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Efficient numerical procedures were found for the solution of shock wave interactions in gas dynamics. The wave interactions were idealized as point interactions and were thus equivalent to the solution of Riemann problems. The equation of state was taken in a very general form, as tabular data. The essential problem solved was the use of tabular equation of state data for description real materials and the efficient solution of Riemann problems in this context. (KR)

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Enhanced Resolution Concepts in Large Scale Scientific Computing

Final Report

James Glimm

October 31, 1989

U.S. Army Research Office

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ENHANCED RESOLUTION CONCEPTS IN LARGE SCALE SCIENTIFIC COMPUTING

1. Body of Report

1.1. The Problem Studied

The accurate computation of nonlinear waves and discontinuities in fluid motion was the overall problem under consideration. Within this framework, the effect of real equation of state (EOS) properties on nonlinear wave structure was the primary object of study. The main emphasis was the efficiency and computational stability associated with the use of tabular equations of state for the solution of Riemann Problems. Additional consideration was given to two dimensional wave interactions and to the physical basis for the internal structure of nonlinear waves.

1.2. Summary of Most Important Results

The most important conclusion of this study is a proof of feasibility for the use of accurate, tabular equations of state in the exact solution of wave interaction (Riemann) problems. Feasibility had been in question for two essential reasons, both of which were resolved in the course of the present study. Numerical efficiency was the first of the essential issues, and stability or accuracy of computation was the other issue. The resolution of both of these questions will be elaborated upon below.

Riemann problems are by definition the solution of a nonlinear conservation law

$$U_t + F(U)_x = 0$$

with special, scale invariant, initial conditions

$$U(x,t=0) = U_L\,, \quad x < 0$$

$$U(x, t{=}0) = U_R\,, \quad x > 0\,,$$

representing a single jump discontinuity at the origin $x = 0$, connecting two arbitrary states U_L and U_R. They represent the resolution of the interaction of nonlinear waves, which have conceptually come together at $x = 0$ and $t = 0-$. The Riemann problem is important for both the conceptual understanding and the quantitative analysis of nonlinear wave interactions. It is also important for use in modem computational methods, the Random Choice Method [7], Higher Order Godunov methods [6, 11-13], and Front Tracking [4, 8].

Real fluid effects enter this solution through the equation of state, which can be specified in tabular format, or as an analytic or piecewise analytic function, with tabulated and fluid dependent parameters. Of these approaches, the tabular form is perhaps the more general, and is applicable to a larger range of fluid parameter space. Any equation of state presented as an analytic or piecewise analytic function can be easily re-expressed as in tabular format, but the transformation in the other direction is not straightforward. The analytic formulation is either too simple to describe real fluids over an extended parameter range, or it becomes very cumbersome, and not much much simpler than a tabular expression. Over an extended parameter range, the equations of state are produced from a variety of sources, using different theoretical models in different regions, or different experimental data sets. These different regions are then joined by some interpolation preceedure, so that the apparent unity of an analytic expression is illusary, and the tabular approach is actually in better contact with reality. The work reported here used the tabular format, SESAME supported by the Los Alamos National Laboratory [1].

A theoretical analysis [14] systematically developed the relation between equation of state properties and fluid wave structure. As opposed to simple analytic expressions for the EOS, real fluid behavior allows for a number of qualitatively different features, as well as quantitatively important corrections to the wave shapes and speeds. For example the normal sign of convexity of thermodynamic relations is often reversed near a phase transition, leading to split shock waves and to rarefaction or expansive shocks which are physically stable.

The main problem encountered in applying these theoretical ideas to a tabular EOS was numerical efficiency. Each Riemann solution required many evaluations of the EOS table to construct rarefaction wave curves and shock waves used in the solution of the Riemann problem.

The solution of this problem, developed within the research reported here, was to precompute many of the intermediate quantities used in the Riemann solution such as the sound speed, Riemann invariants, and rarefaction wave curves. Moreover, inverted tables were constructed in which these quantities were presented as functions of independent variables actually used in the Godunov iteration solution [5] of the Riemann problem. In carrying out this precomputation, a complication was the presence of phase boundaries, which necessitated special data structures so that inversions and interpolations did not mix distinct fluid phases in an unphysical fashion. The body of this table inversion work is contained in two PhD theses (still in progress as this report is written) [C,D], [15, 16]. A subsidiary aspect of this solution has independent interest: a method for cubic spline approximation in two dimensions, for approximation to a piecewise smooth function with first derivatives that are discontinuous along certain curves in the plane.

A problem anticipated when the work was begun concerned numerical stability of the Riemann solution algorithm. The basis for this concern was a knowledge of problems in the equation of state tables. The problems arise from several causes -- van der Waals loops which give rise to negative sound speeds -- and interpolation problems between distinct regions in the construction of the EOS where unphysical discontinuities in physically measurable quantities may occur. The intended use of the tables for automatic solution of Riemann problems had not been attempted on a large scale and in a systematic fashion before, and so there was some caution expressed as to what would emerge. As it turned out this caution was unfounded. The tables were examined carefully from the point of view of physical consistency. The negative sound speeds did occur, but did not effect the research reported here as those regions of parameter space (or the tables containing them, due to an absence of the Maxwell construction) were avoided. The smoothness of the data in the table did seem to be adequate for use in the Godonuv iteration, which is the basic algorithm for the solution of the Riemann problem. Plotting of data from the tables revealed some waviness in some of the shock Hugoniots which appeared to originate in the data.

Ultimately the major weakness of the tables, as far as the research conducted here was able to determine, was a courseness of the presentation of the data, leading to excessive interpolation between data points. This is, however, easily curable. The data are derived from an algorithm which in principle will construct data at an arbitrary point in the pressure, specific volume parameter space, so that finely spaced data are available in principle if required. Similarly, a Maxwell construction is available to remove van der Waals loops as desired.

A second discovery of this project was the identification of a systematic error in a mathematical methodology for the description of phase transitions. Correct theories, accepted by physicists, and consistent with experiment, were identified, and a survey of promising appproaches was prepared [A,B], [9, 10]. In brief, the internal structure of a phase transition, when modeled at a microscopic level, requires use of an additional variable (the order, or phase field parameter). At a macroscopic level, the intermediate zone between two phases (the "mushy zone") is a microscopic mixture of the two phases, each of which is in local thermodynamic equilibrium.

Questions of principle have been raised relative to existence and uniqueness of solutions of Riemann problems. These questions have important physical and computational implications. For this reason, the physical basis for a nonconvex scalar conservation law was examined, and standard uniqueness criteria of Oleinik were related to fundamental principles of physics (the law of maximum entropy production). This work was due to Aavartsmark [2, 3] and a more detailed version was prepared within the work supported by this grant [E].

1.3. Publications and Technical Reports

A. James Glimm. The Continuous Structure of Discontinuities. Proceedings of Nice Conference. Jan 1988. To Appear.

B. James Glimm. Non Linear Waves: Overview and Problems. Proceedings of IMA Symposium on Non Linear Waves. To Appear.

C. Lisa Osterman Piecewise Smooth Interpolation and the Efficient Solution of Riemann Problems with Phase Transitions. NYU Thesis, In preparation.

D. John Scheuermann. Efficient Solution of the Riemann Problem using a Tabular Equation of State. NYU Thesis, In preparation.

E. Brian Wetton. Unpublished Report.

1.4. Participating Scientific Personnel

1. Lisa Osterman
2. Brian Wetton
3. Hans Klapper
4. John Scheuermann

2. Bibliography

References

1. "An Invitation to Participate in the LASL Equation of State Library," Los Alamos Scientific Report LASL-79-62, Los Alamos National Laboratory.

2. I. Aavartsmark, "Kapillarenergie as Entropiefunktion," Preprint.

3. I. Aavartsmark, "Capillary Energy and Entropy Condition for the Buckley-Leverett Equation," *Contemporary Mathematics*, To Appear.

4. I.-L. Chern, J. Glimm, O. McBryan, B. Plohr, and S. Yaniv, "Front Tracking for Gas Dynamics," *J. Comp Phys.*, vol. 62, pp. 83-110, 1986.

5. A. J. Chorin and J. E. Marsden, *A Mathematical Introduction to Fluid Mechanics*, Springer-Verlag, New York, 1979.

6. P. Colella and P. Woodward , "The piecewise parabolic method (PPM) for gas-dynamics," *J. Comp. Phys.* , vol. 54, p. 174, 1984.

7. J. Glimm, "Solutions in the Large for Nonlinear Hyperbolic Systems of Equations," *Comm. Pure and Appl. Math.*, vol. 18, pp. 697-715, 1965.

8. J. Glimm, C. Klingenberg, O. McBryan, B. Plohr, D. Sharp, and S. Yaniv, "Front Tracking and Two Dimensional Riemann Problems," *Advances in Appl. Math.*, vol. 6, pp. 259-290, 1985.

9. J. Glimm, "The Continuous Structure of Discontinuities," in *Proceedings of Nice Conference*, Jan 1988.

10. J. Glimm, *Nonlinear Waves: Overview and Problems*, To Appear.

11. B. van Leer, "Toward the ultimate difference scheme, II," *J. Comp. Phys.*, vol. 14, pp. 361-370, 1974.

12. B. van Leer, "Toward the ultimate difference scheme, III, IV," *J. Comp. Phys.*, vol. 23, pp. 263-275, 276-299, 1977.

13. B. van Leer, "Toward the ultimate difference scheme, V," *J. Comp. Phys.*, vol. 32, pp. 101-136, 1979.

14. R. Menikoff and B. Plohr, "Riemann Problem for Fluid Flow of Real Materials," *Rev. Mod. Phys.*, vol. 61, pp. 75-130, 1989.

15. Lisa Osterman, "Piecewise Smooth Interpolation and the Efficient Solution of Riemann Problems with Phase Trabsitions," NYU Ph. D. Thesis, In Preparation.

16. J. Scheuermann, "Efficient Solution of the Riemann Problem Using a Tabular Equation of State," NYU Ph. D. Thesis, In Preparation.