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NATIONAL LABORATORY

Advanced Three-Dimensional Eulerian Hydrodynamic Algorithm Development

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Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The purpose of this project is to investigate, implement, and evaluate algorithms that have high potential for improving the robustness, fidelity and accuracy of three-dimensional Eulerian hydrodynamic simulations. Eulerian computations are necessary to simulate a number of important physical phenomena ranging from the molding process for metal parts to nuclear weapons safety issues to astrophysical phenomena such as that associated with a Type II supernovae. A number of algorithmic issues were explored in the course of this research including interface/volume tracking, surface physics integration, high resolution integration techniques, multilevel iterative methods, multimaterial hydrodynamics and coupling radiation with hydrodynamics. This project combines core strengths of several Laboratory divisions. The project has high institutional benefit given the renewed emphasis on numerical simulations in Science-Based Stockpile Stewardship and the Accelerated Strategic Computing Initiative and LANL's tactical goals related to high performance computing and simulation.

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Background and Research Objectives

Eulerian hydrodynamic calculations are characterized by the fixed frame of the computational mesh. Lagrangian hydrodynamics where the mesh deforms at the material velocity have a long history at Los Alamos National Laboratory (LANL) and are well-suited to a number of research efforts. The chief difference between calculations performed in these two frames of reference (Lagrangian versus Eulerian) is the smearing of material boundaries associated with the Eulerian calculations. A depiction of the differences in Eulerian and Lagrangian computational grids is given in Figure 1. The specific physical phenomena that Eulerian computations can simulate is vorticity, which is associated with large scale mixing. Vorticity when associated with the Lagrangian frame of reference will cause the computational mesh to tangle destroying the underlying calculation. The ability of Eulerian computations to provide the fidelity necessary for useful calculation can be traced to a number of algorithmic advances made during the 1970s and 1980s. In particular, the use of interface tracking provides Eulerian calculations with Lagrangian-like resolution of material interfaces. However, these methods are quite ad hoc and need to be put on firmer theoretical and algorithmic footing.

The purpose of this project is to investigate, implement, and evaluate algorithms that have high potential for significantly improving the fidelity and effectiveness of three dimensional (3-D) Eulerian hydrodynamic simulations. Existing 3-D Eulerian codes are actively used for 3-D simulations in areas such as nuclear safety, theater missile defense, and conventional munitions. In addition Eulerian computations are needed to compute the pouring/solidification in the molding process for metal parts. In particular the dynamics and physics at the air-metal interface is of critical importance. Additional applications can be found in diverse fields from solid state physics to astrophysics. In astrophysics, the detailed calculation of the mechanism of a Type II supernovae is dependent upon the physics captured by Eulerian hydrodynamics. Details of the observed light curve and explosion mechanism can be simulated through detailed Eulerian hydrodynamic computations.

Useful as they are, the codes are fundamentally limited by their basic algorithms. Our objectives in conducting this research are detailed below, but can be explained compactly as work on methods that can significantly impact the robustness, fidelity and accuracy of Eulerian computations or provide capability that does not currently exist. The objectives are given as follows:

- improved fidelity of the direct computation of interface dynamics through better integration algorithms,

- more accurate and flexible computation of interface physics through extension of the continuum surface force (CSF) model,

- improved natural coupling of physical phenomena through the alleviation of operator splitting used in the algorithmic implementation of integration schemes, and

- more intimate physical coupling of phenomena by the development of algorithms that respect the nature of the coupling.

Importance to LANL's Science and Technology Base and National R&D Needs

This work will benefit a wide range of current and future programs, although it will not replace or augment existing programmatic efforts, which are directed at maintaining current capabilities, making incremental improvements, and supporting users. Other efforts are directed toward development for specific program applications, while this work should lead to generalizable algorithms and models that lend themselves to a wide range of applications such as those detailed above.

The 3-D Eulerian hydrocodes at the Laboratory address many of the Nation's most difficult and complex technical challenges. These codes form a significant part of the basis for the *Theory, Modeling, and High Performance Computing* core competency of the Laboratory. They are used to model a broad range of physical problems, including studies of nuclear safety, theater missile defense lethality, and armor/anti-armor technology. In addition, these codes have application to problems in astrophysics, biotechnology, and industrial processes. Improvements to the algorithms for 3-D Eulerian codes will provide advanced application code technology for the DOE Accelerated Strategic Computing Initiative (ASCI).

Scientific Approach and Accomplishments

Below, we will detail various aspects of the algorithmic accomplishments made during the course of this research project.

Interfacial Computational Physics

We first discuss the broad area of focus which we denote as "interfacial computational physics." This is to provide an emphasis on the dynamics and physics of the material interface whose computation is the hallmark of Eulerian hydrodynamics. Novel volume tracking algorithms have the potential to improve the fidelity and efficiency of 3-D simulations for low- and high-speed flow regimes. One approach is to make a truer approximation to the transport operator. An example is unsplit advection. Methods are currently based on dimensional splitting. Figure 2 shows the difference in split versus unsplit integration of volume fractions. Unsplit advection methods can reduce error because of better corner coupling. In Figure 3 the difference in results and symmetry preservation are demonstrated for the compression and subsequent expansion of a sphere adiabatically.

Furthermore, we are interested in the solution of incompressible flows possessing densities that vary both discontinuously and smoothly. Smooth density variations might be caused by temperature effects, whereas abrupt variations are present at immiscible fluid interfaces. If interfaces are present, we wish to model their gross topological changes. The design of an incompressible flow algorithm that maintains solution accuracy and simulation robustness in the presence of density variations presents challenges, especially if the variations are discontinuous and topologically complex.

We construct robust, accurate, high-fidelity methods for computing such flows. We focus on algorithms for the solution of the pressure equation, and its numerical linear algebra, as well as interfacial physics such as surface tension. Also developed are algorithms for multidimensional advection and volume tracking.

Geometric Volume Tracking

New algorithms for the volume tracking of interfaces have been developed (Pub. 3). The algorithm is based upon a well-defined, second-order geometric solution of a volume evolution equation. The method utilizes local discrete material volume and velocity data to track interfaces of arbitrarily complex topology. A linearity-preserving, piecewise linear interface geometry approximation ensures that solutions generated retain second-order spatial accuracy. Second-order temporal accuracy is achieved by virtue of a multi-dimensional, unsplit time-integration scheme. We detail our geometrically based solution method, in which material volume fluxes are computed systematically, with a set of simple geometric tasks. We then interrogate the method by testing its ability to track interfaces through large (yet controlled) topology changes, whereby an initially simple interface configuration is subjected to vortical flows. Numerical results for these strenuous test problems provide evidence for the algorithm's improved solution quality and accuracy.

Volume tracking methods have enjoyed widespread use and success since the mid-1970s, yet they possess solution algorithms that are too often perceived as being heuristic and without mathematical formalism. Part of this misperception lies in the difficulty of applying standard, hyperbolic, partial-differential-equation (PDE) numerical analysis tools, which assume algebraic formulations, to a method that is largely geometric in nature (hence the more appropriate term **volume tracking**). To some extent the lack of formalism in volume tracking methods, manifested as an obscure underlying methodology, has impeded progress in evolutionary algorithmic improvements.

Basic features of volume tracking methods. It is first instructive to review the common features of most volume tracking methods. Figure 4 shows a computational lifecycle of a volume tracking integration step detailed below. To begin, fluid volumes are initialized in each computational cell from a specified interface geometry. This task requires computing fluid interface volumes in each cell containing the interface (hereafter referred to as *mixed* cells). Exact interface information is then discarded in favor of the discrete volume data. The volume data is traditionally retained as volume fractions (denoted as f hereafter), whereby mixed cells will have a volume fraction f between zero and one, and cells without interfaces (*pure* cells) will have a volume fraction f equal to zero or unity. Since a unique interface configuration does not exist once the exact interface location is replaced with discrete volume data, detailed interface information cannot be extracted until an interface is *reconstructed.* The principal reconstruction constraint is local volume conservation, i.e., the reconstructed interface must truncate cells with a volume equal to the discrete fluid volumes.

Interfaces are "tracked" in volume tracking methods by evolving fluid volumes forward in time with solutions of an advection equation. At any time in the solution, exact interface locations are not known, i.e., a given distribution of volume data does not guarantee a unique interface. Interface geometry must be inferred, based on local volume data and the assumptions of the particular algorithm, before interfaces can be reconstructed. The reconstructed interface is then used to compute the volume fluxes necessary to integrate the volume evolution equations. Typical implementations of these algorithms are one-dimensional, with multi-dimensionality traditionally acquired through operator splitting **[1,2]**.

Interfaces are subsequently "tracked" by evolving fluid volumes in time with the solution of a standard advection equation. At any time in the solution, an exact interface location is not known, i.e., a given distribution of volume fraction data does not guarantee a unique interface topology. Interface geometry is instead inferred (based on assumptions of the particular algorithm) and its location is "reconstructed" from local volume fraction data. Interface locations are then used to compute the volume fluxes necessary for the advective term in the volume evolution equation. Volume fluxes are therefore approximated geometrically rather than algebraically. Typical implementations of these algorithms are one-dimensional, with multi-dimensionality built up through operator splitting. The assumed interface geometry, interface reconstruction, and volume flux calculation typically comprise the unique features of a given volume tracking method.

Our piecewise-linear volume-tracking algorithm, as implemented, is straightforward, simple, and extensible. This is accomplished by drawing upon the extensive literature available in the field of computational geometry [**3**]. The algorithm is robust, second-order accurate (in time and space), and is constructed from a set of simple geometric functions.

Continuum Surface Force Model

Other examples of novel algorithms are surface tension models for simulation of interfacial flow and subgrid methods for following discrete material property changes, such as phase changes, fracturing, or explosive reaction fronts. The fidelity of reaction front simulations may also be improved with the use algorithms such as "hourglass filters" to damp spurious modes (Pub. 2).

Our current models for interfacial surface tension begin with methodology established in the continuum surface force (CSF) method [**4**]. The basic premise of the CSF method to model physical processes specific to and localized at fluid interfaces (e.g, surface tension) by applying the process to fluid elements everywhere within interface transition regions. Figure 5 shows the basic concept in a graphical form. Surface processes are replaced with volume processes whose integral effect properly reproduces the desired interface physics. This approach falls under the general class of immersed interface methods whose origin dates back to the pioneering work of Peskin [**5**]. The CSF method lifts all topological restrictions without sacrificing accuracy, robustness, or reliability. It has been verified extensively in 2-D flows through its implementation in a classical algorithm for free surface flows, where complex interface phenomena such as breakup and coalescence have been modeled.

In the CSF model, surface tension is reformulated as a volumetric force. The surface delta function was proposed in the original CSF model by the characteristic (color) function uniquely identifying each fluid in the problem. If a wide stencil is used, then the force resulting will be nonlocal. We currently force the surface force to be zero in cells not containing the interface, which causes the CSF to be zero only within the interface transition region. A proper discrete Dirac delta function insures that the CSF is normalized to recover the conventional description of surface tension.

Despite the success of the CSF model and related immersed interface methods, there are outstanding issues. If these issues can be resolved adequately, a wider range of surface tension-driven flows will be modeled reliably. For example, improved forms for the Dirac delta function, displaying better convergence and smoothness properties, are needed. Our current numerical results are very sensitive to the discrete form used, indicating that the quality of CSF model relies heavily on the quality of the form used. Recent results motivate the use of other kernels, such as the Peskin or higher-order kernel (Pub. 8).

Perhaps the most stringent test for a surface tension model is a test of the ability to maintain an equilibrium (minimal energy) configuration. A 2-D or 3-D static drop is such an example. Here a perfectly spherical drop is placed in a lighter-density background fluid, and all forces are ignored except the drop interfacial surface tension. The drop should remain stationary, as the net surface tension force is zero. An incompressible flow solution for this system, however, generates false flow dynamics (dubbed "parasitic currents") that can grow with time (sometimes unbounded). The source of these currents originates in part with the surface tension model, as the computed pressure gradient at the drop interface does not exactly cancel the surface tension force.

High Resolution Flow Solvers

The development of flow solvers that are well-matched to the characteristic of the interfacial computational physics requires several goals as defined below. These principles guide our development aimed at providing practical, but powerful Eulerian algorithms (Pub. 1).

Accuracy is defined as the quality of deviating slightly from fact. For our purposes, this definition is refined as the measured error for a given solution. There is also a distinction between order of accuracy and numerical accuracy. For reasonable grid resolution, methods with a higher order of accuracy can be accompanied by significantly larger numerical error than the lower order method. This naturally leads to our next definition.

Fidelity is defined as exact correspondence with fact. A solution that possesses fidelity is one that is physically meaningful. A method is considered to be high-fidelity when it produces solutions that are accurate relative to the computational resources (the mesh size) applied to them. For example, interface tracking mechanisms can increase solution fidelity by maintaining interface discontinuities as the interface is advected and/or undergoing topological change.

Robustness is the property of being powerfully built or sturdy. A robust method will not fail in a catastrophic manner, but rather "degrade gracefully." Robustness implies that the algorithm can be used with confidence on a difficult problem. The degree to which the degradation is graceful is subject to interpretation. A robust method should produce physically reasonable results beyond the point where accuracy is expected or achieved.

We choose a basic method which does not employ operator splitting and has at least second-order accuracy. While this provides an adequate basis for development it is not sufficient for our purposes. The maintenance of a compact material interface provides for a continual singular problem. This gives a continual source of oscillatory behavior in the solution requiring great care and extra measures to assure high fidelity and reasonable efficiency.

The first of these measures is the control of error accumulation. By carefully formulating our discrete problem, the errors can be made to be local in time and accumulate at a far lower level than standard implementations. Without this care, solutions can be polluted by the signature of past errors integrated over all previous time steps. These problems can be fatal to the point where variations in fluid properties are orders of magnitude.

Our second measure to provide the robustness needed for a variety of applications is discrete filtering. This algorithm cleans up errors that are associated with spurious features not recognized by our discrete operators. Without this, the spurious features can interact with the desirable part of the solution, polluting it. Together with error control, filtering can provide exceedingly high resolution solutions for extreme circumstances while not having to make compromises in the calculation of the material interfaces. We should note that for the most part the lack of compact material interfaces and the physics associated with them alleviates the necessity of the measures discussed here.

Another issue is the construction of truly multidimensional advection algorithms which are ideally suited for general 3-D grids. Over the last twenty years, methods for higher-order monotone advection have become accepted and are ubiquitous in the computational fluid dynamics literature [**6**]. When able to reliably suppress nonphysical oscillations, monotone methods have supplanted first-order upwinding schemes. The design and understanding of these methods for data that varies in one dimension is well developed. Most often multidimensional applications of monotone schemes are derived from an operator-split application of the basic one-dimensional method.

Our starting point is multi-dimensional "k-exact" methods devised by Barth [7]. We specifically embrace Barth's approach for deriving a reconstruction based upon least-squares methodology. Barth applies monotonicity after the minimization process, following standard principles. The problem, however, is that the definition and application of monotonicity is not part of a minimization process, and therefore remains tied to the one-dimensional process. We show that if monotonicity considerations are recast as constraints in the minimization processes, the resulting reconstruction is truly multidimensional, i.e., the difference between a constrained (monotonic) and unconstrained (nonmonotonic) reconstruction can be interpreted as a geometric "limiter" that is in general a vector (Pub. 10).

Rather than impose scalar monotonic constraints subsequent to the reconstruction, our monotonicity imposition will assume the form of an inequality constraint and can be interpreted as a vector "correction" to the unconstrained reconstruction. We show that basic one-dimensional slope limiter ideas can be recast as constraints, in a multidimensional reconstruction. We also discuss a powerful weighted-least-squares approach that incorporates expected numerical error into the interpolation process. Two-dimensional numerical results are given to substantiate the benefits of the basic methodology underlying our approach.

Another aspect of the many one-dimensional methods is the ability to design the level of numerical dissipation into the methods through the choice of the limiter. This freedom enables the method to possess discrete properties best suited for the physical and mathematical structure of the waves being transported. We developed an approach to applying data dependent weights to a least squares/minimization formalism that recovers much of the functionality of the family of classical limiters. Our method allows a fairly wide degree of flexibility in tailoring the dissipation inherent in the multidimensional interpolation process.

Multilevel Iterative Methods

Next, we consider the efficiency of our computations in an asymptotic sense. Solutions to the linear systems arising from the pressure equation can also be obtained with a multigrid (MG) algorithm [8]. Use of a MG algorithm is desirable because of its attractive scaling. The operation count for classical, direct-linear-algebra solution techniques (e.g., Cholesy) scales like N^3. This scaling improves to N^2 for banded solvers that take advantage of the structure of the linear system. MG scales linearly with N. Thus, MG (where it works) will eventually provide the fastest route to a solution as the grid is refined. We find that our MG algorithm converges quickly to a solution in most cases, but fails on occasion with flows having interfaces possessing large density variations and complex topology (e.g., a drop splashing into a pool).

Our current solution to the MG robustness problem is to employ the symmetric MG algorithm to precondition a standard conjugate gradient (CG) method. Experimentation has proven the utility of combining these two methods. This combined MG-CG method usually scales like a MG (rather than the less efficient CG scaling). We have found it to be quite robust. It is an important step in designing a robust method that consistently exhibits MG-like scaling. Figure 6 shows the relative improvement that can be achieved for difficult elliptic problems through this approach. Given our success with this approach we have examined these concepts for nonlinear problems.

Nonlinear problems are ubiquitous in physics and their efficient solution is of great practical interest. In particular nonlinear initial value problems present a unique set of challenges especially with respect to the efficiency of the solution. It is our intention to investigate Newton-Krylov methods which have shown great promise in solving a wide class of nonlinear problems. Newton's method is a traditional approach for solving nonlinear problems efficiently while Krylov (subspace) methods extend CG-type algorithms to nonsymmetric and indefinite linear systems.

It is well known that the efficiency of the Newton-Krylov methods is critically dependent on the effectiveness of the preconditioner. Traditional preconditioning [typically ILU(n)] shows less than optimal scalability, practically limiting time step size and mesh size (approximately $N^{3/2}$). Storage becomes an increasing issue with ILU(n) as the degree of fill-in increases (n increases). Our intention is to investigate the potential of multigrid preconditioning to alleviating this shortcoming. Furthermore, the basis of a simple nonlinear iteration such as a Picard iteration (based on a multigrid solver) can serve to precondition Newton's method implemented with a matrix-free Newton-Krylov algorithm (Pub. 7).

It has been shown that Generalized Minimum Residual (GMRES) has advantageous properties for Newton-Krylov. The Krylov vectors are well behaved and the convergence is monotone. When GMRES is used as the Krylov method, the issues regarding the scaling of work and storage are especially critical. This is due to the required storage of the Krylov vectors and the increase in work per iteration associated with the orthogonalization process in the Arnoldi algorithm. The multigrid algorithm in addition to its scalability can also be more effective per iteration than other typical preconditioners and should reduce the raw number of linear iterations significantly, reducing storage needs greatly for large problems (Pubs. 5, 6). We are interested in combining multigrid with Newton-Krylov in order to give better performance.

We have demonstrated this basic approach on several problems of general interest. These include Burgers' equation, Navier-Stokes equations and a Marshak (radiation, nonlinear diffusion) wave. In each case the combined multigrid-Newton-Krylov method has shown excellent scaling, extreme robustness and algorithmic simplicity.

Applications of the Research

Much of the research done in the course of this project has been applicable to Telluride, a simulation code for casting and solidification. Below, we show a demonstration of the capabilities enhanced in Telluride through this research effort.

A pure copper casting, produced at the LANL (Sigma) foundry starting in 1985, has been chosen for a Telluride validation simulation. This casting, referred to as a "chalice", is a test part for the foundry, for which ample experimental data of the mold filling and solidification process is available. The representation of the chalice in Telluride is shown in Figure 7. The chalice casting consists of a thick hemispherical shell which is "gated" at its pole with a cylindrical "hot top". The hot top serves to continuously supply liquid metal to the hemispherical shell during filling/solidification (to avoid shrinkage defects).

A cylindrical graphite crucible containing 400 grams of the molten copper, superheated by 200 °C, is positioned above the cylindrical hot top. The entire crucible/mold/part system is enclosed in a coil furnace containing an inert gas (5 psi argon). The chalice mold (uncoated H-490 graphite) is initially heated to roughly the melting temperature of copper (1083 °C). The molten copper is then allowed to fall under gravity into the mold cavity through a 3/8-inch (diameter) pour hole in the hot top. Power to the furnace coils was shut off 10 minutes to allow the metal to cool down and solidify. Although the data is not available, we estimate the molten copper to have entered the hot top at a velocity of approximately 15.7 inches/sec, filling the entire mold cavity in about 1.6 seconds. Time to complete solidification is approximately 10 minutes, as the molten copper begins cooling immediately after entering the mold. In fact, without the mold being heated, it was found experimentally to "cold shut", i.e., portions of the copper solidified before the entire mold cavity was filled adequately.

Current Telluride simulations are performed in two separate steps: (1) isothermal filling of the mold cavity (neglecting heat transfer), and (2) cooling/solidifying of the quiescent liquid copper subsequent to fill. These two separate simulations will soon be combined into one integrated simulation, in which fluid flow, heat transfer, and solidification will be modeled simultaneously. For the current simulations, only one quadrant of the full geometry is simulated. The geometric model and computational mesh are generated with a commercial software package called I-DEAS. The current (fairly coarse) mesh consists of 6480 unstructured hexahedral elements.

For the mold-filling simulation, the mold cavity is initially filled with a background fluid representing the argon gas. At time zero a stream of liquid copper at the centerline having the diameter of the pour hole is introduced from the top via an in-flow boundary condition. The in-flow velocity is about 15.7 inches/sec. Out-flow boundary conditions are applied on the top boundary near the outer edge to allow venting of the background fluid as the mold is filled, since all fluids are assumed incompressible. Surface tension is neglected because both the Weber and Bond numbers (measures of the relative importance of inertial and gravity forces compared to surface tension) are much greater than unity. The flow is also assumed to be inviscid, as the Reynolds number of the falling liquid metal stream is higher than 8,000. The liquid copper/argon interface is tracked with the Telluride volume tracking algorithm based largely on the research conducted in this project, which assumes the interface to be locally piecewise planar. The incompressible flow algorithm is a nominally second-order-accurate, cell-centered scheme that borrows heavily from Godunov algorithms developed for high speed flows and contains numerous refinements developed during this research project.

For the heat transfer/solidification simulation, the mold cavity is assumed to be initially full of quiescent liquid copper (perfectly filled) at 1270 C. Because only one 90 degree quadrant is simulated, elements along the two vertical symmetry planes are assumed insulated. The top horizontal plane of the hot top is also assumed insulated because of its proximity (1 inch) to the (hot) crucible. For the inner hemispherical surface (adjacent to the graphite mold) a convective heat transfer boundary condition is used with a heat transfer coefficient (h) of 25 W/(m^2-K). For the outer surfaces, a coefficient h equal to 15 W/(m^2-K) is used, which corresponds to experimental heat transfer coefficient values in stationary air. The surface physics associated with the soldification process is modeled using an extension of the CSF model.

Coupling Radiation and Hydrodynamics

One goal of this effort is to develop a system of equations that can accurately predict, at a reasonable computational cost, nonrelativistic strongly radiative inviscid flows. We began with an asymptotic analysis of the coupled radiation-hydrodynamics system of equations. Previously, only the asymptotics of the radiation transport had been studied. By looking at the coupled system, we can identify the magnitude of the material opacity required for the equilibrium, isothermal, and streaming regimes.

The coupled system uses a source-term treatment that is based on the development of Mihalas and Klein [**9**]. The system has the following properties:

- The equations are correct to $O(v/c)$, where v is a characteristic velocity and c is the speed of light. The $O(v/c)$-corrections are sufficient to ensure that the equations have the correct asymptotic behavior.
- The equations identified with the transport of mass, momentum, and total energy are written in conservation form. The conservation property is necessary so that numerical methods based on these equations can predict correct shock speeds given sufficient entropy production in the numerical method.
- A multigroup treatment of radiation can be easily employed.

Note that ensuring that the equations are correct to $O(v/c)$- is sufficient, but not necessary, to obtain the correct asymptotic behavior. With this in mind, we studied several simplified source-term treatments. These treatments are no longer correct to $O(v/c)$-, but have all of the other desirable properties outlined above and are much simpler to implement.

A dispersion analysis of the coupled equations, with a P_1-treatment of radiation, was shown to be consistent with our asymptotic results. The dispersion analysis also showed that the coupling must be a function of **only** two parameters; namely, the momentum and total energy depositions. Less obvious is that numerical discretizations should retain this property to avoid spurious modes. Moreover, in certain popular forms of the governing equations, the two-parameter formulation leads to $O(v^2/c^2)$-terms. Even though the equations are correct to only $O(v/c)$, these terms must be retained; otherwise, in the equilibrium regime, our analysis shows that the wave structure of the coupled system is incorrect.

In addition, we developed numerical methods that closely couple the evolution of hydrodynamics with radiation. Current numerical methods "split" the evolution of the radiation and hydrodynamic fields. For example, in the first stage of a time-step, the radiation field is updated with the hydrodynamic variables held constant. Then, the hydrodynamic variables are updated using the new radiation field. Although the split approach is modular and easy to implement, there are disadvantages:

- High-resolution methods for predicting shock evolution require a reasonable estimation of the local wave structure. Radiation can have a large effect on the hydrodynamic wave structure, but current split methods ignore this effect. Unless a problem-dependent, unnecessarily large amount of artificial dissipation is added, the split methods will have overshoots at shocks (Gibb's phenomenon) and may allow nonphysical, entropy-violating shocks ("expansion shocks").

- Current split methods are at best first-order accurate.
- To ensure conservation, and hence to be able to compute the correct shock speed, the coupling terms must be evaluated identically between each split system.
- In state-space, a split approach may only be able to approximate a certain fixed point (for example, an equilibrium point) as a limit-cycle process.

We have begun to address all but the last issue. For equations that govern the equilibrium regime, two types of coupled-flux solvers were developed and implemented into a conservative code. Numerical results show that both of the solvers eliminate overshoots, approximate expansions correctly, compute the correct shock speed, and were easily incorporated into a second-order framework. Future research will focus on extending these ideas to nonequilibrium radiation hydrodynamics.

Adaptive Riemann Solvers

At the heart of many modern methods for solving the equations of hydrodynamics is the Riemann solver. The Riemann solution is the initial value problem resulting from two constant discontinuous states. Its exact or approximate solution is a means of introducing physically motivated regularizing terms (i.e. artificial viscosity) into the numerical solution of hydrodynamic equations at discontinuities. The solution of the Riemann problem, while well developed as a method, has several flaws with respect to interesting applications. These are that many Riemann solvers can admit nonphysical entropy violating solutions, and the inability of the basic framework to be extended to nonanalytic equations of state for general material. Additionally, methods specifically focused on strongly shocked flows are lacking. Here, we address these concerns with a new approach outline below.

The basic structure of the solution to the Riemann problem is essential to understanding the construction of this solver. A discontinuity between two piecewise constant states evolves into a self-similar solution. The three conservation relations then create three waves: two nonlinear waves, either shocks or rarefactions, and a linear contact wave. Figure 8 shows a representation of the Riemann problem in space/time and pressure-velocity form. This form is used in constructing this approximate Riemann solver. The pressure and velocity are constant across the contact discontinuity, making them convenient for the parametrization of the Riemann solution.

In the years following World War II there was considerable effort in establishing the properties of materials under extreme conditions. Similar efforts were undertaken in both the United States and the Soviet Union. Among the many important results to arise from this effort was the U_s-U_p parametrization of the shock Hugoniot. The U_s-U_p description of the shock Hugoniot has a remarkable capacity to reduce shock data from shock wave experiments.

The U_s-U_p equation is $U_s = A + B\,U_p$ where U_s is the shock speed, U_p is the particle velocity or the jump in velocity across the shock, with A and B being fitting coefficients. Intuition and experimental evidence shows that A is the sound speed of the unshocked material. The definitions can be refined via thermodynamic arguments . Using this form the pressure is given by a quadratic relation in particle velocity by inserting it into the Rankine-Hugoniot equation for momentum, $p_S = p_0 + r_0\,U_s\,U_p$.. This quadratic relation can be analytically evaluated forming the basis of our Riemann solution.

When solving the equations of gas dynamics the flow is defined by the conservation equations and the equation of state (EOS). The EOS in its simplest form for isentropic flow has the form of the dependence of the pressure, p, on the specific volume, V, $p(V)$. An assumption in this case is that $pV<0$, so that the resulting system is hyperbolic. Of nearly equal importance is the assumption of the convexity of the EOS expressed as $pV^2 > 0$. With the convexity of the EOS it is assured that shocks are compressive and rarefactions are expansive. Thus, the fluid structures in the resulting solution(s) are constructed in an entropy satisfying manner.

While the assumption about the convexity is critical in the construction of solutions (analytic or numerical), it is rarely employed to improve the quality of an approximate solution. We describe a process where the degree of convexity of the EOS is used to improve the accuracy of the approximation to the solution of the equations of gas dynamics (Pub. 4). Viewed in another fashion, this solver is designed to carry with it a two-parameter version of the local equation of state.

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Figure 1. A comparison of Eulerian and Lagrangian frames of reference. On the left is the initial configuration which remains unchanged in the Eulerian frame, but will move to reflect material motion in the Lagrangian frame. On the far right are two potential Lagrangian cell configurations, "boomerang" and "bowtie" cells which can lead to computational difficulties.

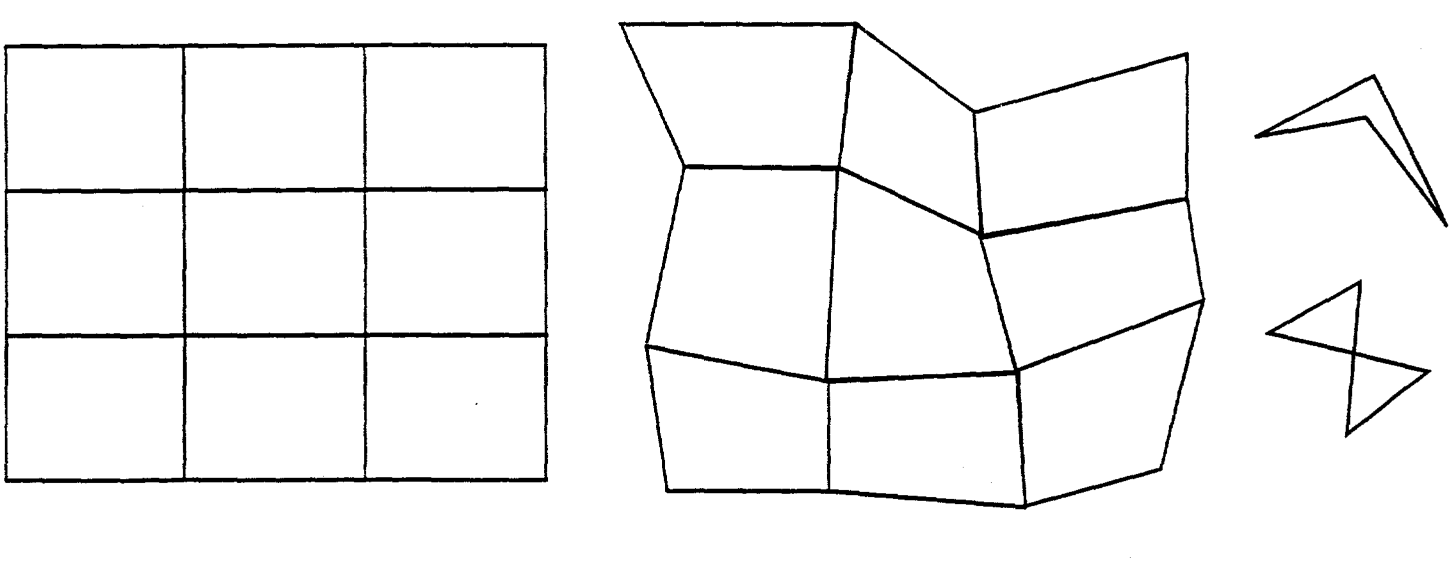

Figure 2a. A comparison of "split" versus "unsplit" spatial integration for volume tracking. The split integration is shown in a sequence of two passes, first in the upward (a) then in the left to right directions (b). The unsplit integration (c) has both directions integrated simultaneously. Note that the inferred geometric operations are more involved in the unsplit method.

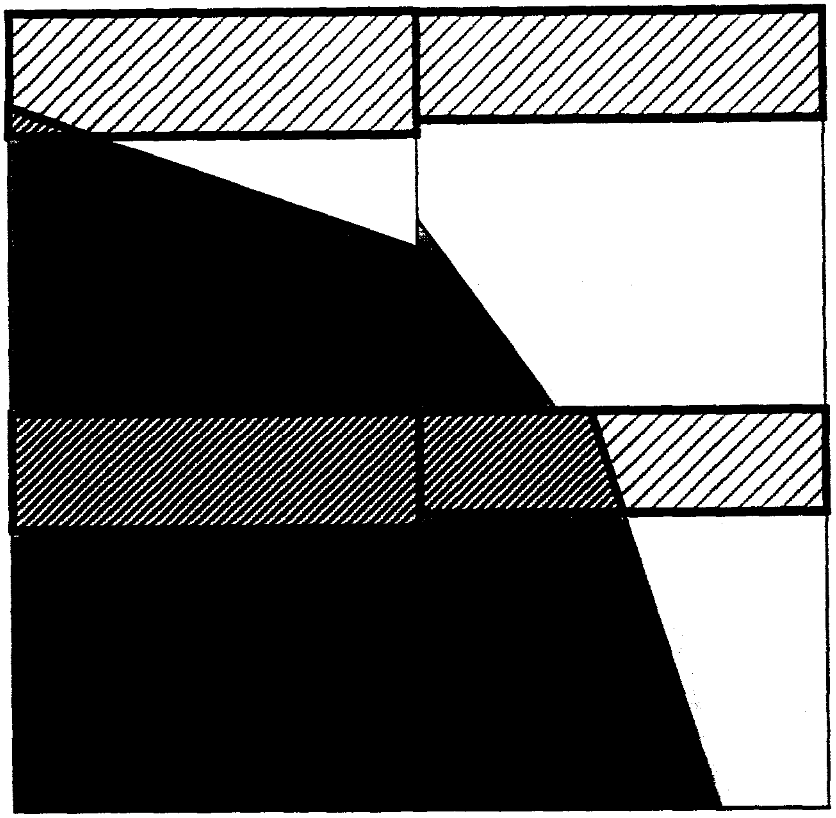

Figure 2b

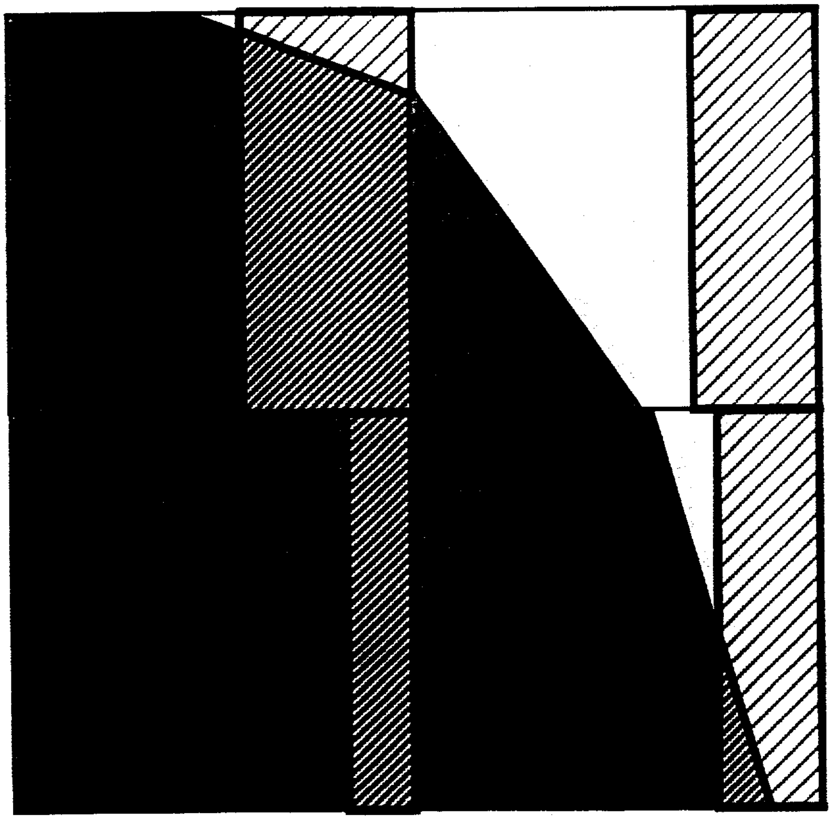

Figure 2c

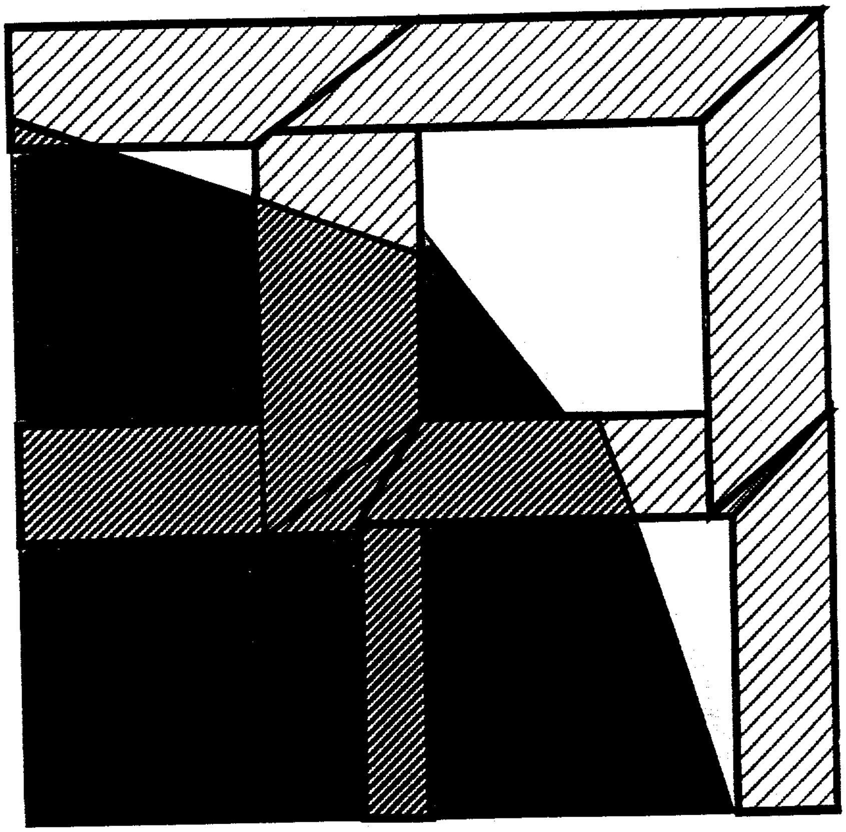

Figure 3a. Some sample results computed using split (a) and unsplit (b) volume integrators in a cylindrical geometry. The circles shown are spheres that have been compressed to a radius of about 20% of their initial radius and returned to their initial configuration. The unsplit results (b) demonstrate superior symmetry as the velocity field is purely radial in this case. With the unsplit method, the sphere is in virtually the same position on the two axes, while there is a greater than 10% difference with the split integration technique (a).

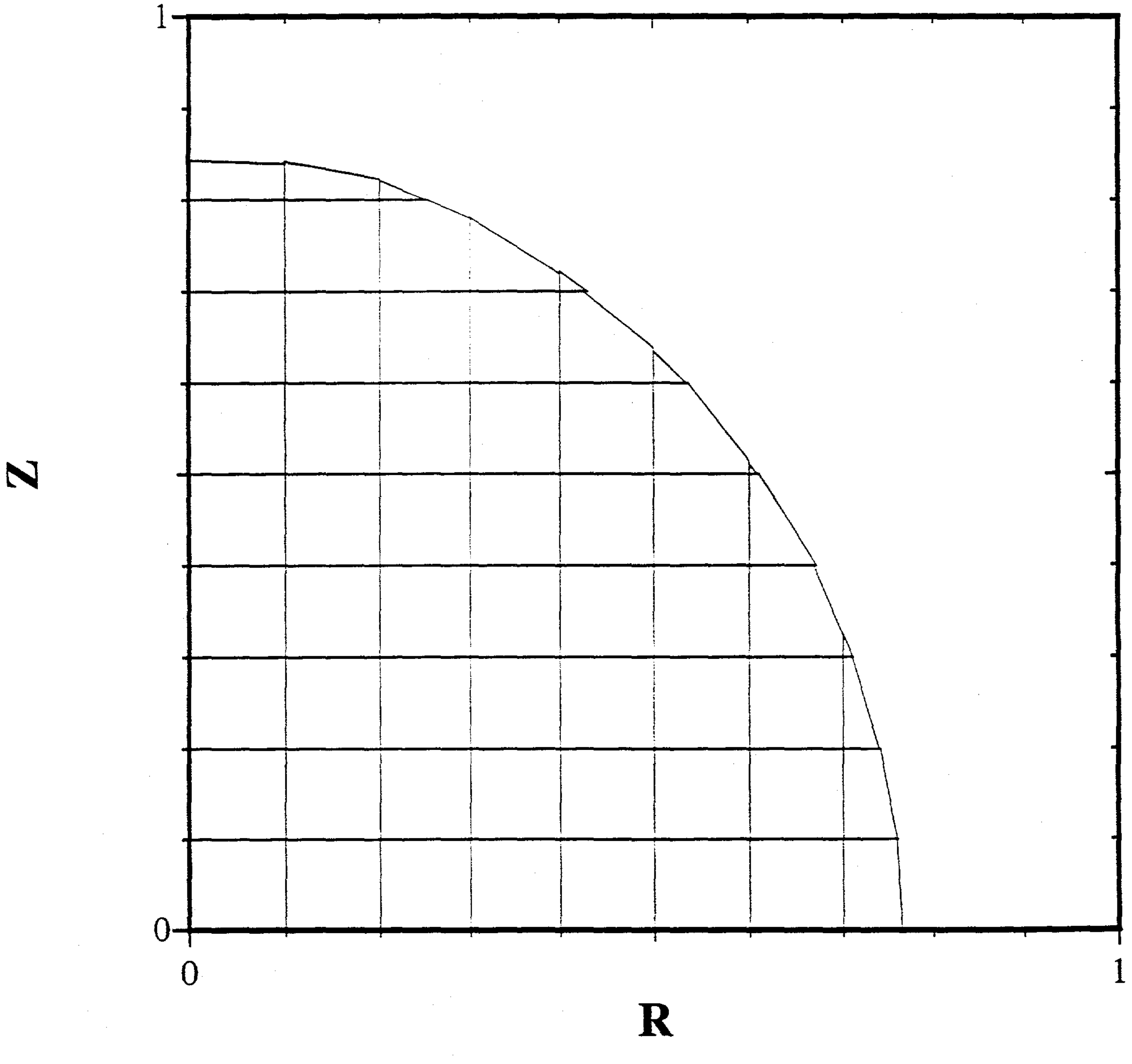

Figure 3b

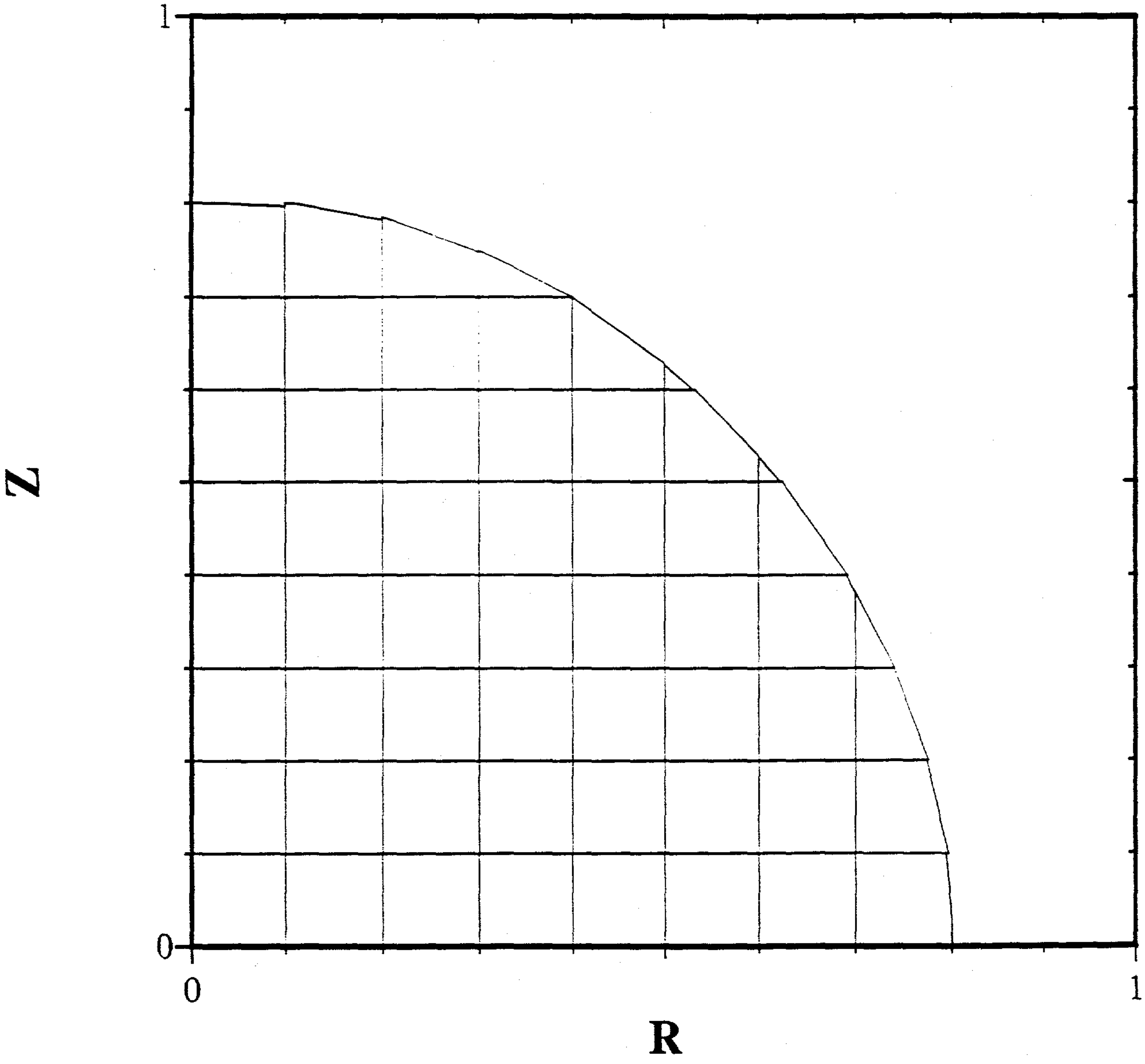

Figure 4. A diagram showing the "lifecycle" of a volume tracking method. Initially the method takes volumes of material on a computational grid and reconstructs an interface of assumed shape (typically linear). Using this reconstructed interface, the volumes are transported by the material velocity to new locations. At this point the process can begin again with the advanced time distribution of volumes.

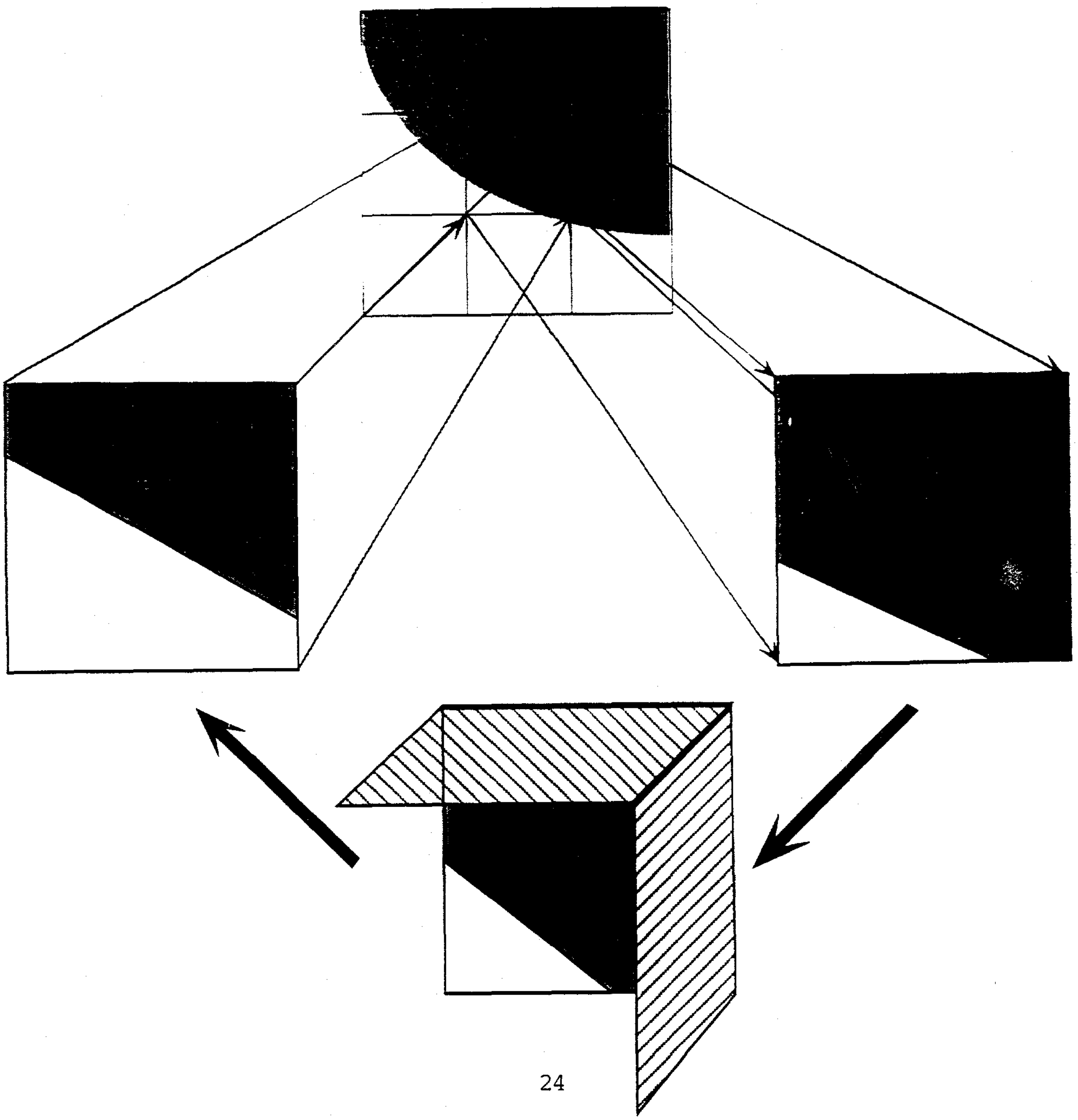

Figure 5. A diagram explaining the basic premise of the continuum surface force method. A force is to be applied to the surface of a region and must be computed. In order to do this, the force is converted from a surface force to a volume force, which is well-suited toward control volume-based physics integrators. This involves the selection of functions that transfer the surface force to a volumetric force in a manner that minimizes errors.

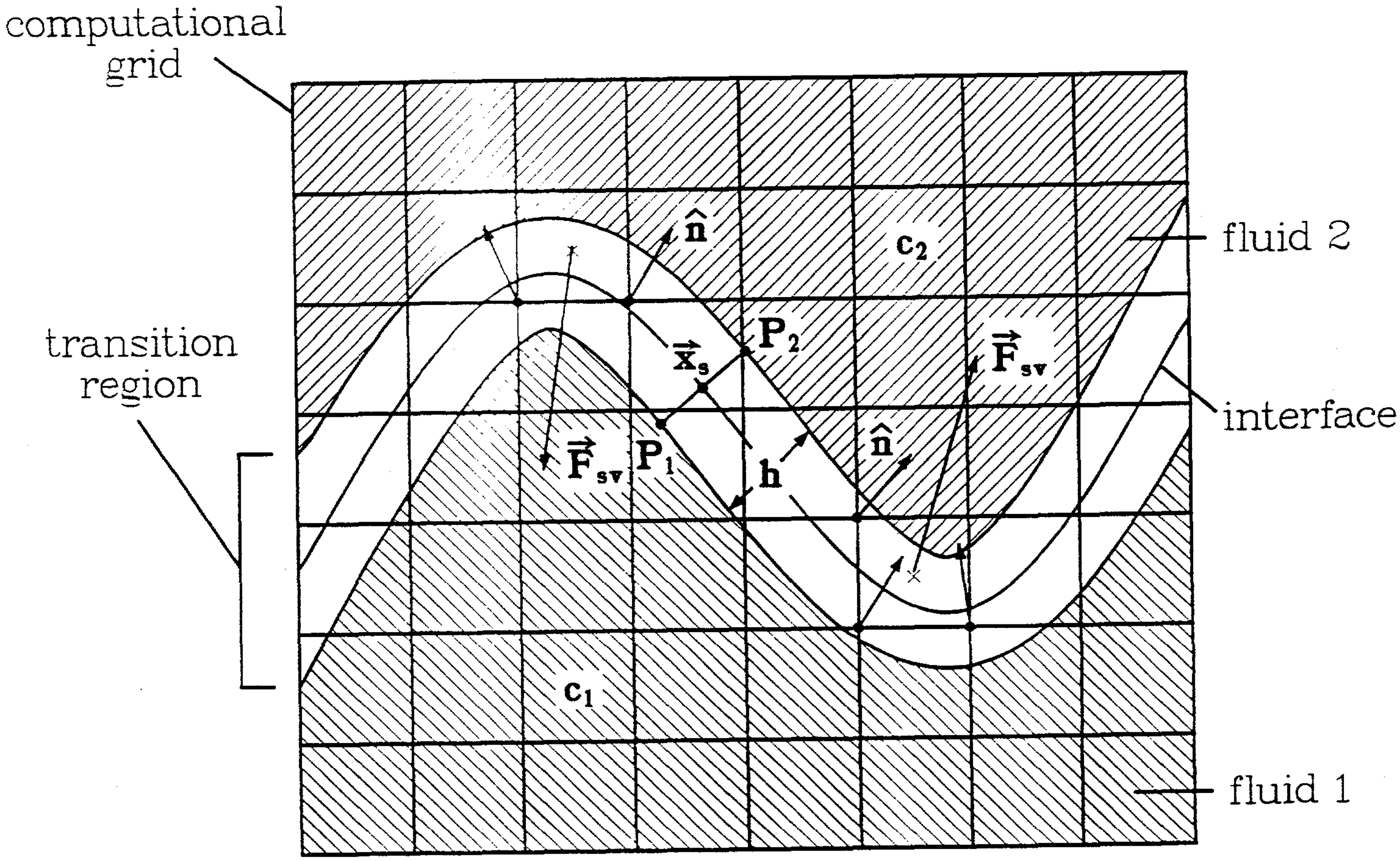

Figure 6a. The graphs show the amount of work required to invert a linear system based on the solution of a radiation diffusion (Marshak) wave with discontinuous coefficients spanning 10 orders of magnitude. (a) shows standard multigrid and (b) shows using multigrid to precondition a Krylov subspace solver. Simply using the same method to precondition rather than solve the linear system results in a factor of seven savings in computational cost.

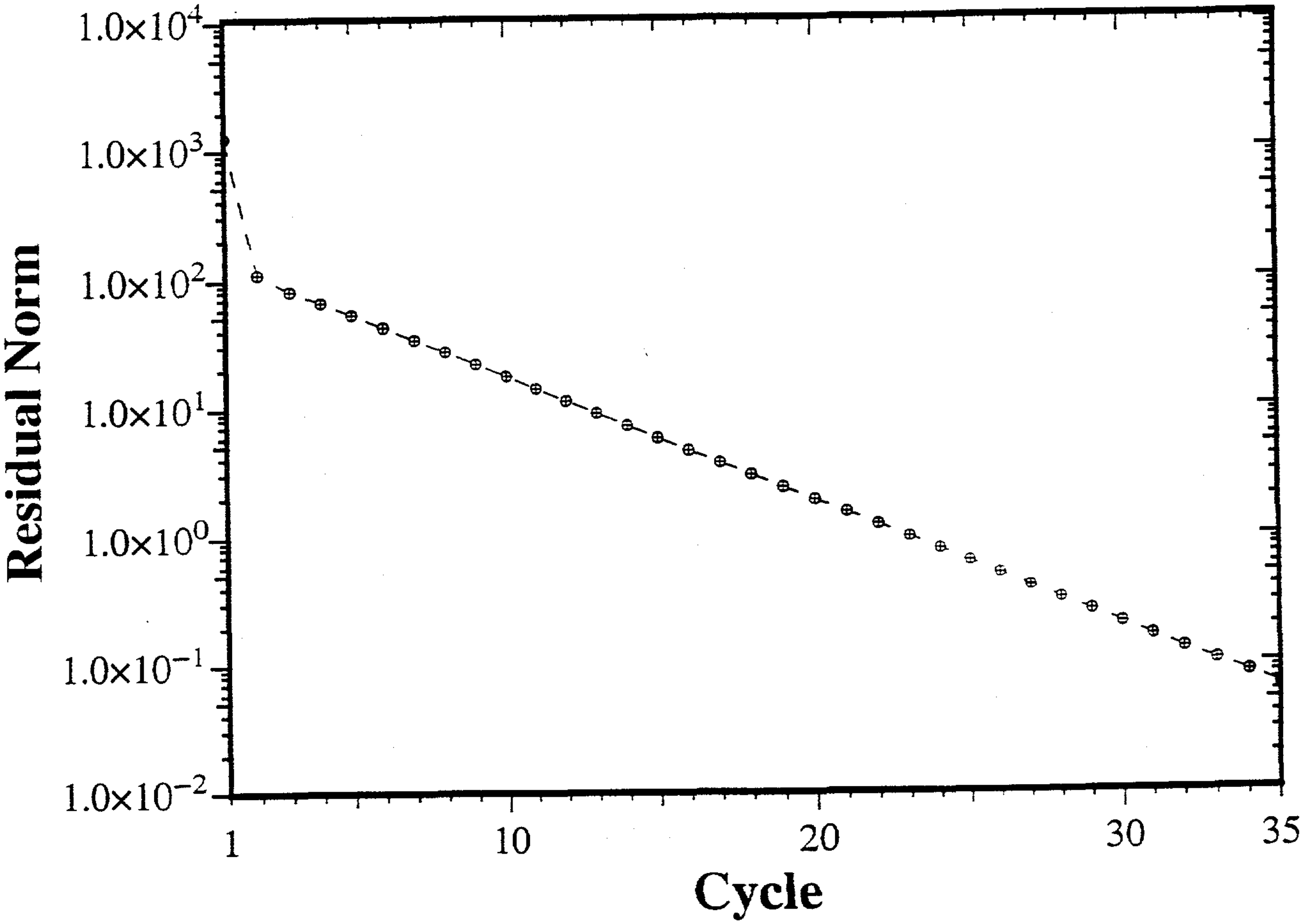

Figure 6b

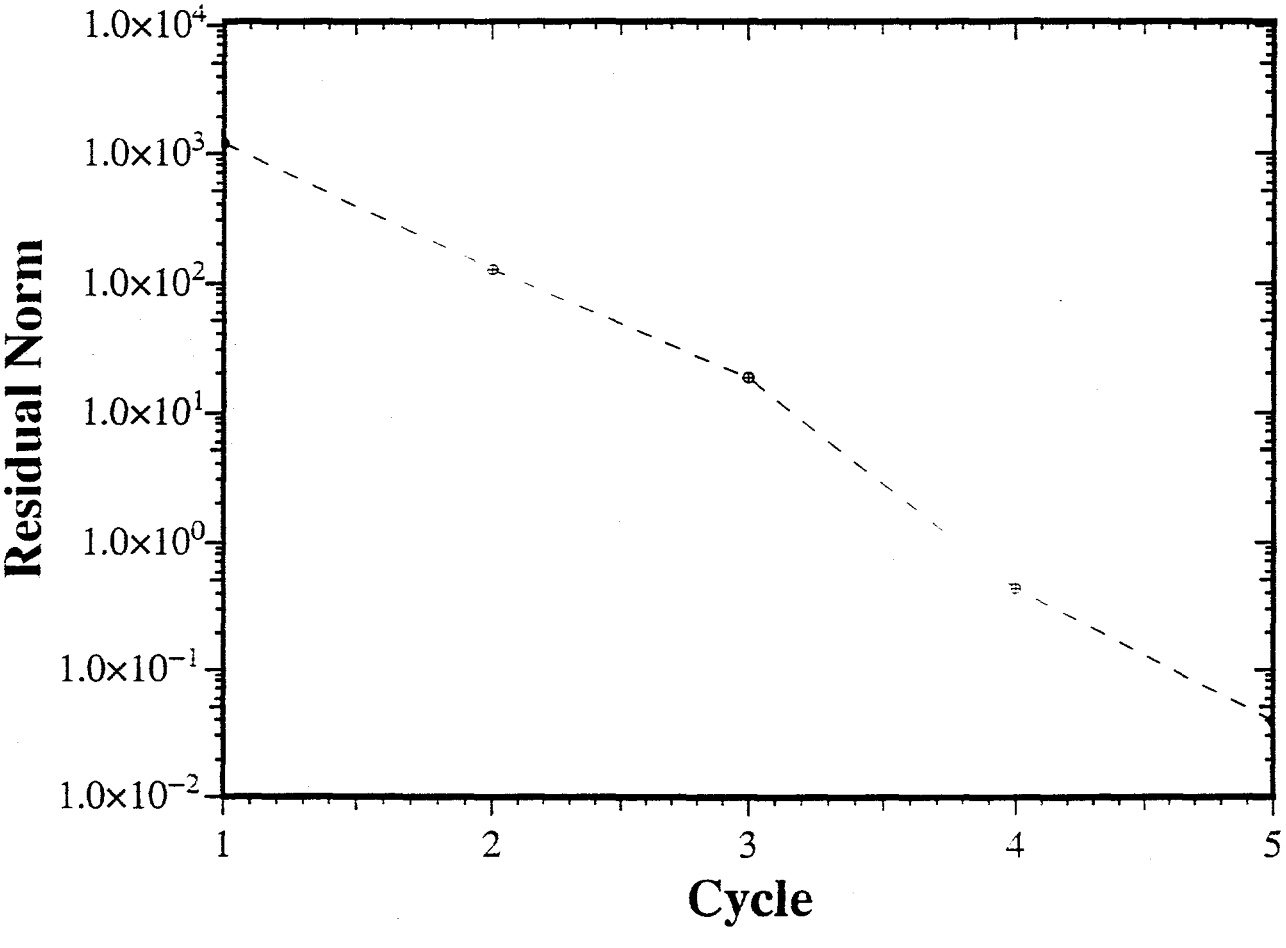
1.0×10⁴
1.0×10³
1.0×10²
1.0×10¹
1.0×10⁰
1.0×10⁻¹
1.0×10⁻²
Residual Norm
1
2
3
4
5
Cycle

Figure 7. A picture of the computational grid used for the chalice pouring and solidification simulation computed using Telluride.

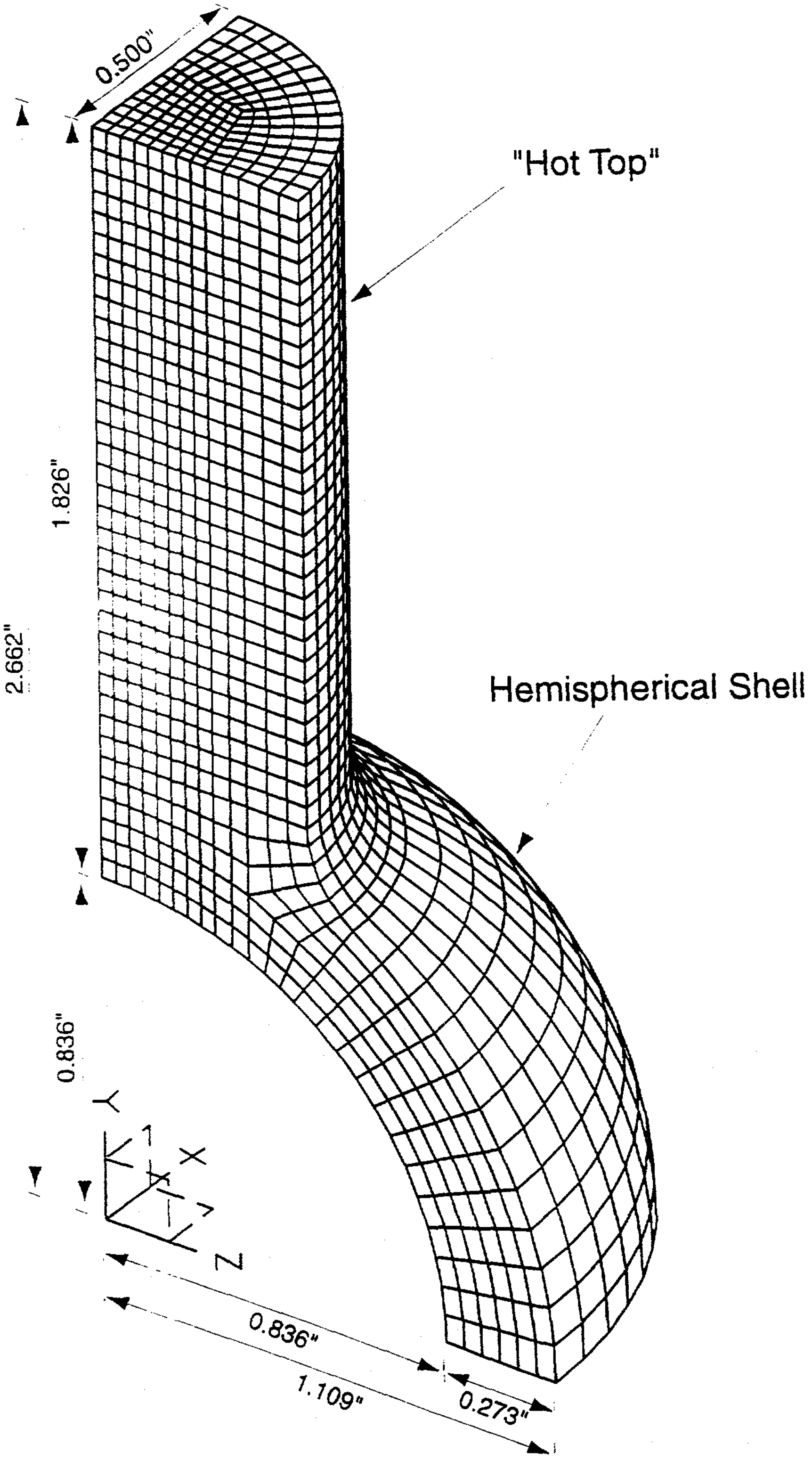

Fig. ~~1~~ 7. Computational mesh (6480 cells) used for TELLURIDE simulation of copper chalice mold filling. Note that the computational model is 1/4 of the full physical model.

Figure 8a. A pictorial representation of the Riemann problem. (a) shows the Feynmann diagram of the wave structure for a classical shock tube problem. A diaphragm breaks and a wave pattern emerges with a shock wave followed by a material discontinuity followed by a release wave. (b) shows this system parametrically in pressure-velocity space, which is employed to compute an adaptive approximate Riemann solution.

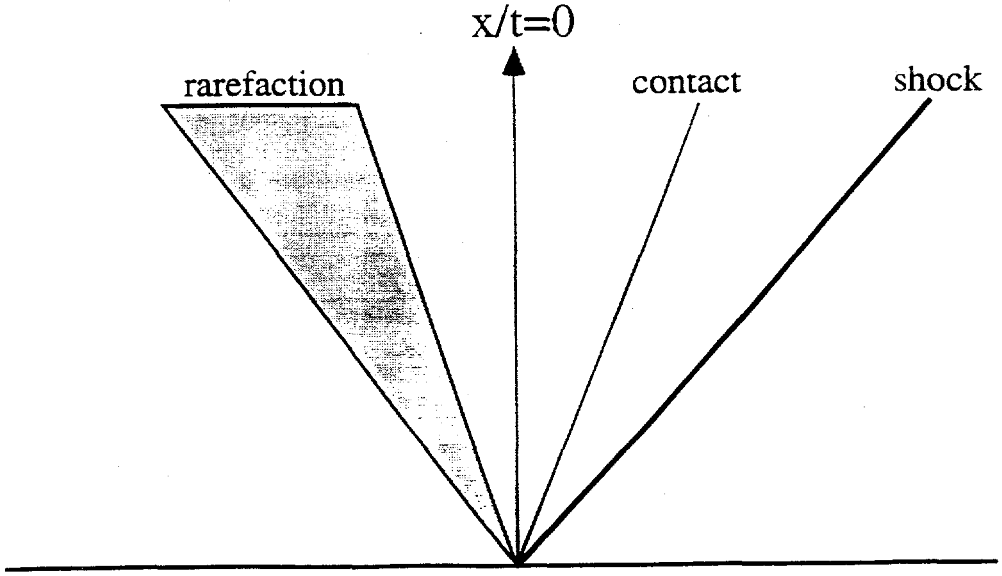

Figure 8b