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DIFFRACTION PATTERNS AND VORTEX ROLLUP

J. Glimm

Courant Institute of Mathematical Sciences

New York University

251 Mercer Street

New York 10012

New York

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1. Introduction

There have been ^{three} main developments to come from the research supported in this project. These concern:

- Riemann problems and nonlinear wave interactions for real materials, including material strength properties.
- Riemann problems and chaotic mixing for conservation laws in general.
- Development of three dimensional and parallel processing front tracking algorithms.

Most of the work performed under this project has focused on the first of these developments.



2. Wave Interactions for Real Materials

Real material properties define nonlinear terms in the equations of continuous media. They determine the nonlinear waves, wave interactions and wave diffraction patterns which the media support. The study of Riemann problems for nonlinear elasticity produced several interesting results, and clarified the mathematical issues associated with material strength computations. A series expansion in powers of the deviatoric (i.e. shear as opposed to compressive) strain identified standard models of constitutive relations as the leading order nonlinear term [2]. The analysis retained full rotation covariance and allowed an arbitrary form for the isotropic (pressure) contributions to the equation of state. In particular, the isotropic strains were not assumed to be small. Thus this treatment of small deviatoric strain seems to be more fundamental than other analyses available in the literature. It explained why only one shear parameter (the shear modulus) is used to characterize material strength, rather than the two parameters predicted to be necessary on group invariance grounds. In fact a second parameter will arise if higher order terms in the deviatoric strain are retained.

Wave curves and the Riemann solution were examined, assuming the above constitutive law. A special rotational symmetry observed by Ting and Tang [12] for the half space (Goursat) Riemann problem was found not to occur for the full Riemann problem [3], but enough was left from this symmetry to allow a simplification of the solution for the Riemann problem.

The theoretical analysis of the Riemann solution led to a numerical algorithm for its solution. The idea was to break the waves and solution variables into blocks corresponding to pressure and shear, respectively. Within each block a solution procedure of Godunov type was used. Because of the reduction to subblocks, the nonlinear root solving, which is the crucial step in the Godunov iterative algorithm, takes place in a lower dimensional space (one dimension for pressure waves and one or two dimensions for shear waves -- depending on whether the deformation is uniaxial and the material is

isotropic). This reduction in dimension is essential for construction of a robust algorithm. In fact the algorithm was fully successful in the isotropic uniaxial case only, in which case the two Godunov iterations occur in one dimensional spaces [3]. One dimensional root solving can be based on monotonicity and betweenness properties, and can be guaranteed to be robust in the large. The full determination of a robust algorithm for the general case is still an open problem.

The umbilic point predicted by Ting and Tang [12] was found to lie well outside the yield surface, and thus in the plastic deformation region, for many common materials [4]. Since the equations used to predict the occurrence of the umbilic point were purely elastic, the physical validity of this phenomena remains undetermined. One dimensional front tracking for elastic waves was tested, and compared to finite difference (higher order Godunov) solutions. The latter were found to be highly diffusive. The very stiff equation of state for metals (i.e. the small compressibility) makes the wave structure close to linear, and leads to much larger values of artificial diffusion than is commonly observed in gas dynamics computations. For this reason the advantages of front tracking for these problems is especially striking [4].

A second aspect of real materials considered within this project was the solution of Riemann problems with a real equation of state. An equation of state (EOS) is a functional relation between the thermodynamic variables (e.g. density, pressure, temperature, specific internal energy and specific entropy) that describe the state of a gas. Two of these variables are independent and the equation of state describes the remaining quantities when any two are given.

The Los Alamos National Laboratory program SESAME is a comprehensive EOS which supports 97 materials and is derived from a variety of analytic models and experimental data bases. On a rectangular grid of densities and temperatures, the pressure and specific internal energy are given at each grid point (ρ, T) . Pressures and energies at intermediate densities and temperatures are found by interpolation. An implementation of

the SESAME program into our gas dynamics code has been completed, [11]. Efficiency considerations are important, and were addressed by the precomputation of quantities used repeatedly.

The following quantities are important to the Riemann solution and are precomputed and tabulated: the entropy, S , the adiabatic and Grueneisen coefficients γ and Γ , and the Riemann invariant

$$r = \int (\rho c)^{-1} dP \mid_{S = \text{const}} .$$

Furthermore, the originally specified variables ρ and T are not convenient for all aspects of the Riemann solution, and so additional tables with inverted independent variables (ρ, e) , (ρ, S) , and (P, S) are constructed. The inversions are constructed by a bisection method.

In the case of phase transitions, the inversions and especially the Riemann solution is complicated by discontinuities in derivatives of the thermodynamic variables across phase boundaries, see [1].

3. General Theory of Conservation Laws

As a minor, or side aspect, of the work on this project, the general theory of conservation laws was considered. The reason for this part of the study was that some parts of this subject were being approached incorrectly by the workers in this area, and we judged it useful to identify and explain promising directions for research. The work on the general theory of conservation laws identified [8] a long standing error in the modeling of phase transitions, and revised common ideas about uniqueness and well posedness of solutions [9]. A survey of the striking recent progress in Riemann problems was given [7], which placed this work in its appropriate scientific context.

4. Chaotic fluid Mixing

Chaos was not considered within the work of this project, but it does provide the motivation for the final part of this report, three dimensional front tracking. Statistical theories of chaotic fluid mixing were developed. The program here is to derive equations for the interaction of elementary mixing modes and from this, to derive a statistical model model which predicts mixing rates in the turbulent (chaotic) region. The program is showing steady progress [10] and it appears that it will reach its major goals. Further analysis of the chaotic mixing region will require three dimensional front tracking, and parallel computing, which we now discuss.

5. Three Dimensional Front Tracking and Parallel Computing

The second main thrust of the work performed under this contract has been the development of three dimensional front tracking capabilities. This activity was begun only in the closing stages of this project, and publications completed dealt only with conceptual questions of organization of data bases [5,6]. This early work has been continued, and considerable progress has been achieved with both surface and volume grids and topological connectedness component labeling algorithms for front tracking in three dimensions. For example the component labeling computation is based on a hash table of triangle locations in each grid block, and is currently taking about 18 CPU minutes per meg-triangle (million triangles) on a sun-4. After optimization of this routine, we anticipate times of 3-5 CPU minutes. Parallel computation, with nodes several times faster than a sun-4 would then give this routine an acceptable timing (in seconds) per time step.

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7. Scientific Personnel Supported by AFOSR grant 88-0025

Xavier Garaizar

Yuefan Deng

John Grove

Qiang Zhang

John Lownegrub

John Scheuermann

Brian Wetton

Lisa Coulter

Samuel Figueroa