Numerical analysis and the scientific method

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The computer has given rise to a new mode of scientific practice, and today computational science stands beside theory and experiment as a fundamental methodology. The impact of the computer revolution on science can be projected from current trends. The demands to be made on computing methodologies will be reviewed. One of the demands is an ongoing need for excellence in computational methodologies. Generic difficulties encountered in meeting these challenges will be discussed. Recent work of the authors and others will be reviewed in this context.

1. The computer revolution

The ages of history are demarcated as much by the rise and fall of ideas and technology as by the rise and fall of empires and nations. In this sense the computer age is a turning point for human events, as was the earlier industrial revolution based upon mechanical energy. With a narrower focus, we consider the impact of the computer revolution on science. Turning points in science are marked by the introduction of new ideas and new tools, and especially by developments which are both tools and ideas. With the invention of calculus, the electron microscope, and DNA sequencing, one finds an ability to formulate, understand, and solve a range of problems which had previously been inaccessible. Judged from this perspective, the computer revolution will have an impact on science at least as large as did these three examples.

Very large parts of science are described in terms of mathematical equations. In most cases the solutions to these equations cannot be obtained without recourse to numerical computation. In the thirty years since the advent of mainframe computers, an impressive range of problems have been solved with the aid of computers. Running a modern wind tunnel to test airfoil designs costs 150 million dollars per year. Supercomputers can explore a much larger range of ideas than can actually be tested, and expensive test facilities can be reserved for the most promising designs. In fact, a broad range of two-dimensional fluid-flow problems are under reasonable scientific control, due primarily to progress on numerical computation on these problems. The list of such successes could be extended to considerable length. Looking to the future, there can be little doubt that the mathematization of various subfields of biology is impending. As indications we can cite the recent computer-assisted determination of the three-dimensional structure of the polio and cold viruses [1, 2], computer simulation of the heart with natural and artificial valves [3], and algorithms for the analysis of DNA sequences [4].

Computers can also be used as an experimental tool to explore the unknown. Feigenbaum discovered universal order in the behavior of chaos [5, 6] through computer experiments, a development which has stimulated and rejuvenated several branches of mathematics and physics.

Computers can simulate experimentally difficult or unattainable parameter ranges, such as the conditions in the interior of the sun or a few microseconds after the big bang origin of the universe. They can also simulate undesirable

parameter ranges such as occur in safety studies to avoid accidents in chemical or nuclear reactors. There have been three types of limits proposed for the ultimate scope of the computational method. However, it is not clear how firm these limits will turn out to be, and in the authors' judgment, it is no more possible to set ultimate limits on the scope of the computational methodology in science than it is to set limits on the scope of future progress in theory or experiment. It has been proposed that fundamental physical limits such as the speed of light will limit the speed of future computers. However, the development of parallel computers, which do many operations concurrently, may permit an end run around this problem. A class of combinatorial problems, known as NP-complete problems, are effectively outside of practical computation. The extent to which the important problems which fall into this class can be restricted to subproblems which do not lie in this class or can be otherwise modified so as to be effectively computable is not known. Finally, it has been proposed that problems with producing complex computer code in debugged and reliable form may provide an outer limit for the use of computers to solve certain types of problems. Again, there are several strategies which may mitigate this problem. We mention in particular portable operating systems and software tools, high-level languages and standardized calling sequences, and modular libraries to allow interchangeability of reliable software components which can be used and thus tested through time in a variety of applications.

There is no shortage of current limits. For all of its astonishing successes, scientific computation provides much less than science and technology need. In most important scientific applications, the solutions are undercomputed relative to the scientific requirements. The gap between needs and performance is often substantial (and includes almost all three-dimensional problems). Narrowing this gap will depend on progress in both hardware and computational methodologies. To assess the current achievements and shortfalls of specific computational methods is like trying to decide whether a glass of water is half full or half empty. It can perhaps wryly be observed that those with responsibility for supporting and maintaining a code tend to believe that it is correct and adequate; those who use it tend to believe that the code is rather imperfect, but can nevertheless serve as a guide to the wise scientist or engineer; and those who develop new methods tend to be acutely aware of the flaws in existing codes.

2. The method of scientific computing

What are the methodologies which define scientific computing as a distinct approach to science, complementing the traditional approaches of theory and experiment? Scientific computing begins with mathematical modeling, whereby essential features of a scientific problem are expressed in terms of mathematical equations. Typically, important compromises and judgments are made at this stage. In order to carry out later computational steps, unimportant and sometimes important problem features must be suppressed. These judgments lead to a sequence of models which capture different aspects of the same problem. The different models may be integrated hierarchically in that a fine-scale model may be used to set the parameters of a coarser model, or they may be integrated only in the final judgments of the scientist or engineer using them.

After the mathematical equations have been formulated, they must be cast in a form suitable for numerical computation. This usually requires that they be discretized in one way or another. The key step is the formulation of a solution algorithm to solve the discretized equations. This step is so important that it often influences the preceding steps of model formulation and discretization.

The next stage is testing and validation of the solution algorithm. Validation may be accomplished by the following methods: comparison with known analytic solutions, comparison with previously validated computations, comparison with laboratory experiments, and internal consistency checks. Such internal checks include convergence under mesh refinement, analysis of solution errors, and analysis of diagnostic data. Truncation errors and convergence rates can be analyzed mathematically. Occasionally there may be a mathematical convergence theorem for the solution algorithm.

The final stage in scientific computing is to use a validated and debugged code for scientific or engineering purposes.

The preceding outline for scientific computing would strike most practitioners as glib, as it omits all discussion of difficulties. We focus on the difficulties inherent in the solution algorithm stage. Dealing with these difficulties defines the subject of numerical analysis.

Typical methodological difficulties, as they manifest themselves to a user, show the following symptoms: slow convergence, nonconvergence, numerical instabilities, and numerical simulation of spurious physical effects. Nonconvergence is normally the sign of an incorrect algorithm, but in listing it here, we have in mind more subtle possibilities, such as solution convergence in an L_p norm, while solution values at specific points (L_∞ convergence) may be invalid. The trap is easy to fall into, since the solution value at some singular point (such as a crack tip) may be both the most important and the least convergent part of the solution. The discretization process is a modification of the mathematical equations and consequently of the physics or problem formulation which the equations represent. In some cases the original physical process is unstable or only weakly stable to changes in the equations or equation parameters. In such cases, there is the danger that numerical discretization errors may grossly change the nature of the solution. Even for stable physics, these errors may change the solution quantitatively to an unacceptable degree.

The symptoms which a user may observe as a sign of poor performance typically have their origin in difficulties inherent in the original mathematical equations and their solutions. In general, finite-difference and finite-element methods give satisfactory performance when computing smooth solutions to regular problems in a space of not too high a dimension. We want to emphasize two somewhat unrelated types of problem difficulties. The first has to do with rapid solution variation, large space or time derivatives, and jump discontinuities or other solution singularities. Such features are ubiquitous. They arise in and give rise to boundary layers. Chemical reactions are a typical source of multiple time scales, also known as stiff systems. Problems with multiple material interfaces or shock waves have discontinuous solutions. To explain this point more fully, we note that the shock width in gas dynamics is of the order of a mean free path, which is about 10^{-5} cm and far smaller than the macroscopic dimensions of typical flow fields. The pressure gradient within the shock might then be of the order of 10^{7} or more using dimensional units appropriate to the problem. Likewise, a flame front width could be 10^{-2} cm, but such numbers are highly problem-dependent. For example, in an oil reservoir fire flood, the flame width could be 20 feet, and still small compared to macroscopic dimensions. Chemical reaction rates within a single problem can easily vary by a factor of 10^{10} because of their exponential dependence on activation energies. The importance of discontinuities and singularities has long been recognized by the community working on hyperbolic equations. However, they are just as important for elliptic problems such as steady-state elasticity or multi-fluid incompressible flow, due to crack tips, corners, and material or phase boundaries, a fact which appears to have been given less emphasis than it deserves.

The second major class of problem difficulties we discuss has to do with the occurrence of a large or infinite number of essential degrees of freedom. Problems having these features arise in the study of turbulence, statistical mechanics and equations of state, quantum field theory, and stochastic partial differential equations. This class of difficulties is the more intractable of the two, and the examples of scientific studies [7–12] which can be cited fall far short of the systematic needs for computational solutions in these areas due to slow convergence. Looking ahead to our proposed methodology for the first class of problems, we observe that the problems with an infinite number of degrees of freedom are also very difficult from a theoretical point of view, and that theoretical ideas have not yet provided the means to devise numerical methods with the required enhanced capabilities or convergence properties.

3. The Grand Unified Scheme (GUS)

As a general principle, we propose the maximal use of analytic knowledge of solution properties. This principle has been successfully used in the case of smooth solutions, where the known solution regularity is used to devise higher-order methods which give accelerated convergence. For the case of solution singularities, which give rise to the first class of difficulties mentioned in the previous section, we propose maximal use of analytic knowledge of those solution singularities. Perhaps paradoxically, the solution singularities can be a source of problem simplification, in that the idealized or asymptotic behavior in the neighborhood of the singularity may possess a simpler structure or higher symmetry than does the full solution. Thus the singularity may be an opportunity for theoretical progress; there may also be a considerable body of knowledge concerning the singularities. Our proposal is to use this body of knowledge within the numerical algorithm itself, and where necessary to create the required knowledge. An instance of this circle of ideas is the vortex method, which uses vortices to represent idealized fluid elements in (for example) shear layers and turbulent flow fields [9, 10, 13–17]. Related ideas are the interface methods based on boundary integral methods [18, 19], and conformal mapping [20].

The Grand Unified Scheme is a version of the general principles discussed above, suitable for compressible reactive fluid flow. These ideas are an outgrowth of work carried out over several years with many colleagues, and were presented in preliminary form in [21]. The scheme could also be called the Kitchen Sink Scheme (KSS) because the main idea is to use everything. There are four main components to this scheme, and we discuss each briefly in this section. The four components are: interior schemes, front tracking, automatic mesh refinement, and automatic asymptotic reactive chemistry (or automatic mode selection).

High-quality interior schemes have been built around two ideas: flux limiters to control overshoots and numerical oscillations and approximate Riemann solvers to achieve upwind differencing [22–25].

The main idea of front tracking is to introduce, as an independent computational degree of freedom, the surfaces of jump discontinuity which may occur within a solution. This method will be explained in more detail in the following section.

Automatic mesh refinement is the idea of using fine grids in regions where the solution is singular or rapidly varying, coupled with coarse grids in regions where the solution has a regular behavior. This method has given rise to a large ongoing enterprise, from which we cite representative works [26–29].

Automated asymptotics or automated mode selection for reactive chemistry is the proposal to determine the ambient conditions from the neighbors of a given mesh block and on the basis of these conditions to determine rate-limiting reactions and simplified chemistry, so that the rapid reactions are replaced by frozen or quasi-steady-state conditions. A hierarchy of time scales would be identified,

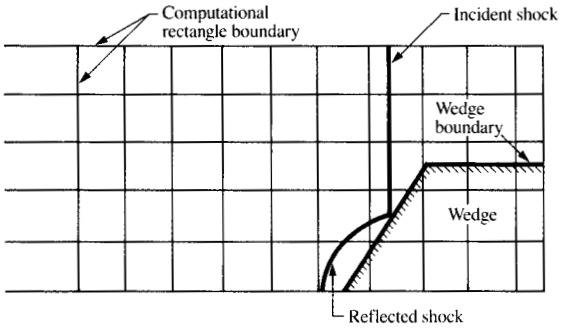

Figure 1

The grids used by front tracking for a shock on ramp problem. A regular two-dimensional grid is superimposed on a one-dimensional front (grid). The latter consists of the incident and reflected shock, the ramp boundary, and the boundary of the computational rectangle.

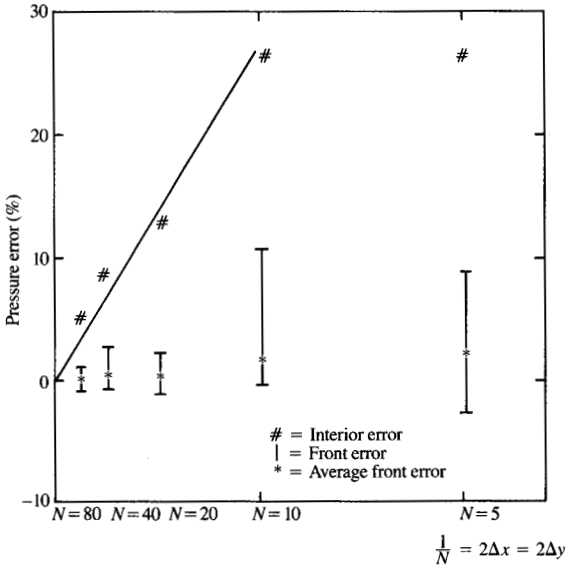

Figure 2(a)

Convergence under mesh refinement in the two-dimensional computation. Convergence of the front and interior schemes. The pressure errors in the interior and at the front are shown for $N \times N$ grids at the time indicated by Figure 2(a). The # signs represent the interior error, where

$$\text{Interior error} = 100\% \times \frac{\int_0^s \int_0^s |P_{2d} - P_{1d}| dxdy}{\int_0^s \int_0^s P_{\text{initial data}} dxdy} .$$

The front error (error bars) gives the range of the errors at the front, defined as

$$\text{Front error} = 100\% \times \frac{P_{2d} - P_{1d}}{[P]} ,$$

where $[P]$ is the pressure jump at the front in the one-dimensional computation at the same time. The asterisks represent the error of the average pressure behind the front, namely

$$\text{Front error (average pressure)} = 100\% \times \frac{P_{2d\ \text{average}} - P_{1d}}{[P]} .$$

and in this hierarchy, the rapid times would be treated as quasi-steady-state, the intermediate times would be treated implicitly, while the slowest times would be treated explicitly and the transients for these time scales would be fully and accurately resolved.

There have been several attempts to date to implement this unified proposal. In [30], the modern interior schemes were successfully combined with a limited version of front tracking. In [31], automatic mesh refinement was successfully added to the above. However, efforts to combine mesh refinement with modern interior schemes in the absence of tracking led to spurious waves generated by strong shocks at the boundaries of the fine meshes. For a problem which does not contain strong shocks, the successful combination of mesh refinement with a high-quality interior scheme has been obtained [32]. The automated analysis of critical modes and solution asymptotics as proposed above is an ambitious undertaking and has not been attempted to date.

Hybrid schemes have obvious software complexity problems which will be mentioned below. More serious are the scientific difficulties. Here we would like to stress the problems of a fundamental mathematical nature. Riemann problems define the scale-invariant large time solution asymptotics to leading order and pose a number of problems both for their behavior in the large and their behavior in higher dimensions [33, 34]. Such considerations have inspired a study of Riemann problems in a variety of physical contexts and have led to the discovery of new and striking mathematical phenomena [35–39], including shocks which violate most proposed physical admissibility conditions. A related problem is the hyperbolic problem with an embedded elliptic region, a notoriously difficult problem which arises in a variety of contexts including transonic flow, elasticity, oil reservoirs, multi-phase flow, and the relativistic hydrodynamics of a quark-gluon plasma [40–45].

4. Front tracking

Front tracking can be most adequately described by a picture. In **Figure 1** we show the grids used for a front tracking solution. Note that there is a regular two-dimensional grid covering a channel, including the wedge, which is an obstacle in the channel. The front includes a shock wave incident on the wedge, the channel walls, and the wedge, as well as the inlet and outlet surfaces. It is represented by a lower-dimensional (one-dimensional) grid, which moves in time, using velocities derived from the jump conditions (the Riemann problem) of gas dynamics.

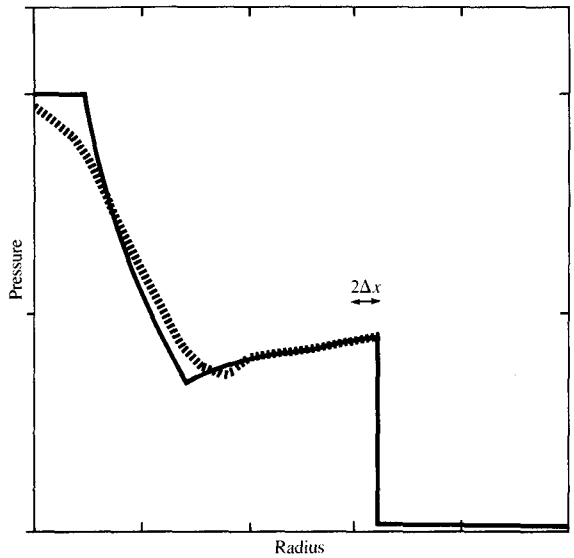

Figure 2(b)

Comparison of one- and two-dimensional computations for a cylindrically symmetrical detonation front computation. A plot of pressure vs. radius is shown. The solid curve shows the results obtained by the one-dimensional random choice computation. The vertical lines represent the range of pressure values in the two-dimensional front tracking solution at a fixed radius as the angle varies. Thus the vertical lines show the range of angular dependence on the solution. The grid is 40 by 40.

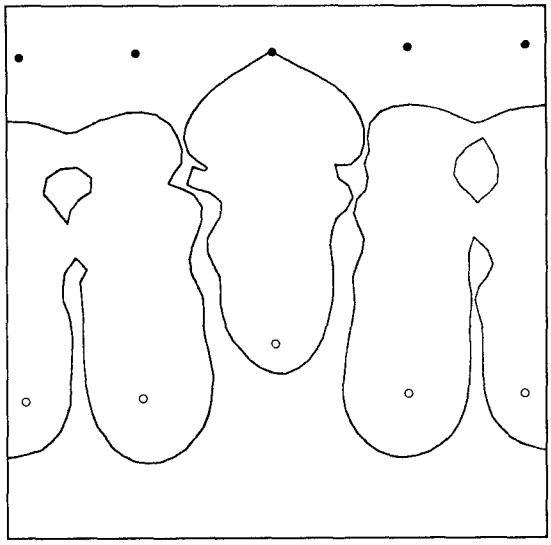

Figure 3

Automated bifurcation of tracked fronts illustrated in a jet pinch-off instability in an oil reservoir study. Here water has been injected into five wells located at the bottom of the figure, and oil is produced at five wells located at the top of the figure. The reservoir parameters represent stable displacement, and so the water-oil interface does not finger. However, for these parameters, the oil is more mobile, and consequently forms a jet between the injection wells.

The plan to use front tracking was initiated by O. McBryan and one of the authors seven years ago; a clear and early statement of the method and the scientific program is contained in [46]. This program was developed and implemented in a series of more than 40 papers by the authors, Oliver McBryan, and other co-workers; see, for example, [46–53]. In these papers, proof of principle and scientific validation has been established. Validation has been accomplished by comparison to analytic solutions, laboratory experiments, elementary one-dimensional calculations, and previously validated computer codes, as well as convergence under mesh refinement. These tests have been conducted in the context of a variety of different applications. In **Figure 2** we show convergence under mesh refinement and comparison of a two-dimensional computation to a simpler one-dimensional (radially symmetric) computation for a cylindrically symmetrical detonation front, in work by B. Bukiet [47].

At the outset the concept of front tracking was considered to be hopelessly wrong, and the plan to initiate this approach in a serious way prompted considerable controversy. The concerns were of three types: This method might not work scientifically, it was too complicated to implement, and it might never be able to handle problems of even moderate engineering complexity. Actually there was a record of previous attempts with this method, which provided encouragement that the method was fundamentally sound [54–56]. The scientific validation was discussed above. Various numerical issues such as the coupling scheme between the interior and the front have been examined but deserve further study. Local behavior in the neighborhood of co-dimension two-intersection points of tracked discontinuities also needs further study.

The software complexity issues were handled through a strategy which is different from that normally employed in computational fluid dynamics and which might be worthy of consideration by others. These issues have been [57, 58] and will be discussed elsewhere.

On the basis of this success with scientific validation and control of software complexity, it can be stated that a proof of scientific principle for front tracking has been achieved. Next we discuss the transition of the front tracking method from benchmark validation studies to problems of moderate engineering complexity. A central research issue involved in this transition is the ability to allow bifurcations or changes in front topology due to the interaction or crossing of tracked waves. This program is partially complete, and we report on progress achieved by co-workers.

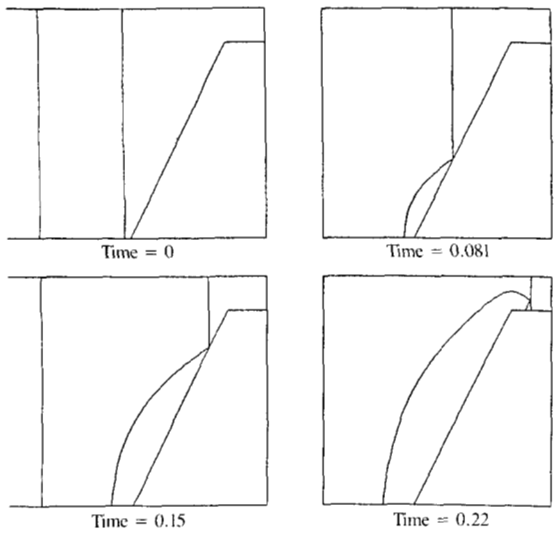

Figure 4

Bifurcations of front topology in a shock on ramp problem. An incident shock hits a ramp and undergoes bifurcation to a regular reflection. When the regular reflection node reaches the top of the ramp, a bifurcation to a Mach-type node occurs. This Mach triple point is degenerate in that the reflected wave has zero strength at the triple point. The grid here is 30 by 30.

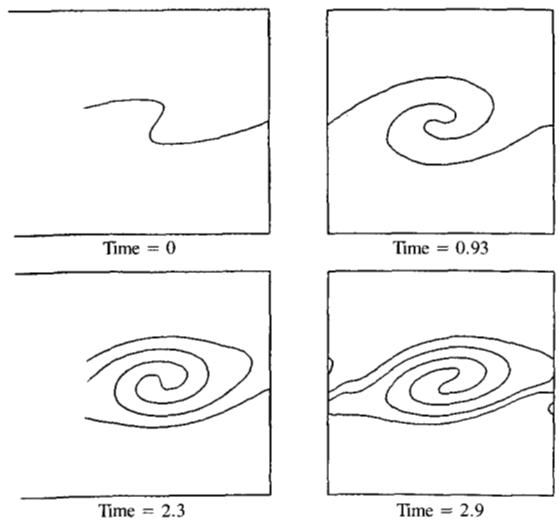

Figure 5

Compressible Kelvin-Helmholtz roll-up, including passage of the front through a periodic boundary. The grid is 40 × 40 and the relative Mach number between the upper and lower fluids is one.

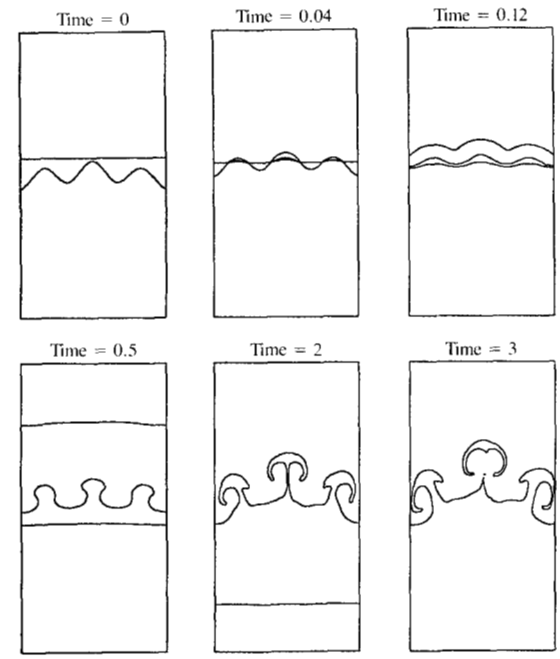

Figure 6

A series of frames showing a shock contact collision interaction. Both gases are polytropic with $\gamma = 1.4$. The pressure ratio across the incident shock is 100, and the density ratio (above to below) across the original contact is 2.86. The grid is 40 × 80. This figure was taken from unpublished work of J. Grove.

In **Figure 3** we show a computation of a line drive well configuration taken from an oil reservoir study in which the jet pinch-off instability leads to successive front bifurcation [53].

In **Figure 4** we show successive stages in the front topology as a shock wave hits a ramp, forms a regular reflection, and finally a Mach stem [48].

In **Figure 5** we show Kelvin-Helmholtz roll-up for compressible gas dynamics, with the tracked slip line exiting and reappearing through periodic boundaries [48].

In **Figure 6** we show successive stages in front topology as a shock wave hits a contact in initiation of Meshkov instability, taken from unpublished work of J. Grove [59]. There are two remarkable points in this computation. One is the change in front topology which occurs within the computation, a transition which has always been regarded as a significant obstacle to the use of this method. The other concerns contiguous waves, as discussed in the next paragraph.

There have been several definitive achievements of the front tracking effort. First we mention a calculation of Grove [59] in which a contact separates highly compressible

($\gamma = 1.1$) SF_6 from air (see **Figure 7**). When hit from a shock on the air side, the transmitted shock in the SF_6 and the contact itself lie almost on top of each other, making this problem virtually impossible to compute correctly by standard methods. Grove's solution, calculated easily on a 20×20 grid, shows the efficacy of front tracking.

J. Jones [60] determined the leading-order endothermic effect of radial cooling on reactive chemistry in curved detonation fronts. This piece of asymptotic analysis solved a major open problem in reactive hydrodynamics; it was prompted by the requirement of front tracking for analytic knowledge of solution behavior.

King, Lindquist, and Reyna [61] solved a 20-year-old problem posed by Ratchford [62], a leading petroleum engineer. They showed that finite-difference methods can duplicate the phenomena of viscous fingering with immiscible displacement and capillary diffusion, as is observed in laboratory experiments. This achievement resulted from the need for a benchmark calculation for comparison to front tracking studies [51].

5. Conclusions

Science requires computational methods with enhanced capabilities which go beyond currently available techniques. A promising strategy for meeting these needs is to use methods which are adapted to known solution behavior. An outline for pursuing this strategy in the context of compressible reactive flow has been presented. Work directed at implementing this strategy has been discussed, with an emphasis on the front tracking program.

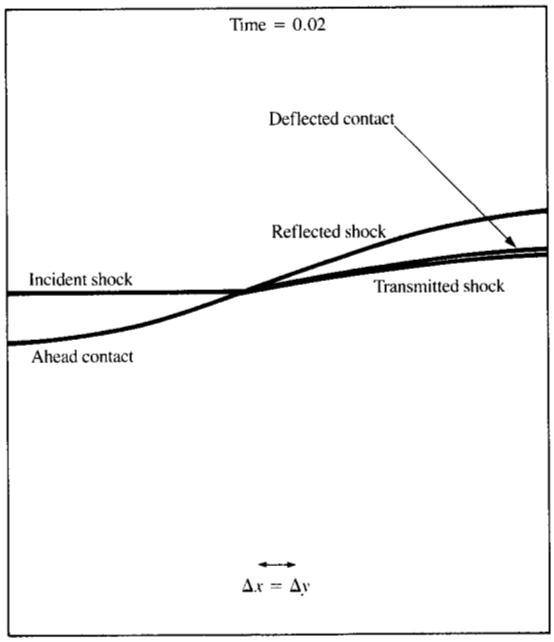

Figure 7

A blowup of a subregion of a shock contact collision, showing the incident shock colliding with the ahead contact discontinuity, producing reflected and transmitted shocks. This figure was taken from unpublished work of J. Grove.

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