SESSION B

Tuesday, October 20, 1992

1:30 p.m.

Algorithm Development II

Papers:

1. Advanced Multi-Material Eulerian Algorithms on Generalized Meshes
   - J. Mike McGlaun (SNL)

2. Dense Matrix Computation on Parallel Computers
   - David Womble, Bruce Hendrickson (SNL)

3. Numerical Modeling of Two-Dimensional Magnetogasdynamics Flow in Eulerian-Lagrangian Variables
   - Anatoliy Zubov, et al (Chelyabinsk)

4. Discrete Models for Mathematical Modeling of Kinetic Processes Concomitantly with Continuous Medium Dynamics
   - Ahmed Gadzhiev (Chelyabinsk)

5. MIMOZA Code for Solving Problems in Continuum Mechanics
   - ~~Vadim Zmushko~~ (Arzamas)

   Given by Safronov

SESSION B

Algorithm Development II

Advanced Multi-Material Eulerian Algorithms on Generalized Meshes

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Eulerian algorithms for modeling the motion of compressible media have advanced tremendously in the last few years. High-order accurate schemes for modeling continuous and discontinuous flow are on a much firmer mathematical foundation. Unfortunately the algorithms are routinely developed for the motion of a single fluid on uniform, rectangular mesh. Many important problems involve multiple, immiscible solids and it is often advantageous to use more general meshes.

This talk describes our work to extend the Eulerian algorithms to model the motion of multiple, immiscible solids on arbitrary-connectivity meshes. The arbitrary-connectivity mesh is constructed from hexahedra. An arbitrary number of hexahedra can share a common vertex.

Extending the algorithms to multiple, solid materials introduces several complications. Some of the algorithms easily extend while others do not. Some new algorithms must be developed, e.g. algorithms to model the interfaces between the immiscible fluids.

The arbitrary connectivity mesh complicates extending the algorithms and developing software to implement the algorithms. Most algorithms must be generalized to accommodate an arbitrary number of neighbor cells. The data structures are much more complex, so concepts such as left-side and right-side neighbors loose their meaning.

This work performed at Sandia National Laboratories supported by the U.S. DOE under contract #DE-AC04-76DP00789.

SESSION B

Algorithm Development II

Dense Matrix Computations on Parallel Computers

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Abstract: Dense linear systems of equations are quite common in science and engineering, arising in boundary element methods, least squares problems and other settings. Massively parallel computers will be necessary to solve the large systems required by scientists and engineers, and scalable parallel algorithms for the linear algebra applications must be devised for these machines. A critical step in these algorithms is the mapping of matrix elements to processors. In this paper, we study the use of the relatively new, torus--wrap mapping in general dense matrix algorithms, from both theoretical and practical viewpoints. We prove that, under reasonable assumptions, this assignment scheme leads to dense matrix algorithms that achieve (to within a constant factor) the lower bound on interprocessor communication. We also show that the torus--wrap mapping also allows algorithms to exhibit less idle time, better load balancing and less memory overhead than the more common row and column mappings. Finally, we discuss practical implementation issues, such as compatibility with BLAS levels 1, 2, and 3, and present the results of implementations of several dense matrix algorithms. These theoretical and expermental results are compared with those obtained from more traditional mappings.

SESSION B

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Numerican Modeling of Two-Dimentional Magnetogasdynamics Flow in Eulerian-Langrangian Variables - Anatoliy Zubov, et al. (Chelyabinsk)

Numerical Modeling of Two-Dimensional Magnetogasdynamics Flow in Eulerian-Lagrangian Variables

V.E. Neuvazhaev, V.D. Frolov, A.D. Zubov
(VNIITF, Chelyabinsk-70)

Annotation

This report introduces a procedure for numerically calculating two-dimensional flows of thermally conducted gas in complex systems. The procedure is generalized in the case of gravitational magnetic gas dynamics. It is based on the Eulerian-Lagrangian description of motion with a specially-located reaction-rate vector in mobile coordinates. In order to implement the implicit, finite-difference technique, a method of splitting along the lines of physical processes and directions is used.

Presented are several results from the calculations of a number of applied problems that were solved using the TIGR software package. This includes problems on the evolution of axially symmetric perturbations in the A.I. Pavlovsky cascade magneto cumulative generator, as well as problems on the gravitational compression of a homogeneous gas cloud.

Numerical Modeling of Two-Dimensional Magnetogasdynamics Flow in Eulerian-Lagrangian Variables

V.E. Neuvazhaev, V.D. Frolov, A.D. Zubov
(VNIITF, Chelyabinsk-70)

The TIGR technique is a generalization /1/ of the arbitrary Euler family of coordinate technique that was described earlier in /2/. Based on /1/ an analogous technique of /3/ was developed at the VNIITF.

The complete system of equations for magnetogasdynamics taking into account radiant heat conduction, and solved by the TIGR technique look like /4/:

$$\frac{d\rho}{dt} + \rho \cdot \mathrm{div}\, u - o: \qquad (1)$$

$$\frac{du}{dt} + \frac{1}{\rho} \cdot \mathrm{grad}P = -\frac{1}{4\pi\rho} \cdot [H \cdot \mathrm{rot}H]; \qquad (2)$$

$$\frac{dH}{dt} = \mathrm{rot}\,[u \cdot H] - \mathrm{rot}\,(\chi \cdot \mathrm{rot}H); \qquad (3)$$

$$\mathrm{div}H = 0; \qquad (4)$$

$$\frac{dE}{dt} + \frac{1}{\rho} \cdot \mathrm{div}u = \frac{1}{\rho}\,\mathrm{div}\,(æ \cdot \mathrm{grad}T) + \frac{\chi}{\rho}(\mathrm{rot}H)^2 \qquad (5)$$

where the equation of state of a substance and the kinetic coefficients are determined by the relationship: $P = P(\rho,T)$, $E = E(\rho,T)$, $æ = æ(\rho,T)$, $\sigma = \sigma(\rho,T)$, $\chi = c^2 / 4\pi\sigma$, ρ is the density of a substance, E is the specific internal energy, P is pressure, u is reaction rate, æ is the coefficient of radiant thermal conduction, σ is the coefficient of electrical conductivity, H is the stress level of the magnetic field, and T is temperature.

The TIGR technique employs a mixed Eulerian-Lagrangian method of describing the motion of gas. One family of coordinate lines, coinciding with the separation boundaries, is Lagrangian, while the other is Eulerian. This method makes it possible to monitor the separation boundaries and simply calculate the overflow of the substance in layers. Thus, the curvilinear coordinate system is linked with the movement of boundaries over time and is mobile.

The Eulerian system of coordinate lines represents a set of straight lines (rays) that do not intersect the regions of the solution.

Motion equations of a continuous medium are recorded in these mobile curvilinear coordinates and take into account the fact that along the boundaries that coincide with the Lagrangian family of coordinate lines, the corresponding contra variant component vector of reaction rate is preserved continuously. Such expansion makes it possible to not have to isolate the separation boundary during computation.

Equations of continuity (1), motion (2), magnetic field (3) and energy (5) are solved according to a splitting-by-vector method: "angular" (Eulerian) and radial (Lagrangian). The resulting implicit algebraic equation, after the linearization of nonlinear terms, is solved by a trial run.

In an overwhelming number of applications the configurations of the magnetic field can be limited to two frequent occurrences:

-- two components of velocity (reaction rate) and two components of the magnetic field, lying in the same plane as the vector of velocity;

-- two (or three) components of velocity and one component of the vector of magnetic strength, perpendicular to the vector of velocity.

The following are examples relating to both the first and second: Z and θ-pinch, expansion of the plasma in the external field, a gravitational collapse of the magnetoactive interstellar cloud, magnetic cumulation, various thermonuclear devices and the like.

In the case of a "poloidal" magnetic field it is advantageous to use a representation of the field through the vector potential, since, in this case, to determine the field it is sufficient to solve the equation for the only null component of the vector potential.

The bibliography describes methods of magnetogasdynamics (MGD) calculations that use Lagrangian and Eulerian difference meshes and explicit diagrams of the first and second order of precision. However, it already appears to be illogical to use implicit diagrams in one-dimensional problems. The presence of additional (to sound) Alfven velocity dictated by the magnetic pressure leads to a situation in which the condition for Courant stability typical in explicit diagrams turns out to be a one time increment more rigid. Therefore, it makes more sense, when solving magnetogasdynamics problems, to employ implicit methods. If one takes into account the fact, that coefficients of migration (thermal conduction and electric conduction) can also alter in a problem of several different orders of magnitude, then the diffused parts of the equation, which are non-linear in the case of variable coefficients of migration, should be approximated by implicit expressions. However, the difference diagram, even for systems equations describing one-dimensional gas dynamics flows with thermal conduction, cannot generally be reduced to three point equations. In the case of multidimensional flows, either iteration methods or fractional increment methods are used /5/.

The stability condition of a separate trial run method for a number of practical and interesting problems is too rigid; however, it can be avoided in the so called method of combined runs (6), in which dynamics, kinetics and electrodynamics equations are solved concomitantly by Newton iterations at the first stage, while at the second stage energy equations are solved, and a record is made of the dissipative processes.

The isothermic process relates to the first group of equations traditional for the TIGR technique for algorithms of separate (sequential) runs. It can be demonstrated that the use of isothermic process for calculating MGD flows restricts the range of unconditional stability. Therefore the TIGR software stipulates envisages a transfer to an algorithm of combined runs /6/. This made it possible to increase the implicitness of the most difference diagram and thus avoid limitations on its stability.

In the TIGR technique the thermal conduction equation is solved by the diagram of fission by direction. The difference equation is written down on a nine-point template. The equations for the vector potentials in the case of the "longitudinal" (poloidal for particular symmetry) magnetic field and equations for the strength field in the case of the "transverse" (azimuthal) magnetic field have two types of two-dimensional diffusion equations. Therefore the notorious methods of solving difference equations can be taken advantage of.

In the case of axisymmetry the gas dynamics flow is invariant relative to the Galilean type transformation of migration along the axis of symmetry. A difference solution can have this property. Theoretic analysis allowed us to to change the difference approximation of the TIGR diagram such that the numerical solution also satisfied the condition of invariability relative to the Galilean transformation. The significance of this question increases as the perturbations of the magnetic and gravitational fields are recorded.

In order to verify the workability of the MGD TIGR technique along with theoretical research on approximations and stability of the difference diagrams used, a number of control calculations of flows with magnetic fields were conducted. Several of the test calculations dealt with one-dimensional flows, such as the motion of MGD shock waves, a fall in the arbitrary MGD jump and Joule's energy release. Also conducted were calculations of two-dimensional problems from a rather general class of motion with a uniform deformation characterized by the linear relationship of the coordinate to the velocity. Such precise solutions to MGD systems equations are very useful in theoretical analyses of multi-dimensional motions. Moreover, they represent a rather non-trivial class of solutions used for testing programs of numerical modeling of multi-dimensional continuous medium flows. In-depth research on this class of MGD flows was conducted in papers /7/ and /8/ by V.A. Simonenko and one of the authors of this report.

When the indicated relationship of the field of reaction rates to the coordinates, and specific conditions for the flow parameters exist, the system of MGD equations is reduced to an autonomous system of typical difference quadratic equations, after the solution of which, the flow parameters appear according to explicit formulae. In particular, it is possible to derive a model of a MGD-type flow with a uniform deformation, in which there would be an arbitrary number of shells in the shape of coaxial elliptic cylinders, whose semiaxis would change over time by law, as the solution to the above mentioned dynamic system determines. The magnetic field is axial.

Records can be made within the framework of the condition of a uniform deformation and other physical effects, such as diffusion of the magnetic field, thermal conduction, the state of having multi components, auto-gravitation and the like. The value of such solutions lies in that there exist motions with cumulative characteristics that conform to the adiabatic compression of the substances finite masses. This demonstrates, in particular, that the multi-dimensional flow in and of itself does not exclude the possibility of achieving singular states. Here it would be appropriate to recall the issue raised by E.I. Zababkin regarding the dissymmetry of initial data which might distort the focusing, but does not eliminate fact of unlimited cumulation /9/. It turns out that motions with a uniform deformation can lead to a collapse which for the most part were exact solutions of three-dimensional equations of continuous medium mechanics. This suggests that deviations in the second harmonic from one-dimensional symmetry does not exclude achieving optimal states /7/.

Analyses of the asymptotic behavior of the class of flows of near singularities being studied corroborate and generalize the earlier obtained asymptotics as a multi-dimensional case for self-similar motions (see /10/). For example, the gas spheroid (an eclipsoid with two identical semiaxes can have three different extreme modes of compression: 1) focusing on a segment of the axis, 2) focusing on the disk and 3) focusing on a point (generally asymmetrical). Given this, the limit flow corresponds to the focusing on the axis with cylindrical symmetry, while it corresponds to the focusing on the disk with oblate symmetry. In the third instance where the focusing is on the center, there is generally asymmetry.

Such solutions have an independent value for understanding a range of physical phenomena, e.g. the compression of various systems, several astrophysical processes, and others. They can also be used for testing and calibrating algorithms, and for programs for the mathematical modeling of gas dynamics phenomena.

Also interesting is a subclass of multi-dimensional finite motions with a uniform deformation. Pulsation in the vicinity of a balanced state could, under certain conditions,

acquire a stochastic property, which, in principle, enables one to regard such flow as turbulent flow.

Currently it is fairly well understood that the onset mechanism of turbulent motion from the laminar flow is not related only to the dissipative quality of the system. Examples of flows described in /7/ and /8/ show that complex and complicated, i.e. essentially turbulent, motion can arise in "ideal" Hamiltonian systems as well. Several types are known that make a transition from regularity to chaos. These are the so called "turbulence scenarios" that are based on the doubling frequencies phenomena, the **[TN] bifurcation, intermittence and the like. However, all of these have only a highly specialized behavior and use considerably dissipating properties of the selected flow model. The primary cause for the appearance of turbulence is, in our opinion, not necessarily related to dissipating factors, and this is substantiated by the flow examples given in this paper.

It is important to stress that unlike the popular system at Lawrence, which is only an approximate convection model, motions with a uniform deformation represent precise solutions to the equations in quotient derivatives of continuous medium mechanics.

The calculation of the development of two-dimensional axially assymmetric perturbations in explosive magneto cumulative (MC) generators serves as an example for how the TIGR technique is applied.

One of the most successful constructions of explosive MC-generators that produce magnetic fields with an order of 10^{17} **[TN] is the cascade MC-generator, developed by A.I. Palovsky et al. /11/-/13/. A multi-entry, multistratal spool solenoid made of insulated copper wire serves as the cylindrical liner. After the shock waves have passed from the external charge, the explosive solenoid becomes a conducting shell that compresses the magentic field. Several internal coaxially arranged cascades work analogously to this shell, and at time zero represent a composite cylinder made of densely packed insulated copper wires, laid lengthwise in an axial direction and coated with an epoxy compound.

In addition to the function of protecting the nappe which is occupied by the magnetic field and a detector against the breakdown of substances in streams, the cascades effectively suppress the instability which is developing during the compression process.

Studies have shown the optimal number of cascades to be used in experimental systems work to be three. Also important is the selection of the location for the cascades. This is so that the perturbations in the shape of the previous cascade do not manage to progress to such an extent that they will affect succeeding cascades.

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Considering the complexity and high cost of the experimental projects, it is becoming increasingly important to create a physical, mathematical model for perturbation development that would enable one to adequately describe the phenomenon. For this purpose, the TIGR technique includes a sufficiently complete description of the necessary thermodynamic and electromagnetic properties of the pertinent substances in all the states that are manifested in the processes.

The TIGR program was used to conduct comparative calculations of Kiddor's model problems (see /11/) on the compression of the magnetic flow using the copper cylindrical liner in a one-dimensional formulation, while calculating various physical processes (the compressionability of the liner and the diffusion of the magnetic field) and various approximations (equations of state and forms of conduction functions).

Moreover, comparative calculations on the development of **[TN] -Taylor instability were conducted in an analogous liner system studied both theoretically and numerically by Somon /15/.

A two-dimensional calculation of the first cascade MK-generator was conducted /11/-/13/ using the TIGR program. V.A. Simonenko, V.F. Kuropatenko and research fellows A.A. Karpikov and V.I. Mamyshev at the VNIIEF participated in the formulation of the calculation and discussion of the results.

The calculations showed that in the process of magnetocumulative motion changes take place in the curvature (even twice) at points along the internal boundaries of the shell: concavity becomes convexity and vice versa. This "flipping" effect is supported by experimental data. Moreover, the temporal scales of the change in the surface phase, obtained in the calculation, are in keeping with the experiment.

With the aid of numerical calculations using the TIGR technique a contemporary theoretical astrophysics problem, i.e. the gravitational compression of a rotating gas cloud was studied /16/.

For numerical calculations on gravitating continuous medium dynamics, a method for solving law of small numbers equations on a curvilinear TIGR mesh has been devised. It is based both on the method and diagram of determining the correction being stabilized. A conservative difference approximation was used to solve the impulse equation which preserved the local (in each Lagrangian layer) point of motion quantity.

Numerical modeling of a homogeneous axisymmetric collapse performed by a various authors (note Larson's /17/ and Charnuter's /18/ pioneer work) with the help of the

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most varied gas dynamics techniques, is today still leading to alternative solutions to this occurrence during the process of calculating either disk or ring structures.

Numerical calculations of the gravitational compression of a rotating gas cloud using the TIGR Eurlerian-Lagrangian technique corroborate the focusing in the disk at a time interval being determined by a precise solution with a uniform deformation.

Motions with a uniform deformation /7/-/8/ do not only provide an adequate test for the problem, but also are adequate for determining natural conditions, to wit: null initial velocity; boundary conditions matched with a precise solution; solid-state rotation; a cloud spheroid given a constant initial density and temperature. These motions represent a precise solution, within which the initial spheroid (in particular, a sphere) collapses on the infinitely thin disk in the equatorial plane.

Within the framework of the accepted physical and mathematical model an occurrence of a ring structure was observed in the calculation done on the TIGR Eulerian mesh (along every time increment the difference mesh in the Lagrangian radial direction was revived). This is explained by the diffusion of the mass and the angular sequence through the boundaries of the Lagrangian mesh. (The diffusion has a difference origin, see Norman, et al.)

In the calculations, even without the readjustment in the mesh, the mass and the angular sequence inside each Lagrangian layer is exactly preserved. The collapse is accompanied by a cyclical sequencing reflected off the equatorial surface of the shock waves in ever decreasing temporal and spatial scales. An earlier description of this mode of cumulation in a model with other parameters was published by Norman et al. /18/.

Among other supplements to the TIGR software package we note the following:

-- numerical research on the effects of radiant dissymmetry and thickness non-uniformity in the shell on the degree of compression and the form of the target in the relationship between the amplitude and the length of the perturbation wave when the shell target is compressed by laser radiation /20/;

-- numerical research on the development of **[TN] -Taylor unstable separation boundaries of liquefiable mediums in similar energy release problems /21/.

In addition to the current inclusion into the TIGR program of the possibility of recording the spread of energy in a tri-temperature approximation, the TIGR is part of a greater computer software program call TIGR-OMEGA, in which it is possible to record a multitude of other physical processes.

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Currently, the possibilities for using the TIGR code program created in our institute are expanding. The program describes magnetogasdynamics and plasma processes and is used for modeling new classes of phenomena. This pertains specifically to the physical and mathematical modelling of processes taking place during the interaction of the plasma with the wall and the diverter plates in the ITER Tokamak /22/ and during "explosions" of the plasma against the wall (the so called "instability explosion").

There are several different theoretical studies this topic (for theoretical analyses done, see, for example, /23/) and several experiments imitating explosions have been conducted.

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SESSION B

Algorithm Development II

Discrete Models for Mathematical Modeling of Kinetic Processes Concomitantly with Continuous Medium Dynamics - Ahmed Gadzhiev (Chelyabinsk)

B-4

Discrete Models for the Mathematical Modeling of Kinetic Processes Concomitantly with Continuous Medium Dynamics

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Introduction

This report presents an overview of the methods and programs developed in the Department of Numerical Methods and Kinetic Processes of the VNIITF. Discussed are: the one-dimensional KIT method and the two dimensional TIGR-OMEGA and FENIKS methods.

The report is presented on behalf of the group of individuals who developed the herein examined methods.

The authors of the KIT method are: L.F. Varganova, A.D. Gadzhiev, V.M. Gribov, B.E. Neuvazhaev, O.S. Shirokovskaya and V.G. Yakovlev.

The authors of the TIGR-OMEGA method are: N.N. Bokov, A.D. Gadzhiev, V.M. Gribov, A.D. Zubov, K.A. Mustafin, V.E. Neuvazhaev, V.N. Pisarev, S.B. Serov, V.D. Florov, O.S. Shirokovskaya.

The authors of the FENIKS method are: A.D. Gadzhiev, V.V. Gadzhieva, S.N. Lebedev, V.N. Pisarev, A.A. Shestakov.

It should be noted that in the USSR the first methods and software packages for the mathematical modeling of kinetic processes concomitantly with continuous medium dynamics in a one-dimensional formulation were developed at the M.V. Kel'dysh IPM AS USSR under the guidance of A.N. Tikhonov and A.A. Samarsky. This knowledge base was employed in developing the new methods.

I. The one-dimensional method and the software package KIT

Processes modeled:

-- gas dynamic motions taking into account turbulent agitation (TP). Model TP is of a diffused type;

-- radiant thermal conduction;

-- break-off temperature ($T_i \neq T_e \neq T_\phi$)

-- production, multiplication, absorption and transfer of neutrons in a multiple group approximation taking into account the anisotropy of diffusion;

--the kinetics of nuclei in neutrons and thermonucelar reactions, and in energy release;

-- production and transfer of γ- quanta in a multiple-group approximation taking Compton scattering anisotropy into account;

-- the transfer of radiation in a multiple group approximation, kinetic and diffusion models;

-- the transfer of energy and impulse of high-speed charged particles in a multiple group approximation taking anisotropy diffusion into account.

Problem solving methods:

An implicit method with a separate run [1] is used to solve gas dynamics equations, while an implicit diagram with a scalar run is used to solve thermal conduction equations.

An implicit diagram in conjunction with a matrix run method is employed to solve a system of energy equations in a three-dimensional approximation. Diagrams based on S_π and DS_π methods are used to solve kinetic equations. In order to ensure a positive solution and an acceptable monotony, the combination of diagrams of the first and second order of precision are used.

A DS_π based method is also used to calculate the transfer of charged particles. Given that in this instance the matrix of the system of difference equations is not trigonal, it is suggested that a splitting method be used in conjunction with iterations along the collision integral [2].

Thermal physical properties of particles and neutron constants:

For solving equations of state $\Gamma=\Gamma(\rho,T)$, $\varepsilon=\varepsilon(\rho, T)$, as well as equilibrium path lengths of radiation $1=1(\rho,T)$ the software package uses a special library of data that works both with an analytical form and with matrices of equations of state and transit.

Neutron constants are calculated in the following manner: first, the neutron flow ranges are calculated by using the Monte Carlo method with the spectral constants NAS

[3]. Then, either the isotropic or anisotropic group constants are calculated while adhering to the averaging spectra of the system ranges.

2. Two-dimensional method and the software package TIGR-OMEGA

Processed modeled:

-- gas dynamic motion taking into account turbulent agitation;

-- radiant thermal conduction;

-- break-off temperature ($T_I \neq T_e \neq T_\phi$)

-- production, multiplication, absorption and transfer of neutrons in a multiple group approximation taking into account diffusion anisotropy;

-- kinetics of nuclear reactions, energy release;

-- transfer of γ- quanta and α-particles in a one-group kinetic approximation.

Problem solving methods:

The technique applies the Eulerian-Lagrangian description of motion. The calculated geometry is described by either a quasispherical or quasicylindrical system of coordinates, or by a combination thereof.

Gas dynamics and conductiveness is calculated by an implicit difference diagram and applies the method of splitting along physical processes and spatial variables [4].

Both the two-dimensional equation and the system of gas dynamics equations are recorded in mixed Eulerian-Lagrangian curvilinear coordinates. A local system of coordinates with the spherical coordinates O, Φ (polar and azimuthal angles) are introduced in the set $\{\Omega\}$ of the flight directions of the particles.

$$\Omega = \varepsilon \cdot \vec{\omega}_1 + \eta \cdot \vec{\omega}_2 + \mu \cdot \vec{\omega}_3,$$

where $\varepsilon = \sqrt{1-\mu^2}\cos\phi$. $\eta = \sqrt{1-\mu^2}\sin\phi$, $\mu = \cos\theta$.

If we orient the polar axis $\vec{\omega}_3$ along the radius-vector $\vec{r}$, then we will obtain a record of the kinetic equation during which a two-dimensional equation transforms into a one-dimensional spherical symmetrical equation in the spherical symmetry hypothesis. This approach is used in the T_1 method.

In the second approach, we orient the polar axis $\vec{\omega}_3$ axis of symmetry Z. $\vec{\omega}_1$ lies on the plane R, Z. In these coordinates the transfer equation look like this:

$$\frac{\Delta}{\Delta t}(R \cdot R_x \cdot \underline{N}_g) + \frac{\Delta}{\Delta z}[R \cdot R_2 \cdot (\underline{\nu} + \mu) \cdot N_g] + \frac{\Delta}{\Delta x}[R \cdot \xi \cdot R_4 \cdot \mu) \cdot N_9] -$$

$$\underline{\Delta} - (R_Z \cdot \eta \cdot N_g) + R \cdot Rx \cdot \alpha_g N_g - R \cdot R_x \cdot (S_g + r_g)$$
$$\Delta\phi$$

It can be seen that there is no maximum transition to the spherical symmetry. The DS_π method is used to solve this equation [5,6].

In the T_1 method the unknown function $N(r, z, \mu, \phi, t)$ taking into account its precision along ϕ, is represented in the form of an infinite row according to the trigonometrical system of the function $\{T_1 = \cos\phi\}$, a difference diagram of the DS_π method type is constructed along the remaining variables [7].

The mesh in the set $\{\Omega\}$ is constructed by dividing the surface of the unit sphere into equal areas and by using quadrants that ensure a diffusion limit, thus creating a "tortoise" mesh.

The kinetics equation is solved by runs along channels in the Z direction.

As an example of numerical calculations using TIGR-OMEGA, we will give calculations of a thermonuclear detonation in dense plasma taken from the study [8]

3. The two-dimensional method and the software package FENIKS

The package is designed to provide mathematical modeling of continuous medium dynamics and kinetic processes in two-dimensional axisymmetrical systems with complex geometry and large deformations.

Processes modeled:

-- gas dynamic motion;
-- computation of elastoplastic and durable properties of materials (discrete and kinetic models of mechanical failure);
-- radiant thermal conduction;
-- break-off temperature ($T_I \neq T_e \neq T_\phi$)
-- production, multiplication, absorption and migration of neutrons in multiple group isotropic and anisotropic approximations;
-- kinetics of nuclear reactions, energy release;
-- migration of energy and impulse of α-particles and γ-quanta in a single group approximation;
-- migration of thermal radiation in a P_1 approximation.

Several principles that form the basis of the FENIKS technique:

a) Calculation by region.

The entire system is broken into grid-like regions within each of which a regular mesh is constructed out of quadrangles. This approach makes it possible to describe physical systems that are complex both in terms of their geometry and their composition.

In both the gas dynamics and thermal conductivity programs, the calculations are done by mesh regions with an interchange of boundary conditions along the internal boundaries. In gas dynamics the heavy regions take on pressure as a boundary condition, and the lighter regions normal composite velocity. In thermal conduction the interchange takes places either in the temperature and the heat flow, or in a sort of linear combination depending upon the properties of the [numerical] solution.

The neutron migration equation is solved in the entire system by using a transparent sequencing of all the cells of the mesh regions [9].

Kinetic equations are solved by region.

b) Using an arbitrary Lagrangian-Eulerian description of the motion of the environment by applying a quadrangle mesh. Re-adjustable meshes are used to allow for solutions with large deformations to be found.

If the mesh undergoes major deformations during the solution process, then the calculation of that step consists of two stages: the Lagrangian stage and the stage of reconstructing the mesh with a recalculation of the mesh values. The software has two means of recalculating values. The first is a method which takes into account the convective flows through the boundaries of the cells during the movement of the mesh to its new position [10]. The second approach is the method of fractional engineering [11].

When large deformations are present, it is not always possible to describe the boundaries dividing the medium with Lagrangian lines. Therefore, in FENIKS all the substances are described by mass concentrations

$$c_i = \frac{m_i}{m},$$ where m_i is the mass of substance i and m is the mass of the entire cell.

The presence of three different substances are allowed within one calculated cell that are characterized by their thermodynamic properties and neutrino-nuclear constants. The concentrations allow one to make a rough description of the behavior of the contact boundaries over time. There is a mechanism embedded in the algorithms for calculating values that prevents excess diffusion of substances as the cells are being reconstructed.

The method of fractional engineering is used, as a rule, for a significant overlappping of tasks. It is a method of calculating convective flows during only slight changes in the mesh.

Problem solving methods.

When the FENIKS software package was created, new implicit "ROMB" diagrams were developed for solving various types of equations of computational physics. The necessity of such a development was dictated by the fact that the traditional implicit nine-point difference diagram on meshes with considerable deformations leads to large inaccuracies. In the "ROMB" diagrams, just as in the DS_π method of solving the migration equation, the approximation is constructed within the boundaries of one cell, whereby values of unknown functions are used in the centers and along the edges of the mesh cells.

"ROMB" [12-18] diagrams have been built for solving

equations of thermal conduction,

equations of thermal conduction taking into account the [temperature] break-off ($T_1 \neq T_e \neq T_\phi$),

typical hyperbolic systems equations,

gas dynamics equations,

equations of migration in P and in quasidiffusion approximations,

migration equations of heat radiation in the P_1 approximation.

Numerical studies [14-18] conducted have confirmed that the "ROMB" diagram ensures satisfactory precision on meshes with large deformations.

In FENIKS gas dynamics equations are computed by using the implicit-explicit "RID" [17] technique, thermal processes by using the "ROMB" diagram [15], [18], and migration equations by using the difference diagram based on the DS_π method.

The "RID" technique incorporates both an explicit diagram and the ability to determine the pressure at a given moment in time by using the solution to a diffusion-type equation derived by the linearization of both systems equations of gas dynamics recorded for viscous pressure and equations of state. The "ROMB" diagram is used to solve equations for pressure.

The simplicity of approximating boundary conditions and one-time calculations of thermal conduction in the mesh cell when using the "ROMB" diagram should be noted.

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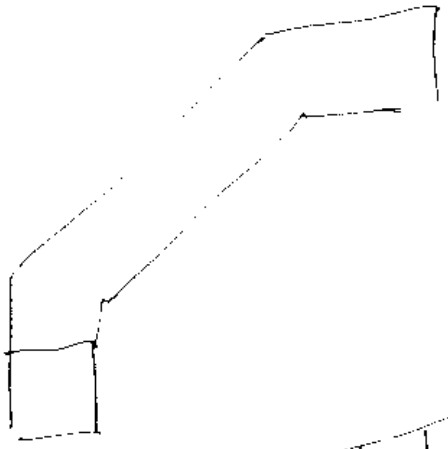
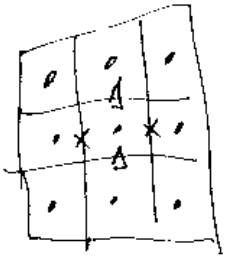


Romb → allows 3 dimensional extension.



Uses ADI solution technique.
implicit

SESSION B

Algorithm Development II

MIMOZA Code for Solving Problems in Continuum Mechanics

Sofronov I.D., Vinokurov O.A., Zmushko V.V.,
Pletenev F.A., Saraev V.A.

Abstract

The MIMOZA code is intended for two and three-dimensional problems in hydrodynamics: elastic-plastic material properties, heat conduction and other physical processes can be included. The main principles that served the base for MIMOZA are as follows: splitting by physical processes; splitting the solution region into subregions (computation regions); applying regular quadrangular and hexahedral grids for two-dimensional and three-dimensional calculations, respectively, with the motion of these grids not necessarily coinciding with the material motion; using problem-oriented languages to specify data and to control the computations. MIMOZA is oriented to a class of problems where the number of points ranges from 10,000 to 100,000. MIMOZA codes allow to perform a wide spectrum of calculations and to describe highly sheared flows.

1. broken down to sub-programs. Initially necessary because of small address space.

2. splitting physical processes. (carried to its logical end)

"D methodology"

~100K zones seems to be a limit.

2D problems can be done with the 3D code.

- MIMOZA is written in Fortran using the swift preprocessor.
- They archive output for at least 10 years.
- MIMOZA is now a standard for linking between their codes.
- They commonly use 10 processors. They also farm some work out to distributed processors.

MIMOZA Code

for Solving Problems in Continuum Mechanics

Sofronov I.D., Vinokurov O.A., Zmushko V.V.,
Pletenev F.A., Saraev V.A.

much smaller team of people. up to speed only over the last 3-4 years.
2L, 1E ~200K lines (expected to grow) SIGMA (2 years) ~ 1 million lines.

Introduction

The MIMOZA code is intended for two and three-dimensional problems in hydrodynamics: elastic-plastic material properties, heat conduction and other physical processes can be included. The code /1/ was designed for ELBRUS-2 computers based on SIGMA code that successfully runs on BESM-6 since 1967. The main principles that served the base for MIMOZA and had been verified within SIGMA are as follows: splitting by physical processes; splitting the solution region into subregions (computation regions); applying regular quadrangular and hexahedral grids for two-dimensional and three-dimensional calculations, respectively, with the motion of these grids not necessarily coinciding with the material motion; using problem-oriented languages to specify data and to control the computations. MIMOZA is oriented to a class of problems where the number of points ranges from 10,000 to 100,000. MIMOZA codes allow to perform a wide spectrum of calculations and to describe highly sheared flows.

For two-dimensional and three-dimensional hydrodynamics

MIMOZA is a descendant of SIGMA. transition to FORTRAN
they require two independent solution methods.
nuclear tests yield integral characteristics

equations, MIMOZA uses Eulerian - Lagrangian technique, which is now the most efficient one for calculations of high distorted flows. For two-dimensional case, the whole solution region is split into subregions. A regular quadrangular grid is constructed in each subregion. The effect of the computational subregions on those sharing boundaries with them is accounted via inner boundary conditions /3/. Two-dimensional equations are solved in two stages: Eulerian and Lagrangian. For the Lagrangian stage the nodes are considered frozen in the material and move with it. For the Eulerian stage, a new difference grid is constructed where severe distortions of the previous grid are removed if possible. Then the values are mapped from the previous grid to the new one. The solution for the system of three-dimensional hydrodynamics equations bases on equations written in Lagrangian - Eulerian coordinates with one Eulerian and two Lagrangian variables /4/. The family of coordinate surfaces corresponding to the fixed Eulerian variable consists of planes. The same routines as in two-dimensional case are used in each plane for grid design, value mapping and boundary condition exchanges between subregions.

Two-dimensional hydrodynamics equations

1. Splitting into subregions

Splitting the whole solution region into subregions for

one-dimensional gas-dynamic equations is proposed in /3/. This method is ported to two and three-dimensional cases in SIGMA/2/ and MIMOZA, respectively. Usually, physical characteristics differ from one subregion to another. For boundaries between adjacent subregions, sliding lines are automatically introduced that is the lines on which the following requirements are supposed: pressure equality and normal velocity component continuity. Inner boundary conditions can be specified without sliding, with friction etc. The algorithm for sliding line computation is to divide the contact surfaces into "light" and "heavy" (slave and master) that is those for which pressure or velocity are taken as boundary conditions. The stability conditions for such algorithm depend on boundary cell masses and Courant numbers and are not restrictive /5/. Splitting into subregions permits to cover a geometrically complex region with a rectangular grid, calculate easily the inter-material sliding, select the grid that is the most suitable for the flow nature.

2. Lagrangian stage calculations

For Lagrangian stage, the gas motion is described by the following differential equations:

$$\frac{d\bar{u}}{dt} = -\frac{1}{\rho}\,\mathrm{grad}(p+Q) \quad ;$$

$$\frac{d\bar{x}}{dt} = \bar{u} \quad ;$$

$$\frac{d\rho}{dt} = -\rho \cdot \mathrm{div}\bar{u} \quad ;$$

$$\frac{d\varepsilon}{dt} = -(p+Q)\cdot\frac{d(1/\rho)}{dt} \quad ;$$

$$p = P(\rho,\varepsilon) \ ,$$

where $\bar{x} = (x,y)$, $\bar{u} = (u,\omega)$.

Quadratic viscosity is computed as :

$$Q_{i-\frac{1}{2},j-\frac{1}{2}} = \begin{cases} 0 \ , & \text{if} \quad \rho^{n+1} < \rho^n \ ; \\ 2Bh^2(\rho^{n+1})^3\left\{\dfrac{(\rho^n - \rho^{n+1})^2}{\tau^n \cdot \rho^n \cdot \rho^{n+1}}\right\}, & \text{if} \quad \rho^{n+1} \geqslant \rho^n \ . \end{cases}$$

Here B is the viscosity coefficient, τ - time step, h - typical cell size. For system integration, a difference scheme is used which is based on D scheme /6/ and its extension reported in /7/. In other words, we take a fully conservative scheme and then add spherical test corrections. The time step is selected as follows:

$$\tau_{cq} = \min_{i,k}\left\{\frac{0.7\cdot h_{i,k}}{C_{V_{i,k}}} \ , \ \frac{V_{i,k}}{8B\cdot|V_{i,k}|}\right\} .$$

where $C_{V_{i,k}}$ - sound speed, $V_{i,k}$ - amount of cell rotation, with respect to the symmetry axis. A smoothing procedure similar to that reported in /8/ is used to suppress short wave perturbations. Smoothing is accomplished by the fourth - order operator with respect to velocity components relatively normal to grid lines: $\bar{u}_n^{new} = [\,I - (\eta\cdot\partial)^2]\,\bar{u}_n^{old}$.

The difference approximation for A has the form:

$$(A u)_k = \frac{2}{M_k}\left[M_{k+\frac{1}{2}}(u_{k+1} - u_k) - M_{k-\frac{1}{2}}(u_k - u_{k-1})\right]$$

where M_k - planar mass of grid nodes (the sum of planar masses of cells with the given nodes being their vertices); $M_{k+\frac{1}{2}}, M_{k-\frac{1}{2}}$ - planar masses of cells, k - index along the grid line, η - smoothing coefficient.

3. Eulerian stage calculations

Moving quadrangular grids in MIMOZA which are not related to material allow to perform calculations with strong distortions. After the Lagrangian stage is completed, a new difference grid is constructed. It computes all thermodynamic values and velocities from the previous grid.

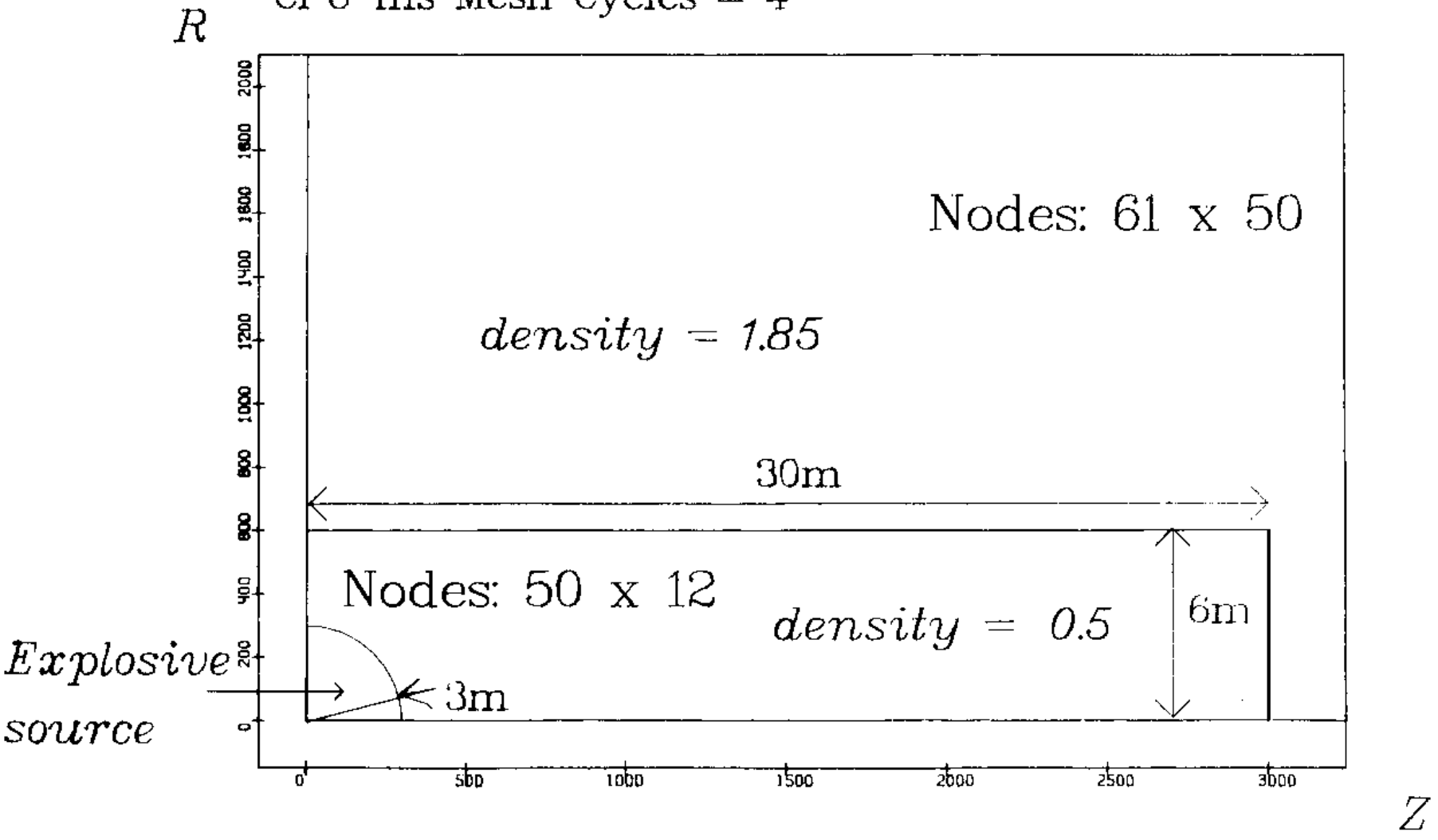
Two approaches are used to construct a new grid in MIMOZA. For the first approach, the node coordinates of the new grid are usually obtained from the previous grid nodes which are the nearest neighbours of the given node. Several algorithms exist for such grid construction and the algorithm number should be specified when initialization is performed and can be changed when computing. These algorithms will be further referred to as local. For the second approach, all internal grid nodes are constructed from specified nodes of a region boundary.

Grid construction with local algorithms

At present, MIMOZA contains about 30 algorithms which are used to reconfigure the grid. The position of some points may be never changed that is they remain Lagrangian. The most frequent algorithms include those which conserve (a) straight

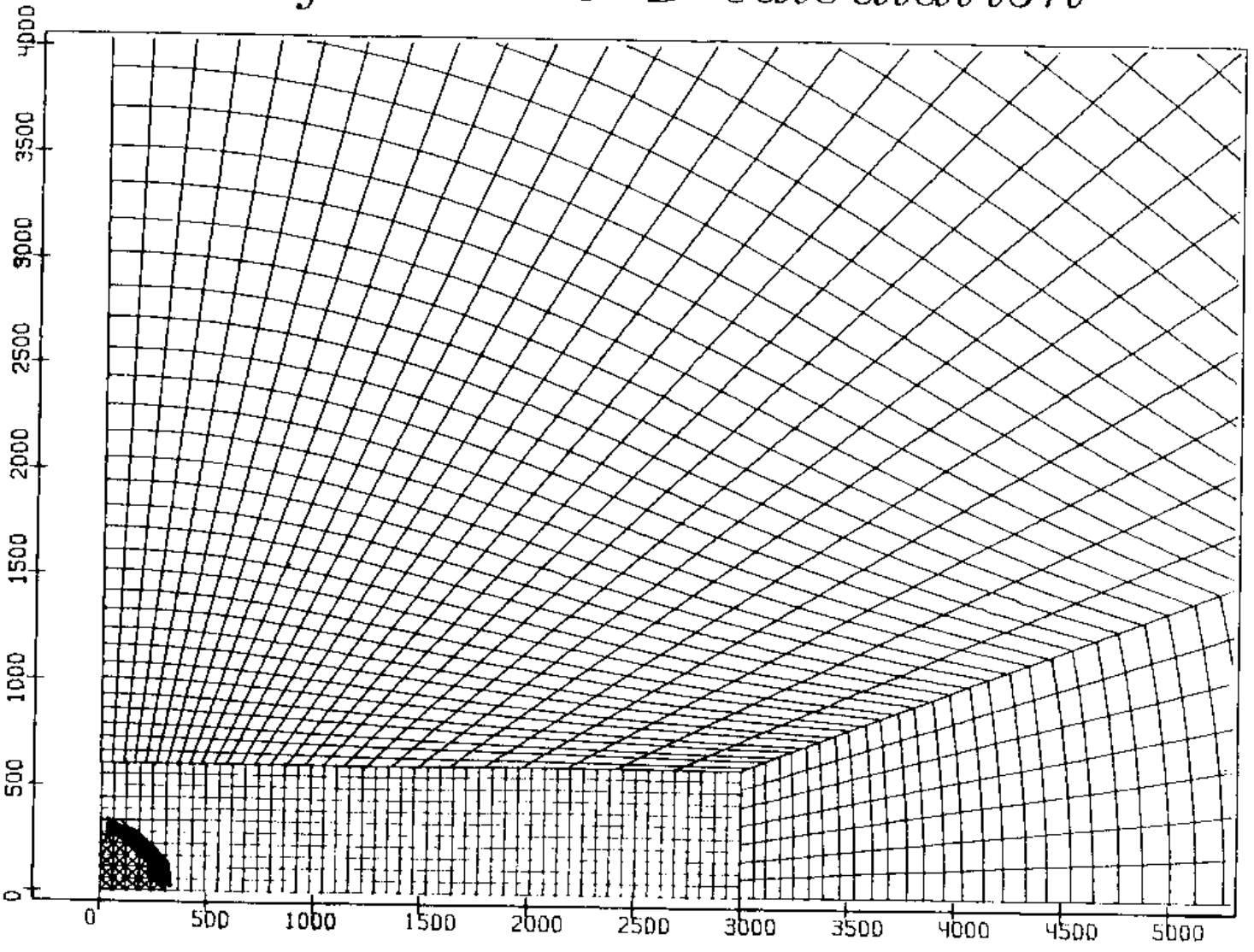
• "elimination of chemical waste"

Total ELBRUS–2 CPU Time 40 hours
Number of nodes = 3650
CPU ms Mesh Cycles = 4

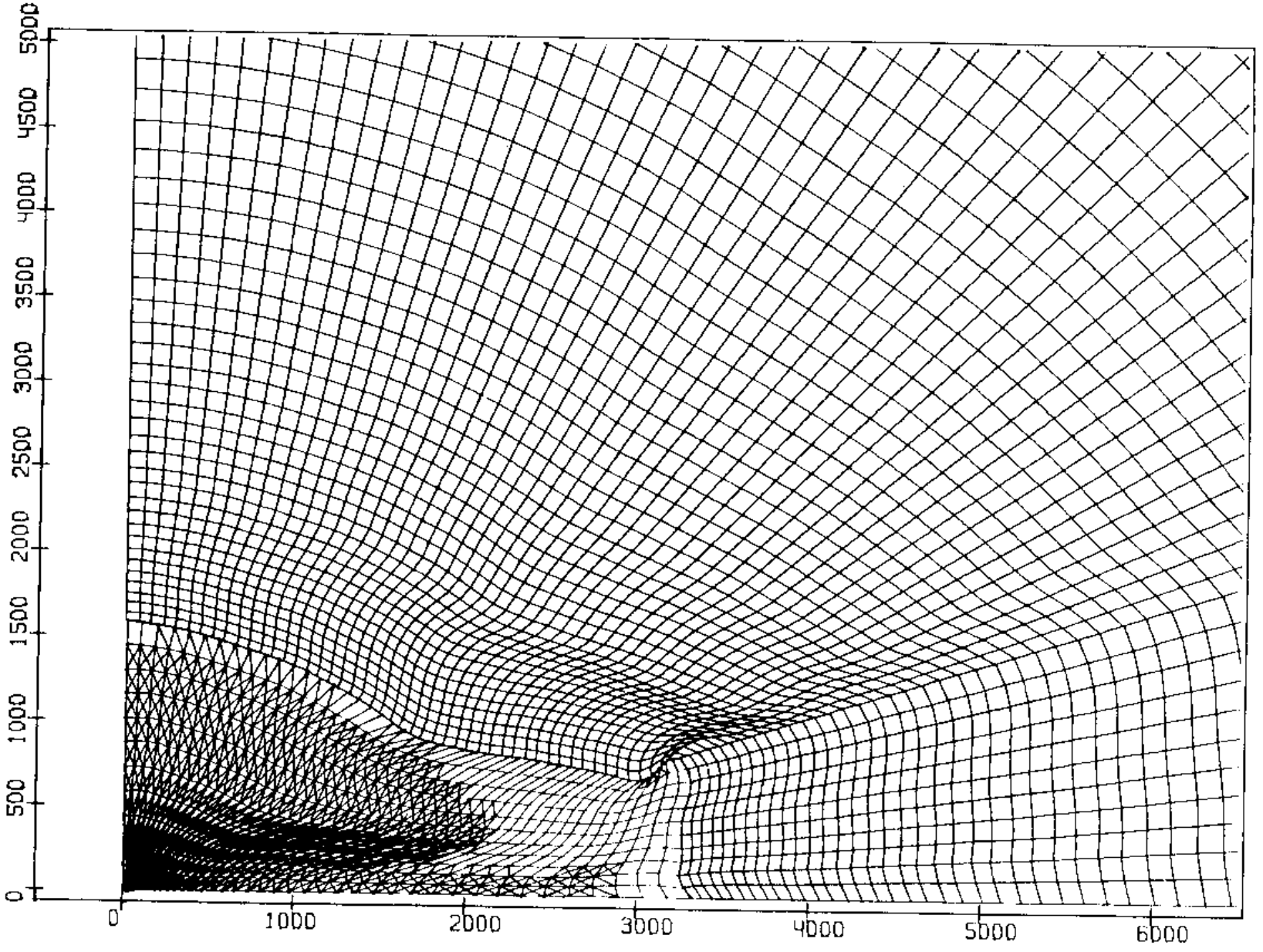


Explosive yield 100kt

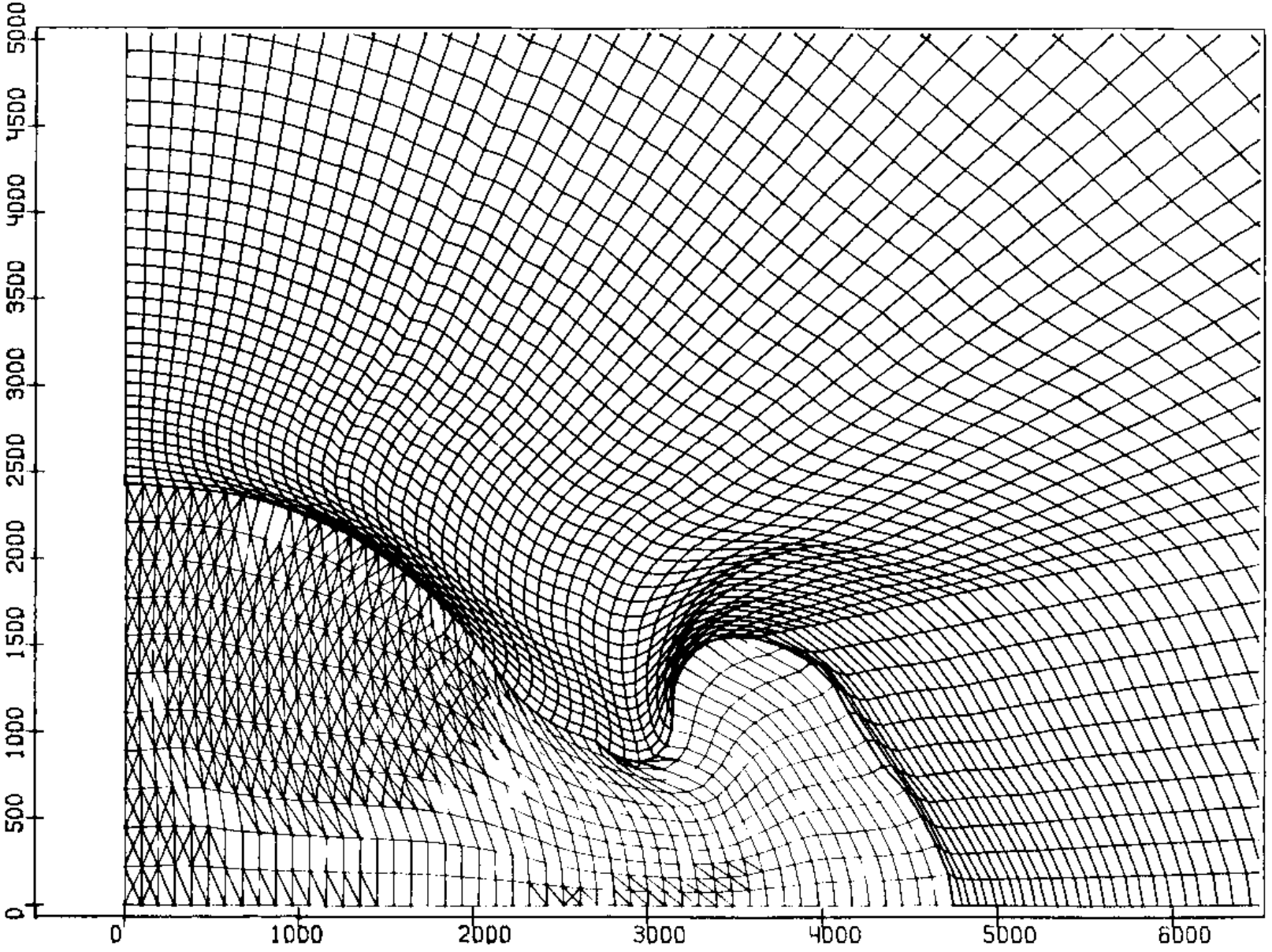
Initial grid and explosive source for the 2–D calculation



Grid and explosive source at 6.5ms.



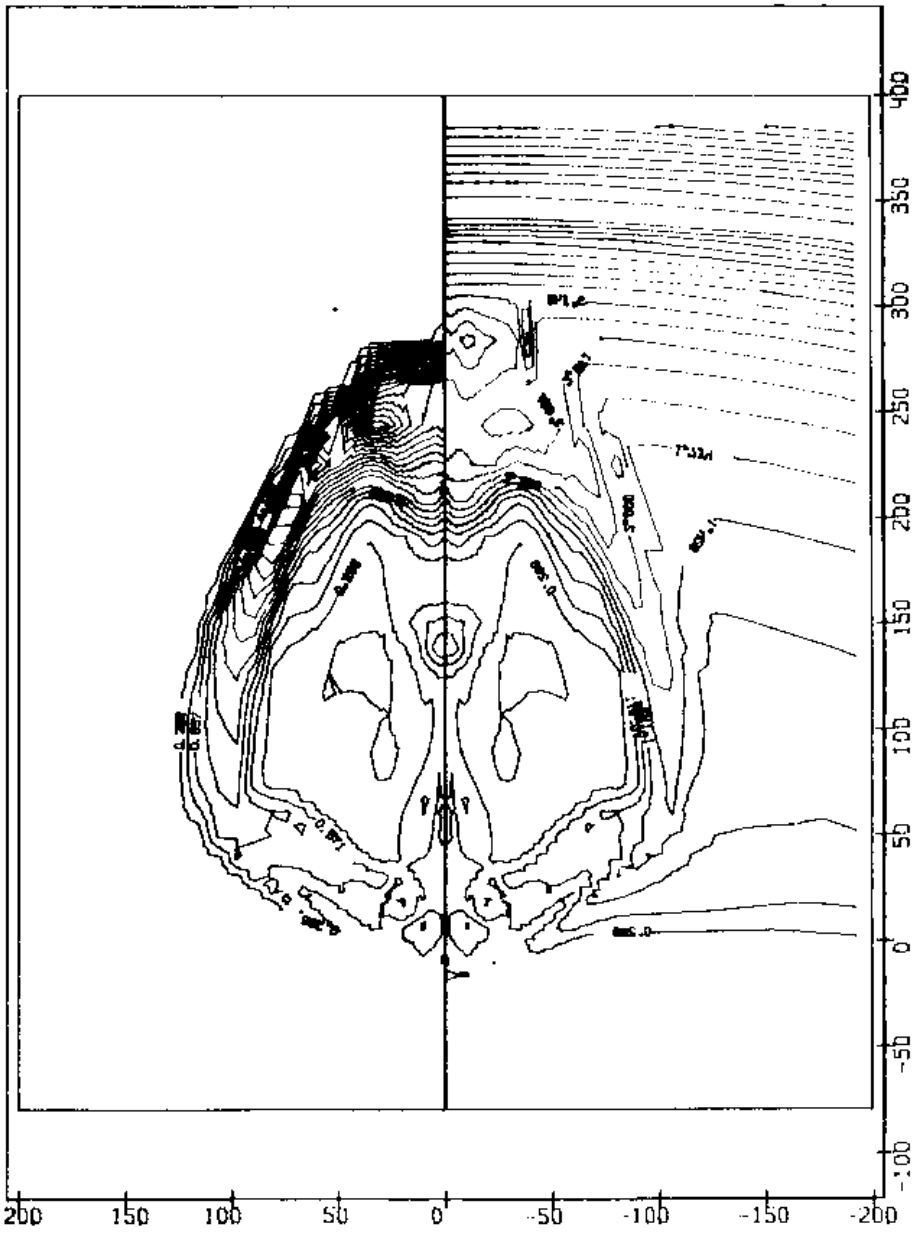
Grid and explosive source at 19.0ms.



Ion temperature

levels:

0.285714 1.714286
3.142857 4.571429

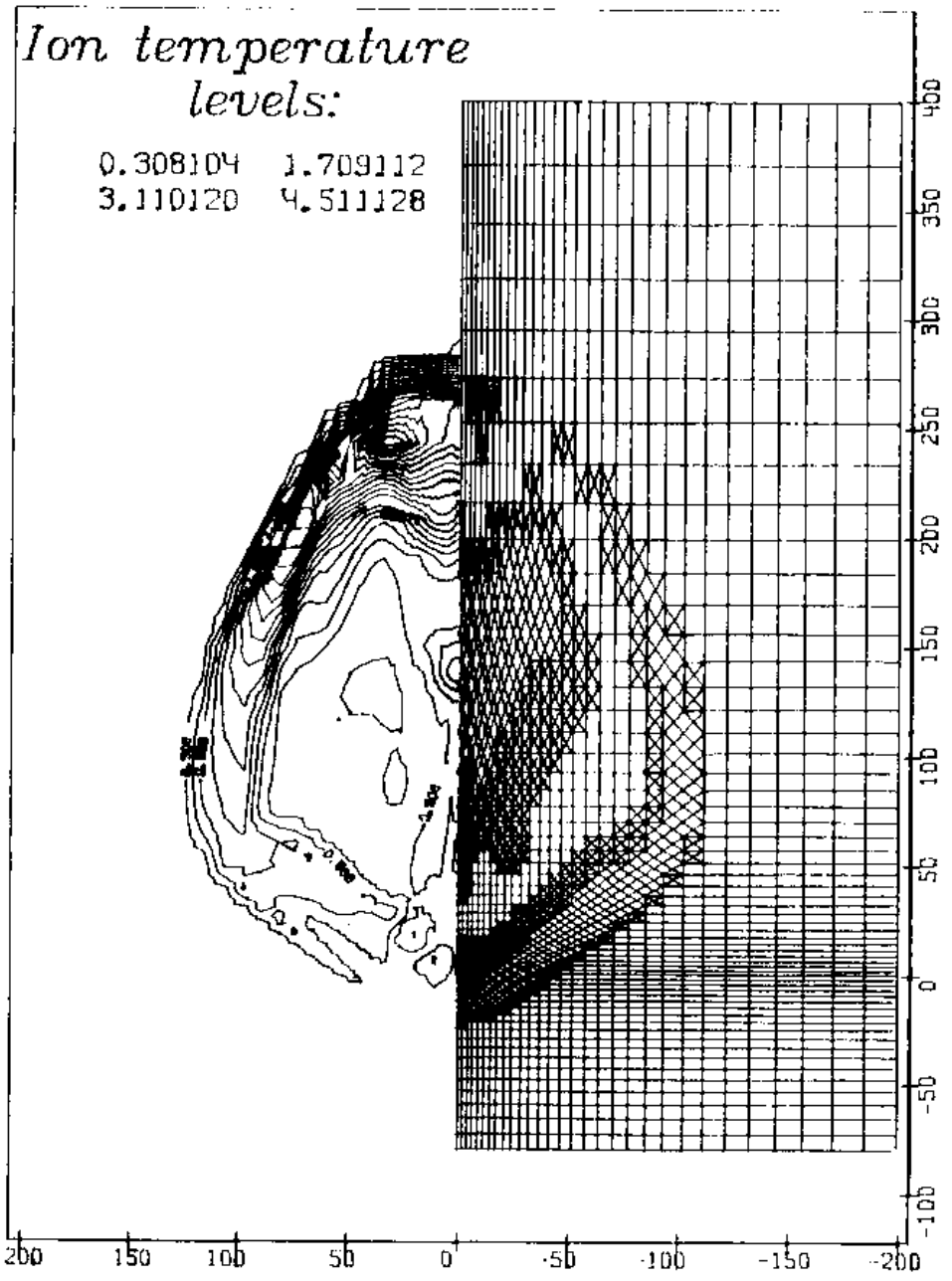


Electron temperature

levels:

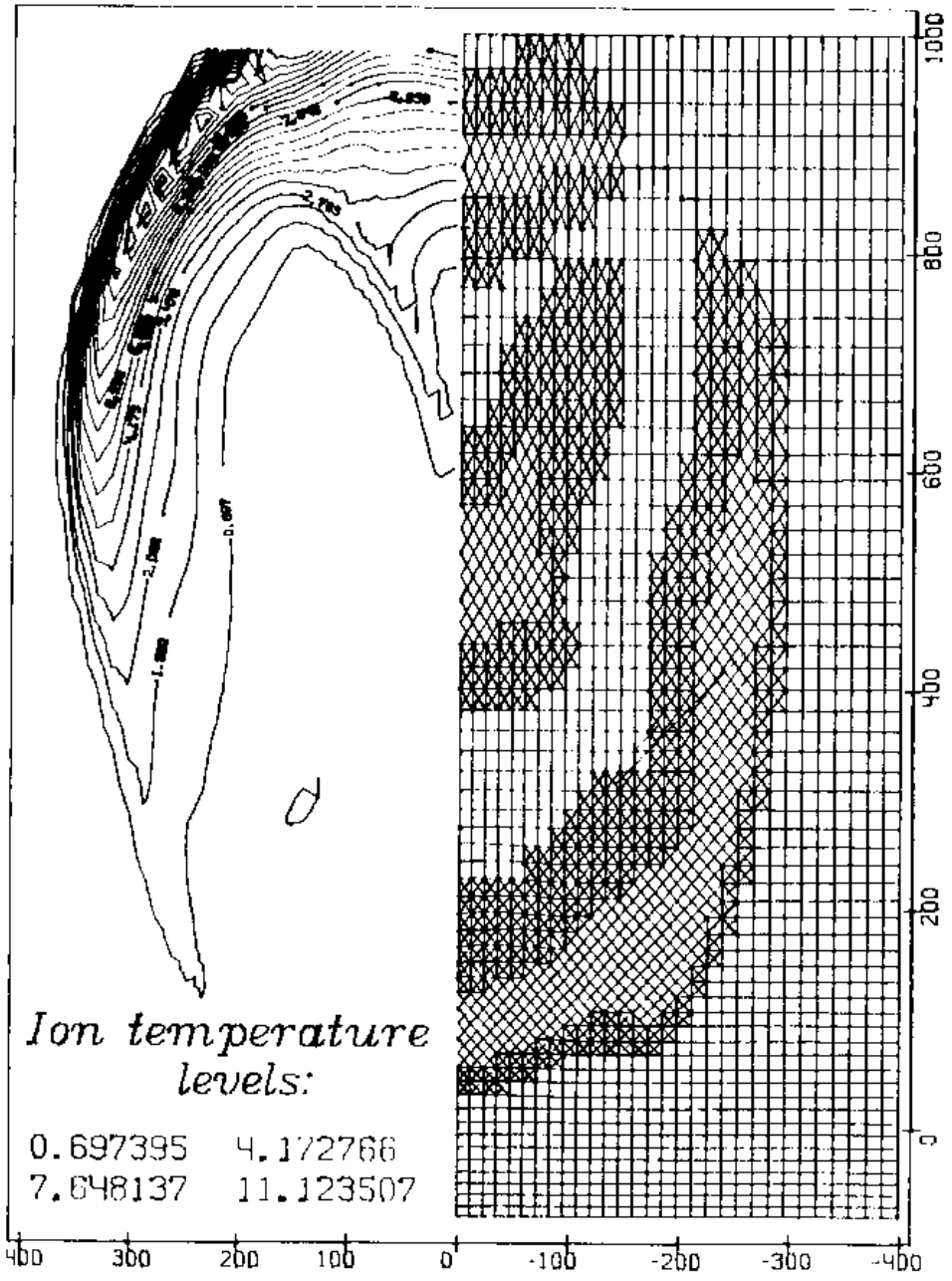
0.285714 1.714286
3.142857 4.571429

Time 10.0



Time 10.0

Localization regions molecules, neutral atoms, simple and double atomic ions

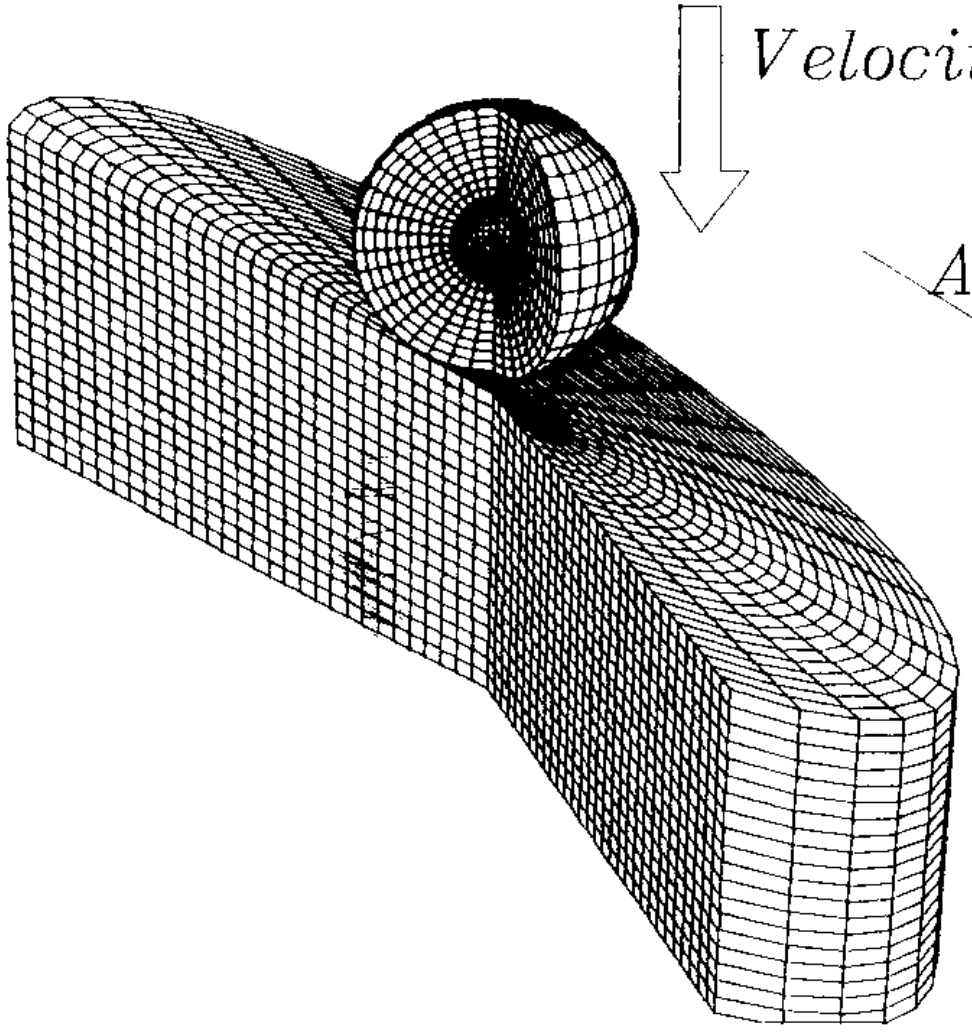


Time 40.0

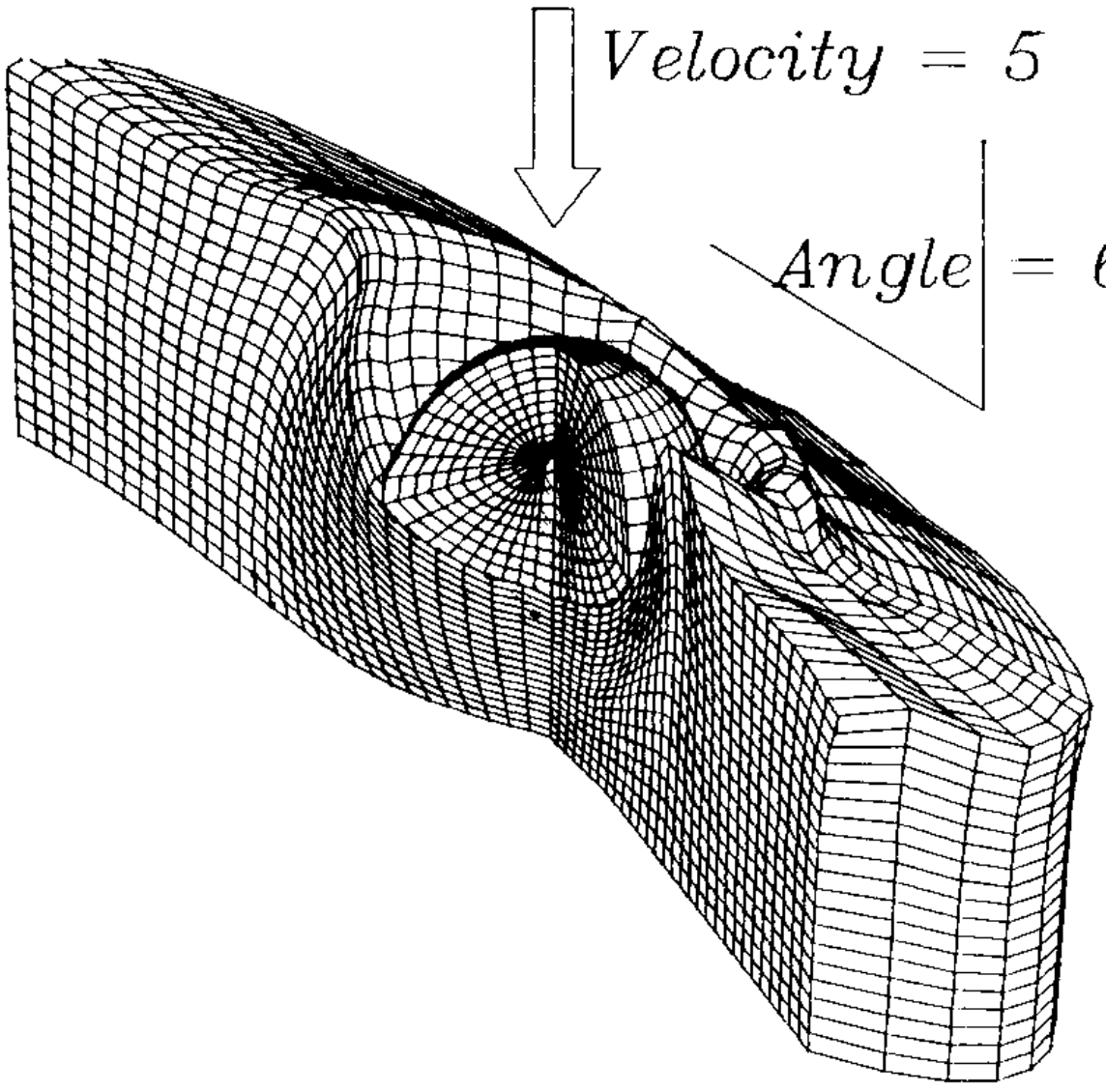
Localization regions molecules, neutral atoms, simple and double atomic ions

uranium ball on an aluminum plate

3D calculation of the body impact.



3D calculation of the body impact.



Chernobyl yields ~~~

D-methodology ~Grigory or Nicolai Alexander...

- Alexander Dimitriev. Sofronov was hired by him in 1955. Very gifted but shy.
- linear & angular viscosity. reference to Shulte
- ... "my archive ...." Sofronov.
- D-methodology lab, a small but dynamic group.

~~~

They do employ a smoothing operator.

They tried 300,000 points but it took so long that they try to limit themselves to 100,000 points.

~~~

Occasionally they use a "global advection"

lines from one of the families on the difference grid, (b) equal or specified ratios for distances between difference grid nodes, (c) equal angles at which line segments of a difference grid are observed from a given point. These algorithms often allow to construct an acceptable grid and maintain its configuration for a broad class of geometries when computations proceed though it requires considerable efforts. A set of more complex algorithms is also available which provides a higher automatization level but each algorithm has its own scope.

Configuring a grid from boundary points. To configure regular quadrangular grids inside a region using boundary points, a simplified algorithm from /9/ is used. The lines of one family only are consecutively constructed starting from two opposite boundaries. The algorithm is based on geometry considerations.

Value remapping

The values specified on a difference grid when rezoning it are recomputed using the FCT algorithm ideas similar to those from /10/. The algorithm relies upon directional splitting and using a one-dimensional higher accuracy algorithm. Higher accuracy is achieved by introducing in-cell distribution for the values to be remapped which differs from the constant. The distribution is introduced so that convective terms should be recomputed with a second order

accuracy on smooth solutions.

Let ν_1,ν_2,ν_3 be the values of a quantity contained in three consecutive cells. Then the distribution of this quantity in the average cell is selected as follows:

1. $\nu_1 < \nu_2 < \nu_3$; in this case $\Delta\nu = \min(\nu_3-\nu_2,\nu_2-\nu_1)$;

$$\nu(x) = \begin{cases} \nu_2-\Delta\nu\cdot 0.5, & \text{if } x \leqslant (x_2+x_3)\cdot 0.5 \\ \nu_2+\Delta\nu\cdot 0.5, & \text{if } x > (x_2+x_3)\cdot 0.5 \end{cases}$$

2. $\nu_3 < \nu_2 < \nu_1$; in this case $\Delta\nu = \min(\nu_1-\nu_2,\nu_2-\nu_3)$;

$$\nu(x) = \begin{cases} \nu_2+\Delta\nu\cdot 0.5, & \text{if } x \leqslant (x_2+x_3)\cdot 0.5 \\ \nu_2-\Delta\nu\cdot 0.5, & \text{if } x > (x_2+x_3)\cdot 0.5 \end{cases}$$

In all other cases the in-cell quantity distribution is assumed to be constant. Further a usual "donor" cell algorithm is used.

Three - dimensional hydrodynamics equations

Consider differential equations of motion in coordinates including two Lagrangian and one Eulerian variables. These equations are used for difference approximation:

$$\frac{\partial u}{\partial \tau} + \frac{\omega}{R}\cdot\left(\frac{\partial u}{\partial \theta} - \omega\right) = -\frac{1}{\rho}\cdot\frac{\partial p}{\partial R} ;$$

$$\frac{\partial v}{\partial \tau} + \frac{\omega}{R}\cdot\frac{\partial v}{\partial \theta} = -\frac{1}{\rho}\cdot\frac{\partial p}{\partial z} ;$$

$$\frac{\partial \omega}{\partial \tau} + \frac{\omega}{R}\cdot\left(\frac{\partial \omega}{\partial \theta} + u\right) = -\frac{1}{\rho R}\cdot\left(\frac{\partial p}{\partial \theta} - \frac{\partial R}{\partial \theta}\cdot\frac{\partial p}{\partial R} - \frac{\partial z}{\partial \theta}\cdot\frac{\partial p}{\partial z}\right) ;$$

$$\frac{\partial R}{\partial \tau} = u - \frac{\partial R}{\partial \theta}\cdot\frac{\omega}{R} ;$$

$$\frac{\partial z}{\partial \tau} = v - \frac{\partial z}{\partial \theta}\cdot\frac{\omega}{R} ,$$

where u,v,w - corresponding velocity vector components in original cylindrical coordinates with respect to variables r,z,θ.

The explicit difference scheme approximating these equations is constructed so that it should be equivalent to the two - dimensional D scheme /4/ if the motion exists which does not depend on the variable θ. Convective terms occurring due to one Eulerian variable are approximated in "upstream" manner to ensure the approximation stability. Density and internal energy variations are computed on a single time step in two stages: Lagrangian and Eulerian. For Lagrangian stage, the cell boundaries are assumed to move with material and cell masses remain unchanged, which is achieved by introducing an additional Lagrangian variable. For Eulerian stage the convection terms and quantities obtained from Lagrangian stage are used to compute the values on angularly fixed difference grid.

This method for numerical three - dimensional hydrodynamics calculations consists of splitting the region into sheets, each of them corresponding to a certain value of the Eulerian variable (angle), thus the task is divided into multiple two - dimensional tasks exchanging data. Data from one sheet are sometimes sufficient, for example, for rezoning the grid on a sheet, remapping values to a new difference grid. In this case, the code uses the same computation modules

as for the two - dimensional case.

The code organization

The MIMOZA is written using FORTRAN pre-processor SWIFT /11/ which allows to obtain various code modifications from the same source.

The code comprises a service procedure kernel and a set of handling and computation routines, the call sequence for these routines can be specified with a command language. The main routine controls the code operation by analyzing the command language using service subroutines. The service subroutines are divided into two groups. The first one relates to the lexical analyzer which assists in operating the command language. The second group includes routines for local database operation.

Local database

For dynamic operation of FORTRAN grid arrays they are put into a single common block array. Each sub-array is identified with its name and the number of a computation subregion which it relates to. Service subroutines permit to find sub-array locations, to create and to remove them. Since the local database operation is simple, users can easily write their own computation or handling modules by exploiting the code capabilities.

Command language

The command language consists of instructions and

instruction data. Data frequently consist of key parameters which must be ordered according to syntax. Initialization instruction can be taken as an example of the instruction where information is relatively hard to specify.

Computations and interrupts

Transition from one time step to another is accomplished by computational routines. Each computation routine has a standard name: PROGO1, PROGO2 etc. Each computation region may have its own set of computation routines which can be changed with special instructions. The COMPUTE instruction performs a call within a computation subroutine loop through computation routines specified in computational regions. Prior to COMPUTE instruction complete computation conditions can be specified and any potential action can be provided at a given time step at any time.

Initial data calculation

The RND instruction allows to calculate the initial data for a wide spectrum of two - dimensional problems. For three - dimensional problems, geometry specification is restricted. In MIMOZA, the RND data specification language is based on its predecessor from SIGMA/10/. The RND data are divided into a list of geometric objects, region boundary geometry description, regional information. The list of geometric objects includes descriptions of points, straight lines, circles and lines (curves which consist of straight line

segments and arcs). Geometric object identifiers consist of characters and digits,with the first character specifying the object type: T - point, P - straight line, K - circle, L - line. A point may be determined by coordinates, intersection of straight lines, intersection of a straight line and a circle, intersection of circles and so on. The lines are specified with a list of bending points on a curve and objects which connect them.

Region description

Region descriptions rely upon previously specified simple geometric objects. For each region, its boundaries, the point locations along the boundary must be specified and algorithms for configuring the grid inside the region should be given. Some descriptions can be omitted, then the routine selects descriptions by default. In addition to region geometry initial and boundary conditions should be set. The whole specified information is controlled and full diagnostic data are generated if an error occurs.

Numerical examples

Problem 1. Figures 1 - 3 show initial geometry and computational results for an explosion produced in a cylinder cavity filled with a material having a density lower as compared to the surrounding density. Initially, energy was uniformly distributed in a spherical source. Gas dynamics was computed for the cavity and elastic- plastic properties were

considered for the surrounding material. The grid is rezoned and values are mapped for each time step. It is seen that the grid remains reliably regular even though strong distortions are observed. The region of initial energy release was traced with concentrations; the level of 0.5 is shown in figures. Till later times, the calculations were performed by moving to a spherical grid.

Problem 2. To illustrate the computational capabilities for Eulerian problems including ionization kinetics and medium dissociation consider a powerful explosion (like "Teak") produced in model atmosphere at a high altitude. The kinetics includes time variations of molecule , atoms, molecular and atomic ions concentrations. Figure 4 shows ion and electron temperatures. Areas of material non-equilibrium state are clearly observed on the plot. Figures 5 and 6 show localization regions for molecules (black), neutral atoms (blue), simple (green) and double (red) atomic ions. Highly non-equilibrium medium state is indicated by a high level ionization observed in areas where the temperature is less then 0.5 eV.

Problem 3. Three - dimensional calculations for a spherical body impacting a plane target at an angle. The angle between velocity and normal of obstacle is $\alpha = 60^{o}$, initial velocity is $u = 5$. Initial target density is 2.7 and that of the ball is 18.7. Both regions used the following equation of

state

$$p(\rho_o, \varepsilon) = \begin{cases} -Prt, & \text{if } p_1 < -Prt \\ \text{else} & p_1 \end{cases}$$

where $p_1 = \frac{\rho_o \cdot C_o^2}{C_n} \cdot \left[\left(\frac{\rho}{\rho_o} \right)^{C_n} - 1 \right] + C_\gamma \cdot \rho \cdot (\varepsilon - \varepsilon_n)$,

$$\varepsilon_n = \frac{\rho_o \cdot C_o^2}{C_n} \cdot \left[C_n - 1 - \frac{\rho}{\rho_o} \cdot C_n + \left(\frac{\rho}{\rho_o} \right)^{C_n} \right]$$

where ρ_o- initial material density. The constants are given in the table:

	ρ_o	C_o	C_n	C_γ	Prt
body	18.7	2.88	3.4	1.33	0.5
target	2.7	5.5	3.5	1.33	0.2

Figures 7 and 8 show the grid for initial time and for the time where the ball has penetrated the target deep enough. The void inside the ball has disappeared.

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