2DE - A Two-Dimensional Eulerian Hydrodynamic Code for Computing One Component Reactive Hydrodynamic Problems
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2DE - A Two-Dimensional Eulerian Hydrodynamic Code for Computing One Component Reactive Hydrodynamic Problems

by

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ABSTRACT

This report is a description of a code for the IBM 7030 computer for computing two-dimensional reactive hydrodynamic problems in cylindrical geometry using a modification of Gentry's finite difference analogs of the Eulerian equations of motion for a compressible fluid.

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I. INTRODUCTION

This study was undertaken to determine if the Eulerian approach to reactive hydrodynamic problems might be useful in solving reactive flow, one-component problems which result in severe distortion of a Lagrangian mesh. The problem of interest was the failure of a nitromethane detonation wave, with a numerically resolved reaction zone, caused by side rarefactions. The numerical method described in this report will compute the nitromethane failure problem.

The finite difference analogs of the Eulerian equations of motion for a compressible fluid described in this report are similar to the FLIC method described by Gentry, Martin and Daly\(^1\) which was an outgrowth of the work of Rich\(^2\). The OIL method for velocity weighting in the mass flux phase of the calculation was found to be the best method described in the literature. The OIL method was developed by M. Walsh's group at General Atomic Division of General Dynamic Corporation. It was first described in a report written by W. E. Johnson.\(^3\) The densities used in the mass flux were treated as the new Lagrangian densities rather than old Eulerian ones. This was first found to be useful by Gentry.\(^4\)

Since reactive hydrodynamic problems require as much numerical resolution as possible, the code (called 2DE) was written to make maximum use of the large capacity disk storage of the IBM 7030 (STRETCH) computer. The maximum height of the mesh is 3000 cells, and the maximum number of cells is 200,000. The numerical calculations require sufficient time to permit the data transfer between the disk and core memory to be overlapped.
This report describes the method used in complete detail. It also presents sufficient details for a coder to be able to follow and change the code. The latter information is not of interest to the casual reader.

II. THE HYDRODYNAMIC EQUATIONS

The partial differential equations for nonviscous, nonconducting, compressible fluid flow in cylindrical coordinates are

\[
\frac{\partial \rho}{\partial t} + \frac{U \partial \rho}{\partial R} + \frac{V \partial \rho}{\partial Z} = -\rho \left( \frac{\partial U}{\partial R} + \frac{\partial V}{\partial Z} + \frac{U}{R} \right) \quad \text{Mass}
\]

\[
\rho \left( \frac{\partial U}{\partial t} + \frac{U \partial U}{\partial R} + \frac{V \partial U}{\partial Z} \right) = -\frac{\partial P}{\partial R} \quad \text{Momentum}
\]

\[
\rho \left( \frac{\partial V}{\partial t} + \frac{U \partial V}{\partial R} + \frac{V \partial V}{\partial Z} \right) = -\frac{\partial P}{\partial Z} \quad \text{Energy}
\]

The equations are written in finite-difference form appropriate to a fixed (Eulerian) mesh of cells and used to determine the dynamics of the fluid. The fluid is moved by a continuous mass transport method.

The first of the above equations, that of mass conservation, is automatically satisfied. The momentum and energy equations are treated as follows: In the first step, the contributions to the time derivatives which arise from the terms involving pressure are calculated. The mass is not moved at this step; thus the transport terms are dropped. Tentative new values of velocity and internal energy are calculated for each cell.
In the second step, the mass is moved according to the cell velocity. The mass which crosses cell boundaries carries with it into the new cells appropriate fractions of the mass, momentum, and energy of the cells from which it came. This second step accomplishes the transport that was neglected in the first step.

In the third step, the amount of chemical reaction is determined, and the new cell pressure is computed using the HOM equation of state. The equations we shall difference are of the form

\[
\frac{\partial V}{\partial t} = - \frac{\partial (P+q)}{\partial R}
\]

\[
\frac{\partial U}{\partial t} = - \frac{\partial (P+q)}{\partial Z}
\]

\[
\frac{\partial I}{\partial t} = - \frac{\partial VR}{R} \frac{\partial VR}{\partial R} - \frac{1}{R} \frac{\partial VR}{\partial R} + 2 \frac{\partial q}{\partial R} - \frac{\partial VR}{\partial Z} - \frac{\partial U}{\partial Z} + U \frac{\partial q}{\partial Z}
\]

III. THE CODING EQUATIONS AND TECHNIQUES

Problem Boundaries

- Axis
- Piston (Constant Input) Boundary
- Continuum
- Cell Sides

Continuum

Continuum

Continuum

Continuum

2

3

4

1
The Initial Problem Setup

Cell Quantities

- \( \rho \) - CM - cell density
- \( I \) - CI - cell energy
- \( P \) - CP - cell pressure
- \( T \) - CT - cell temperature
- \( W \) - CW - cell mass fraction
- \( U \) - CU - cell z velocity
- \( V \) - CV - cell r velocity
- \( \hat{\rho} \) - RHOT - tilde density

Intermediate Quantities

- \( q \) - Q1, Q2, Q3, Q4 - Viscosities (locations also used as \( \Delta \) quantities in mass movement)
- \( V' \) - CMB - 1/\( \rho \) (location also used as \( \Delta M \) in mass movement)
- \( \hat{U} \) - CUB - cell z velocity tilde
- \( \hat{V} \) - CVB - cell r velocity tilde
Phase I. Equation of State and Reaction

The pressure and temperature are calculated from the density, internal energy, and cell mass fraction of undecomposed explosive using the HOM\(^5\) or ideal gas equation of state. \(^6\)

1. Test to determine if \(\Delta V'/V', \Delta I/I, \Delta W/W\) from the previous cell and the present cell are less than 0.0005, and if they are, use the previous cell \(P\) and \(T\).

2. If an HOM iteration error occurs and if \(W\) is > 0.5, resolve with \(W = 1.0\). If \(W\) is < 0.5, resolve with \(W = 0.0\). Print the cell \(W, P, T\) and a comment each time the HOM error occurs.

Knowing \(T\) we calculate \(W\) using the Arrhenius rate law

\[
\frac{dW}{dt} = Z^*W e^{-E^*/R_g T}
\]

where \(Z^*\) is the frequency factor, \(E^*\) the activation energy, \(R_g\) the gas constant, and \(\delta t\) the time increment. In difference form this is

\[
W^{n+1} = W^n - \delta t Z^*W^n e^{-E^*/R_g T^{n+1}}
\]

1. If cell temperature is less than \(\text{MINWT(1000)}\) reaction is not permitted.
2. If \(CW\) is less than \(\text{GASW(0.02)}\) set \(CW = 0\).
3. Do not react for first \(\text{VCNT (25)}\) cycles.

Phase I, II are skipped if \(\rho_{1j}^n < \text{MINRHO} + (\rho_0 - \text{MINRHO})(W_{1j}^n)\).

This is for handling free surfaces, eliminating false diffusion. \(\text{MINRHO} = 0.5\).
Phase II. Viscosity and Velocity

A. Viscosity Equations

\[ Q_{ij}^n = q_{i-\frac{1}{2},j}^n = Q_{j-1,i,j}^n \]

except on boundary 1 when \( Q_{ij} = 0 \) or on piston boundary when

\[ Q_{ij}^n = \begin{cases} K(p_{ij}^n + \text{MAPP})(\text{UAPP} - U_{ij}^n) & \text{if } \text{UAPP} > U_{ij}^n, \\ 0 & \text{if } \text{UAPP} < U_{ij}^n \end{cases} \]

\[ Q_{ij}^{n+1} = q_{i,j-\frac{1}{2}}^n = Q_{i,j-1}^n \]

except on axis boundary when \( Q_{ij}^{n+1} = 0 \).

\[ Q_{ij}^{n+1} = q_{i+\frac{1}{2},j}^n = \begin{cases} K(p_{ij+1,j}^n + \text{MAPP})(U_{ij+1,j}^n - U_{ij,j}^n) & \text{if } U_{ij,j}^n > U_{ij+1,j}^n, \\ 0 & \text{if } U_{ij,j}^n < U_{ij+1,j}^n \end{cases} \]

except on a continuative boundary 3 when \( Q_{ij}^{n+1} = 0 \).

\[ Q_{ij}^{n+1} = q_{i,j+\frac{1}{2}}^n = \begin{cases} K(p_{ij,j+1}^n + \text{MAPP})(V_{ij,j+1}^n - V_{ij,j}^n) & \text{if } V_{ij,j}^n > V_{ij,j+1}^n, \\ 0 & \text{if } V_{ij,j}^n < V_{ij,j+1}^n \end{cases} \]

except on a continuative boundary 4 when \( Q_{ij}^{n+1} = 0 \). MAPP, UAPP, PAPP are piston applied values of mass, particle velocity and pressure. Also calculated in the viscosity section are:

\[ P_1 = P_{i-1,j}^n \]

except at piston when \( P_1 = \text{PAPP} \) or on continuative boundary 1 when

\[ P_1 = P_{i,j}^n \]
\[ P_2 = P_{i,j-1}^n \]

except on axis when \( P_2 = P_{i,j}^n \)

\[ P_3 = P_{i+1,j}^n \]

except on continuative boundary 3 when \( P_3 = P_{i,j}^n \)

\[ P_4 = P_{i,j+1}^n \]

except on continuative boundary 4 when \( P_4 = P_{i,j}^n \)

**B. Velocity Equations**

\[
\begin{align*}
\bar{u}_{i,j}^n &= U_{i,j}^n - \frac{\delta t}{\rho_{i,j} \delta z} \left[ (P+q)^n_{i+\frac{1}{2},j} - (P+q)^n_{i-\frac{1}{2},j} \right] \\
&= U_{i,j}^n - \frac{\delta t}{\rho_{i,j} \delta z} \left\{ P_{i+\frac{1}{2},j} + q_{i+\frac{1}{2},j} - P_{i-\frac{1}{2},j} - q_{i-\frac{1}{2},j} \right\} \\
P_{i+\frac{1}{2},j}^n &= \frac{(P_{i,j}^n + P_{i+1,j}^n)}{2} = \frac{(P_{i,j}^n + P_3)}{2} \\
\bar{v}_{i,j}^n &= V_{i,j}^n - \frac{\delta t}{\rho_{i,j} \delta z} \left\{ \frac{1}{2}(P_{i,j}^n + P_{i,j}^n - P_1) + q_{i+\frac{1}{2},j} - q_{i-\frac{1}{2},j} \right\} \\
&= U_{i,j}^n - \frac{\delta t}{\rho_{i,j} \delta z} \left\{ \frac{P_{i,j}^n + P_{i,j}^n - P_1}{2} + Q_{i,j} - Q_{i,j} \right\} \\
\bar{w}_{i,j}^n &= W_{i,j}^n - \frac{\delta t}{\rho_{i,j} \delta z} \left\{ \frac{1}{2} \left[ \sum_j \left( S_{j+\frac{1}{2}} (P_{i,j}^n - P_{i-1,j}^n) - S_{j-\frac{1}{2}} (P_{i,j}^n - P_{i+1,j}^n) \right) \right] \\
&= \frac{1}{\delta r} \left[ q_{i,j}^n + q_{i,j}^n - q_{i,j}^n \right] \\
&= \frac{1}{\delta r} \left[ q_{i+\frac{1}{2},j}^n - q_{i-\frac{1}{2},j}^n \right] \\
&= \frac{1}{\delta r} \left[ q_{i,j}^n - q_{i+\frac{1}{2},j}^n \right]
\end{align*}
\]
\[ S_{j+\frac{1}{2}} = 2n(j+1) \delta r \delta z \quad V'_j = 2n(j+\frac{1}{2}) \delta r \delta z \]

\[ \varphi^n_{ij} = \frac{8t}{\rho^n_{ij} \delta r} \left\{ \frac{1}{2j+1} \left[ (j+1)(P^n_{i,j,j+1}-P^n_{j,j}) -(j)(P^n_{i,j,j}-P^n_{i,j}) \right] \right. \]

\[ + \left. \frac{q^n_{i,j+\frac{1}{2}} - q^n_{i,j-\frac{1}{2}}}{J} \right\} \]

\[ = \frac{8t}{\rho^n_{ij} \delta r} \left\{ \frac{j(P^n_{4}-P^n_{2})+P^n_{i,j}}{2j+1} + \frac{Q^n_{i,j}-Q^n_{i,j}}{J} \right\} \]

**Phase III. Internal Energy and \( \rho \)**

**A. Piston Energy Constraint**

For the first VCNT cycles the internal energy is calculated from

\[ \mathcal{I}^n_{ij} = \frac{1}{2}(P^n_{ij}+Q^n_{ij})(V^n_{ij} - \frac{1}{\rho^n_{ij}}) + \mathcal{I}_0 \quad V'_o > \frac{1}{\rho^n_{ij}} \]

\[ \mathcal{I}^n_{ij} = \mathcal{I}^n_{ij} \quad V'_o < \frac{1}{\rho^n_{ij}} \]

**B. \( \rho \) Calculation**

\[ \rho^n_{ij} = \rho^n_{ij} \left[ 1 - \frac{8t}{2\delta r}(V^n_{i,j+1}-V^n_{i,j}) - \frac{8t}{2\delta z}(U^n_{i+1,j}-U^n_{i-1,j}) \right] \]

On piston boundary, \( U_{i-1,j} = \text{UAPP} \)

On axis boundary, \( V_{i-1,j} = V_{ij} \)

On boundary 3, \( U_{i+1,j} = U_{ij} \)

On boundary 4, \( V_{i,j+1} = V_{ij} \)
On boundary 1, \( U_{i-1,j} = U_{i,j} \)

For \( \rho_{ij}^n < \text{MINRHO} + (\rho_o - \text{MINRHO})(w_{ij}^n) \), \( E_{ij}^n = I_{ij}^n \), and the rest of Phase III is skipped.

\[ \gamma_{ij} = \gamma_{ij}^n = \frac{\Delta t}{\rho_{ij}^n v_j} \left\{ p_{ij}^n(S_{j+\frac{1}{2}}^r v_{ij}^n + S_{j-\frac{1}{2}}^r v_{ij}^n) - \frac{1}{2} q_{i-\frac{1}{2},j}^n (S_{j-\frac{1}{2}}^r v_{ij}^n + S_{j+\frac{1}{2}}^r v_{ij}^n) \right\} 
\]

\[ \gamma_{ij} = \frac{\Delta t}{\rho_{ij}^n v_j} \left\{ p_{ij}^n(S_{j+\frac{1}{2}}^r v_{ij}^n + S_{j-\frac{1}{2}}^r v_{ij}^n) - \frac{1}{2} q_{i-\frac{1}{2},j}^n (S_{j-\frac{1}{2}}^r v_{ij}^n + S_{j+\frac{1}{2}}^r v_{ij}^n) \right\} 
\]

\[ E_{ij} = E_{ij}^n = \frac{\Delta t}{\rho_{ij}^n v_j} \left\{ p_{ij}^n(S_{j+\frac{1}{2}}^r v_{ij}^n + S_{j-\frac{1}{2}}^r v_{ij}^n) - \frac{1}{2} q_{i-\frac{1}{2},j}^n (S_{j-\frac{1}{2}}^r v_{ij}^n + S_{j+\frac{1}{2}}^r v_{ij}^n) \right\} 
\]

\[ s_{ij}^r = 2n(j+\frac{1}{2}) \delta r \delta z \quad v_j^t = 2n(j+\frac{1}{2}) \delta r^2 \delta z \quad s_j^z = 2n(j+\frac{1}{2}) \delta r^2 \]
\[ \tilde{V}_{1,j+\frac{1}{2}}^n = \frac{1}{4}(V_{1,j}^n + \tilde{V}_{1,j}^n + V_{1,j+1}^n + \tilde{V}_{1,j+1}^n) \]

\[ \tilde{V}_{1,j+\frac{1}{2},j}^n = \frac{1}{4}(U_{1,j}^n + \tilde{U}_{1,j}^n + U_{1,j+1}^n + \tilde{U}_{1,j+1}^n) \]

\[ \tilde{V}_{1,j}^n = \frac{1}{2}(V_{1,j}^n + \tilde{V}_{1,j}^n) \quad \tilde{U}_{1,j}^n = \frac{1}{2}(U_{1,j}^n + \tilde{U}_{1,j}^n) \]

\[ V_{1} = (V_{1,j-1}^n + V_{1,j-1}^n) \text{ except on axis boundary when } V_{1} = (V_{1,j}^n + V_{1,j}^n). \]

\[ V_{2} = (V_{1,j+1}^n + V_{1,j+1}^n) \text{ except on continuative boundary 4 when } V_{2} = (V_{1,j}^n + V_{1,j}^n). \]

\[ U_{1} = (U_{1-1,j}^n + U_{1-1,j}^n) \text{ except on piston boundary when } U_{1} = 2U_{APP} \]

\[ U_{1} = (U_{1,j}^n + U_{1,j}^n) \text{ and on continuative boundary 1 when } U_{1} = (U_{1,j}^n + U_{1,j}^n). \]

\[ U_{2} = (U_{1+1,j}^n + U_{1+1,j}^n) \text{ except on continuative boundary 3 when } U_{2} = (U_{1,j}^n + U_{1,j}^n). \]

\[ TEMP_{1} = (V_{1,j}^n + V_{1,j}^n) \quad TEMP_{3} = (U_{1,j}^n + U_{1,j}^n) \]

\[ \tilde{V}_{1,j+\frac{1}{2}}^n = \frac{1}{4}(TEMP_{1} + V_{2}) \quad \tilde{V}_{1,j-\frac{1}{2}}^n = \frac{1}{4}(TEMP_{1} + V_{1}) \]

\[ \tilde{U}_{1,j+\frac{1}{2}}^n = \frac{1}{4}(TEMP_{3} + U_{2}) \quad \tilde{U}_{1,j-\frac{1}{2}}^n = \frac{1}{4}(TEMP_{3} + U_{1}) \]

\[ \tilde{V}_{1,j}^n = \frac{1}{2}(TEMP_{1}) \quad \tilde{U}_{1,j}^n = \frac{1}{2}(TEMP_{3}) \]

\[ \tilde{V}_{1,j+1}^n = \frac{1}{2}(V_{2}) \quad \tilde{V}_{1,j-1}^n = \frac{1}{2}(V_{1}) \]

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\[ \tau_{ij}^n = I_{ij} - \frac{8t}{n \rho_{ij}} \left( \frac{p_{ij}^n}{2(2j+1)\delta r} [ (j+1)(\text{TEMP1}+v2)-(j)(\text{TEMP1}+v1) ] \right) \\
+ \frac{Q_4_{ij}}{2(2j+1)\delta r} [ (j+\frac{3}{2})(v2)-(j+\frac{1}{2})(\text{TEMP1}) ] \\
- \frac{Q_2_{ij}}{2(2j+1)\delta r} [ (j-\frac{1}{2})(v1)-(j+\frac{1}{2})(\text{TEMP1}) ] \\
+ \frac{1}{4\delta z} \left[ p_{ij}^n (u2-u1)+Q_3_{ij} (u2-\text{TEMP3})+Q_1_{ij} (\text{TEMP3}-u1) \right] \] \\
\]
\[ = I_{ij} - \frac{8t}{n \rho_{ij}} \left( \frac{p_{ij}^n}{6r} [ v2-v1+ \frac{v2+2\text{TEMP1}+v1}{2j+1} ] \right) \\
+ \frac{Q_4_{ij}}{6r} [ v2-\text{TEMP1}+ \frac{2v2}{2j+1} ] \\
- \frac{Q_2_{ij}}{6r} [ v1-\text{TEMP1}- \frac{2v1}{2j+1} ] \]
\[ + \frac{1}{8z} \left[ p_{ij}^n (u2-u1)+Q_3_{ij} (u2-\text{TEMP3})+Q_1_{ij} (\text{TEMP3}-u1) \right] \]

Total energy

\[ E_{ij}^n = \tau_{ij}^n + \frac{1}{2} \left[ (v_{ij}^n)^2+(0_{ij}^n)^2 \right] \]

Phase IV. Mass Movement

The viscosities, Q1 through Q4 are no longer needed, and their storage locations are used to store the changes in various physical quantities as the mass is moved. Mass is not moved unless the pressure of the cell from which the mass moves is greater than PREPR (0.0005).

Q1 - $\Delta E$ change in energy
Q2 - $\Delta W$ change in mass fraction
Q3 - $\Delta PV$ change in V momentum

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Q4 - ΔPU change in U momentum
CMB - ΔM change in mass

Mass movement across side 2

1. For an axis cell Q1 = Q2 = Q3 = Q4 = CMB = 0 and no mass is moved.

\[ \Delta = \frac{(v_{i,j}^n + v_{i,j-1}^n) \frac{8t}{\delta r}}{(v_{i,j}^n - v_{i,j-1}^n) (8t/5r) + 1} \]

2. \( \Delta \geq 0 \), DM = \( (\rho_{i,j}^n)^{2j+1} \Delta \), mass moves from cell \( i,j-1 \) to cell \( ij \).

\[
\begin{align*}
Q1_{ij} &= E_{i,j-1}^n (DM) \\
Q2_{ij} &= W_{i,j-1}^n (DM) \\
Q3_{ij} &= \varphi_{i,j-1}^n (DM) \\
Q4_{ij} &= \psi_{i,j-1}^n (DM) \\
\text{CMB}_{i,j} &= \text{DM}
\end{align*}
\]

3. \( \Delta < 0 \)

\[ \text{DM} = (\rho_{ij}^n)^{2j+1} \Delta \), mass moves from cell \( ij \) to cell \( i,j-1 \).

\[
\begin{align*}
Q1_{ij} &= E_{i,j}^n (DM) \\
Q2_{ij} &= W_{i,j}^n (DM) \\
Q1_{i,j-1} &= Q1_{i,j-1} - E_{i,j-1}^n (DM) \\
Q2_{i,j-1} &= Q2_{i,j-1} - W_{i,j-1}^n (DM)
\end{align*}
\]
Mass movement across side 1

1. For a piston boundary cell we have

\[
\Delta = \frac{(U_{i,j} + U_{i,j}^n)(8t/8z)}{2(U_{i,j}^n - U_{i,j})(8t/8z) + 1}
\]

For \( \Delta < 0 \) no mass is moved.
For \( \Delta \geq 0 \), DM = (MAPP)\( \Delta \), mass moves from piston to cell i,j.

\[
Q_{1_{i,j}} = Q_{1_{i,j}} + EAPP(DM)
\]

\[
Q_{2_{i,j}} = Q_{2_{i,j}} + WAPP(DM)
\]

\[
Q_{3_{i,j}} = Q_{3_{i,j}} + VAPP(DM)
\]

\[
Q_{4_{i,j}} = Q_{4_{i,j}} + UAPP(DM)
\]

\[
CMB_{i,j} = CMB_{i,j} + DM
\]

2. For continuative boundary 1 cell

\[
\Delta = (U_{i,j}^n)(8t/8z)
\]

\[
DM = (\rho_{i,j})\Delta
\]
\[ Q_{1 ij} = Q_{1 ij} + E_{1 ij}^n(DM) \]
\[ Q_{2 ij} = Q_{2 ij} + W_{1 ij}^n(DM) \]
\[ Q_{3 ij} = Q_{3 ij} + U_{1 ij}^n(DM) \]
\[ Q_{4 ij} = Q_{4 ij} + \eta_{1 ij}^n(DM) \]
\[ \text{CMB}_{ij} = \text{CMB}_{ij} + DM \]
\[
\Delta = \frac{(\eta_{1 ij}^n + \eta_{1 i-1,j}^n) S_t}{S_z (\eta_{1 ij}^n - \eta_{1 i-1,j}^n)(S_t/S_z) + 1}
\]

3. \( \Delta \geq 0 \)

\[ \text{DM} = (\rho_{i-1,j}^n)(\Delta) \] mass moves from cell \( i-1,j \) to cell \( ij \).
\[ Q_{1 ij} = Q_{1 ij} + E_{1-1,j}^n(DM) \]
\[ Q_{2 ij} = Q_{2 ij} + W_{1-1,j}^n(DM) \]
\[ Q_{3 ij} = Q_{3 ij} + U_{1-1,j}^n(DM) \]
\[ Q_{4 ij} = Q_{4 ij} + \eta_{1-1,j}^n(DM) \]
\[ \text{CMB}_{ij} = \text{CMB}_{ij} + DM \]

4. \( \Delta < 0 \)

\[ \text{DM} = (\rho_{ij}^n)\Delta \] mass moves from cell \( ij \) to cell \( i-1,j \).
Mass movement on side 3

Except on the continuative boundary 3, this mass movement is taken care of by the mass movement across side 1 of the cell directly above.

On the boundary

\[ \Delta = (\bar{u}^n_{ij})(\partial t/\partial z) \]

\[ DM = (\rho^n_{ij})\Delta \]

\[ Q_{1ij} = Q_{1ij} - E^n_{ij}(DM) \]

\[ Q_{2ij} = Q_{2ij} - W^n_{ij}(DM) \]

\[ Q_{3ij} = Q_{3ij} - V^n_{ij}(DM) \]

\[ Q_{4ij} = Q_{4ij} - \bar{U}^n_{ij}(DM) \]

\[ CMB_{ij} = CMB_{ij} - DM \]

Mass movement on side 4

Except on the continuative boundary 4, this mass movement is taken...
care of by the mass movement across side 2 of the cell on its right.

On the boundary

\[ \Delta = \frac{\bar{V}_{ij} \text{St}}{\delta r} \]

a) \( \Delta \geq 0 \) mass moves out of cell \( ij \).

\[ \begin{align*}
\Delta M &= (\rho_{ij}^n) \left( 2j + 2 - \Delta \right) \frac{\Delta}{2j + 3} \\
Q_{1ij} &= Q_{1ij} - B_{ij}^n (DM) \\
Q_{2ij} &= Q_{2ij} - W_{ij}^n (DM) \\
Q_{3ij} &= Q_{3ij} - \bar{V}_{ij}^n (DM) \\
Q_{4ij} &= Q_{4ij} - \bar{V}_{ij}^n (DM) \\
\text{CMB}_{ij} &= \text{CMB}_{ij} - \Delta M
\end{align*} \]

b) \( \Delta < 0 \) mass moves into cell \( ij \).

\[ \begin{align*}
\Delta M &= (\rho_{ij}^n) \left( 2j + 2 - \Delta \right) \frac{\Delta}{2j + 1} \\
Q_{1ij} &= Q_{1ij} - B_{ij}^n (DM) \\
Q_{2ij} &= Q_{2ij} - W_{ij}^n (DM) \\
Q_{3ij} &= Q_{3ij} - \bar{V}_{ij}^n (DM) \\
Q_{4ij} &= Q_{4ij} - \bar{V}_{ij}^n (DM) \\
\text{CMB}_{ij} &= \text{CMB}_{ij} - \Delta M
\end{align*} \]
Phase V. Repartition

Add on mass moved quantities

For \( \rho_{ij}^n > \text{MINGRHO} + (\rho_0 - \text{MINGRHO})(w_{ij}^n) \)

\[
\rho_{ij}^{n+1} = \rho_{ij}^n + \text{CMB}_{ij}
\]

\[
w_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(\rho_{ij}^n w_{ij}^n + Q2_{ij})
\]

\[
v_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(v_{ij}^n \rho_{ij}^n + Q3_{ij})
\]

\[
u_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(u_{ij}^n \rho_{ij}^n + Q4_{ij})
\]

\[
i_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(i_{ij}^n \rho_{ij}^n + Q1_{ij}) - \frac{1}{2CMB}(v_{ij}^{n+1})^2 + (u_{ij}^{n+1})^2
\]

For \( \rho_{ij}^n \leq \text{MINGRHO} + (\rho_0 - \text{MINGRHO})(w_{ij}^n) \)

\[
\rho_{ij}^{n+1} = \rho_{ij}^n + \text{CMB}_{ij}
\]

\[
w_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(\rho_{ij}^n w_{ij}^n + Q2_{ij})
\]

\[
v_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(v_{ij}^n \rho_{ij}^n + Q3_{ij})
\]

\[
u_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(u_{ij}^n \rho_{ij}^n + Q4_{ij})
\]

\[
i_{ij}^{n+1} = \frac{1}{\rho_{ij}^{n+1}}(i_{ij}^n \rho_{ij}^n + Q1_{ij}) - \frac{(Q3_{ij})^2 + (Q4_{ij})^2}{2CMB_{ij}}
\]
IV. THE PISTON OR CONSTANT INPUT BOUNDARY

To obtain a smooth initial piston profile it was found necessary to set the internal energy of the cells for the first VCNT (25) cycles to

\[ I - I_o = \frac{1}{2}(P + Q_3)(V_o' - V') \]

Another method which did not require initially adjusting the internal energy to obtain a smooth initial piston profile was to feed in the last 10 cells of a previously calculated flat topped shock as the starting conditions of a new calculation.

Steady-State Reaction Zone Piston

The steady-state piston was computed by iteration for a given detonation velocity by using the amount of reaction that has occurred in a cell near the piston to determine the proper piston density, energy and particle velocity.

Used axis cell of fifth layer to get Piston W. For fast reaction it was found necessary to use a lower W for Piston W by multiplying by a constant (WPISF).

1. Given a W, assume a V'.
2. Find Pr from \( P_r - P_o = (\rho_o)^2(D)^2(V_o' - V') \), the Rayleigh Line.
3. Calculate I from \( I - I_o = \frac{1}{2}(P_r)(V_o' - V') \).
5. Iterate on V' until \( P_r - P \) is less than \( 1 \times 10^{-5} \).
6. Calculate \( U = \sqrt{(P_o - P_o)(V_o' - V')} \) and assign it to UAPP, assign \( 1/V' \) to MAPP, assign \( I + \frac{1}{2}(MAPP)(UAPP)^2 \) to EAPP.

V. THE DISK STORAGE AND USAGE

The calculation proceeds as if the layers in the z direction are on a barrel - the last layer at nth cycle is followed by the first at n+1th cycle. There are two barrels - one containing the cell quantities and
one containing the intermediate quantities. The intermediate quantity barrel has four layers around it.

For an eight layer problem the layers labeled A, B, C, ... H, the calculation proceeds as follows:

<table>
<thead>
<tr>
<th>Pass through loop</th>
<th>Phase of Calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>I \ A</td>
</tr>
<tr>
<td>2.</td>
<td>II \ B  \ A</td>
</tr>
<tr>
<td>3.</td>
<td>III \ C  \ B  \ A</td>
</tr>
<tr>
<td>4.</td>
<td>IV \ D  \ C  \ B  \ A</td>
</tr>
<tr>
<td>5.</td>
<td>V  \ E  \ D  \ C  \ B  \ A</td>
</tr>
<tr>
<td>6.</td>
<td>\ F  \ E  \ D  \ C  \ B  \ A</td>
</tr>
<tr>
<td>7.</td>
<td>\ G  \ F  \ E  \ D  \ C</td>
</tr>
<tr>
<td>8.</td>
<td>\ H  \ G  \ F  \ E</td>
</tr>
<tr>
<td>9.</td>
<td>\ H  \ G  \ F  \ E  \ D</td>
</tr>
<tr>
<td>10.</td>
<td>\ H  \ G  \ F  \ E</td>
</tr>
<tr>
<td>11.</td>
<td>\ H  \ G  \ F</td>
</tr>
<tr>
<td>12.</td>
<td>\ H  \ G</td>
</tr>
<tr>
<td>13.</td>
<td>\ H</td>
</tr>
</tbody>
</table>

write on disk

After thirteen passes the time is incremented, plotting and printing are done, and the cycle is started over again.

The skipping of various parts of the calculation is controlled by changing branch instructions to NOP's and vice versa.

The barrel operation is described below:

1. When all the layers can be held in core. \( \text{NMRD} \leq \text{NSCMAX} \)

When phase V has been completed for a layer, it is transmitted to the disk and to the proper core location for the next cycle, e.g.

8 layers in core

A B C D E F G H

after phase V on A is completed

A B C D E F G H A'
after phase V on B is completed

A B C D E F G H A' B' etc.

When the top of core storage is reached, the next layer goes at the
bottom of cell storage, e.g. for an 8 layer calculation in a 10 layer
capacity core, we have

initially |A|B|C|D|E|F|G|H| | |

after 1 complete cycle

|C'|D'|E'|F'|G'|H'|G|H|A'|B'|

after 2 complete cycles

|E''|F''|G''|H''|G'|H'|A''|B''|C''|D''|

2. When all the layers will not fit in core (NMRD > NSCMAX),
e.g., 8 layers in 6 layer capacity

initially |A|B|C|D|E|F|

after phase V of A is completed, A goes to disk, and G is read in

|G|B|C|D|E|F|

after phase V of B is completed, B goes to disk and H is read in

|G|H|C|D|E|F|

after phase V of H has been calculated, H goes to disk and F is read in

|E'|F'|A'|E'|C'|D'|

The number of layers required for the calculation increases with time at
a rate characteristic of the problem. Graphing and printing use the same
technique, except that graphing uses all the layers.

VI. INPUT FORMATS

<table>
<thead>
<tr>
<th>Card</th>
<th>Col.</th>
<th>Format</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1-72</td>
<td>72H</td>
<td>Problem description</td>
</tr>
<tr>
<td>2</td>
<td>1-18</td>
<td>E0.1.11.3</td>
<td>Delta R</td>
</tr>
<tr>
<td></td>
<td>19-36</td>
<td>E0.1.11.3</td>
<td>Delta Z</td>
</tr>
<tr>
<td></td>
<td>37-54</td>
<td>E0.1.11.3</td>
<td>Delta T</td>
</tr>
<tr>
<td>3</td>
<td>1-18</td>
<td>E0.1.11.3</td>
<td>Activation Energy</td>
</tr>
<tr>
<td></td>
<td>19-36</td>
<td>E0.1.11.3</td>
<td>Frequency</td>
</tr>
<tr>
<td></td>
<td>37-54</td>
<td>E0.1.11.3</td>
<td>Minimum temp. to burn</td>
</tr>
<tr>
<td>Card</td>
<td>Col.</td>
<td>Format</td>
<td>Data</td>
</tr>
<tr>
<td>------</td>
<td>------</td>
<td>--------</td>
<td>------</td>
</tr>
<tr>
<td>4</td>
<td>1-18</td>
<td>E0.1.11.3</td>
<td>V' for equation of state = ( \frac{1}{\rho_o} )</td>
</tr>
<tr>
<td></td>
<td>19-36</td>
<td>E0.1.11.3</td>
<td>Initial cell pressure</td>
</tr>
<tr>
<td></td>
<td>37-53</td>
<td>E0.1.11.3</td>
<td>Initial cell temperature</td>
</tr>
<tr>
<td>5</td>
<td>1-18</td>
<td>E0.1.11.3</td>
<td>Piston detonation velocity</td>
</tr>
<tr>
<td></td>
<td>19-36</td>
<td>E0.1.11.3</td>
<td>Piston initial volume guess</td>
</tr>
<tr>
<td></td>
<td>37-54</td>
<td>E0.1.11.3</td>
<td>Viscosity constant</td>
</tr>
<tr>
<td>6</td>
<td>1-6</td>
<td>V1*5</td>
<td>0 for HOM, 1 for ideal gas</td>
</tr>
<tr>
<td></td>
<td>7-12</td>
<td>V1*5</td>
<td>0 for no reaction, 1 for reaction</td>
</tr>
<tr>
<td></td>
<td>13-18</td>
<td>V1*5</td>
<td>Number of cycles between prints</td>
</tr>
<tr>
<td></td>
<td>19-24</td>
<td>V1*5</td>
<td>Number of cycles between graphs</td>
</tr>
<tr>
<td></td>
<td>25-30</td>
<td>V1*5</td>
<td>Number of cycles between disk dumps</td>
</tr>
<tr>
<td></td>
<td>31-36</td>
<td>V1*5</td>
<td>Graph type (see below)</td>
</tr>
</tbody>
</table>

7 + following cards - equation of state cards for HOM or ideal gas
- for HOM - 4 cards for solid parameters, then 5 cards for gas parameters
- for ideal gas - 1 card

<table>
<thead>
<tr>
<th>Card</th>
<th>Col.</th>
<th>Format</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>1-18</td>
<td>E0.1.11.3</td>
<td>Gamma</td>
</tr>
<tr>
<td></td>
<td>19-36</td>
<td>E0.1.11.3</td>
<td>Q</td>
</tr>
<tr>
<td></td>
<td>37-54</td>
<td>E0.1.11.3</td>
<td>C_v</td>
</tr>
<tr>
<td>8 or 16</td>
<td>1-5</td>
<td>V0*5</td>
<td>Number of mesh set up cards</td>
</tr>
<tr>
<td>9 or 17</td>
<td>1-5</td>
<td>V0*5</td>
<td>Z min</td>
</tr>
<tr>
<td>to end</td>
<td>6-10</td>
<td>V0*5</td>
<td>Z max</td>
</tr>
<tr>
<td></td>
<td>11-15</td>
<td>V0*5</td>
<td>R min</td>
</tr>
<tr>
<td></td>
<td>16-20</td>
<td>V0*5</td>
<td>R max</td>
</tr>
<tr>
<td></td>
<td>21-32</td>
<td>E0.1.6.2</td>
<td>Density</td>
</tr>
<tr>
<td></td>
<td>33-44</td>
<td>E0.1.6.2</td>
<td>Internal energy</td>
</tr>
<tr>
<td></td>
<td>45-58</td>
<td>E0.1.6.2.1</td>
<td>U velocity with flag</td>
</tr>
<tr>
<td></td>
<td>59-72</td>
<td>E0.1.6.2.1</td>
<td>V Velocity with flag</td>
</tr>
</tbody>
</table>

Cells in the mesh that are not within the limits of any card are set empty with \( \sigma=\Gamma=U=V=W=0 \) and \( P=P_0 \).
The individual cell flags that are set by the input cards are described below:

1. To put a continuative boundary on side 1 set U flag on CU which is a 2.
2. To put a continuative boundary on side 3 set V flag on CU which is a 1.
3. To put an axis boundary on side 2 set U flag on CV which is a 2.
4. To put a continuative boundary on side 4 set V flag on CV which is a 1.
5. To put a piston boundary on side 1 set T flag on CU which is a 4.

To keep mass from flowing from cell i+1,j into cell i,j or from cell i,j into cell i+1,j set continuative boundary on side 3 of cell i,j and set continuative or piston boundary on side 1 of cell i+1,j.

A cell may not be both on boundaries 1 and 3 or on boundaries 2 and 4.

The flag conventions used for initial problem set-up are described below:
VII. THE ISOPLOT SUBROUTINE

ISOPLOT is a plotting program which produces graphs of isotherms, isobars, etc., on the 4020. The input consists of the x and y coordinates and a function value (temperature, pressure, etc.) at each point in a two-dimensional lattice, the boundaries on x and y for the graph, the number of lattice points in the x direction, the total number of lattice points, the number of words in core between the x coordinate of one cell and the x coordinate of the next cell in the x direction (the difference is assumed to be the same as that between y's and function values), and the numerical difference of the function value between two isolines.

The calling sequence is:
LVI, $15, 5+1$
B, ISOPLOT $P$

, NCELL  Total # of lattice points
, X    address of x coordinate
, NXDIFF  # words between successive x coordinates
, Y  y coordinate address
, NXCELL  # of lattice points in x direction
, F  address of function
, DELTA  difference between isolines
, XYB  location of 4 words giving x, y boundaries

example: 4 x 5 lattice of values

. . . . $x_{20}, y_{20}, p_{20}$
. . . .
. . . .
. . . .
. . . .

$x_1, y_1, p_1$  $x_4, y_4, p_4$

with x's, y's, and p's arranged in core as follows:

X  DR(N),(20)
Y  DR(N),(20)
P  DR(N),(20)

and x range from 0 to 3, y range from 0 to 4, plotting lines every .1.

XYB  DD(N),0.
     DD(N),3.
     DD(N),0.
     DD(N),4.
DELTA  DD(N),.1.

The calling sequence is then:
Note: Whether the x, y, and P's are stored as vectors or in individual blocks, the x coordinate of the next cell in the y direction must be (NXCELL)(NXDIFF) words away (e.g., \( x_5 \) is four words from \( x_1 \): stored \( x_1, x_2, x_3, x_4, x_5 \)).

The method:

The quantities for four points are brought in:

\[
\begin{align*}
x_2 & \quad y_2 & \quad P_2 & \quad x_3 & \quad y_3 & \quad P_3 \\
2 & \quad & \quad & 4 & \quad & \quad \\
-1 & \quad -1 & \quad -1 & \quad -1 \\
x_1, y_1, P_1 & \quad x_4, y_4, P_4
\end{align*}
\]

Determine if an isoline crosses side 1.

A. \( P_1 < P_4 \)

(integer part \((P_1/DELT) + 1\)) \( \text{DELT} = \text{PT} \)

If \( \text{PT} < P_4 \) a line crosses side 1, and we find the coordinates of the point at which it crosses:

\[
x' = \left( \frac{x_4 - x_1}{P_4 - P_1} \right) + x_4
\]
B. \[ P_1 > P_4 \]

\[ PT = (\text{integer part} \, \frac{P_4}{\text{DELT}}) + 1 \text{DELT} \]

If \( PT < P_1 \) a line crosses side 1 at

\[ x' = (PT - P_1) \frac{(x_4 - x_1)}{(P_4 - P_1)} + x_1 \]

\[ y' = (PT - P_1) \frac{(y_4 - y_1)}{(P_4 - P_1)} + y_1 \]

We then proceed to find out which other side this isoline crosses. It crosses side 2 if \( P_1 < PT < P_2 \) or \( P_1 = 0 > P_2 \). The coordinates of the point at which it crosses are:

\[ x'' = (PT - P_2) \frac{(x_1 - x_2)}{(P_1 - P_2)} + x_2 \]

\[ y'' = (PT - P_2) \frac{(y_1 - y_2)}{(P_1 - P_2)} + y_2 \]

Having found the point, a vector is drawn from \((x', y')\) to \((x'', y'')\) using a 4020 draw vector subroutine.

\( PT \) is incremented by \( \text{DELT} \), and if \( PT < P_4 \) another line crosses side 1. One then goes back to find out what other side this line crosses. This continues until \( PT > P_4 \), then one moves to side 2 to see if any lines cross side 2. The lines crossing side 2 are connected to sides 3 or 4 since lines from side 1 to side 2 have already been drawn. Similarly lines between sides 3 and 4 are drawn.
LITERATURE CITED


