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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Extensive simulations of chemically reactive magneto-hydrodynamic flows have been performed at the Naval Research Laboratory. The paper discusses briefly the numerical scheme and the use of virtual disc storage. It shows how the data flow for the computation of chemical reactions is organized to achieve an optimal computing speed. As an example the plasma flow around the earth is simulated. The results show a detailed structure, therefore demonstrating the almost complete lack of diffusion.

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CONTENTS

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NUMERICAL SIMULATIONS OF MAGNETO-HYDRODYNAMIC CHEMICALLY REACTIVE FLOWS IN THREE-DIMENSIONS ON A VECTOR COMPUTER

I. Introduction

Large numerical simulations of three dimensional flows have been performed at the Naval Research Laboratory. The limitations of the present day computers with a word storage of about 10^6 words and a speed of about 10^7 operations/sec impose severe restrictions on the kind of problems one can do in a reasonable time on a computer.

The storage restriction can be somewhat alleviated by using discs as an intermediate storage. But still relative coarse resolution of 15-30 meshpoints per dimension is a serious drawback. It can be partially overcome by using an appropriate coordinate system and a closely connected difference scheme.

The requirements on a good numerical scheme in multidimension can be stated as follows:

1) at least second order in space and preferably also in time

2) as non- diffusive as possible

3) the convection terms have to be monotonic. This implies the use of a (nonlinear) hybridization with a first order scheme

4) adjusted coordinate system, stretched mesh

5) all points should be closely connected. This excludes in 3-D the use of a leapfrog scheme.

6) the scheme should be non-time split

7) the scheme should be conservative to the extent possible.

Many problems require a transport of many chemical species which react chemically with each other at one meshpoint. The resulting ordinary differential equations are generally stiff. The scheme used here is a second order predictor, corrector method.

In chapter II the hydrodynamic scheme will be briefly explained with a 1-D example. Chapter III shows the implementation of the scheme in a 3-D code. Specially the problem of keeping the magnetic fields divergence free and the problem of high characteristic speeds are discussed. Chapter IV presents the numerical scheme for the ordinary differential equations and shows the data flow. Chapter V gives an overall flowchart for a multifluid code and for interweaving computations, writing and reading discs. Chapter VI shows the results of 3-D computations for the plasma flow around the earth. The example demonstrates clearly that even with a coarse resolution it is possible to get detailed results.

II. One dimensional example

The numerical scheme (PHOENIX) presented here is the simplest possible second order scheme. The hydrodynamic variables, density and pressure are defined at meshpoints and time t, the velocities as defined at midpoints and time $t - \frac{dt}{2}$, the magnetic fields are given at the same points in space as the velocities, but at time t. PHOENIX is an explicit code, therefore the time step limitation is given by the Courant condition.

The scheme will be explained on the one dimensional continuity equation for the number density in cartesian coordinates

$$\frac{\partial n}{\partial t} = - \frac{\partial}{\partial x} (nv)$$

Let us define the following operators

$$m^{\pm}(f_j) = \frac{1}{2} (f_j + f_{j \pm 1})$$

$$\nabla^+(f_j) = f_{j+1} - f_j$$

$$\nabla^-(f_j) = f_j - f_{j-1}$$

$$pdm^-(v, f) = (m^- - \eta \, sign \, (v) \, \nabla^-)f$$

and

$$f^{\pm} = f_{j \pm 1}$$

where η is the diffusion coefficient. The numerical scheme for solving the continuity equation can be written as

$$\hat{n} = n - \frac{dt}{dx} \nabla^+ (v \, pdm^-(v,n))$$

where "^" denotes the value at $t + dt$.

The PDM operator, the so called partial donor cell operator, will now be explained. The diffusion coefficient η has to be chosen such that n remains monotonic. This means that the convected n_j has to be bounded by n_{j+1}, and n_{j-1}. One can easily see that $\eta = 0$ gives no diffusion and $\eta = 1/2$ the donor cell method. The partial donor cell method [1] determines η nonlinearly. One should remark here that this method gives no clipping for $v = 0$, in contrasts to flux corrected transport [2,3] FCT. The method can be easily used to hybridize higher order schemes [4]. In the PHOENIX scheme the formula for $\eta \, \nabla f$ is

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$$\eta \nabla f = \frac{1}{2} \, \text{sign} \, (\nabla f) \, \max \left[0, |\nabla f| \right.$$

$$- \beta/4 \Big(\text{sign} \, (\nabla f^+) + \text{sign} \, (\nabla f) \Big) (1 + \text{sign}(v)) \, |\nabla f^+|$$

$$- \beta/4 \left. \Big(\text{sign} \, (\nabla f^-) + \text{sign} \, (\nabla f) \Big) (1 - \text{sign} \, (v)) \, |\nabla f^-| \right]$$

where $\beta = .8$ is usually used to maintain a small amount of diffusions.
($\beta = 0$ the donor cell). One may also note that an extremum, the maximum
diffusion, is taken in order to avoid overshoots.

PHOENIX uses velocities and pressure as variables. The momentum and energy
equation are solved in the same fashion as explained above. It is easy to
conserve total mass numerically. All other physical quantities like
momentum or total energy are conserved to the order of the scheme. Energy
conservation is used as a check. Theoretically the nonconservation is small,
but not necessarily in practice because of the occurrence of discontinuities.

In general, it is not advisable to conserve total energy
numerically because the error in computing the pressure (temperature) can
become very large. The temperature is a critical variable for reactions and
radiation and has to be as accurate as possible. A scheme which does not
conserve total energy numerically has to loose energy in order to be stable.
In order to show that the code works properly in one dimension, the numerical
solution of a diaphram problem as posed by Sod [5] has been used as a test.
The parameters are as follows

$P_1 = 1.$	$P_2 = .1$
$\rho_1 = 1.$	$\rho_2 = .125$
$v_1 = 0$	$v_2 = 0$
$\gamma_1 = 1.4$	$\gamma_2 = 1.4$

The resulting machnumber is 1.62. Figures 1,2,3 show the densities, presures
and velocities after the shock traveled a quarter of the mesh (t=.147 sec).
One solid line gives the analytic solution of the Riemann problem, the other
solid line shows the results of a high resolution calculation with 180 meshpoints,
the dashed the results for 25 meshpoints. One can see that the results for the
high resolution case are quite good. For the low resolution case the main
features are still represented. This is the kind of resolution one will find
in a typical 3-D calculation.

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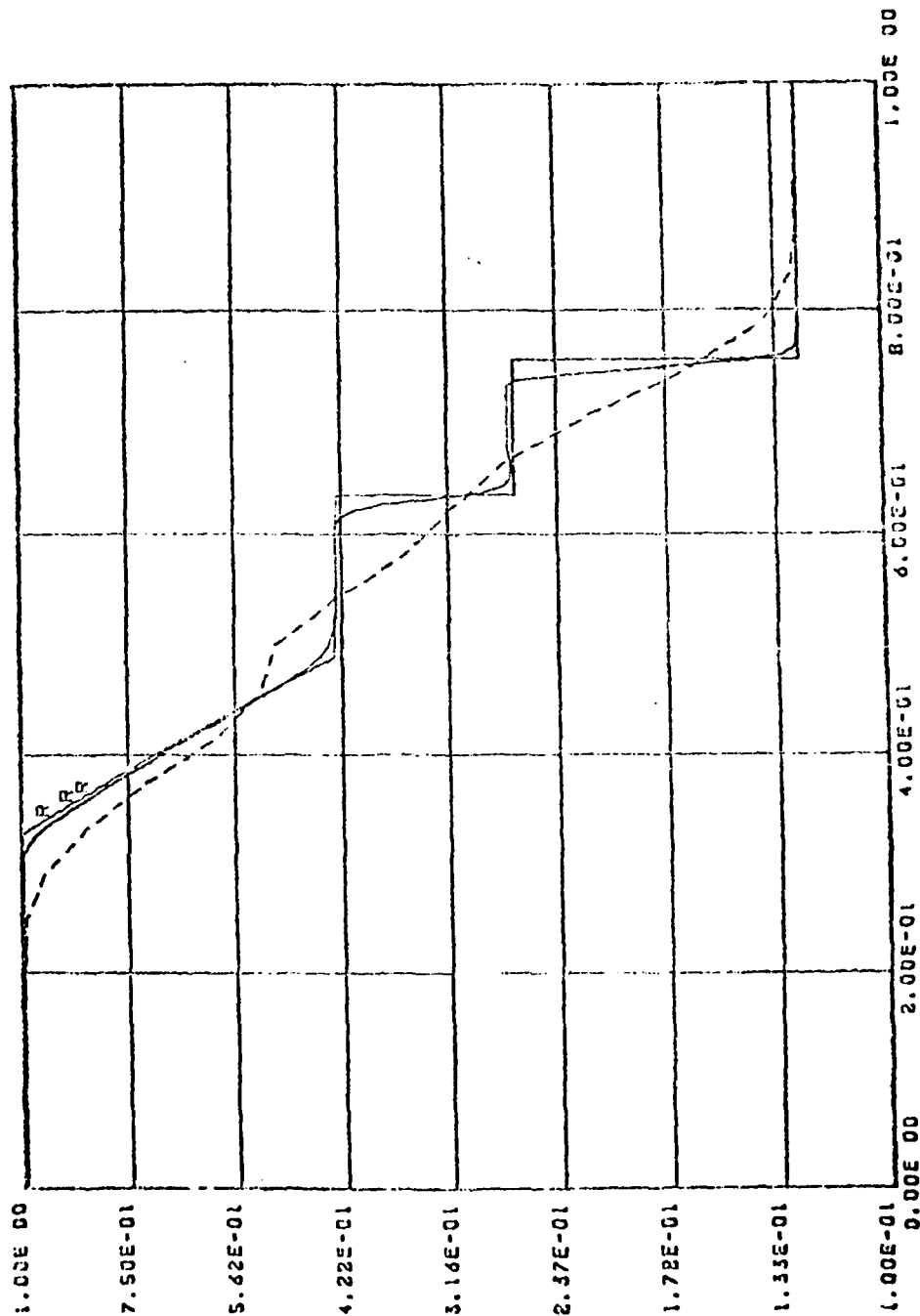
Fig. 1 — Diaphragma at .147 sec: density profiles

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Fig. 2 — Diaphragma at .147 sec: pressure profiles

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Fig. 3 — Diaphragma at .147 sec: velocity profiles

III. Extension to two and three dimensions

The PHOENIX scheme can be easily extended to two and three dimensions, but several points should be made.
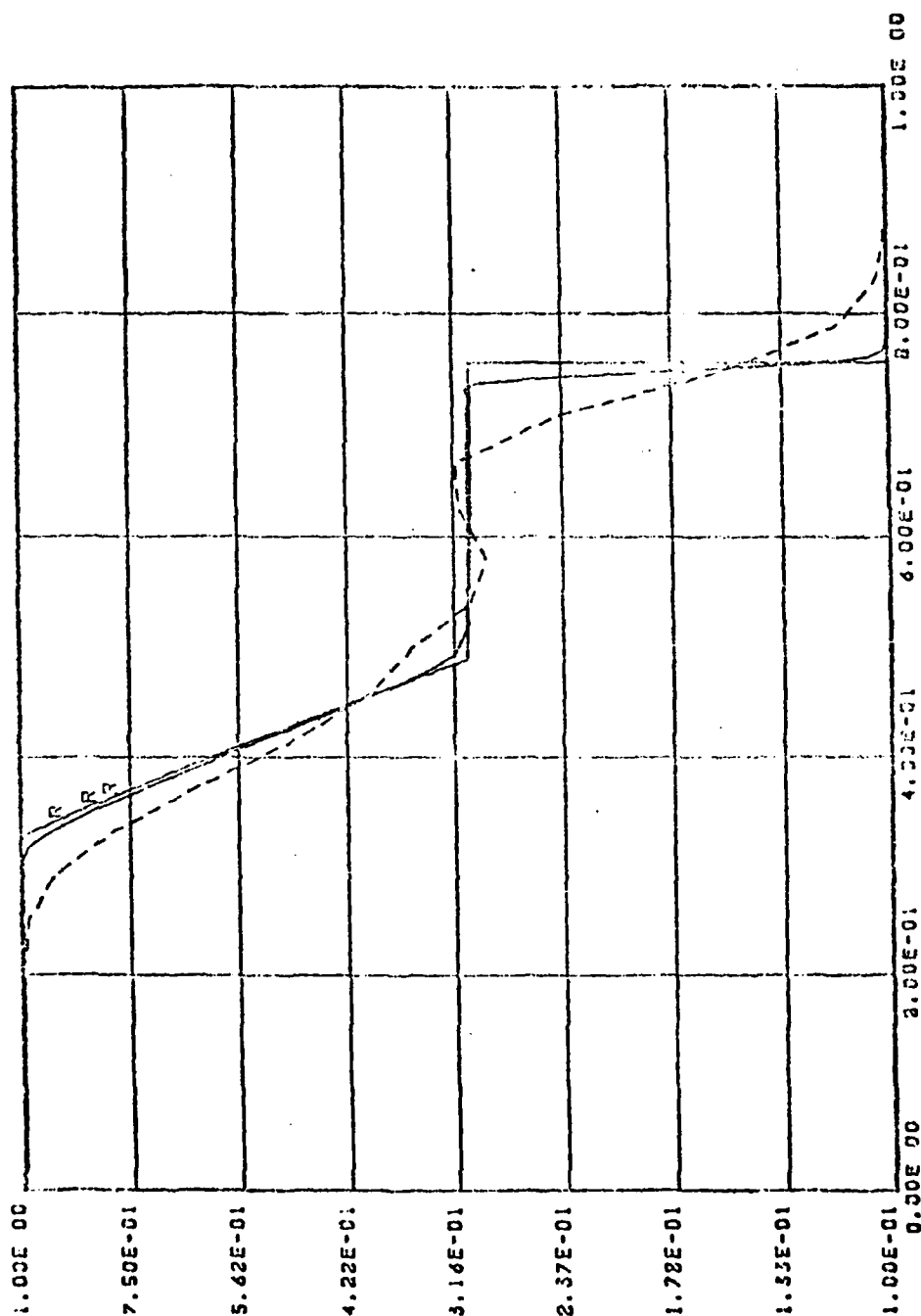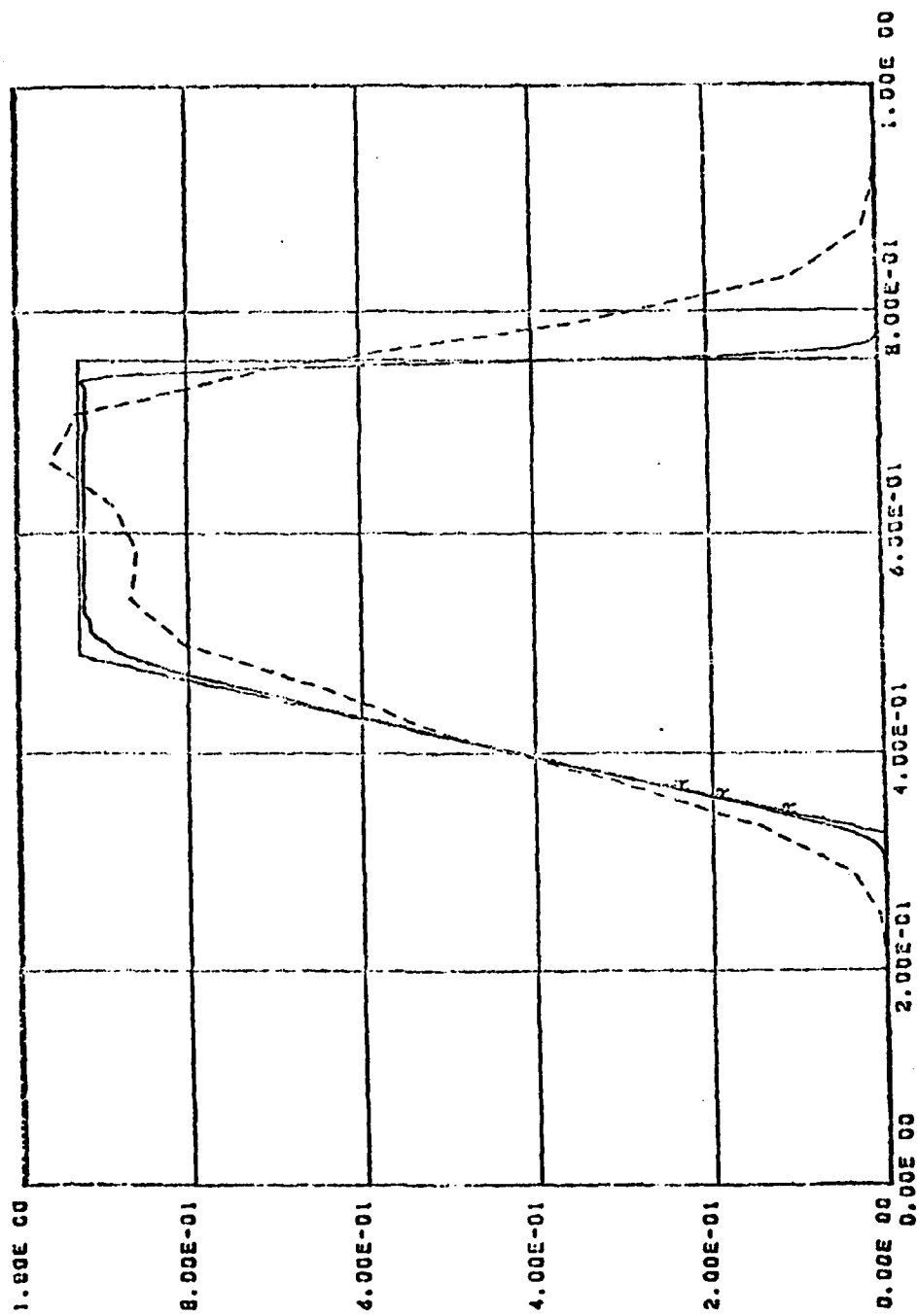
Shockwidths should be constant in the number of points over which the shockfront is computed. The shock should not be more than 4 meshpoints wide. In general the meshspacing is not the same for different directions, therefore, it follows that, the artificial shock pressure used in the code is not isotropic in physical space. PHOENIX gives a shockwidth of 2-3 meshspacing. In a magnetohydrodynamic flow the magnetic field has to remain numerically divergence free. This can be achieved in two ways, either one computes the vector potential or one uses the curl of the electric fields to advance B. In many 2-D problems the first approach is useful because there is only one component of the vector potential. In 3-D the latter approach is more suitable. The PHOENIX scheme computes the electric fields in the magnetic field calculation. This approach avoids the taking of second derivatives which may introduce numerical noise. In the compuation of the electric field the PDM operator is used. It results in a resisitivity which causes B to be monotonic (compare [2]).

In most real MHD problems there exists regions where the Alfven speed $c_\alpha = B^2/4\pi\rho$ is high, therefore requiring very small timesteps. The time step can be increased in two ways, either by using an implicit scheme for computing B or by limiting the characteristic velocity to a velocity $c_{\ell im}$ The first approach is feasible in 2-D. It involves solving implicity a diffusion equation with an diffusion coefficient c_α^2 dt . The second approach consists of increasing the density perpendicular to B by a factor $1 + c_\alpha^2/c_{\ell im}^2$, thus decreasing the accelerations perpendicular to the magnetic field. The limiting velocity $c_{\ell im}$ should be larger than any physical velocity involved.

IV. Chemical reactions

The ordinary differential equations resulting from chemical reactions at each meshpoint can be written as

$$\frac{dy}{dt} = -ay + b$$

where y represents the species array. The coefficient a and b depends also on time via species concentrations. Assuming a, b to be constant during a timestep t, the exact solution is

$$y = \left[y_0 + \frac{a}{b} (e^{at} - 1) \right] e^{-at}$$

The numerical approximation to this exact solution was chosen such that it will give the correct asymptotic solution

$$y = \frac{a}{b} \qquad \text{for } at \gg 1$$

In order to acchieve this e^{at} is approximated by

$$e^{at} = 1 + at + \frac{1}{2} a^2 t^2$$

(Some integration schemes use

$$e^{at} \approx (1 + \frac{1}{2} at)/(1 - \frac{1}{2} at)$$

which will lead to ocillations for at $\gg$ 1)

As a, b are time dependent one has to use a predictor and corrector step.

Predictor step

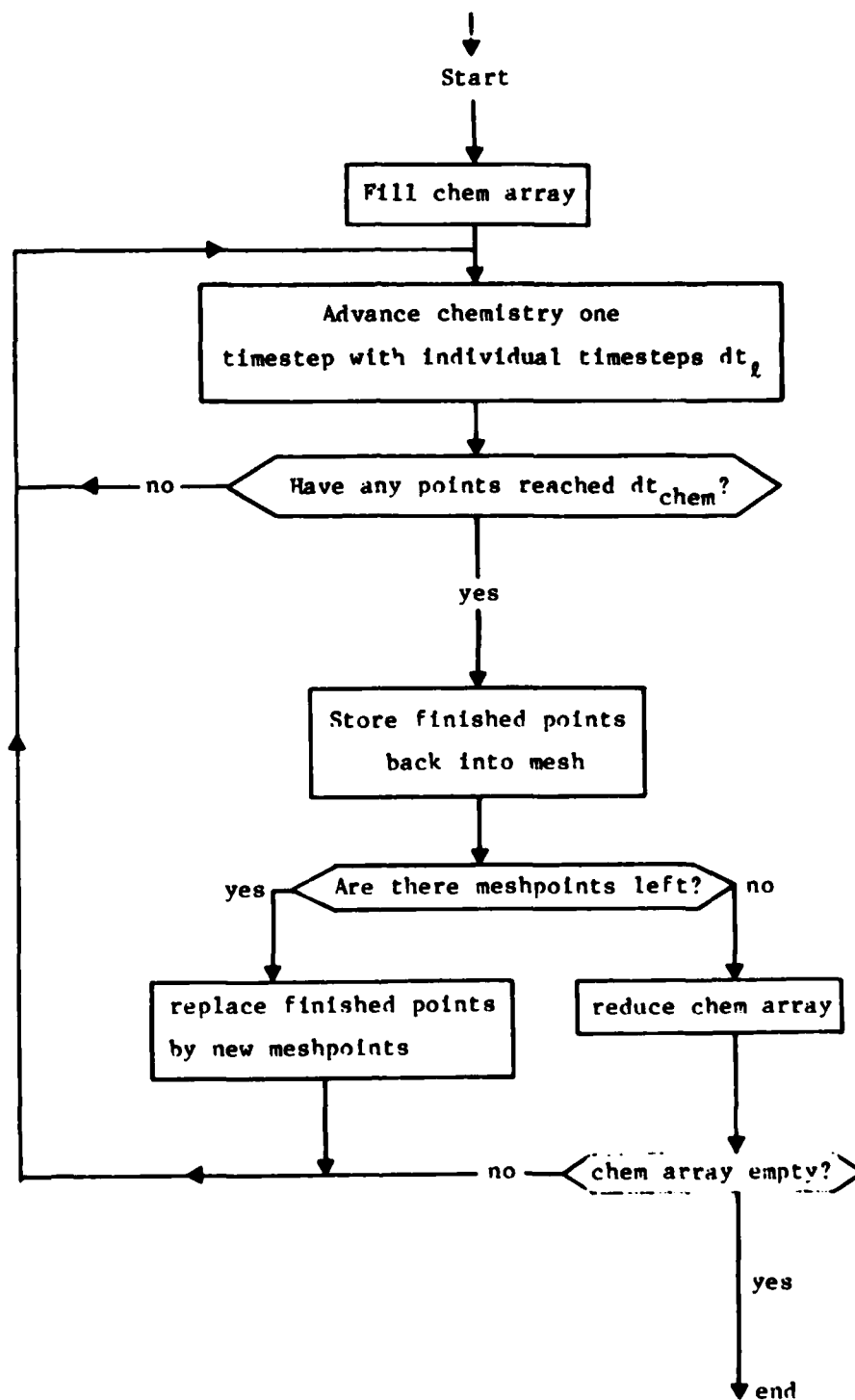$$y^e = (y_0 + b_0 (1 + \frac{1}{2} a_0 t)t)/(1 + a_0 t + \frac{1}{2} a_0 t^2)$$

Corrector step

$$y^i = (y_0 + \frac{1}{2} (b_0 + b_e (1 + a_e t))t)/(1 + \frac{1}{2} (a_0 + a_e (1 + a_e t))t)$$

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The difference betwen y^e and y^i determines the time step.

The setting up of the differential equations and the coding for the numerical integration is achieved by an interpretive program ARIS [6]. The input to this program are the chemical reactions and reaction energies. The resulting FORTRAN code is completely vectorized. Decisions are made by the use of sign functions rather than IF statements. This permits great improvements in speed as the sign function statements are vectorized.

The chemical reactions have to be solved at every meshpoint for a certain time interval t_{chem}. As the species concentrations and temperature are different at every meshpoint the number of timesteps needed for a given error varies from point to point. As the computations are fairly complicated, the number of auxiliary arrays is large, therefore the simultaneous solutions are set up for an array of length $m < n$ where n is the number of meshpoints. Usually $m = 200$. The data flow is shown in the following flowchart

10

Start

Fill chem array

Advance chemistry one
timestep with individual timesteps dt_ℓ

no — Have any points reached dt_{chem}?

yes

Store finished points
back into mesh

yes — Are there meshpoints left? — no

replace finished points
by new meshpoints

reduce chem array

no — chem array empty?

yes

end

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In this way the chem array is always filled until the last point is completed. This optimization achieves an efficiency of about 75% of the maximum speed (about 3.10^7 op/sec at the ASC of Texas Instruments).

V. Flow charts and data flow

The following flowchart gives the general computational scheme for solving the magnetohydronamic equations for one timestep. As the PHOENIX scheme is explicit, the timestep has to be determined by the Courant condition. Furthermore, the stability conditions require that first all ρ p, $\vec{B}$ computed, afterwards the velocities are updated. In addition, a limiting velocity c is used here

$$dt < \beta \min (dx/(\overset{*}{c} + v))$$

$$\overset{*}{c} = \sqrt{\gamma P/\rho} \qquad\qquad \text{for neutral}$$

$$\overset{*}{c} = \sqrt{\gamma P/\rho} + \min (c^2, \frac{B^2}{4\pi\rho}) \qquad \text{for plasma}$$

$$\rho = \rho - dt \nabla(\rho v)$$
$$p = p - dt \; (\nabla p v) + (\gamma - 1)p\nabla v)$$

Plasma? — no

yes

$$B = B + dt \; \nabla x \; (B \; x \; v)$$
$$v = v + \frac{dt \; B \; x \; S}{4\pi \; (\rho + B^2/(4\pi c^2))}$$

$$\hat{v} = v - dt((v\nabla)v + \frac{1}{\rho} \nabla P)$$

Plasma? — no

yes

$$\hat{v}_\perp = v_\perp + \frac{\hat{v}_\perp - v_\perp}{1 + B^2/(4\pi\rho c^2)}$$

Shock

$$v = \hat{v} - \frac{dt \; \nabla q}{\rho}$$
$$P = P - dt(\gamma - 1)q\nabla v$$

out
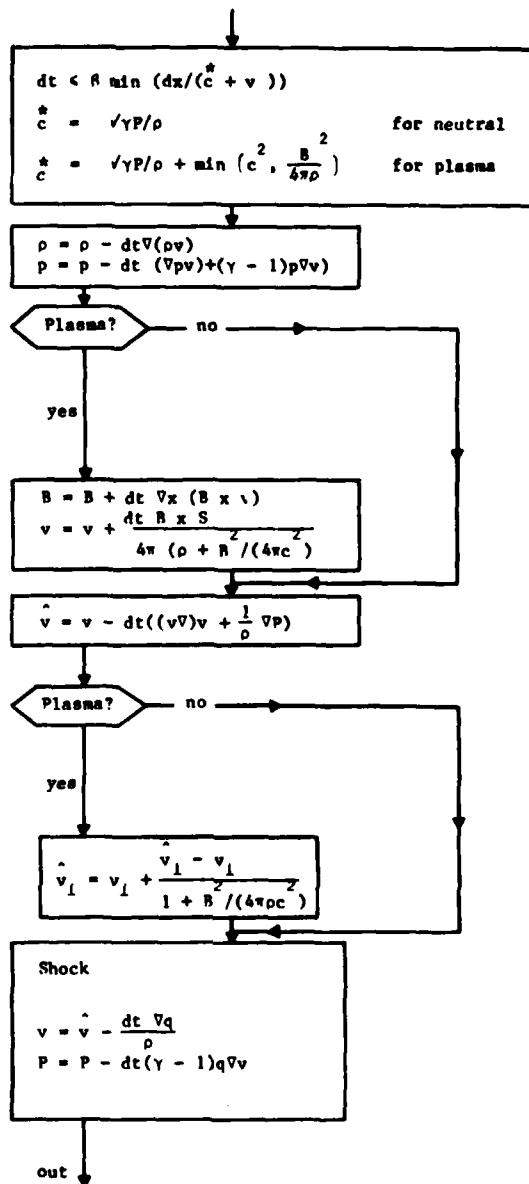
In a multifluid code each of the fluids can have their own timestep. They interact with each other through collision terms. The chemistry is called independently.

Some of our large simulations require a data base which exceeds the available core storage of about 10^6 words. This requires the use of disks as an intermediate storage. The computation is done for one plane in the third dimension at one time.

PDM (or FCT) requires the code to keep at least 5 planes in core. PHOENIX, because of the definition of v_3 at midpoints, needs one more plane.

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The reading and writing has to be done simultaneously with the computations. This adds two more planes. Therefore 8 planes have to be in core. The restriction on the number of points $n_1 \times n_2$ is therefore given by

$$8 \times L_{var} \times n_1 \times n_2 < core - auxilary\ variables$$

where L_{var} is the total number of variables used.

PDM (or FCT) require the computation of higher order differences. For the third direction these computations have to be repeated. This increases the number of computations by about 10%.

There are about 150 operations per point and variable. The time per operation on the ASC of Texas Instruments is about 3×10^{-8} sec, therefore the computing time per point and variable is $\approx 5\ 10^{-6}$ sec. Assume $n_1 \times n_2 = 650$, and the number of variables to be 30, such that $\ell_{var} \times n_1 \times n_2 \approx 2 \times 10^4$. This gives $\approx .1$ sec per plane. For 50 planes this will give 5 sec per timestep.

The I/O operations are done in one I/O instruction without using additional buffer storage. The correctness of the data transfer is checked after completion.

The core storage is used in a revolving fashion. If L is the index to reference a 2-D plane, then the 2-d planes of all variables for -L- are stored as one sequential block. The start index for such a block is given by
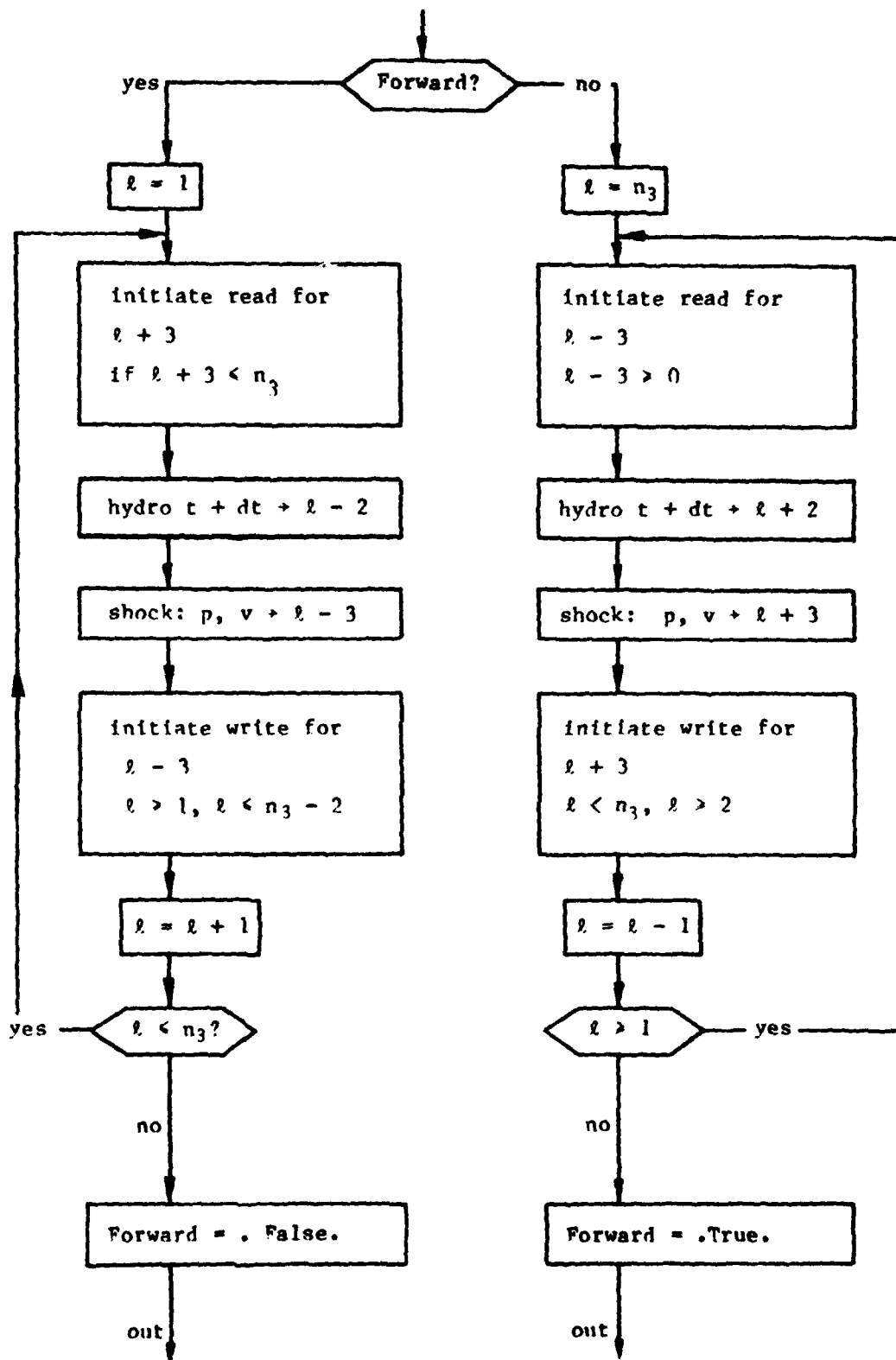
$$Lf(L) = L_{var} \times n_1 \times n_2 \times mod(L + 7, 8) + 1$$

The address of one special variable n, is then given by

$$L_{varn}(L) = Lf(L) + (n - 1) \times n_1 \times n_2$$

To be able to write a comprehensible program the names of physical variables are set with equivalences.

In order to save I / O operations, the hydrodynamic calculation can run forward or backward in the third dimension. These are always the first or last three planes in core. The following flow chart will show the data flow

14

Forward?

yes — no

left branch (yes):

$\ell = 1$

initiate read for
$\ell + 3$
if $\ell + 3 < n_3$

hydro $t + dt \rightarrow \ell - 2$

shock: $p, v \rightarrow \ell - 3$

initiate write for
$\ell - 3$
$\ell > 1, \ell < n_3 - 2$

$\ell = \ell + 1$

$\ell < n_3?$ — yes

no

Forward = .False.

out

right branch (no):

$\ell = n_3$

initiate read for
$\ell - 3$
$\ell - 3 > 0$

hydro $t + dt \rightarrow \ell + 2$

shock: $p, v \rightarrow \ell + 3$

initiate write for
$\ell + 3$
$\ell < n_3, \ell > 2$

$\ell = \ell - 1$

$\ell > 1$ — yes

no

Forward = .True.

out

VI. 3-D example

As an illustration of the capabilities of the 3-D MHD code, the
interaction of the solarwind with the earth dipole field has been computed. [7],
[8] The earth dipole field is formed by placing a current loop in one of the
cells. A solar wind is then introduced at the left x boundary. It has a
velocity of 400 km/sec and carries a density of 5 particles/cm^3. In the
example shown it carries also a southward field of -2γ . The length unit is
one earthradius. The computation shown required about half an hour of
computing time and simulated two hours in real time (about 2000 time steps).
The mesh is 29 x 21 x 21 $\approx$ 13000 points. Several difficulties arose during
the runs. The main one involved the internal boundary at the earth. This
problem produced large currents due to the sharp field curvature and low
resolution. This was solved by massloading the cells around the earth, and not
allowing the mass to move.

One other interesting phenomena occurred. The plasma sheet behind the
earth contains opposite fields. The configuration is physically unstable to
resistive instabilities, resulting in reconnection of field lines. Although
the code is nearly diffusion free, this occurred during test runs showing up
as reconnections of the magnetic field lines, a result that is thought to
cause magnetic substorms when physically initiated. [8]

The Figs. 4 and 5 show density and pressure in the noon-midnight meridional
plane. The lines display the actual grid used. One can see the density
increase at the bowshock by about a factor of 3. The machnumber is about 3.
Also one can see a slight increase in density in the plasma sheet which is
about about one cell wide. The pressure graph shows the structure a bit
clearer. It also shows the side lobes of higher pressure.

These results show clearly that one can keep detailed structures even
with a relative coarse resolution. They also demonstrate the almost complete
lack of diffusion.

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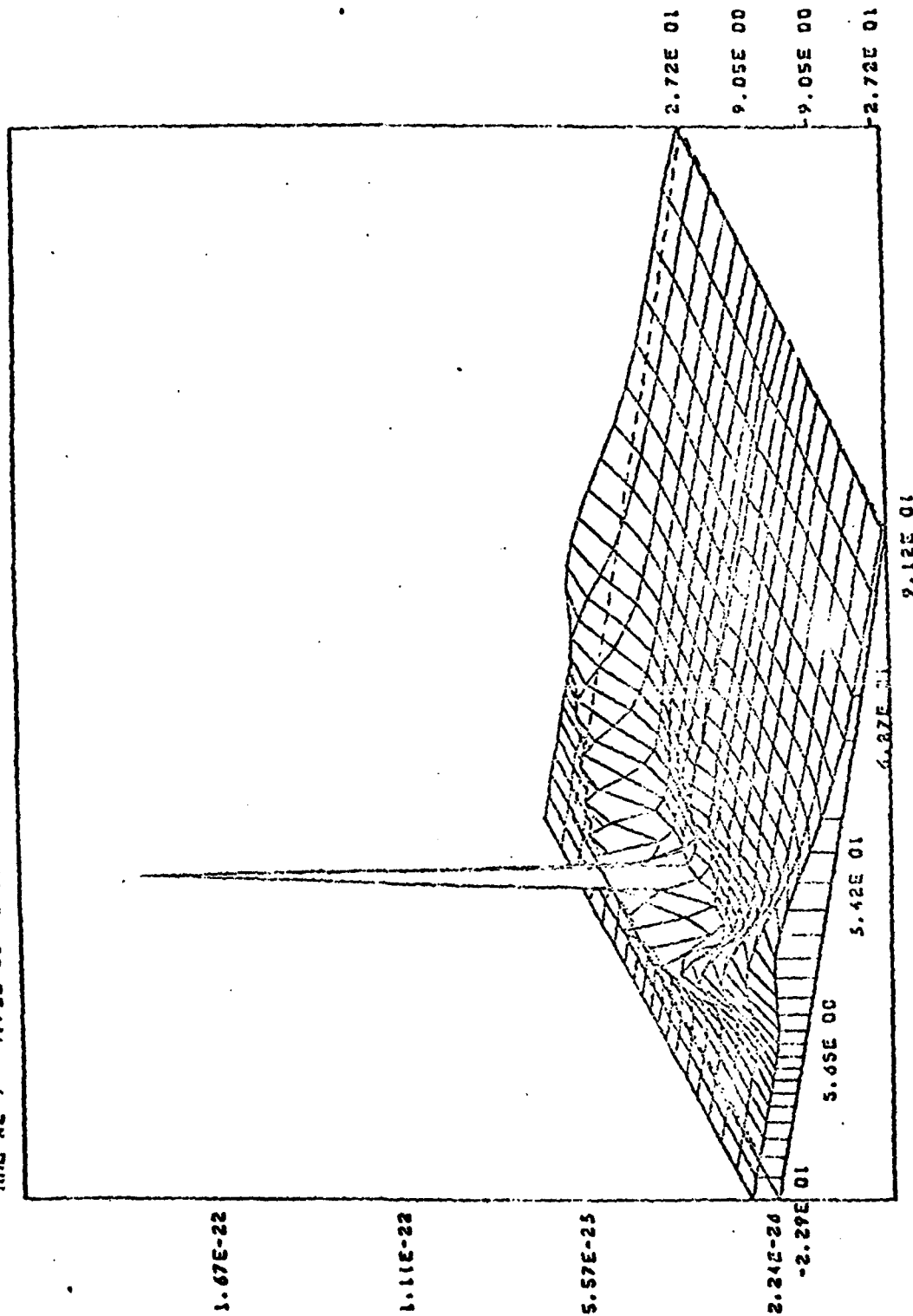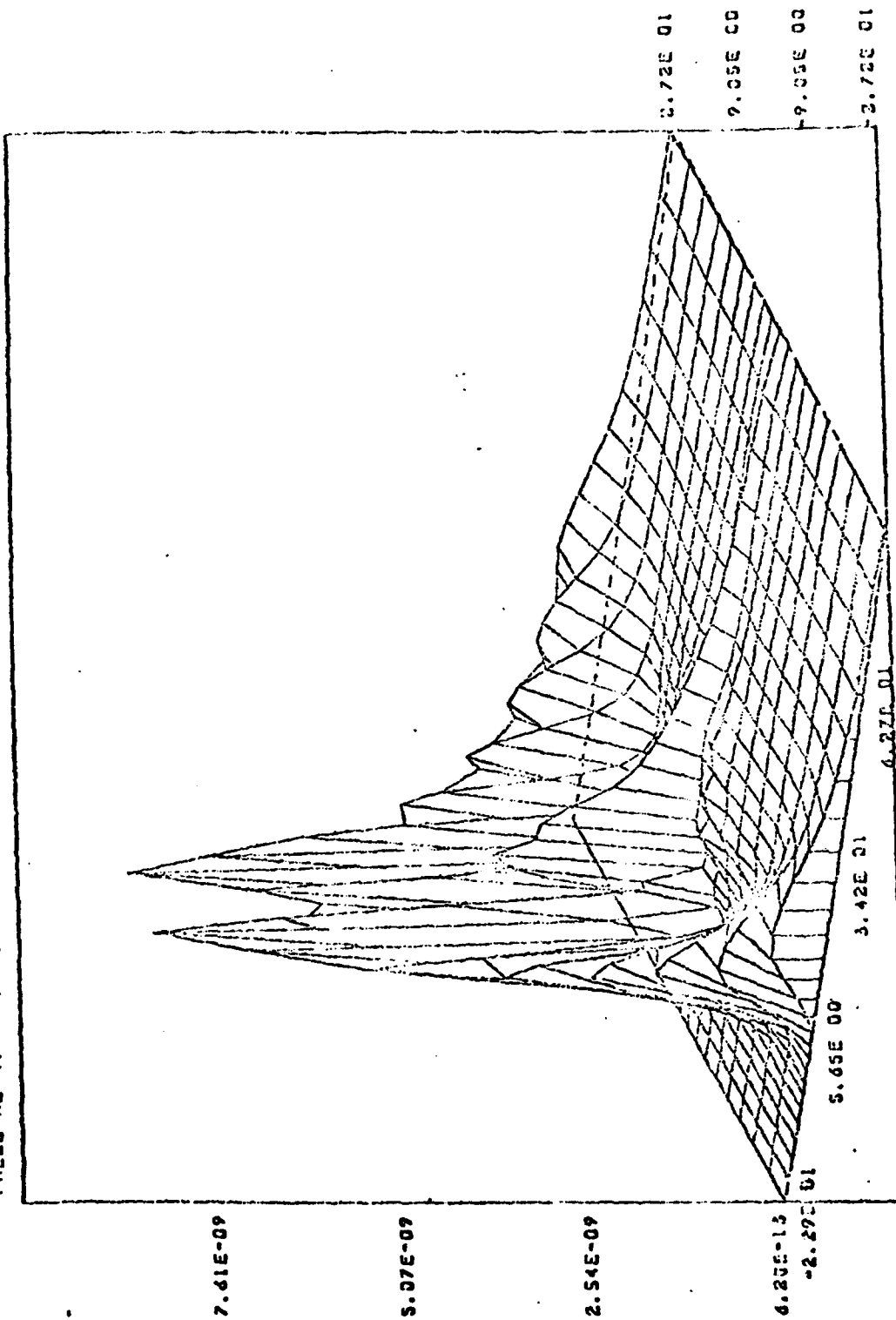Fig. 4 — Bow shock with IMF = -2γ: density plot

Fig. 5 — Bow shock with IMF = -2γ: pressure plot

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VII. Conclusion

It is possible to perform realistic 3-D simulations with present day computers.

The use of an adjusted coordinate system in combination with a numerical scheme which closely connects neighboring points can give detailed structures even with a relative coarse resolution. The non diffusivity will keep those structures during a calculation. The use of virtual disc storage can al least partially overcome the limitations of the core storage. The optimization achieved by the vectorization of the chemical reactions makes it possible to do realistic 3-D flow problems which involve many species and their interactions.

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