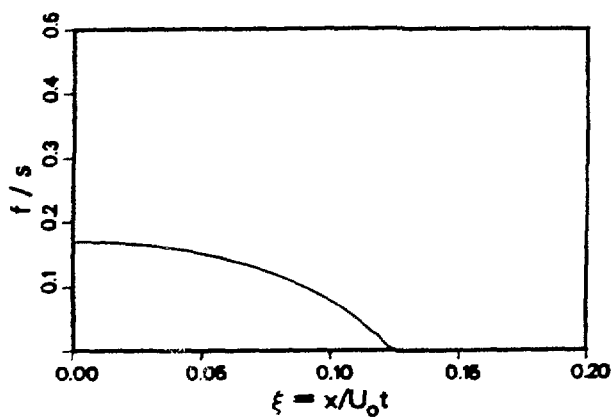
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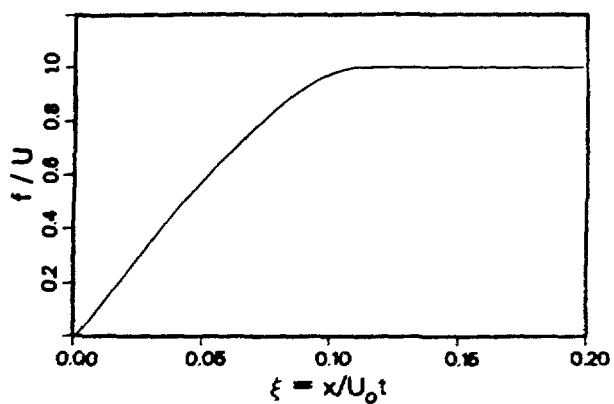
a)



b)



c)



d)

Fig. 1. Universal functions describing self-similar growth of Kelvin-Helmholtz instability-mixing layer.

- a) turbulent kinetic energy function ($k = U_0^2 f$)
- b) turbulent shear stress function ($k_{xy} = U_0^2 f$)
- c) mixing-length function ($s = (U_0 t) f$)
- d) velocity function ($U = U_0 f$)

U_0 represents half of the total velocity jump across the layer.

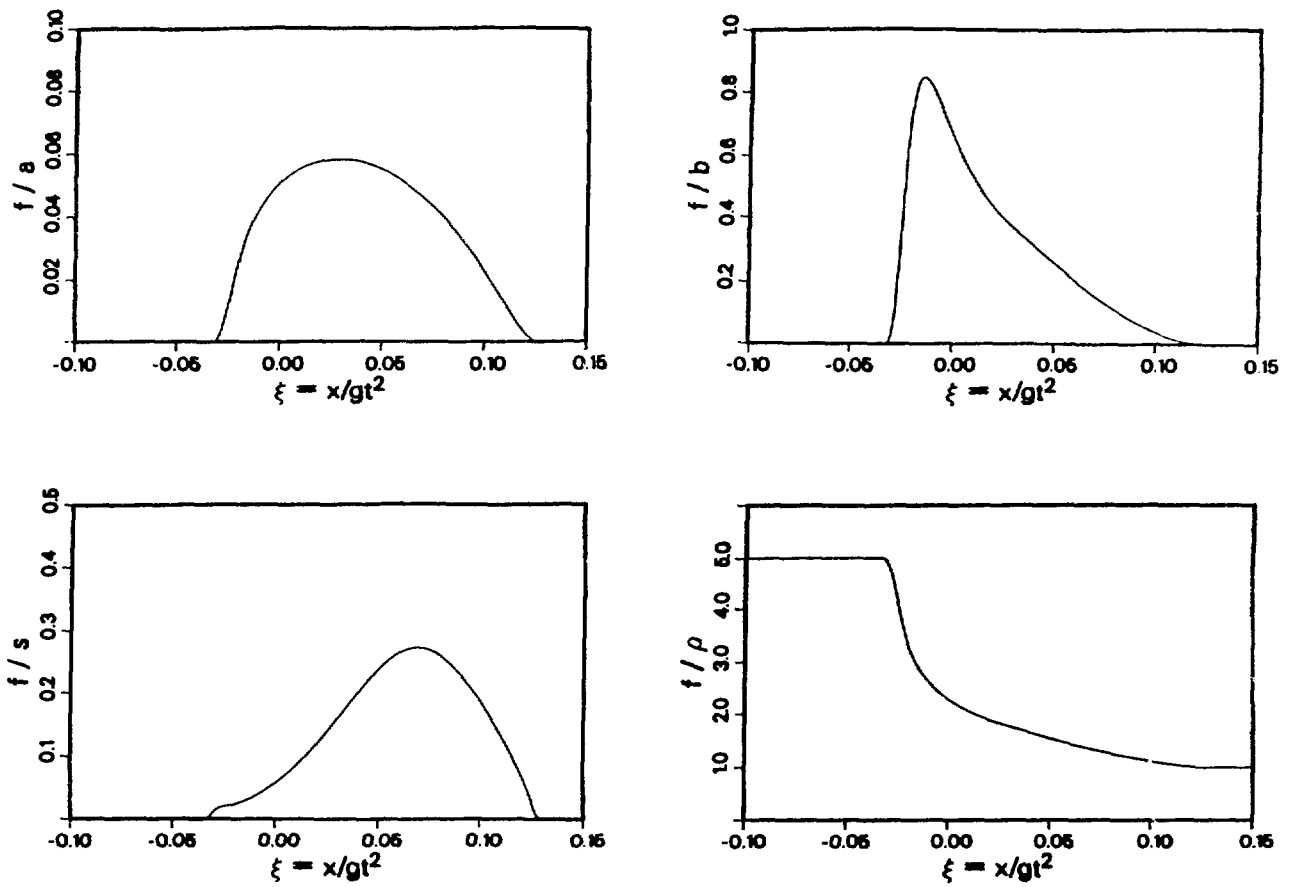


Fig. 2. Universal functions describing self-similar growth of Rayleigh-Taylor-instability-driven mixing layer.

a) interpenetrational mass flux function

$$\left(a = \overline{\rho' u'} / \bar{\rho} = (gt)f \right)$$

b) density fluctuation self-correlation function

$$\left(b = \frac{\overline{\rho'^2}}{\bar{\rho}} = \rho_{ref} f \right)$$

c) mixing-length function ($s = (gt^2)f$)

d) density profile function ($\rho = \rho_{ref} f$)

g represents the constant acceleration applied to the system to accelerate the fluid toward the left-hand side.

SECOND ORDER SCHEME FOR REACTING FLOWS. APPLICATION TO DETONATION

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RESUME

Grâce à la solution approchée du problème de Riemann généralisé, le schéma de Van Leer pour les écoulements compressibles est étendu au cas des écoulements réactifs.

La qualité des résultats obtenus est due essentiellement à l'absence de pseudoviscosité et à la résolution simultanée des équations d'Euler et de la cinétique chimique.

ABSTRACT

The approximate solution of the generalized Riemann's problem for reacting fluids allows the extension of Van leer's scheme to reacting flows. The presentation will describe this new scheme.

The given examples will show very good improvements in comparison with the classical methods applied for reacting flows. The main reasons are the absence of pseudoviscosity in this new scheme, and the fact that the reaction rate is used in the generalized Riemann's problem's solution.

I - INTRODUCTION

There have been many improvements [1, 6, 7, 8] in the numerical schemes developed for solving the equations of ideal compressible flows. Up to now those schemes have not been extended to the more complex reacting flows.

Thus the numerical study of reacting fluids was limited to the chemical reactions at fixed hydrodynamical conditions for the small scale computation or to the hydrodynamics with simplified models of combustion (C-J, ZND) for the large-scale computations.

If not, the results are not reliable and even for some coarse grids unphysical solutions are obtained [5]. The main reason is that hydrodynamics and kinetics were uncoupled such that, since characteristic times are different but not enough for neglecting the smaller one (kinetics), fine grids and small CFL are needed. And this is not the best solution for large-scale computations.

In the following we will show how to extend Van Leer's scheme to reacting fluids and how then some of the difficulties above are solved.

In section 2 we begin by introducing our notations, listing the equations of inviscid compressible reacting flows and giving the new tools necessary for such flows. Then section 3 will be a description of the numerical scheme, while the front tracking method will be the object of section 4. Finally, the numerical results are given in section 5, and the section 6, as conclusion, will tell how this method is included in our actual approach of the detonation and what are the next developments.

II - THE REACTING FLOWS

Since the scheme will be used for large scale computations; we assume a simplified model for the reacting flows. Namely only two species are taken into account, unburnt explosive and burnt products, the first one being transformed into the second one by one irreversible chemical reaction. Moreover the viscosity and diffusion effects are neglected. Thus the system we will have to solve is given by the following equations :

$$\frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial r} + \rho \frac{\partial v}{\partial r} + \chi \rho v = 0$$

$$\frac{\partial r}{\partial t} + v \frac{\partial v}{\partial r} + \frac{1}{\rho} \frac{\partial P}{\partial r} = 0$$

$$\frac{\partial E}{\partial t} + v \frac{\partial E}{\partial r} + \frac{1}{\rho} \frac{\partial (Pv)}{\partial r} + \chi \frac{Pv}{\rho} = 0,$$

$$\frac{\partial \omega}{\partial t} + v \frac{\partial \omega}{\partial r} = f(P, \rho, \omega);$$

where ρ is the density, v the fluid velocity, P the pressure, E the total specific energy, ω the mass fraction of burnt products, t is the time and r is the space

variable ; χ is a function of r given by the geometry :

$$\chi(r) = \begin{cases} 0 & \text{planar symmetry} \\ \frac{1}{r} & \text{cylindrical symmetry} \\ \frac{2}{r} & \text{spherical symmetry} \\ \frac{A'(r)}{A(r)} & \text{flow through a duct of section } A(r) \end{cases}$$

For the kinetics, the function $f(P, \rho, \omega)$ is any of the commonly used reaction rate.

The total energy E is given by :

$$E = e + \frac{1}{2} v^2$$

where e is the sum of the internal energy and chemical energy.

The last equation, the equation of state, is then chosen as

$$e(P, \rho, \omega) = \frac{P + \gamma P^0}{(\gamma + 1) \rho} - \frac{\gamma P^0}{(\gamma - 1) \rho} + (1 - \omega) q$$

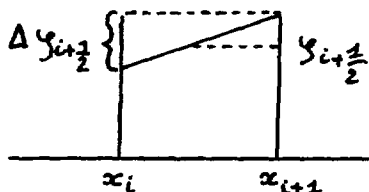
with γ , P^0 and ρ^0 functions of ω and q the amount of heat released by the reaction.

There are many ways to choose γ , P^0 and ρ^0 . We may, for example suppose that they are known for $\omega = 0$ and $\omega = 1$; and then, we compute them for $\omega \in] 0, 1 [$ in order to recover a given pressure distribution $P(\omega)$ in the ZND reaction zone.

III - THE NUMERICAL SCHEME

The scheme is essentially the same as the one presented by Van Leer [8]. It is divided into two steps ; we first apply a Lagrangean scheme and then remap the solution into the operating grid.

The solution is represented in each mesh zone by a linear function. Indeed, in order to get second order accuracy, we have in each zone, not only the mean value, but also the increment for the density, the velocity, the total energy and the mass fraction of burnt products.



The remapping is not changed by the introduction of the kinetics and is done by least squares fitting.

On the other hand the lagrangean step is quite different. First, at each mesh point, the interaction of the two contiguous zones is solved by looking at the solution of the corresponding generalized Riemann's problem for which the reaction rate equation has already been introduced [4]. Then if the equations of conservation of mass, momentum and energy are integrated as previously in each zone, we have yet to consider the reaction rate equation :

$$\frac{\partial \omega}{\partial t} + v \frac{\partial \omega}{\partial r} = \frac{d\omega}{dt} = f(P, \rho, \omega)$$

In order to have here also second order accuracy we must evaluate the mean value in time of $f(P, \rho, \omega)$. Thus we first calculate the mean values in time $\bar{P}$ of P and $\bar{\rho}$ of ρ and after that the usual forms of f allow us to integrate exactly the approximate equation :

$$\frac{d\omega}{dt} = f(\bar{P}, \bar{\rho}, \omega).$$

Finally in order to avoid the oscillations which appear with second order schemes, the same monotonicity algorithms are applied as in the original Van Leer's scheme [8].

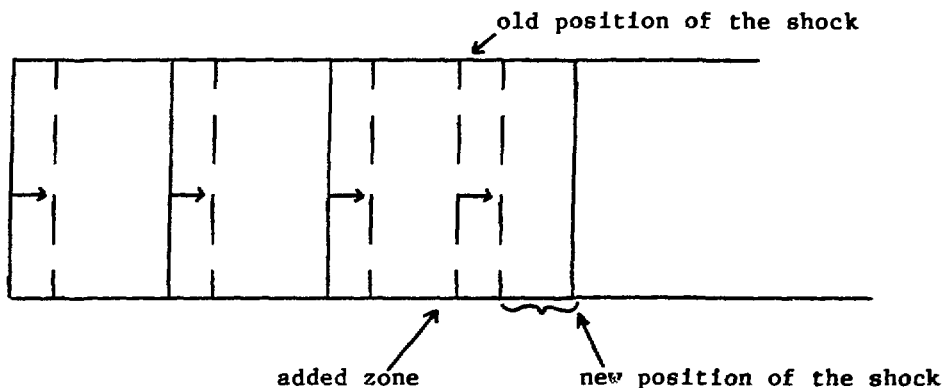
IV - THE FRONT TRACKING METHOD

In order to study shock to detonation transition it is essential to compute the shock as well as possible. One of the best way is to use a front tracking methode in order to know with a good accuracy the position and the intensity of the shock. This is not only useful for solving the flow downstream but may also be a great advantage for some kinetics which take the intensity of the initial shock as a parameter.

Such a method is quite difficult in multidimensional computations but much easier to develop in monodimensional configurations. Moreover Van Leer's scheme is particularly appropriate for a front tracking method.

At each time step the Eulerian grid is modified in order to include the position of the shock as a mesh point. Actually it will be the last point of the computational grid then the solution of the generalized Riemann's problem [4] at this node determines the speed of the shock and its time-derivative which allow us to compute the position of the shock as well as the state on the shock at the next time step.

Since we know the old and the new grid, there will be no change for the remapping step. On the other hand, the Lagrangean step will be done as previously except that one zone must be added, the zone corresponding to the mass of explosive crossed by the shock during the time step.



In this zone the mean values of ρ , U , E and w are given by the conservation laws. In each step the slopes in the zone behind the shock are defined in order to get back the right state on the shock.

V - NUMERICAL RESULTS

The method above has been tested on several numerical simulations. We show here the results for four such computations.

The first one is the comparison between the method presented here and the direct integration of a ZND detonation followed by a centered rarefaction wave. At The initial we have at right a ZND reaction zone and at left the explosive is at rest. The right boundary is at rest and we look at the solution when the shock

which has been tracked, reaches the left boundary. On picture 1 we have plotted the results for P , ρ , v and ω . The numerical solution is given by the circles, while the squares represent the "exact" solution. The reaction zone is 2 millimeters large and there are 4 points per millimeter.

The three other computations are the study of a cylindrical shock to detonation transition. At the initial time the explosive is at rest and some energy is added in a few zones near the center. Picture 2 shows the profiles for P and ω at different times for a 1-D computation with 125 points. Picture 3 is the same as picture 2 except that the front tracking method has been used. The speed of the shock versus time is also in this case plotted on picture 4. Finally picture 5 gives the isocontours for P , ρ , v and ω at the end of a 2-D computation using the 1-D scheme in alternating directions on a 100 x 100 grid.

For the first computation f is given by :

$$f(P, \rho, \omega) = \sqrt{1 - \omega} (a P^\alpha + b P^\beta),$$

in order to get a finite reaction zone. Otherwise we have chosen :

$$f(P, \rho, \omega) = (1 - \omega) (a P^\alpha + b P^\beta).$$

In both cases the equation of state is the same and gives :

$$P_{cj} = 365.2 \cdot 10^9, \quad P_{vn} = 549.2 \cdot 10^9 \quad (\text{CGS})$$

VI - CONCLUSION

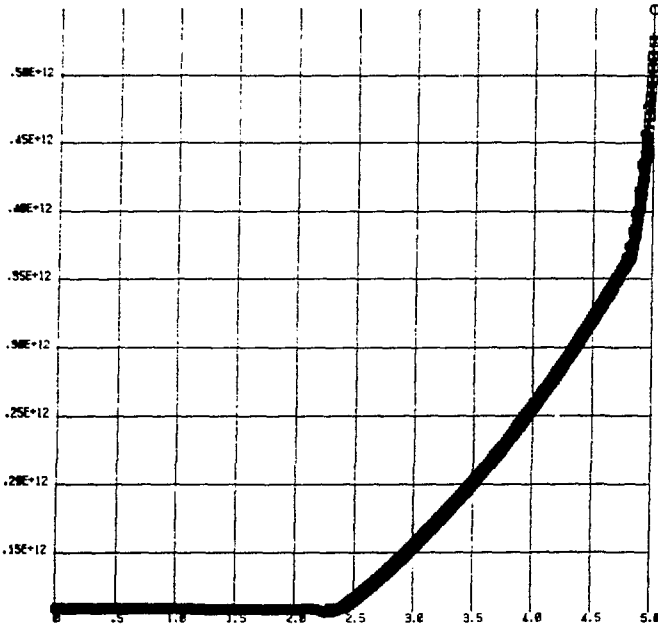
The results presented above show that it is now possible to introduce better treatments for large-scale computations of flows with explosives (see also [2]). Actually depending on the explosive several methods are possible. For fast explosives a front tracking method for the detonation front [3] is probably the best

solution, while for explosives with large reaction zone, the above method is well suited. Moreover the 1-D computations for such explosives have shown that even in this case a front tracking method for the inert shock is very useful. This can be done also in 2-D. Finally, in order to unify the treatments, it appears that the next step could be a method with a front tracking for a reactive front followed by a still reactive flow.

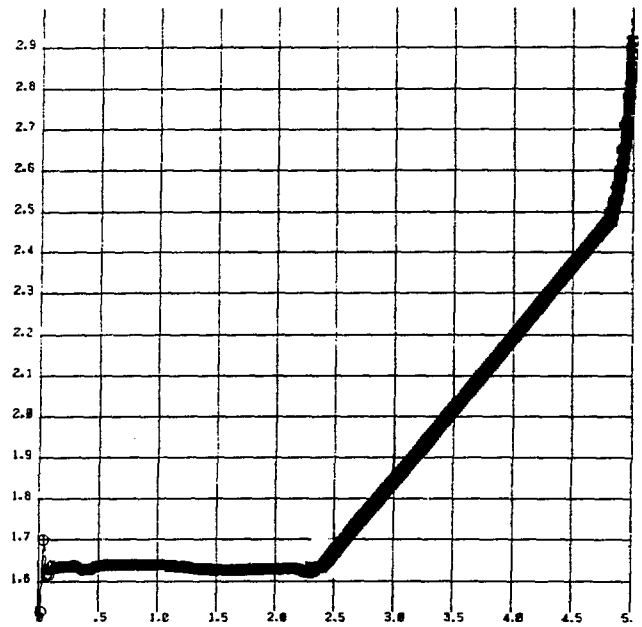
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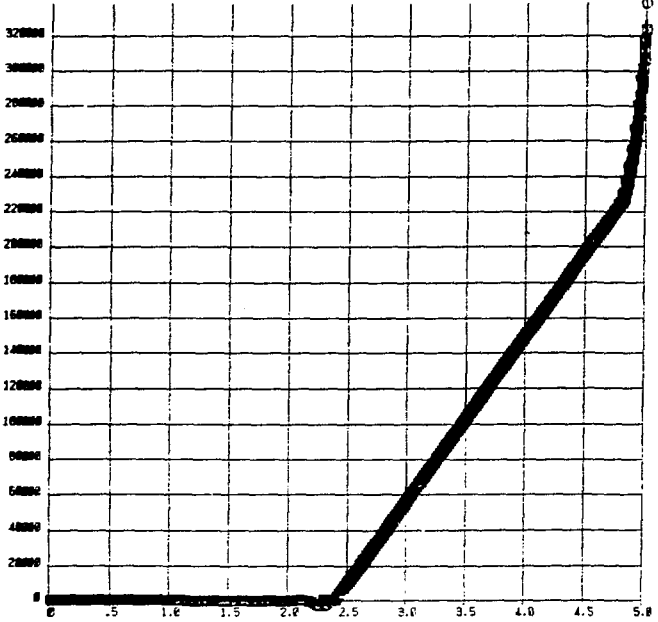
PRESSURE



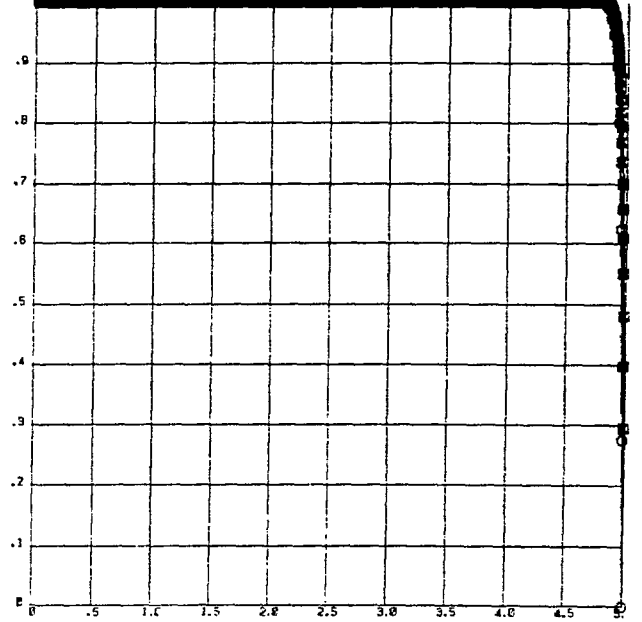
DENSITY



VELOCITY



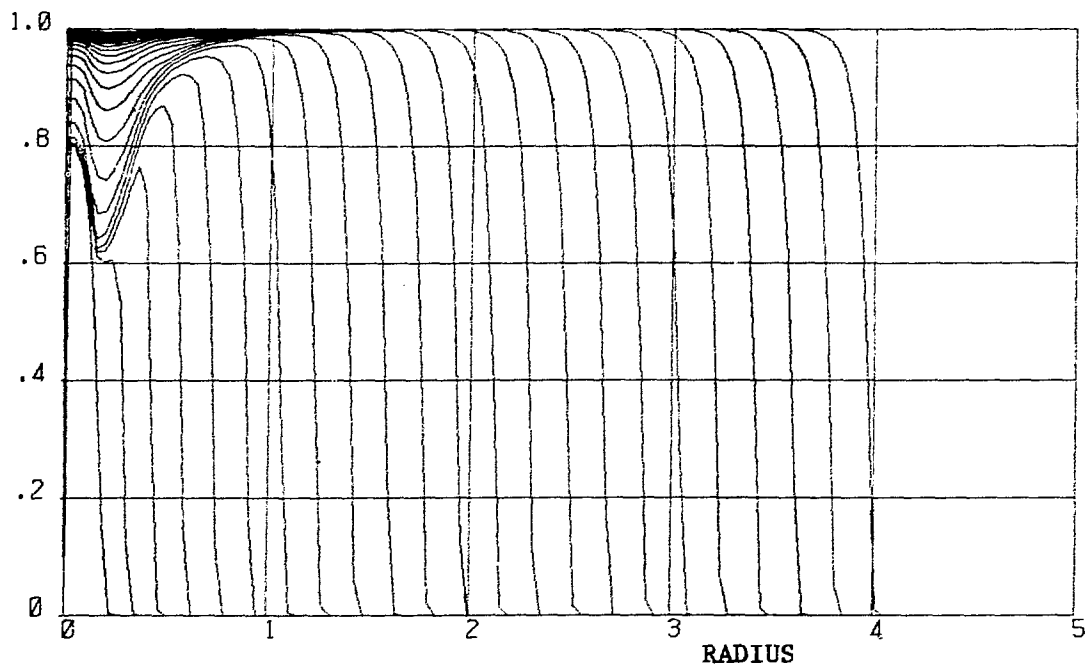
BURNT FRACTION



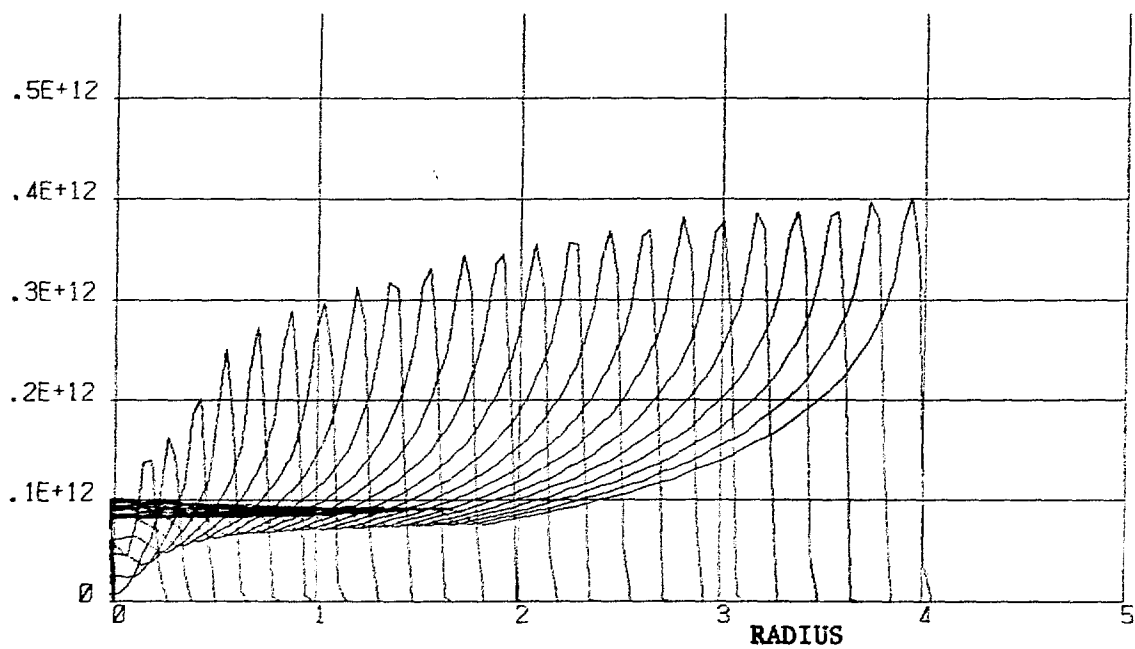
1. Z N D DETONATION

(SYSTEM OF UNITS : C G S)

BURNT FRACTION



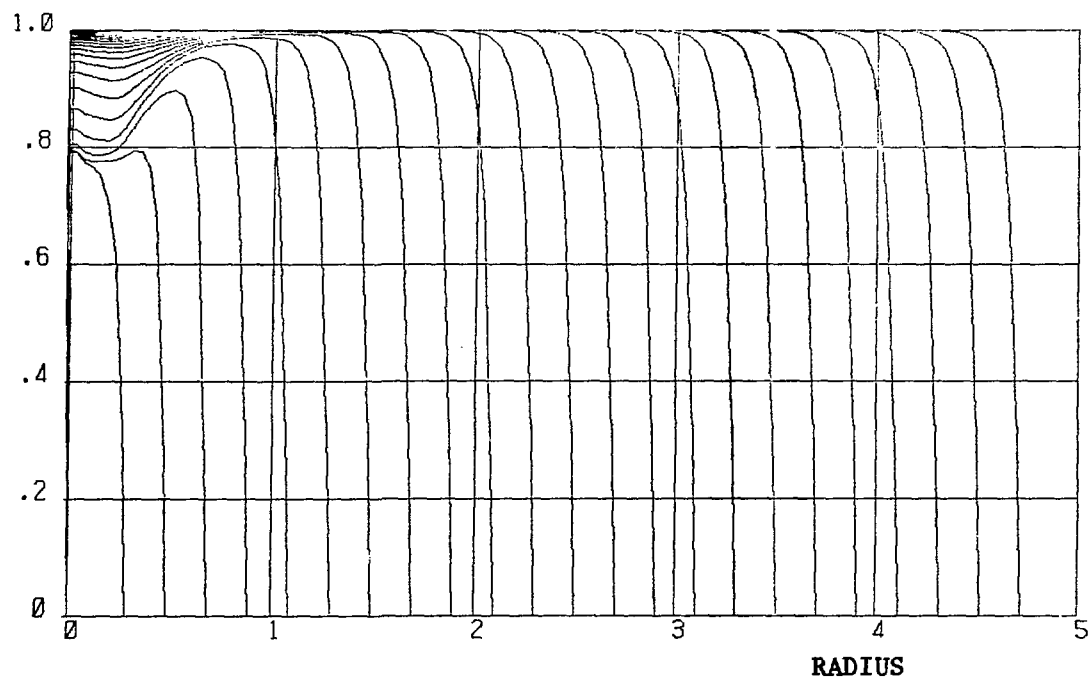
PRESSURE



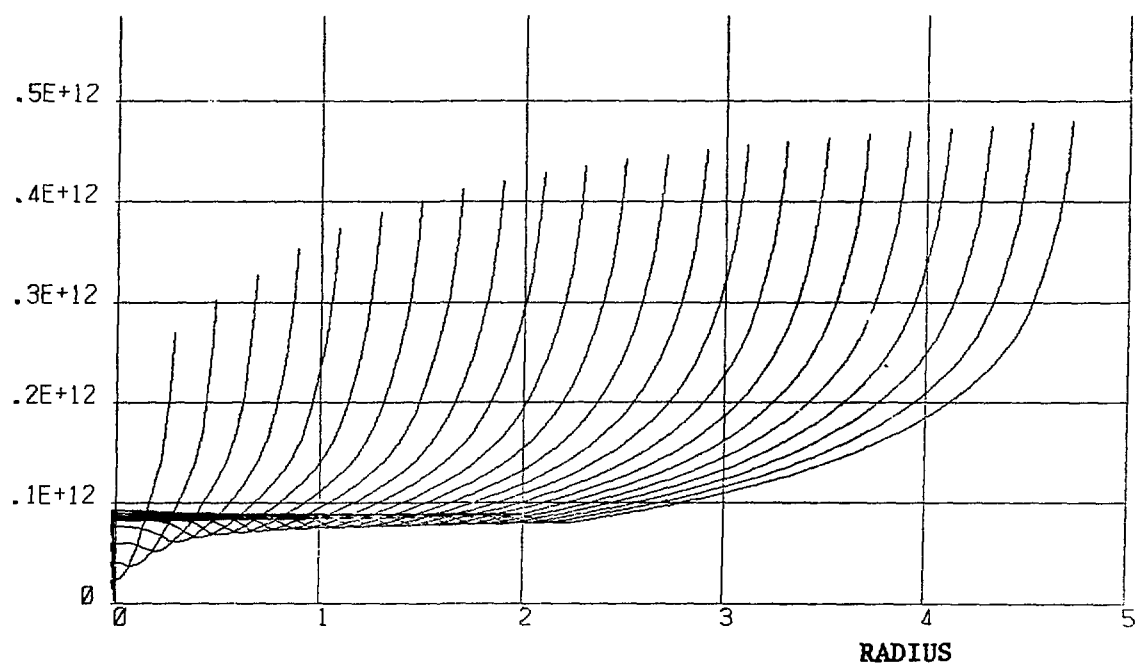
2. 1-D INITIATION

(SYSTEM OF UNITS : C G S)

BURNT FRACTION

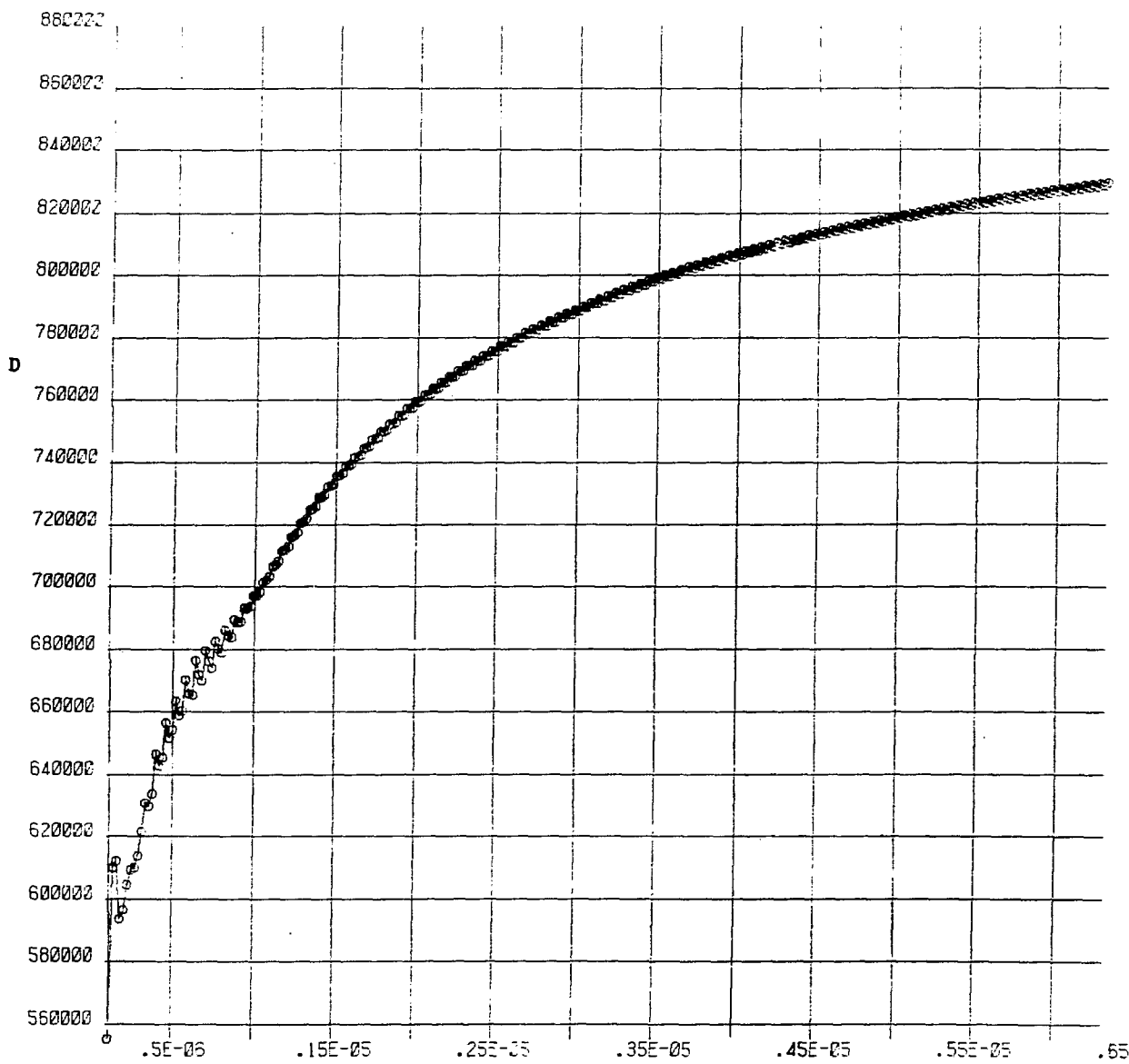


PRESSURE



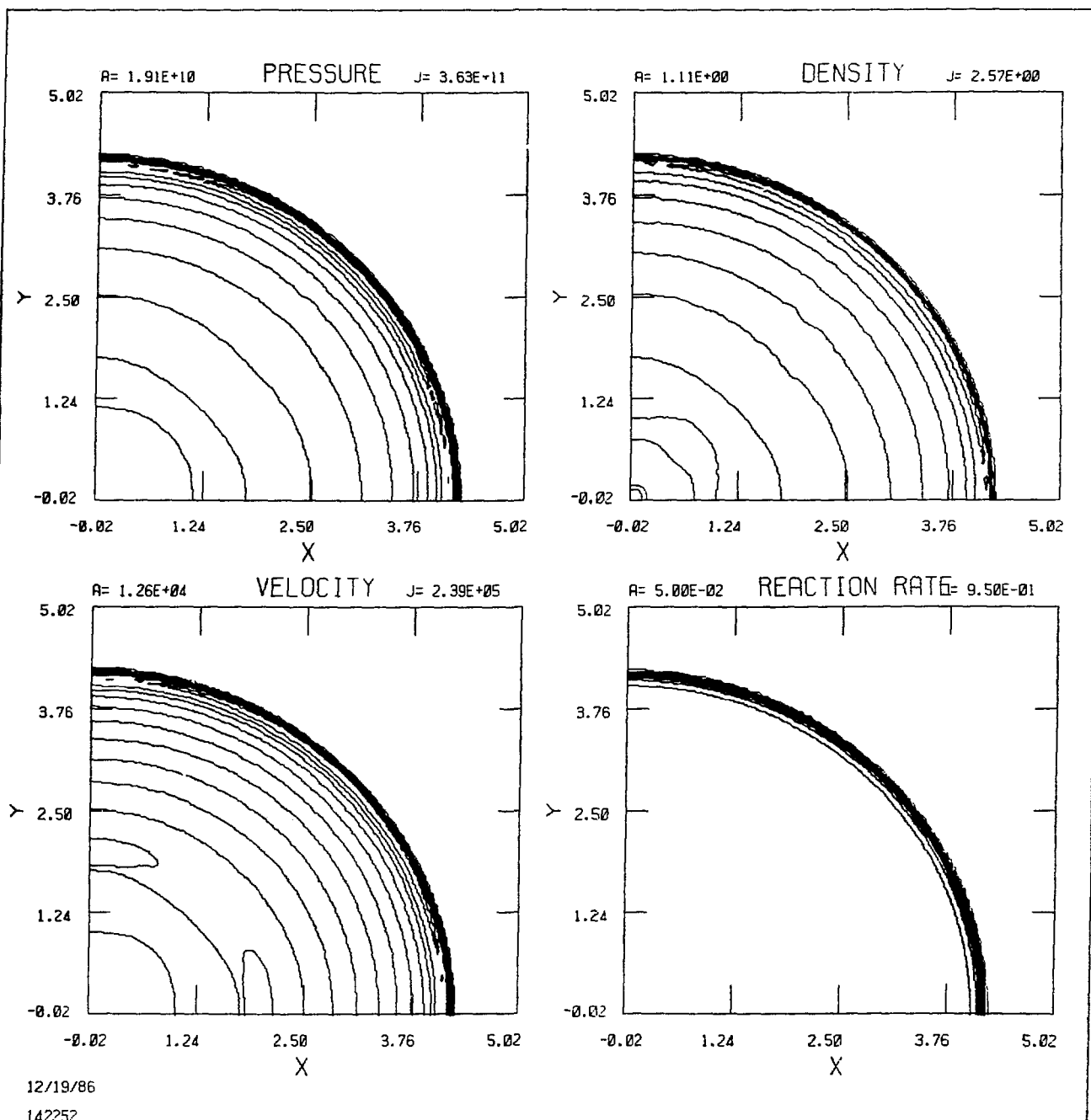
3. 1-D INITIATION WITH FRONT TRACKING

(SYSTEM OF UNITS : C G S)



4. SHOCK'S SPEED

(SYSTEM OF UNITS : C G S)



5. 2-D INITIATION
(SYSTEM OF UNITS : C G S)

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INTRODUCTION

The GAIA computer code is developed for time-dependent, compressible, multimaterial fluid flow problems, to overcome some drawbacks of traditional 2-D Lagrangian codes. The initial goals of robustness, entropy accuracies, efficiency in presence of large interfacial slip, have already been achieved.

The general GODUNOV approach is applied to an arbitrary time-varying control-volume formulation. We review in this paper the Riemann solver, GODUNOV's cartesian and curvilinear moving grid schemes and an efficient grid generation algorithm. We finally outline a possible second-order accuracy extension.

1. - AN ITERATIVE RIEMANN SOLVER

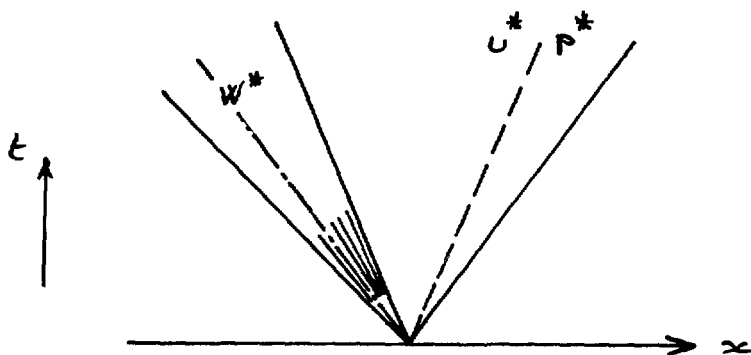
Widespread usage of Godunov's schemes in hydrodynamics has been limited by the cost and the complexity of the Riemann problem. It appeared recently that approximate solutions may be used with equal success.

1.1. Approximate relationship : $U_s = C_o + s U_p$

Dukowitz's simple and efficient Riemann solver /9/ relies on the two-shock approximation and the experimental relationship $U_s = C_o + s U_p$ relating the shock velocity to the corresponding fluid velocity. This solver provides the pressure P^* and the fluid velocity U^* at the contact discontinuity of the Riemann solution. It is consequently well-suited for lagrangian schemes.

1.2. Simplified equation of state

Considering a Godunov moving grid scheme, the complete Riemann solution is necessary to get the hydrodynamic state "seen" by a grid point moving at an arbitrary velocity W^* . This requires a complete equation of state.



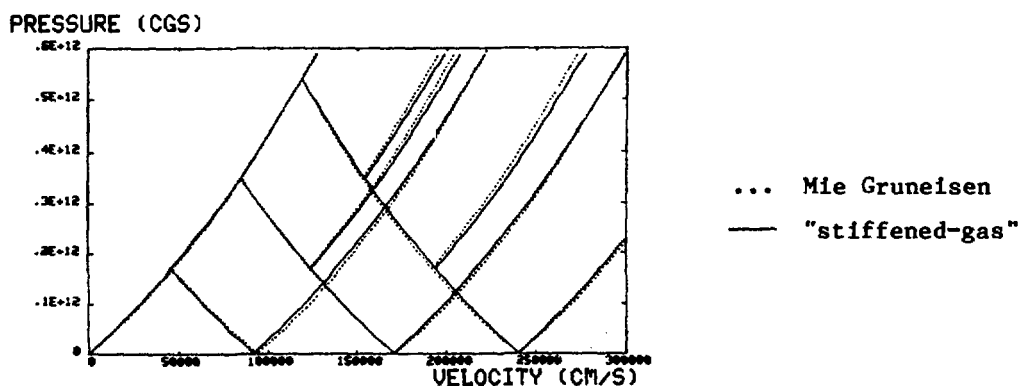
The Riemann solver used in the GAIA code operates on the "stiffened-gas" equation of state (Harlow, Amsden, /4/)

$$(1) \quad P = c_o^2 (\rho - \rho_o) + (\gamma - 1) \rho \epsilon \quad (1)$$

where P is the pressure, ρ is the density and ϵ is the internal energy per unity of mass.

The form $\epsilon(P, \rho) = \frac{P + \gamma P_o}{(\gamma - 1)\rho}$ is equivalent to (1) where $P_o = \frac{1}{\gamma} \rho_o c_o^2$ is spall pressure and γ polytropic coefficient. The corresponding Riemann solver algorithm is iterative as in the case of perfect gas, but quite affordable when used in traditional hydrodynamic computations.

Remark : The "stiffened-gas" equation of state is a zeroth-order development of the Gruneisen equation of state constructed on the approximate Hugoniot $U_s = C_o + sU_p$. It constitutes a good approximation for solids, as illustrated for iron by the following shock-release diagram.



1.3 Extension to mixtures

A specific solver is required for cells containing several materials. An extended form of the "stiffened-gas" equation of state has been designed for that

purpose by A. Bourgeade, B. Scheurer and the author.

Considering two species A and B with their respective equation of state

$$\varepsilon_A(P, \rho) = \frac{P + \gamma^A P_o}{(\gamma^A - 1)\rho}, \quad \varepsilon_B(P, \rho) = \frac{P + \gamma^B P_o}{(\gamma^B - 1)\rho},$$

introducing λ the mass fraction of A, an equation for the mixture of the two species can be stated as

$$\varepsilon(P, \rho, \lambda) = \lambda \varepsilon_A(P, \rho) + (1-\lambda) \varepsilon_B(P, \rho).$$

The equivalent "stiffened-gas" formulation is

$$(2) \quad \varepsilon(P, \rho, \lambda) = \frac{P + \Gamma(\lambda) P_o(\lambda)}{(\Gamma(\lambda) - 1)\rho}$$

$$\text{with } \Gamma(\lambda) = 1 + \frac{(\gamma^A - 1)(\gamma^B - 1)}{(1-\lambda)(\gamma^A - 1) + \lambda(\gamma^B - 1)}, \quad P_o(\lambda) = \frac{\Gamma(\lambda) - 1}{\Gamma(\lambda)} \left((1-\lambda) \frac{\gamma^B P_o^B}{\gamma^B - 1} + \lambda \frac{\gamma^A P_o^A}{\gamma^A - 1} \right).$$

2. - 2-D MOVING GRID GODUNOV'S SCHEMES

In the algorithms /1/ and /6/, convective and non-convective fluxes are computed simultaneously using the complete Riemann solver solution. Then it is not necessary to decompose the scheme in a lagrangian phase and a remapping phase. The general methodology is summarized here.

2.1. Cartesian scheme

The unsteady two-dimensional Euler equations

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x} F(U) + \frac{\partial}{\partial y} G(U) = 0$$

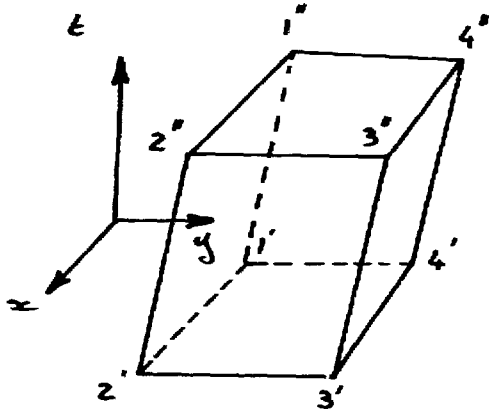
$$\text{where } U = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \end{pmatrix} \quad F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho e + p)u \end{pmatrix} \quad G(U) = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho e + p)v \end{pmatrix}$$

can be written in integral form using the divergence theorem

$$\iint U \, dx \, dy + F \, dy \, dt + G \, dt \, dx = 0.$$

An application of this formula to the closed surface (1', 2', 3', 4', 1'', 2'', 3'', 4'') delimited by the four vertices of an arbitrary moving cell during a time-step Δt leads to

$$(3) \quad U^* Q^* = U_0 Q_0 - Q_{12} - Q_{23} - Q_{34} - Q_{41}$$



relating the unknowns U^* at time Δt to four numerical fluxes and the corresponding known quantities U_0 at the initial time.

Using the following notations

$$Q^* = \iint_{(1'', 2'', 3'', 4'')} dx \, dy, \quad Q_0 = \iint_{(1', 2', 3', 4')} dx \, dy$$

$$Q_{ij} = \iint_{ij} dx \, dy, \quad \Phi_{ij} = \iint_{ij} dy \, dt, \quad \Psi_{ij} = \iint_{ij} dt \, dx$$

the expression of a numerical flux is

$$Q_{ij} = U_{ij} Q_{ij} + F_{ij} \Phi_{ij} + G_{ij} \Psi_{ij}$$

Defining average positions of vertices over the time-step Δt

$$x_i = \frac{1}{2} (x_i' + x_i''), \quad y_i = \frac{1}{2} (y_i' + y_i'')$$

the area appearing in the numerical flux Q_{ij} are approximated by

$$\Phi_{ij} = \Delta t (y_j - y_i)$$

$$\Psi_{ij} = \Delta t (x_i - x_j)$$

$$Q_{ij} = \frac{1}{2} [(x_j'' - x_i')(y_i'' - y_j') - (x_i'' - x_j')(y_j'' - y_i')].$$

Introducing a moving grid velocity W_{ij}^* that satisfies

$$Q_{ij} = \Delta t \, l_{ij} W_{ij}^* \quad \text{with} \quad l_{ij} = [(x_j - x_i)^2 + (y_j - y_i)^2]^{\frac{1}{2}}$$

the numerical flux becomes

$$Q_{ij} = U_{ij} \Delta t \, l_{ij} W_{ij}^* + F_{ij} \Delta t (y_j - y_i) - G_{ij} \Delta t (x_j - x_i)$$

or, using direction cosines

$$\alpha_{ij} = -(y_j - y_i)/l_{ij}, \quad \beta_{ij} = (x_j - x_i)/l_{ij}$$

$$Q_{ij} = \Delta t \, l_{ij} (U_{ij} W_{ij}^* - F_{ij} \alpha_{ij} - G_{ij} \beta_{ij}).$$

An extended form is

$$(4) \quad Q_{ij} = \Delta t \, l_{ij} \begin{pmatrix} R & (W_{ij}^* - N) \\ RU & (W_{ij}^* - N) - \alpha P \\ RV & (W_{ij}^* - N) - \beta P \\ RE & (W_{ij}^* - N) - NP \end{pmatrix}_{ij} \quad (4)$$

$$\text{with } N_{ij} = \alpha_{ij} U_{ij} + \beta_{ij} V_{ij}.$$

Such an expression could have been written directly. The precise derivation has been detailed for use in the more complex curvilinear case. Parameters denoted with capital letters $(R, U, V, P, E)_{ij}$ are obtained by resolution of an one dimensional problem in direction normal to the cell edge with left and right states given by these at the centers of the adjacent cells.

Density, pressure and normal component of velocity $(R, P, N)_{ij}$ "seen" by a cell edge during its displacement at velocity W_{ij}^* are extracted from the self-similar Riemann solution.

The tangential component of velocity is obtained by the comparison of the grid velocity to the contact discontinuity velocity

$$T_{ij} = \begin{cases} T_{ij}^L, & \text{if } W_{ij}^* < U^* \\ T_{ij}^R, & \text{if } W_{ij}^* > U^* \end{cases}$$

giving the cartesian components of velocity necessary in (4)

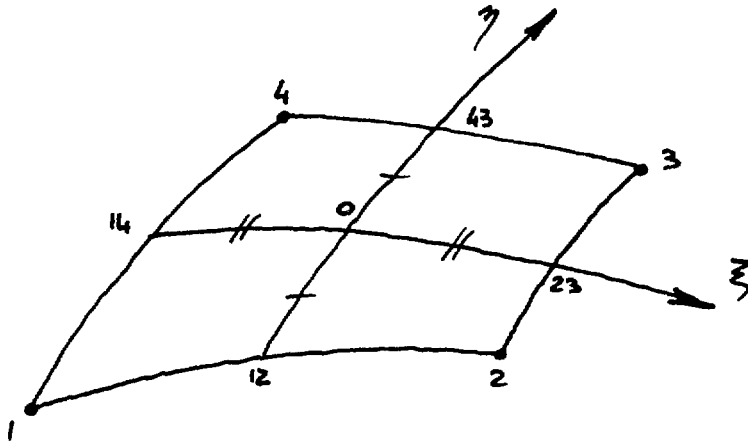
$$(5) \quad U_{ij} = N_{ij} \alpha_{ij} + T_{ij} \beta_{ij}, \quad V_{ij} = N_{ij} \beta_{ij} - T_{ij} \alpha_{ij}.$$

This completes the general description of the cartesian scheme.

2.2. Curvilinear scheme

a) Local curvilinear coordinate system

A local curvilinear coordinate system is defined for each cell delimited by its four vertices (1, 2, 3, 4) at the initial time.



The following notations hold for the rest of the paper :

- direction cosines

$$\alpha' = \frac{1}{\sqrt{g_{11}}} \frac{\partial x}{\partial \xi}, \quad \beta' = \frac{1}{\sqrt{g_{11}}} \frac{\partial y}{\partial \xi}$$

$$\alpha'' = \frac{1}{\sqrt{g_{22}}} \frac{\partial x}{\partial \eta}, \quad \beta'' = \frac{1}{\sqrt{g_{22}}} \frac{\partial y}{\partial \eta}$$

- angle between coordinate lines

$$\alpha = \cos(\xi, \eta) = \alpha' \alpha'' + \beta' \beta''$$

$$\beta = \sin(\xi, \eta) = \alpha' \alpha'' - \beta' \beta''$$

- velocity components

. cartesian : u, v

$$\text{. contravariant : } \mu = \frac{1}{\beta} (u \beta'' - v \alpha''), \quad v = \frac{1}{\beta} (v \alpha' - u \beta')$$

$$\text{. "intrinsic" : } \mu^k = u \alpha' + v \beta', \quad v^k = u \alpha'' + v \beta''$$

$$v^n = v \alpha' - u \beta', \quad \mu^n = u \beta'' - v \alpha''$$

b) (μ^k, v^k) Euler equations

From the unsteady two-dimensional Euler equations in plane or axisymmetric geometry

$$(6) \quad \frac{\partial [Q(y) \rho u]}{\partial t} + \frac{\partial [Q(y) (\rho u^2 + p)]}{\partial x} + \frac{\partial [Q(y) \rho u v]}{\partial y} = 0$$

$$(7) \quad \frac{\partial [Q(y) \rho v]}{\partial t} + \frac{\partial [Q(y) \rho u v]}{\partial x} + \frac{\partial [Q(y) (\rho v^2 + p)]}{\partial y} = -p \frac{dQ}{dy}$$

with $Q(y) = 1$ or $Q(y) = y$

one can derive evolution equations for the tangential velocity component to each coordinate line.

$$\begin{aligned} \alpha'(6) + \beta'(7) & \frac{\partial [Q(y)\rho(u\alpha' + v\beta')]}{\partial t} + \frac{\partial}{\partial x} [Q(y)p\alpha' + Q(y)\rho u(u\alpha' + v\beta')] \\ & + \frac{\partial}{\partial y} [Q(y)p\beta' + Q(y)\rho v(u\alpha' + v\beta')] \\ & - P \left[\frac{\partial \alpha' Q(y)}{\partial x} + \frac{\partial \beta' Q(y)}{\partial y} \right] \\ & - \left[\rho u Q(y) \left(u \frac{\partial \alpha'}{\partial x} + v \frac{\partial \alpha'}{\partial y} \right) + \rho v Q(y) \left(u \frac{\partial \beta'}{\partial x} + v \frac{\partial \beta'}{\partial y} \right) \right] = 0 \end{aligned}$$

$$\begin{aligned} \alpha''(6) + \beta''(7) & \frac{\partial [Q(y)\rho(u\alpha'' + v\beta'')]}{\partial t} + \frac{\partial}{\partial x} [Q(y)p\alpha'' + Q(y)\rho u(u\alpha'' + v\beta'')] \\ & + \frac{\partial}{\partial y} [Q(y)p\beta'' + Q(y)\rho v(u\alpha'' + v\beta'')] \\ & - P \left[\frac{\partial \alpha'' Q(y)}{\partial x} + \frac{\partial \beta'' Q(y)}{\partial y} \right] \\ & - \left[\rho u Q(y) \left(u \frac{\partial \alpha''}{\partial x} + v \frac{\partial \alpha''}{\partial y} \right) + \rho v Q(y) \left(u \frac{\partial \beta''}{\partial x} + v \frac{\partial \beta''}{\partial y} \right) \right] = 0 \end{aligned}$$

Introducing the curvature of the coordinate lines and angle variations, the corresponding integral formulation is (for the complete set of equations)

$$\begin{aligned} \iint_S \rho Q(y) \sqrt{g} d\xi d\eta - \iint_S \rho v^n Q(y) \sqrt{g_{11}} d\xi dt \\ + \iint_S \rho \mu^n Q(y) \sqrt{g_{22}} d\eta dt = 0 \end{aligned}$$

$$\begin{aligned} \iint_S \rho \mu^k Q(y) \sqrt{g} d\xi d\eta - \iint_S \rho \mu^k v^n Q(y) \sqrt{g_{11}} d\xi dt \\ + \iint_S (p\beta + \rho \mu^k \mu^n) Q(y) \sqrt{g_{22}} d\eta dt \\ - \iiint_V P \frac{\partial}{\partial \xi} \left(\frac{\sqrt{g} Q(y)}{\sqrt{g_{11}}} \right) d\xi d\eta dt \\ - \iiint_V \rho v \left[\mu K_{\eta=cste} + v \left(K_{\xi=cste} + \frac{1}{\sqrt{g_{22}}} \frac{\partial [\eta, \xi]}{\partial \eta} \right) \right] \beta Q(y) \sqrt{g} d\xi d\eta dt = 0 \end{aligned}$$

$$\begin{aligned} \iint_S \rho v^k Q(y) \sqrt{g} d\xi d\eta - \iint_S (p\beta + \rho v^k v^n) Q(y) \sqrt{g_{11}} d\xi dt \\ + \iint_S (\rho v^k \mu^n) Q(y) \sqrt{g_{22}} d\eta dt \\ - \iiint_V P \frac{\partial}{\partial \eta} \left(\frac{\sqrt{g} Q(y)}{\sqrt{g_{22}}} \right) d\xi d\eta dt \end{aligned}$$

$$\begin{aligned} - \iiint_V \rho \mu \left[v K_{\xi=cste} + \mu \left(K_{\eta=cste} - \frac{1}{\sqrt{g_{11}}} \frac{\partial [\eta, \xi]}{\partial \xi} \right) \right] \beta Q(y) \sqrt{g} d\xi d\eta dt = 0 \end{aligned}$$

$$\iint_S \rho e Q(y) / g \, d\xi d\eta - \iint_S (\rho e + p) v^n Q(y) / g_{11} d\xi dt + \iint_S (\rho e + p) \mu^n Q(y) / g_{22} d\eta dt = 0$$

c) (ξ, η) numerical scheme

The following curvilinear moving grid scheme can then be derived from the above integral equations, as in the cartesian case.

$$[\rho]^\circ I^\circ - [\rho] I_\circ - \tau[\rho]_{12} \{ [v^n]_{12} - [\beta v^*]_{12} \} I_{12} + \tau[\rho]_{43} \{ [v^n]_{43} - [\beta v^*]_{43} \} I_{43} + \tau[\rho]_{23} \{ [\mu^n]_{23} - [\beta \mu^*]_{23} \} I_{23} - \tau[\rho]_{14} \{ [\mu^n]_{14} - [\beta \mu^*]_{14} \} I_{14} = 0$$

$$[\rho \mu^k]^\circ I^\circ - [\rho(\mu + \alpha v)]_\circ I_\circ - \tau[\rho \mu^k]_{12} \{ [v^n]_{12} - [\beta v^*]_{12} \} I_{12} + \tau[\rho \mu^k]_{43} \{ [v^n]_{43} - [\beta v^*]_{43} \} I_{43} + \tau[\rho(\beta \mu^n + \alpha v^k)]_{23} \{ [\mu^n]_{23} - [\beta \mu^*]_{23} \} I_{23} - \tau[\rho(\beta \mu^n + \alpha v^k)]_{14} \{ [\mu^n]_{14} - [\beta \mu^*]_{14} \} I_{14} - \tau\{ [p]_{14} - [p]_{23} \} \frac{1}{2} (\beta_{23} I_{23} + \beta_{14} I_{14}) - \tau[\rho v]_\circ \{ ([\mu]_\circ - [\mu^*]_\circ) [K_{\eta=\text{cste}}]_\circ + ([v]_\circ - [v^*]_\circ) [K_{\xi=\text{cste}} + \frac{1}{\sqrt{g_{22}}} \frac{\partial[\eta, \xi]}{\partial \eta}]_\circ \} \beta_\circ I_\circ = 0$$

$$[\rho v^k]^\circ I^\circ - [\rho(v + \alpha \mu)]_\circ I_\circ - \tau[\rho(\beta v^n + \alpha \mu^k)]_{12} \{ [v^n]_{12} - [\beta v^*]_{12} \} I_{12} + \tau[\rho(\beta v^n + \alpha \mu^k)]_{43} \{ [v^n]_{43} - [\beta v^*]_{43} \} I_{43} + \tau[\rho v^k]_{23} \{ [\mu^n]_{23} - [\beta \mu^*]_{23} \} I_{23} - \tau[\rho v^k]_{14} \{ [\mu^n]_{14} - [\beta \mu^*]_{14} \} I_{14} - \tau\{ [p]_{12} - [p]_{43} \} \frac{1}{2} (\beta_{12} I_{12} + \beta_{43} I_{43}) - \tau[\rho \mu]_\circ \{ ([\mu]_\circ - [\mu^*]_\circ) [K_{\eta=\text{cste}} - \frac{1}{\sqrt{g_{11}}} \frac{\partial[\eta, \xi]}{\partial \xi}]_\circ + ([v]_\circ - [v^*]_\circ) [K_{\xi=\text{cste}}]_\circ \} \beta_\circ I_\circ = 0$$

$$[\rho(\epsilon + \frac{q^2}{2})]^\circ I^\circ - [\rho(\epsilon + \frac{q^2}{2})]_\circ I_\circ - \tau\{ [\rho(\epsilon + \frac{q^2}{2})]_{12} ([v^n]_{12} - [\beta v^*]_{12}) + [\rho v^n]_{12} \} I_{12} + \tau\{ [\rho(\epsilon + \frac{q^2}{2})]_{43} ([v^n]_{43} - [\beta v^*]_{43}) + [\rho v^n]_{43} \} I_{43} + \tau\{ [\rho(\epsilon + \frac{q^2}{2})]_{23} ([\mu^n]_{23} - [\beta \mu^*]_{23}) + [\rho \mu^n]_{23} \} I_{23} - \tau\{ [\rho(\epsilon + \frac{q^2}{2})]_{14} ([\mu^n]_{14} - [\beta \mu^*]_{14}) + [\rho \mu^n]_{14} \} I_{14} = 0$$

Hydrodynamic quantities appearing in the numerical fluxes are determined by resolution of 1-D Riemann problems. Normal and tangential velocity components on one side of a cell edge take the curvature of the coordinate lines into account, considering (μ^k, v^n) [resp. (v^k, μ^n)] as constants along a ξ -line [resp. η -line]. In axisymmetric geometries I_0 , I^0 and I_{1j} are respectively cell volumes at old and new time-level and surface of the curved edge (1j) at the initial time.

2.3 - Second-order accuracy extension

We are working now on a second-order accuracy extension of this method.

The complete set of 2-D curvilinear moving grid hydro equations is first splitted into two 1-D hyperbolic systems

$$\frac{\partial}{\partial t} \psi' + A' \frac{\partial}{\partial \xi} \psi' = B'$$

$$\frac{\partial}{\partial t} \psi'' + A'' \frac{\partial}{\partial \eta} \psi'' = B''$$

with
$$\psi' = \begin{pmatrix} \mu_k^n \\ v_k^n \\ \rho \\ p \end{pmatrix}, \quad \psi'' = \begin{pmatrix} v_k^n \\ \mu_k^n \\ \rho \\ p \end{pmatrix}.$$

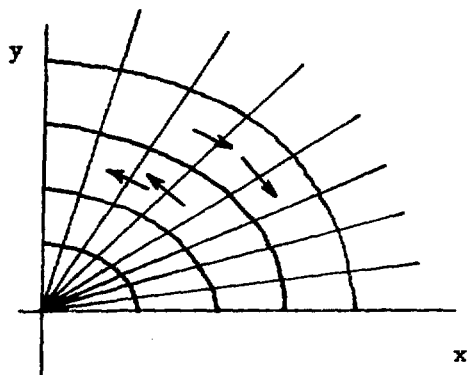
Roe's general second order method /8, 10/ is then applied to each system to derive antidiffusion fluxes.

3. - GRID GENERATION ALGORITHMS

Any grid motion that satisfies the stability condition of the explicit moving grid scheme can be used in a GAIA computation.

A simple algorithm is particularly well-suited for quasi 1-D cylindrical and spherical problems. The grid points are assumed to move in the most lagrangian way along fixed angular directions. This is done by first solving the radial Riemann problems of the 2-D grid, next interpolating the resulting fluid velocities at the grid points, and finally moving these grid points along the fixed directions with the correct velocity. The complete formula using the curvature of the cell edges are not reported here.

Such a grid motion behaves as lagrangian in the radial direction, as eulerian in the transverse direction. Since the discontinuities of tangential velocity are disregarded, interfacial slips are taken into account without particular care.



4. - NUMERICAL RESULTS

- (a) The first example fig. 1 is the shock tube problem used by Sod /7/. The tube extends from $x = 0$ to $x = 1$ and is divided into 100 equal cells. A perfect gas is initially at rest with $p = 1$, $\rho = 1$ for $0 \leq x < .5$, $p = .1$, $\rho = 0.125$ for $0.5 \leq x < 1$ with $\gamma = 1.4$.

The problem is run with lagrangian and eulerian grids using the second-order scheme. Reduced diffusion appears in both lagrangian and eulerian limits.

- (b) The second example fig. 2 illustrates the convergence of the Godunov method when used in reactive flow.

The stationary reaction zone of a plane 1-D detonation wave is solved using equation of state (2) for the mixture of condensed and gaseous components. One can check the good agreement with the Z.N.D model. The numerical points are well aligned along the Rayleigh line between the C.J state and the von Neumann spike. The pressure-burn fraction profile is also in agreement with the EOS dependent theoretical solution.

- (c) The 2-D capabilities of the GAIA code are illustrated fig.3 by the computation of a hypersonic flow around a compressible sphere. Such a calculation was first presented by Noh /2/ with the Coupled Eulerian-Lagrangian code.

An unique computational domain is now considered. Very important slip is noticeable on the flow velocity diagrams. However, no particular smoothing is applied to the interfaces and the logical grid connectivity is maintained during the whole calculation.

CONCLUSIONS

Designed for applied physics problems, the GAIA hydrodynamic computer code offers specific advantages over its Lagrangian, Coupled Eulerian-Lagrangian or Arbitrary Lagrangian-Eulerian counterparts [2, 3, 5, 11].

Thanks to curvilinear coordinates, this code provides cheap computations for quasi 1-D flows, requiring few grid points in the transverse direction.

In truly 2-D flows :

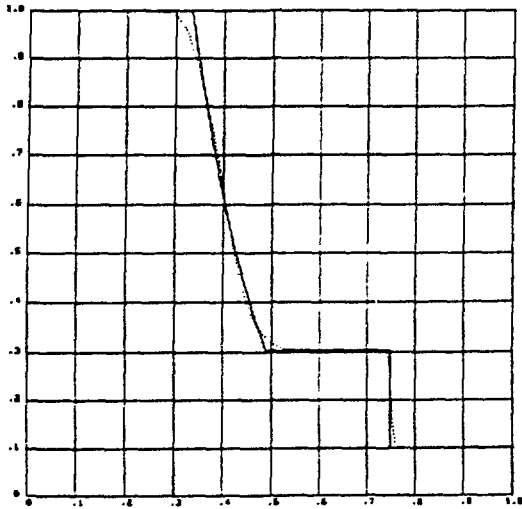
- shocks are well resolved especially at the interfaces,
- the moving grid scheme allows continuous rezone without excessive numerical diffusion, a dramatic contribution to the overall code robustness,
- slip lines can be handled without specific treatment using a simple connected grid.

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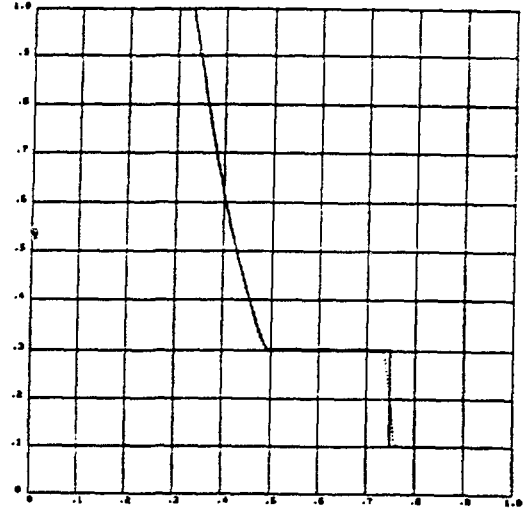
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FIGURE 1

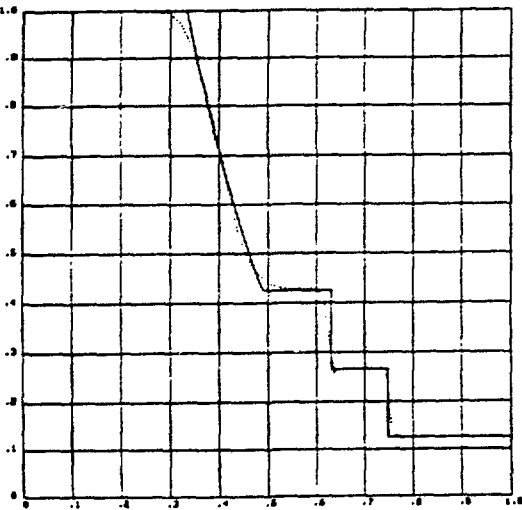
SLP PROFILE-03



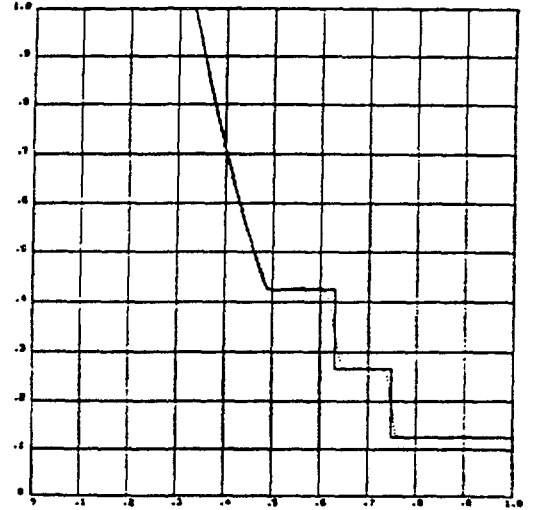
SLP PROFILE-02



SLP PROFILE-04



SLP PROFILE-01



LANGRANGIAN : MIN-MOD LIMITER

EULERIAN : SUPERBEE LIMITER

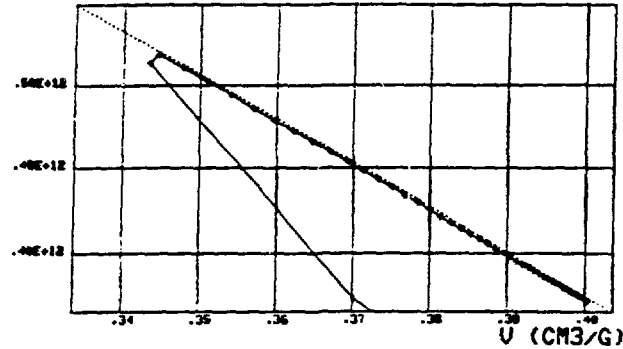
HYDRODYNAMIQUE G A I A
 DETONIQUE
 1-3
 EXPLASIF FICTIF
 PUN=254 KGRS, PCJ=335 KGRS

DETONO = 1.844 (G/CM)
 PCJ = 8850. (R/S)
 GUPVPCJ = 2.31
 MAILLAGE: 4. COUCHES/CM
 C.F.L. : .9

RESOLUTION
 ZONE DE REACTION
 STATIONNAIRE

LAMB=	.000	PMAT=	.28E+07	U=	.41E+01
LAMB=	.000	PMAT=	.45E+09	U=	.28E+03
LAMB=	.012	PMAT=	.63E+11	U=	.68E+06
LAMB=	.151	PMAT=	.37E+12	U=	.28E+06
LAMB=	.261	PMAT=	.51E+12	U=	.28E+06
LAMB=	.351	PMAT=	.58E+12	U=	.28E+06
LAMB=	.440	PMAT=	.51E+12	U=	.31E+06
LAMB=	.521	PMAT=	.56E+12	U=	.31E+06
LAMB=	.584	PMAT=	.48E+12	U=	.30E+06
LAMB=	.638	PMAT=	.48E+12	U=	.30E+06
LAMB=	.688	PMAT=	.48E+12	U=	.30E+06
LAMB=	.735	PMAT=	.47E+12	U=	.30E+06
LAMB=	.762	PMAT=	.47E+12	U=	.30E+06
LAMB=	.792	PMAT=	.48E+12	U=	.30E+06
LAMB=	.818	PMAT=	.48E+12	U=	.30E+06
LAMB=	.841	PMAT=	.48E+12	U=	.30E+06
LAMB=	.851	PMAT=	.44E+12	U=	.27E+06
LAMB=	.870	PMAT=	.44E+12	U=	.27E+06
LAMB=	.884	PMAT=	.43E+12	U=	.27E+06
LAMB=	.897	PMAT=	.43E+12	U=	.27E+06
LAMB=	.910	PMAT=	.43E+12	U=	.28E+06
LAMB=	.928	PMAT=	.44E+12	U=	.28E+06
LAMB=	.945	PMAT=	.41E+12	U=	.28E+06
LAMB=	.959	PMAT=	.41E+12	U=	.28E+06

PRESSION (CGS) — DROITE DE RAYLEIGH



(P-PCJ)/(PUN-PCJ) — SOLUTION THEORIQUE

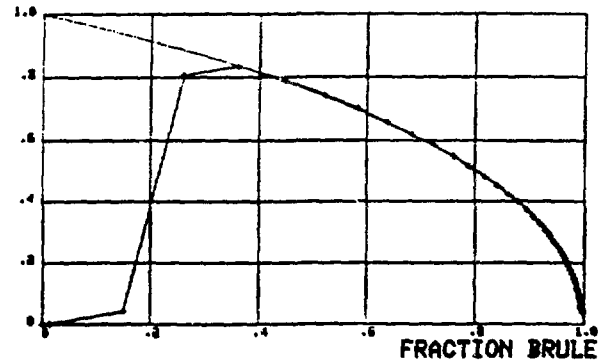
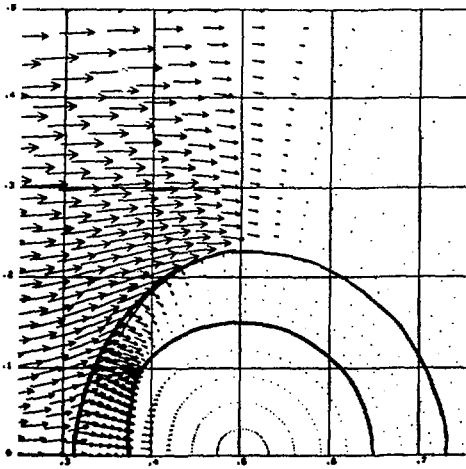


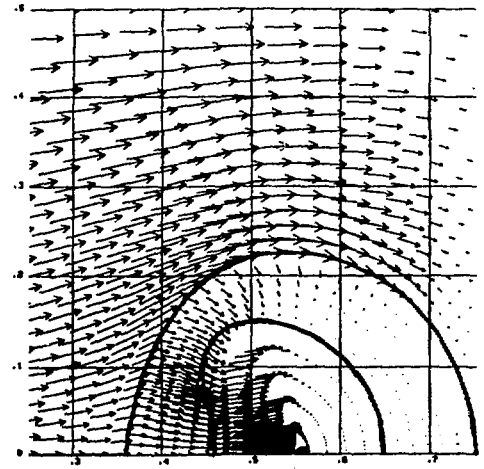
FIGURE 2

FIGURE 3

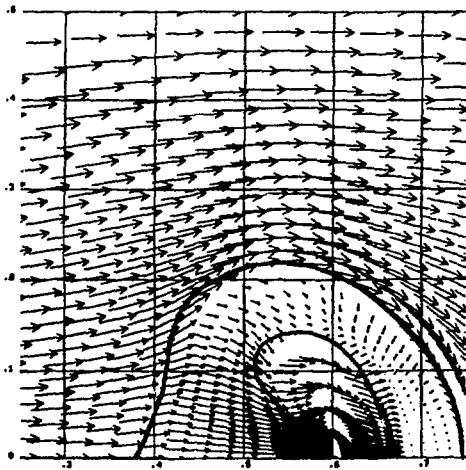
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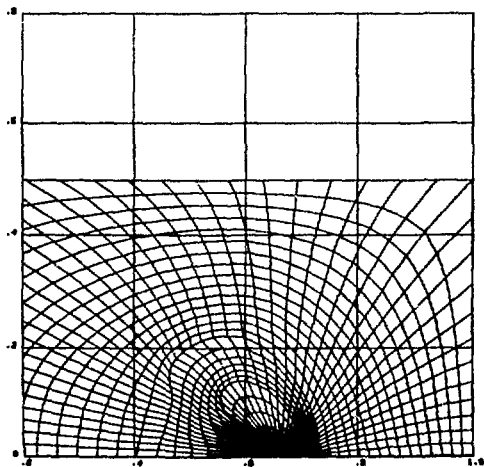
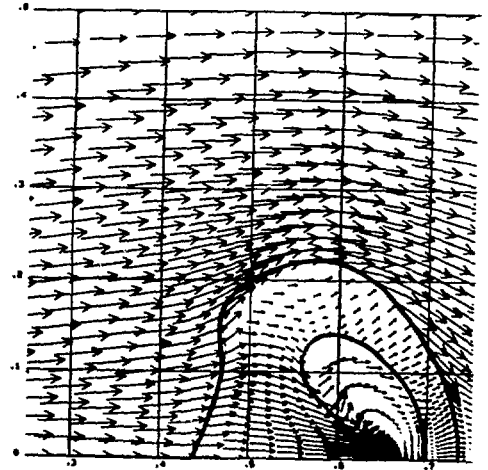
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063211003



FINAL TIME GRID

FRONT TRACKING FOR A TWO-DIMENSIONAL DETONATION FRONT

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FRANCE

RESUME

Ce papier présente une méthode qui permet, dans le cas des explosifs très rapides, de représenter et de faire avancer le front de détonation. Cette méthode a été appliquée aux détonations C-J et permet de retrouver le bon écoulement aval tout en imposant un état C-J sur le front. Le schéma numérique utilisé est celui de Van Leer ; il a été étendu à la dimension deux par la méthode des directions alternées.

ABSTRACT

Even for very reactive explosives it is difficult to get, in numerical computations, accurate pressures behind the detonation front. For two-dimensional computations, especially when the scheme used for solving the flow's equation is Eulerian with an alternate directions sweep, many geometrical difficulties arise. The method presented here is one solution to this problem. The front is represented by segments parallel to the axes and is redefined after each sweep.

Van Leer's scheme is used for solving the flow's equation. The given examples will show that we can get with this method almost as good results as in one-dimensional computations.

1 - INTRODUCTION

Front tracking methods have shown their interest in many 1-D computations. Unfortunately their extension to 2-D problems is not easy and the difficulties have hindered their development. This paper will describe one 2-D front tracking method for detonation front.

The choice of the method has been determined by the numerical scheme used for solving the flow's equations. Namely the Euler equations are solved on a

regular grid by an alternate directions sweep. Each sweep is the application of Van Leer's scheme [1] in the appropriate direction. Thus the front is defined after each sweep and it is built of segments parallel to the axes. This explain the complexity of the method.

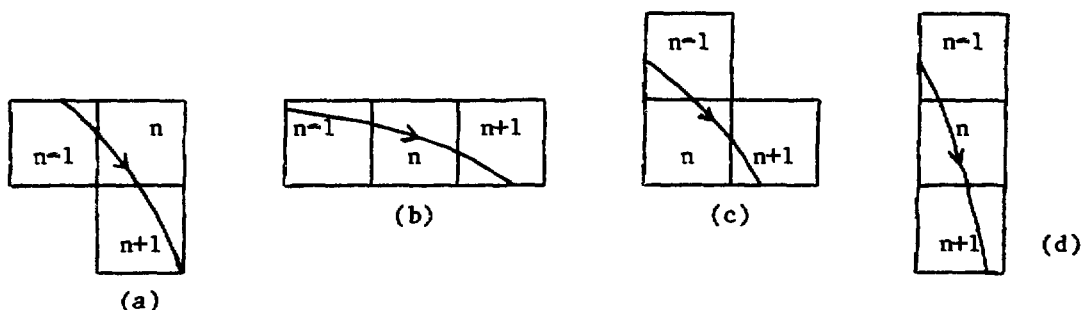
Four steps are used in order to define the front, its curvature and its normal directions. These steps are presented in Section 2. Section 3 will describe the three different ways used to solve the Euler equations : for burnt cells, mixed cells and newly burnt volumes. The results for C-J detonations are presented in Section 4. Finally Section 5 is the conclusion.

2 - FRONT DISCRETISATION

In this section the distribution of burnt products is supposed to be known for each cell. From these data a broken line is built through all the mixed cells, i.e. all cells where burnt products and unburnt explosive can be found. This line will be the detonation front approximation and will be used for the following computations. It is built in four steps.

The detonation front is a discontinuity line going through only some of the cells. The first question to solve is thus to determine those cells, the mixed cells. In our approach we suppose that for each point of the front the normal vector has positive coordinates. Thus if we go from left to right and from top to bottom, the front is going into a mixed line through the top side or the left side and going out through the right side or the bottom side ; and we can number the mixed cells as follows.

The first mixed cell is the top mixed cell of the first column. If we know a mixed cell and its number the next mixed cell is either the cell below or the cell to the right. The last mixed cell is on the bottom line and has no mixed cell on the right.

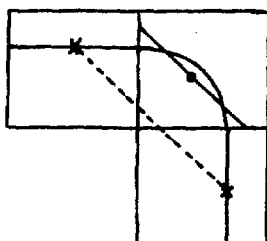


The second step is based on this result : all the lines going through a cell from the left side to the right side and defining two zones of constant surface have a common point on the vertical median.



Thus in the mixed cell of type b or d we define a point of the front by supposing that this front is straight in the cell.

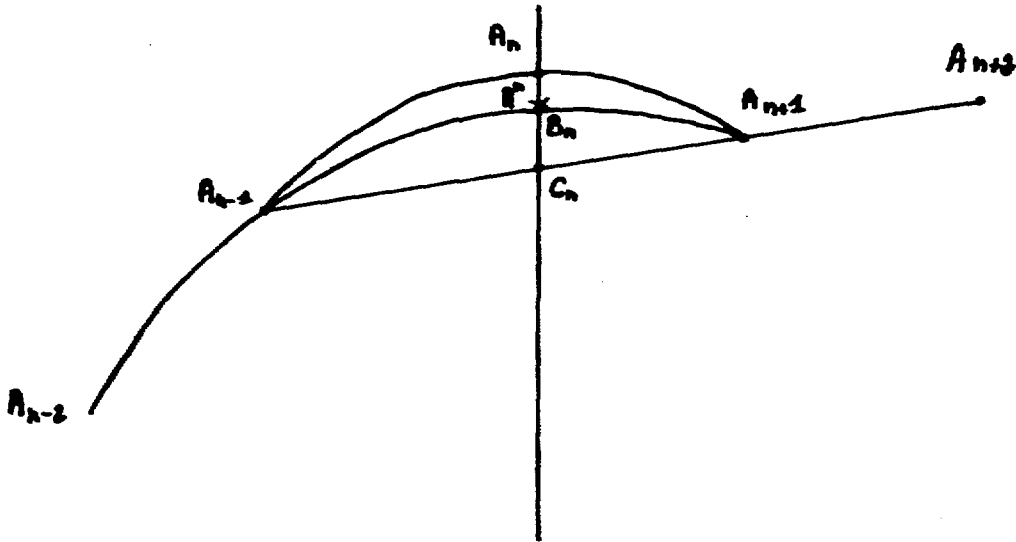
For the other cells, either a point has been defined in the previous cell either we can get a point as above by considering the two cells together. A second point is defined by considering, now, the next cell. Finally there is only one segment parallel to the segment defined by the two previous points and delimiting the right surface for the burnt products. The mid-point on that segment will be the point associated to the cell.



All these points determine a line which, except when the front is a straight line, needs to be smoothed. The smoothing will allow to define a normal direction and a curvature but it will in no way change the distribution of detonation products.

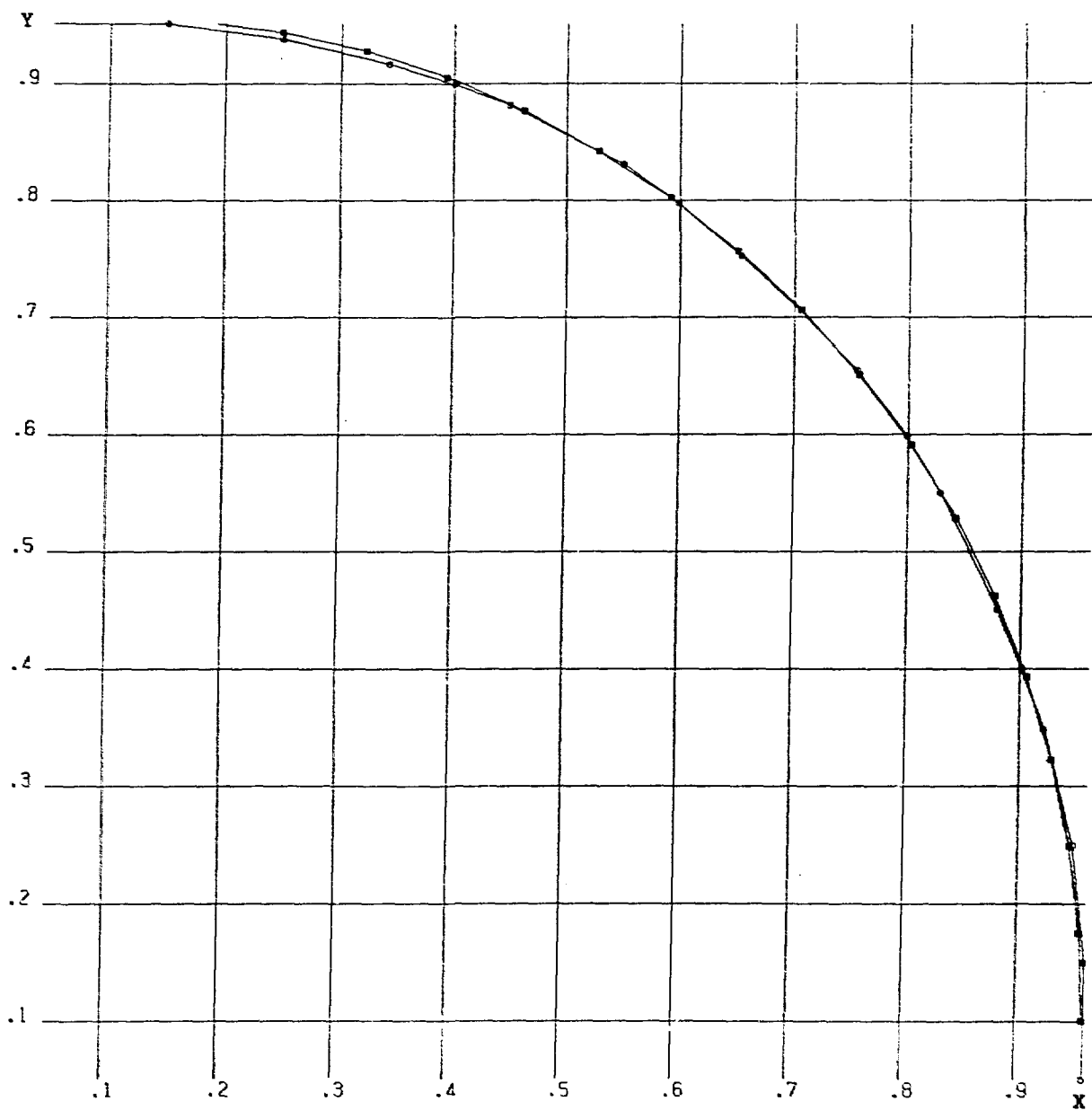
Let A_n be the point defined for the mixed cell of index n . The circle going through the points A_{n-1} , A_{n+1} determines a normal direction and a curvature for the detonation front at point A_n . Let thus Δ_n be the normal line through A_n . Then B_n is the point of Δ_n such that A_{n-2} , A_{n-1} , B_n , A_{n+1} are, in this order, on a same circle. We define in the same way the point C_n with Δ_n and the points A_{n+1} , A_{n+2} .

The smoothing will replace A_n by the mid-point A_n^n of the segment between A_n and the mid-point of $B_n C_n$, when all the points $B_n C_n$ have been defined. This smoothing can be applied many times.



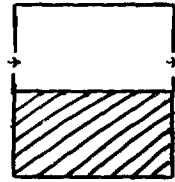
Once everything has been done we get for each mixed cell, a point, a normal direction and a curvature. This will allow us to define the geometry on which the numerical scheme will be applied, and then to advance the front in the right direction.

If the mixed cell is in configuration (b) or (d) the front will be represented in this cell by an horizontal or vertical straight line.

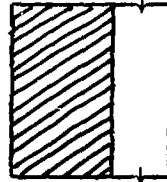


THE SMOOTHED FRONT AND THE THEORETICAL FRONT

($\Delta x = 0.1$)



(b)



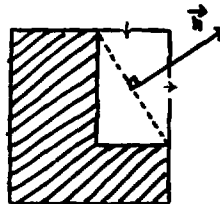
(d)

In case of configuration (a), the burnt products are represented by a rectangle in the lower left corner of the mesh :



(a)

Finally in case of configuration (c), the unburnt explosive is represented by a rectangle in the upper right corner of the mesh :

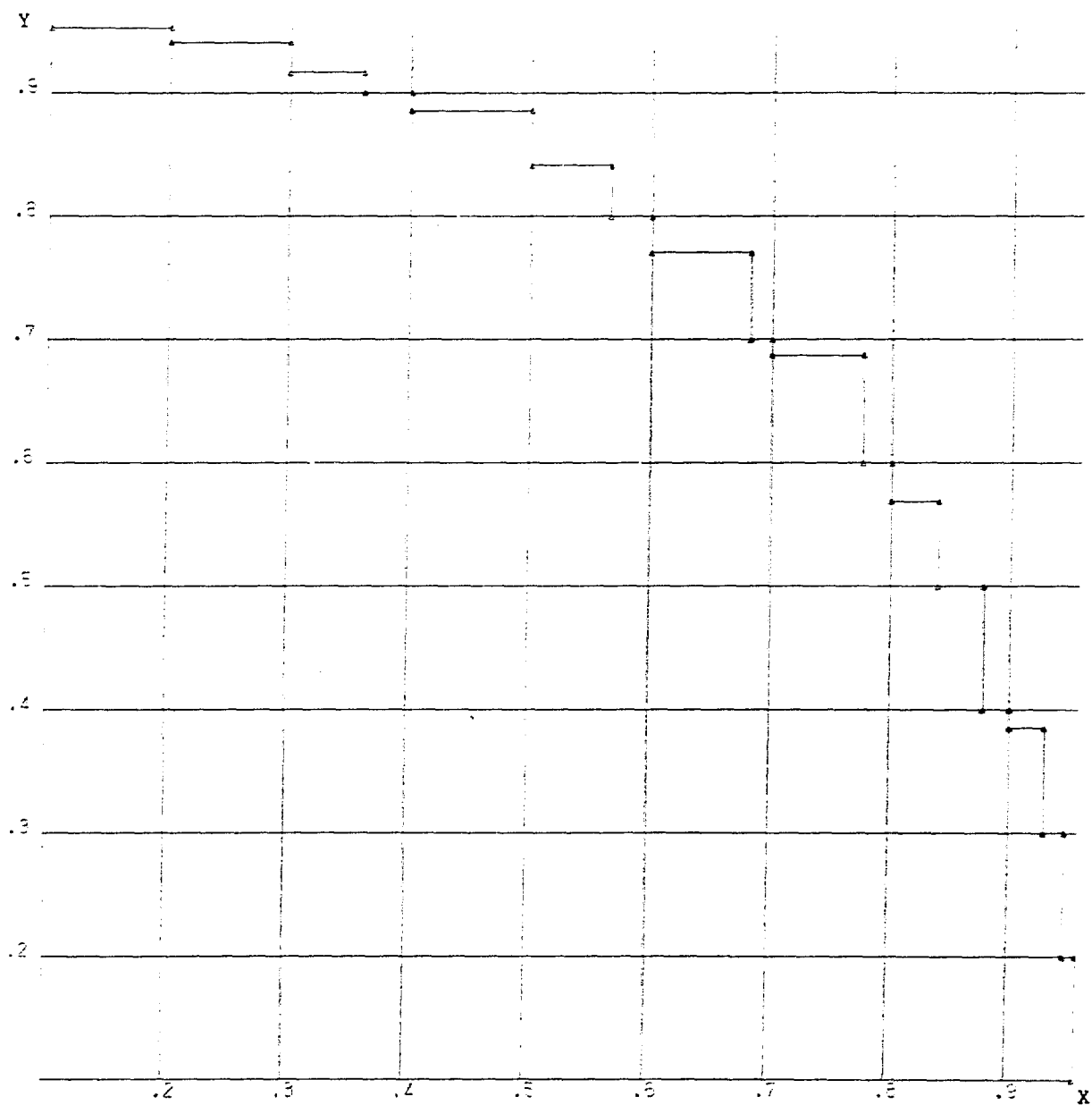


(c)

In the two last cases the rectangles are defined in order that the NW-SE diagonal and the normal direction defined for the mesh are perpendicular. At the end the detonation front will be represented by a broken line whose segments are all parallel to the horizontal or vertical directions.

3 - FRONT'S PROPAGATION AND COUPLING WITH VAN LEER'S SCHEME

We have made the hypothesis that at initial time the explosive is at rest, but we have still to solve the Euler equations for the burnt products. The method chosen is an alternate directions method where each monodimensional sweep makes use of Van Leer's scheme [1]. Moreover in order to keep second order accuracy, a computation will be decomposed in a certain number of iterations. One iteration is the



THE DISCRETIZED FRONT

succession of an horizontal sweep, a vertical sweep with the same time-step, a second vertical sweep for another time-step and finally a second horizontal sweep with this same time-step.

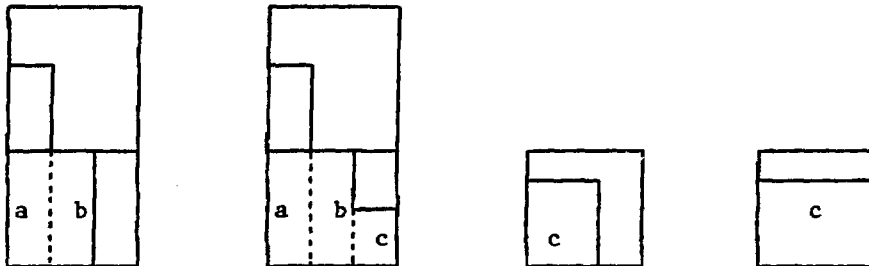
Horizontal sweep and vertical sweep are similar such that we need only to know how to do a vertical sweep for example.

For all completely burnt cells the sweep will consist of a simple application of Van Leer's scheme.

For mixed cells it is much more complex since we have to consider not only the products burnt at the initial time but also the products burnt during the time-step.

Let us handle first the already burnt products.

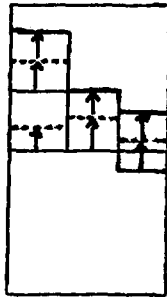
Thus for a vertical sweep the burnt products in each mixed cell are vertically cut into one, two or three parts, as shown below for every occurring case :



Then mass, momentum and total energy are distributed in each of these portions by using the slopes of these quantities in the horizontal direction. Finally the Lagrangean step of Van Leer's scheme can be applied at each of the portions a, b or c, by solving the appropriate Riemann's problems at the top and using a common Riemann's problem for the bottom.

Only the portions b and c are bounded by the front. In these portions the front is translated by using the vertical component of the front speed. This will determine two new zones, corresponding to products burnt during the time step. In these zones we can define mean values for the density, the velocity and the specific total energy by using the conservation laws. On the other hand, the slopes will be determined in order to get the right states on the front. Only the vertical components of the gradients are thus defined.

Finally all the quantities above are remapped in the right cell of the Eulerian grid. Moreover the newly burnt zones will allow to define the new distribution of burnt products. In the totally burnt cells the gradients have been defined by the remapping step, while for the mixed cells the gradients will be determined after definition of the new geometry of the front in order to get again the right states on the front.



4 - RESULTS

The method presented above has been tested on three different configurations.

The first example is the case of a plane C-J detonation front making an angle of 45° with the horizontal and vertical lines. The boundary conditions have been chosen in order to keep, as well as possible, the flow monodimensional. At the initial the burnt products are in a triangle $(5,5,5\sqrt{2})$. After 50 iterations, i.e. 100 time-steps, the front is still a quasi straight line and the results are quite as good as in 1-D computations.

The two other examples are the study of C-J cylindrical or spherical detonations. At the initial time only $\frac{1}{10000}$ of the cell in the lower left corner is burnt, its pressure is P_{CJ} , its density ρ_{CJ} , its velocity U_{CJ} . After more than hundred iterations, the detonation "front" which should be a circle is represented with its theoretical position on picture 1. We can see that the difference is relatively small and it is mostly explained by the difficulty to represent the front when only a few cells are burnt. In both cases, spherical or cylindrical geometry, the detonation front is the same. For the hydrodynamic quantities, which are different, the isocontours are plotted on pictures 2 and 3. We can notice that except small perturbations on the front and on the boundaries, the spherical or cylindrical properties of the flow are well preserved.

For the three computations the burnt products have been considered as a polytropic gas with adiabatic coefficient :

$$\gamma = 3.$$

The detonation front progresses with a speed whose modulus is

$$D_{cJ} = 8000 \text{ m/s}$$

and whose direction is normal to the front. The C-J state on the front is

$$P_{cJ} = 2.4 \cdot 10^{10}, \quad \rho_{cJ} = 2 \cdot 10^3, \quad U_{cJ} = 2 \cdot 10^3$$

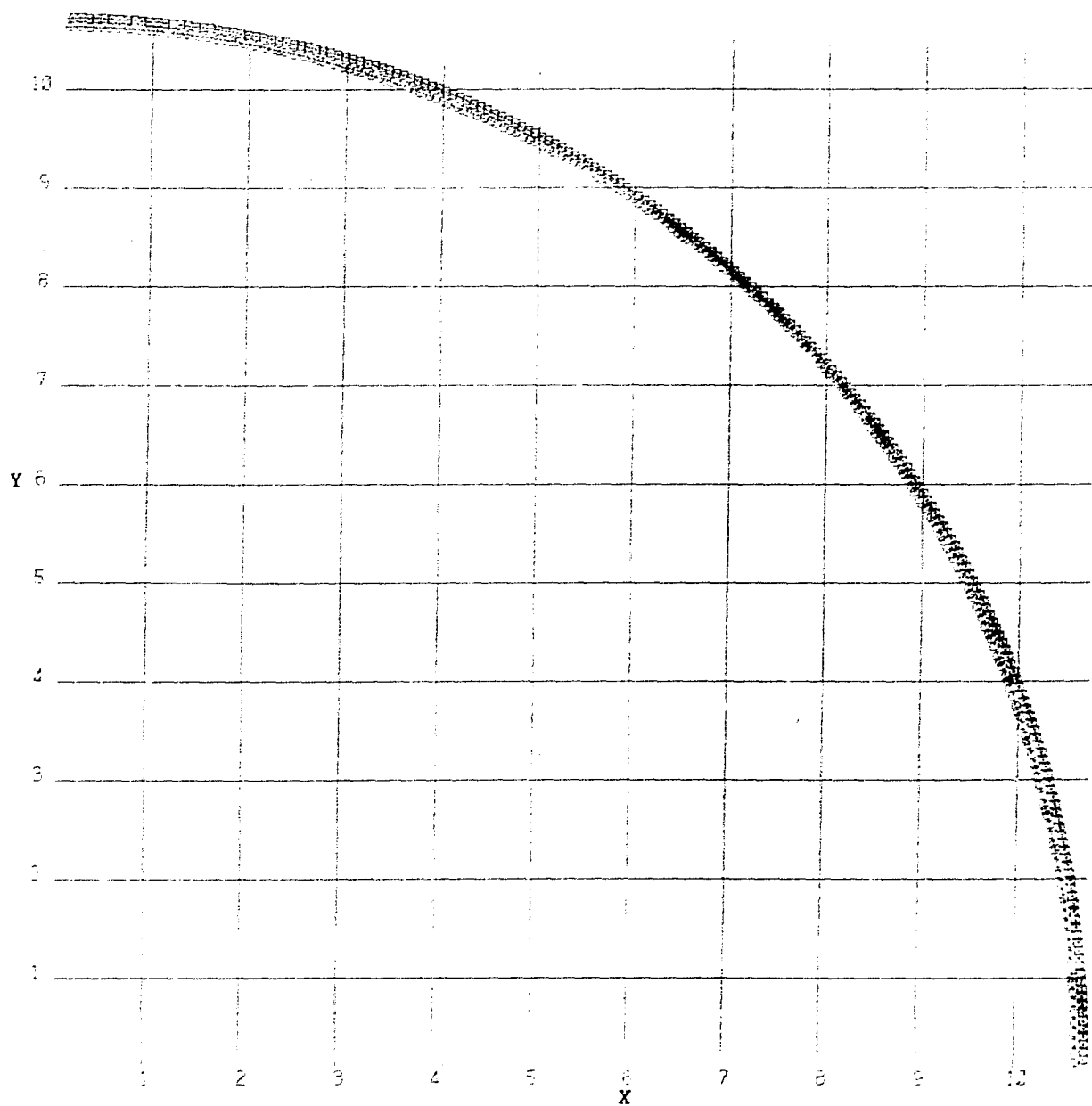
The unit system used here is the international system (SI : kg, m, s).

5 - CONCLUSION

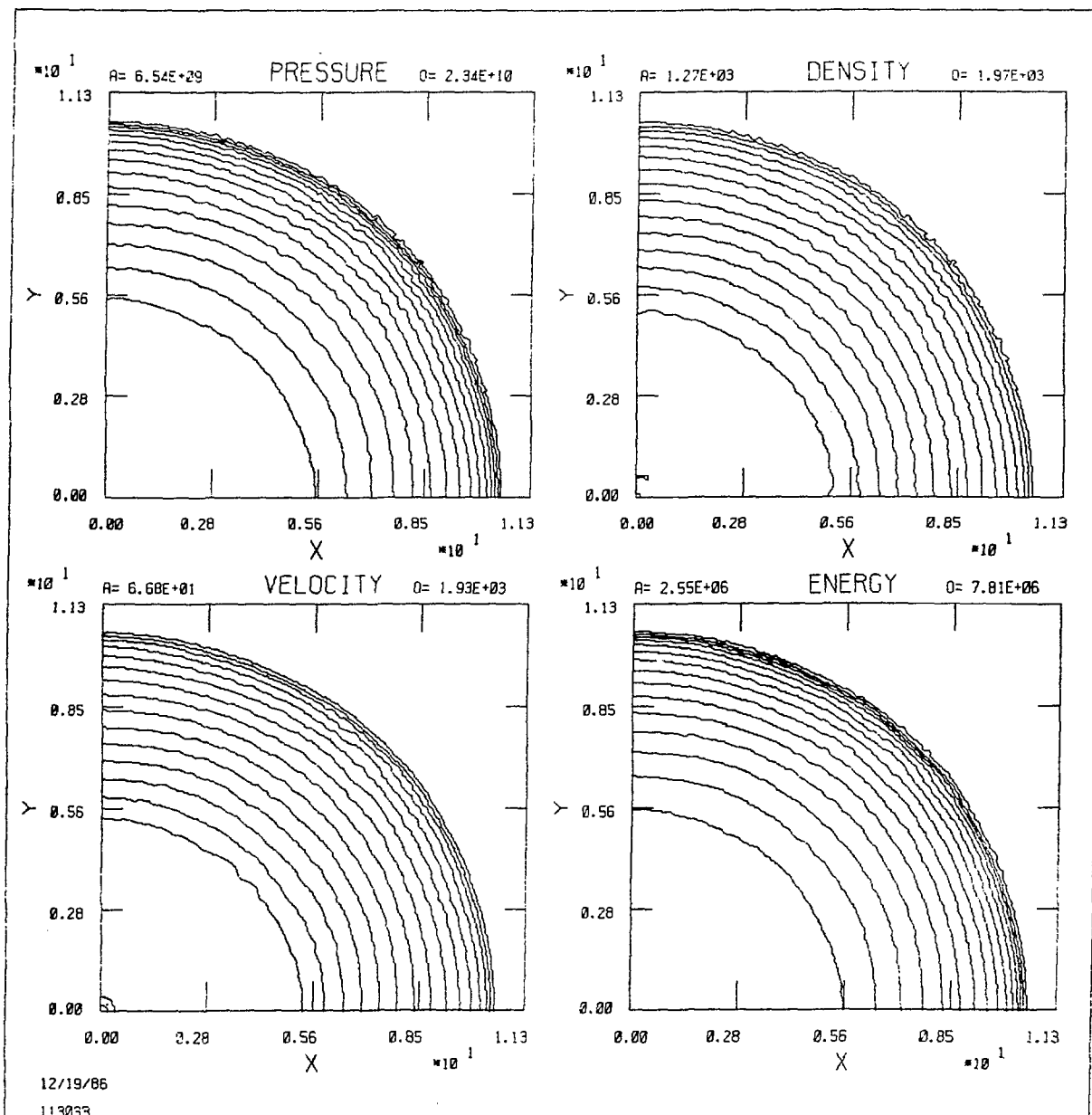
This paper has shown that it was possible to develop a front tracking method even for an Eulerian alternate directions method. This method can be easily extended to the case of shocks or of reactive shocks and then it can allow us to develop new methods for studying the behaviour of many kinds of explosive (see [2]).

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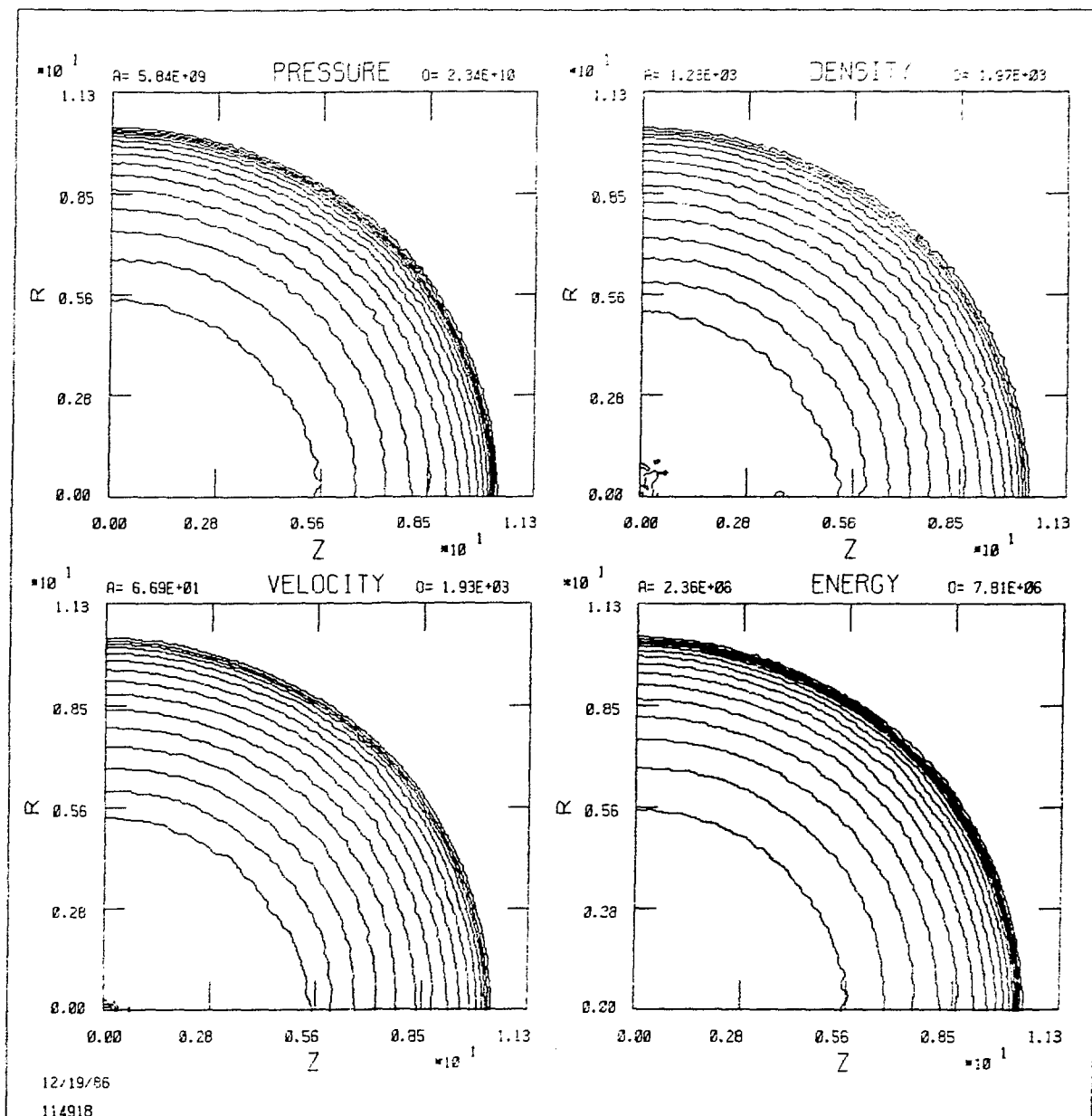
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To appear with this paper.



1 - THEORETICAL (□) AND COMPUTED (○) FRONT



2 - ISOCONTOURS IN THE CYLINDRICAL CASE
(S.I UNIT SYSTEM)



3 - ISOCONTOURS IN THE SPHERICAL CASE

(S.I UNIT SYSTEM)

NEW MODELLINGS OF MATERIAL BEHAVIOR IN THE EULERIAN HYDRODYNAMIC CODE CEE

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ABSTRACT

New constitutive equations have been added to the standard hydrodynamic behavior in the eulerian hydrodynamic code CEE. We can now compute elastic-plastic materials, and some attempts have been made to model fracture, Bauschinger effect and shear handing. An updated resolution of the equation of energy has also been implemented in order to improve the modelling of thermal softening through increased accuracy in temperature computation.

Several simulations of theoretical and experimental geometries are presented which show the interest of the new constitutive equations and the improvements in temperature evaluation.

Notations

P	pressure	ρ	density
ρ_0	normal density	e	specific internal energy
$\alpha \beta$	indices (from 1 to 3)	$s_{\alpha\beta}$	stress deviator
$\sigma_{\alpha\beta}$	stress tensor	$\delta_{\alpha\beta}$	Kronecker tensor
μ	shear modulus	Y	elastic limit
$e_{\alpha\beta}$	strain deviator	$d_{\alpha\beta}$	strain rate deviator
$\Omega_{\alpha\beta}$	rotation rate tensor	E	specific total energy
u_α	velocity	x_α	coordinate
E_c	specific kinetic energy	Δt	time increment
Δx	space increment	i	space index
n	time index	D	detonation velocity
f_i^n	if $f = f(x,t)$; $f_i^n = f(i \Delta x, n \Delta t)$		
γ	polytropic gamma		

1. INTRODUCTION

CEE is an eulerian hydrodynamic code designed in the late 70's [1] to compute unsteady flows of compressible materials in 2D geometries. As we had to compute more and more weak shocks and low velocities, it turned out that the hydrodynamic behavior assumed for the materials became unrealistic, especially for metals. We thus updated the code in order to take into account elastic-plastic constitutive equations.

We also tested the modelling of fracture and Bauschinger effect, and some attempts were made to simulate shear-handing.

This being done, a problem arose in the modelling of thermal softening : we observed that in certain circumstances, mostly in severe release waves, the temperatures were overevaluated, which could be a serious drawback when thermal softening is modelled as a function of temperature. This difficulty, which has been encountered in other codes similar to CEE [2] , has been overcome by the simultaneous resolution of the equations of total and kinetic energy after an idea already proposed in [2]. The method we used, which is slightly different from that of reference[2], will be developed thereafter.

In the second part of the paper we present several computations of theoretical and experimental geometries which show the interest of the new constitutive equations and the improvements in temperature evaluation.

2. NUMERICS

We will not discuss here on the implementation of the elastic-plastic constitutive equations which have already been presented in detail in [3][4] . Two different models are available :

- elastic perfectly plastic
- model of Steinberg et al[5] .

The simulation of the Bauschinger effect has been realized for 1D flows with the model described in [5] which assumes a linear variation of the shear modulus under unloading to account numerically for this effect.

The fracture of materials is modelled by a simple limit stress in tension : beyond this limit, full fracture is assumed in the computations (i.e. the stress is reduced to zero and a void opens freely).

We restrict here our presentation of the physical and numerical hypothesis on constitutive equations and we will focus our attention on the modifications of the resolution of the equation of energy.

2.1 Equation of energy

The computation of energy is made in CEE in the subroutine which solves the equation of conservation of total energy :

$$\frac{\partial PE}{\partial t} + \frac{\partial PE u_{\alpha}}{\partial x_{\alpha}} = \frac{\partial \sigma_{\alpha\beta} u_{\beta}}{\partial x_{\alpha}}$$

The pressure in the cells is obtained via an equation of state as a function of density and internal energy.

$$P = P(\rho , e)$$

Since only E is known, e has to be computed by a difference between total and kinetic energy :

$$e = E - \frac{1}{2} \sum_{\alpha=1}^3 u_{\alpha}^2 \quad (1)$$

U is computed in the subroutine which solves the equation of momentum. This procedure is equivalent to the simultaneous resolution of the equations of total and kinetic energy. This last one is not effectively solved, but an analysis similar to that of reference [2] shows that the scheme we should use to obtain the same result is an order 1 discretisation of the equation of kinetic energy with additional meaningless terms of the same order.

As a consequence, the kinetic energy evaluated in (1) is underestimated and the internal energy, hence the temperature, is overestimated. This phenomena is particularly severe in regions undergoing severe release waves.

In order to improve the evaluation of the temperatures, we decided to solve effectively the equation of kinetic energy together with the equation of total energy, following the method proposed in [2].

In [2] the following equation is solved (for simplicity, we restrict us to one dimension in the next lines)

$$\frac{\partial \rho E_c}{\partial t} + \frac{\partial \rho u E_c}{\partial x} = -u \frac{\partial \sigma}{\partial x} \quad (2)$$

After some tests we found more convenient to solve :

$$\frac{d(\rho E_c)}{dt} = \rho u \frac{du}{dt} \quad (3)$$

We use the explicit scheme of CEE; the complete resolution of (3) is then :

1 equation of momentum

$$\left(\frac{du}{dt}\right)_i^n = -\frac{1}{\rho_i^n} \frac{\sigma_{i+1/2}^n - \sigma_{i-1/2}^n}{\Delta x} \quad (4)$$

$$u_i^{n+1} = u_i^n + \left(\frac{du}{dt}\right)_i^n \Delta t \quad (5)$$

2 compute intermediate value of u

$$\hat{u}_i = \theta u_i^n + (1 - \theta) u_i^{n+1} \quad (6)$$

$$0 \leq \theta \leq 1$$

3 equation of kinetic energy

$$E_{c,i}^{n+1} = E_{c,i}^n + \hat{u}_i \left(\frac{du}{dt}\right)_i^n \Delta t \quad (7)$$

Several values of θ were studied; the most interesting ($\theta = 0, 1/2, 3/4, 1$) will be presented thereafter. $\theta = 1$ and $\theta = 1/2$ are special values; the first one gives the normal discretisation of equation (2) with the standard scheme of CEE; $\theta = 1/2$ determines the exact variation of E_c corresponding to the increment of u between u_i^n , and u_i^{n+1} .

3. TESTS

3.1 Release wave in detonation products

Before presenting the tests on experimental geometries, we will first show a theoretical test we performed in order to compare the schemes.

This test is the detonation of a semi infinite plate of explosive (Fig. 1).

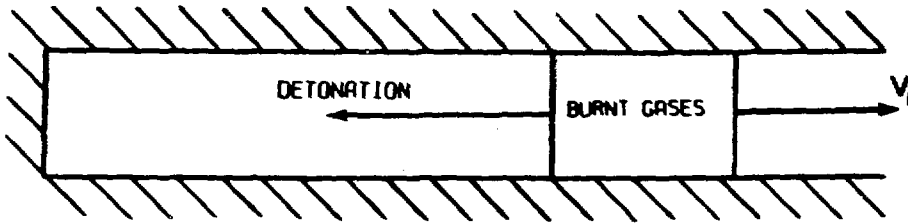


FIGURE 1 TEST 1 : PLANE DETONATION

The equation of state of burnt explosive is a perfect gas law ($P = (\gamma - 1) \rho e$). The observed quantities are the peak pressure on the detonation front and the limit velocity of expansion of burnt gases in the void.

These quantities are :

$$P_m = \frac{\rho_0 D^2}{\gamma + 1}$$

$$V_l = \frac{D}{\gamma - 1}$$

We chose $\rho_0 = 1.84 \text{ g/cm}^3$ $T_0 = 300 \text{ K}$ $\gamma = 3.15$ $D = 8700 \text{ m/s}$
thus $P_{\max} = 335.6 \text{ kbar}$ and $V_{\lim} = 4046 \text{ m/s}$.

The different schemes are compared on Fig. 2 and Fig. 3.

On Fig. 2, we can see the importance of the choice of θ on the final results. The maximum pressure increases continuously with θ . With $\theta = 3/4$, we obtain a value of P_m close to that of the standard scheme. The advantage of the modified scheme appears on Fig. 3. Contrary to the standard case where the velocities are above the theoretical velocity, this value is well reproduced in all the computations with the effective resolution of the equation of kinetic energy.

In general, the various tests we made convinced us that the modified scheme with $\theta = 3/4$ was relatively close to the standard scheme in the computation of shocks; with a better resolution in the computation of release waves. The experiments we present in the next paragraphs will then be computed either with the standard scheme or with the modified scheme and $\theta = 3/4$.

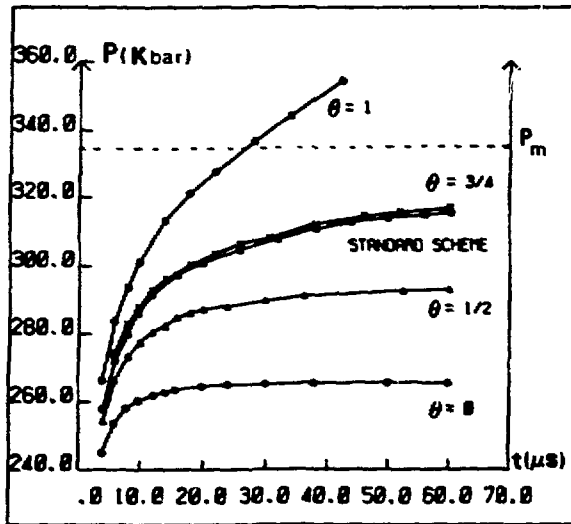


FIGURE 2 PEAK PRESSURE ON DETONATION FRONT

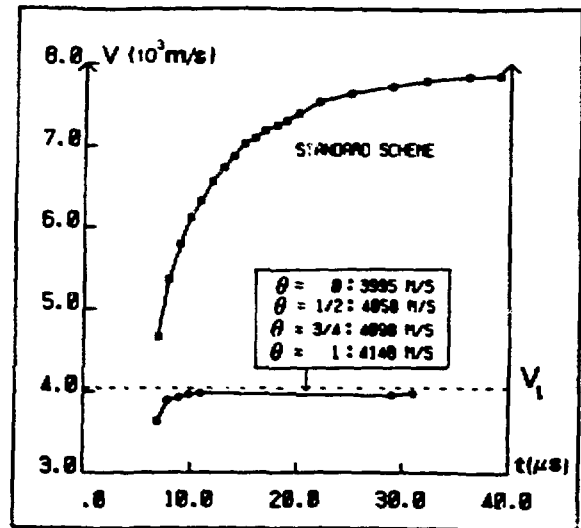


FIGURE 3 EXPANSION VELOCITY OF BURNT GASES

3.2 Numerical treatment of elastoplasticity and fracture

The computations we present now are simulations of impacts of semi-infinite plates of thickness e_p on semi-infinite plates of the same material of thickness e_c . The recorded quantity is the velocity of the free surface of the target. The characteristics of the experiments are summarized in table I.

	Aluminum	Uranium
Impact velocity (m/s)	412	143
e_p (mm)	0.76	1.534
e_c (mm)	12.7	3.018

Table I

The computations were performed with the standard resolution of equation of energy. The mesh size is 0.1 mm.

Our results are compared on Fig. 4 and Fig. 5 with experimental data published in [6] and [7].

On Fig. 4 we can see with aluminum the importance of taking elastoplastic behavior into account. With uranium, the 4 curves of Fig. 5 show the progressive improvements in the restitution of the experiments when we introduce successively the elastoplastic behavior, the Bauschinger effect and the simulation of fracture.

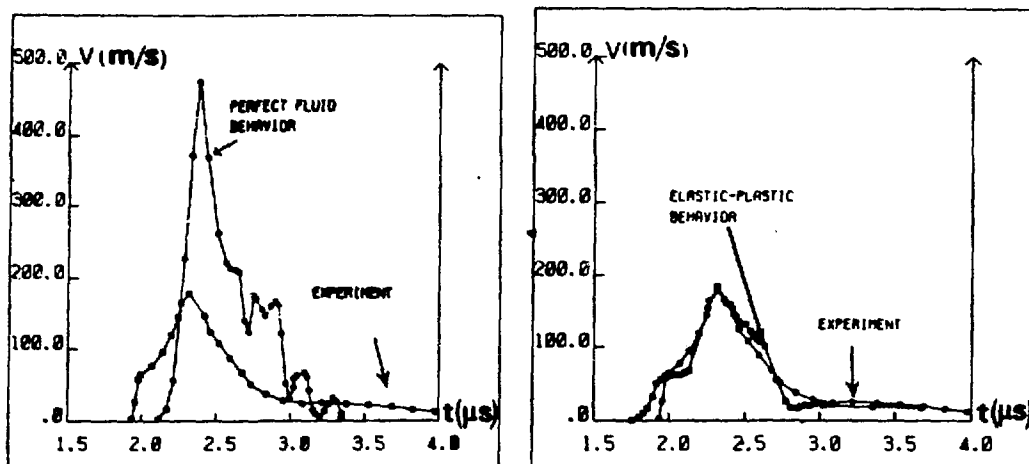


FIGURE 4 PLATE IMPACT INFLUENCE OF CONSTITUTIVE EQUATION FOR ALUMINUM

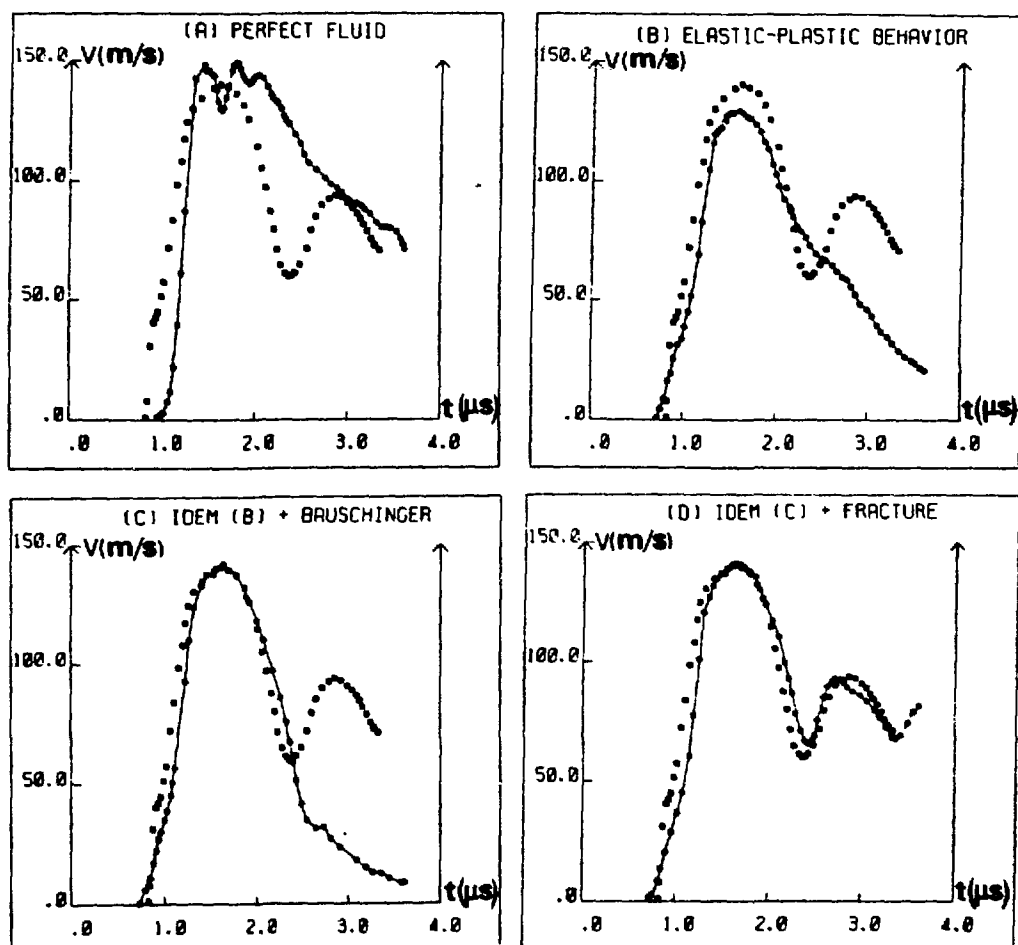


FIGURE 5 PLATE IMPACT INFLUENCE OF CONSTITUTIVE EQUATION FOR URANIUM

• • EXPERIMENT

—•— COMPUTATION

3.3 Computation of metal singularities

In this paragraph, we study the influence of plastic strains on the ejection of mass out of micronic defects under shocks loading. Experiments have been presented in [8] and [9] which show an important decrease of the ejected mass with increasing melting temperature. We have tried to evidence this observation numerically. The geometry of the defects is shown on Fig. 6.

A plane sustained shock is applied on the defect to simulate the explosive loading of the experiment. The numerical and experimental results are plotted on Fig. 7.

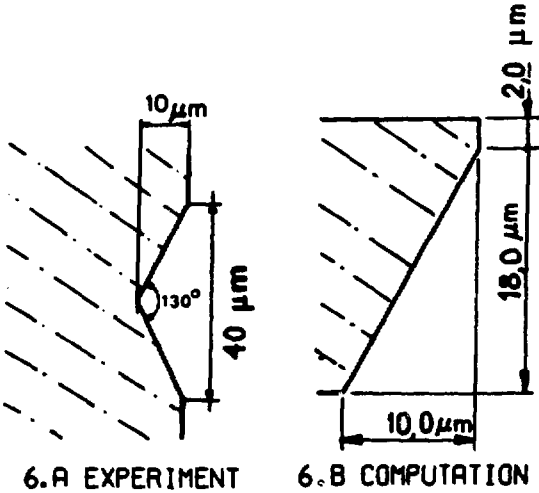


FIGURE 6 GEOMETRY OF THE DEFECTS

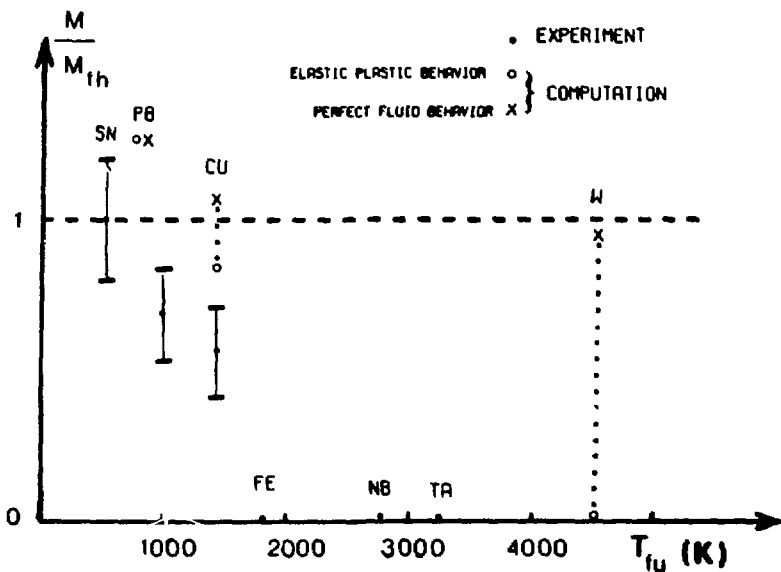


FIGURE 7 EJECTED MASSES

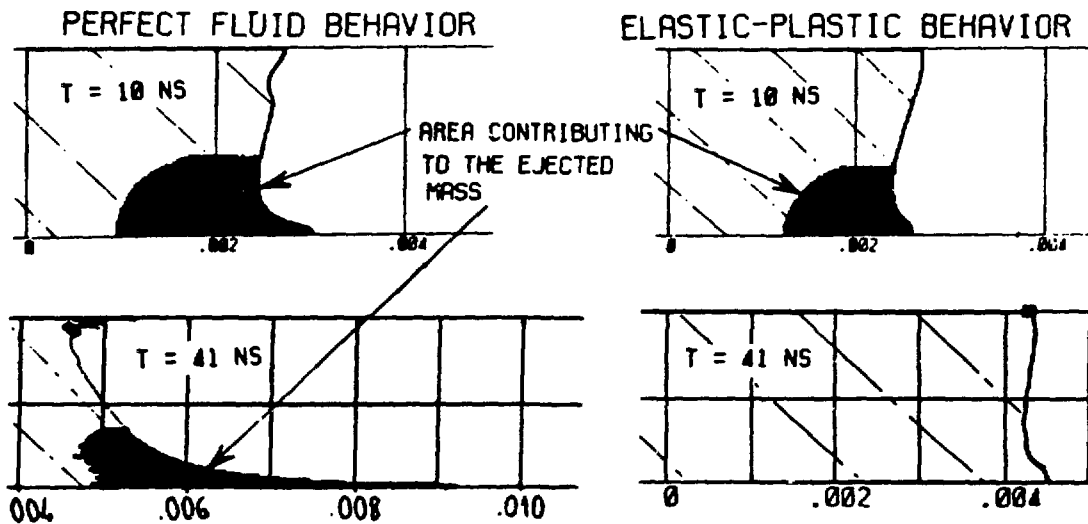


FIGURE 8 INFLUENCE OF THE CONSTITUTIVE EQUATIONS

We can see that the introduction of plastic stresses in the computations improves the numerical results .

This effect must be taken into account to simulate the experimental influence of the melting temperature on mass ejection. On Fig. 8, we can see more clearly the influence of the plastic stresses : at the early stages of the computations the jets develop similarly in hydrodynamic and elastoplastic calculations, but though the jet keeps on developing in the first case, the plastic stresses lower down the fastest particles in the second case and finally no matter is ejected.

3.4 Influence of energy evaluation

The last example we want to present now is the computation of a shaped charge named S2 (see [10]).

Two computations have been performed : one with standard resolution of the equation of energy, the other with the modified scheme and $\theta = 3/4$.

In both case, we find good agreement between computations and experiments, as far as velocities are concerned. For instance we find 7030 m/s and 6930 m/s for jet trip velocity respectively with standard and modified schemes, to be compared with 7100 m/s in the experiment.

Great differences appear however in temperature computations (see Fig. 9). The differences are such that the jet remains solid with the modified resolution when it melts with standard scheme. The temperatures computed with the modified scheme are also much closer to the measured ones (see [10])

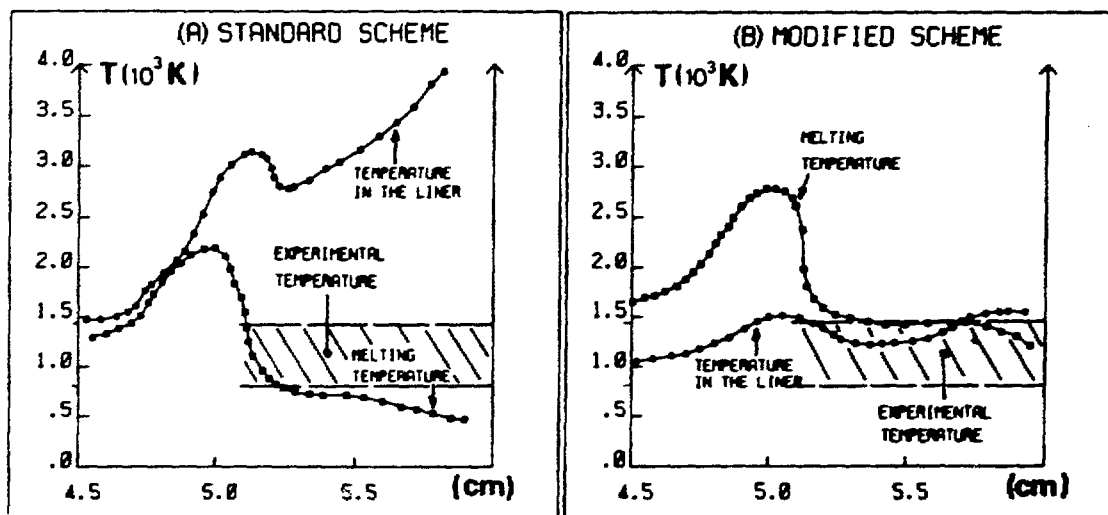


FIGURE 9 TEMPERATURES OF COPPER VS ABSCISSA AT A 0.45 MM RADIUS ($T = 7.5 \text{ MUS}$)

4. FUTURE TRENDS - CONCLUSIONS

With the new constitutive equations available in CEE and the improvement in temperature evaluation we have obtained with the modified resolution of the equation of energy, we have at our disposition an eulerian code which allows us to compute very distorted flows of various materials in a large range of pressures and velocities. Our efforts will be now to update the modelling of fracture; some work is presently done to simulate shear handing. As can be seen in Fig. 10 to 12, the results are encouraging since we can already obtain plugging in the computation of cylinder impacts which is in agreement with experimental observations [11] .

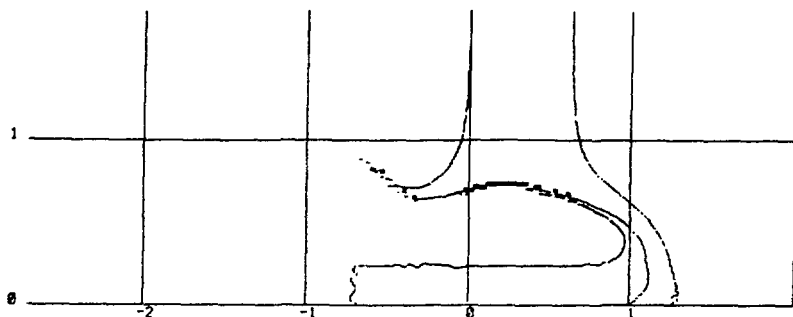


FIGURE 10 IMPACT OF STEEL CYLINDER VS TITANIUM TARGET AT 455 M/S . PERFECT FLUID BEHAVIOR

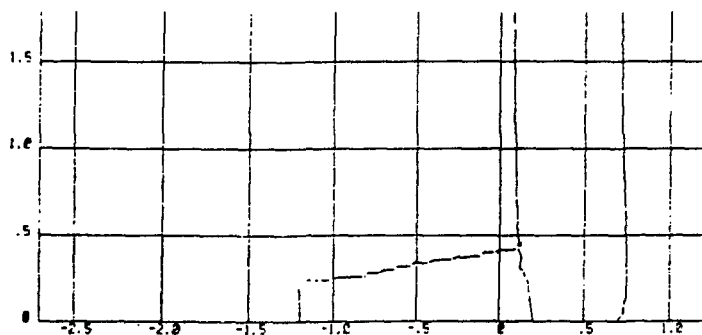


FIGURE 11 IMPACT OF STEEL CYLINDER VS TITANIUM TARGET AT 455 M/S . ELASTIC PLASTIC BEHAVIOR

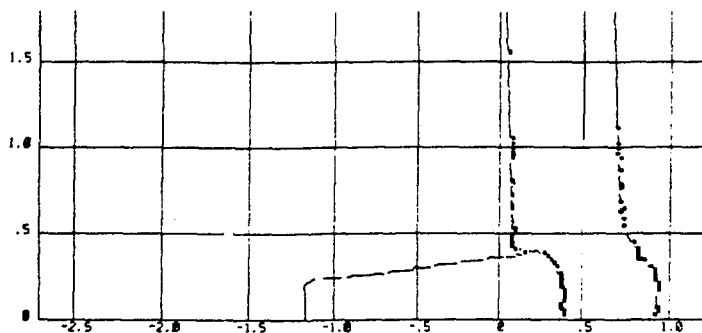


FIGURE 12 IMPACT OF STEEL CYLINDER VS TITANIUM TARGET AT 455 M/S . ELASTIC PLASTIC BEHAVIOR
SHEAR BANDING IN TITANIUM

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ADAPTIVE MESH EXPERIMENTS IN 1D HYDRODYNAMICS

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This is a preliminary study for a 2D hydrodynamic adaptive mesh algorithm. We try to give some arguments to answer the question : is a really useful 2D adaptive mesh algorithm feasible ?

For this prospective study we deliberately choosed some simplifications :

- the algorithm is uncoupled from the hydro-scheme. This allows to introduce it in an existing code, whatever the hydro scheme. We demonstrate this by using it with schemes as different as Von Neumann-Richtmyer scheme and Godunov scheme, among others.
- It is automatically switched on. The new mesh is so calculated as to serve for a few time steps.
- The algorithm by itself is fully explicit.

All this reduces the cost to an acceptable value (less than twice that of the standard scheme in most cases).

On this algorithm, we studied the effect of some variations :

- The structure function : a combination of first and second derivatives of hydrodynamic quantitatives, such as density, energy, presure, or other.
- The smothing of the structure function, which provides smootheness of the grid (ratio of succesive cells) and flattenning in the neighborhood of discontinuities.
- The rythm of adaptation, automatic or not.
- Special grid features, such as time filtering or boundary refinement, to catch new discontinuities emerging from the walls.

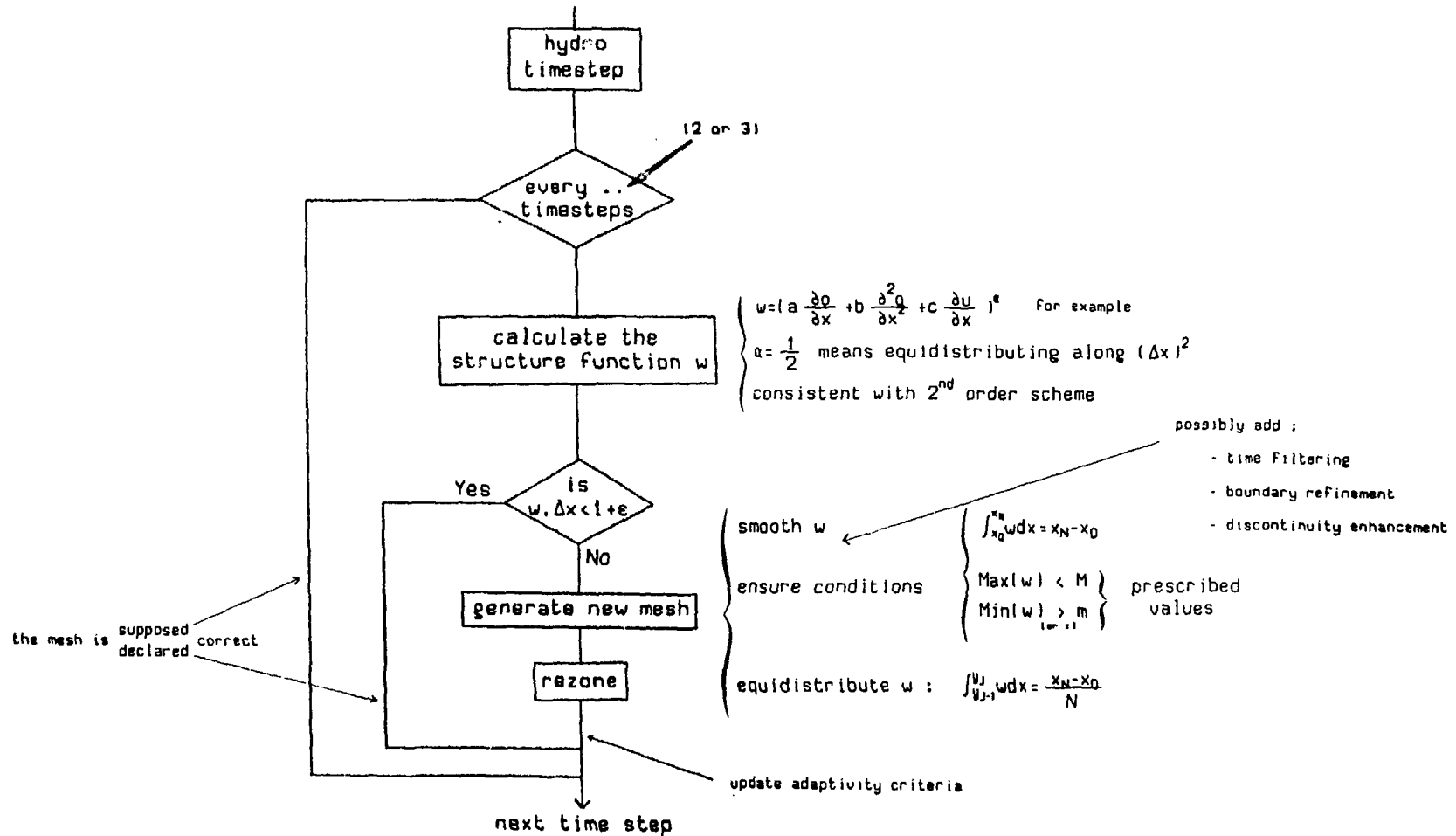
Furthermore, we try to answer some questions that arise, such as :

- Does adaptive mesh modify the scheme itself, especially concerning boundary conditions ?
- How to maintain a proper control of the time step, when a sudden change in the grid make it change rapidly ?

We illustrate all these questions by numerical tests with Sod shock tube problem, with multiple reflection of shocks on the wall and on the contact discontinuity.

It shows that it seems possible to construct a simple 2D algorithm and obtain good results, even with a scheme that is not the best possible, such as the standard Von Neumann-Richtmyer or its 2D analogous.

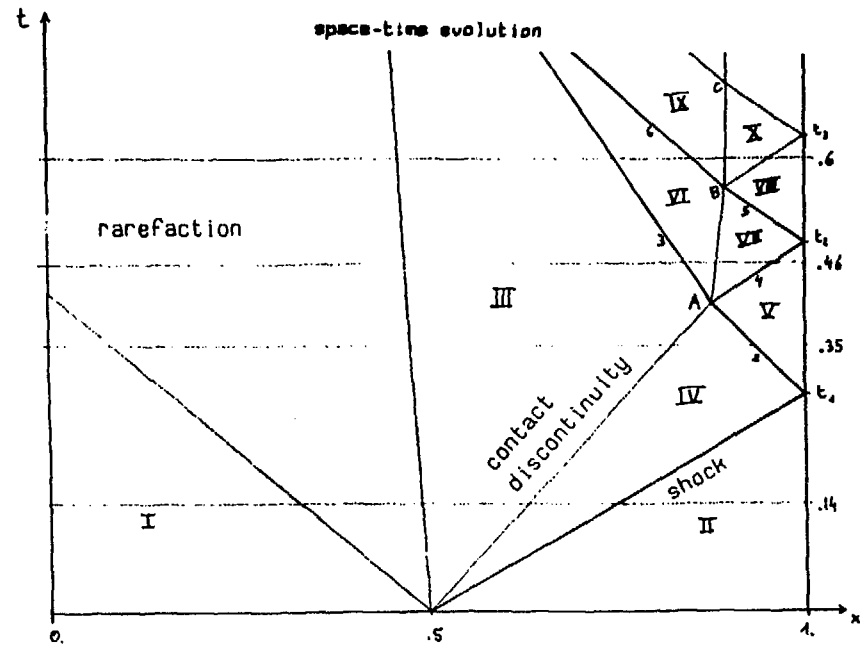
SKETCH OF THE ALGORITHM



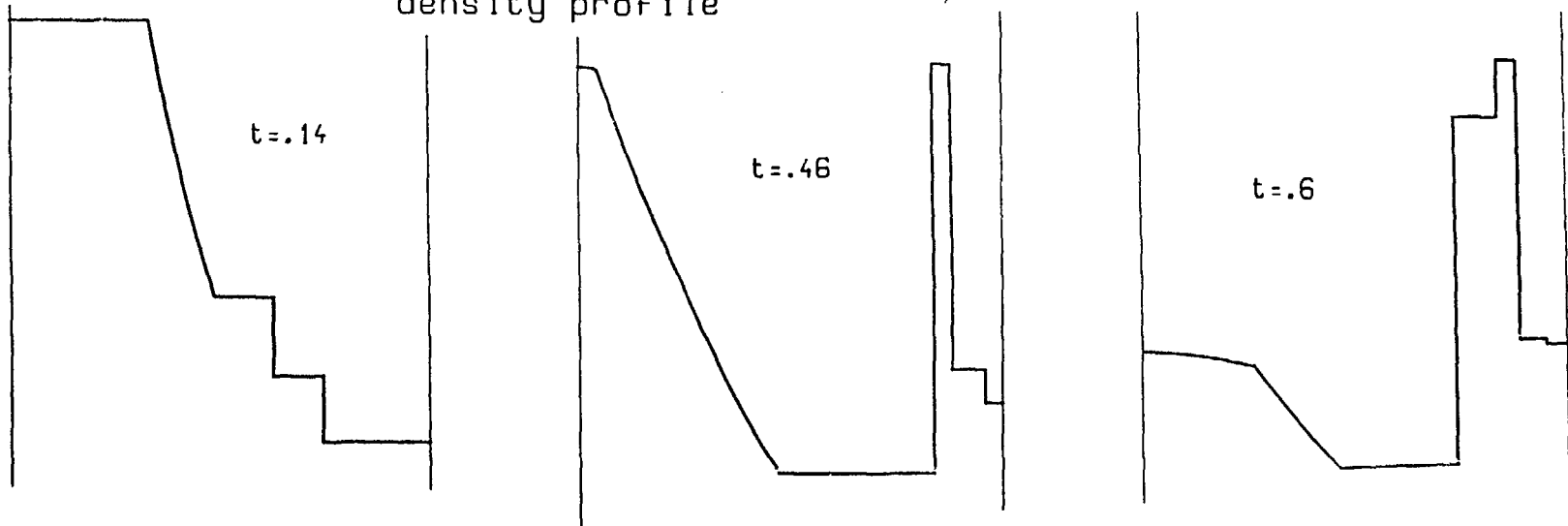
SOD SHOCK TUBE

perfect gas $\gamma=7/5$

constant states	ρ	p	u
I	1.	1.	0.
II	.125	.1	0.
III	.4263	.3031	.9275
IV	.2656		
V	.509	.780	0.
VI	.872	.864	.107
VII	.548		
VIII	.589	.955	0.
IX	.945	.966	.012
X	.593		

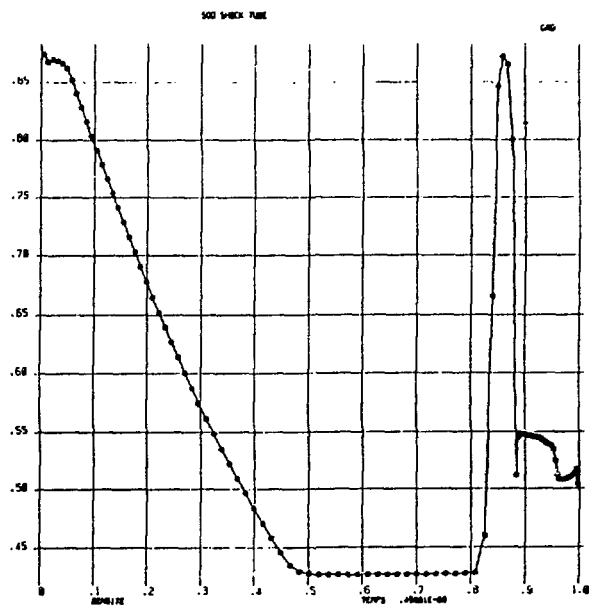
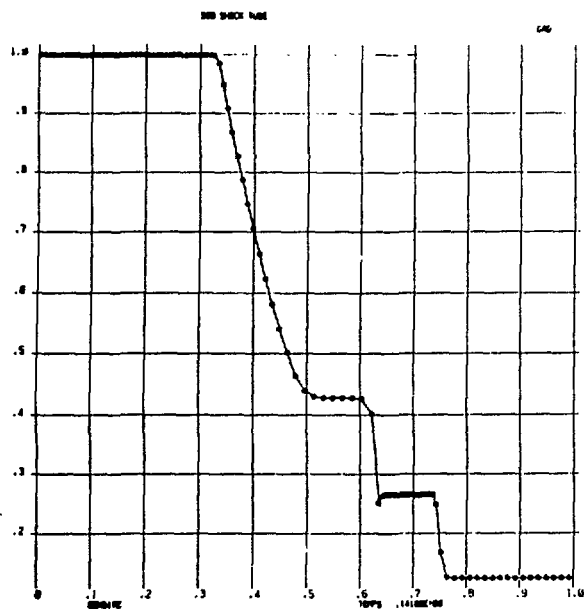


density profile

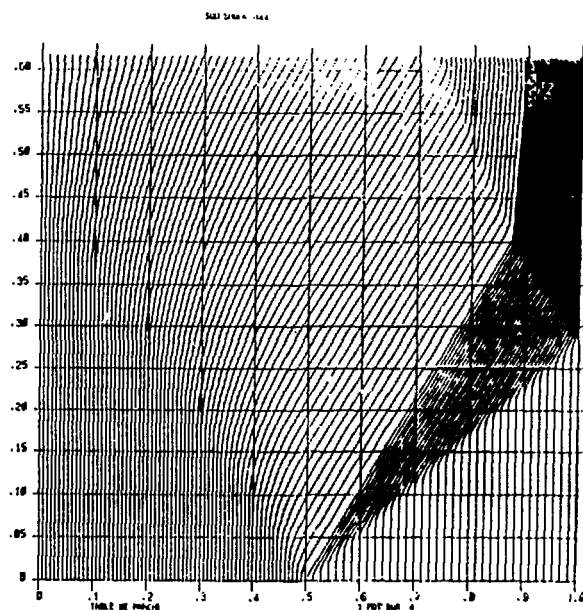
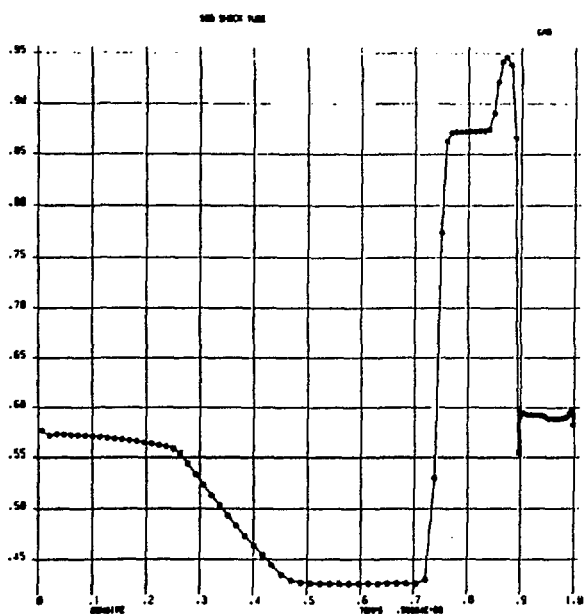


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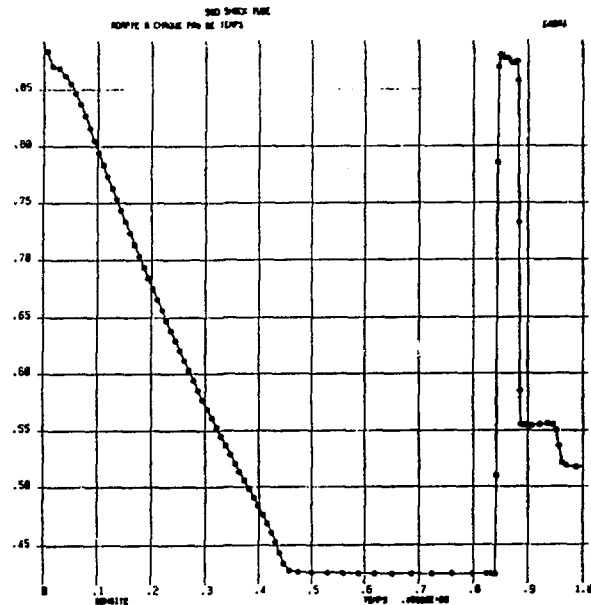
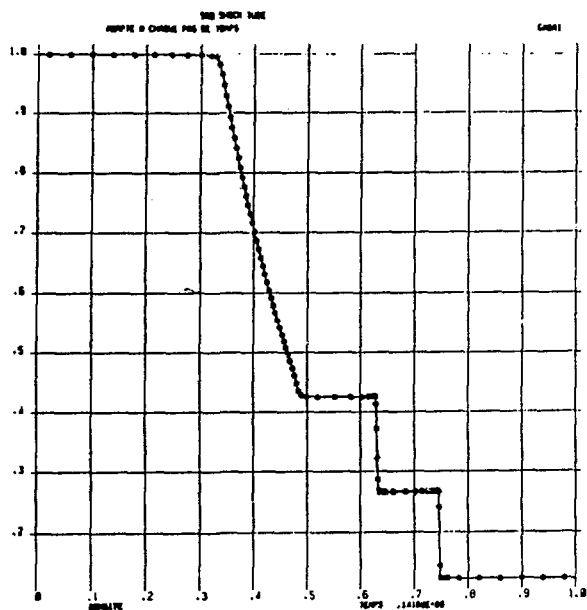
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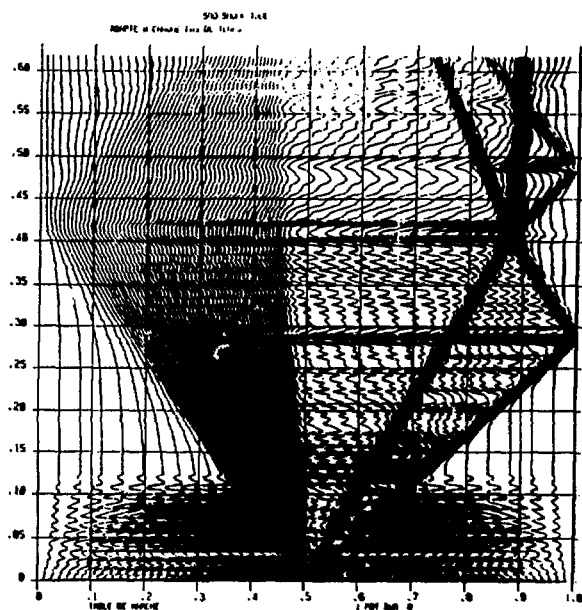
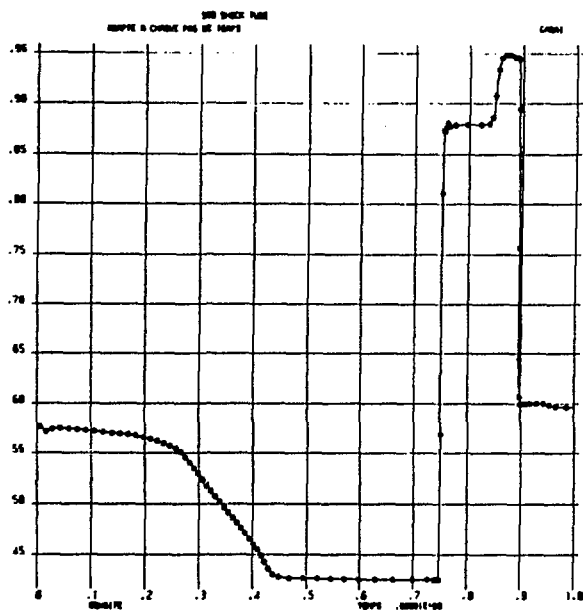
POST-PROCESSED 2ND ORDER
GODUNOV-TYPE SCHEME



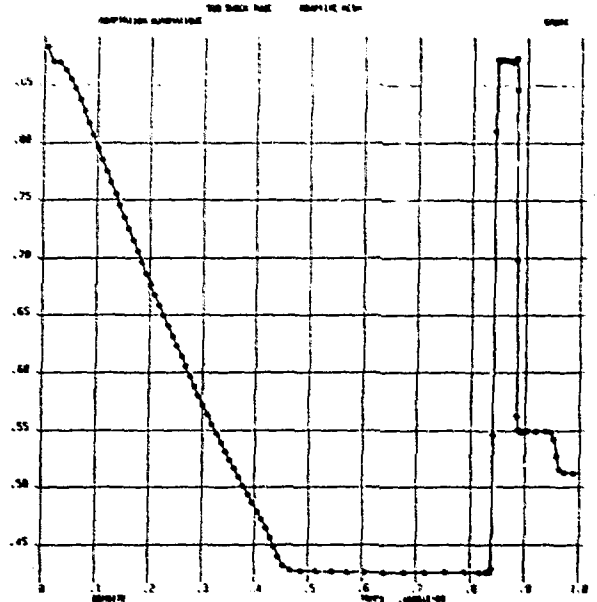
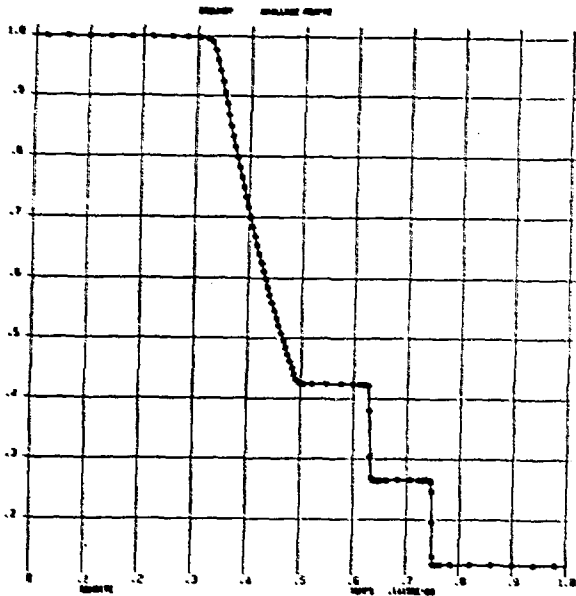
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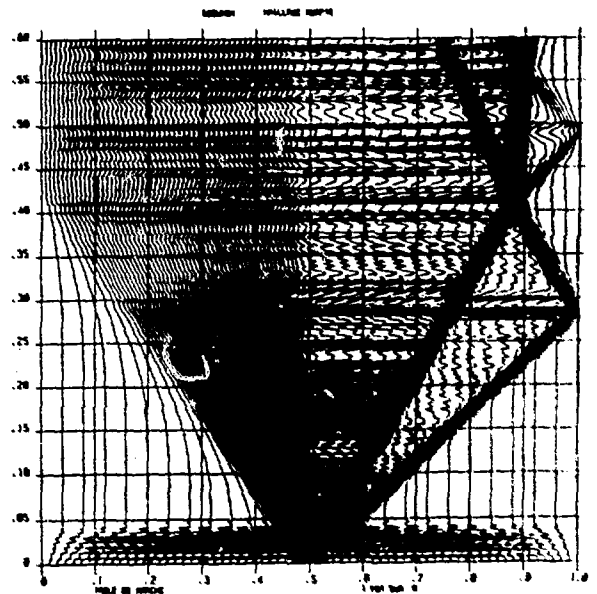
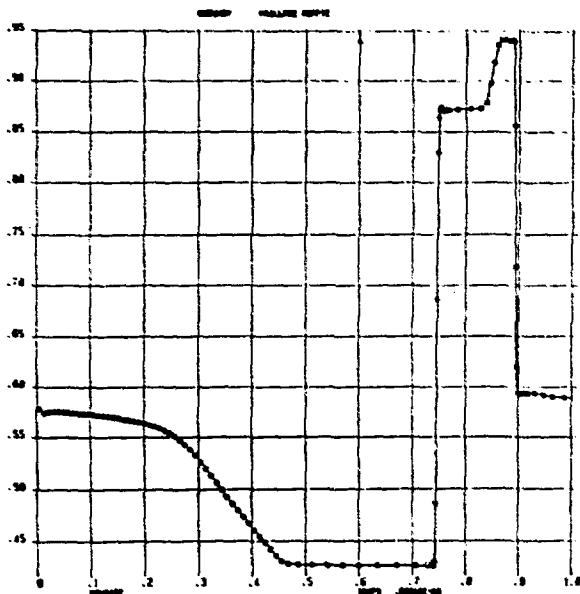
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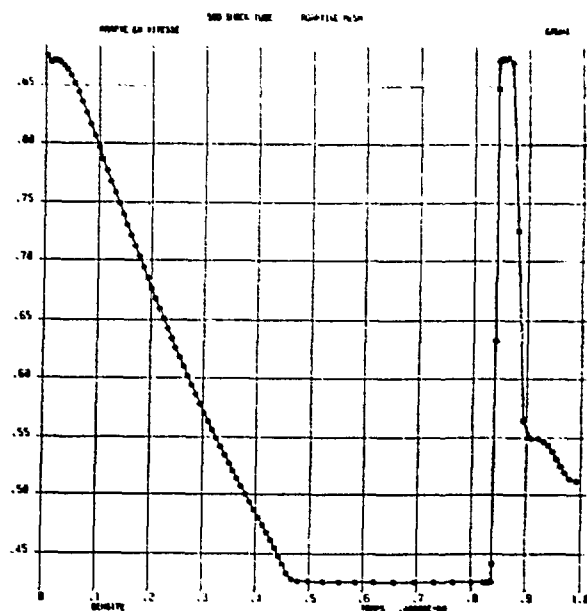
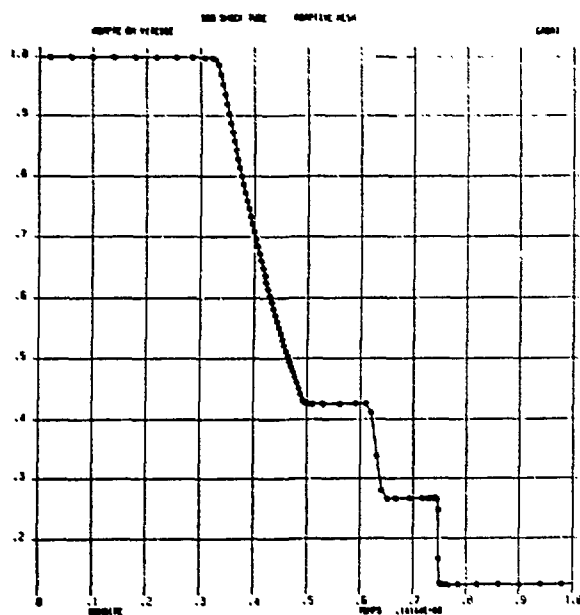
ADAPTED AUTOMATICALLY
(EVERY 6.5 IN THE MEAN)



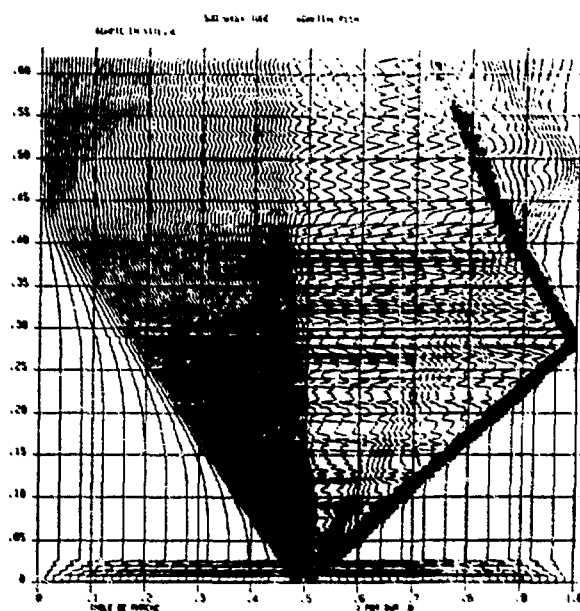
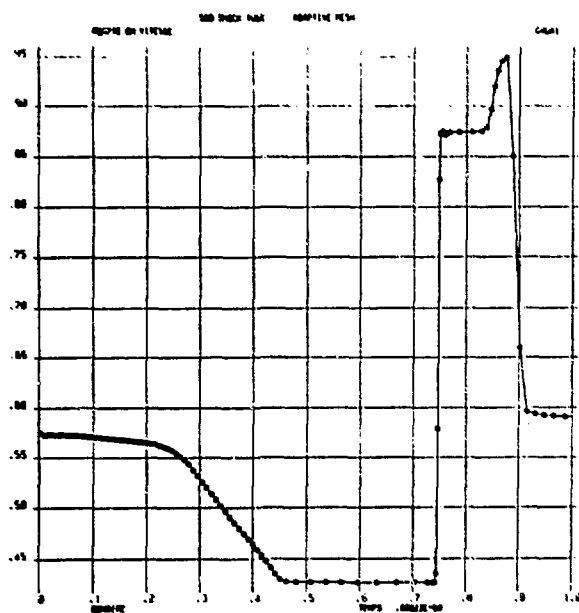
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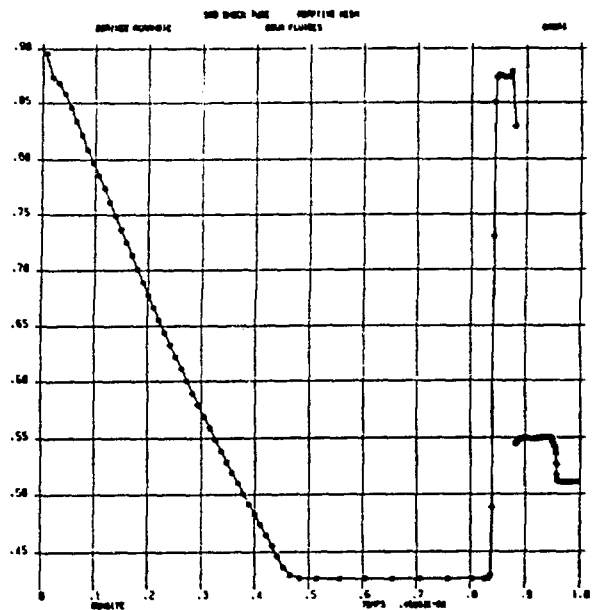
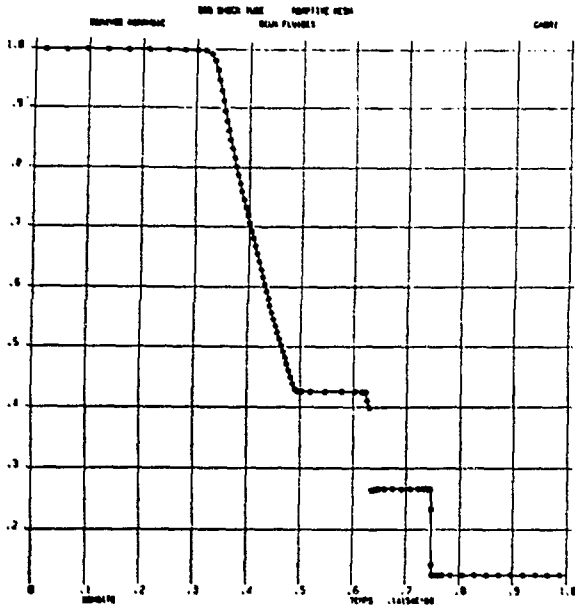
ADAPTED ACCORDING TO VELOCITY



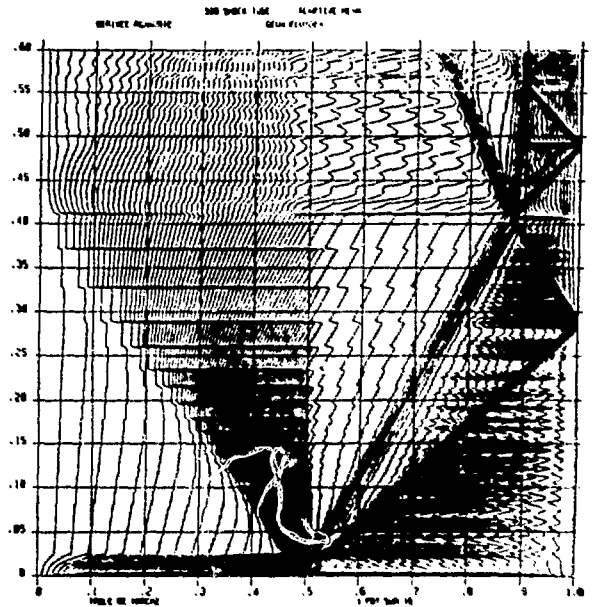
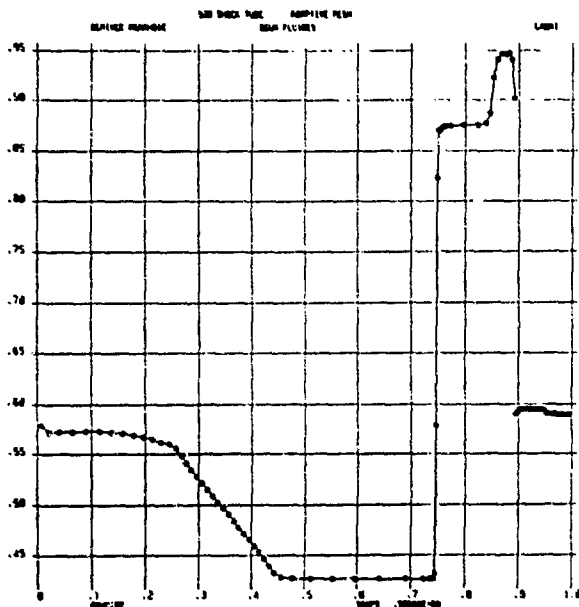
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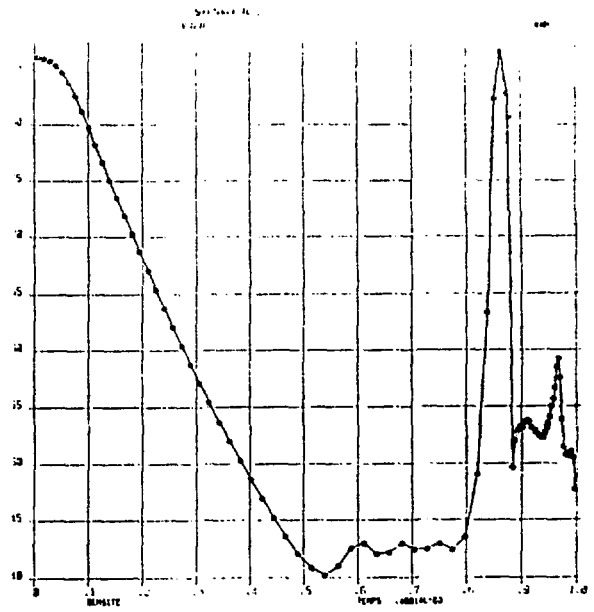
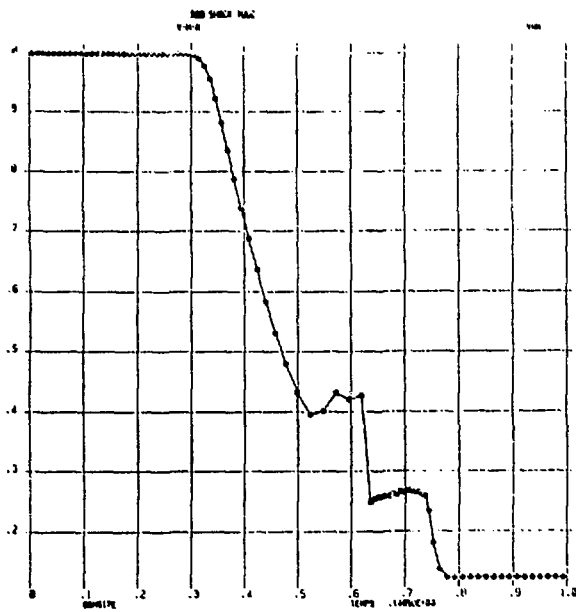
TWO MATERIALS SEPARATELY ADAPTED



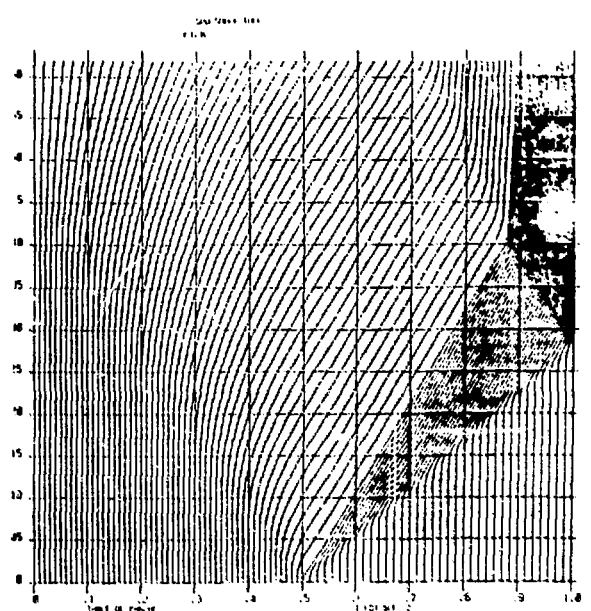
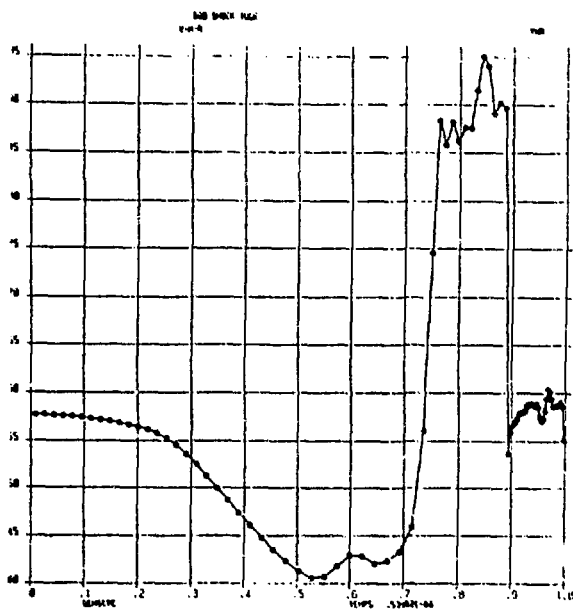
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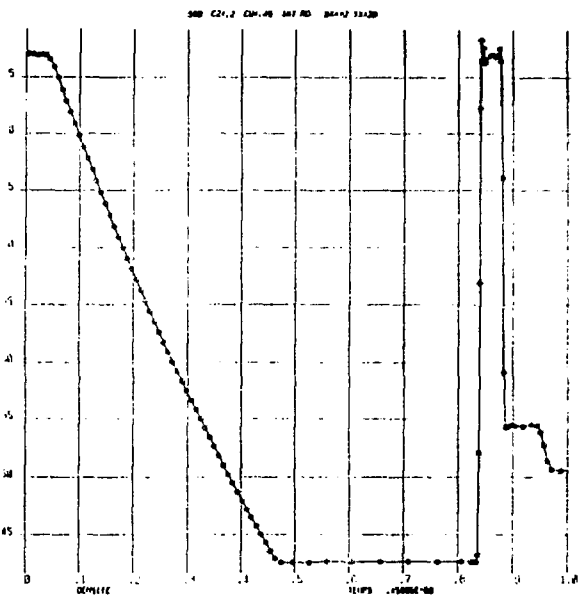
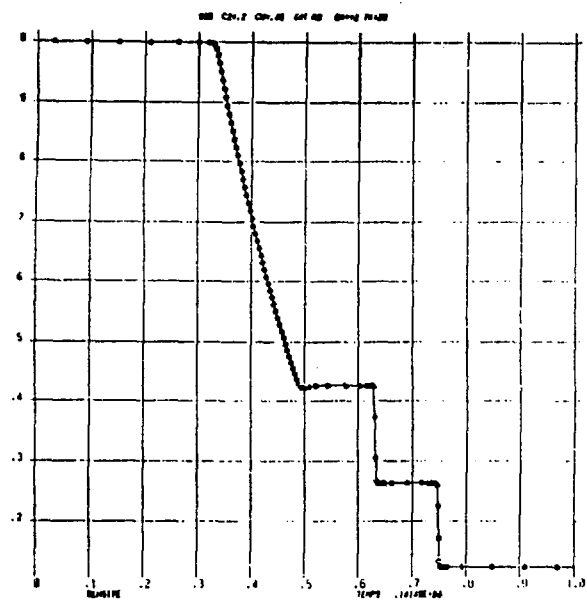
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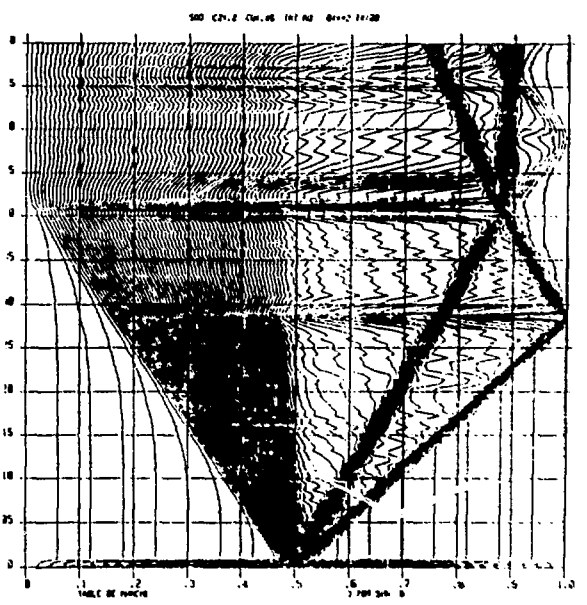
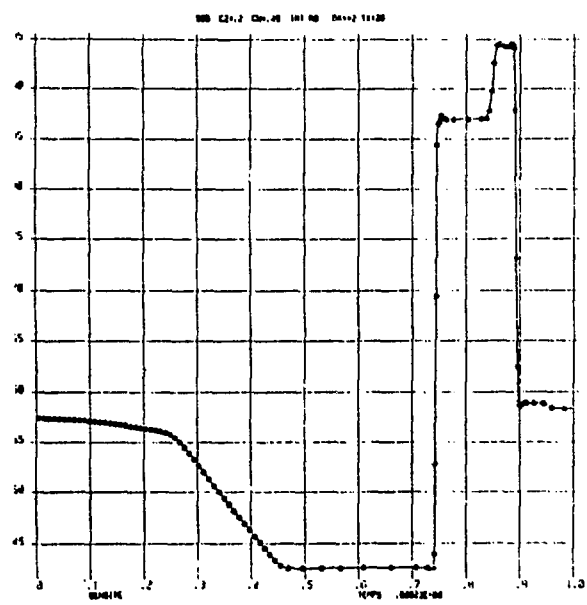
VON NEUMANN-RICHTMYER SCHEME



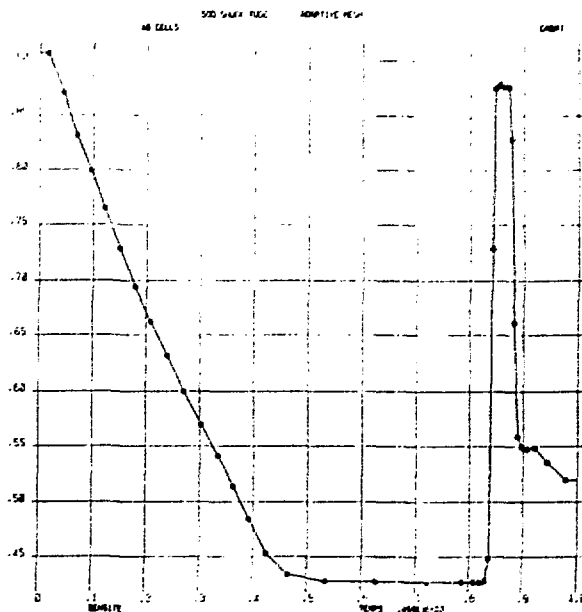
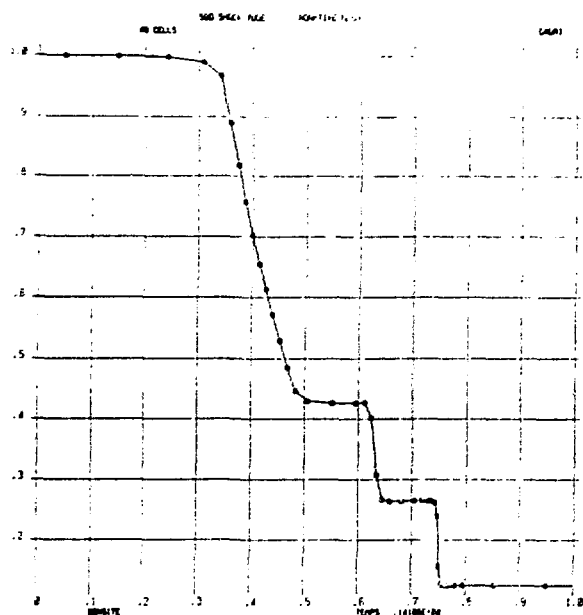
ADAPTED AUTOMATICALLY



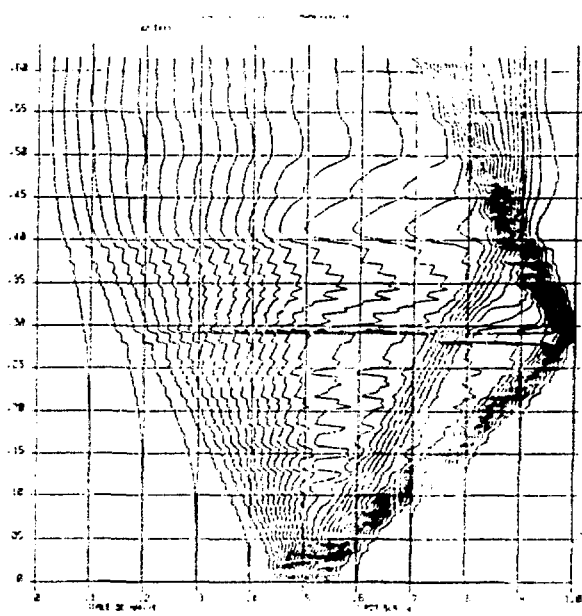
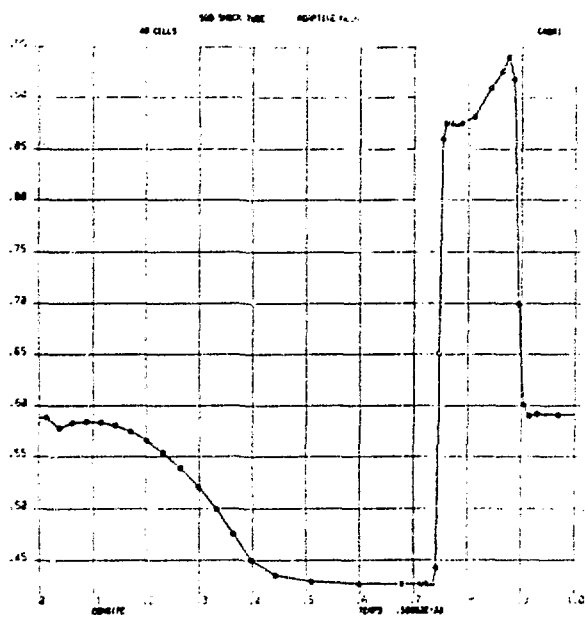
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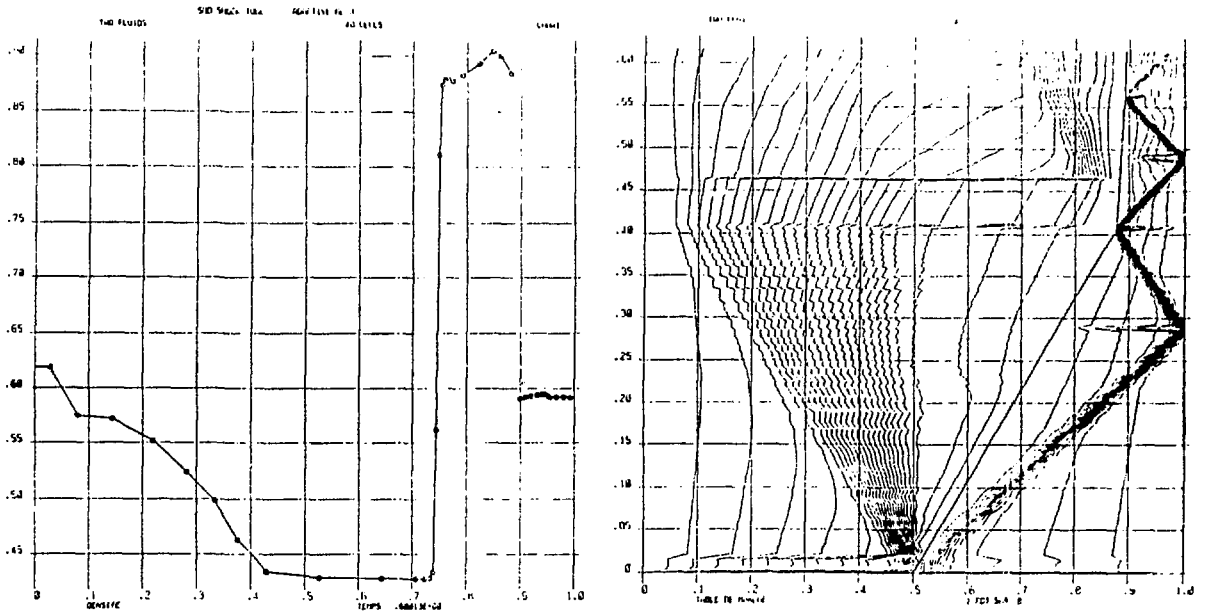
ONLY 40 CELLS



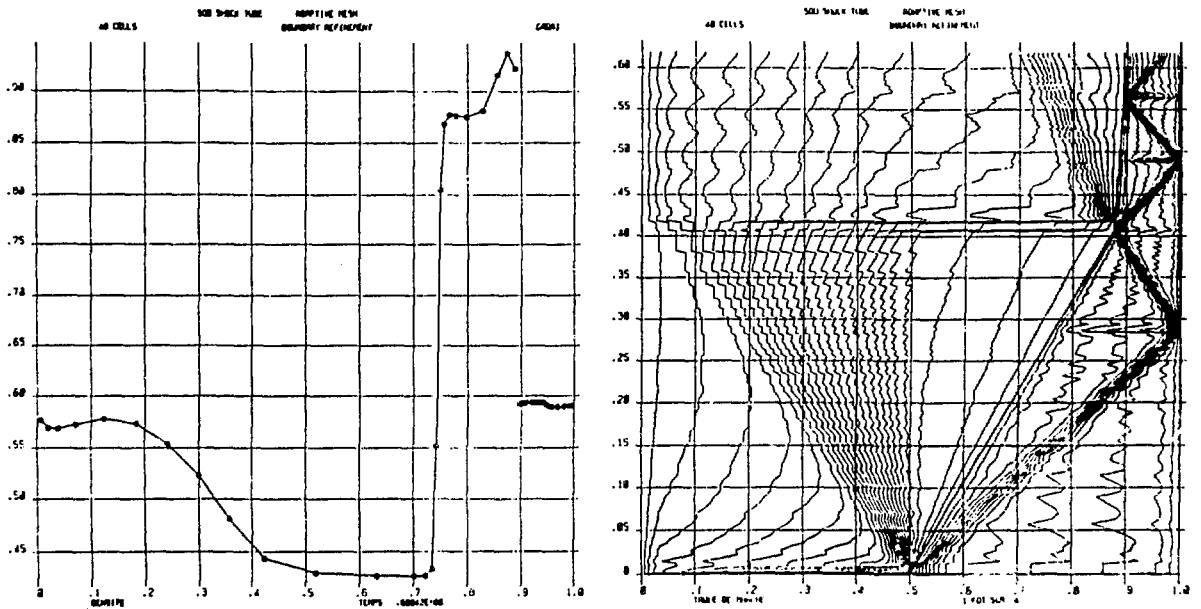
POST-PROCESSED 2ND ORDER GODUNOV-TYPE SCHEME



WITHOUT BOUNDARY REFINEMENT

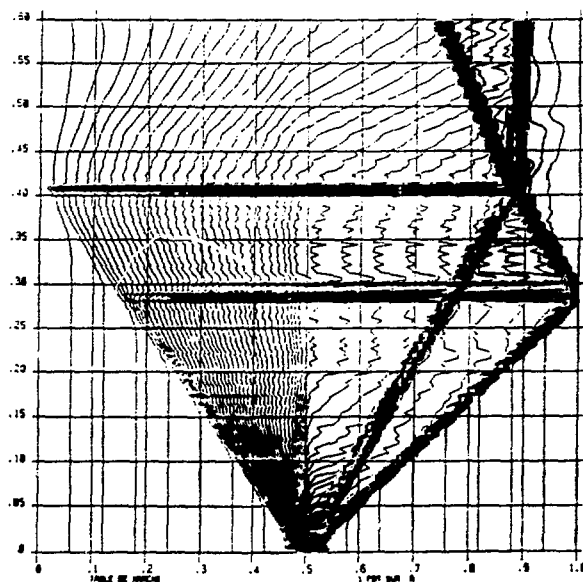
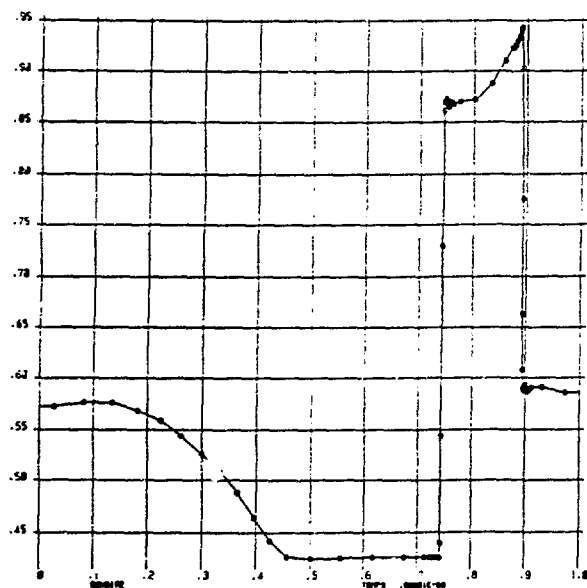


WITH BOUNDARY REFINEMENT



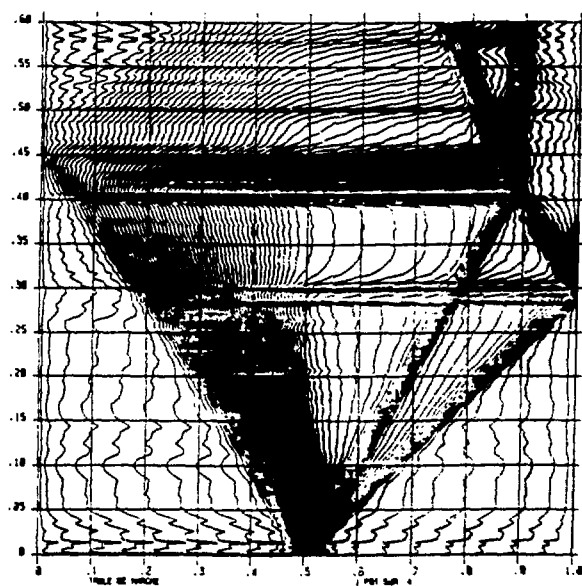
PATHOLOGY

adapted according to 2^{nd} derivative : the discontinuities tend to split

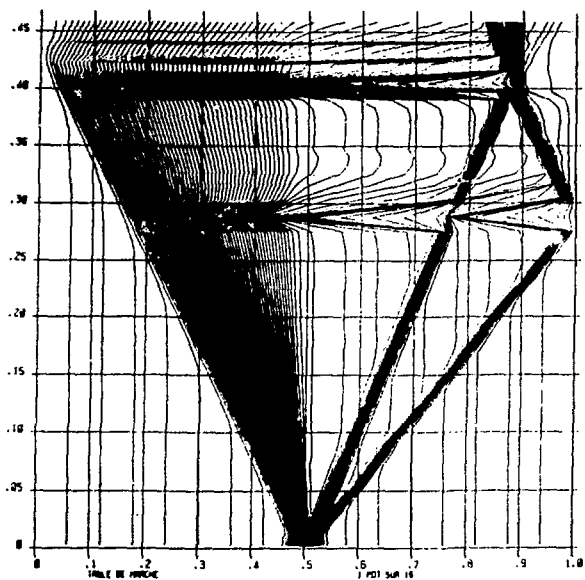


automatically switched adaptive mesh does not allow time filtering

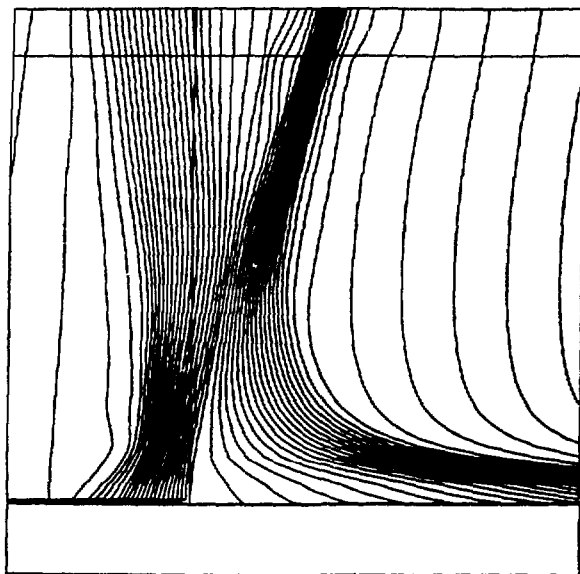
the mesh is refined behind the discontinuity more than ahead



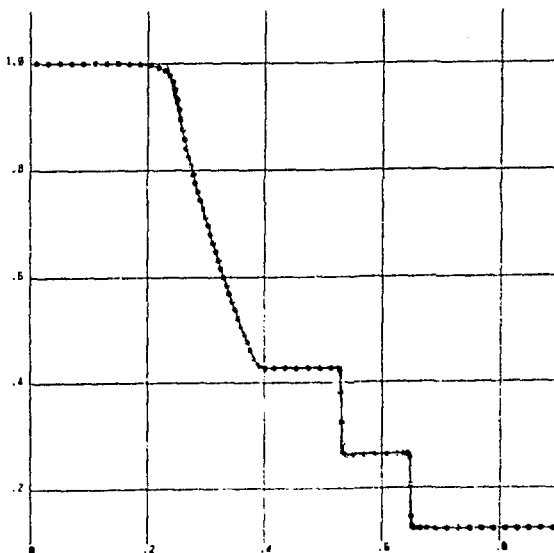
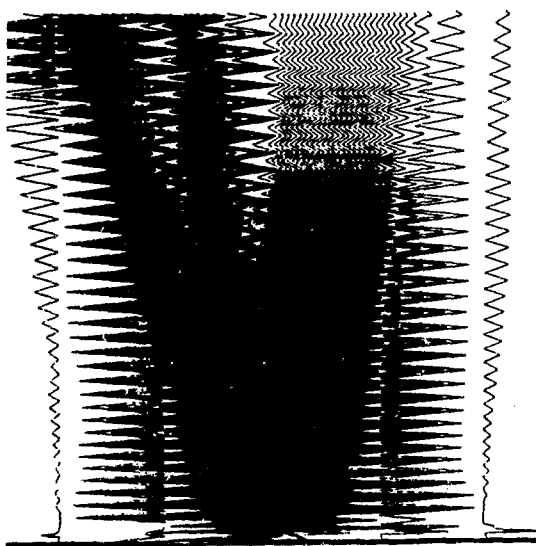
no time filtering



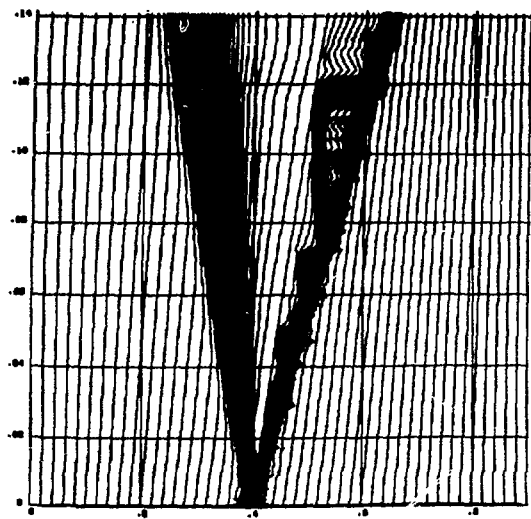
the time filtering is switched off at the 1st time step
but not at the second



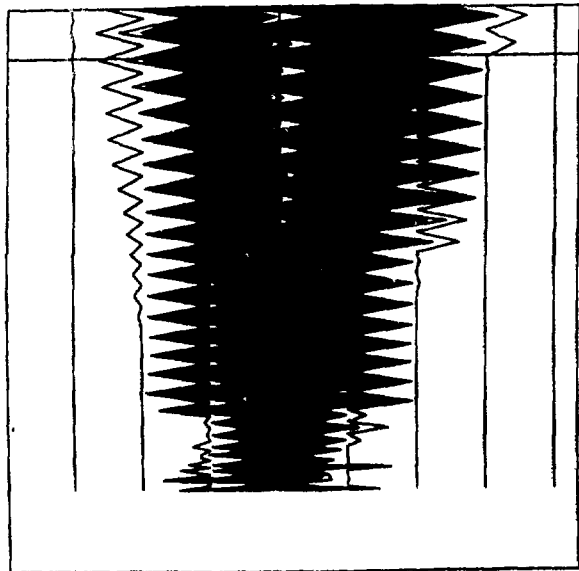
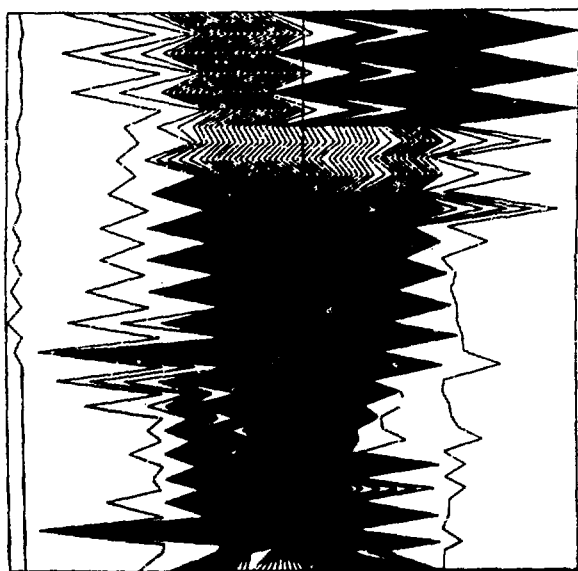
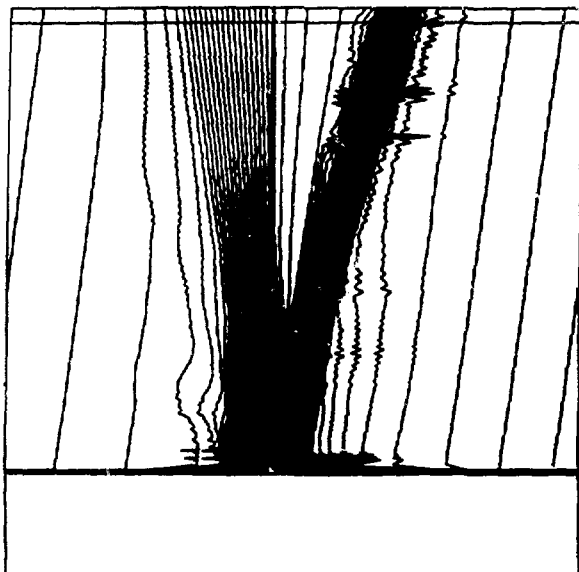
a bad grid does not guarantee bad profiles



too many mesh points : they stay on non-existent structures



instabilities of the grid



A QUADRATIC ANALYSIS OF LINEAR TRANSPORT EQUATIONS

D. VERWAERDE

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BP. 7 - 77181 COUNTRY

ABSTRACT

Performing transport computations on Lagrangian mesh is often difficult, because finite elements or finite differences methods are not directly implementable. One way to get ride of this is to formulate the problem in terms of even parity flux problem : The equation is then elliptic and a quadratic analysis is possible.

We introduce here this analysis , use it to point out some properties and we perform a continuous finite element method in this formalism.

1 - MATHEMATICAL PROPERTIES

We confine our study to the linear mono kinetic equation written :

$$(1) \quad \vec{\Omega} \cdot \vec{\nabla} \phi + \Sigma_T \phi = \frac{\Sigma_d}{4\pi} \int_{S_2} \phi(\vec{x}, \vec{\Omega}) d\vec{\Omega} + Q(\vec{x})$$

Where $\vec{x} \in E \subset \mathbb{R}^3$, $\vec{\Omega} \in S_2$ (i.e. $|\vec{\Omega}| = 1$, $\vec{\Omega} \in \mathbb{R}^3$), ϕ is the flux, Q the heterogenous source, Σ_T the total cross-section and Σ_d the scattering cross section.

We denote ∂E the domain boundary and $\vec{n}$ the normal-unit pointing out of E on ∂E ; ∂E may be cut into two continuous pieces noted ∂E_1 and ∂E_2 .

On the domain boundary, we add conditions to (1) such as :

$$(2) \quad \left\{ \begin{array}{ll} \phi(\vec{x}, \vec{\Omega}) = 0 & \vec{x} \in \partial E_1, \vec{\Omega} \cdot \vec{n} < 0 \\ \phi(\vec{x}, \vec{\Omega}) = \phi(\vec{x}, -\vec{\Omega}) & \vec{x} \in \partial E_2 \end{array} \right.$$

In this first paragraph, we are going to look at a weak formulation for the problem and derive properties of the solution and its asymptotical behaviour.

1.1 - A WEAK FORMULATION FOR THE PROBLEM

As it is now usual, we define the even parity flux ϕ^+ and the odd parity flux ϕ^- by :

$$(3) \quad \phi^+(\vec{x}, \vec{\Omega}) = \frac{1}{2} [\phi(\vec{x}, \vec{\Omega}) + \phi(\vec{x}, -\vec{\Omega})] ; \quad \phi^-(\vec{x}, \vec{\Omega}) = \frac{1}{2} [\phi(\vec{x}, \vec{\Omega}) - \phi(\vec{x}, -\vec{\Omega})]$$

and the even parity flux problem by :

$$(4) \quad \left\{ \begin{array}{l} -\vec{\Omega} \cdot \vec{\nabla} \left[\frac{1}{\Sigma_T} \vec{\Omega} \cdot \vec{\nabla} \phi^+ \right] + \Sigma_T \phi^+ = S \left(\equiv Q + \frac{\Sigma_d}{4\pi} \int_{S_2} \phi^+(\vec{x}, \vec{\Omega}) d\vec{\Omega} \right) \text{ in } E \\ \vec{\Omega} \cdot \vec{\nabla} \phi^+ - \Sigma_T \phi^+ = 0 \text{ on } \partial E_1 \text{ with } \vec{\Omega} \cdot \vec{n} < 0 \\ \vec{\Omega} \cdot \vec{\nabla} \phi^+ + \Sigma_T \phi^+ = 0 \text{ on } \partial E_1 \text{ with } \vec{\Omega} \cdot \vec{n} > 0 \\ \vec{\Omega} \cdot \vec{\nabla} \phi^+ = 0 \text{ on } \partial E_2. \end{array} \right.$$

1.1.1 - Formulation

As the even parity flux problem is an elliptic problem, we define the bilinear formulation :

Definition 1 : $D = \text{Ex}S_2$ and $B = \partial \text{Ex}S_2$

$$(6) \quad \left\{ \begin{array}{l} V = \{u \in L^2(D) : (\vec{\Omega} \cdot \vec{\nabla} u) \in L^2(D) \text{ and } (|\vec{\Omega} \cdot \vec{n}|^{\frac{1}{2}} u) \in L^2(B), u \text{ is even for } \vec{\Omega}\} \\ L(\psi^+) = \int_D S \psi^+ d\vec{x} d\vec{\Omega} \\ a(\phi, \psi^+) = \int_D \left(\frac{1}{\Sigma_T} (\vec{\Omega} \cdot \vec{\nabla} \psi^+) \cdot (\vec{\Omega} \cdot \vec{\nabla} \phi^+) + \Sigma_T \phi^+ \psi^+ \right) d\vec{x} d\vec{\Omega} + \int_B |\vec{\Omega} \cdot \vec{n}| \phi^+ \psi^+ d\gamma \\ \text{A weak formulation of the problem (4) is :} \\ \text{Find } \phi^+ \text{ in } V \text{ such as for all } \psi^+ \text{ in } V : a(\phi^+, \psi^+) = L(\psi^+) . \end{array} \right.$$

Proposition 1

- V is an Hilbert space ; the Hilbert norm on V , $\| \cdot \|$, is : $\|u\|^2 = \int_D [(\vec{\Omega} \cdot \vec{\nabla} u)^2 + u^2] d\vec{x} d\vec{\Omega} + \int_B |\vec{\Omega} \cdot \vec{n}| u^2 d\gamma$
- L is a continuous linear form ;
- a is a bilinear continuous form ; it is also symmetric and V -elliptic.

Proof : a proof for the proposition 1 is given in the ref. 6.

1.1.2 - A solution to the problem (6)

The weak formulation (6) is a convenient way to draw out properties for the solution of the transport equation :

Proposition 2 The weak problem (6) has an unique solution if $\Sigma_T > \Sigma_d$; this solution is positive if Q is positive.

Proof : We denote $\Phi^+ = \frac{1}{4\pi} \int_{S_2} \phi^+(\vec{x}, \vec{\Omega}) d\vec{x}d\vec{\Omega}$; the general bilinear form $a(\phi^+, \psi^+) = \int_D \Sigma_d \phi^+ \psi^+ d\vec{x}d\vec{\Omega}$ is symmetric, continuous and V-elliptic $(\|\phi^+\|_{L^2(D)} < \|\phi^+\|_{L^2(D)}) : a(\phi^+, \phi^+) = \int_D \Sigma_d (\phi^+)^2 d\vec{x}d\vec{\Omega} > \min(1, \Sigma_T - \Sigma_d, \frac{1}{\Sigma_T}) \|\phi^+\|^2$; the Lax-Milgram theorem gives an unique solution to (6).

Positivity of ϕ^+ : let us define :

$$(\phi^+)_+ = \max(0 ; \phi^+) > 0 \text{ and } (\phi^+)_- = \max(0 ; -\phi^+) > 0$$

Then $\phi^+ = (\phi^+)_+ - (\phi^+)_-$ and :

$$(\phi^+)_+ \cdot (\phi^+)_- \equiv 0, (\vec{\Omega} \cdot \vec{\nabla}(\phi^+)_+) \cdot (\vec{\Omega} \cdot \vec{\nabla}(\phi^+)_-) \equiv 0.$$

a $((\phi^+)_+ - (\phi^+)_-, (\phi^+)_-) = \int_D \Sigma_d ((\phi^+)_+ - (\phi^+)_-, (\phi^+)_-) d\vec{x}d\vec{\Omega} = \int_D Q(\phi^+)_- d\vec{x}d\vec{\Omega} > 0$ using the different properties of $(\phi^+)_+$ and $(\phi^+)_-$, it comes :

$$a((\phi^+)_-, (\phi^+)_-) = \int_D \Sigma_d ((\phi^+)_-, (\phi^+)_-) d\vec{x}d\vec{\Omega} < 0$$

The V-ellipticity gives : $\min(1, \Sigma_T - \Sigma_d, \frac{1}{\Sigma_T}) \|(\phi^+)_-\|^2 < 0$ and : $(\phi^+)_- \equiv 0$.

1.1.3 - A fundamental property of V

If the geometrical domain E has what we call Poincaré's Property, an interesting result can be shown :

Definition 2 : Poincaré's Property

We say that the domain E has the Poincaré's Property if for each point $\vec{x}$ in E and each direction $\vec{\Omega}$ in S_2 the right line starting in $\vec{x}$ and directed by $\vec{\Omega}$, intersects the vacuum boundary ∂E_1 .

Proposition 3 : fundamental inequality in V :

We assume that E has the Poincaré's property and that E is convex and bounded ; then there's a strictly positive constant C such as for each u in V :

$$\int_D \frac{1}{\Sigma_T} (\vec{\Omega} \cdot \vec{\nabla} u)^2 d\vec{x}d\vec{\Omega} + \int_B |\vec{\Omega} \cdot \vec{n}| u^2 d\gamma > C \cdot \int_D \Sigma_T u^2 d\vec{x}d\vec{\Omega}$$

Proof : see reference 6.

This fundamental inequality has two consequences :

- The V-ellipticity of the general form can be re-written :

$$a(\phi^+, \phi^+) = \int_D \Sigma_d (\phi^+)^2 d\vec{x} d\vec{\Omega} > \min(1, \Sigma_T - \Sigma_d + \frac{C}{2} \Sigma_T, \frac{1}{2\Sigma_T}) \|\phi\|^2$$

So, when Σ_d is closed to Σ_T , the even-parity flux problem has a solution.

- Critical size

The constant C is defined as : $\min(\frac{1}{d}, \frac{2}{d^2})$ with d : diameter of E. For $\Sigma_d > \Sigma_T$ (over critical case) the fundamental inequality shows that for d littler than dmax, the general bilinear form is V-elliptic ; dmax can be associated to the critical size of E.

1.2 - ASYMPTOTIC BEHAVIOUR OF THE SOLUTION OF (6)

In ref. 2, E.E. Lewis shows in slab geometry that the P0 angular approximation of the even parity flux problem is the diffusion equation. We extend this property to the general case and study the asymptotic behaviour of the solution of (6) in two important situations : opacous medium and void.

1.2.1 - A PO angular approximation for (6)

The "diffusion approximation" of the angular flux $\phi(\vec{x}, \vec{\Omega})$ of the transport problem is the P1 angular developpement :

$$\phi(\vec{x}, \vec{\Omega}) = \Phi(\vec{x}) + 3 \vec{\Omega} \cdot \vec{J}(\vec{x}) + O(\vec{\Omega}^2)$$

When we apply this approximation to the even parity flux, we get the P0 approximation : $\phi^+(\vec{x}, \vec{\Omega}) = \Phi^+(\vec{x}) + O(\vec{\Omega}^2)$ which we plug into the formulation (6). It comes :

Proposition 4 : The diffusion approximation is defined by :

$$\begin{aligned} V &= \{u \quad V : u \quad P_0(\vec{\Omega})\} = H^1(E) \\ a(\phi^+, \phi^+) &= 4\pi \int_E \left(\frac{1}{3\Sigma_T} \sum_{i=1}^3 \frac{\partial \phi^+}{\partial x_i} \cdot \frac{\partial \phi^+}{\partial x_i} + \Sigma_T \phi^+ \phi^+ \right) d\vec{x} + \frac{4\pi}{2} \int_{\partial E_1} \phi^+ \phi^+ d\gamma \\ L(\phi^+) &= 4\pi \int_E S \phi^+ d\vec{x} \\ \text{"Find } \phi^+ & \in H^1(E) : \text{ for each } \psi^+ \text{ in } H^1(E) : \\ a(\phi^+, \psi^+) &= L(\psi^+) \end{aligned}$$

Proof : see reference 6.

This diffusion approximation can be interpreted in the distributions formalism : ϕ^+ is then a distribution which is the solution of the diffusion equation (7) :

$$(7) \quad \left\{ \begin{array}{l} -\frac{1}{3} \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(\frac{1}{\Sigma_T} \cdot \frac{\partial \phi^+}{\partial x_i} \right) + \Sigma_T \phi^+ = S \text{ in } E, \\ \frac{1}{3\Sigma_T} \cdot \frac{\partial \phi^+}{\partial n} + \frac{1}{2} \phi^+ = 0 \text{ on } \partial E_1 \text{ and } \frac{\partial \phi^+}{\partial n} = 0 \text{ on } \partial E_2. \end{array} \right.$$

The proposition 4 or its distribution interpretation (7) proves that diffusion is only an internal approximation of the even parity flux problem : Using this results, it will be easier to build compatible approximations of transport and diffusion.

1.2.2 - Asymptotic behaviour in opacous medium

In ref. 4, one shows that the asymptotic behaviour of transport equation solution in opacous medium is given by a diffusion equation. Such a result can also be proved for the solution of the even parity flux problem ; A proof is given in ref. 6 :

Proposition 5 : We assume that cross sections are growing like Σ_T/ε and Σ_d/ε , that the difference $(\Sigma_T - \Sigma_d)/\varepsilon$ can be written $\gamma \cdot \varepsilon$ (γ is a bounded function) and that the heterogeneous source is $\varepsilon^{n+1} \cdot Q$ (with $\varepsilon > 0$). Let ϕ_ε^+ the unique solution of : find ϕ_ε^+ in V such that for each ψ^+ in V :

$$(8) \quad \varepsilon \int_D \frac{1}{\Sigma_T} (\vec{\Omega} \cdot \vec{\nabla} \phi_\varepsilon^+) (\vec{\Omega} \cdot \vec{\nabla} \psi^+) d\vec{x} d\vec{\Omega} + \int_B |\vec{\Omega} \cdot \vec{n}| \phi_\varepsilon^+ \psi^+ d\gamma + \frac{1}{\varepsilon} \int_D \Sigma_T (\phi_\varepsilon^+ - \Phi_\varepsilon^+) \psi^+ d\vec{x} d\vec{\Omega} + \varepsilon \gamma \int_D \Phi_\varepsilon^+ \psi^+ d\vec{x} d\vec{\Omega} = \varepsilon^{1+n} \int_D Q \psi^+ d\vec{x} d\vec{\Omega}$$

Let u_0 the unique solution of :

$$-\frac{1}{3} \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(\frac{1}{\Sigma_T} \frac{\partial u_0}{\partial x_i} \right) + \gamma u_0 = Q \text{ in } E, \\ u_0 = 0 \text{ on } \partial E_1, \quad \frac{\partial u_0}{\partial n} = 0 \text{ on } \partial E_2,$$

Let u_1 the unique solution of :

$$-\frac{1}{3} \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(\frac{1}{\Sigma_T} \frac{\partial u_1}{\partial x_i} \right) + \gamma u_1 = 0 \text{ in } E, \\ u_1 = -\frac{2}{3\Sigma_T} \cdot \frac{\partial u_0}{\partial n} \text{ on } \partial E_1, \quad \frac{\partial u_1}{\partial n} = 0 \text{ on } \partial E_2.$$

Then, there is a bounded function g of Q , such that we have :

$$\|\phi_\varepsilon^+ - \varepsilon^n (u_0 + \varepsilon u_1)\|_{L^2(D)} < C \cdot \varepsilon^{2+n} \cdot \|g\|_{L^2(D)}$$

One can say that this result is classical ; but quadratic analysis is a convenient way to show it, without any other theorem.

1.2.3 - Asymptotic behaviour in void

When one uses even parity flux equation to solve transport problems, many questions are often asked about solution behaviour in void because of the term $1/\Sigma_T$. This behaviour is studied in ref. 7 and here we only give the main result :

Proposition 6 : We assume that cross sections goes to zero like ϵ . Σ_T and $\epsilon \Sigma_d$ (with

$$(9) \left\{ \begin{array}{l} \epsilon > 0 \right\} \quad \text{Let } \phi_\epsilon^+ \text{ the unique solution of: "Find } \phi_\epsilon^+ \text{ in } V, \text{ such for each } \psi^+ \text{ in } V: \\ \int_D \frac{1}{\epsilon \Sigma_T} (\vec{\Omega} \cdot \vec{\nabla} \phi_\epsilon^+) (\vec{\Omega} \cdot \vec{\nabla} \psi^+) d\vec{x} d\vec{\Omega} + \int_B |\vec{\Omega} \cdot \vec{n}| \phi_\epsilon^+ \psi^+ d\vec{x} d\vec{\Omega} \\ + \int_D (\epsilon \Sigma_T \phi_\epsilon^+ \psi^+) d\vec{x} d\vec{\Omega} = \int_D (Q + \epsilon \Sigma_d \Phi_\epsilon^+) \psi^+ d\vec{x} d\vec{\Omega} \end{array}$$

Then, the solution ϕ_ϵ^+ verifies :

- $\|\phi_\epsilon^+\|_{L^2(D)} < 4d \|Q\|_{L^2(D)}$ (d : diameter of E , for $\epsilon < 1$)
- There is a bounded function g in $L^2(D)$ such as :

$$\|\phi_\epsilon^+ - (\phi_0 + \epsilon \phi_1)\|_{L^2(D)} < \epsilon^2 \|g\|_{L^2(D)}$$

with ϕ_0 , the solution of : $\vec{\Omega} \cdot \vec{\nabla} \phi_0 = 0$

(Transport equation in void), and with ϕ_1 solution of :

- $-\vec{\Omega} \cdot \vec{\nabla} \left[\frac{1}{\Sigma_T} \cdot \vec{\Omega} \cdot \vec{\nabla} \phi_1 \right] = Q$ in $\text{Ex}S_2 = D$
- $\vec{\Omega} \cdot \vec{n} > 0 : \frac{1}{\Sigma_T} (\vec{\Omega} \cdot \vec{\nabla} \phi_1) + \phi_0 = 0$ on B
- $\vec{\Omega} \cdot \vec{n} < 0 : \frac{1}{\Sigma_T} (\vec{\Omega} \cdot \vec{\nabla} \phi_1) - \phi_0 = 0$ on B

Proposition 6 proves that the asymptotic behaviour of ϕ_ϵ^+ is ϕ_0 , the solution of transport problem in void : Even parity equation can also be used in transparent medium.

1.3 - CONVERGENCE OF ITERATIVE PROCESSES

Quadratic analysis will also be a convenient way to study convergence of iterative processes : classical process or diffusion synthetic acceleration method (ref. 10). In ref. 8 or 9, results are given in slab geometry by using spectral analysis : they are generalized here.

1.3.1 - A criterion for convergence

As it usual in quadratic analysis, we introduce the J functional coupled with the problem (6) :

Definition 3 : The J fonctionnal is defined on V by $(\psi^+ \in V)$:

$$(10) \quad \left\{ \begin{array}{l} J(\psi^+) = \frac{1}{2} a(\psi^+, \psi^+) = \frac{1}{2} \int_D \Sigma_d \bar{\psi}^+ \cdot \psi^+ d\vec{x} d\vec{\Omega} = \int_D Q \psi^+ d\vec{x} d\vec{\Omega} \\ (\bar{\psi}^+ = \frac{1}{4\pi} \int_{S_2} \psi^+(\vec{x}, \vec{\Omega}) d\vec{\Omega}) \\ \text{The unique solution of (6) is also the unique solution of :} \\ \text{"Find } \phi^+ \text{ in V", minimizing } J(\psi^+). \end{array} \right.$$

J will be used to evaluate a distance between an element u in V and ϕ^+ :
 $J(u) - J(\phi^+) = d(u, \phi^+) > 0$.

1.3.2 - Analysis of the classical process

First, we define the classical process :

Definition 4 : Classical Process

$$(11) \quad \left\{ \begin{array}{l} \text{Let } \phi_0^+ \text{ in } L^2(E) ; \text{ for } n > 1 \text{ we define } \phi_n^+ \text{ as the unique solution of the} \\ \text{problem : "find } \phi_n^+ \text{ in V such as for all } \psi^+ \text{ in V } (\phi_{n-1}^+ = \frac{1}{4\pi} \int_D \phi_{n-1}^+(\vec{x}, \vec{\Omega}) d\vec{\Omega}) \\ a(\phi_n^+, \psi^+) = \int_D \Sigma_d \phi_{n-1}^+ \psi^+ d\vec{x} d\vec{\Omega} + \int_D Q \psi^+ d\vec{x} d\vec{\Omega} \text{".} \end{array} \right.$$

Using quadratic analysis, we show in ref 6 the :

Proposition 7 : Let $(\phi_n^+)_{n \in \mathbb{N}}$ defined in (11). Then :

- $\forall n \in \mathbb{N} : J(\phi_n^+) < J(\phi_{n-1}^+)$
- $\lim_{n \rightarrow \infty} \phi_n^+ = \phi^+$.

According to our criterion, ϕ_n^+ is "closer" to ϕ^+ than ϕ_{n-1}^+ . We will say that ϕ_n^+ is "better" than ϕ_{n-1}^+ .

1.3.3 - Analysis of the "diffusion synthetic acceleration method"

We can define the accelerated process as :

Definition 5 : Accelerated-Process

- Let Φ_0^+ in $L^2(E)$; for $n > 1$, we define ϕ_n^+ as :
- $\tilde{\phi}_n^+$, the unique solution of the problem : "Find $\tilde{\phi}_n^+$ in V , such as for all ψ^+ in V ": $a(\tilde{\phi}_n^+, \psi^+) = \int_D \Sigma_d \Phi_{n-1}^+ \cdot \psi^+ d\vec{x} d\vec{\Omega} + \int_D Q \psi^+ d\vec{x} d\vec{\Omega}$
 - Let $\tilde{\Phi}_n^+ = \frac{1}{4\pi} \int_{S_2} \tilde{\phi}_n^+(\vec{x}, \vec{\Omega}) d\vec{\Omega}$ and d_n the unique solution of the "diffusion problem" :
 "Find d_n in $H^1(E)$, such as for all ψ^+ in $H^1(E)$ ":
 $a(d_n, \psi^+) = \int_E \Sigma_d \cdot d_n \psi^+ d\vec{x} = \int_E \Sigma_d (\tilde{\Phi}_n^+ - \Phi_{n-1}^+) \psi^+ d\vec{x}$
- (11) • Then ϕ_n^+ is defined as $\tilde{\phi}_n^+ + d_n$.

Here also, we use quadratic analysis to show (in ref. 6) :

Proposition 8 : Let $(\phi_n^+)_n$ N defined in (11). Then :

- $n \in N, J(\tilde{\phi}_n^+ + d_n) < J(\tilde{\phi}_n^+) < J(\phi_{n-1}^+)$;
- $\lim_{n \rightarrow +\infty} \tilde{\phi}_n^+ = \lim_{n \rightarrow +\infty} (\phi_n^+ + d_n) = \phi^+$.

Two conclusions can be drawn out of this last proposition :

- a) according to our criterion, the diffusion synthetic acceleration solution $(\tilde{\phi}_n^+ + d_n)$ is "closer" to ϕ^+ than ϕ_n^+ : so, convergence is accelerated.
- b) "diffusion synthetic acceleration" gives an iterative process which converges to ϕ^+ , for all kinds of domain E , with or without vacuum boundary.

But, one question (at least) remains : what is the speed of convergence !

Next property gives a partial answer to it :

Proposition 9 : Let $(\phi_n^+)_n$ N , defined in (11). We assume "opacous medium conditions" as in proposition 5, and $n = -2$. It comes :

$$J(\tilde{\phi}_n^+) - J(\tilde{\phi}_n^+ + d_n) = (J(\tilde{\phi}_n^+) - J(\phi^+))(1 + \varepsilon^2 F(\phi^+)), \text{ where } F(\phi^+) \text{ is a bounded function of } \phi^+.$$

For proof, see ref. 6.

Proposition 9 shows that, when ε goes to zero, the "diffusion synthetic acceleration" solution goes to ϕ^+ , according to our criterion J .

II - NUMERICAL SOLUTION

In the first part, we used quadratic analysis to prove some mathematical properties of even parity flux problem. Because V is closed to a Sobolev space and the problem is elliptic, we can approximate V with standard finite elements methods used to approximate $H^1(D)$.

2.1 - A CONFORM FINITE ELEMENTS METHOD

We want to build a method which preserves the fundamental link between even parity flux and diffusion equations. This is why every admissible triangulation of D (or finite element method on D) must be the cartesian (resp. tensorial) product of a triangulation (resp. F.E.) of E and a triangulation (resp. F.E.) of S_2 .

A general method has been built in ref. 5 for r.z geometry. To get a clearer talk, we are going to build a method on the spherical case.

2.1.1 - A triangulation of $D : T_{IM}$

As it is usual in this case, D is the product of two intervals $[0, R]$ and $[0, 1]$. A triangulation of $[0, R]$ is :

$0 \leq i \leq I, \quad 0 = r_0 < \dots < r_1 < r_{i+1} < \dots < r_I = R$ and we note $h_i = \sup_{0 \leq i \leq I-1} r_{i+1} - r_i$.

A triangulation of $[0, 1]$ is :

$0 \leq m \leq M, \quad 0 = \mu_0 < \dots < \mu_M = 1, \quad \mu_m = m/M$

A cell of D is noted $K = [r_i ; r_{i+1}] \times [\mu_m, \mu_{m+1}]$. Its diameter is noted h .

2.1.2 - A C^0 finite element method

To approximate V , we define V_h :

$V_h = \{u_h \in C^0(D) : K \in T_{IM}, u_h|_K = P_1(r_i, r_{i+1}) \times P_1(\mu_m, \mu_{m+1})\}$

V_h can also be defined by :

$V_h = \{u_h \in C^0(D) : K \in T_{IM}, u_h|_K \in Q_1(K)\}$

For V_h , freedom degrees will be summits of cells K .

The approximating problem is :

$$(12) \quad \left\{ \begin{array}{l} \text{"Find } \phi_h^+ \text{ in } V_h, \text{ such as for all } \psi_h^+ \text{ in } V_h \\ a(\phi_h^+, \psi_h^+) = L(\psi_h^+) \end{array} \right.$$

2.1.3 - Rate of convergence

Let C et M the constants defining the ellipticity and continuity of a . Then it comes :

- $a(\phi^+, \psi_h) = L(\psi_h) = a(\phi_h, \psi_h)$; so :
 - $a(\phi^+ - \phi_h^+, \psi_h) \equiv 0$ for each ψ_h
 - $C \|\phi^+ - \phi_h^+\|^2 \leq a(\phi^+ - \phi_h^+, \phi^+ - \phi_h^+)$
 $\leq a(\phi^+ - \phi_h^+, \phi^+ - \chi_h)$ for each χ_h
 $\leq M \|\phi^+ - \phi_h^+\| \cdot \|\phi^+ - \chi_h\|$
- so : $\|\phi^+ - \phi_h\| \leq \frac{M}{C} \inf_{\chi_h \in V_h} \|\phi^+ - \chi_h\|$

If we use a result on Sobolev approximation, we have :

$\inf_{\chi_h \in V_h} \|\phi^+ - \chi_h\| \leq h.C' \cdot \|\phi^+\|_{H^2(D)}$. So we have the :

$\chi_h \in V_h$

Proposition 10

If the solution ϕ^+ is in $H^2(D)$ and the triangulation is regular, then :
the rate of convergence of ϕ_h^+ to ϕ^+ :

$$\|\phi^+ - \phi_h^+\| \leq h.C \cdot \|\phi^+\|_{H^2(D)}$$

and, in the $L^2(D)$ space :

$$\|\phi^+ - \phi_h^+\|_{L^2(D)} \leq h^2.C \cdot \|\phi^+\|_{H^2(D)}.$$

To point out the last rates of convergence (13) and (14) we assumed that ϕ^+ is in $H^2(D)$, which is not generally true.

2.1.4 - Method for resolution

To compute the numerical solution, we build two symmetric matrices : the first one to discretize equation (12) and the second one to approximate the general bilinear form. These two matrices are factorized by using a Cholesky method.

2.2 - NUMERICAL RESULTS

2.2.1. - Numerical solution when $\Sigma_d = 0$

The first problem which was numerically solved is the case $\Sigma_d = 0$, where we get analytical solutions. We started with $Q \equiv 1$, and looked at the norm $L^2(E)$ of the difference between ϕ_h^+ and ϕ^+ . We made two observations about it :

- this norm goes to 0 when h goes also to 0.
- the speed of convergence is only $O(h)$;

This result does not verify the inequality (14). In fact, ϕ^+ is not in $H^2(D)$, for some second partial derivatives are not in $L^2(D)$ because of the singularity in $r = R$ and $\mu = 0$.

2.2.2 - Computation of fundamental inequality constant

An interesting comparison can be obtained in computing the fundamental inequality constant (proposition 3) and in comparing it to the theoretical result :

$$C_0 > \min\left(\frac{1}{d}, \frac{2}{d^2}\right) \text{ with } d, \text{ diameter of } E.$$

To perform the comparison, we choose the numerical values :

- for R : $R = 1$, so that $d = 2$.
- $\Sigma_T = 1$ everywhere.

then, the estimation of the minimal value of C_0 is $1/2$.

We give here the result of the numerical estimation of C_0 , computed with different values of Σ_d :

Σ_d	0.5	1.	1.5
THEORETICAL BOUND	0.5	0.5	0.5
NUMERICAL VALUE	0.9950	0.9948	0.9949

The numerical values lead us to think that a better evaluation of the theoretical value of C_0 could be made.

2.2.3 - Asymptotic behaviour of solution in opacous medium

We want to numerically observe the convergence of the solution of the even parity-flux problem when the medium becomes more and more opacous (proposition 5). In order to do it, we choose :

- for R , $R = 1$,
- for the source : $\varepsilon.Q$, with $Q = 1$,
- for $\Sigma_T(\varepsilon) = 1/\varepsilon$,
- for $\Sigma_d(\varepsilon) : 1/\varepsilon - \gamma.\varepsilon$ with $\gamma = .5$

For different values of ε (decreasing from 1 to 10^{-4}) we compute :

- the norm L^2 of the difference $(\phi^+ - \Phi_D)$,
- the norm L^1 of the function ϕ^+ . It comes :

(Φ_D is the solution of the asymptotic diffusion equation)

ε	$\ \phi^+ - \Phi_D\ _{L^2}$	$\ \phi^+\ _{L^1}$
1.000	.312 10^{-1}	.2080
0.500	.159 10^{-1}	.1435
0.100	.229 10^{-2}	.0771
0.05	.932 10^{-3}	.0678
0.01	.745 10^{-3}	.0601
10^{-3}	.353 10^{-4}	.0584
10^{-4}	0.	.0583

There is a good agreement between the theoretical result (proposition 5) and computation.

CONCLUSION

The even parity flux equation was a new equation for us. This is why, before coding, we developed a theoretical approach of the problem. This mathematical formulation gave us interesting properties which lead us to study the link between diffusion flux and even parity flux. So, we generalized some well known properties of acceleration of convergence for iterative processes.

Then, we developped a continuous finite element method which preserves the fundamental link between even parity flux and diffusion. But, such a method can be too "rigid" and is very efficient only if the general solution is sufficiently smooth. Perhaps, a new finite element, taking into account the singularity of the solution would give a speedier convergence of numerical problems.

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USE OF THE CHEBYSHEV-LEGENDRE QUADRATURE SET IN DISCRETE-ORDINATE CODES

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ABSTRACT

The Chebyshev-Legendre (C-L) quadrature set has been implemented in the neutron transport section of the TWODANT code. The C-L quadrature set has two advantages as compared to other quadrature sets. First, it is possible to *easily* generate S_N orders up to S_{100} with weights that are positive. TWODANT has been used to carry out calculations with as many as 10,000 discrete directions with the C-L quadrature set. Second, a product C-L set of order N will integrate *exactly* all the terms in the scattering source arising from P_{N-1} scattering. For example, the S_4 set will correctly integrate all scattering source terms if a P_3 scattering approximation is used. In TWODANT, users normally use the current S_8 quadrature set in the belief that P_3 scattering will be treated correctly. The S_8 set consists of some 40 directions and many times results in problem models that require excessive computer memory. The C-L S_4 set integrates exactly all the source terms associated with a P_3 expansion and consists of only 16 discrete directions. The results of test calculations, using both the current set and the C-L set in TWODANT, indicate that when high-order scattering is not significant, the two sets give answers that are in good agreement.

I. INTRODUCTION

Despite all the work that has been published on discrete-ordinate quadrature sets, the criteria used to judge if one set is "better" than another has never been unambiguously established. In this paper, the requirement that the quadrature be capable of integrating the greatest number of spherical harmonics and products of spherical harmonics will be shown to be critically important for the exact treatment of forward peaked anisotropic scattering. This type of scattering occurs for fast neutrons and for gamma-ray photons. The Chebyshev-Legendre quadrature set examined in Refs. 1 and 2 will be shown to be efficient for the integration of the spherical harmonics; and hence, the quadrature set of choice for highly anisotropic scattering. Two simple sample problems exhibiting forward peaked scattering are examined. The results obtained from these sample calculations point out clearly the need for this type of quadrature set for this class of problem. A third test problem, a uranium cylinder, is studied; and it is found that the new quadrature set is superior for this simple problem also. This quadrature set has been implemented in the unclassified code TWODANT.³

II. BACKGROUND

The coordinate system used in this discussion is indicated in Fig. 1. This is the system for a cylindrical problem. In x-y geometry, η is the y-direction cosine, μ is the x-direction cosine, and ξ is the z-direction cosine.

If the scattering transfer probability is assumed to be represented by a finite Legendre polynomial expansion

$$\sigma_s(E' \rightarrow E) = \sum_{n=0}^N \frac{2n+1}{4\pi} P_n(\mu_0) \sigma_{sn}(E' \rightarrow E) \quad .$$

The multigroup-transport equation becomes

$$\nabla \cdot (\Omega \psi_g) + \sigma_{tg} \psi_g = \sum_{h=1}^G \sum_{n=0}^N (2n+1) \sigma_{snh \rightarrow g} \sum_{k=0}^n R_n^k \psi_{nh}^k + \text{SOURCE TERMS} \quad .$$

Here

$$R_n^k = \sqrt{\frac{(2 - \delta_{k0})(n-k)!}{(n+k)!}} P_n^k(\eta) \cos k\omega \quad ,$$

and

$$\int_{-1}^1 d\eta \int_0^\pi d\omega R_n^k(\eta, \omega) R_m^\ell(\eta, \omega) = \frac{2\pi}{2n+1} \delta_{nm} \delta_{k\ell} \quad .$$



The expansion coefficients ψ_n^k are given by

$$\psi_n^k = \int_{-1}^1 d\eta \int_0^\pi d\omega R_n^k \frac{\psi}{2\pi} .$$

$$\sum_{k=1}^G \sigma_{smk \rightarrow g} \psi_{mk}^{\ell} \quad .$$
$$\omega_p R_m^L(\eta_p, \omega_p) \quad ,$$

and summed over all discrete directions p . If the discrete representation is to correctly model the analytic result, then the discrete directions must be chosen such that all the products

$$R_n^k R_m^\ell, n, m \leq N ; k \leq n ; \ell \leq m ,$$

are integrated correctly! If this is the case, then the orthogonality of the R functions is preserved.

III. CHEBYSHEV-LEGENDRE QUADRATURE SET

The integral operator for integration over all solid angle is given by

$$\int_0^\pi \sin \phi \, d\phi \int_0^{2\pi} d\omega .$$

If $\cos \phi = \eta$ and $\cos \omega = y$, then the integral becomes

$$2 \int_{-1}^1 d\eta \int_{-1}^1 \frac{1}{\sqrt{1-y^2}} dy .$$

It is well known that the y integration can be accomplished accurately with the equal weight Gauss-Chebyshev quadrature set. In fact, polynomials in y up to y^m , where $m \leq 2n_c - 1$, are integrated exactly (here n_c order of the Chebyshev quadrature). In a similar fashion, the η integral is exact for polynomials up to η^ℓ when the Gauss-Legendre quadrature set is used. $\ell \leq 2n_L - 1$ where n_L is the order of the Legendre quadrature set.

In the y integral, the quadrature points are given by

$$y_i = \cos \omega_i, \omega_i = \frac{(2i-1)\pi}{2n_c}, \quad i = 1, \dots, n_c .$$

The equal weights are

$$w_{ci} = \frac{\pi}{n_c} .$$

The weights and quadrature points for the Legendre quadrature set are well known and are tabulated.

Notice that the values of ω are equally spaced between 0 and 2π . If the weights for the y integration are normalized by dividing by 2π , and the weights in the η integration are normalized by dividing by 2, then the normalized Chebyshev weights w_c and the normalized Legendre weights w_L are given by

$$w_{ci} = \frac{1}{n_c}, \quad w_{Lj} \rightarrow \frac{w_{Lj}}{2}, \quad i = 1, \dots, n_c ; \quad j = 1, \dots, n_L .$$

The point weights associated with the two-dimensional integration is then the product of the j -th η level Legendre weight and the i -th Chebyshev weight. For a true

product set that is consistent, we take $n_c = n_L = n_q$. n_q will be chosen an even integer. This is the square or product Chebyshev-Legendre quadrature set.

Will this quadrature set correctly integrate

$$\int_{-1}^1 d\eta \int_0^\pi d\omega R_n^k(\eta, \omega) R_m^\ell(\eta, \omega) = \frac{2\pi}{2n+1} \delta_{nm} \delta_{k\ell} \quad ,$$

for all n, k, ℓ , and $m \leq N$ where N is the scattering order? The answer is yes! Integrals of the form

$$\int_0^\pi \cos kw \cos \ell w dw \quad k + \ell \leq 2N \quad ,$$

can be written

$$2 \int_{-1}^1 \frac{ay^1 + by^2 + \dots + cy^{k+1}}{\sqrt{1-y^2}} dy \quad .$$

Notice that the integrand is now a polynomial in y of maximum order $k+1$. This can be shown by noting that

$$\cos kw = a(\cos \omega)^k + b(\cos \omega)^{k-2} + \dots + c(\cos \omega)^M \quad ,$$

and since $y = \cos kw$

$$\cos kw = ay^k + by^{k-2} + \dots + cy^M \quad .$$

Here, $M = 0$ for k even and $M = 1$ for k odd.

Since the integral over w leads to a $\delta_{k\ell}$, the integral over η has the form

$$\int_{-1}^1 P_n^k(\eta) P_m^\ell(\eta) d\eta \quad , \quad n + m \leq N \quad .$$

The highest power of η appearing in the integrand of the integral above is η^{n+m} , and the integrand is a polynomial in η .

Now, if the quadrature n_q is related to the scattering order by $n_q = N + 1$, then the integration is exact for polynomial integrands of order $2n_q - 1$ or $2N + 1$. The integrands involved are polynomials of maximum order $2N$; hence, the integrals are computed exactly! This means, for example, that an S4 Chebyshev-Legendre (C-L) square or product quadrature will treat exactly P3 scattering.

IV. RESULTS AND CONCLUSIONS

The square geometry and the cross sections for each of the two sample problems is shown in Fig. 2. The leakage problem has a small absorption cross section while

the average flux problem is a pure scattering problem. A plot of the differential scattering cross section for both problems is shown in Fig. 3. Notice that both differential cross sections are strongly forward peaked.

Figure 4 is a plot of the average flux in the system as a function of the number of discrete-ordinate directions for the average flux cross-section set. Figure 5 is a plot of total leakage as a function of the number of discrete-ordinate directions for the leakage cross sections. In average flux problem, the current production set, which is the default set in TWODANT, yields divergent results for both S4 and S6 ordinates. Convergence finally occurs at S8 or forty directions. The square C-L quadrature set yields a reasonable value with only 16 directions (S4 square set). The triangular C-L set is similar to the square C-L set but uses Chebyshev integration of order 2 (2 points) on the η level with the largest value of η , Chebyshev integration of order 4 (4 points) on the η level with the next largest value of η , and so on. In two dimensions, an SN square set has N^2 points and an SN triangle set has $(N)(N+2)/2$ points. The triangular set can rigorously only yield correct results for P1 scattering. It can be seen from the results; however, that the triangular set result approaches the square set result as the number of directions becomes large. The current production set, which is also a triangular set, seems to exhibit a constant offset with respect to the C-L sets even for a large number of directions (up to S16). Similar observations apply for the leakage results shown in Fig. 5.

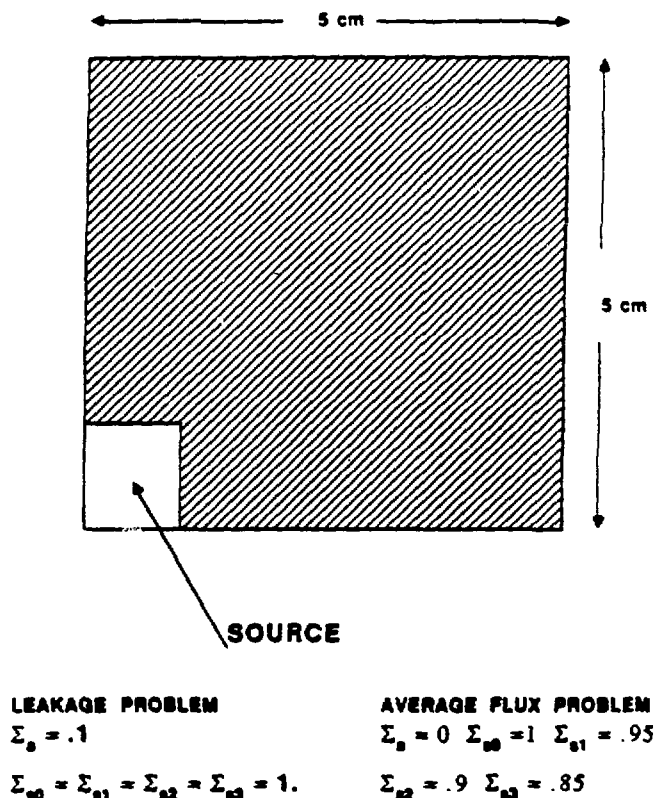


Fig. 2. Test Problem Geometry.

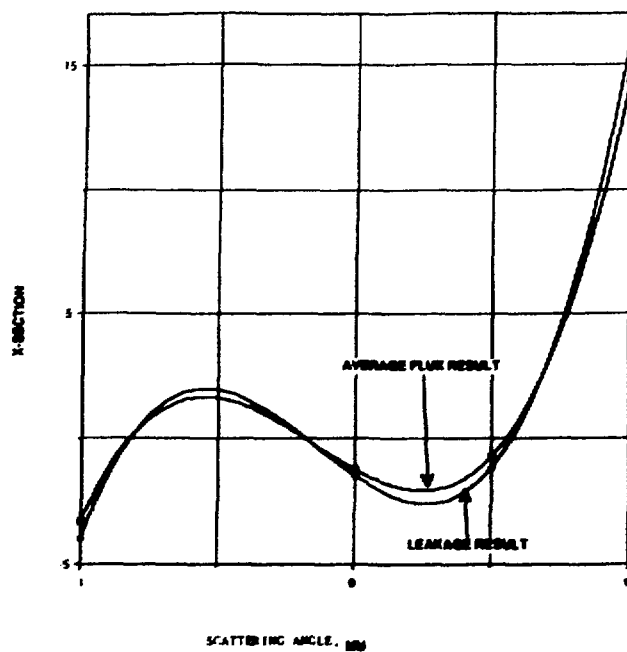


Fig. 3. Scattering X-Section vs. Angle Cosine.

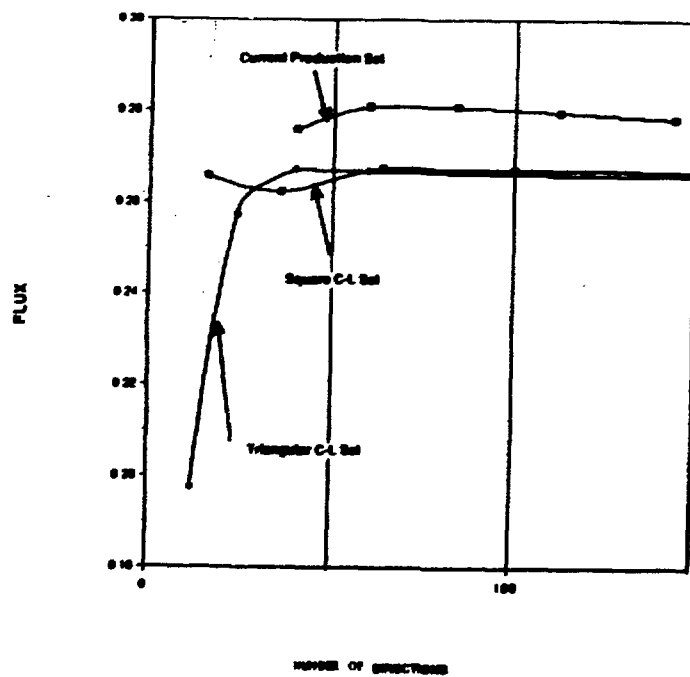


Fig. 4. Average Flux vs. Number of Directions.

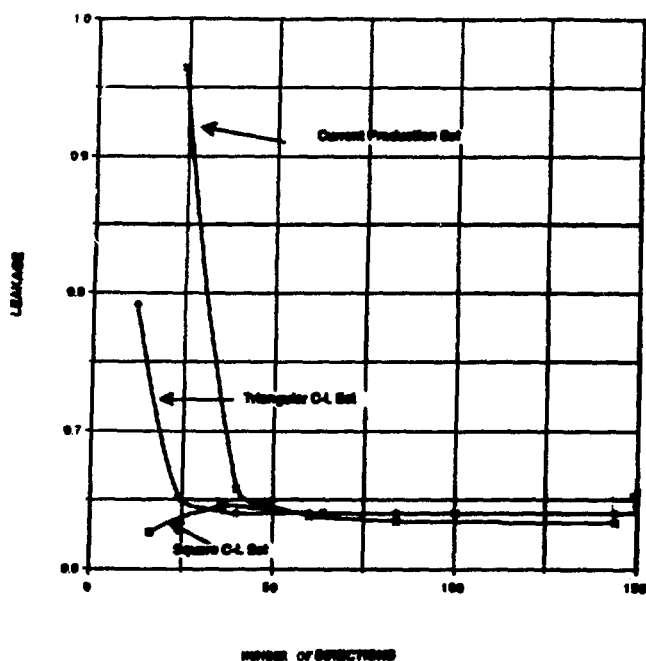


Fig. 5. Leakage vs. Ordinate Directions.

In Fig. 6 and the excess reactivity, multiplication constant -1 , is plotted versus the number of discrete directions for a pure uranium cylinder. P3 scattering is assumed. In Fig. 7, the transport correction to the self-scatter cross section has been used to make the comparison easier. The transport correction has little or no effect on the C-L set, but results in a smoother result for the TWODANT production set. Again, the C-L set approaches the asymptotic result more quickly as the angular mesh is refined as compared to the production set. A constant offset is once again seen between the two sets.

The new square C-L quadrature set yields results in agreement with the default quadrature set in TWODANT when anisotropic scattering is small. The C-L set is seen to be significantly better than the default set in problems where forward peaked scattering is large. If there is any question that high-order P3 scattering is important, the S4 square C-L set should be used instead of the S8 default set. The S4 square C-L set consists of 16 directions while the default S8 set consists of 40 directions. This difference will result in a large savings in storage and a decrease by a factor of 2.5 in the neutronic run time.

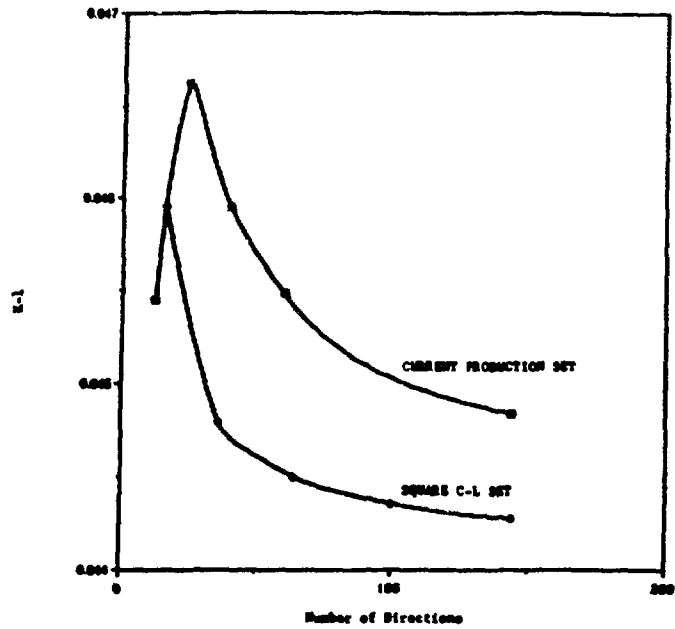


Fig. 6. Excess Reactivity vs. Discrete Directions.

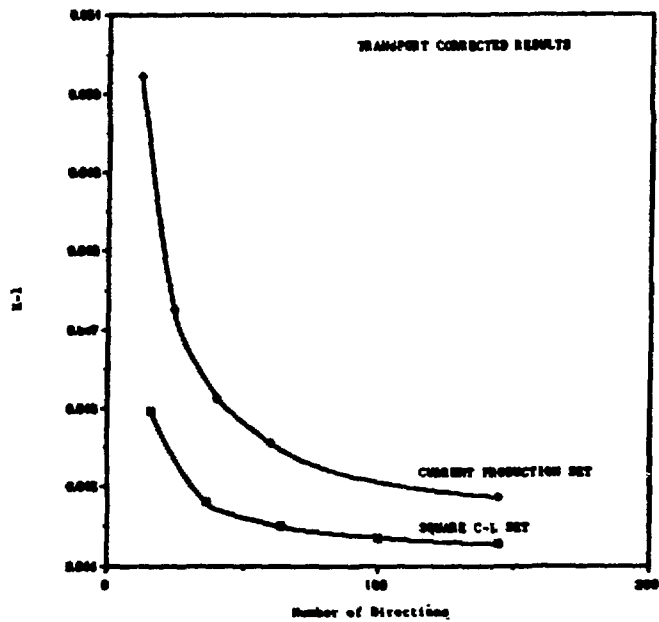


Fig. 7. Excess Reactivity vs. Discrete Directions—Transport Corrected Results.

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LONG DISTANCE PROPAGATION WITH DFE : A DISCONTINUOUS FINITE ELEMENT SCHEME

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We consider the one-dimensional BOLTZMANN equation in its time-dependant form it can be written as usual

$$(1) \quad \frac{1}{v} \frac{\partial \Phi}{\partial t} + \mu \frac{\partial \Phi}{\partial r} + \frac{1-\mu^2}{r} \frac{\partial \Phi}{\partial \mu} + \sigma \Phi = S(\Phi) + Q_0$$

where the flux Φ depends on r , μ and t , respectively the distance from the center, the cosine of deflection angle and the time.

σ is the total interaction cross-section.

Q_0 is an external source term.

and S the so-called scattering source terme depending on Φ .

In the treatment of the propagation of a point like source, in media where scattering is not important, the unscattered flux has to be calculated if possible analytically, keeping the numerical solution for the collided flux.

Thus it was done and equation (1) was solved with a discontinuous finite element method DFE in space and direction and a centered Crank-Nicholson scheme in time.

Over the domain Ω defined by

$$\begin{aligned} 0 &< r < R \\ -1 &< \mu < +1 \end{aligned}$$

we can integrate equation (1), after multiplying by a set of trial functions $\Phi_k \in Q_1$.

It comes

$$\frac{1}{v} \int \frac{\Phi_{j+1} - \Phi_j}{\Delta t} \psi_K r^2 dr d\mu + \int \mu \frac{\partial \Phi^m}{\partial r} \psi_K r^2 dr d\mu + \int (1-\mu^2) r \frac{\partial \Phi^m}{\partial \mu} \psi_K dr d\mu + \int \sigma \Phi^m \psi_K r^2 dr d\mu$$

$$= \int S(r, \mu, t) \psi_K r^2 dr d\mu + \int Q_0 \psi_K r^2 dr d\mu$$

with $\Phi^m = \frac{1}{2} (\Phi_j + \Phi_{j+1})$

j being the index of time t_j

$$t_{j+1} = t_j + \Delta t$$

$$\psi_K \in Q_1 \quad 1, r, \mu, r\mu$$

This equation can be solved by a mesh sweeping method over a regular r, μ grid.

APPLICATION

Corresponding to a ponctual source term

$$Q \propto \frac{\delta(r) \delta(t)}{4\pi r^2}$$

the uncollided flux can be written as :

$$\frac{1}{4\pi r^2} e^{-\int_0^r \sigma(r') dr'} \delta(t - \frac{r}{v}) \delta(1-\mu)$$

The DFE scheme used here is suitable for expanding the first collision source term on the spatial mesh. This term has the following expression.

$$S(\Phi_i)_{\text{uncollided}} = \frac{1}{t_{j+1} - t_j} \int_{t_j}^{t_{j+1}} dr e^{-\int_0^r \sigma(r') dr'} [Y(r - vt_j) - Y(r - vt_j - v\Delta t)]$$

where Y is the Heaviside function

The uncollided flux gives raise to a front wave source, propagating with a speed v and a spatial width defined by the 2 Y functions.

We used this method to treat a benchmark problem given at the last CEA-LOS ALAMOS encounter in Bruyères-le-Chatel.

It was a 2 groups neutron-gamma coupled problem where a pulse of high energy neutrons was emitted at the center of the following system.

Air	Leak	Iron	Sand	Tuff	
138.57	.16	1.27	100.	100.	in cm

The neutron-speed is taken equal to 5.4797 cm per ns.

The diffusion source term is developed in Legendre polynomials until order 4.

The following pictures exhibit the scalar γ flux function of the radius at 2 different times, i.e.

$$t = 40 \text{ ns and } 50 \text{ ns}$$

compared to values given by the TIMEX code.

In both cases, the shape is almost the same, except at 50 ns where the region with leak and iron shells shows large negative fluxes (not drawn) in TIMEX which are not present in the DFE treatment.

We give also, the γ flux, function of time at a fixed radius $R = 200$ cm in the Sand. We see the shoulder centered at approximately 30 ns due to the γ created in the iron shell and having been scattered. This bump comes before the neutron gamma peak corresponding to γ created in the medium.

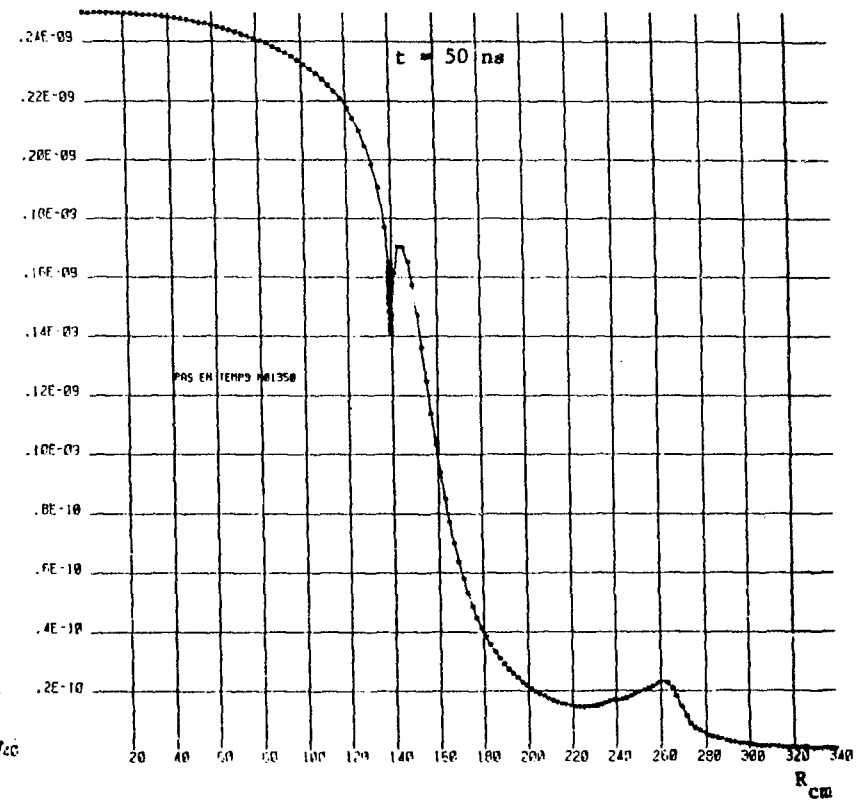
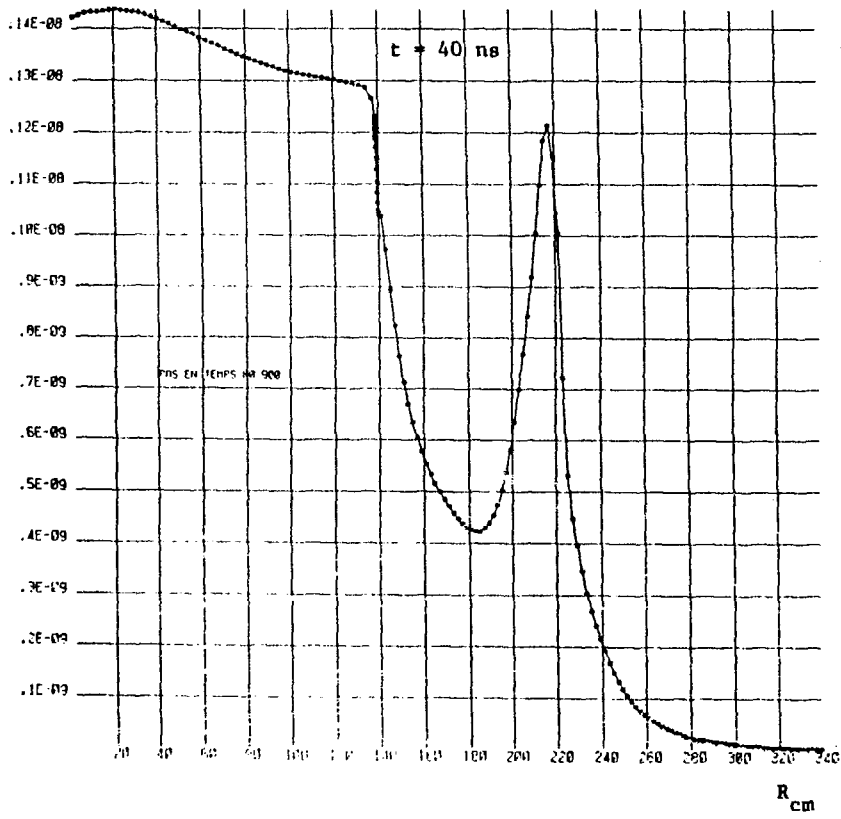
The accuracy of the method which has been tested on other cases allows us to study long distance propagation problems without introducing numerical shifts between the wave front and the other related phenomena.

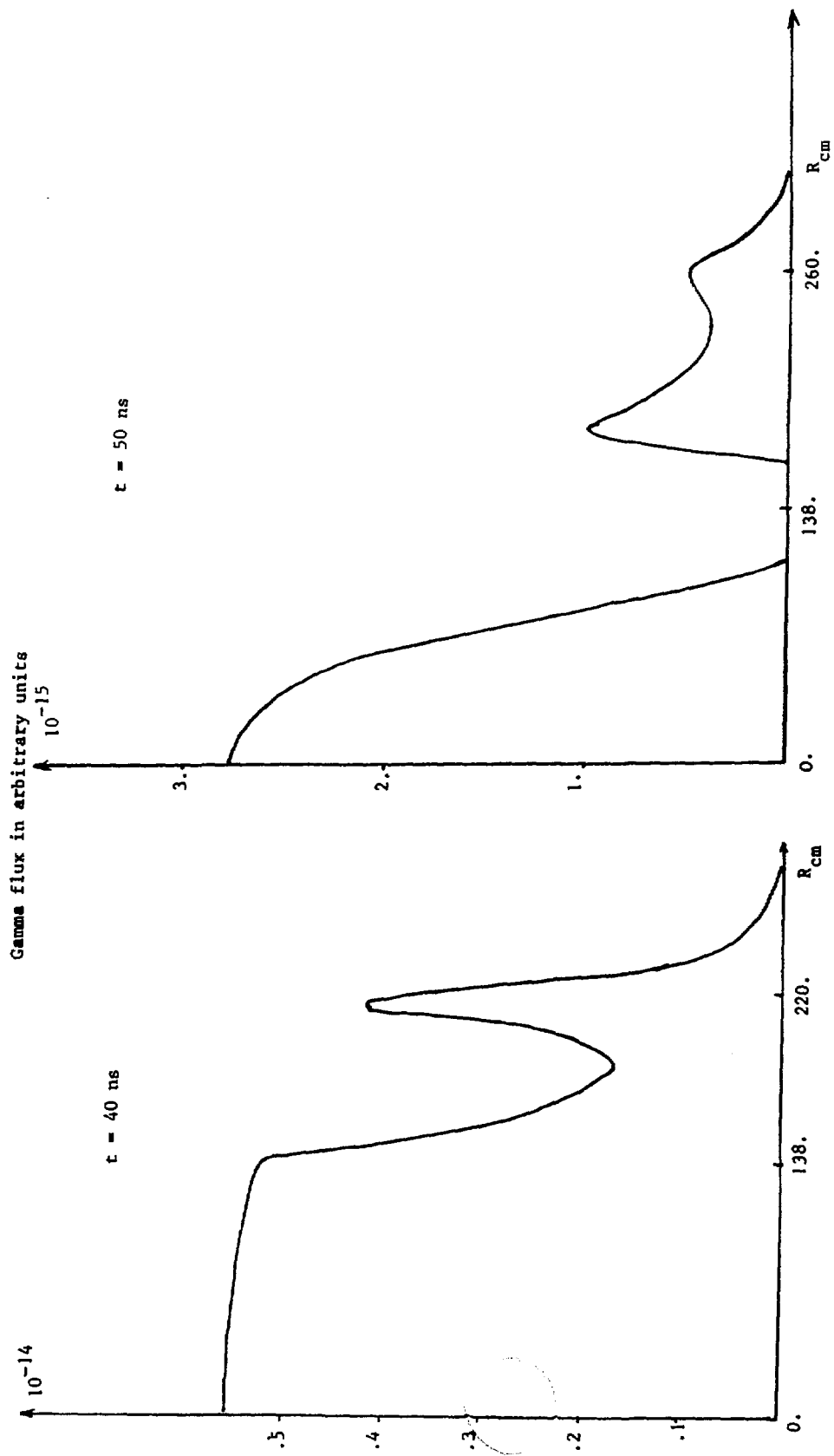
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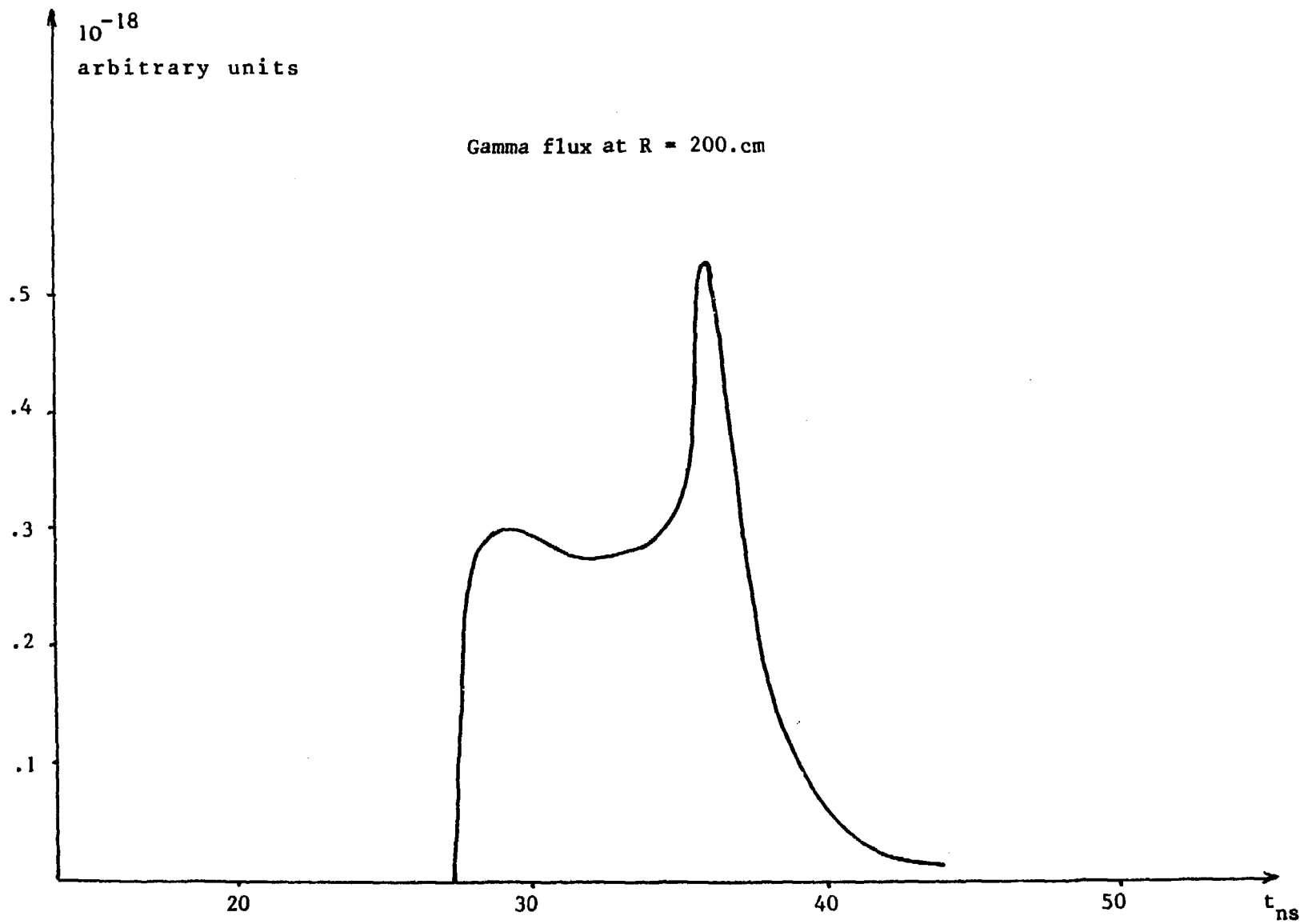
DFE RESULTS

Gamma flux in arbitrary units



TIMEX RESULTS

DFE RESULTS



COMPARISON OF TWO MODELS OF RAYLEIGH-TAYLOR INDUCED TURBULENT MIXING

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ABSTRACT

Turbulent mixing of two species occurs in a variety of natural and technological phenomena such as diffusion of pollutants in the atmosphere or oceans, combustion, astrophysics and inertial confinement fusion (ICF). We compare here two turbulence models in the special case of Rayleigh-Taylor instability induced turbulent mixing in a variety of experiments for one-dimensional mean-flows.

I/ INTRODUCTION

For some years, the use of turbulence models was devoted to single fluid, incompressible flow. Even if tensor models were first proposed¹, "k- ϵ " models, composed of equations for the turbulent kinetic energy and its dissipation rate^{2,3} were soon preferred, for the sake of simplicity and computing cost. These models were mostly used for shear layers⁴. Recently, more sophisticated models were proposed for reacting⁵ and compressible flows. Also, models for instability-induced turbulence have been developed, including the effect of large density gradients in the mean flow^{5,6,7}. Mixtures are described either with a two field approach⁸, or with a turbulent mixture model^{9, 10, 11, 12}.

Our purpose here is to compare two models for turbulent mixtures, in the special case of less studied Rayleigh-Taylor (RT) instability induced turbulent mixing, but of great interest in ICF configurations. The detailed description of the different phases of the mixing is out of reach in real situations, and we therefore rely instead on statistical models.

In both models one starts with the Navier-Stokes equations and, having separated each variable into mean and fluctuating parts, one obtains a set of equations for a variety of turbulent correlations expressed as products of the fluctuating variables. TURGAU has been developed at Limeil^{9,14,15} and is specifically designed for applications in ICF calculations. It contains the usual mean flow equations with the turbulent correlations modeled by first gradient laws and one equation for the transport of turbulent kinetic energy. BHL, developed in collaboration at Los Alamos and Limeil^{6, 12}, was conceived with broader applications in mind, and has several additional turbulence transport equations for the other second-order correlations.

Section II is devoted to the theoretical comparison of the two models, and we show that TURGAU can be deduced from BHI, provided we make a number of approximations, among which quasi-isotropy of the turbulent kinetic energy, and stationary turbulent mass fluxes.

Numerical applications are considered in Section III. We address the problem of initialization in time-dependent circumstances, of the presence of shocks in the mean-flow, and present results for shock-tube experiments.

II/ PRESENTATION OF THE MODELS

BHI Model is intended to generalize models for incompressible flow in three different ways : it is specifically designed for handling instability driven turbulence creation ^{6,12} (Rayleigh-Taylor, Kelvin-Helmoltz, coherent two-field instabilities, including both exponential growth and self-similar regime for the fluctuating energy; it allows for large Mach Number mean-flow ¹² ; in the case of a small level of turbulence, it reduces to a two-field statistical model, therefore includes the limiting case of "ordered" two-field interpenetration¹².

At this stage of development, our main assumption is that the turbulent Mach number ($\sqrt{k}/C$) is small. In other words, we preclude here the case of supersonic interpenetration of the different materials. Fortunately, this is true for a large variety of flows.

The technique used here is to derive transport equations for the following turbulent correlations : Reynolds tensor $\bar{\rho} k_{ij}$ ($\bar{\rho} u_i u_j - \bar{\rho} \tilde{u}_i \tilde{u}_j$), turbulent mass flux A_i ($\bar{\rho}' u_i$), density self correlation B (ρ'^2), and for the corresponding equations for the dissipation correlations D_{ij} ($\overline{\partial u_i' / \partial x_k} \partial u_j' / \partial x_k}$), Da_i ($\overline{\partial \rho' / \partial x_k} \partial u_i' / \partial x_k}$), and D_B ($\overline{\partial \rho' / \partial x_k} \partial \rho' / \partial x_k}$). An equation for the correlation $\bar{\rho}' I'$, where I is the specific internal energy, is not required for the type of applications we want to study here.

TURGAU model was derived independently and is aimed at the more practical applications of ICF calculations. It is therefore simpler and is composed of an evolution equation for the turbulent kinetic energy k .

We present the BHI equations¹² in the special case of a 1D mean-flow allowing for RT-instability driven turbulence. From them, we deduce TURGAU equations.

$$\frac{\partial \bar{\rho}}{\partial t} + r^{-\alpha} \frac{\partial r^{\alpha} \bar{\rho} \tilde{u}_r}{\partial r} = 0, \quad (1)$$

$$\frac{\partial \bar{\rho} \tilde{u}_r}{\partial t} + r^{-\alpha} \frac{\partial r^{\alpha} \bar{\rho} \tilde{u}_r^2}{\partial r} = - \frac{\partial \bar{P}}{\partial r} - r^{-\alpha} \frac{\partial r^{\alpha} \bar{\rho} k_r}{\partial r}, \quad (2)$$

$$\frac{\partial \bar{\rho}}{\partial t} \tilde{I} + r^{-\alpha} \frac{\partial r^{\alpha} \bar{\rho} \tilde{u}_r \tilde{I}}{\partial r} = -\bar{P} r^{-\alpha} \frac{\partial \bar{u}_r r^{\alpha}}{\partial r} - r^{-\alpha} \frac{\partial r^{\alpha} S_r}{\partial r} + \epsilon, \quad (3)$$

$$\frac{\partial \bar{\rho} \tilde{c}}{\partial t} + r^{-\alpha} \frac{\partial r^{\alpha} \bar{\rho} \tilde{c} \tilde{u}_r}{\partial r} = -r^{-\alpha} \frac{\partial r^{\alpha} i_r}{\partial r}, \quad (4)$$

$$S_r = -C_s \tilde{c} (1-\tilde{c}) A_r \tilde{I} - C_{\mu s} s \sqrt{k} \bar{\rho} \frac{\partial \tilde{I}}{\partial r}, \quad (5)$$

$$i_r = C_i \tilde{c} (1-\tilde{c}) A_r - C_{\mu i} s \sqrt{k} \bar{\rho} \frac{\partial \tilde{c}}{\partial r}, \quad (6)$$

$$\frac{\partial \bar{\rho} k}{\partial t} + r^{-\alpha} \frac{\partial \bar{\rho} k \tilde{u}_r r^{\alpha}}{\partial r} + 2 \bar{\rho} k_r \frac{\partial \tilde{u}_r}{\partial r} =$$

$$\frac{2}{\rho} A_r \frac{\partial \bar{P}}{\partial r} + r^{-\alpha} \frac{\partial}{\partial r} [\alpha_k r^{\alpha} C_{\mu} D^{-\frac{1}{2}} \bar{\rho} k \frac{\partial k}{\partial r}] + \frac{2}{3} C_k D^{\frac{1}{2}} \frac{\partial \tilde{u}_r}{\partial r} - \epsilon,$$

$$\begin{aligned} \frac{\partial \bar{\rho} k_{\perp}}{\partial t} + r^{-\alpha} \frac{\partial \bar{\rho} k_{\perp} \tilde{u}_r r^{\alpha}}{\partial r} &= r^{-\alpha} \frac{\partial}{\partial r} [r^{\alpha} C_{\mu} D^{-\frac{1}{2}} \bar{\rho} k_r \frac{\partial k_{\perp}}{\partial r}] + C_w D^{\frac{1}{2}} \bar{\rho} \left(\frac{k_r - 2 k_{\perp}}{3} \right) \\ &- \frac{4}{3} C_K D^{\frac{1}{2}} \frac{\partial \tilde{u}_r}{\partial r} - \epsilon_{\perp}, \end{aligned} \quad (8)$$

$$\frac{\partial A_r}{\partial t} + r^{-\alpha} \frac{\partial A_r \tilde{u}_r r^{\alpha}}{\partial r} + k_r \frac{\partial \bar{\rho}}{\partial r} - \bar{\rho} r^{-\alpha} \frac{\partial}{\partial r} (r^{\alpha} A_r^2 / \bar{\rho}^2) - r^{-\alpha} A_r \frac{\partial}{\partial r} (r^{\alpha} A_r / \bar{\rho})$$

$$+ A_r \frac{\partial \tilde{u}_r}{\partial r} = r^{-\alpha} \frac{\partial}{\partial r} [2 r^{\alpha} C_{\mu a} D^{-\frac{1}{2}} \bar{\rho} k_r \frac{\partial A_r / \bar{\rho}}{\partial r}] + \frac{B}{\bar{\rho}} 2 \frac{\partial \bar{P}}{\partial r} - C_a D^{\frac{1}{2}} A_r, \quad (9)$$

$$\begin{aligned} \frac{\partial B}{\partial t} + r^{-\alpha} \frac{\partial r^{\alpha} B \tilde{u}_r}{\partial r} + B \frac{\partial \tilde{u}_r}{\partial r} + 2 A_r \frac{\partial \bar{\rho}}{\partial r} - \frac{A_r}{\bar{\rho}} \frac{\partial B}{\partial r} - 2 B \frac{\partial A_r / \bar{\rho}}{\partial r} \\ = r^{-\alpha} \frac{\partial}{\partial r} (r^{\alpha} C_{\mu B} D^{-\frac{1}{2}} \bar{\rho} k_r \frac{\partial B}{\partial r}) - C_B D^{\frac{1}{2}} B, \end{aligned} \quad (10)$$

where α ($= 0, 1, 2$) is the geometry index, k is twice the turbulent kinetic energy per unit mass, k_r the component of k_{ij} along the mean-flow motion, $k_{\perp}$ the orthogonal component, A_r the turbulent mass flux along the mean motion, s the local turbulent

length scale and $\tilde{c}$ the mean concentration of one of the materials. We also have

$$\varepsilon = C_{\mu} s \sqrt{k} D,$$

and

$$\varepsilon_{\perp} = C_{\mu} s \sqrt{k} D_{\perp},$$

where D and $D_{\perp}$ are respectively the contraction of the D_{ij} tensor, and its difference with the component D_{rr} of D_{ij} along the mean motion.

The dissipation equations are lengthy and complicated, but formally similar to those of k_r , $k_{\perp}$, A_r and B . They are not crucial for our demonstration, and we therefore omit them here. They can be found elsewhere¹².

To compare BHI to TURGAU, we start with Eqs.(1-10) in which we first approximate¹ the correlation D as $\alpha_D k s^{-2}$. In the special case of RT induced turbulent mixing, it is known¹³ that the turbulence length scale remains a fraction of the turbulent mixing zone (TMZ) thickness L . We therefore state

$$L(t) = \alpha_s s, \quad (11)$$

where L can also be interpreted as an integral length scale.

The second approximation is to assume a quasi-steady state in Eq. (9), and to balance the production term due to the presence of a mean-density gradient and the dissipation of A_r . This means that turbulence is in late stage, and precludes any description of the exponential growth stage of k ⁶, as well as any triggering mechanism for the turbulence growth due to corrugations of the interface or nonhomogeneities in the flow when accelerated¹². Another crucial approximation is needed, that is that the turbulence is quasi-isotropic. This implies that the coefficient C_w in Eq.(8) is very large, and we can seek an expression for k_{ij} as

$$k_{ij} = \frac{1}{3} k_{kk} \delta_{ij} + \frac{\varepsilon_{ij}}{C_w}. \quad (12)$$

Using Eq. (12) in the general equation for k_{ij} ^{6, 8, 12}, and keeping only the lowest order terms of C_w^{-1} , we obtain an equation for k after contraction. We multiply the resulting equation by δ_{ij} , and subtract it from the initial uncontracted equation. We obtain

$$\varepsilon_{ij} = -\frac{3}{\sqrt{\alpha_D}} s \sqrt{k} \left[\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{1}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right]. \quad (13)$$

From the balance in the A_r equation, and the lowest-order form of Eq.(12), we

deduce that

$$A_r = -\alpha_A s \sqrt{k} \frac{\partial \bar{\rho}}{\partial r}, \quad (14)$$

with

$$\alpha_A = (3 C_a \alpha_D^{-\frac{1}{2}})^{-1}.$$

Inserting Eqs.(12) and (13) in Eqs.(2), (7) and (8), and Eq.(14) in Eqs.(5) and (6), we obtain

$$\frac{\partial \bar{\rho}}{\partial t} \tilde{u}_r + r^{-\alpha} \frac{\partial r^{\alpha} \bar{\rho} \tilde{u}_r^2}{\partial r} = - \frac{\partial \bar{P}}{\partial r} - r^{-\alpha} \frac{\partial}{\partial r} \left[r^{\alpha} \left(\frac{2}{3} \bar{\rho} k - \frac{4}{3} \alpha_v L \sqrt{k} \bar{\rho} \frac{\partial \tilde{u}_r}{\partial r} \right) \right], \quad (15)$$

$$\frac{\partial \bar{\rho} \tilde{c}}{\partial t} + r^{-\alpha} \frac{\partial r^{\alpha} \bar{\rho} \tilde{c} \tilde{u}_r}{\partial r} = r^{-\alpha} \frac{\partial}{\partial r} \left(r^{\alpha} \alpha_c L \sqrt{k} \bar{\rho} \frac{\partial \tilde{c}}{\partial r} \right), \quad (16)$$

$$\begin{aligned} \frac{\partial \bar{\rho} k}{\partial t} + r^{-\alpha} \frac{\partial r^{\alpha} \bar{\rho} k \tilde{u}_r}{\partial r} = & - \left(\frac{4}{3} \alpha_v L \sqrt{k} \bar{\rho} \frac{\partial \tilde{u}_r}{\partial r} + \frac{2}{3} \bar{\rho} k \right) \frac{\partial \tilde{u}_r}{\partial r} \\ & + r^{-\alpha} \frac{\partial}{\partial r} \left(r^{\alpha} \alpha_k L \bar{\rho} \sqrt{k} \frac{\partial k}{\partial r} \right) - \alpha_R L \frac{1}{\bar{\rho}} \sqrt{k} \frac{\partial \bar{\rho}}{\partial r} \frac{\partial \bar{P}}{\partial r} - \alpha' \bar{\rho} k^{3/2} L^{-1}, \end{aligned} \quad (17)$$

where

$$\alpha_v = 3 \alpha_s^{-1} \alpha_D^{-\frac{1}{2}},$$

$$\alpha_c = (C_1 \alpha_A + C_{\mu 1}) \alpha_s^{-1},$$

$$\alpha_R = (3 C_a \alpha_D^{\frac{1}{2}} \alpha_s)^{-1}, \quad (18)$$

and

$$\alpha' = C_{\mu} \alpha_s.$$

The approximation given in Eqs.(12-13) may fail when shocks are present in the flow. In Eqs.(15) and (17), the value of k_r is then limited between (.1k) and (1.2k). Also, in the stable case of pressure and density gradients of same sign, k should not decrease. The corresponding term in Eq. (17) is then truncated as

$$P_{RT} = \alpha_R L \frac{1}{\bar{\rho}} \sqrt{k} \left| \frac{\rho_A - \rho_B}{L} \frac{\partial \bar{P}}{\partial r} \right| \tilde{c} (1 - \tilde{c}) \text{ when } \frac{\partial \bar{\rho}}{\partial r} \frac{\partial \bar{P}}{\partial r} < 0, \quad (19)$$

$$P_{RT} = 0 \text{ when } \frac{\partial \bar{\rho}}{\partial r} \frac{\partial \bar{P}}{\partial r} > 0,$$

where ρ_A and ρ_B are the densities at the boundaries of the TMZ.

Noticing that $\bar{u}_r = \tilde{u}_r - A_r/\bar{\rho}$, we transform Eq. (3) to obtain

$$\begin{aligned} \frac{\partial \rho \tilde{I}}{\partial t} + r^{-\alpha} \frac{\partial r^{\alpha} \bar{\rho} \tilde{u}_r \tilde{I}}{\partial r} = - \bar{P} r^{-\alpha} \frac{\partial \tilde{u}_r}{\partial r} - \bar{P} r^{-\alpha} \frac{\partial}{\partial r} \left(\alpha_R \frac{L \sqrt{k}}{\bar{\rho}} \frac{\partial \bar{\rho}}{\partial r} \right) \\ + r^{-\alpha} \frac{\partial}{\partial r} \left(\alpha_T L \sqrt{k} \bar{\rho} \frac{\partial \tilde{I}}{\partial r} \right) + \alpha' \bar{\rho} k^{3/2} L^{-1}, \end{aligned} \quad (20)$$

where

$$\alpha_T = (C_s \alpha_A + C_\mu) \alpha_s^{-1}.$$

Equations (1), (15-20) are constituting the version of TURGAU used for our numerical comparisons with BHL. A equation of state is added to both models to close the equations. A temperature equilibrium for the two material is assumed in TURGAU, not in BHL.

III/ NUMERICAL APPLICATION

III.1 - Initialization

BHL and TURGAU¹⁴ are implanted in one-dimensional Lagrangian hydro-codes and mixing takes place with constant mass per cell. Enhancement of turbulent mixing due to shock waves cannot be treated rigorously by the simple current numerical schemes of BHL and TURGAU but, for the purpose of our comparison, this is not crucial. As TURGAU does not calculate the initial phases of Rayleigh-Taylor instability (i.e. linear and non-linear growth), turbulent mixing has to be initialized, with phenomenological rules and experimental data if available. In the exemple shown, where the details of the rupture of the membrane separating the gases are unknown, a mixing length L , over which $B = A_t^2 \bar{\rho}^2 (A_t : \text{Atwood number})$ and k the local turbulent kinetic energy per unit mass, constitute the initialization of BHL. In Turgau, the TMZ is initialized over a width L with a triangular profile of k , straddling the interface with a maximum at $k_{\max}$. There is no term for density fluctuations B and the time and value of initialization are critical. As a guideline, we estimate k and L using the growth rates of Rayleigh-Taylor instability in its non-linear phase, where the wavelengths and amplitudes of the initial contact surface perturbations are forgotten. Numerical and experimental results¹³, extrapolated to the case of the shock-induced Rayleigh-Taylor instability, suggest that $k = (0.06 A_t V)^2$, $L = 0.12 A_t V t$, where t is the time elapsed since the shock accelerated the contact surface to the velocity V . The integrated turbulent kinetic energy initialized over the width L is approximately $0.5(\rho_A + \rho_B)kL$,

and because it is abruptly injected in the calculation, a transient numerical phase occurs after initialization. The values of k , L and K should in principle be adjusted after that phase.

We present the results of the calculation of the TMZ for 4 experiments : a low Mach number shock tube experiment ^{10,11}, a cylindrical implosion ¹¹, and high Mach number shock tube experiments ¹⁵.

The coefficients for BHI are : $C_A = C_B = 1$, $C_k = 0$, $C_w = 2.5$, $C_\mu = C_{\mu A} = C_{\mu B} = 0.1$ plus others ¹²; for TURGAU, $\alpha_c = \alpha_k = \alpha_T = 0.1$, $\alpha_v = 0.05$, $\alpha' = 4$ and $\alpha_R = 6$. The integral scale of turbulence in TURGAU is L . At initialization, the two gases have not yet mixed, but soon afterwards, the thickness based on the concentration catches up with L . The two values are shown on figures 1a and 1c.

III.2. Low Mach number shock tube experiments

An air-helium contact surface is accelerated and decelerated by a shock wave of initial Mach number 1.3 in air. The computational grid, made of 200 cells for BHI and 300 for TURGAU extends over 33.8 cm in air and 16.9 cm in helium. The acceleration takes place at 760 μ s, the TMZ is initialized at 800 μ s for TURGAU with $k_{\max} = 10^{-3} v^2 = 5 \cdot 10^5 \text{ cm}^2/\text{s}^2$, $L = 0.25 \text{ cm}$ which is consistent with the guideline above. The initial TMZ thickness for BHI is 0.25 cm as measured before the reflected shock, and $k(\text{initial}) = 0$. Figure 1a shows the trajectory and the thickness of the TMZ and Figure 1b gives $k_{\max}$ and K as calculated by TURGAU. Note that the TMZ thickness is 1 cm instead of 0.25 cm at 1000 μ s for a correct final value of 4.5 cm and that the transient phase between 800 and 900 μ s create an unphysical rise of $k_{\max}$ before the rises due to reflected shocks at 1010 and 1180 μ s. Figures 2a,b,c, show the trajectory, thickness and $k_{\max}$ as calculated by BHI with error bars representing the experimental results. BHI is able to reproduce the measured growth of the TMZ with very little initial turbulence, because of the additional equation for B , when TURGAU needs a large amount of k . In fact, for flows with long coasting phases between shocks, the results of BHI are quite insensitive to the initial value of k .

III.3. Cylindrical implosion

With only a x - t diagram published ¹¹, we chose a 3.6 cm outer layer of air, with an external pressure of 7.0 bars from 0 to 30 μ s and decreasing to 1 bar (also the initial pressure) from 30 to 150 μ s and a 6 cm radius cylindrical region of helium. Initialization was at 50 μ s over $L = 0.2 \text{ cm}$ with $k_{\max} = 10^{-3} v^2 = 8 \cdot 10^6 \text{ cm}^2/\text{s}^2$ for TURGAU. Results are shown on Figure 1c,d. In the case of BHI, with an air layer of 3.0 cm, initialization was made at 0 μ s with $L = 0.2 \text{ cm}$. Thickness, trajectory and $k_{\max}$ are shown on Figures 2d,e,f, again with the error bars from the experiments.

As shown on figures 1d and 2f, both models correctly predict a slow rise of $k_{\max}$, due to the pressure and velocity gradients existing behind a converging cylindrical shock, before the steep rise due to the expanding reflected shock at 75 μ s.

III.4 High Mach number shock tube experiments

In the experiments¹⁵, a Mach 4.5 shock wave propagating in CO₂ at $1.52 \cdot 10^4$ cgs accelerates a CO₂-helium or CO₂-argon contact surface thus creating the TMZ which is then decelerated by the reflected shocks. Because of the high Mach number and low initial pressures, thick unsteady boundary layers in the shock tube make the flow more two-dimensional. This cannot be simulated in the two models, but it is nevertheless useful to examine the effects in the calculation of the high Mach number and of the different Atwood numbers after compression by the incident shock ($A_t = -0.85$ for CO₂/He and -0.45 for CO₂/A). The computational grid extends over 250 cm on the CO₂ side and 152 cm on the helium (argon) side, as in the experiment. In the calculation, the CO₂/He (respectively CO₂/A) contact surface accelerates at 2350 μ s to $V = 1.45 \cdot 10^5$ cm/s (10^5 cm/s) and the first reflected shock slows down the TMZ at 3200 μ s (3650 μ s). In TURGAU, the CO₂/He TMZ is initialized at 2800 μ s with $k_{\max} = 5 \cdot 10^{-4} v^2 = 10^7$ cm²/s² over $L = 1$ cm while the CO₂/A TMZ starts at 2800 μ s with lower values: $k_{\max} = 2.5 \cdot 10^{-4} v^2 = 0.25 \cdot 10^7$ cm²/s² over $L = 0.5$ cm in order to take in account the difference in Atwood number. Results are shown on figures 1e for the TMZ thickness L and 1f for $k_{\max}$. Note the artificial rise of $k_{\max}$ between 2800 and 3000 μ s for CO₂/He.

The experimental data¹⁵, before the reflected shock ($L = 3.5$ cm for CO₂/He and $L = 2.5$ cm for CO₂/Ar) and after (very large thickening in both cases) do not indicate such a strong dependance on the Atwood number. Finally, the results obtained with BHI, with an initialization at $t = 2300$ μ s with $L = 2.1$ cm for argon and at $t = 2500$ μ s with $L = 3.5$ cm for helium are shown on figures 2g and 2h for the TMZ thickness for CO₂/A and CO₂/He and figure 2i for $k_{\max}$ in the case CO₂/He. Note that in these preliminary calculations the coarseness of the grid creates the abrupt changes of L at 2500 μ s for CO₂/A.

IV- CONCLUSION

The comparison of the two codes shows that the additional equation for the density fluctuations B in the modelisation of BHI is crucial for the calculation of the very rapid thickening of the TMZ during its deceleration by reflected shocks, behavior that models with only one equation for k (and even ϵ) such as TURGAU cannot reproduce. However, when shock waves are not dominant in the mean flow, both models should perform similarly. In spite of the encouraging results when some data are available, we have to emphasize the problem of the initialization due to the difficulty of getting relevant measurements in ICF target implosion.

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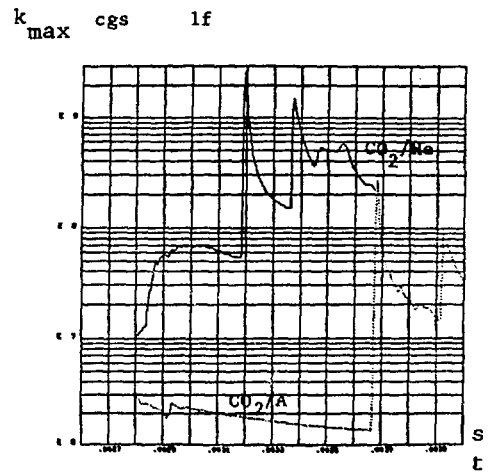
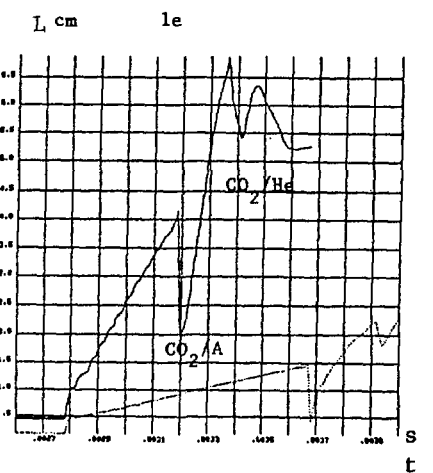
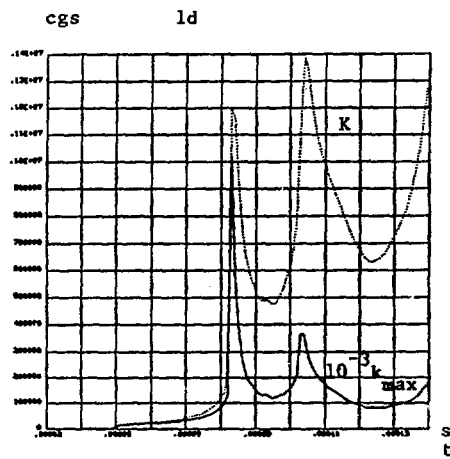
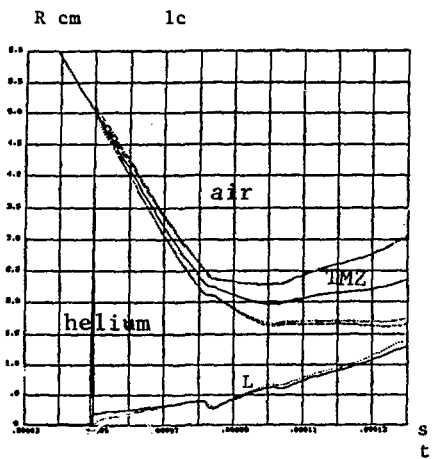
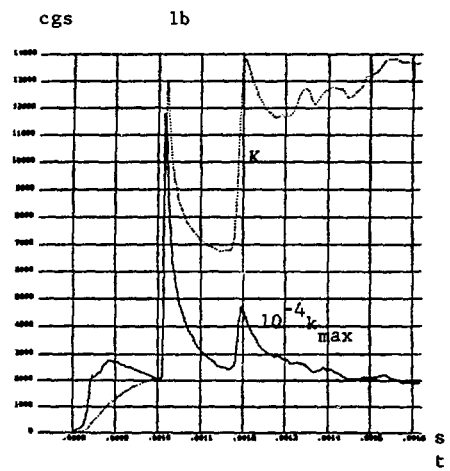
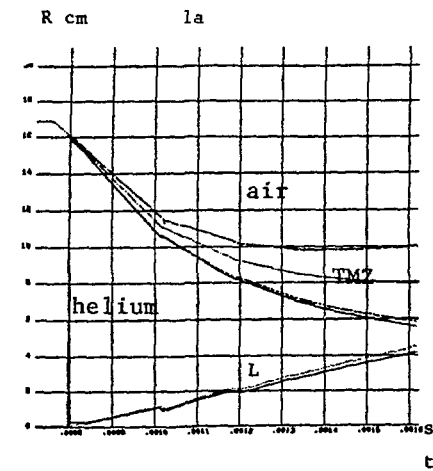


FIGURE 1 : TURGAU' results

1a,b : air/helium shock tube

1c,d : air/helium cylinder,

1e,f : CO_2 shock tube

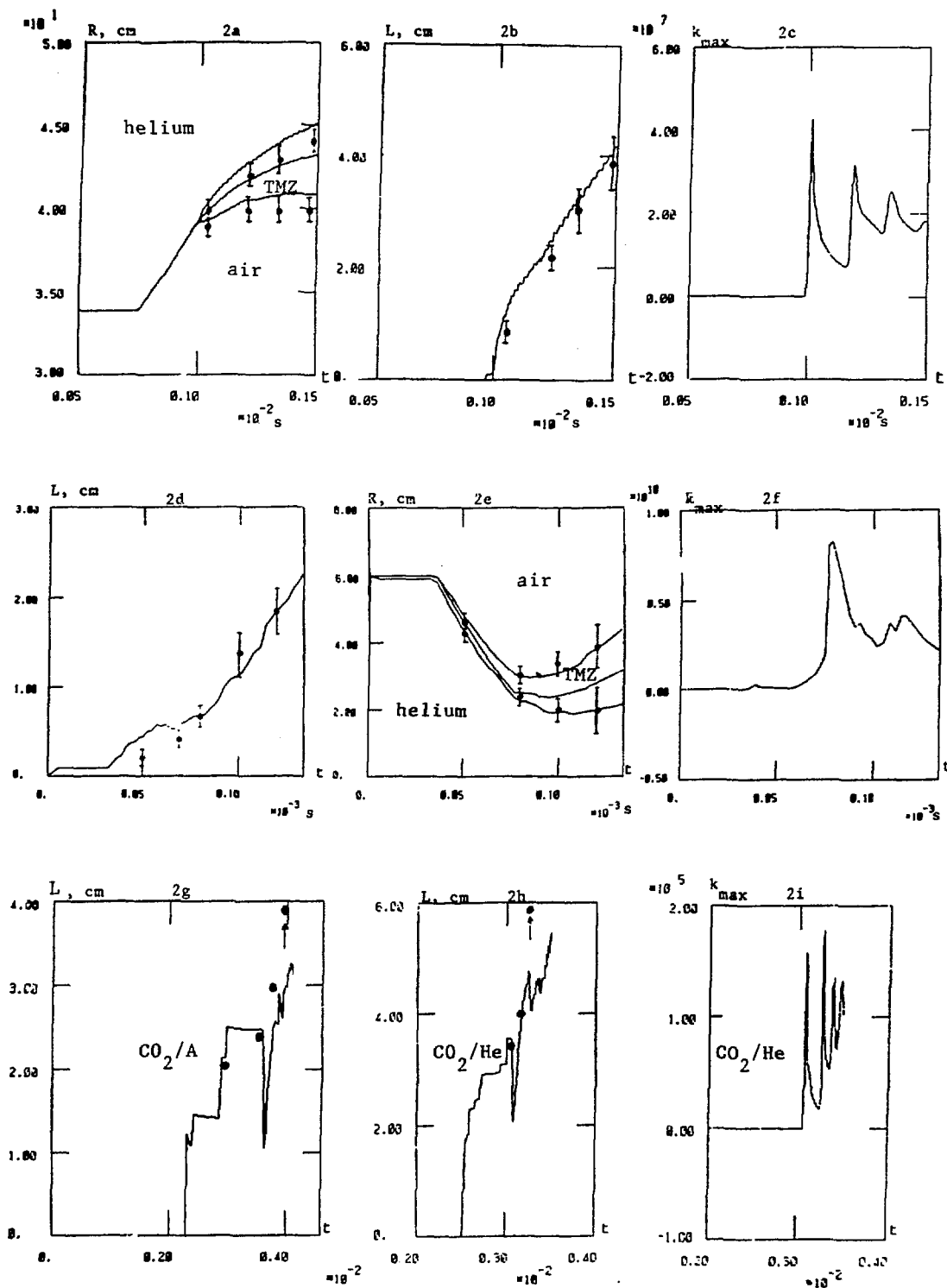


FIGURE 2 : BHI results

2a,b,c : air/helium shock tube 2d,e,f : air/helium cylinder 2g,h,i : CO_2 shock tube

AN ALTERNATIVE SOLUTION TO THE NUMERICAL MODELING OF MIXING

BY RAYLEIGH-TAYLOR INSTABILITY

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ABSTRACT

We propose a simple evolution modelisation of the mixture area induced by Rayleigh-Taylor instabilities at two fluid interfaces. The mixing has been assumed heterogeneous and we have taken into account the kinetic energy supplied to each fluid by relative motion of the other, via a single parameter. The model has been introduced in a 1-D lagrangian code : some results are shown for the definition and the interpretation of experimental devices.

INTRODUCTION

In order to study the evolution of a mixture area induced by small defects Rayleigh-Taylor instabilities at the interface between two different density species, we proposed a simple model with a single parameter /1/ but which alters the main flow which would be obtained if it had been computed a priori without defects. With an expression easier than the most complex turbulent mixing models we expect from this model a reasonably good approach of the influence of the mixture in very different fields. In our previous paper, the equations and also the numerical modelisation were proposed connected with a specific 1-D experiment in a convergent geometry for which the species were practically incompressible.

In order to take into account the compressibility of the species we propose here an extension of the equations formerly quoted to this area and also an extension to 2-D or 3-D geometries. We show how the compressible model has been introduced in a 1-D Lagrangien code using a finite difference method and how it is expected to be introduced in a 2-D Eurlian code.

From some experimental results and also from 1-D simulations we express some comments about the analysis which can be done from mixture area involvements created by instabilities.

NOMENCLATURE

k	parameter of the model
e	mixture internal energy $\left(e = \frac{1}{\rho} (\omega_1 e_1 + \omega_2 e_2) \right)$
e_i	species internal energy
$\vec{e}_j$	unit vectors of the coordinate system
$\vec{F}_i$	external volume forces applied to the system
N	1-D parameter ($N=0,1,2$ for plane, cylindrical or spherical geometry)
p	mixture pressure
p_i	species pressure
t	time
T_i	species temperature
$\vec{u}, u_j$	mean velocity of the mixture and component $\vec{u} = \frac{1}{\rho} (\omega_1 \vec{u}_1 + \omega_2 \vec{u}_2)$
$\vec{u}_i$	mean velocity of the species
$\vec{V}$	grid velocity
$\vec{V}_i^2$	mean square transversal velocity of a species
$\vec{W}, W_j$	auxiliary velocity of the mixture and components
γ	external acceleration field
$\frac{\delta}{\delta t}$	time derivative along the grid velocity $\vec{V} \left(\frac{\delta}{\delta t} = \frac{\partial}{\partial t} + \vec{V} \times \vec{\nabla} \right)$
λ	auxiliary factor in the mixture
ρ	mass density of the mixture ($\rho = \omega_1 + \omega_2$)
ρ_i	mass density of a species
σ	volume fraction of species 1 ($\sigma = \omega_1 / \rho_1$)
ω_i	species bulk density

SUBSCRIPTS :

$i = 1,2$ denoting each species
 $j = 1,3$ denoting the coordinates

1 - EQUATIONS

1-1 - Modelisation assumptions

As it had been proposed in /1/, the model is simply coming from a relation written for the motion of a bubble in a steady infinite, incompressible fluid ; so it is possible to take into account the kinetic energy induced to the surrounding fluid by the motion of the bubble via a single parameter. The mixtures that we are studying are supposed to be heterogeneous, every species producing on the other a kinetic energy of this kind, caused by their relative motions.

. The two species are not different in their nature so the model is symmetrical.

. Though the mixture is heterogeneous, the basic equations are homogenized with the main motion so we can carry out numerical computation practically as if it was a pure material.

. The two species move each other with their own average velocity field, the consequence is that the mixture boundaries with the pure species are clearly separated . On the other side the two species still obey to their own equations of state .

According to a thermodynamical point of view we assume that the two species are locally at the same pressure. In the compressible area, two extreme assumptions are used for heat exchanges between the two species (thermal isolation or temperature equilibrium).

1-2 - Mathematical formulation

The concept of the mathematical formulation is similar to the one expressed in /1/ : it is built by writing the integral conservation laws for the mixture then by homogenizing them. We assume that for any volume Ω in the mixture we can find a volume Ω_i belonging to each species i (Fig.1).

Obviously, we get :

$$\Omega = \Omega_1 + \Omega_2$$

and, by definition :

$$\left. \begin{aligned} \omega_1 \Omega &= \rho_1 \Omega_1 \\ \omega_2 \Omega &= \rho_2 \Omega_2 \end{aligned} \right\} \quad (1-1)$$

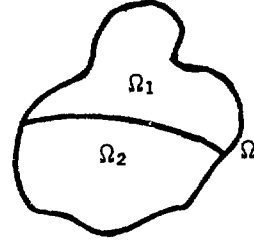


Fig 1

TRANSVERSAL VOLUME KINETIC ENERGY

Considering a spherical bubble of volume Ω_B ascending with a velocity $\vec{V}_B$ in an infinite incompressible fluid at rest of density ρ_F , this bubble induces to the fluid by its motion a kinetic energy K such as

$$K = \frac{1}{2} k \rho_F \Omega_B \vec{V}_B^2 \quad (1-2)$$

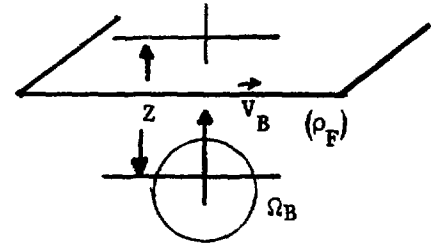


Fig.2

in which $k \approx 1/2$

Also, the kinetic energy per unit length in a plane at a distance Z in the direction of motion $\vec{V}_B$ decreases like $1/Z^2$, and then the main part of the energy stays in the vicinity of Ω_B .

By analogy, for the present problem, we assume that a small volume Ω_1 mainly influences the volume Ω_2 of the other species and reciprocally.

In terms of transversal volume kinetic energy induced by a species over an other, we will write :

$$\left\{ \begin{aligned} \frac{1}{2} \omega_1 \vec{V}_1^2 &= \frac{1}{2} k \rho_1 \frac{\omega_2}{\rho_2} (\vec{U}_2 - \vec{U}_1)^2 && \text{for the species 1} \\ \frac{1}{2} \omega_2 \vec{V}_2^2 &= \frac{1}{2} k \rho_2 \frac{\omega_1}{\rho_1} (\vec{U}_2 - \vec{U}_1)^2 && \text{for the species 2} \end{aligned} \right. \quad (1-3)$$

in which k is now an adjustable parameter.

We write now the set of equations governing the mixture in terms of general orthogonal curvilinear coordinates ; the position $\vec{X}$ of a particle is denoted by :

$$\vec{X} = \sum_{i=1}^3 X_i \vec{e}_i$$

Each variable depends on $\vec{X}$ and t .

MASS CONSERVATION

$$\frac{\delta}{\delta t} (\omega_i) + \omega_i \cdot \text{div} (\vec{V}) + \text{div} (\omega_i (\vec{U}_i - \vec{V})) = 0 \quad (i=1,2) \quad (1-4)$$

MIXTURE EQUATIONS OF MOTION

$$\rho \left[\frac{\delta}{\delta t} (u_j) + (\vec{U} - \vec{V}) \cdot \vec{\text{grad}} (u_j) \right] + \text{div} \left(\lambda^2 \omega_1 \omega_2 \rho \vec{W}_j \right) \quad (1-5)$$

$$+ \rho \sum_{m=1}^3 \sum_{l=1}^3 \left(u_m u_l + \lambda^2 \omega_1 \omega_2 W_m W_l \right) v_{jl} (\vec{e}_k) + Q_j$$

$$= \sum_{n=1}^2 \left[- \vec{\text{grad}} \left(\frac{\omega_i}{\rho_i} p_i \right) + \frac{\omega_i}{\rho_i} \cdot \vec{F}_i \right] \cdot \vec{e}_j \quad (j = 1,3)$$

Q_j is a sophisticated term depending on the velocity $\vec{V}_i^2$ ($i=1,2$). For the 1-D case (in which X_1 is the main coordinate) we get $Q_1 = -\frac{N}{2x_1} \sum_{i=1}^2 \omega_i \vec{V}_i^2$

KINETIC ENERGY OF THE MIXTURE

$$\frac{1}{2} \rho \left[\frac{\delta}{\delta t} (\vec{u}^2 + \vec{W}^2) + (\vec{u} - \vec{V}) \cdot \vec{\text{grad}} (\vec{u}^2 + \vec{W}^2) \right] + \frac{1}{2} \text{div} (\vec{\Phi})$$

(1-6)

$$= \sum_{i=1}^2 \left[- \vec{\text{grad}} \left(\frac{\omega_i}{\rho_i} p_i \right) + \frac{\omega_i}{\rho_i} \cdot \vec{F}_i \right] \cdot \vec{u}_i$$

$$\text{where } \phi = \lambda^2 \rho \omega \left[2 \omega_1 \omega_2 \vec{u} \cdot \vec{W} + \lambda \omega_1 \omega_2 (\omega_1 - \omega_2) \vec{W}^2 \right. \\ \left. + k \lambda \rho \omega^2 \left(\rho_2 \frac{\omega_1^2}{\rho_1} - \rho_1 \frac{\omega_2^2}{\rho_2} \right) \right]$$

ENERGY CONSERVATION

We have dealt with the two following thermodynamical assumptions (the reality is probably located between them).

I - Thermal isolation

$$\frac{\delta}{\delta t} (e_i) + (\vec{u}_i - \vec{V}) \cdot \vec{\text{grad}} (e_i) = - \frac{p_i}{\rho_i} \text{div} (\vec{u}_i) \quad (i=1,2) \quad (1-7-1)$$

II - Temperature equilibrium

$$\frac{\delta}{\delta t} (e) + (\vec{u} - \vec{V}) \cdot \vec{\text{grad}} (e) + \frac{1}{\rho} \text{div} \left[\lambda \omega_1 \omega_2 (e_2 - e_1) \vec{W} \right] \quad (1-7-2)$$

$$T_1 = T_2 = - \frac{1}{\rho} \sum_{i=1}^2 \frac{\omega_i}{\rho_i} p_i \text{div} (\vec{u}_i)$$

PRESSURE EQUILIBRIUM

$$p_1 = p_2 = p \quad (1-8)$$

VOLUME COMPATIBILITY

$$\frac{\omega_1}{\rho_1} + \frac{\omega_2}{\rho_2} = 1 \quad (1-9)$$

EQUATIONS OF STATE

For each species i, we get

Equation of state

$$\rho_i = \rho_i (p_i, T_i) \quad (1-10)$$

Caloric equation of state

$$e_i = e_i (p_i, T_i) \quad (1-11)$$

AUXILIARY EQUATIONS

In order to close the set of equations, we assume that both mean velocities of the species are locally in the same direction, that is to say :

$$\vec{u}_1 // \vec{u}_2 \quad (1-12)$$

so we can write

$$\vec{u} // \vec{w} \quad (1-13)$$

The relations between the different celerities are :

$$\vec{w} = \frac{1}{\lambda \rho} (\vec{u}_2 - \vec{u}_1) \quad (1-14)$$

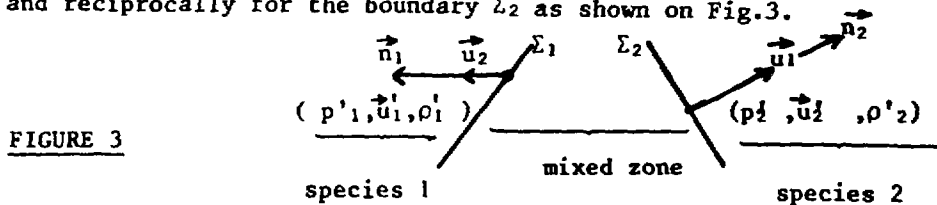
with
$$\lambda = \left[\omega_1 \omega_2 + k\rho \left(\rho_1 \frac{\omega_1}{\rho_2} + \rho_2 \frac{\omega_1}{\rho_1} \right) \right]^{-1/2}$$

and, then

$$\begin{aligned} \vec{u}_1 &= \vec{u} - \lambda \omega_2 \vec{w} \\ \vec{u}_2 &= \vec{u} + \lambda \omega_1 \vec{w} \end{aligned} \quad (1-15)$$

BOUNDARY CONDITIONS

Assuming that the mixture is heterogeneous we will write that the mixture boundary Σ_1 with the pure species 1 is moving at the velocity of the bubbles of the species 2 and reciprocally for the boundary Σ_2 as shown on Fig.3.



From the classical relationships of discontinuity in mechanics we can set the following expressions ($\vec{n}_1$ is the normal at the boundary Σ_1 and is borne by $\vec{u}_2$, $\vec{n}_2$ is the normal at the boundary Σ_2 and is borne by $\vec{u}_1$).

$$\left\{ \begin{aligned} \vec{u}_1' \cdot \vec{T} &= 0 \quad \forall \vec{T} \text{ so that } \vec{T} \cdot \vec{n}_1 = 0 \\ \rho_1' (\vec{u}_1' - \vec{u}_2) &= \rho (\vec{u} - \vec{u}_2) \\ p_1' &= p + \rho \left(1 - \frac{\rho}{\rho_1'}\right) (\vec{u} - \vec{u}_2)^2 \end{aligned} \right. \quad \text{at } \Sigma_1 \quad (1-16-1)$$

and ,

$$\left\{ \begin{aligned} \vec{u}_2' \cdot \vec{T} &= 0 \quad \forall \vec{T} \text{ so that } \vec{T} \cdot \vec{n}_2 = 0 \\ \rho_2' (\vec{u}_2' - \vec{u}_1) &= \rho (\vec{u} - \vec{u}_1) \\ p_2' &= p + \rho \left(1 - \frac{\rho}{\rho_2'}\right) (\vec{u} - \vec{u}_1)^2 \end{aligned} \right. \quad \text{at } \Sigma_2 \quad (1-16-2)$$

INITIAL CONDITIONS

In the majority of the works which are encountered it is difficult to estimate the initial conditions of a mixture area created by small defects Rayleigh Taylor instabilities. It is usually supposed that these small defects quickly get outside the linear phasis, and that the initial thickness of the mixture area is practically negligible and the velocities as well. Additionally, the volume fraction of each species are taken to be equal to 0.5. Nevertheless, if the initial concentration profile velocities and thickness are known, they may be introduced in the code; at first we have considered the initialization of a mixing zone which would be initially created by a shock wave at the interface of the two species as studied in /2/.

2 - OUTLINES OF THE NUMERICAL COMPUTATION

We briefly explain how the introduction on a finite difference lagrangian 1-D code has been carried out and how the introduction in a Eurlian 2-D code is expected.

In 1-D geometry we have adopted a classical finite difference lagrangian code. For a given time, the mixing is initialized at the contact surface of both species as shown on Fig.4.

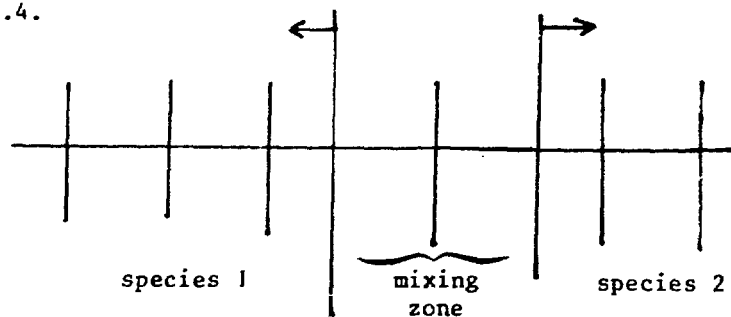


Fig.4 GRID

The cells which have not been reached by the mixing area are still computed with a classical method; the cells which have been reached by the mixing area are not "Lagrangian" and, for that reason, they are computed by a specific method. The mixing area is related to a particular grid which is bound with the grid velocity V . The transport masses are treated just on the separations between the cells defining the mixing area.

As the boundaries of the mixture are moving we need to gather the cells in the pure species which neighbour the mixture at certain times, we also need to double the cells which belong to the mixture and which are near the boundaries. The specific treatment of energy equations requires a Newton method more sophisticated than the usual treatment connected with a pure species because we have to set the mixing thermodynamical equilibrium at each time step as it has been described just above (pressure equilibrium, etc...).

In order to study an anisotropic evolution of a mixing zone around a 2-D contact surface, we have considered the model introduction in an Eulerian 2-D code by using the alternate direction method. Presently, the numerical transfer methods / 3 / and SLIC / 4 / that we have fit to specific calculation of mixing zone evolution, are entered in 2-D numerical test codes.

3 - COMMENTS ABOUT EXPERIMENTAL RESULTS

To show the possibilities of such a modelisation and to attempt to assess the results that we got, by comparing them to the experimental results, we focus our interest here to three kinds of studies on the mixtures created by Rayleigh Taylor instabilities, involving different physical fields.

The first work includes the studies of Youngs and al./5/ where they have studied incompressible fluid mixture under atmospheric pressure. The second work is addressed to the results obtained by Andronov and al./6/ on mixtures of two gases in a shock tube ; in this case compressibility is certainly influent and we get an evolution of velocities much greater than in the first work. At last the third work is supposed to study the development of a mixing area between a fluid and a gas in a convergent geometry in an area which is very different from the two previous ones.

FLUID-FLUID MIXTURE

In a previous paper / 1 / we have shown an experimental set-up allowing to study the development of a mixture area created between two fluids in a convergent geometry.

The use of the model in a field limited to this configuration (where fluids are considered as incompressible) makes us able to estimate approximatively the parameter k of the model from several experiments. We got

$$k = 1.5$$

The experimental results only provided the evolution versus time of the boundaries, up and down of the mixture. We had to optimize the initial conditions of the mixture (a priori unreachable because of the diaphragm extraction), mainly on the thickness, the concentration and the celerity.

Some results are shown on graphs 1. If we consider the model proposed with the simplest assumptions which are :

- . Fluids are incompressible
- . Geometry is 1-D and plane
- . The exterior forces are such that $\vec{F}_i = \rho_i \gamma \vec{x}_1$ ($i = 1, 2$)
where γ is a constant and uniform acceleration field.

We have found the following evolution laws for the celerity :

$$\frac{du_1}{dt} = \frac{\sigma(1-\sigma)^2}{k + \sigma(1-\sigma)} \cdot \frac{\rho_1 - \rho_2}{\sigma\rho_2 + (1-\sigma)\rho_1} \cdot \gamma \quad (3-1)$$

$$\frac{du_2}{dt} = - \frac{\sigma}{1-\sigma} \frac{du_1}{dt}$$

where σ is the volume fraction of the species 1. When the evolution around the contact surface is symmetrical we get $\sigma = \frac{1}{2}$ and the previous relations become

$$\frac{du_1}{dt} = \alpha \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2} \gamma, \quad \frac{du_2}{dt} = - \frac{du_1}{dt} \quad (3-2)$$

$$\text{where } \alpha = \frac{1}{4k+1}$$

This last expression is classical and similar to the ones used by Youngs and al./5/ in which the parameter α had been primarily found from some series of experiments and was equal to :

$$\alpha = 0.14 \quad (3-3)$$

For $k = 1.5$ we find here (with (3-2)) a value of α very close to 0.14.

Since the value of α turned out to be as low as 0.12 /5/, a rigorous comparison will require to take account of the flow disymmetry around the contact surface of the two fluids (viz. the volume fractions) by using the expressions (3-1).

At this standpoint we can only assume that the results that we got on both sides are quite fit since performed on similar experiments (for which we don't take account of the side effects).

GAS - GAS MIXTURE

In order to test the results of the model for mixture between two gases we pay our attention to an experiment in a shock tube proposed by ANDRONOV and al./6/.

Some important differences occur between the present model (which assumes an heterogeneous model and therefore discontinuous concentrations through the mixing boundaries) and a turbulent mixing zone classical model which involves a continuous concentration evolution.

From an experimental point of view the undesirable effects due to the shock tube sides or the diaphragm which have a tendency to attenuate the amplitude of concentration variations are not taken into account in the computation ; so we have only an approximative approach to the real mixing zone thicknesses. Comparison would have been better if we could have removed the undesirable effects.

To illustrate this point of view in connection with the considered experiment / 6 / for an air-helium mixture, we have carried out calculations for some different values of the parameter k . The mixing thickness has been approximately initialized at 4 mm when the contact surface begins to slow down.

On the graph 2 we have shown the mixing zone thickness evolution for $k=1$ and $k=0.7$ because it is obvious that the value of $k=1.5$ is not adequate for this kind of mixture. For these two values it appears that the calculation provides thicknesses less important than the ones which have been reported in the experiment. We have not attempted to decrease the parameter k anymore because a perfect fit would have been insignificant. As a matter of fact the numerical simulations neither take into account the sides effects (and diaphragm) nor the actual initial conditions (we have set the initial evolution velocity to 0).

FLUID - GAS MIXTURE

In order to get a purely evolving mixing zone created by Rayleigh-Taylor instabilities we must pay attention to an experimental set up which leads to get rid of undesirable influences of the sides or diaphragm which divides the two steady species. The metallic layer implosion on a gas cavity visualized by a X-ray radiography makes possible to phase them out. Unfortunately, in that kind of experimental set up, the contact surface observations are poor ; so we prefer to use statistical methods to interpret radiographs, they lead to histograms showing the considered surfaces related to density steps.

To give an example, we have simulated with a 1-D code the iron layer implosion on a gas (D 2) and we have drawn the numerical histograms : the first corresponds to a flow without mixing area and the others to flows with a mixture related to $k=0.7$, 1 , 1.5 (graph 3) ; these computations have been carried out to imagine the kind of configurations that we could get experimentally. The four histograms have been drawn at the same time and for the same lagrangian space window around the contact surface.

When the parameter k is decreasing the mixing zone thickness is increasing, differences on the histogram general shape effectively occur, showing that intermediate densities between the two species become more and more conspicuous.

Although the mixing zone thickness has not evolved a lot (for example we get for $k=0.7$ a mixture mass of 50 g and a thickness of 2.7mm) the differences between the simulations are remarkable.

CONCLUSION

We have described an alternative model with a single parameter to calculate the mixing area evolution created by Rayleigh-Taylor instabilities at the surface contact of two species. The mixing equations have been written with a general expression, they have been introduced in a 1-D code and they are presently tested on a 2-D code.

As usual in every model the parameter requires to be fit on experiments. We have investigated three kinds of experiment which could make conspicuous the mixing area created by Rayleigh-Taylor instabilities for very different physical fields. It would be interesting to have more elaborate experiments which would lead to estimate with accuracy the mixing zone lengths and also the mixing internal structure. We have the feeling that a simple model such as the one we have realized could be a first step to reach the understanding of this physical phenomenon and also it could help us to define some experiments.

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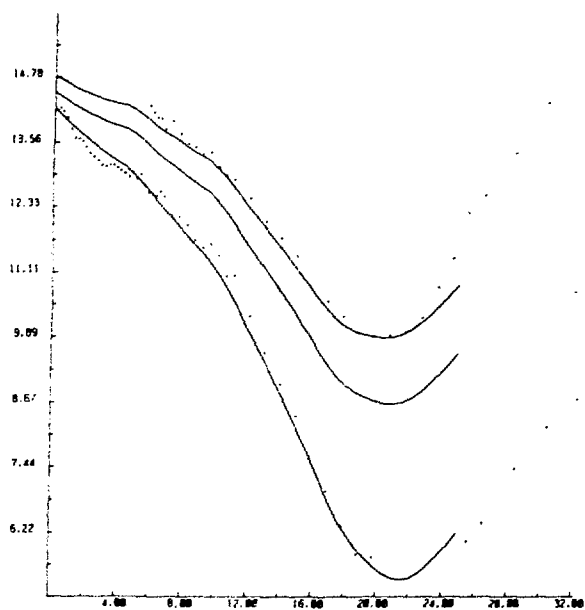
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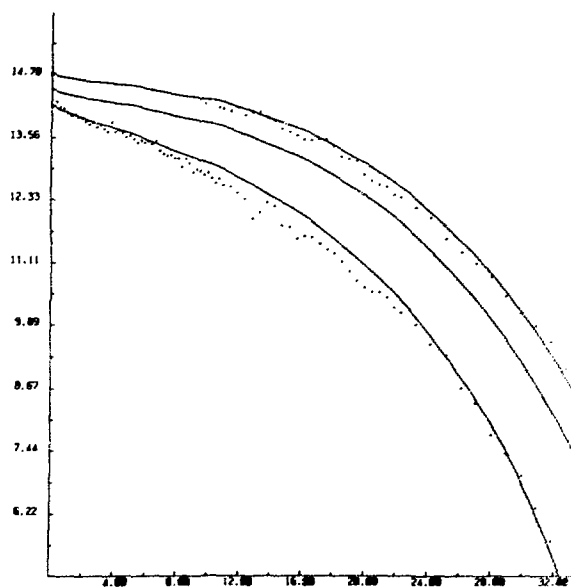
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ACKNOWLEDGMENT

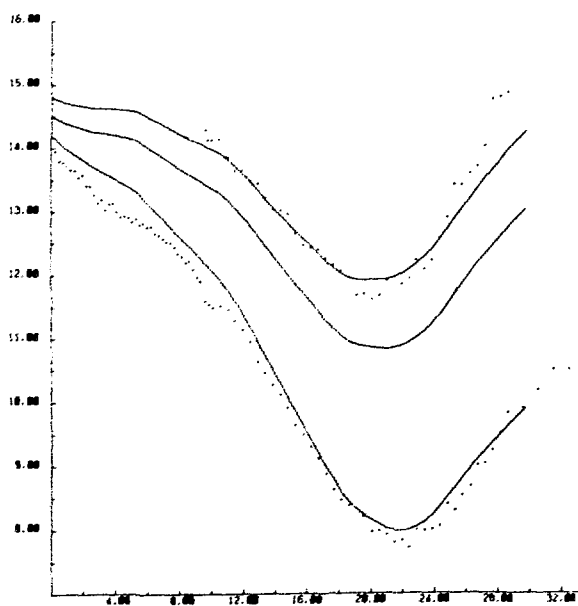
We thank N CARION for his contribution at the conception of the 1-D code and
P VIBERT and F TORCOL for their suggestions about experimental problems.



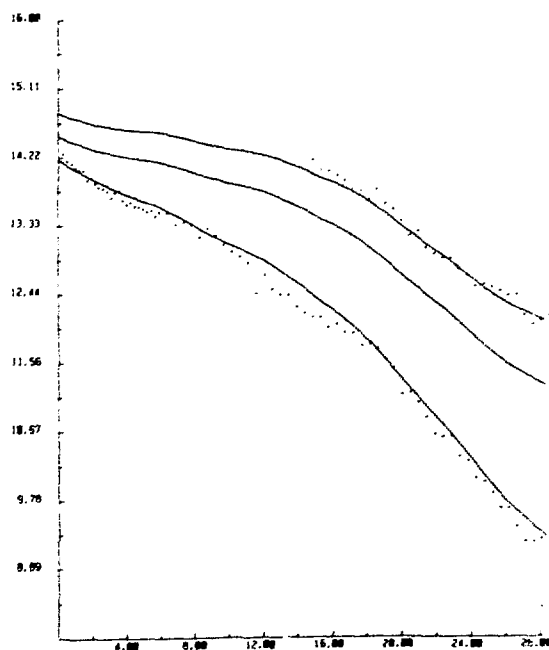
DIIODOMETHANE + WATER



DIIODOMETHANE + WATER



IODOETHANE + WATER



IODOETHANE + WATER

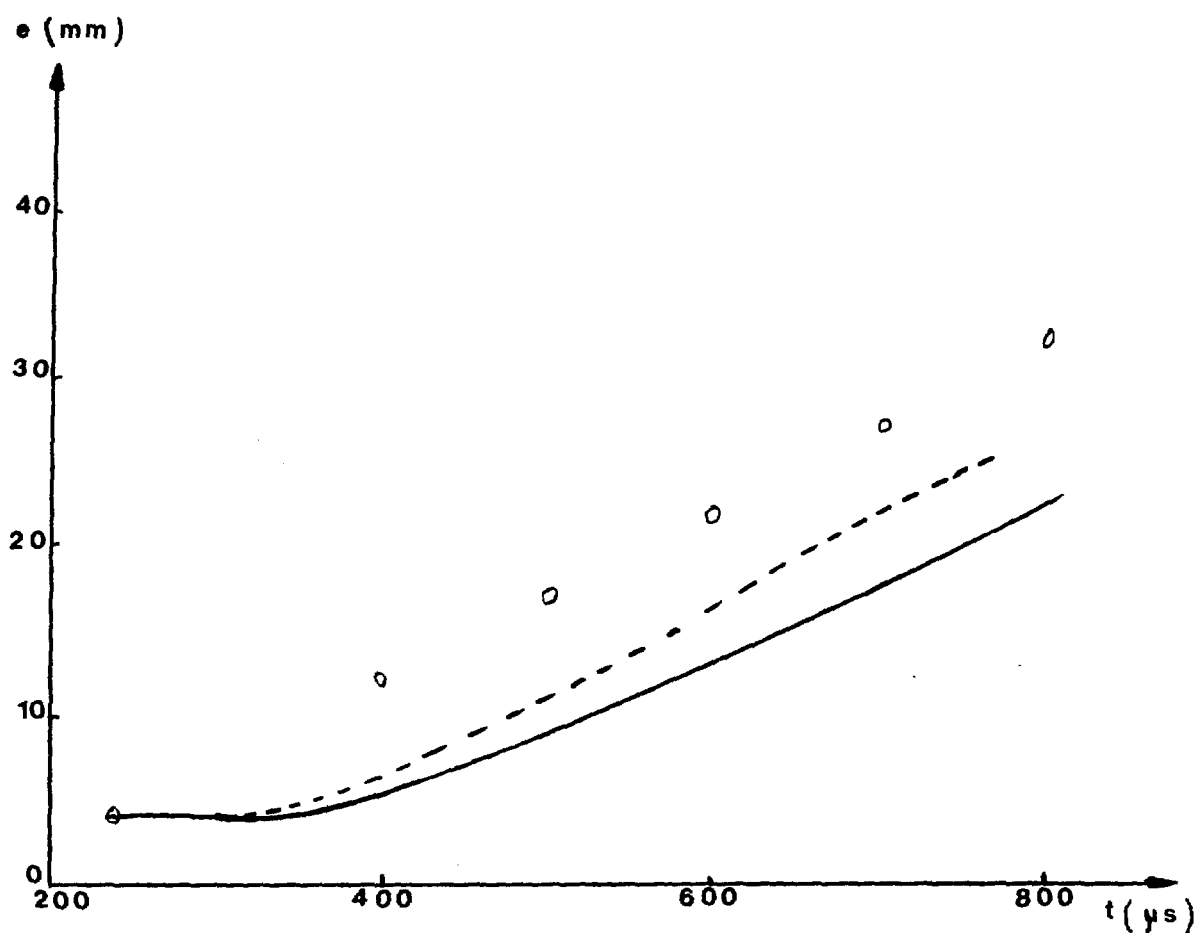
RADII VS TIME

* EXPERIMENT

— COMPUTATION

GRAPH 1 : MIXING ZONE EVOLUTION

FROM CONVERGENT GEOMETRY EXPERIMENTS / 1 /

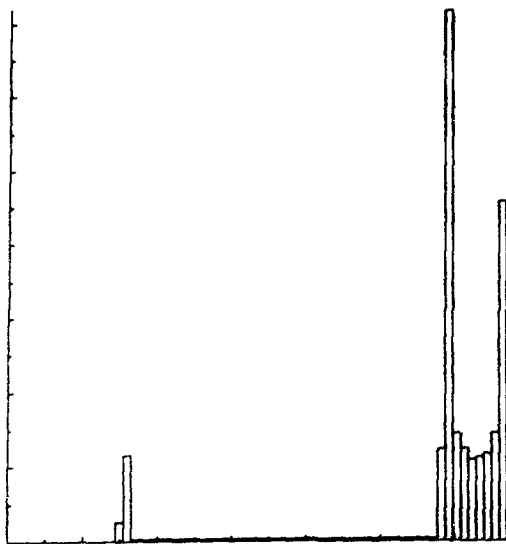


0 experimental data /5/

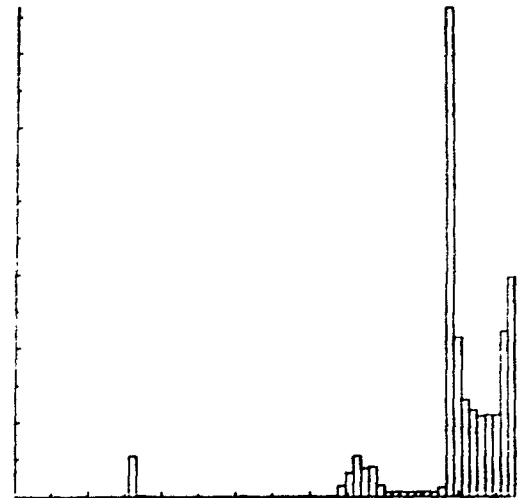
Present model — k=1

---- k=0.7

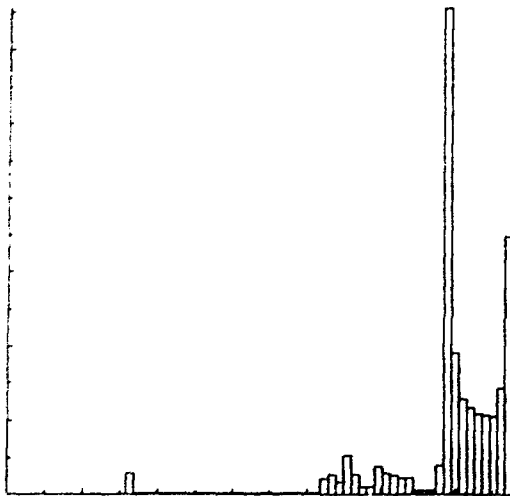
GRAPH 2 : AIR-HELIUM MIXING ZONE
THICKNESS VS TIME



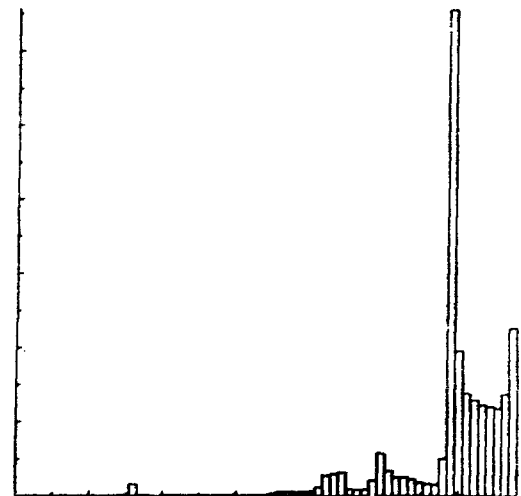
a) Pure hydrodynamic



b) $k = 1.5$



c) $k = 1$



d) $k = 0.7$

GRAPH 3 : NUMERICAL HISTOGRAMS

SURFACE VS DENSITY $S (\rho)$

a) pure case without mixing zone

b) c) d) with a mixing zone

EAD-EP : COMPUTATION OF ELASTOPLASTIC FLOW, WITH A SECOND ORDER
OCCURATE EULERIAN CODE

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1 - INTRODUCTION

To begin, we recall the characteristics of the 2-dimensional EAD code [1]
(E.A.D. : Euler Anti Diffusion) :

This code computes multifluid flows involving great deformation, including
treatment of interfaces and free surfaces, in an eulerian grid.

- . The eulerian grid is rectangular.
- . Interfaces between materials are tracked with the SLIC method [2]
involving mixed cells.
- . Free boundaries are handled via the "fictive fluid" technique [3].
- . All quantities are cell-centered at i, j .
- . Appropriate averaging is used to evaluate quantities at $(i+\frac{1}{2}, j)$ or
 $(i, j+\frac{1}{2})$.
- . Each fractionnary step is itself decomposed into 2 phases. First is
an explicit predictor Lagrangian phase using the grid which
coincides at t with the eulerian grid $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$. This predictor
phase gives us quantities at $t + \frac{\Delta t}{2}$ in the eulerian grid.

The corrector phase is constituted by :

- a projection from $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ to $[x_i, x_{i+1}]$
- a lagrangian scheme on $[x_i, x_{i+1}]$ using the pressure and velocity
computed in the predictor phase

- a projection phase from $[x_i, x_{i+1}]$ to $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$
- a correction by antidiffusion via a FCT technique [4].

This phase gives us the quantities at $t + \Delta t$ in the eulerian grid. Therefore we obtain a second order accurate scheme in time and a "quasi" second order accurate scheme in space.

Using these E.A.D. features as background, we are going to solve the following problem : to compute at each time $t = n \Delta t$ and in each cell of the eulerian grid : density ρ , velocity $\underline{v}$, specific total energy e and eulerian stress tensor $\underline{g}$, satisfying the equations which we shall describe in the following sections.

2 - EQUATIONS TO BE SOLVED

We recall the basic equations of conservation of mass, momentum and energy :

$$\frac{D}{Dt} \rho + \rho \Delta \cdot \underline{v} \quad (1)$$

$$\rho \frac{D}{Dt} \underline{v} = \nabla \cdot \underline{g} + \underline{X} \quad (2)$$

$$\rho \frac{D}{Dt} e = \nabla \cdot (\underline{g} \times \underline{v}) + \underline{X} \cdot \underline{v} \quad (3)$$

with :

- ρ : density
- $\underline{v}$: velocity
- e : specific total energy
- $\underline{X}$: body force per volume unit
- $\underline{g}$: stress tensor
- $\frac{D}{Dt}$: material derivative

System (1), (2), (3) has to be completed by a constitutive law relating $\underline{g}$ to $\underline{v}$ which we shall now describe.

We use a generalized Hook's law deduced from the theory of hypoelasticity :

$$\underline{\underline{\sigma}}^V = 2\mu \underline{\underline{F}} + \lambda (\text{tr } \underline{\underline{F}}) \underline{\underline{\delta}} \quad (4)$$

where
$$\sigma_{ij}^V = \frac{D}{Dt} \sigma_{ij} + \sigma_{jp} \Omega_{pi} + \sigma_{ip} \Omega_{pj} \quad (5)$$

and
$$\underline{\underline{F}} = \frac{1}{2} (\underline{\underline{V}} \underline{\underline{V}} + \underline{\underline{V}} \underline{\underline{V}}^T)$$

is the rate of deformation tensor.

$$\underline{\underline{\Omega}} = \frac{1}{2} (\underline{\underline{V}} \underline{\underline{V}} - \underline{\underline{V}} \underline{\underline{V}}^T)$$

is the rate of rotation tensor.

Superscript T denotes transposition. λ and μ are Lamé's coefficients, characteristic of the continuum.

Tensor σ^V can be seen to be obtained from tensor $\underline{\underline{T}}$ by taking its Jaumann's derivative.

We denote M a point of the flow field, let us consider the rectangular Cartesian frame of reference (M, x_1, x_2, x_3) . We call (x'_1, x'_2, x'_3) a rectangular frame, the origin of which is the volume element centered at M at time t, and which is moving with the medium. Let x'_1 coincide with x_1 at time t. If we denote by a' the quantities referred to the rotating axes x' , Jaumann defines its pseudo-derivative by :

$$\underline{\underline{\sigma}}^V = \lim_{dt \rightarrow 0} \frac{1}{dt} (\underline{\underline{\sigma}}' (t + dt) - \underline{\underline{\sigma}}' (t)) \quad (6)$$

We can remark that for a pre-stressed body performing a rigid-body rotation, $\underline{\underline{F}}$ and $\underline{\underline{\sigma}}^V$ vanishes identically, hence (6) is verified. Note that neither $\frac{\partial}{\partial t} \underline{\underline{\sigma}}$ nor $\frac{D}{Dt} \underline{\underline{\sigma}}$ vanishes identically in this case, which shows the necessity of Jaumann's pseudo derivative.

Let us show that (5) and (6) are equivalent. We call $\underline{\underline{R}}$ the rotation matrix which gives the coordinates of a vector in (x'_i) as a function of its coordinate in (x_i) . We have :

$$\underline{\underline{R}} = \underline{\underline{\delta}} + \underline{\underline{\Omega}} dt + O(dt)^2 \quad (7)$$

But $\underline{\sigma}'(t) = \underline{\sigma}(t)$ and we obtain :

$$\underline{\sigma}^V = \frac{1}{dt} (\underline{R}^{-1} \underline{\sigma}(t + dt) \underline{R} - \underline{\sigma}(t) + O(dt)^2) \quad (8)$$

where
$$\underline{\sigma}(t + dt) = \underline{\sigma}(t) + \frac{D}{Dt} \underline{\sigma} \cdot dt + O(dt)^2 \quad (9)$$

Using (7), (8) and (9) a few calculations give (5). Finally with system (1), (2), (3), (4), (5), we have the equations to be solved in the elastic case. The elasto-plastic case is postponed until section 4.

3 - DISCRETISATION IN THE ELASTIC CASE

For simplicity we shall restrict ourselves to the case of plane geometry with coordinates x, z (the modifications in the case of cylindrical geometry are straightforward). We assume the medium to be infinite in the y direction in 3D coordinates (x, y, z) .

For symmetry considerations, we have :

$$v_y = 0 \quad (10)$$

and
$$\sigma_{xy} = \sigma_{yx} = \sigma_{yz} = \sigma_{zy} = 0 \quad (11)$$

The cell centers are assumed to be indexed by $[i, j]$, where i denotes the index along x and j along z . The space step is denoted Δx (resp. Δz).

We have now to split the system of equations according to the alternate direction scheme.

We separate it into two sub-systems which contain only V_x for the first half step in x and only V_z for the 2nd half-step in z . In this way, we obtain one-dimensional motion for the lagrangian step.

We discretise the momentum and energy equations in the following way :

$$\begin{aligned} (Q_x)_{ij}^{n+1} - (Q_x)_{ij}^n = \Delta t \{ \Delta z ((\sigma_{xx})_{i+\frac{1}{2},j}^n - (\sigma_{xx})_{i-\frac{1}{2},j}^n) \\ + \Delta x ((\sigma_{xz})_{i,j+\frac{1}{2}}^n - (\sigma_{xz})_{i,j-\frac{1}{2}}^n) \} \end{aligned} \quad (12)$$

$$(Q)_{ij}^{n+1} - (Q_z)_{ij}^n = 0$$

$$(E_t)_{ij}^{n+1} - (E_t)_{ij}^n = \Delta t \{ \Delta z ((v_x \sigma_{xx})_{i+\frac{1}{2},j}^n - (v_x \sigma_{xx})_{i-\frac{1}{2},j}^n) \\ + \Delta x ((v_x \sigma_{xz})_{i+\frac{1}{2}}^n - (v_x \sigma_{xz})_{i,j-\frac{1}{2}}^n) \}$$

for the first half step in x , and

$$(Q_x)_{ij}^{n+1} - (Q_x)_{ij}^n = 0$$

$$(Q_z)_{ij}^{n+1} - (Q_z)_{ij}^n = \Delta t \{ \Delta z ((\sigma_{zz})_{i+\frac{1}{2},j}^n - (\sigma_{zz})_{i-\frac{1}{2},j}^n) \\ + \Delta x ((\sigma_{zz})_{i,j+\frac{1}{2}}^n - (\sigma_{zz})_{i,j-\frac{1}{2}}^n) \} \quad (13)$$

$$(E_t)_{ij}^{n+1} - (E_t)_{ij}^n = \Delta t \{ \Delta z (v_z \sigma_{xz})_{i+\frac{1}{2},j}^n - (v_z \sigma_{xz})_{i-\frac{1}{2},j}^n \\ + \Delta x ((v_z \sigma_{zz})_{i,j+\frac{1}{2}}^n - (v_z \sigma_{zz})_{i,j-\frac{1}{2}}^n) \}$$

for the second half step in z , where :

$$\sigma_{i+\frac{1}{2},j} = \frac{\sigma_{ij} \cdot m_{i+1,j} + \sigma_{i+1,j} \cdot m_{ij}}{m_{i+1,j} + m_{ij}} \quad (14)$$

$$v_{i+\frac{1}{2},j} = \frac{\rho_{ij} \cdot v_{ij} \cdot \Delta x_{i+1,j} + \rho_{i+1,j} \cdot v_{i+1,j} \cdot \Delta x_{ij}}{\rho_{ij} \Delta x_{i+1,j} + \rho_{i+1,j} \Delta x_{ij}} \quad (15)$$

Note that this scheme is a first order accurate only ; however it becomes second order accurate after the antidiffusion correction.

We now turn to discretization of the constitutive law (4) which we write, in view of (8) and (9) :

$$\underline{\sigma}(t + \Delta t) = \underline{R} [\underline{\sigma}(t) + \Delta t \{ 2\mu \underline{E} + \lambda(\text{tr } \underline{E}) \delta \}] \underline{R}^{-1} + O(dt^2) \quad (16)$$

We also split this relation into two sub-systems according to the same method as for the conservation laws, and we obtain after a few calculations, for our explicit scheme :

$$\begin{aligned}
 (\sigma_{xx})_{ij}^{n+1} - (\sigma_{xx})_{ij}^n &= \Delta t \left\{ \frac{\lambda + 2\mu}{\Delta x} ((v_x)_{i+\frac{1}{2},j}^n - (v_x)_{i-\frac{1}{2},j}^n) \right. \\
 &\quad \left. - \frac{(\sigma_{xz})_{ij}^n}{\Delta z} ((v_x)_{i,j+\frac{1}{2}}^n - (v_x)_{i,j-\frac{1}{2}}^n) \right\} \\
 (\sigma_{yy})_{ij}^{n+1} - (\sigma_{yy})_{ij}^n &= \Delta t \cdot \frac{\lambda}{\Delta x} \cdot \{ (v_x)_{i+\frac{1}{2},j}^n - (v_x)_{i-\frac{1}{2},j}^n \} \\
 (\sigma_{zz})_{ij}^{n+1} - (\sigma_{zz})_{ij}^n &= \Delta t \left\{ \frac{\lambda}{\Delta x} ((v_x)_{i+\frac{1}{2},j}^n - (v_x)_{i-\frac{1}{2},j}^n) \right. \\
 &\quad \left. + \frac{(\sigma_{xz})_{ij}^n}{\Delta z} ((v_x)_{i,j+\frac{1}{2}}^n - (v_x)_{i,j-\frac{1}{2}}^n) \right\} \\
 (\sigma_{xz})_{ij}^{n+1} - (\sigma_{xz})_{ij}^n &= \frac{\Delta t}{\Delta z} \left(\mu - \frac{1}{2} ((\sigma_{zz})_{ij}^n - (\sigma_{xx})_{ij}^n) \right) \cdot ((v_x)_{i,j+\frac{1}{2}}^n \\
 &\quad - (v_x)_{i,j-\frac{1}{2}}^n)
 \end{aligned} \tag{17}$$

for the first half step in x

$$\begin{aligned}
 (\sigma_{xx})_{ij}^{n+1} - (\sigma_{xx})_{ij}^n &= \Delta t \left\{ \frac{\lambda}{\Delta z} ((v_z)_{i,j+\frac{1}{2}}^n - (v_x)_{i,j-\frac{1}{2}}^n) \right. \\
 &\quad \left. + \frac{(\sigma_{xz})_{ij}^n}{\Delta x} ((v_z)_{i+\frac{1}{2},j}^n - (v_x)_{i-\frac{1}{2},j}^n) \right\} \\
 (\sigma_{yy})_{ij}^{n+1} - (\sigma_{yy})_{ij}^n &= \Delta t \cdot \left\{ \frac{\lambda}{\Delta z} ((v_z)_{i,j+\frac{1}{2}}^n - (v_z)_{i,j-\frac{1}{2}}^n) \right\} \\
 (\sigma_{zz})_{ij}^{n+1} - (\sigma_{zz})_{ij}^n &= \Delta t \cdot \left\{ \frac{\lambda+2\mu}{\Delta z} ((v_z)_{i,j+\frac{1}{2}}^n - (v_z)_{i,j-\frac{1}{2}}^n) \right. \\
 &\quad \left. - \frac{(\sigma_{xz})_{ij}^n}{\Delta x} ((v_z)_{i+\frac{1}{2},j}^n - (v_z)_{i-\frac{1}{2},j}^n) \right\} \\
 (\sigma_{xz})_{ij}^{n+1} - (\sigma_{xz})_{ij}^n &= \frac{\Delta t}{\Delta x} \left(\mu - \frac{1}{2} ((\sigma_{xx})_{ij}^n - (\sigma_{zz})_{ij}^n) \right) ((v_z)_{i+\frac{1}{2},j}^n \\
 &\quad - (v_z)_{i-\frac{1}{2},j}^n)
 \end{aligned} \tag{18}$$

For the second half step in z, where the velocity is interpolated using (15).

However in the multifluid case it is necessary to be able to compute λ and μ in a mixed cell $[i,j]$ in order to use (17) and (18).

We call α_{ij} the proportion of volume of material α in cell $[i,j]$.

We take :

$$\lambda_{ij} = \sum_{\alpha} \alpha_{ij} \lambda^{\alpha} \quad (19)$$

and
$$\mu_{ij} = \sum_{\alpha} \alpha_{ij} \mu^{\alpha} \quad (20)$$

We give the following justification : the deformation of a cell, determined by λ_{ij} and μ_{ij} , is directly a function of the proportion of volume of materials contained by the cell (for the "fictive fluids" on the free boundaries we take $\lambda = \mu = 0$).

Now we can describe our algorithm in the elasto-plastic case.

4 - ALGORITHM IN THE ELASTO-PLASTIC CASE

In the elasto-plastic case, tensor $\underline{s}$ is restricted to belong to some plasticity domain. In the following, we shall consider only the plasticity domain defined by Von Mises' criterion.

After a lagrangian phase on the cell $[x_i, x_{i+1}]$ using (17) and (18) we have computed the variation $\Delta\sigma$ of the stress tensor from t to $t + dt$, in the deformed cell $[x'_i, x'_{i+1}]$. We compute the quantities in the eulerian cell by :

$$\Delta\sigma[x'_{i-\frac{1}{2}}, x'_{i+\frac{1}{2}}] = \frac{m_D}{m_G + m_D} \Delta\sigma[x'_{i-1}, x'_i] + \frac{m_G}{m_G + m_D} \Delta\sigma[x'_i, x'_{i+1}] \quad (21)$$

where m_G and m_D are the respective mass of the left and right half cells of $[x'_{i-\frac{1}{2}}, x'_{i+\frac{1}{2}}]$. This formula results from numerical experiments, in order to avoid diffusion.

In each cell of the eulerian grid we have computed the stresses $\tilde{\underline{s}}_{ij}^{n+1}$ and we apply Von Mises' criterion of plasticity. We call Y_0 the elastic limit, which depends on the material.

. First case :

$$\text{tr} [(\tilde{\underline{s}}_{ij}^{n+1})^2] \leq \frac{2}{3} Y_0^2. \text{ The deformation is elastic and}$$

$$\underline{\sigma}_{ij}^{n+1} = \tilde{\underline{\sigma}}_{ij}^{n+1}$$

. Second case :

$\text{tr} [(\tilde{s}_{ij}^{n+1})^2] \geq \frac{2}{3} Y_0^2$. The deformation is plastic

p_{ij}^{n+1} is computed from the equation of state and we come back to the plasticity domain by

$$\tilde{s}_{ij}^{n+1} = \sqrt{\frac{2/3 Y_0^2}{\text{tr} [(\tilde{s}_{ij}^{n+1})^2]}} \tilde{s}_{ij}^{n+1}$$

Then we compute σ_{ij}^{n+1} using :

$$\underline{\sigma} = \underline{s} + p \underline{\delta}$$

For a mixed cell we have chosen to define the plastic limit by :

$$Y_{0ij} = \max_{\alpha} Y_0^{\alpha}$$