METHODS IN COMPUTATIONAL PHYSICS

Advances in Research and Applications

Edited by

Berni Alder

Sidney Fernbach

Manuel Rotenberg

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Preface

With the present-day availability of large scale digital computers comes the possibility of numerically solving systems of partial differential equations never attempted before. Even the simplest one-dimensional, time-dependent system being run routinely on standard computers today would have required so many man-hours of effort a few years ago that its solution was not even attempted.

The present volume of this series on computational aspects of physical problems is concerned with current techniques for numerically solving problems primarily in nonviscous, compressible fluid motion. These techniques have been developed for solution on digital computers over a period of 15 years or so. Some of the methods described are more useful than others; the methods of limited use are included because we feel that in these early years of the development of the computer as a mathematical tool, even the less successful heuristic methods should be exposed to public view for consideration.

The first four chapters involve methods which use Lagrangian or Eulerian coordinates, or a mixture of both in several space dimensions. The next two chapters illustrate the use of some of these same techniques along with the added complexity of elastic-plastic media. The two chapters which follow use the method of characteristics in both one- and two-space dimensional problems. The next chapter is devoted to the now well-known particle-in-cell method. The last chapter is devoted to viscous incompressible fluid flow. It is included because in it is discussed a new method for attacking such problems.

Volume 4 of this series will also be devoted to hydrodynamics, but from a more applied point of view.

BERNI ALDER
SIDNEY FERNBACH
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June, 1964

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Two-Dimensional Lagrangian Hydrodynamic Difference Equations[1]

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I. Introduction

THE FIRST HYDRODYNAMICAL INITIAL VALUE PROBLEMS that were tried on a computer were one-dimensional (one space dimension, the added time dimension always being understood). In one dimension the arguments in favor of a Lagrangian over an Eulerian formulation are almost overwhelming. Once Richtmyer and von Neumann had introduced artificial viscosities into the theory, the production of a relatively accurate and stable Lagrangian code was quite straightforward. Eulerian codes in general are not as accurate and have additional troubles. When the problem of interest contains several different materials they tend to diffuse across material interfaces at nonphysical rates. A second difficulty is that if the system is compressed, definition is lost due to the fixed-in-space nature of the coordinates in Eulerian codes, in contrast to the fixed-in-the-material nature of the coordinates in Lagrangian codes. In general, the structure of a problem can be better defined by Lagrangian coordinates. These arguments all apply to the interior of the system.

[1] This work was performed under the auspices of the U. S. Atomic Energy Commission.

Occasionally the boundary conditions are such that it will be preferable to use an Eulerian system, but this is rare.

With this Lagrangian background in one dimension, the first two-dimensional codes were naturally Lagrangian also. All of the previous reasons for preferring a Lagrangian formulation still hold true but one of them has to be qualified. In two dimensions a new process enters in, namely, turbulence. In one dimension, if one has a suitable Lagrangian coordinate system, i.e., one that defines the system well, then as time progresses it will usually continue to define the system well. In two dimensions the situation is somewhat reversed. A Lagrangian coordinate system that initially defines the system well everywhere will often transform into one with areas of poor definition. Usually the trouble can be attributed to turbulence. Lagrangian codes give believable results when the areas of poor definition are not significant to the general behavior of the system. In the final section of this article there are a few more comments on this subject, which are related directly to a small sample problem given there.

The artificial viscosity of Richtmyer and von Neumann has been generalized here into a tensor artificial viscosity in two dimensions. This was done partly in an attempt to alleviate the turbulence problem and partly just to produce a better representation of a shock. This development had an interesting side effect. The tensor viscosity produces equations for the one-dimensional cylindrical and spherical cases which differ from those produced by the usual procedure of treating the Richtmyer–von Neumann viscosity as a scalar. In practice these tensor viscosity equations give different results for multiple shock systems but are in essential agreement with the scalar viscosity equations for single shock systems.

II. Definitions, Notation, and Transformation Relations

For convenience a few relations connecting Eulerian coordinates with Lagrangian coordinates will be discussed first. Eulerian coordinates are the ones which are most familiar in physics. In addition, Eulerian expressions serve as shorthand for longer Lagrangian equivalents. Before differencing, of course, everything is put in Lagrangian form (see Fig. 1):

$R(k, l, t)$ = Eulerian coordinate, may be either Cartesian or cylindrical,

$Z(k, l, t)$ = Eulerian coordinate, always Cartesian,

$\mathbf{R}$ = the vector (R, Z),

k = Lagrangian coordinate,

l = Lagrangian coordinate,

j = Jacobian of transformation.

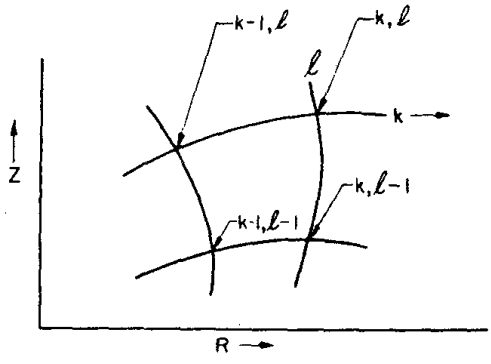

FIG. 1. Lagrangian coordinate network for differencing.

If $R_k = \partial R/\partial k$, $R_l = \partial R/\partial l$, etc., then $j = R_k Z_l - R_l Z_k$ = area Jacobian.

Let

$$\hat{R} = \begin{cases} R \text{ for cylindrical coordinates,} \\ 1 \text{ for Cartesian coordinates,} \end{cases}$$

then a "volume Jacobian" may be defined as

$$J = \hat{R}j .$$

Consider the conversion of an Eulerian derivative into a Lagrangian derivative:

$$\frac{\partial}{\partial R} = \left(\frac{\partial k}{\partial R}\right)\frac{\partial}{\partial k} + \left(\frac{\partial l}{\partial R}\right)\frac{\partial}{\partial l},$$

$$\frac{\partial}{\partial Z} = \left(\frac{\partial k}{\partial Z}\right)\frac{\partial}{\partial k} + \left(\frac{\partial l}{\partial Z}\right)\frac{\partial}{\partial l}.$$

Expressions for $\partial k/\partial R$, ..., $\partial l/\partial Z$, in terms of R_k, ..., Z_l can be found as follows. For arbitrary g,

$$\frac{\partial g}{\partial k} = R_k \frac{\partial g}{\partial R} + Z_k \frac{\partial g}{\partial Z},$$

$$\frac{\partial g}{\partial l} = R_l \frac{\partial g}{\partial R} + Z_l \frac{\partial g}{\partial Z}.$$

Let $g = k$, then one can solve for $\partial k/\partial R$ and $\partial k/\partial Z$. Similarly $g = l$ gives $\partial l/\partial R$ and $\partial l/\partial Z$. The result of this is

$$\frac{\partial k}{\partial R} = \frac{Z_l}{j}, \qquad \frac{\partial l}{\partial R} = -\frac{Z_k}{j},$$

$$\frac{\partial k}{\partial Z} = -\frac{R_l}{j}, \qquad \frac{\partial l}{\partial Z} = \frac{R_k}{j},$$

which gives

$$\frac{\partial}{\partial R} = \frac{Z_l}{j}\frac{\partial}{\partial k} - \frac{Z_k}{j}\frac{\partial}{\partial l},$$

$$\frac{\partial}{\partial Z} = -\frac{R_l}{j}\frac{\partial}{\partial k} + \frac{R_k}{j}\frac{\partial}{\partial l}.$$

Define a vector $\bar{\mathbf{R}}$ lagging $\mathbf{R}$ by 90° as the "normal vector" to $\mathbf{R}$:

$$\bar{\mathbf{R}} = (Z, -R) = \text{normal vector to } \mathbf{R}.$$

Note that

$$\bar{\mathbf{R}}_1 \cdot \bar{\mathbf{R}}_2 = \bar{\mathbf{R}}_1 \cdot \bar{\mathbf{R}}_2, \qquad \bar{\mathbf{R}}_1 \cdot \mathbf{R}_2 = -\mathbf{R}_1 \cdot \bar{\mathbf{R}}_2.$$

A useful vector operator can be defined as

$$\mathbf{D} = \frac{1}{j}\left[\bar{\mathbf{R}}_l \frac{\partial}{\partial k} - \bar{\mathbf{R}}_k \frac{\partial}{\partial l}\right] = \frac{1}{j}\left[\frac{\partial}{\partial k}(\bar{\mathbf{R}}_l \ldots) - \frac{\partial}{\partial l}(\bar{\mathbf{R}}_k \ldots)\right].$$

Then

$$\nabla f = \mathbf{D}f,$$

$$\nabla \cdot \mathbf{f} = \frac{1}{\hat{R}}\mathbf{D} \cdot (\hat{R}f).$$

Lagrangian time derivatives, that is, partial derivatives with k and l held fixed, will be written as follows:

$$u(k, l, t) = \frac{\partial R}{\partial t} = R_t = \dot{R} = R \quad \text{velocity},$$

$$v(k, l, t) = \frac{\partial Z}{\partial t} = Z_t = \dot{Z} = Z \quad \text{velocity},$$

$$\mathbf{u} = \text{the vector } (u, v).$$

At this point we can deduce some relations for later use:

$$
\begin{aligned}
j &= \mathbf{R}_k \cdot \bar{\mathbf{R}}_l \,, \\
j_t &= \mathbf{R}_{kt} \cdot \bar{\mathbf{R}}_l + \mathbf{R}_k \cdot \bar{\mathbf{R}}_{lt} \\
&= \bar{\mathbf{R}}_l \cdot \mathbf{R}_{kt} - \bar{\mathbf{R}}_k \cdot \mathbf{R}_{lt} \,, \\
j_t &= \bar{\mathbf{R}}_l \cdot \mathbf{u}_k - \bar{\mathbf{R}}_k \cdot \mathbf{u}_l = j\mathbf{D} \cdot \mathbf{u} \,. \qquad (1)
\end{aligned}
$$

In cylindrical coordinates

$$\nabla \cdot \mathbf{u} = \frac{u}{R} + \mathbf{D} \cdot \mathbf{u} \,.$$

Substituting from (1) for $\mathbf{D} \cdot \mathbf{u}$, we obtain

$$\nabla \cdot \mathbf{u} = \frac{R_t}{R} + \frac{j_t}{j} = \frac{(Rj)_t}{Rj} \,.$$

Therefore

$$\nabla \cdot \mathbf{u} = \frac{J_t}{J} \,. \qquad (2)$$

Since $J = j$ for Cartesian systems, (2) reduces to (1) and thus is valid for both coordinate systems.

To complete the discussion of the transformation relations, the connection between Eulerian and Lagrangian time derivatives may be deduced as follows.

Let g be an arbitrary function, then

$$\frac{\partial g}{\partial t} = \frac{\partial g}{\partial t}\bigg|_{\mathbf{R}} + \frac{\partial g}{\partial R} R_t + \frac{\partial g}{\partial Z} Z_t \,.$$

Thus

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t}\bigg|_{\mathbf{R}} + (\mathbf{u} \cdot \nabla) \,.$$

Some further notation and definitions:

p = pressure,
ρ = density,
$\tau = \rho^{-1}$ = specific volume,
ϵ = specific internal energy,
S = entropy,
$M = \rho^0 J^0$ = mass constant (a superscript 0 means $t = 0$),
$\epsilon(s)$ = specific internal energy introduced through an external source,
$E = M\epsilon$.

III. Conservation Equations

The differential formulation of the system is given in this section. The various differential equations are commented on and related to each other but not in any fundamental sense; that is, with the exception of the development of an artificial viscosity, we assume the basic differential equations are known and proceed from there. Thus Eqs. (3)–(6) are considered defining equations. Equations (7)–(9) are relations deduced from these defining equations.

Mass equation:

$$\tau = J/M\,. \tag{3}$$

This follows directly from the mass conservation equation as it is more usually written,

$$(\rho J)_t = 0,$$

and therefore

$$\rho J = \rho^0 J^0 = M\,.$$

Differential momentum equation:

$$\rho \mathbf{u}_t + \nabla p + \frac{\rho}{M}\left[\frac{\partial}{\partial k}(\hat{R}\bar{\mathbf{R}}_l q_A) - \frac{\partial}{\partial l}(\hat{R}\bar{\mathbf{R}}_k q_B)\right] = 0\,. \tag{4}$$

The hydrodynamic equations use a tensor artificial viscosity to smooth out shock discontinuities; q_A is to be thought of as a "one-dimensional" viscosity associated with the $\bar{\mathbf{R}}_l$ direction while q_B is a "one-dimensional" viscosity associated with the $\bar{\mathbf{R}}_k$ direction.[2]

Internal energy equation:

$$\frac{\partial \epsilon}{\partial t} - \frac{\partial \epsilon(s)}{\partial t} + p\frac{\partial \tau}{\partial t} + \frac{q_A(\bar{\mathbf{R}}_l \cdot \mathbf{u}_k)}{\rho j} + \frac{q_B(-\bar{\mathbf{R}}_k \cdot \mathbf{u}_l)}{\rho j} = 0\,. \tag{5}$$

The equation of total energy conservation (7) demonstrates the self-consistency of the terms containing q_A and q_B in the momentum and internal energy equations.

Equation of state: The quantity p which appears in the conservation equations is computed from a known function of ϵ and τ. Thus one has given equations (or tables) of the form

$$p = p(\epsilon, \tau)\,. \tag{6}$$

[2] A complete discussion of the tensor artificial viscosity will be found in Section IV.

Total energy conservation equation: From the momentum and internal energy equations, we have

$$\rho\mathbf{u}\cdot\left\{\mathbf{u}_t+\frac{\nabla p}{\rho}+\frac{1}{M}\left[\frac{\partial}{\partial k}(\hat{R}\bar{\mathbf{R}}_l q_A)-\frac{\partial}{\partial l}(\hat{R}\bar{\mathbf{R}}_k q_B)\right]\right\}$$
$$+\rho\left\{\epsilon_t-\epsilon(s)_t+p\tau_t+\frac{q_A}{\rho j}(\bar{\mathbf{R}}_l\cdot\mathbf{u}_k)+\frac{q_B}{\rho j}(-\bar{\mathbf{R}}_k\cdot\mathbf{u}_l)\right\}=0\,.$$

Rearranging and using

$$\rho\tau_t=\frac{\tau_t}{\tau}=\frac{J_t}{J}=\nabla\cdot\mathbf{u}\,,$$

we obtain

$$\rho[\mathbf{u}\cdot\mathbf{u}_t+\epsilon_t-\epsilon(s)_t]=-\mathbf{u}\cdot\nabla p-p\nabla\cdot\mathbf{u}$$
$$-\frac{\mathbf{u}}{J}\cdot\frac{\partial}{\partial k}(\hat{R}\bar{\mathbf{R}}_l q_A)-\frac{q_A\hat{R}}{J}\bar{\mathbf{R}}_l\cdot\frac{\partial\mathbf{u}}{\partial k}$$
$$+\frac{\mathbf{u}}{J}\cdot\frac{\partial}{\partial l}(\hat{R}\bar{\mathbf{R}}_k q_B)+\frac{q_B\hat{R}}{J}\bar{\mathbf{R}}_k\cdot\frac{\partial\mathbf{u}}{\partial l}\,.$$

Use

$$-\mathbf{u}\cdot\nabla p-p\nabla\cdot\mathbf{u}=-\nabla\cdot(p\mathbf{u})=-\frac{1}{J}\left[\frac{\partial}{\partial k}(\hat{R}p\bar{\mathbf{R}}_l\cdot\mathbf{u})-\frac{\partial}{\partial l}(\hat{R}p\bar{\mathbf{R}}_k\cdot\mathbf{u})\right]$$

and collect terms:

$$\rho\{\tfrac{1}{2}\mathbf{u}^2+\epsilon-\epsilon(s)\}_t=-J^{-1}\left\{\frac{\partial}{\partial k}[(p+q_A)\mathbf{u}\cdot(\hat{R}\bar{\mathbf{R}}_l)]-\frac{\partial}{\partial l}[(p+q_B)\mathbf{u}\cdot(\hat{R}\bar{\mathbf{R}}_k)]\right\}.$$

Integrate over a radian slice in cylindrical coordinates or over a unit thick slab in Cartesian coordinates:

$$\int_{K_1}^{K_2}\int_{L_1}^{L_2}\{\tfrac{1}{2}\mathbf{u}^2+\epsilon-\epsilon(s)\}_t\rho J\,dk\,dl=-\int_{K_1}^{K_2}\int_{L_1}^{L_2}\left\{\frac{\partial}{\partial k}[(p+q_A)\mathbf{u}\cdot(\hat{R}\bar{\mathbf{R}}_l)]\right.$$
$$\left.-\frac{\partial}{\partial l}[(p+q_B)\mathbf{u}\cdot(\hat{R}\bar{\mathbf{R}}_k)]\right\}dk\,dl\,. \tag{7}$$

This is the desired total energy conservation expression. Note that q_A and q_B appear only in integrals over the boundaries of the system as must be required for a satisfactory artificial viscosity.

Integrated momentum equation:

$$\frac{d}{dt}\int M\mathbf{u}\,dk\,dl=\int J\rho\mathbf{u}_t\,dk\,dl=-\int J\nabla p\,dk\,dl-\int\frac{\partial}{\partial k}(\hat{R}\bar{\mathbf{R}}_l q_A)\,dk\,dl$$
$$+\int\frac{\partial}{dl}(\hat{R}\bar{\mathbf{R}}_k q_B)\,dk\,dl\,. \tag{8}$$

It is seen that q_A and q_B will again only appear in integrals over the boundary of the system. This would not be true for a scalar q in the case of cylindrical coordinates.[3]

Angular momentum equation:

$$\frac{d}{dt}\int \mathbf{R} \times M\mathbf{u}\, dk\, dl = \int \mathbf{R} \times J\rho\mathbf{u}_t\, dk\, dl$$

$$= -\int \Big\{\mathbf{R} \times (J\nabla p) - \mathbf{R} \times \frac{\partial}{\partial k}(\hat{R}\bar{\mathbf{R}}_l q_A) + \mathbf{R} \times \frac{\partial}{\partial l}(\hat{R}\bar{\mathbf{R}}_k q_B)\Big\}\, dk\, dl$$

$$= -\int \mathbf{R} \times J\nabla p\, dk\, dl - \int \frac{\partial}{\partial k}(\mathbf{R} \times \bar{\mathbf{R}}_l \hat{R} q_A)\, dk\, dl + \int \frac{\partial}{\partial l}(\mathbf{R} \times \bar{\mathbf{R}}_k \hat{R} q_B)\, dk\, dl + \int \mathbf{R}_k \times \bar{\mathbf{R}}_l \hat{R}(q_A - q_B)\, dk\, dl\,. \tag{9}$$

For angular momentum things do not turn out so well. There is a term containing $(q_A - q_B)$ which is integrated over the volume of the system. This will be commented on in the next section.

IV. Tensor Artificial Viscosity

In order to integrate the hydrodynamic equations by replacing them with finite difference equations, a mechanism must be introduced to smooth out the discontinuities which occur when shocks are present. Von Neumann and Richtmyer (1950) first solved this problem in one dimension by introducing an artificial viscosity which spread shock discontinuities out over a specified number of zones.

Essentially they constructed an artificial medium whose final behavior, after experiencing smoothed-out shock waves, was sufficiently like that of the true medium that it could be used in physical equations in place of the true medium.

This artificial medium was defined as follows: Consider a plane shock in the R direction only, no motion in the Z direction. Under these

[3] We are integrating over a radian slice in cylindrical coordinates. If the total volume of the system were integrated over, then a scalar q would also only appear in surface integrals.