LAUR 02-892

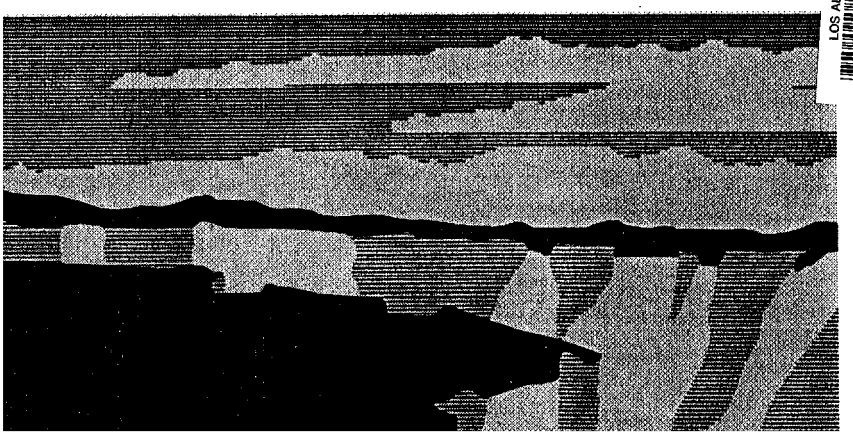
Approved for public release; distribution is unlimited.

Title: Grid Adaptation and Remapping for Arbitrary Lagrangian Eulerian (ALE) Mathods

Author(s): Giovanni Lapenta
Plasma Theory Group, Theoretical Division
University of California, Los Alamos National Laboratory
Los Alamos, NM 87545, USA

Submitted: 8th International Conference on Numerical Grid Generation in Computational Field Simulations
June2-6, 2002 Honolulu, Hawaii, USA

Group Address Theoretical Biology and Biophysics Group
Los Alamos National Laboratory Los
Alamos, New Mexico 87545



Grid Adaptation and Remapping for Arbitrary Lagrangian Eulerian (ALE) Methods

Giovanni Lapenta
Plasma Theory Group, Theoretical Division
University of California, Los Alamos National Laboratory
Los Alamos, NM 87545, USA
lapenta@lanl.gov

Abstract

Methods to include automatic grid adaptation tools within the Arbitrary Lagrangian Eulerian (ALE) method are described. Two main developments will be described. First, a new grid adaptation approach is described, based on an automatic and accurate estimate of the local truncation error. Second, a new method to remap the information between two grids is presented, based on the MPDATA approach.

Introduction

The Arbitrary Lagrangian Eulerian (ALE) [2] method solves hyperbolic equations by splitting the operators is two phases.

First, in the *Lagrangian phase*, the equations under consideration are written in a Lagrangian frame and are discretized [6]. In this phase, the grid moves with the solution, the velocity of each node being the local fluid velocity.

Second, in the *Eulerian phase*, a new grid is generated and the information is transferred to the new grid. The advantage of considering this second step is the possibility of avoiding mesh distortion and tangling typical of pure Lagrangian methods.

The second phase of the ALE method is the primary topic of the present communication. In the Eulerian phase two tasks need to be completed. First, a new grid need to be created (we will refer to this task as *rezoning*). Second, the information is transferred from the grid available at the end of the Lagrangian phase to the new grid (we will refer to this task as *remapping*).

New techniques are presented below for the two tasks of the Eulerian phase: rezoning and remapping.

Rezoning

The rezoning task of the ALE method requires to generate a new adaptive grid that best describes the system and minimizes the local truncation error for the discretized equations. Below, we describe a new approach to grid adaptation based on an accurate estimate of the local truncation error.

Operator Recovery Computation of the Local Truncation Error

We have recently proposed an accurate technique for approximating the local truncation error [4]: the operator recovery method. Our aim is to derive an error indicator, not a mathematically rigorous a-posteriori error estimator (i.e. an error definition that converges to the actual truncation error).

The operator recovery method can be descibed for a general multi-dimensional non-linear partial differential equation (PDE):

$$\mathbb{A}(q) = \mathbb{X}(q) \tag{1}$$

Equation (1) summarizes the most general PDE for an unknown function $q(\mathbf{x})$ defined on the multidimensional space $\mathbf{x}$. The operator $\mathbb{X}$ summarizes all the spatial operators, of any degree and possibly non-linear; the operator $\mathbb{A}$ summarizes all other terms, such as time dependent terms, source terms or linear and non-linear homogeneous terms.

Equation (1) is discretized in space on a grid with N nodes $\mathbf{x}_i$:

$$\mathbb{A}_i = X_i(q_1, \ldots, q_N) \tag{2}$$

The two sides of the equation are evaluated at $\mathbf{x}_i$; to achieve this goal, the operator $\mathbb{A}$ is simply evaluated in $\mathbf{x}_i$, while the operator $\mathbb{X}$, differential in space, is discretized using a suitably chosen discretization scheme to obtain X_i.

From the discretized field q_i and from the discretized operator X_i applied to q_i defined only on the grid points, it is possible to reconstruct two functions defined everywhere in the continuum space $\mathbf{x}$:

$$\begin{aligned} \widetilde{q}(\mathbf{x}) &= \mathcal{L}\{q_i\} \\ \widetilde{X_q}(\mathbf{x}) &= \mathcal{L}\{X_i(q_1, \ldots, q_N)\} \end{aligned} \tag{3}$$

where $\mathcal{L}$ is the operator representing the multilinear (e.g., linear in 1D, bilinear in 2D) interpolation from the grid points.

The local truncation error is defined as the residual of the application of the exact operators upon the interpolation reconstruction of the solution of the discretized equation:

$$e = \mathbb{A}(\widetilde{q}(\mathbf{x})) - \mathbb{X}\widetilde{q}(\mathbf{x}) \tag{4}$$

Recalling that the operator $\mathbb{A}$ commutes with any spatial operator and particularly with the linear interpolation operator $\mathcal{L}$, it follows:

$$\mathbb{A}(\widetilde{q}(\mathbf{x})) = \widetilde{X_q}(\mathbf{x}) \tag{5}$$

Using eq.(5), the definition of the local truncation error becomes:

$$e = \widetilde{X_q}(\mathbf{x}) - \mathbb{X}\widetilde{q}(\mathbf{x}) \tag{6}$$

which defines the local truncation error as the difference between the linear interpolation of the discretized operator applied to the discretized field $\widetilde{X_q}(\mathbf{x})$ and the exact differential operator applied to the linear interpolation of the discretized field $\widetilde{q}(\mathbf{x})$.

The local truncation error in each cell i is defined as the L_2 nrom:

$$e_i = \left(\frac{1}{V_i}\int_{V_i} T^2 dV\right)^{1/2} \tag{7}$$

where e_i is the average local truncation error over cell i and V_i is the cell volume.

Variational Grid Adaptation Based on Error Indicators

We have recently proposed a new approach to variational grid adaptation based of the local truncation error computed above [4]. The method can be constructed starting from the following theorem proven in Ref. [4]

THEOREM:*In a optimal grid, defined as a grid that minimizes the local truncation error according to the minimzation principle*

$$\int_{\mathcal{V}} \mid e \mid d^N x\,, \tag{8}$$

the product of the local truncation error in any cell i by the cell volume V_i (given by the Jacobian $J = \sqrt{g}$) is constant:

$$e_i V_i = \text{const} \tag{9}$$

The equidistribution theorem is applied solving the following Euler-Lagrange equations:

$$g^{ij}\frac{\partial}{\partial\xi^i}\left(e\frac{\partial x^i}{\partial\xi^j}\right)=0 \tag{10}$$

This approach creates a grid where e_iV_i is constant. Note that the equations above are identical to the equations used by the Winslow's variable diffusion method. The primary innovation is that the monitor function is now directly linked with the local truncation error instead of being left undefined. In the typical implementations of the Winslow's variable diffusion method, the merit function is defined heuristically by the user. The use of the operator recovery error indicator proposed here results in a more accurate scheme [4].

Remapping

The remapping phase can be considered simply an advection step [1], where the interpolation between two grids is modeled with an advection equation. Below we present the advection equation equivalent to the interpolation task of the remapping phase. Then the MPDATA [7] method is used to dicretize the remapping equation. The application of the MPDATA method requires some relevant modifications and extension to the formalism published in [7].

Remapping: Formulation of the Problem

One can assume that the grid moves from the old grid $\mathbf{x}^0$ to the new $\mathbf{x}^1$ as: $\mathbf{x}(\boldsymbol{\xi},t)$ with a constant velocity: $\mathbf{v}=\frac{\partial\mathbf{x}}{\partial t}$. We assume further that the mapping from physical to natural coordinates changes as the grid moves. The cell volume, which is defined as: $G(\boldsymbol{\xi},t)=\det(\frac{\partial\mathbf{x}}{\partial\boldsymbol{\xi}})$, changes in time also.

In the derivation below we limit the scope to 1D, the extension to 2D being tedious but straightforward. The correct equation for remapping based on advection is:

$$\frac{\partial G\psi}{\partial t}=\frac{\partial}{\partial\xi}\cdot(u\psi) \tag{11}$$

This is the equation that we need to solve using MPDATA. It differs from all the models considered in the review paper [7] in two ways:

1. The determinant of the metric tensor of the mapping G is time dependent, a case not considered before. The time dependence is very

benign, as the grid velocity is assumed to be constant in time. For example in 1D the variation of G in time is linear. Taylor series in time are therefore convergent.

2. The determinant of the metric tensor of the mapping G is not particularly smooth in space, as grid spacing can jump arbitrarily from cell to cell. The assumption of analiticity of G is unacceptable, requiring special care in handling Taylor series in space. Only within a cell, they do converge.

In the 1D case, the application of the donor cell to eq.(12) is straightforward:

$$\psi_i^1 G_i^1 = \psi_i^0 G_i^0 + \left(u_{i+1/2} \psi^0_{i+1/2(upwind)} - u_{i-1/2} \psi^0_{i-1/2(upwind)} \right) \qquad (12)$$

where

$$u_{i+1/2} \psi_{i+1/2(upwind)} = \mathbb{F}[\psi_i^0, \psi_{i+1}^0, -u_{i+1/2}] \qquad (13)$$

and $\mathbb{F}$ is defined as in [7]:

$$\mathbb{F}(\psi_L, \psi_R, U) \equiv \begin{cases} U\psi_L \text{ if } \mathrm{U} > 0 \\ U\psi_R \text{ if } \mathrm{U} < 0 \\ 0 \text{ otherwise} \end{cases} \qquad (14)$$

Note that we have used the fact that the velocity in eq.(12) has the opposite sign than usual advection, as appropriate for remapping.

Equation (13) includes two sources of second order errors: one is coming from the explicit Euler discretization of the time derivative and one from the upwind discretization of the spatial derivative. The two errors can be treated separately, in a *dividi et impera* approach.

Modified Equation Approach - Spatial Error

For simplicity, we assume here that the system is 1D. If we consider the spatial error alone, we have:

$$\frac{\partial G\psi}{\partial t} = F \qquad (15)$$

where $F = \partial \psi u / \partial \xi$. We then proceed to discretize F in space:

$$\left. \frac{\partial G\psi}{\partial t} \right|_i = (F_{i+1/2} - F_{i-1/2}) \qquad (16)$$

note that eq.(17) is second order accurate, until we introduce upwinding to approximate $F_{i\pm1/2}$. The exact expression of $F_{i\pm1/2}$ would be: $F_{i\pm1/2} =$

$u_{i\pm1/2}\psi_{i\pm1/2}$ but the upwind method approximates:

$$F_{i+1/2} = \mathbb{F}[\psi_i^0, \psi_{i+1}^0, -u_{i+1/2}] \tag{17}$$

and similarly for $F_{i-1/2}$. Consequently an error is committed:

$$\delta F_{i\pm1/2} = u_{i+1/2}\delta\psi_{i\pm1/2} \tag{18}$$

where $\delta\psi_{i\pm1/2} = \psi_{i\pm1/2} - \psi_{i\pm1/2(upwind)}$.

To fix the ideas, let us consider $i+1/2$ and assume $u_{i+1/2} > 0$; the expression for $\delta\psi_{1+1/2}$ is:

$$\delta\psi_{i+1/2} = \psi_{i+1/2} - \psi_{i+1} \tag{19}$$

Now we apply the crucial MPDATA machinery, the modified equation approach, but with a new twist. We Taylor series expand around $i + 1/2$, instead of the usual i. The reason is that G is potentially non-analytic requiring special care in dealing with the Taylor series expansion. Centering around i and using it beyond cell i would be forgetting that G might jump from cell to cell. Furthermore, we can approximate first derivatives better in $i + 1/2$ than in i. Finally, we need to center in $i + 1/2$ because that is the exact value we assume as reference.

Performing the Taylor expansion, it follows :

$$\delta\psi_{i+1/2} = \psi_{i+1/2} - \left[\psi_{i+1/2} + \left.\frac{\partial\psi}{\partial x}\right|_{i+1/2}(x_{i+1} - x_{i+1/2})\right] \tag{20}$$

recalling that $G_{i+1} = 2(x_{i+1} - x_{i+1/2})$, it follows:

$$\delta\psi_{i+1/2} = \left.\frac{\partial\psi}{\partial x}\right|_{i+1/2}\frac{G_{i+1}}{2} \tag{21}$$

which provides the final result for the expression of the error as provided by the modified equation approach.

The derivative can be approximated using the cell centered values of ψ: $\left.\frac{\partial\psi}{\partial x}\right|_{i+1/2} = (\psi_{i+1} - \psi_i)/(x_{i+1} - x_i)$. Note that this approximation is perfectly justified, as $\psi(x)$ is analytic (it is G that is not). Recalling again the definition of G, the final expression, generalized for any sign of the node velocity $u_{i+1/2}$ is

$$\delta\psi_{i\pm1/2} = -\frac{\psi_{i+1} - \psi_i}{G_{i+1} + G_i}G_{i+1/2(upwind)} \tag{22}$$

that provides the approximation to the correction that we have to introduce in the second step of MPDATA, coming from the spatial truncation error alone:

$$\delta F_{i+1/2} = -2\frac{\psi_{i+1} - \psi_i}{G_{i+1} + G_i}(u_{i+1/2} G_{i+1/2(upwind)}) \tag{23}$$

where $G_{i+1/2(upwind)} = \mathbb{F}(G_i, G_{i+1}, -\text{sign}(u_{i+1/2}))$.

As usual to make the MPDATA correction similar to the donor cell step, we divide and multiply by $\psi_{i+1/2(upwind)}$, and replace it in the denominator with the averaged value. Following that procedure, the contribution of the spatial error to the correction velocity for the second step of the MPDATA method is:

$$V^A_{i+1/2} = \frac{|u_{i+1/2}| G_{i+1/2(upwind)}}{0.5(G_{i+1} + G_i)} \frac{\psi_{i+1} - \psi_i}{\psi_i + \psi_{i+1}} \tag{24}$$

Note that the contribution V^A is related to, but differs from, the corresponding expression in eq.(8) or in eq.(29a) of [7] for the presence of the factor: $G_{i+1/2(upwind)}/0.5(G_{i+1} + G_i)$ that becomes crucially important for very non-smooth grids.

Of course, the complete expression will need also the contribution of the truncation error due to the discretization of the time derivative.

Modified Equation Approach - Time Error

The computation of the truncation error coming from the explicit Euler discretization of the time derivative in eq.(12) is much simpler and more closely related to the usual derivations in Ref. [7].

Basically the task is simple: to generalize the derivation in section 3.1 of Ref. [7] to the case where v is constant in time (but not in space) but G is variable both in space and time (time variation of G was never considered within the MPDATA approach). But the procedure follows closely eqs.(20-25) of Ref. [7]. Here is the algebra:

We discretize eq.(12) using explicit Euler:

$$\frac{G^1\psi^1 - G^0\psi^0}{\delta t} = \frac{\partial u\psi}{\partial \xi} \tag{25}$$

Expanding in Taylor series around time level 0 (an harmless task since G is analytic in time, while it was not in space), with trivial straightforward algebra, one gets the following modified equation:

$$\frac{\partial \psi G}{\partial t} - \frac{\partial u\psi}{\partial \xi} = -\frac{\delta t}{2}\frac{\partial^2 G\psi}{\partial t^2} \tag{26}$$

Next step is to eliminate the time derivatives transforming them in spatial derivative using the modified equation itself. To eliminate the second order derivative, we derive the equation above in time:

$$\frac{\partial^2 \psi G}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial G\psi}{\partial t}\right) = \frac{\partial}{\partial t}\left(\frac{\partial u\psi}{\partial \xi}\right) + \mathcal{O}(\delta t) = \frac{\partial}{\partial t}\left(u\frac{\partial \psi}{\partial t}\right) + \mathcal{O}(\delta t) \quad (27)$$

Using furthermore that:

$$G\frac{\partial \psi}{\partial t} = \frac{\partial u\psi}{\partial \xi} - \psi\frac{\partial G}{\partial t} + \mathcal{O}(\delta t) \quad (28)$$

it follows :

$$\frac{\partial \psi G}{\partial t} - \frac{\partial u\rho}{\partial \xi} = -\frac{\delta t}{2}\frac{\partial}{\partial \xi}\left[\frac{u}{G}\frac{\partial u\psi}{\partial \xi} - \frac{u\psi}{G}\frac{\partial G}{\partial t}\right] \quad (29)$$

Now a crucial algebraic step, that is peculiar to remapping. The derivative of G with respect of time can be expressed in an interesting way. Recalling that $G = \partial x/\partial \xi$:

$$\frac{\partial G}{\partial t} = \frac{\partial}{\partial \xi}\frac{\partial x}{\partial t} = \frac{\partial u}{\partial \xi} \quad (30)$$

Using this result, eq.(30), the modified equation becomes:

$$\frac{\partial \psi G}{\partial t} - \frac{\partial u\psi}{\partial \xi} = -\frac{\delta t}{2}\frac{\partial}{\partial \xi}\left[\frac{u}{G}u\frac{\partial \psi}{\partial \xi}\right] \quad (31)$$

This equation is the final result, to be compared with eq.(25) of Ref. [7]. Indeed, it is identical, exept for the absence of the $\nabla \cdot \mathbf{u}$ term. This lead directly to the correction in the second MPDATA step coming from the time truncation error:

$$V^B_{i+1/2} = -\frac{u^2_{i+1/2}}{0.5(G_{i+1} + G_i)}\ \frac{\psi_{i+1} - \psi_i}{\psi_i + \psi_{i+1}} \quad (32)$$

where δt can be assumed to be 1. This contribution ought to be added to the spatial contribution $V^A_{i+1/2}$ to get the complete expression.

Summary of the MPDATA Scheme for 1D Remapping

In the first step, the donor step is applied:

$$\psi^*_i G^*_i = \psi^0_i G^0_i + \mathbb{F}[\psi^0_i, \psi^0_{i+1}, -u_{i+1/2}] - \mathbb{F}[\psi^0_{i-1}, \psi^0_i, -u_{i-1/2}] \quad (33)$$

Next the correction velocity is computed as:

$$V_{i+1/2} = \frac{|u_{i+1/2}|G^0_{i+1/2(upwind)} - u^2_{i+1/2}}{0.5(G^0_{i+1} + G^0_i)} \frac{\psi^0_{i+1} - \psi^0_i}{\psi^0_i + \psi^0_{i+1}} \tag{34}$$

Note that the choice of the time level in the equation above is somewhat arbitrary. To second order, it does not change the error, but practical examples have shown that the choice above, which it is to use the original grid values everywhere is best.

The the final step in the MPDATA remapper is another donor step:

$$\psi^1_i G^1_i = \psi^*_i G^*_i - \mathbb{F}[\psi^*_i, \psi^*_{i+1}, V_{i+1/2}] + \mathbb{F}[\psi^*_{i-1}, \psi^*_i, V_{i-1/2}] \tag{35}$$

The approach followed above does not appear to have any problem to be extended to 2D or 3D. We shall see.

Results

We consider the classic spherical 1D implosion test proposed by Noh [5]. The gas initially has $\rho = 1$, $e = 10^{-4}$ and uniform velocity $u = -1$ (except in the center where $u(r = 0) = 0$). The gas has $\gamma = 5/3$. The problem represents a serious challenge for Lagrangian calculations and the solution is known to suffer from serious wall heating due to the use of artificial viscosity to capture shocks. Note that we are not using artificial heat conduction (Noh, 1987), a tool to remove the wall heating problem, precisely to highlight the trouble of Lagrangian calculations for the present case .

The results of an ALE calculation using the adaptive grid is compared with a reference standard Lagrangian calculation.

Figure 1 show the density at the end of the Lagrangian and ALE calculation. The use of adaptive grid results in a much improved solution. The reason for the improvement is explained by the better description of the shock achieved by the adaptation. As noted in Dorfi's benchmark, the adaptation results in a sharper shock. In the present case this sharper resoluition results also in a considerable reduction of the wall heating, as explained in the original paper by Noh (Noh, 1987). Such reduction explains why the improvement in the present case is more relevant than in the previous case shown (Dorfi's benchmark).

References

[1] J.K. Dukowicz, J.R. Baumgardner, *J. Comput. Phys.*, **160**, 318 (2000).

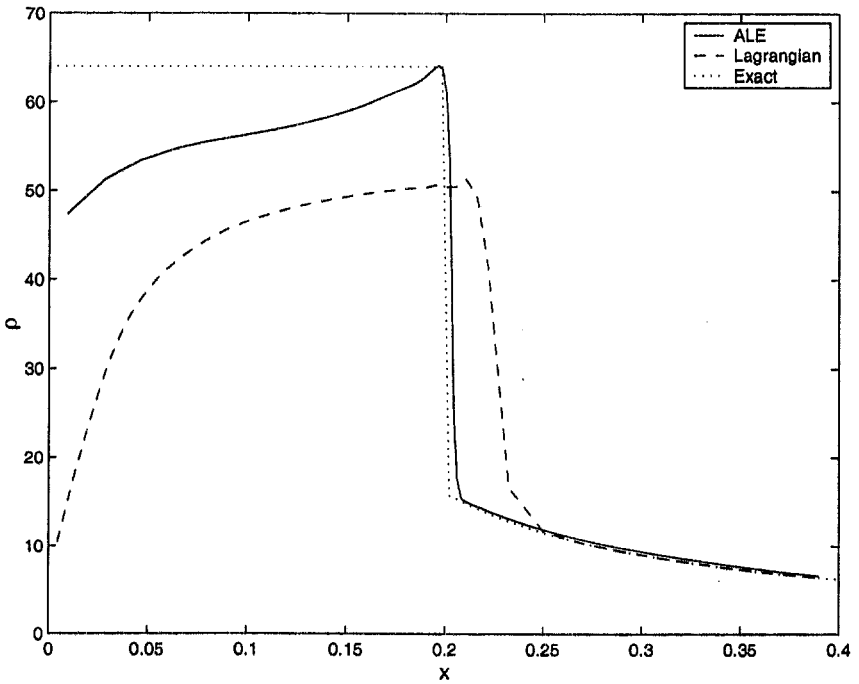


Figure 1. Gas Dynamics - Noh's spherical benchmark: comparison of the density at the end ($t = 0.6$), for a Lagrangian (dashed) and ALE (solid line) calculation. The exact solution is also shown (dotted line).

[2] C.W. Hirt, A.A. Amsden, J.L. Cook, *J. Comput. Phys.*, **14**, 227 (1974).

[3] J.U. Brackbill, *J. Comput. Phys.*, **108**, 38 (1993).

[4] G. Lapenta, *J. Comput. Phys.*, submitted.

[5] W.F. Noh, *J. Comput. Phys.*, **72**, 78 (1987).

[6] M.S. Shashkov, *Conservative finite-difference methods on general grids* (CRC Press, Boca Raton, 1996).

[7] P.K. Smolarkiewicz, L.G. Margolin, *J. Computat. Phys.*, **140**, 459-480 (1998).