Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Computational Physics 198 (2004) 265–277
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

The repair paradigm and application to conservation laws

Mikhail Shashkov *, Burton Wendroff

Theoretical Division, T-7, Los Alamos National Laboratory, MS-B284, Los Alamos, NM 87545, USA

Received 24 September 2003; received in revised form 22 December 2003; accepted 9 January 2004
Available online 20 February 2004

Abstract

Repair is a conservative, post-processing procedure to be used in numerical methods for hyperbolic conservation laws in order to preserve certain qualitative characteristics of the numerical solution, such as positivity of density and internal energy, by means of redistribution of conserved quantities such as mass, momentum and total energy among the cells of the mesh. In this paper we describe the repair paradigm and prove several theorems which form a theoretical foundation for the repair procedures. We consider two applications of repair and present corresponding numerical results. The first application deals with improving properties of the remapping (conservative interpolation) stage of arbitrary Lagrangian–Eulerian (ALE) methods for the gas dynamics equations, in which the solution is conservatively transferred from one mesh to another. One requirement for remapping is that the interpolated density and internal energy on the new mesh have to stay positive. Another desirable property is that the remapping procedure should not create new extrema for the velocity field. For various reasons these properties may not be satisfied, especially for high-order methods. Repair plays a supplemental role by bringing gas dynamics quantities into physically justified bounds. Another application of repair is to improve the quality of numerical methods for advection of some scalar tracer field with prescribed divergence-free velocity field, in which case the advection equation can be written as a conservation law, and therefore the total amount of tracer is conserved. We show how the repair procedure allows us to reduce oscillations in a numerical solution obtained by a formally high-order method. Repair offers an alternative to more classical methods of reducing oscillations and maintaining positivity.

AMS: 65N05; 65N10; 65N15; 80A20

Keywords: Mass redistribution; Repair; Remapping; Advection

1. Introduction

The repair algorithm introduced in [2] is a post-processing procedure designed to improve the quality of an efficient accurate numerical remapping method presented there. In this work we analyze repair in greater detail, present variants of it along with some mathematical justification, and apply it to advection.

* Corresponding author. Tel.: +1-505-667-4400; fax: +1-505-665-5757.
E-mail addresses: shashkov@lanl.gov, misha@t7.lanl.gov (M. Shashkov), bbw@lanl.gov (B. Wendroff).

0021-9991/$ - see front matter © 2004 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcp.2004.01.014

The need for conservative remapping occurs in the context of an Euler solver that has produced density, velocity, and energy on some grid, and these need to be transferred to another grid so as to conserve mass, momentum and energy.

Consider first masses. Suppose the initial grid defines cells C_i having masses $m_i > 0$, areas $|C_i| > 0$, and mean densities $\rho_i \equiv m_i/|C_i|$. Move the vertices a little bit (not the boundaries), producing new cells C_i'. An incremental remapping algorithm will assign masses m_i' to each cell C_i' so that total mass is conserved. The algorithm can have two forms. In one, a nonnegative mass matrix (i.e., with nonnegative elements) $m_{ij} \geqslant 0$ is constructed that assigns a mass to each of the sub-partition sets $C_{ij} \equiv C_i' \cap C_j$. This is done by extending the ρ_i to a function $\rho(x) \geqslant 0$ defined on the whole domain such that the integral of $\rho(x)$ over each C_i is m_i and then setting m_{ij} to be the integral of $\rho(x)$ over C_{ij}. The new masses m_i' are then defined by

$$m_i' = \sum_{j:|C_i' \cap C_j| \neq 0} m_{ij}. \tag{1}$$

But then it is also true that

$$m_i = \sum_{j:|C_j' \cap C_i| \neq 0} m_{ji}. \tag{2}$$

This form of remapping is developed in detail in [1], in [2] it is called remapping by exact integration. Another remapping that plays a major role in [2] and [4] has the general form

$$m_i' = m_i + \sum_j F_{ij},$$

where the *flux* matrix F_{ij} is anti-symmetric. Remapping, whether by exact integration or by the above general flux form must be *consistent*, that is if the ρ_i are constant, $\rho_i = A$ for all i, then $\rho_i' = A$ for all i.

Now, the mass matrix form implies a flux form, since

$$m_i' = m_i + \sum_j m_{ij} - m_i = m_i + \sum_j m_{ij} - \sum_j m_{ji} = m_i + \sum_j (m_{ij} - m_{ji}),$$

so that in this case $F_{ij} = m_{ij} - m_{ji}$.

A flux form will not in general lead to a nonnegative mass matrix, although we can set

$$m_{ij} = \{F_{ij}, i \neq j, F_{ij} > 0\},$$

$$m_{ij} = \{0, i \neq j, F_{ij} \leqslant 0\},$$

$$m_{ii} = m_i + \sum_{j, F_{ij} < 0} F_{ij}.$$

The problem is that the m_{ii} could be negative.

Now suppose that another conserved quantity like momentum has also been remapped from the first grid to the second. Restrict attention to one dimension. If the momenta are P_i and velocities are u_i, then for the original grid $u_i \equiv P_i/m_i$, and on the new grid $u_i' \equiv P_i'/m_i'$. Similarly, if total energy E_i and specific internal energy e_i and kinetic energy $\frac{1}{2}m_i u_i^2$ on the original grid are related by $E_i \equiv m_i(e_i + \frac{1}{2}u_i^2)$, then on the new grid this becomes $E_i' \equiv m_i'(e_i' + \frac{1}{2}(u_i')^2)$. Since E_i' is the remapped variable, e_i' is defined by $e_i' \equiv (E_i' - \frac{1}{2}m_i'(u_i')^2)/m_i'$.

We consider the following questions. First, if the ρ_i satisfy certain bounds, say

$$\rho_i^{\min} \leqslant \rho_i \leqslant \rho_i^{\max},$$

can we adjust the m_i' so that total mass remains conserved and

$$\rho_i^{\min} \leqslant \rho_i' \leqslant \rho_i^{\max}, \tag{3}$$

where $\rho_i' \equiv m_i'/|C_i'|$. Second, if the u_i satisfy certain bounds, say

$$u_i^{\min} \leqslant u_i \leqslant u_i^{\max},$$

can we adjust the P_i' so that total momentum remains conserved and

$$u_i^{\min} \leqslant u_i' \leqslant u_i^{\max}. \tag{4}$$

Third, if the internal energies e_i satisfy certain bounds, say

$$e_i^{\min} \leqslant e_i \leqslant e_i^{\max},$$

can we adjust the E_i' so that total energy remains conserved and the new internal energies satisfy

$$e_i^{\min} \leqslant e_i' \leqslant e_i^{\max}. \tag{5}$$

In several dimensions bounds would be applied to each velocity component and the kinetic energy becomes the sum of the kinetic energies corresponding to each velocity component.

1.1. Main result

The process of adjustment is what is called repair in [2], and we shall show that under reasonable assumptions about the bounds the masses can be repaired so that (3) holds. If a nonnegative mass matrix exists then momentum also can be repaired so that (4) holds. If these repairs are made first, then if the total kinetic energy of the new grid is not larger than the total kinetic energy of the old grid the energy E_i can be adjusted so as to satisfy the *lower bounds* on internal energy.

The existence of the nonnegative mass matrix is crucial for the theory, but the difficulty we face is that after repair of masses we just have assigned masses m_i and m_i'. The m_i might come from a density, but the m_i' might not, as in [2]. This raises a new question, namely, do there exist masses $m_{ij} \geqslant 0$ such that for given $m_i > 0$ and $m_i' > 0$

$$m_i = \sum_j m_{ji}, \tag{6}$$

$$m_i' = \sum_j m_{ij}, \tag{7}$$

$$m_{ij} = 0 \quad \text{if } |C_i' \cap C_j| = 0. \tag{8}$$

This turns out to be a classical problem in constrained optimization for which there are necessary and sufficient conditions implying the existence of a solution [6].

The repair notion is not restricted to remapping, but it can also be applied to advection schemes, even those that are not conservative. Repair can be used to impose positivity and reduce oscillations. Since even the sophisticated and carefully constructed third-order scheme CENOAC (see Section 8, where numerical examples are given) can lead to negative values, we feel that repair offers an alternative that should be considered. We might also note that doing repair in more than one dimension on unstructured grids is not particularly difficult.

2. Repair of mass

First, choose a *bound-determining neighborhood* $\mathcal{N}_i$ for each cell C_i. For example, this neighborhood might consist of cell C_i itself and all of its nearest neighbors – in the case of a logically rectangular grid in 2D it will be the 3×3 patch with center in cell C_i. We will use the notation $\mathcal{N}_i$ also for the set of indices of cells in the neighborhood.

The first *assumption* about this neighborhood is,

$$|C_i' \cap C_j| \neq 0 \quad \text{if and only if } j \in \mathcal{N}_i, \tag{9}$$

that is, the interior of C_i' is completely covered by the bound-determining neighborhood of cell C_i.

If the bound-determining neighborhood is specified then this condition can be considered as a restriction on the displacements of the vertices of the old cells. In other words, allowable displacements have to be compatible with the definition of bound-determining neighborhood.

The lower and upper bounds $\rho_i^{\min}$, $\rho_i^{\max}$, are

$$\rho_i^{\min} = \min_{j \in \mathcal{N}_i} \rho_j,$$

$$\rho_i^{\max} = \max_{j \in \mathcal{N}_i} \rho_j.$$

The repair process redistributes mass. Its success depends on the following theorem, the proof of which will be given later.

Theorem 1. *Suppose* (9) *holds and mass is conserved. If there exists a cell* C_a' *such that* $m_a' < \rho_a^{\min}|C_a'|$ $(m_a' > \rho_a^{\max}|C_a'|)$ *then there exists a cell* C_b' *such that* $m_b' > \rho_b^{\min}|C_b'|$ $(m_b' < \rho_b^{\max}|C_b'|)$.

There are two ways to redistribute mass, locally or globally.

Note that in applying repair we may leave out those cells for which $C_i = C_i'$.

2.1. Local redistribution

To redistribute mass locally, following [2], we sweep through the cells and check if the new mean density ρ_i' is within its range, if so we do nothing. If the new mean value is out of range we attempt to move it to the extreme value by subtracting or adding mass to nearby cells. Below we give the algorithm for the case when, for some i, $\rho_i' < \rho_i^{\min}$. The case when $\rho_i' > \rho_i^{\max}$ is similar.

If

$$\rho_i' < \rho_i^{\min},$$

then

$$\delta m_i^- \equiv \left(\rho_i^{\min} - \rho_i'\right)|C_i'|$$

is the mass needed to add to this cell to increase the new value up to its lower bound. Conservation requires that this needed mass be taken from other cells. Starting with a *search* neighborhood $\mathcal{S}_i$ consisting of the cells C_j' for j in the bound-determining neighborhood $\mathcal{N}_i$, we compute how much mass can safely be taken from each cell, that is, without violating its local bound. This is

$$\delta m_j \equiv \max\left((\rho_j' - \rho_j^{\min})|C_j'|, 0\right),$$

and the total available mass in the neighborhood is

$$\delta m \equiv \sum_{j \in \mathscr{S}_i} \delta m_j.$$

If there is enough available mass in neighboring cells to provide the mass needed for cell C_i', that is, if

$$\delta m_i^- \leqslant \delta m,$$

then the mass and corresponding density in cells C_i' are increased up to their lower bounds. That is, we set

$$\hat{m}_i = \rho_i^{\min} |C_i'|, \quad \hat{\rho}_i = \rho_i^{\min}.$$

All other cell masses in the neighborhood are decreased proportionally to the mass available in the cell, that is,

$$\hat{m}_j = m_j' - \frac{\delta m_j}{\delta m} \delta m_i^-,$$

for $j \neq i$ and $j \in \mathscr{N}_i$, and clearly the total mass of cell C_i' and its neighbors remains unchanged.

A modified version of this is to set

$$\tau = \min\left(\frac{\delta m_i^-}{\delta m}, 1\right),$$

$$\hat{\rho}_j = (1-\tau)\rho_j' + \tau \rho_j^{\min},$$

and

$$\hat{m}_i = m_i' + \min(\delta m_i^-, \delta m),$$
$$\hat{\rho}_i = \hat{m}_i / |C_i'|.$$

In either case if $\delta m_i^- > \delta m$, that is, not enough mass is available in the search neighborhood to provide the needed mass, then the neighborhood is extended and the process is repeated.

Theorem 1 guarantees that this process will terminate successfully. Indeed, it follows from Theorem 1 that (in this case)

$$\delta M^+ = \sum_{i:\rho_i' > \rho_i^{\min}} (\rho_i' - \rho_i^{\min}) |C_i'| \geqslant \delta M^- = \sum_{i:\rho_i' < \rho_i^{\min}} (\rho_i^{\min} - \rho_i') |C_i'| > 0.$$

For otherwise, if $\delta M^+ < \delta M^-$, since δM^+ exhausts all cells that could possibly contribute mass, there would be at least one cell covered in δM^- that contradicts the theorem. Thus, there is enough mass to repair all cells.

This local procedure does not lend itself readily to parallelization.

2.2. Global redistribution

There are several forms of global redistribution. In all of them we first set each cell C_i' whose density is out of bound to its extremum. Thus, for each i set

$$\hat{\rho}_i = \max(\rho_i^{\min}, \min(\rho_i', \rho_i^{\max})),$$
$$\hat{m}_i = \hat{\rho}_i |C_i'|$$

and

$$\hat{M} = \sum_i \hat{m}_i.$$

Next, let

$$D^+ = \sum_i \left(\hat{\rho}_i - \rho_i^{\min}\right)|C_i'|,$$
$$D^- = \sum_i \left(\rho_i^{\max} - \hat{\rho}_i\right)|C_i'|.$$

Let the original total mass be M and

$$\delta = \hat{M} - M.$$

We now *redefine* the new cell masses m_i'. If $\delta = 0$ then set $m_i' = \hat{m}_i$. If $\delta > 0$ we have to subtract mass from those cells that are above their lower bound, and if $\delta < 0$ we have to add mass to those cells below their upper bound. That is, in the case $\delta > 0$ Theorem 1 guarantees that $D^+ > 0$ and therefore we can set for each i

$$m_i' = \hat{m}_i - (\hat{m}_i - \rho_i^{\min}|C_i'|)\frac{\delta}{D^+},$$

without violating the lower bound, while in the case $\delta < 0$, by the same argument given in the previous section, Theorem 1 guarantees that $D^- > 0$ and we can set for each i

$$m_i' = \hat{m}_i - (\rho_i^{\max}|C_i'| - \hat{m}_i)\frac{\delta}{D^-}.$$

Then

$$\sum_i m_i' = M$$

and all bounds are satisfied.

One problem with this is that there may be unnecessarily large changes in some masses. One alternative is to try to distribute δ uniformly. Thus, in the case $\delta > 0$ let N be the number of cells for which

$$(\hat{m}_i - \rho_i^{\min}|C_i'|) > 0, \tag{10}$$

and for each of those cells let $m_i' = \hat{m}_i - \delta/N$. If no cell drops below its lower bound as a result then these m_i' are optimal in the sense of being the minimizer of the function $\max_i(\hat{m}_i - x_i)$ where the maximum is taken over all i satisfying (10) and the constraints are $x_i \geqslant 0$, $\hat{m}_i - x_i \geqslant 0$, and $\sum(\hat{m}_i - x_i) = \delta$. If some cell drops below its lower bound we can just repeat the process starting at (10). This must terminate, although no longer necessarily with the optimal deviation.

Both of these procedures are easily parallelized.

3. Repair of velocity

The repair method can be applied to any conserved quantity, for example, momentum P. However, we might not be interested in bounds for momentum but rather bounds for velocity, defined as $u = P/m$ (this is for just one component). The velocity bounds $u_i^{\min}$, $u_i^{\max}$ are

$$u_i^{\min} = \min_{j \in \mathcal{N}_i} u_j,$$

$$u_i^{\max} = \max_{j \in \mathcal{N}_i} u_j.$$

Velocity repair proceeds exactly as mass repair, except replacing density everywhere by velocity, mass by momentum, and then area by mass. The following gives conditions for the validity of this process.

Theorem 2. *Suppose mass and momentum are conserved and suppose that there exist* $m_{ij} \geqslant 0$ *such that* (6) *and* (7) *hold and*

$$\text{if } j \notin \mathcal{N}_i \text{ then either } m_{ij} = 0 \quad \text{or} \quad u_i^{\min} \leqslant u_j \leqslant u_i^{\max}. \tag{11}$$

Then if there exists a cell C'_a *such that* $u'_a < u_a^{\min}$ $(u'_a > u_a^{\max})$ *then there exists a cell* C'_b *such that* $u'_b > u_b^{\min}$ $(u'_b < u_b^{\max})$.

Note that the condition on m_{ij} is weaker than requiring (8).
This applies to any conserved quantity A_i with density A_i/m_i.

4. Repair of internal energy

If (total) energy is remapped, internal energy has to be obtained by subtracting the kinetic energy from the energy, and this can lead to negative internal energies. However, if the remapping is dissipative in the sense that the total kinetic energy computed from the remapped and repaired densities and velocities is not greater than the initial total kinetic energy, then repair can be applied to satisfy lower bounds on internal energy without violating energy conservation. This follows from

Theorem 3. *Suppose total energy is conserved, total kinetic energy has decreased, and suppose that there exist* $m_{ij} \geqslant 0$ *such that* (6) *and* (7) *hold and*

$$\text{if } j \notin \mathcal{N}_i \text{ then either } m_{ij} = 0 \quad \text{or} \quad e_i^{\min} \leqslant e_j. \tag{12}$$

Then if there exists a cell C'_a *such that* $e'_a < e_a^{\min}$ *then there exists a cell* C'_b *such that* $e'_b > e_b^{\min}$.

5. Proofs

Consider first Theorem 1. We want to show that not all new densities can be out of bound. Suppose for all i that $\rho'_i \leqslant \rho_i^{\min}$, but for some i $\rho'_i < \rho_i^{\min}$. Then

$$\sum_j m'_j = \sum_j \sum_i |C_{ji}| \rho'_j < \sum_j \sum_i |C_{ji}| \rho_j^{\min}.$$

By (9),

$$\sum_j m'_j < \sum_j \sum_i |C_{ji}| \rho_j = \sum_i \rho_i \sum_j |C_{ji}| = \sum_i m_i,$$

which contradicts mass conservation. So if one new density is less than its lower bound then there must be one that is greater, as claimed.

Consider next Theorem 2. We want to show that not all new velocities can be out of bound. Suppose for all i that $u'_i \leqslant u_i^{\min}$, but for some i $u'_i < u_i^{\min}$. Then

$$\sum_j P'_j = \sum_j m'_j u'_j < \sum_j m'_j u_j^{\min}.$$

By (6), (7) and (11),

$$\sum_j P'_j < \sum_j \sum_i m_{ji} u_j^{\min} \leqslant \sum_j \sum_i m_{ji} u_i = \sum_i u_i \sum_j m_{ji} = \sum_i u_i m_i = \sum_i P_i,$$

which contradicts momentum conservation. So if one new velocity is less than its lower bound then there must be one that is greater, as claimed.

For Theorem 3, let $K = \sum_i \frac{1}{2} m_i u_i^2$, $K' = \sum_i \frac{1}{2} m'_i (u')_i^2$. Then if $e'_i \leqslant e_i^{\min}$ for all i,

$$\sum_j E'_j = \sum_j m'_j e'_j + K' \leqslant \sum_j \sum_i m_{ji} e_j^{\min} + K'.$$

By (12)

$$\sum_j E'_j \leqslant \sum_j \sum_i m_{ji} e_i + K' = \sum_i m_i e_i + K' = \sum_i E_i - K + K'.$$

Therefore, since total energy is conserved, $K \leqslant K'$, contradicting the hypothesis.

6. Existence of a mass matrix

When does the mass matrix $m_{ij} \geqslant 0$ that satisfies (6)–(8) exist? It certainly does if the new and old masses are the result of exact integration of a common nonnegative density function, but that may not be the case. If it does exist then the following is an obvious necessary condition: if

$$C_{i_1} \cup \cdots C_{i_k} \subset C'_{j_1} \cup \cdots C'_{j_l},$$

then

$$\sum_{n=1,k} m_{i_n} \leqslant \sum_{n=1,l} m'_{j_n}$$

and if

$$C'_{i_1} \cup \cdots C'_{i_k} \subset C_{j_1} \cup \cdots C_{j_l},$$

then

$$\sum_{n=1,k} m'_{i_n} \leqslant \sum_{n=1,l} m_{j_n}.$$

Is this a sufficient condition?

Given this condition the m_{ij} can easily be constructed in one dimension. This is not so in two dimensions, but there is an existence theorem.

Once the masses m, m' are given, this question becomes strictly combinatorial. Namely, we are asking if there is a $M \times N$ matrix $A = \{m_{ij}\}$ with nonnegative entries having prescribed positive row sums m'_i and

positive column sums m_i and prescribed zero entries. This is answered in [6, Theorem 2]. Following that paper, let $\mathrm{supp}(A) = \{i, j : m_{ij} \neq 0\}$. For any index set $I = (i_1, \ldots, i_k)$ let I^c be the complementary index set. Let A_{IJ} be the submatrix $\{m_{ij} : i \in I, j \in J\}$. One necessary and sufficient condition for the existence of $m_{ij} > 0$, $(i, j) \in \mathrm{supp}(A)$, is that

$$\sum_{i \in I} m_i \geqslant \sum_{j \in J} m'_j,$$

if $A_{I^c J} = 0$, and equality holds if and only if also $A_{IJ^c} = 0$. Note that since

$$\sum_i m_i = \sum_j m'_j,$$

then

$$\sum_{j \in J^c} m'_i \geqslant \sum_{i \in I^c} m_i.$$

Unfortunately, this result is only of theoretical interest, as these conditions cannot be readily verified in general.

7. An illustrative example

We give a simple example to show the effect of repair for density, velocity and internal energy. The calculation is done as follows. First the conserved quantities mass, momentum and total energy are remapped. Then density is repaired. Now velocity is defined as the ratio of the remapped momentum to the repaired mass, and then repaired. The kinetic energy is then computed from the repaired density and repaired velocity in order to extract internal energy from the remapped total energy, and then the internal energy is repaired.

We have an initial grid in one dimension of four equal intervals with vertices ($x_1 = 0, x_2 = 0.25, x_3 = 0.5, x_4 = 0.75, x_5 = 1$). The new grid vertices are ($x_1 = 0, x_2 = 0.23, x_3 = 0.55, x_4 = 0.75, x_5 = 1$). The initial grid data are

$$\rho_1 = 20, \quad \rho_2 = 20, \quad \rho_3 = 1, \quad \rho_4 = 1,$$

$$m_1 = 5, \quad m_2 = 5, \quad m_3 = 0.25, \quad m_4 = 0.25,$$

$$u_1 = 1, \quad u_2 = 1, \quad u_3 = -1, \quad u_4 = -1,$$

$$e_1 = 16, \quad e_2 = 16, \quad e_3 = 0, \quad e_4 = 0.$$

The remap is done by constructing a piecewise linear function on each original cell for each of the conserved variables mass momentum and total energy, and then integrating that function over the new cells. The slope for each of these is taken to be the *central* divided difference, which of course produces remapped values well out of bound.

The remapped and repaired densities are shown in Fig. 1. The repaired masses are

$$\hat{m}_1 = 4.6, \quad \hat{m}_2 = 5.45, \quad \hat{m}_3 = 0.2, \quad \hat{m}_4 = 0.25.$$

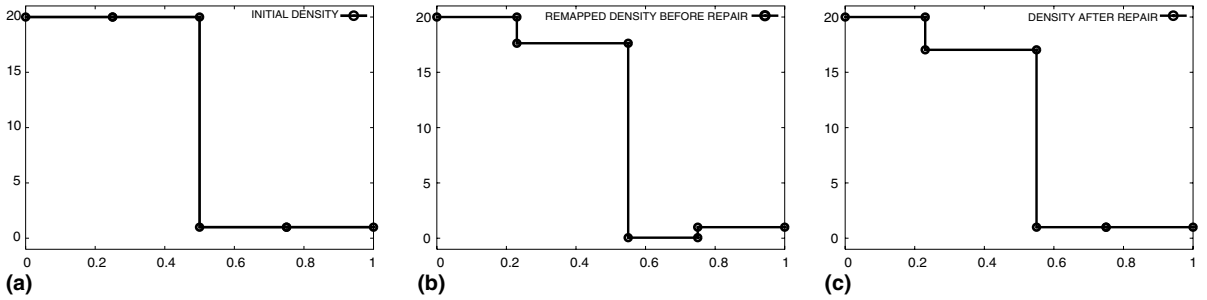

Fig. 1. Density: (a) initial, (b) remapped before repair, (c) after repair.

In this case the mass matrix is easily found:

4.6	0	0	0	4.6
.4	5	.05	0	5.45
0	0	.2	0	.2
0	0	0	.25	.25
5	5	.25	.25	

The initial total kinetic energy is 5.25. After repair of density but before repair of velocity the total kinetic energy has increased to 5.68. After velocity repair it is 5.15.

The density remap and repair process is demonstrated in Fig. 1: (a) the initial density, (b) remapped, (c) repaired. The velocity remap and repair process is demonstrated in Fig. 2: (a) the initial velocity, (b) ve-

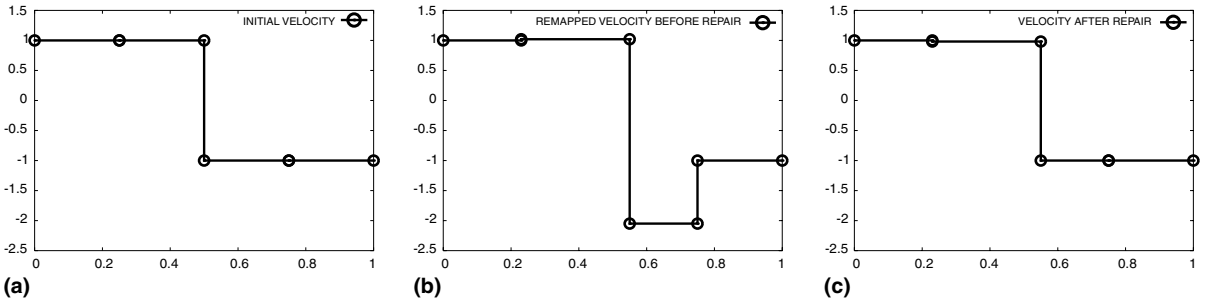

Fig. 2. Velocity: (a) initial, (b) remapped before repair, (c) after repair.

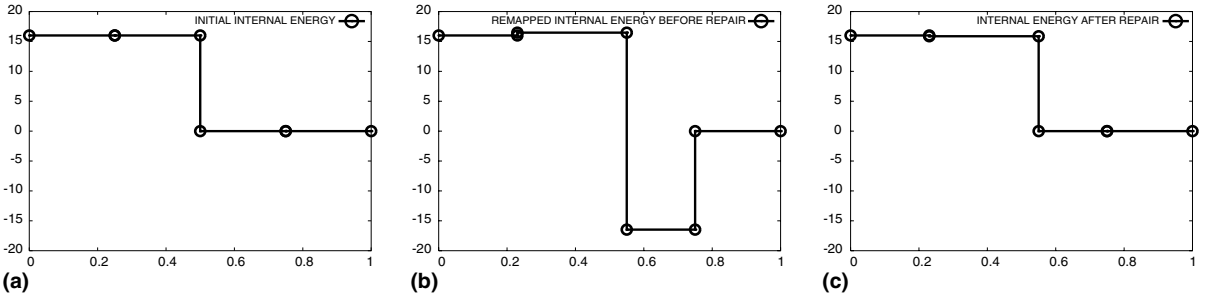

Fig. 3. Internal energy: (a) initial, (b) remapped before repair, (c) after repair.

locity computed using the remapped momentum and repaired mass, and then (c) repaired. The internal energy remap and repair process is demonstrated in Fig. 3: (a) the initial internal energy, (b) computed using the remapped total energy and the repaired density and the repaired velocity, and then (c) repaired.

8. Application to advection

The advection equation (in two dimensions)

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + v\frac{\partial \rho}{\partial y} = 0,$$

and the conservation equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0$$

are equivalent if the given velocity field is divergence-free. A conservative numerical scheme for the conservation equation will conserve mass, but a numerical advection method may not, even if the velocity field is divergence-free. Also, unphysical values can be generated.

This is a well-known difficulty and many ideas have been proposed to avoid it. A discussion of the general approaches via flux-corrected transport and nonlinear filters is given in [5] along with some new methods. Some form of mass redistribution plays an important role in those methods. Repair can be classified as a mass redistribution nonlinear filter, and, not surprisingly, it is similar to such filters proposed in [5].

The global mass repair algorithms can be applied as a post processor at the end of each time step of an advection scheme, and they have the potential to enforce mass conservation as well as reduce oscillations. In Section 2.2 the total mass M was assumed to be the same before and after remapping. If the chosen advection scheme is not conservative we can still take M to be the mass at the beginning of the time step, but in this case we cannot be certain that repair will successfully distribute the mass error and impose the bounds. The discrepancy $|\delta|$ might be too large or the bounds might be too narrow. So the implementation has to allow for this, but typically the mass error is small compared to the mass.

We computed the advection by a rigid rotation of a discontinuous nonegative cone, after three rotations on a 200×200 grid. In Fig. 4(a) the initial data are shown in side-view and as a reference calculation we

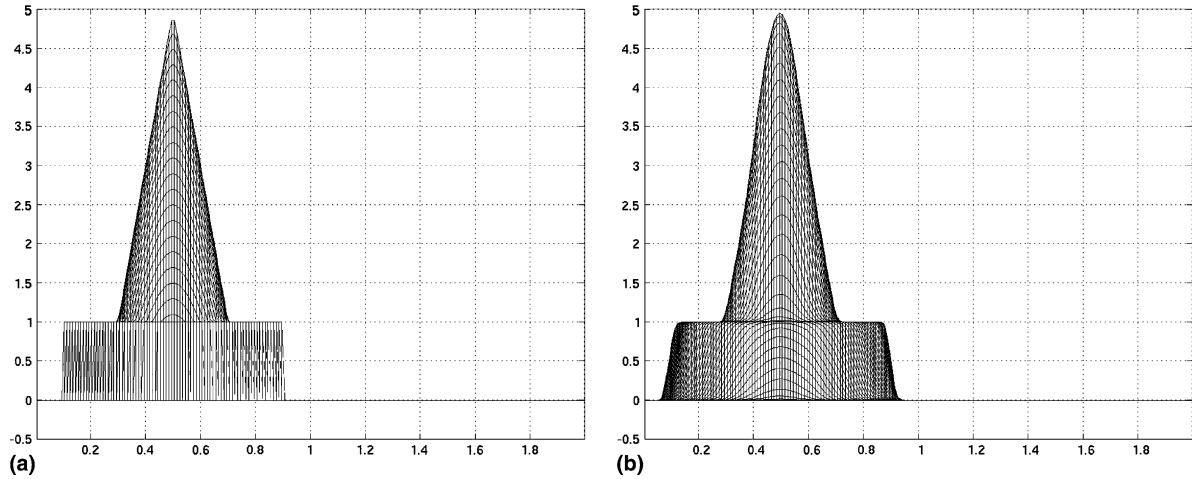

Fig. 4. Discontinuous cone: (a) initial, (b) by CENOAC after three rotations.

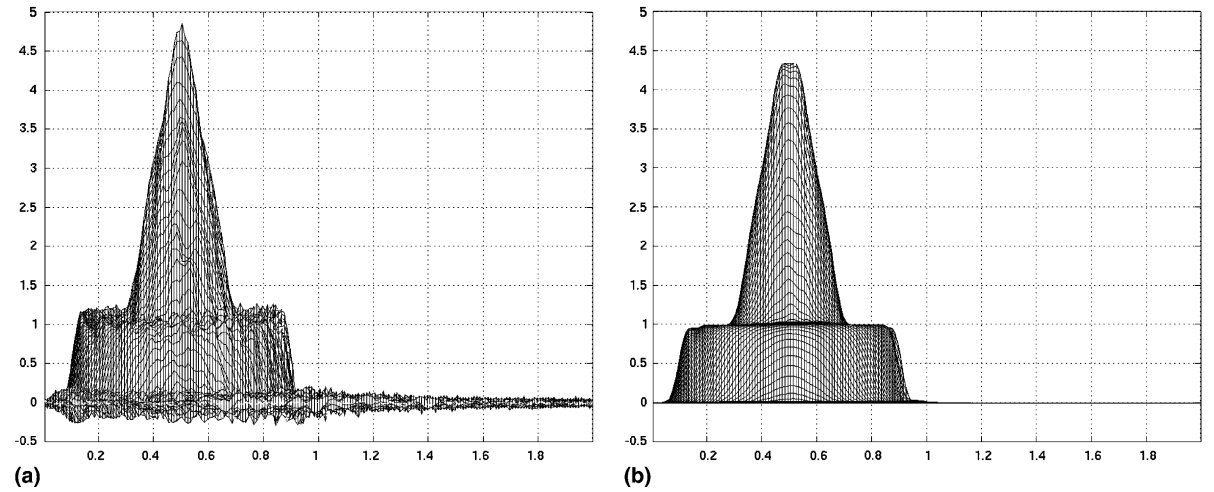

Fig. 5. Discontinuous cone after three rotations: (a) central third order, (b) repaired.

show in Fig. 4(b) the result of a limited version of the third order CENO scheme [3] using artificial compression (CENOAC), as devised by Tariq Aslam (unpublished). This method is excellent for this problem, although there is a 2% mass error and a minimum density equal to -6.3×10^{-5}.

Strictly for illustrative purposes, we have eliminated the flux limiter and removed the upwind bias from the third-order CENO scheme [3], obtaining a very oscillatory central finite difference method that would horrify the authors of CENO but one that clearly shows how repair can work. Before repair, Fig. 5(a), there are negative densities and severe oscillations. After repair, Fig. 5(b) all densities are nonnegative, but some small oscillations remain. The repair has also clipped some off the peak. The repair used the final global variant of Section 2.2.

The running time for unlimited repaired CENO was 507 s, while for the limited upwind CENOAC the running time was 548 s. The central difference scheme, having no limiter steps, took 433 s. One can only say that in this case the computational expense of repair is reasonable.

9. Comments

The hypothesis of Theorem 2 is satisfied if the new masses are obtained by exact integration of a nonnegative density, but that is not readily checked in general. As for Theorem 3, even for this exact integration we do not know if kinetic energy always decreases. There is an alternative procedure that does decrease total kinetic energy, namely, if the new velocity is not defined by remapping momentum but by averaging over the submasses of the nonnegative mass matrix, that is, if

$$u_i' = \frac{\sum_j m_{ij} u_j}{\sum_j m_{ij}},$$

for then, by the Cauchy–Schwarz inequality

$$\begin{aligned}\sum_i m_i'(u_i')^2 &= \sum_i \frac{\left(\sum_j m_{ij} u_j\right)^2}{m_i'} = \sum_i \frac{\left(\sum_j \sqrt{m_{ij}}\sqrt{m_{ij}} u_j\right)^2}{m_i'} \leqslant \sum_i \frac{\sum_j m_{ij} \sum_j m_{ij} (u_j)^2}{m_i'} \\ &= \sum_j \sum_i m_{ij} u_j^2 = \sum_j m_j u_j^2.\end{aligned}$$

Finally, some words of caution about repair as applied to remapping. One method of solving the Euler equations that is popular in certain circles is to start with an orthogonal grid, do a time step with a Lagrangian method, and then remap back to the orthogonal grid. The local repair algorithm gives different results for different ordering of the sweep through the cells, and as a result a solution that should be independent of one of the coordinate variables will get distorted. Repair by global redistribution avoids this, but there remains the issue of the effect of repair on the dynamics of the Euler equations. Some computations of Riemann problems by Raphael Loubere indicate that local repair is ''safe'', but repair by global redistribution is not. This requires further research into ways of keeping locality and 1D symmetry. It is our feeling that for advection, it being a linear problem, and based on the admittedly few examples we have done, repair by global redistribution is a valid process for enforcing bounds and conservation on advection codes, and could be considered as an alternative to various existing that attempt to achieve that goal, as shown above, even as sophisticated a method as CENOAC still produces negative values upon advecting a nonnegative distribution.

Acknowledgements

We would like to thank James C. Scovel for taking an interest in the mass matrix problem and for showing us [6]. We thank also Tariq Aslam for giving us his adaptation of CENO. Thanks also to Milan Kucharik, Raphael Loubere and Len Margolin. This work was performed under the auspices of the US Department of Energy at Los Alamos National Laboratory, under contract W-7405-ENG-36. The authors acknowledge the partial support of the DOE/ASCR Program in the Applied Mathematical Sciences and the Laboratory Directed Research and Development program (LDRD). The authors also acknowledge the partial support of DOEs Accelerated Strategic Computing Initiative (ASCI).

References

[1] J. Dukowicz, J. Baumgardner, Incremental remapping as a transportation/advection algorithm, Journal of Computational Physics 160 (2000) 318–335.
[2] M. Kucharik, M. Shashkov, B. Wendroff, An efficient linearity-and-bound-preserving remapping method, Journal of Computational Physics 188 (2003) 462–471.
[3] X.-D. Liu, S. Osher, Convex eno high order multi-dimensional schemes without field by field decomposition or staggered grids, Journal of Computational Physics 142 (1998) 304–330.
[4] L. Margolin, M. Shashkov, Second-order sign-preserving remapping on general grids, Journal of Computational Physics 184 (2003) 266–298.
[5] A. Oliveira, A. Fortunato, Toward an oscillation-free mass conservative eulerian-lagrangian transport model, Journal of Computational Physics 183 (2002) 142–164.
[6] U. Rothblum, H. Schneider, Scalings of matrices which have prespecified row sums and column sums via optimization, Linear Algebra and Its Applications 114/115 (1989) 737–764.