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2DE - A Two-Dimensional Eulerian Hydrodynamic Code for Computing One Component Reactive Hydrodynamic Problems

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2DE - A Two-Dimensional Eulerian Hydrodynamic Code for Computing One Component Reactive Hydrodynamic Problems

by

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ABSTRACT

This report is a description of a code for the IBM 7030 computer for computing two-dimensional reactive hydrodynamic problems in cylindrical geometry using a modification of Gentry's finite difference analogs of the Eulerian equations of motion for a compressible fluid.

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I. INTRODUCTION

This study was undertaken to determine if the Eulerian approach to reactive hydrodynamic problems might be useful in solving reactive flow, one-component problems which result in severe distortion of a Lagrangian mesh. The problem of interest was the failure of a nitromethane detonation wave, with a numerically resolved reaction zone, caused by side rarefactions. The numerical method described in this report will compute the nitromethane failure problem.

The finite difference analogs of the Eulerian equations of motion for a compressible fluid described in this report are similar to the FLIC method described by Gentry, Martin and Daly,[1] which was an outgrowth of the work of Rich.[2] The OIL method for velocity weighting in the mass flux phase of the calculation was found to be the best method described in the literature. The OIL method was developed by M. Walsh's group at General Atomic Division of General Dynamic Corporation. It was first described in a report written by W. E. Johnson.[3] The densities used in the mass flux were treated as the new Lagrangian densities rather than old Eulerian ones. This was first found to be useful by Gentry.[4]

Since reactive hydrodynamic problems require as much numerical resolution as possible, the code (called 2DE) was written to make maximum use of the large capacity disk storage of the IBM 7030 (STRETCH) computer. The maximum height of the mesh is 3000 cells, and the maximum number of cells is 200,000. The numerical calculations require sufficient time to permit the data transfer between the disk and core memory to be overlapped.

This report describes the method used in complete detail. It also presents sufficient details for a coder to be able to follow and change the code. The latter information is not of interest to the casual reader.

II. THE HYDRODYNAMIC EQUATIONS

The partial differential equations for nonviscous, nonconducting, compressible fluid flow in cylindrical coordinates are

$$\frac{\partial \rho}{\partial t} + U\frac{\partial \rho}{\partial R} + V\frac{\partial \rho}{\partial Z} = -\rho\left(\frac{\partial U}{\partial R} + \frac{\partial V}{\partial Z} + \frac{U}{R}\right) \qquad \text{Mass}$$

$$\rho\left(\frac{\partial U}{\partial t} + U\frac{\partial U}{\partial R} + V\frac{\partial U}{\partial Z}\right) = -\frac{\partial P}{\partial R}$$

Momentum

$$\rho\left(\frac{\partial V}{\partial t} + U\frac{\partial V}{\partial R} + V\frac{\partial V}{\partial Z}\right) = -\frac{\partial P}{\partial Z}$$

$$\rho\left(\frac{\partial I}{\partial t} + U\frac{\partial I}{\partial R} + V\frac{\partial I}{\partial Z}\right) = -P\left(\frac{\partial U}{\partial R} + \frac{\partial V}{\partial Z} + \frac{U}{R}\right) \qquad \text{Energy}$$

The equations are written in finite-difference form appropriate to a fixed (Eulerian) mesh of cells and used to determine the dynamics of the fluid. The fluid is moved by a continuous mass transport method.

The first of the above equations, that of mass conservation, is automatically satisfied. The momentum and energy equations are treated as follows: In the first step, the contributions to the time derivatives which arise from the terms involving pressure are calculated. The mass is not moved at this step; thus the transport terms are dropped. Tentative new values of velocity and internal energy are calculated for each cell.

In the second step, the mass is moved according to the cell velocity. The mass which crosses cell boundaries carries with it into the new cells appropriate fractions of the mass, momentum, and energy of the cells from which it came. This second step accomplishes the transport that was neglected in the first step.

In the third step, the amount of chemical reaction is determined, and the new cell pressure is computed using the HOM equation of state.[5]

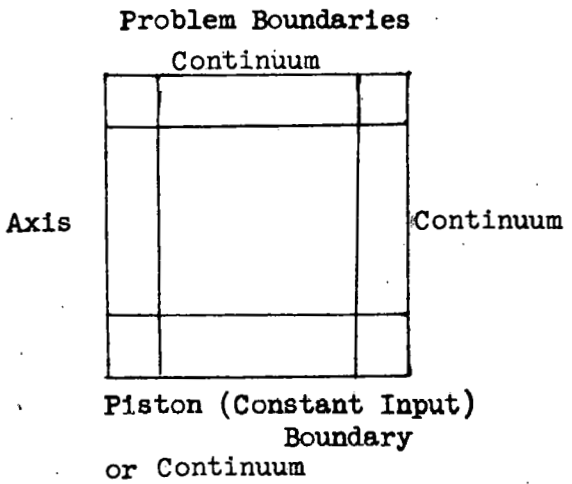
The equations we shall difference are of the form

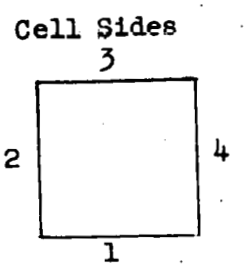
$$\rho\frac{\partial V}{\partial t} = -\frac{\partial(P+q)}{\partial R}$$

$$\rho\frac{\partial U}{\partial t} = -\frac{\partial(P+q)}{\partial Z}$$

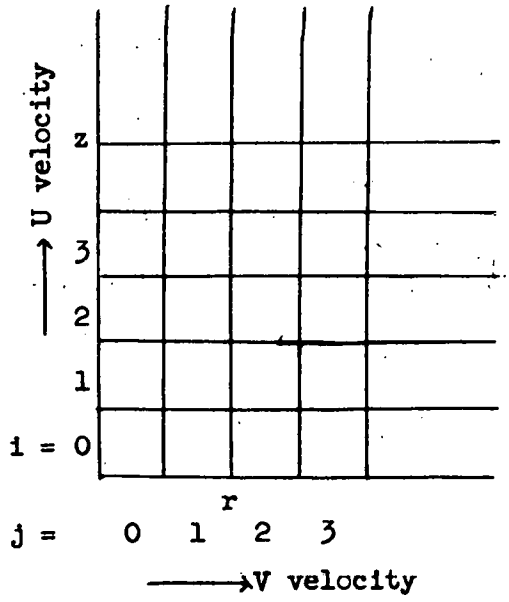
$$\rho\frac{\partial I}{\partial t} = -\frac{P}{R}\frac{\partial VR}{\partial R} - \frac{1}{R}\frac{\partial qVR}{\partial R} + V\frac{\partial q}{\partial R} - P\frac{\partial U}{\partial Z} - \frac{\partial qU}{\partial Z} + U\frac{\partial q}{\partial Z}$$

III. THE CODING EQUATIONS AND TECHNIQUES





The Initial Problem Setup



Cell Quantities

ρ - CM - cell density

I - CI - cell energy

P - CP - cell pressure

T - CT - cell temperature

W - CW - cell mass fraction

U - CU - cell z velocity

V - CV - cell r velocity

$\hat{\rho}$ - RHOT - tilde density

Intermediate Quantities

q - Q1, Q2, Q3, Q4 - Viscosities (locations also used as Δ quantities in mass movement)

V' - CMB - $1/\rho$ (location also used as ΔM in mass movement)

$\tilde{U}$ - CUB - cell z velocity tilde

$\tilde{V}$ - CVB - cell r velocity tilde

Phase I. Equation of State and Reaction

The pressure and temperature are calculated from the density, internal energy, and cell mass fraction of undecomposed explosive using the HOM[5] or ideal gas equation of state.[6]

1. Test to determine if $\Delta V'/V'$, $\Delta I/I$, $\Delta W/W$ from the previous cell and the present cell are less than 0.0005, and if they are, use the previous cell P and T.
2. If an HOM iteration error occurs and if W is > 0.5, resolve with W = 1.0. If W is < 0.5, resolve with W = 0.0. Print the cell W, P, T and a comment each time the HOM error occurs.

Knowing T we calculate W using the Arrhenius rate law

$$\frac{dW}{dt} = Z^{*}We^{-E^{*}/R_{g}T}$$

where Z* is the frequency factor, E* the activation energy, R_g the gas constant, and δt the time increment. In difference form this is

$$W^{n+1} = W^{n} - \delta t\, Z^{*}W^{n}e^{-E^{*}/R_{g}T^{n+1}}$$

1. If cell temperature is less than MINWT(1000) reaction is not permitted.
2. If CW is less than GASW(0.02) set CW = 0.
3. Do not react for first VCNT (25) cycles.

Phase I, II are skipped if $\rho_{ij}^{n} <$ MINGRHO + $(\rho_{o}$-MINGRHO$)(W_{i,j}^{n})$. This is for handling free surfaces, eliminating false diffusion. MINGRHO = 0.5.

Phase II. Viscosity and Velocity

A. Viscosity Equations

$$Q1_{ij} = q^n_{i-\frac{1}{2},j} = Q3_{i-1,j}$$

except on boundary 1 when $Q1_{ij} = 0$ or on piston boundary when

$$Q1_{ij} = \begin{cases} K(\rho^n_{ij}+MAPP)(UAPP-U^n_{ij}) & \text{if } UAPP > U^n_{ij}, \\ 0 & \text{if } UAPP < U^n_{ij} \end{cases}$$

$$Q2_{ij} = q^n_{i,j-\frac{1}{2}} = Q4_{i,j-1}$$

except on axis boundary when $Q2_{ij} = 0$.

$$Q3_{ij} = q^n_{i+\frac{1}{2},j} = \begin{cases} K(\rho^n_{ij}+\rho^n_{i+1,j})(U^n_{ij}-U^n_{i+1,j}) & \text{if } U^n_{ij} > U^n_{i+1,j} \\ 0 & \text{if } U^n_{ij} < U^n_{i+1,j} \end{cases}$$

except on a continuative boundary 3 when $Q3_{ij} = 0$.

$$Q4_{ij} = q^n_{i,j+\frac{1}{2}} = \begin{cases} K(\rho^n_{ij}+\rho^n_{i,j+1})(V^n_{ij}-V^n_{i,j+1}) & \text{if } V^n_{ij} > V^n_{i,j+1} \\ 0 & \text{if } V^n_{ij} < V^n_{i,j+1} \end{cases}$$

except on a continuative boundary 4 when $Q4_{ij} = 0$. MAPP, UAPP, PAPP are piston applied values of mass, particle velocity and pressure. Also calculated in the viscosity section are:

$$P1 = P^n_{i-1,j}$$

except at piston when P1 = PAPP or on continuative boundary 1 when

$$P1 = P^n_{ij}$$

$$P2 = P^n_{i,j-1}$$

except on axis when $P2 = P^n_{ij}$

$$P3 = P^n_{i+1,j}$$

except on continuative boundary 3 when $P3 = P^n_{ij}$

$$P4 = P^n_{i,j+1}$$

except on continuative boundary 4 when $P4 = P^n_{ij}$

B. Velocity Equations

$$\tilde{U}^n_{ij} = U^n_{ij} - \frac{\delta t}{\rho^n_{ij}\delta z}\left[(P+q)^n_{i+\frac{1}{2},j} - (P+q)^n_{i-\frac{1}{2},j}\right]$$

$$= U^n_{ij} - \frac{\delta t}{\rho_{ij}\delta z}\left\{P^n_{i+\frac{1}{2},j}+q^n_{i+\frac{1}{2},j}-P^n_{i-\frac{1}{2},j}-q^n_{i-\frac{1}{2},j}\right\}$$

$$P^n_{i+\frac{1}{2},j} = \frac{(P^n_{ij}+P^n_{i+1,j})}{2} = \frac{(P^n_{ij}+P3)}{2}$$

$$\tilde{U}^n_{ij} = U^n_{ij} - \frac{\delta t}{\rho_{ij}\delta z}\left\{\frac{1}{2}(P^n_{ij}+P3-P^n_{ij}-P1)+q^n_{i+\frac{1}{2},j}-q^n_{i-\frac{1}{2},j}\right\}$$

$$= U^n_{ij} - \frac{\delta t}{\rho_{ij}\delta z}\left\{\frac{P3-P1}{2}+Q3_{ij}-Q1_{ij}\right\}$$

$$\tilde{V}^n_{ij} = V^n_{ij} - \frac{\delta t}{\rho^n_{ij}}\left\{\frac{1}{2V'_j}\left[S^r_{j+\frac{1}{2}}(P^n_{i,j+1}-P^n_{ij})-S^r_{j-\frac{1}{2}}(P^n_{i,j-1}-P^n_{ij})\right]\right.$$

$$\left. + \frac{1}{\delta r}\left[q^n_{i,j+\frac{1}{2}}-q^n_{i,j-\frac{1}{2}}\right]\right\}$$

$$S^r_{j+\frac{1}{2}} = 2\pi(j+1)\delta r\delta z \qquad V'_j = 2\pi(j+\tfrac{1}{2})\delta r^2\delta z$$

$$\tilde{V}^n_{ij} = V^n_{ij} - \frac{\delta t}{\rho^n_{ij}\delta r}\left\{\frac{1}{2j+1}\left[(j+1)(P^n_{i,j+1}-P_{ij})-(j)(P^n_{i,j-1}-P^n_{ij})\right]\right.$$

$$\left. + q^n_{i,j+\frac{1}{2}} - q^n_{i,j-\frac{1}{2}}\right\}$$

$$= V^n_{ij} - \frac{\delta t}{\rho^n_{ij}\delta r}\left\{\frac{j(P4-P2)+P4-P^n_{ij}}{2j+1} + Q4_{ij} - Q2_{ij}\right\}$$

Phase III. Internal Energy and $\hat{\rho}$

A. Piston Energy Constraint

For the first VCNT cycles the internal energy is calculated from

$$\tilde{I}^n_{ij} = \frac{1}{2}(P^n_{ij}+Q3_{ij})(V'_o - \frac{1}{\rho^n_{1j}}) + I_o \qquad V'_o > \frac{1}{\rho^n_{1j}}$$

$$\tilde{I}^n_{ij} = I^n_{ij} \qquad V'_o < \frac{1}{\rho^n_{1j}}$$

B. $\hat{\rho}$ Calculation

$$\hat{\rho}^n_{ij} = \rho^n_{ij}\left[1 - \frac{\delta t}{2\delta r}(V^n_{i,j+1}-V^n_{i,j-1}) - \frac{\delta t}{2\delta z}(U^n_{i+1,j}-U^n_{i-1,j})\right]$$

On piston boundary, $U_{i-1,j} = UAPP$

On axis boundary, $V_{i-1,j} = V_{ij}$

On boundary 3, $U_{i+1,j} = U_{ij}$

On boundary 4, $V_{i,j+1} = V_{ij}$

On boundary 1, $U_{i-1,j} = U_{ij}$

For $\rho^n_{ij} <$ MINGRHO + (ρ_o-MINGRHO)(W^n_{ij}), $E^n_{ij} = I^n_{ij}$, and the rest of Phase III is skipped.

C. Internal Energy Equation

$$\tilde{I}^n_{ij} = I^n_{ij} - \frac{\delta t}{\rho^n_{ij} V'_j} \Big\{ P^n_{ij} (S^r_{j+\frac{1}{2}} \bar{V}^n_{i,j+\frac{1}{2}} - S^r_{j-\frac{1}{2}} \bar{V}^n_{i,j-\frac{1}{2}})$$

$$+ \frac{1}{2} q^n_{i,j+\frac{1}{2}} (S^r_{j+1} \bar{V}^n_{i,j+1} + S^r_j \bar{V}^n_{ij}) - \frac{1}{2} q^n_{i,j-\frac{1}{2}} (S^r_j \bar{V}^n_{ij} + S^r_{j-1} \bar{V}^n_{i,j-1})$$

$$- \bar{V}^n_{ij} S^r_j (q^n_{i,j+\frac{1}{2}} - q^n_{i,j-\frac{1}{2}}) - \bar{U}^n_{ij} S^z_j (q^n_{i+\frac{1}{2},j} - q^n_{i-\frac{1}{2},j})$$

$$+ S^z_j \Big[\bar{U}^n_{i+\frac{1}{2},j} (P^n_{ij} + q^n_{i+\frac{1}{2},j}) - \bar{U}^n_{i-\frac{1}{2},j} (P^n_{ij} + q^n_{i-\frac{1}{2},j}) \Big] \Big\}$$

$$= I^n_{ij} - \frac{\delta t}{\rho^n_{ij} V'_j} \Big\{ P^n_{ij} (S^r_{j+\frac{1}{2}} \bar{V}^n_{i,j+\frac{1}{2}} - S^r_{j-\frac{1}{2}} \bar{V}^n_{i,j-\frac{1}{2}})$$

$$+ \frac{1}{2} q^n_{i,j+\frac{1}{2}} (S^r_{j+1} \bar{V}^n_{i,j+1} - S^r_j \bar{V}^n_{ij})$$

$$- \frac{1}{2} q^n_{i,j-\frac{1}{2}} (S^r_{j-1} \bar{V}^n_{i,j-1} - S^r_j \bar{V}^n_{ij})$$

$$+ S^z_j \Big[P^n_{ij} (\bar{U}^n_{i+\frac{1}{2},j} - \bar{U}^n_{i-\frac{1}{2},j}) + q^n_{i+\frac{1}{2},j} (\bar{U}^n_{i+\frac{1}{2},j} - \bar{U}^n_{ij})$$

$$+ q^n_{i-\frac{1}{2},j} (\bar{U}^n_{ij} - \bar{U}^n_{i-\frac{1}{2},j}) \Big] \Big\}$$

$$S^r_j = 2\pi(j+\tfrac{1}{2})\delta r \delta z \qquad V'_j = 2\pi(j+\tfrac{1}{2})\delta r^2 \delta z \qquad S^z_j = 2\pi(j+\tfrac{1}{2})\delta r^2$$

$$\bar{V}^n_{i,j+\frac{1}{2}} = \frac{1}{4}(V^n_{ij}+\tilde{V}^n_{ij}+V^n_{i,j+1}+\tilde{V}^n_{i,j+1})$$

$$\bar{U}_{i+\frac{1}{2},j} = \frac{1}{4}(U^n_{ij}+\tilde{U}^n_{ij}+U^n_{i+1,j}+\tilde{U}^n_{i+1,j})$$

$$\bar{V}^n_{ij} = \frac{1}{2}(V^n_{ij}+\tilde{V}^n_{ij}) \qquad \bar{U}^n_{ij} = \frac{1}{2}(U^n_{ij}+\tilde{U}^n_{ij})$$

V1 = $(V^n_{i,j-1}+\tilde{V}^n_{i,j-1})$ except on axis boundary when V1 = $(V^n_{ij}+\tilde{V}^n_{ij})$.

V2 = $(V^n_{i,j+1}+\tilde{V}^n_{i,j+1})$ except on continuative boundary 4 when

V2 = $(V^n_{ij}+\tilde{V}^n_{ij})$.

U1 = $(U^n_{i-1,j}+\tilde{U}^n_{i-1,j})$ except on piston boundary when U1 = 2UAPP and on continuative boundary 1 when U1 = $(U^n_{ij}+\tilde{U}^n_{ij})$.

U2 = $(U^n_{i+1,j}+\tilde{U}^n_{i+1,j})$ except on continuative boundary 3 when

U2 = $(U^n_{ij}+\tilde{U}^n_{ij})$.

TEMP1 = $(V^n_{ij}+\tilde{V}^n_{ij})$ TEMP3 = $(U^n_{ij}+\tilde{U}^n_{ij})$

$$\bar{V}^n_{i,j+\frac{1}{2}} = \frac{1}{4}(\text{TEMP1}+\text{V2}) \qquad \bar{V}^n_{i,j-\frac{1}{2}} = \frac{1}{4}(\text{TEMP1}+\text{V1})$$

$$\bar{U}^n_{i+\frac{1}{2},j} = \frac{1}{4}(\text{TEMP3}+\text{U2}) \qquad \bar{U}^n_{i-\frac{1}{2},j} = \frac{1}{4}(\text{TEMP3}+\text{U1})$$

$$\bar{V}^n_{ij} = \frac{1}{2}(\text{TEMP1}) \qquad \bar{U}^n_{ij} = \frac{1}{2}(\text{TEMP3})$$

$$\bar{V}^n_{i,j+1} = \frac{1}{2}(\text{V2}) \qquad \bar{V}^n_{i,j-1} = \frac{1}{2}(\text{V1})$$

$$\tilde{I}^{n}_{ij} = I_{ij} - \frac{\delta t}{\rho^{n}_{ij}}\left\{\frac{P^{n}_{ij}}{2(2j+1)\delta r}\left[(j+1)(TEMP1+V2)-(j)(TEMP1+V1)\right]\right.$$

$$+ \frac{Q4_{ij}}{2(2j+1)\delta r}\left[(j+\tfrac{3}{2})(V2)-(j+\tfrac{1}{2})(TEMP1)\right]$$

$$- \frac{Q2_{ij}}{2(2j+1)\delta r}\left[(j-\tfrac{1}{2})(V1)-(j+\tfrac{1}{2})(TEMP1)\right]$$

$$\left. + \frac{1}{4\delta z}\left[P^{n}_{ij}(U2-U1)+Q3_{ij}(U2-TEMP3)+Q1_{ij}(TEMP3-U1)\right]\right\}$$

$$= I^{n}_{ij} - \frac{\delta t}{4\rho_{ij}}\left\{\frac{P^{n}_{ij}}{\delta r}\left[V2-V1+\frac{V2+2TEMP1+V1}{2j+1}\right]\right.$$

$$+ \frac{Q4_{ij}}{\delta r}\left[V2-TEMP1+\frac{2V2}{2j+1}\right]$$

$$- \frac{Q2_{ij}}{\delta r}\left[V1-TEMP1-\frac{2V1}{2j+1}\right]$$

$$\left. + \frac{1}{\delta z}\left[P^{n}_{ij}(U2-U1)+Q3_{ij}(U2-TEMP3)+Q1_{ij}(TEMP3-U1)\right]\right\}$$

Total energy

$$E^{n}_{ij} = \tilde{I}^{n}_{ij} + \frac{1}{2}\left[(\tilde{V}^{n}_{ij})^{2}+(\tilde{U}^{n}_{ij})^{2}\right]$$

Phase IV. Mass Movement

The viscosities, Q1 through Q4 are no longer needed, and their storage locations are used to store the changes in various physical quantities as the mass is moved. Mass is not moved unless the pressure of the cell from which the mass moves is greater than FREPR (0.0005).

Q1 - ΔE change in energy

Q2 - ΔW change in mass fraction

Q3 - ΔPV change in V momentum

Q4 - ΔPU change in U momentum

CMB - ΔM change in mass

Mass movement across side 2

1. For an axis cell Q1 = Q2 = Q3 = Q4 = CMB = 0 and no mass is moved.

$$\Lambda = \frac{\left(\frac{\tilde{V}^n_{ij}+\tilde{V}^n_{i,j-1}}{2}\right)\frac{\delta t}{\delta r}}{(\tilde{V}^n_{ij}-\tilde{V}^n_{i,j-1})(\delta t/\delta r)+1}$$

2. $\Delta \geq 0$, $DM = (\hat{\rho}^n_{i,j-1})\left(\frac{2j-\Delta}{2j+1}\right)\Delta$, mass moves from cell i,j-1 to cell ij.

$$Q1_{ij} = E^n_{i,j-1}(DM) \qquad Q1_{i,j-1} = Q1_{i,j-1} - E^n_{i,j-1}(DM)$$

$$Q2_{ij} = W^n_{i,j-1}(DM) \qquad Q2_{i,j-1} = Q2_{i,j-1} - W^n_{i,j-1}(DM)$$

$$Q3_{ij} = \tilde{V}^n_{i,j-1}(DM) \qquad Q3_{i,j-1} = Q3_{i,j-1} - \tilde{V}^n_{i,j-1}(DM)$$

$$Q4_{ij} = \tilde{U}^n_{i,j-1}(DM) \qquad Q4_{i,j-1} = Q4_{i,j-1} - \tilde{U}^n_{i,j-1}(DM)$$

$$CMB_{ij} = DM \qquad CMB_{i,j-1} = CMB_{i,j-1} - (DM)$$

3. $\Delta < 0$

$DM = (\hat{\rho}^n_{ij})\left(\frac{2j-\Delta}{2j-1}\right)\Delta$, mass moves from cell ij to cell i,j-1.

$$Q1_{ij} = E^n_{ij}(DM) \qquad Q1_{i,j-1} = Q1_{i,j-1} - E^n_{ij}(DM)$$

$$Q2_{ij} = W^n_{ij}(DM) \qquad Q2_{i,j-1} = Q2_{i,j-1} - W^n_{ij}(DM)$$

$$Q3_{ij} = \tilde{V}^n_{ij}(DM) \qquad Q3_{i,j-1} = Q3_{i,j-1} - \tilde{V}^n_{ij}(DM)$$

$$Q4_{ij} = \tilde{U}^n_{ij}(DM) \qquad Q4_{i,j-1} = Q4_{i,j-1} - \tilde{U}^n_{ij}(DM)$$

$$CMB_{ij} = DM \qquad CMB_{i,j-1} = CMB_{i,j-1} - DM$$

Mass movement across side 1

1. For a piston boundary cell we have

$$\Delta = \frac{\frac{(UAPP + \tilde{U}^n_{ij})}{2}\left(\frac{\delta t}{\delta z}\right)}{(\tilde{U}^n_{ij} - UAPP)(\delta t/\delta z)+1}$$

For $\Delta < 0$ no mass is moved.

For $\Delta \geq 0$, $DM = (MAPP)\Delta$, mass moves from piston to cell ij.

$$Q1_{ij} = Q1_{ij} + EAPP(DM)$$

$$Q2_{ij} = Q2_{ij} + WAPP(DM)$$

$$Q3_{ij} = Q3_{ij} + VAPP(DM)$$

$$Q4_{ij} = Q4_{ij} + UAPP(DM)$$

$$CMB_{ij} = CMB_{ij} + DM$$

2. For continuative boundary 1 cell

$$\Delta = (\tilde{U}^n_{ij})(\delta t/\delta z)$$

$$DM = (\hat{\rho}^n_{ij})\Delta$$

$$Q1_{ij} = Q1_{ij} + E^n_{ij}(DM)$$

$$Q2_{ij} = Q2_{ij} + W^n_{ij}(DM)$$

$$Q3_{ij} = Q3_{ij} + \tilde{V}^n_{ij}(DM)$$

$$Q4_{ij} = Q4_{ij} + \tilde{U}^n_{ij}(DM)$$

$$CMB_{ij} = CMB_{ij} + DM$$

$$\Delta = \frac{\left(\frac{\tilde{U}^n_{ij}+\tilde{U}^n_{i-1,j}}{2}\right)\frac{\delta t}{\delta z}}{(\tilde{U}^n_{ij}-\tilde{U}^n_{i-1,j})(\delta t/\delta z)+1}$$

3. $\Delta \geq 0$

$DM = (\hat{\rho}^n_{i-1,j})(\Delta)$ mass moves from cell i-1,j to cell ij.

$$Q1_{ij} = Q1_{ij} + E^n_{i-1,j}(DM) \qquad Q1_{i-1,j} = Q1_{i-1,j} - E^n_{i-1,j}(DM)$$

$$Q2_{ij} = Q2_{ij} + W^n_{i-1,j}(DM) \qquad Q2_{i-1,j} = Q2_{i-1,j} - W^n_{i-1,j}(DM)$$

$$Q3_{ij} = Q3_{ij} + \tilde{V}^n_{i-1,j}(DM) \qquad Q3_{i-1,j} = Q3_{i-1,j} - \tilde{V}^n_{i-1,j}(DM)$$

$$Q4_{ij} = Q4_{ij} + \tilde{U}^n_{i-1,j}(DM) \qquad Q4_{i-1,j} = Q4_{i-1,j} - \tilde{U}^n_{i-1,j}(DM)$$

$$CMB_{ij} = CMB_{ij} + DM \qquad CMB_{i-1,j} = CMB_{i-1,j} - DM$$

4. $\Delta < 0$

$DM = (\hat{\rho}^n_{ij})\Delta$ mass moves from cell ij to cell i-1,j.

$$Q1_{ij} = Q1_{ij} + E^n_{ij}(DM) \qquad Q1_{i-1,j} = Q1_{i-1,j} - E^n_{ij}(DM)$$

$$Q2_{ij} = Q2_{ij} + W^n_{ij}(DM) \qquad Q2_{i-1,j} = Q2_{i-1,j} - W^n_{ij}(DM)$$

$$Q3_{ij} = Q3_{ij} + \tilde{V}^n_{ij}(DM) \qquad Q3_{i-1,j} = Q3_{i-1,j} - \tilde{V}^n_{ij}(DM)$$

$$Q4_{ij} = Q4_{ij} + \tilde{U}^n_{ij}(DM) \qquad Q4_{i-1,j} = Q4_{i-1,j} - \tilde{U}^n_{ij}(DM)$$

$$CMB_{ij} = CMB_{ij} + DM \qquad CMB_{i-1,j} = CMB_{i-1,j} - DM$$

Mass movement on side 3

Except on the continuative boundary 3, this mass movement is taken care of by the mass movement across side 1 of the cell directly above.

On the boundary

$$\Delta = (\tilde{U}^n_{ij})(\delta t/\delta z)$$

$$DM = (\hat{\rho}^n_{ij})\Delta$$

$$Q1_{ij} = Q1_{ij} - E^n_{ij}(DM)$$

$$Q2_{ij} = Q2_{ij} - W^n_{ij}(DM)$$

$$Q3_{ij} = Q3_{ij} - \tilde{V}^n_{ij}(DM)$$

$$Q4_{ij} = Q4_{ij} - \tilde{U}^n_{ij}(DM)$$

$$CMB_{ij} = CMB_{ij} - DM$$

Mass movement on side 4

Except on the continuative boundary 4, this mass movement is taken

care of by the mass movement across side 2 of the cell on its right.

On the boundary

$$\Delta = \frac{\tilde{V}^n_{ij}\,\delta t}{\delta r}$$

a) $\Delta \geq 0$ mass moves out of cell ij.

$$DM = (\hat{\rho}^n_{ij})\,\frac{(2j+2-\Delta)\Delta}{2j+3}$$

$$Q1_{ij} = Q1_{ij} - E^n_{ij}(DM)$$

$$Q2_{ij} = Q2_{ij} - W^n_{ij}(DM)$$

$$Q3_{ij} = Q3_{ij} - \tilde{V}^n_{ij}(DM)$$

$$Q4_{ij} = Q4_{ij} - \tilde{U}^n_{ij}(DM)$$

$$CMB_{ij} = CMB_{ij} - DM$$

b) $\Delta < 0$ mass moves into cell ij.

$$DM = (\hat{\rho}^n_{ij})\,\frac{(2j+2-\Delta)\Delta}{2j+1}$$

$$Q1_{ij} = Q1_{ij} - E^n_{ij}(DM)$$

$$Q2_{ij} = Q2_{ij} - W^n_{ij}(DM)$$

$$Q3_{ij} = Q3_{ij} - \tilde{V}^n_{ij}(DM)$$

$$Q4_{ij} = Q4_{ij} - \tilde{U}^n_{ij}(DM)$$

$$CMB_{ij} = CMB_{ij} - DM$$

Phase V. Repartition

Add on mass moved quantities

For $\rho_{ij}^{n} > \text{MINGRHO} + (\rho_o - \text{MINGRHO})(W_{ij}^{n})$

$$\rho_{ij}^{n+1} = \rho_{ij}^{n} + CMB_{ij}$$

$$W_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(\rho_{ij}^{n} W_{ij}^{n} + Q2_{ij})$$

$$V_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(\tilde{V}_{ij}^{n} \rho_{ij}^{n} + Q3_{ij})$$

$$U_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(\tilde{U}_{ij}^{n} \rho_{ij}^{n} + Q4_{ij})$$

$$I_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(\rho_{ij}^{n} E_{ij}^{n} + Q1_{ij}) - \frac{1}{2}\left[(V_{ij}^{n+1})^2 + (U_{ij}^{n+1})^2\right]$$

For $\rho_{ij}^{n} \leq \text{MINGRHO} + (\rho_o - \text{MINGRHO})(W_{ij}^{n})$

$$\rho_{ij}^{n+1} = \rho_{ij}^{n} + CMB_{ij}$$

$$W_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(\rho_{ij}^{n} W_{ij}^{n} + Q2_{ij})$$

$$V_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(V_{ij}^{n} \rho_{ij}^{n} + Q3_{ij})$$

$$U_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(U_{ij}^{n} \rho_{ij}^{n} + Q4_{ij})$$

$$I_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}\left(I_{ij}^{n} \rho_{ij}^{n} + Q1_{ij} - \frac{(Q3_{ij})^2 + (Q4_{ij})^2}{2CMB_{ij}}\right)$$

IV. THE PISTON OR CONSTANT INPUT BOUNDARY

To obtain a smooth initial piston profile it was found necessary to set the internal energy of the cells for the first VCNT (25) cycles to

$$I - I_o = \frac{1}{2}(P + Q_3)(V'_o - V')$$

Another method which did not require initially adjusting the internal energy to obtain a smooth initial piston profile was to feed in the last 10 cells of a previously calculated flat topped shock as the starting conditions of a new calculation.

Steady-State Reaction Zone Piston

The steady-state piston was computed by iteration for a given detonation velocity by using the amount of reaction that has occurred in a cell near the piston to determine the proper piston density, energy and particle velocity.

Used axis cell of fifth layer to get Piston W. For fast reaction it was found necessary to use a lower W for Piston W by multiplying by a constant (WPISF).

1. Given a W, assume a V'.
2. Find P_r from $P_r - P_o = (\rho_o)^2(D)^2(V'_o - V')$, the Rayleigh Line.
3. Calculate I from $I - I_o = \frac{1}{2}(P_r)(V'_o - V')$.
4. With V', I, and W, compute P from HOM equation of state.
5. Iterate on V' until $P_r - P$ is less than 1×10^{-5}.
6. Calculate $U = \sqrt{(P-P_o)(V'_o - V')}$ and assign it to UAPP, assign 1/V' to MAPP, assign $I + \frac{1}{2}(MAPP)(UAPP)^2$ to EAPP.

V. THE DISK STORAGE AND USAGE

The calculation proceeds as if the layers in the z direction are on a barrel - the last layer at nth cycle is followed by the first at n+1th cycle. There are two barrels - one containing the cell quantities and

one containing the intermediate quantities. The intermediate quantity barrel has four layers around it.

For an eight layer problem the layers labeled A, B, C, ... H, the calculation proceeds as follows:

Pass through loop	Phase of Calculation					
	I	II	III	IV	V	write on disk
1.	A					
2.	B	A				
3.	C	B	A			
4.	D	C	B	A		
5.	E	D	C	B	A	
6.	F	E	D	C	B	A
7.	G	F	E	D	C	B
8.	H	G	F	E	D	C
9.		H	G	F	E	D
10.			H	G	F	E
11.				H	G	F
12.					H	G
13.						H

After thirteen passes the time is incremented, plotting and printing are done, and the cycle is started over again.

The skipping of various parts of the calculation is controlled by changing branch instructions to NOP's and vice versa.

The barrel operation is described below:

1. When all the layers can be held in core. (NMRD ≤ NSCMAX)

When phase V has been completed for a layer, it is transmitted to the disk and to the proper core location for the next cycle, e.g.

8 layers in core

A B C D E F G H

after phase V on A is completed

A B C D E F G H A'

after phase V on B is completed

A B C D E F G H A' B' etc.

When the top of core storage is reached, the next layer goes at the bottom of cell storage, e.g. for an 8 layer calculation in a 10 layer capacity core, we have

initially |A|B|C|D|E|F|G|H| | |

after 1 complete cycle

|C'|D'|E'|F'|G'|H'|G|H|A'|B'|

after 2 complete cycles

|E"|F"|G"|H"|G'|H'|A"|B"|C"|D"|

2. When all the layers will not fit in core (NMRD > NSCMAX), e.g., 8 layers in 6 layer capacity

initially |A|B|C|D|E|F|

after phase V of A is completed, A goes to disk, and G is read in

|G|B|C|D|E|F|

after phase V of B is completed, B goes to disk and H is read in

|G|H|C|D|E|F|

after phase V of H has been calculated, H goes to disk and F is read in

|E'|F'|A'|B'|C'|D'|

The number of layers required for the calculation increases with time at a rate characteristic of the problem. Graphing and printing use the same technique, except that graphing uses all the layers.

VI. INPUT FORMATS

Card	Col.	Format	Data
1	1-72	72H	Problem description
2	1-18	E0.1.11.3	Delta R
	19-36	E0.1.11.3	Delta Z
	37-54	E0.1.11.3	Delta T
3	1-18	E0.1.11.3	Activation Energy
	19-36	E0.1.11.3	Frequency
	37-54	E0.1.11.3	Minimum temp. to burn

Card	Col.	Format	Data
4	1-18	E0.1.11.3	V_o' for equation of state = $1/\rho_o$
	19-36	E0.1.11.3	Initial cell pressure
	37-53	E0.1.11.3	Initial cell temperature
5	1-18	E0.1.11.3	Piston detonation velocity
	19-36	E0.1.11.3	Piston initial volume guess
	37-54	E0.1.11.3	Viscosity constant
6	1-6	V1*5	0 for HOM, 1 for ideal gas
	7-12	V1*5	0 for no reaction, 1 for reaction
	13-18	V1*5	Number of cycles between prints
	19-24	V1*5	Number of cycles between graphs
	25-30	V1*5	Number of cycles between disk dumps
	31-36	V1*5	Graph type (see below)

7 + following cards - equation of state cards for HOM or ideal gas

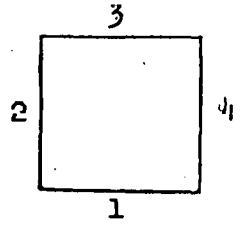
- for HOM - 4 cards for solid parameters, then 5 cards for gas parameters
- for ideal gas - 1 card

7	1-18	E0.1.11.3	Gamma
	19-36	E0.1.11.3	Q
	37-54	E0.1.11.3	C_V
8 or 16	1-5	V0*5	Number of mesh set up cards
9 or 17	1-5	V0*5	Z min
to end	6-10	V0*5	Z max
	11-15	V0*5	R min
	16-20	V0*5	R max
	21-32	E0.1.6.2	Density
	33-44	E0.1.6.2	Internal energy
	45-58	E0.1.6.2.1	U velocity with flag
	59-72	E0.1.6.2.1	V Velocity with flag
			Cells in the mesh that are not within the limits of any card are set empty with ρ=T=I=U=V=W=0 and P=P_o.

Graph type number

0	No graphs
1	Isotherm
2	Isobar
3	Isotherm and Isobar
4	Isopycnic
5	Isopycnic and Isotherm
6	Isopycnic and Isobar
7	Isopycnic, Isobar, and Isotherm

The individual cell flags that are set by the input cards are described below:

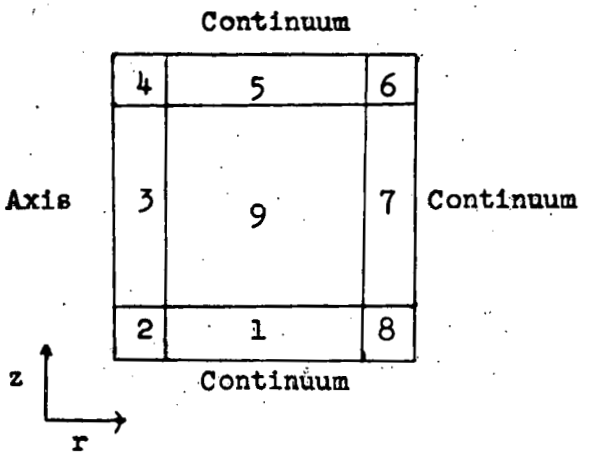


1. To put a continuative boundary on side 1 set U flag on CU which is a 2.
2. To put a continuative boundary on side 3 set V flag on CU which is a 1.
3. To put an axis boundary on side 2 set U flag on CV which is a 2.
4. To put a continuative boundary on side 4 set V flag on CV which is a 1.
5. To put a piston boundary on side 1 set T flag on CU which is a 4.

To keep mass from flowing from cell i+1,j into cell i,j or from cell i,j into cell i+1,j set continuative boundary on side 3 of cell i,j and set continuative or piston boundary on side 1 of cell i+1,j.

A cell may not be both on boundaries 1 and 3 or on boundaries 2 and 4.

The flag conventions used for initial problem set-up are described below:



Region	Flags
1	U flag on CU
2	U flag on CU, U flag on CV
3	U flag on CV
4	U flag on CV, V flag on CU
5	V flag on CU
6	V flag on CU, V flag on CV
7	V flag on CV
8	V flag on CV, U flag on CU
9	No flags

Piston is indicated by a T flag on CU.

VII. THE ISOPLOT SUBROUTINE

ISOPLOT is a plotting program which produces graphs of isotherms, isobars, etc., on the 4020. The input consists of the x and y coordinates and a function value (temperature, pressure, etc.) at each point in a two-dimensional lattice, the boundaries on x and y for the graph, the number of lattice points in the x direction, the total number of lattice points, the number of words in core between the x coordinate of one cell and the x coordinate of the next cell in the x direction (the difference is assumed to be the same as that between y's and function values), and the numerical difference of the function value between two isolines.

The calling sequence is:

```
        LVI,$15,$+1
        B,ISOPLOT$P
        ,NCELL          Total # of lattice points
        ,X              address of x coordinate
        ,NXDIFF         # words between successive x coordinates
        ,Y              y coordinate address
        ,NXCELL         # of lattice points in x direction
        ,F              address of function
        ,DELTA          difference between isolines
        ,XYB            location of 4 words giving x, y boundaries
```

example: 4 x 5 lattice of values

x_{20}, y_{20}, P_{20}

x_1, y_1, P_1 $\quad\quad$ x_4, y_4, P_4

with x's, y's, and P's arranged in core as follows:

```
        X    DR(N),(20)
        Y    DR(N),(20)
        P    DR(N),(20)
```

and x range from 0 to 3, y range from 0 to 4, plotting lines every .1.

```
       XYB  DD(N),0.
            DD(N),3.
            DD(N),0.
            DD(N),4.
     DELTA  DD(N),.1.
```

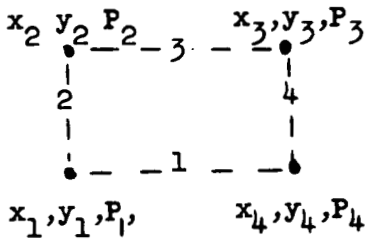
The calling sequence is then:

```
LVI,$15,$+1
B,ISOPLOT$P
,20.
,X
,1.
,Y
,4.
,P
,DELTA
,XYB
```

Note: Whether the x, y, and P's are stored as vectors or in individual blocks, the x coordinate of the next cell in the y direction must be (NXCELL)(NXDIFF) words away (e.g., x_5 is four words from x_1: stored x_1, x_2, x_3, x_4, x_5).

The method:

The quantities for four points are brought in



Determine if an isoline crosses side 1.

A. $P_1 < P_4$

(integer part $(P_1/\text{DELTA})+1)\text{DELTA} = PT$

If $PT < P_4$ a line crosses side 1, and we find the coordinates of the point at which it crosses

$$x' = (PT-P_4)\frac{(x_4-x_1)}{(P4-P1)} + x4$$

$$y' = (PT-P_4)\frac{(y_4-y_1)}{(P_4-P_1)} + y_4$$

B. $P_1 > P_4$

PT = (integer part $(P_4/DELTA)+1)DELTA$

If $PT < P_1$ a line crosses side 1 at

$$x' = (PT-P_1)\frac{(x_4-x_1)}{(P_4-P_1)} + x_1$$

$$y' = (PT-P_1)\frac{(y_4-y_1)}{(P_4-P_1)} + y_1$$

We then proceed to find out which other side this isoline crosses. It crosses side 2 if $P_1 < PT < P_2$ or $P_1 > PT > P_2$. The coordinates of the point at which it crosses are:

$$x'' = (PT-P_2)\frac{(x_1-x_2)}{(P_1-P_2)} + x_2$$

$$y'' = (PT-P_2)\frac{(y_1-y_2)}{(P_1-P_2)} + y_2$$

Having found the point, a vector is drawn from (x',y') to (x",y") using a 4020 draw vector subroutine.

PT is incremented by DELTA, and if $PT < P_4$ another line crosses side 1. One then goes back to find out what other side this line crosses. This continues until $PT > P_4$, then one moves to side 2 to see if any lines cross side 2. The lines crossing side 2 are connected to sides 3 or 4 since lines from side 1 to side 2 have already been drawn. Similarly lines between sides 3 and 4 are drawn.

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