Numerical codes development issues

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Abstract

An overview of the various design choices to be made for a two-dimensional numerical code to simulate heavy ion targets is given. We discuss such issues as the grid structure, rezoning techniques, and the inclusion of material properties to various degrees. This is followed by a brief discussion of the open codes being used in the European heavy ion fusion community with characteristic samples of their application.

Keywords: Hydrodynamics; Ion beams; Numerical techniques

1. INTRODUCTION

The development of the physics of matter heated by heavy ion beams would not be possible without computer codes to simulate the complex flows occurring in such targets. For scientific research, as opposed to industrial or military development, there is an obvious need for open codes where—even if the source code is not available—the equations and input material properties are completely defined, so that the calculations are, in principle, reproducible.

This review is restricted to two-dimensional hydrodynamic codes, and the codes specifically addressed are BIG-2 (Chernogolovka), Caveat [Los Alamos National Laboratory (LANL) code modified at Frankfurt], DUED (Rome), Multi-2D (Madrid and Garching), and SARA-2D (Madrid). This is by no means an exhaustive list; among the notable codes omitted is, for example, ARWEN (Velarde, 1993).

2. THE EQUATIONS

These hydrodynamic codes in principle solve the conservation equations of hydrodynamics, that is, the set

$$\frac{\partial}{\partial t}\rho = -\nabla(\rho\boldsymbol{u})$$

$$\frac{\partial}{\partial t}(\rho\boldsymbol{u}) = -\nabla(\rho\boldsymbol{u}\boldsymbol{u}) - \nabla p$$

$$\frac{\partial}{\partial t}(\rho e) = -\nabla(\rho e\boldsymbol{u}) - \nabla(p\boldsymbol{u}) + \rho w_{\text{deposit}},$$

where ρ, u, and e stand for the density, flow velocity, and total energy of the fluid, respectively, and the pressure $p(\rho, e)$ is calculated from the equation of state. A necessary ingredient for heavy ion targets is the specific deposition w, which is prescribed by the externally applied beam and has to be calculated in a special way. Other physical effects incorporated into some of the codes will be discussed later.

The following sections give a brief overview of the design choices influencing the applicability, accuracy, and efficiency of the codes.

3. MESH DEFINITION

A crucial difference between the codes is the way in which the spatial discretization is done. All of them employ a conventional division of space into cells (in contrast to particle-in-cell methods or the newer smoothed-particle hydrodynamics), but there are many choices along the way that influence the applicability of the codes.

One basic distinction is between structured and unstructured grids. The former have cells that are logically rectangular, that is, a cell may be referenced by two indices and neighboring cells have neighboring index values, just like in a two-dimensional array, although the cell structure may geometrically look quite different from a Cartesian grid. If several such two-dimensional arrays of cells can be joined at their boundaries, one obtains a block-structured grid. Unstructured grids, on the other hand, have no such simple layout: Cells can be joined in arbitrary ways and the program has to keep the neighbor information available by special means such as pointers. The latter codes are, of course, slower but can cope with more complicated geometries.

In addition, the cells may be polygons of different types: In practice, most codes work with quadrangular cells and Multi-2D is the only one which also employs triangles. Triangles provide the advantage of easily discretizing even very complicated target geometries, but are computationally somewhat less accurate, so that they have to be employed with care.

4. REZONING

The time dependence of the numerical grid is another issue. Two limiting cases are provided by Eulerian calculations, in which the grid is simply fixed in space. This provides very efficient and robust calculations, but the resolution cannot adapt to the flow, and, most importantly, material interfaces cannot be followed (except with additional techniques of considerable complexity). The Lagrangian limit, on the other hand, has the grid move exactly with the fluid, which eliminates the deficiencies of the Eulerian approach, but introduces the difficulty of grid distortion. In heavy ion targets, this appears unavoidably, for example, during the motion of plasma out of a partially heated target: The cells near the boundary of the deposition region move very rapidly with respect to their neighbors, so that because these cells are attached to each other, strong distortion occurs. The negative effect on the solution is that for strongly distorted cells the numerical approximations work less accurately, they lead to very small time steps, and may also acquire negative volumes by flipping over two of their corners.

A generally adopted method of solution is that of rezoning. The traditional arbitrary Lagrangian–Eulerian (ALE) technique interpolates between the two limits. A Lagrangian step, where the cells are moved but not with the fluid velocities, is followed by a Eulerian step with transport of conserved quantities between cells. Since this implies, however, that the grid motion be prescribed in some new and arbitrary way, a large variation of solutions adaptable to individual cases is possible; some indications will be given for the individual codes.

Another possibility of dealing with strong grid distortions is that of discrete rezoning: At a fixed time, the code is halted and a new grid is constructed based on the boundaries of the materials at that time and having, of course, better geometry. The hydrodynamic quantities then have to be interpolated onto this new grid with the unavoidable loss of accuracy this entails, so that such a process should not be repeated too often.

5. HYDRODYNAMIC ALGORITHMS

Many modern codes propagate the fluid quantities using methods based on the Godunov method. The essence of the Godunov method is that the cell boundaries, where there are jumps in the hydrodynamic quantities, evolve according to a Riemann problem (the problem of the evolution of a discontinuity in initial conditions) and after the time given by the current time step, the time-developed distributions are mapped back onto the cells. Since the exact solution of the Riemann problem for an arbitrary equation of state is too cumbersome for an algorithm, various approximate methods have been developed and are used in these codes.

The restriction on the usable time step in all codes is the Courant–Friedrichs–Levy criterion: The time step must be so small that neither sound nor fluid motion can propagate through more than one cell during the time step. This also explains the above remark that distorted cells (where usually one dimension shrinks compared to the other) reduce the time step.

6. EQUATIONS OF STATE

All codes allow the use of the SESAME tables (Lyons & Johnson, 1992). For some generic applications, the ideal-gas equation of state is also useful, and while Caveat, being a code with a broader intended application range, incorporates a number of other parametrized equations of state, BIG-2 and DUED also use locally developed equations of state.

7. THERMOCONDUCTIVITY AND VISCOSITY, DIFFERENT TEMPERATURES

Some codes also include thermoconductivity or viscosity. Thermoconductivity requires the use of implicit techniques, since explicitly time-stepping the heat-conduction term would lead to excessively small time steps.

In the same way, different temperatures for ions and electrons are sometimes dealt with, although this is more important for the case of laser irradiation.

8. BEAM DEPOSITION

Ion beam deposition poses a special problem because of the nonlocal transport. An easy way to calculate this, which is used in most codes, is to represent the ion beam as a large number of beamlets, whose path through the grid is followed like in ray tracing. If a beamlet passes a cell, it de-

posits the amount of energy given by its instantaneous energy loss rate (depending on the cell density and temperature) and the length of the cell traversal. This method is easily adapted to various beam geometries and profiles. Another possibility is that of discretizing the beam deposition on a regular grid in space and then interpolating onto the hydrodynamic cells.

9. RADIATION TRANSPORT

Radiation transport in some ways causes problems similar to those in beam deposition, although on a much larger scale, which can only be avoided if a very simple approximation such as radiative thermoconductivity is used. A popular solution is to use ray tracing by following the radiation in a large number of angular groups, adding to or subtracting from the local radiation intensity depending on local conditions. Similar in spirit but quite different in detail is the S_n method, which follows angular groups through finite-difference equations, not rays.

Once such a method has been adopted, it remains to decide whether to use multigroup radiative transport or a simple one-group approximation with averaged opacity. In any case, the opacity has to be obtained from an opacity model, but because of the computational expense, usually a functional interpolation to opacity tables is used.

10. COMPARISONS OF RESULTS

Considering the complexity of the problem, it would be very welcome if more comparisons of the code performance existed. Unfortunately the amount of effort used to do such comparisons for problems which are otherwise uninteresting has prevented a more systematic testing. One test that was quite illuminating was one comparison between calculations done at the Russian Federal Nuclear Center VNIIEF and Multi-2D calculations done at Frankfurt (Maruhn *et al.*, 1998) for a simple cylindrical target irradiated by a heavy ion beam. The results showed very satisfactory agreement in both the geometric evolution of the targets and the time dependence of crucial quantities such as the maximum density or temperature. It only appeared that for longer times, Multi-2D showed somewhat larger damping of the collective motion than did the VNIIEF calculations.

11. THE CODE BIG-2

BIG-2 (Fortov, 1996) was developed by Alexander Shutov, Oleg Vorobiev, and Alexander Ni at Chernogolovka, and is available to others for a fee. It uses a quadrilateral block-structured mesh, a unique rezoning not based on ALE in the sense that there are no separate Lagrangian and Eulerian steps.

BIG-2 contains some advanced grid features that are rarely found: Neighboring blocks can have different resolutions,

that is, one cell can on one of its sides be in contact with several neighbors, which helps it to deal with slide lines, that is, the case of fluid regions flowing past each other with strong relative motion. In addition it can handle void closures, that is, connect cells that collide during the motion of the fluid (like in the case of an imploding hollow cylinder, where cells meet on the axis) which in other codes simply leads to cells spuriously coexisting at the same location.

BIG-2 can use the Chernogolovka equation of state in addition to SEAME and the ideal gas; it contains implicit thermoconductivity but no radiation. It is thus mostly used for the simulation of lower-intensity ion-beam experiments.

12. THE CODE CAVEAT

Caveat was developed at LANL (Addessio *et al.*, 1992) and is available by request. It is part of a collection of codes known as CFDLIB, which also contains variations for magnetohydrodynamics, mixed materials, incompressible flow, and a parallel three-dimensional version. The codes are available by request. In Frankfurt, a relatively simple version was adapted by including new initialization geometries and beam deposition.

Caveat uses a block-structured mesh with quadrilateral cells. Grid adaptation can be done either by a simple ALE variation setting the grid velocities equal to a factor times the fluid velocities (but preserving boundaries), or by an adaptive scheme through the minimization of a functional (Winslow, 1981), which allows, for example, a refinement of the grid near steep gradients of any of the hydrodynamic state variables.

The code's history as a general-purpose code is shown by the large number of equations of state and boundary conditions it can deal with, but in the Frankfurt version, there is neither thermoconductivity or viscosity nor radiation transport, so that in this version it is best suited to lower-energy heavy ion targets.

13. THE CODE DUED

The code DUED (Atzeni, 1986; Atzeni & Guerrieri, 1991, 1993) has as principal author Stefano Atzeni of the University of Rome, with contributions from Letizia Ciampi, Simona Graziadei, Alessandro Guerrieri, and Mauro Temporal, and is available by special arrangement. Its special facilities include flux-limited thermoconductivity, electron–ion relaxation, and especially radiation transport in either a one-group three-temperature or a multigroup flux-limited diffusion approximation, while laser–matter interaction is dealt with using two-dimensional ray tracing, including plasma refraction and inverse bremsstrahlung.

A structured quadrilateral mesh is used and rezoning is done in a discrete way so as to make it particularly well suited to Rayleigh–Taylor instability simulations.

Its unique feature is the emphasis on burn physics, including diffusion of charged fusion product and knocked-on

bulk ions and Monte Carlo neutron transport, which led to many applications in fast-ignition physics, but was also useful in the treatment of the burn phase of conventional pellets.

14. THE CODE MULTI-2D

Multi-2D (Ramis & Meyer ter Vehn, 1992) was originally developed by Rafael Ramis, Julio Ramirez, and Jürgen Meyer-ter-Vehn from Madrid and Munich and then continually enhanced. It is available through an ftp site. The original goal was to be able to do radiation transport very efficiently, and for that purpose a triangular mesh was used, which also allowed the discretization of very complicated target geometries. In its present version, it can use both triangular and quadrilateral cells, albeit only in cylindrical geometry. Reflection symmetry of the target can be also be used to reduce the computation, and the grid motion is based on ALE. The hydrodynamics is based on Richtmyer–Morton and a flux-limited thermoconductivity in the one-temperature limit may be included. The radiation transport is handled by using typically 32 angular groups which are followed using ray tracing.

Multi-2D was thus the first European open code that could calculate radiation transport in hohlraum targets, and it has since been applied to many such target studies as well as to laser target simulations.

15. THE CODE SARA-2D

SARA-2D (Honrubia *et al.*, 1998) was authored by Javier Honrubia and is available by request. The mesh is structured with quadrilateral cells and it uses rezoning features similar to Caveat. Thermoconductivity and radiation transport (one-group, based on the S_n method) are included with separate temperatures for matter and radiation.

This code is also suited to a full simulation of indirectly driven fusion capsules and can follow the development of the pellet up to highest compression.

16. CONCLUSIONS

The five codes discussed show large differences in the physics included and the mesh handling, which makes them suited to different problems. Comparisons of results unfortunately are rare but should be very useful because of the different numerical strategies employed. A comparison with experiment in the heavy ion case at present and in the near future is possible only for relatively modest conditions; simulations of laser targets therefore may be necessary as an intermediate step.

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