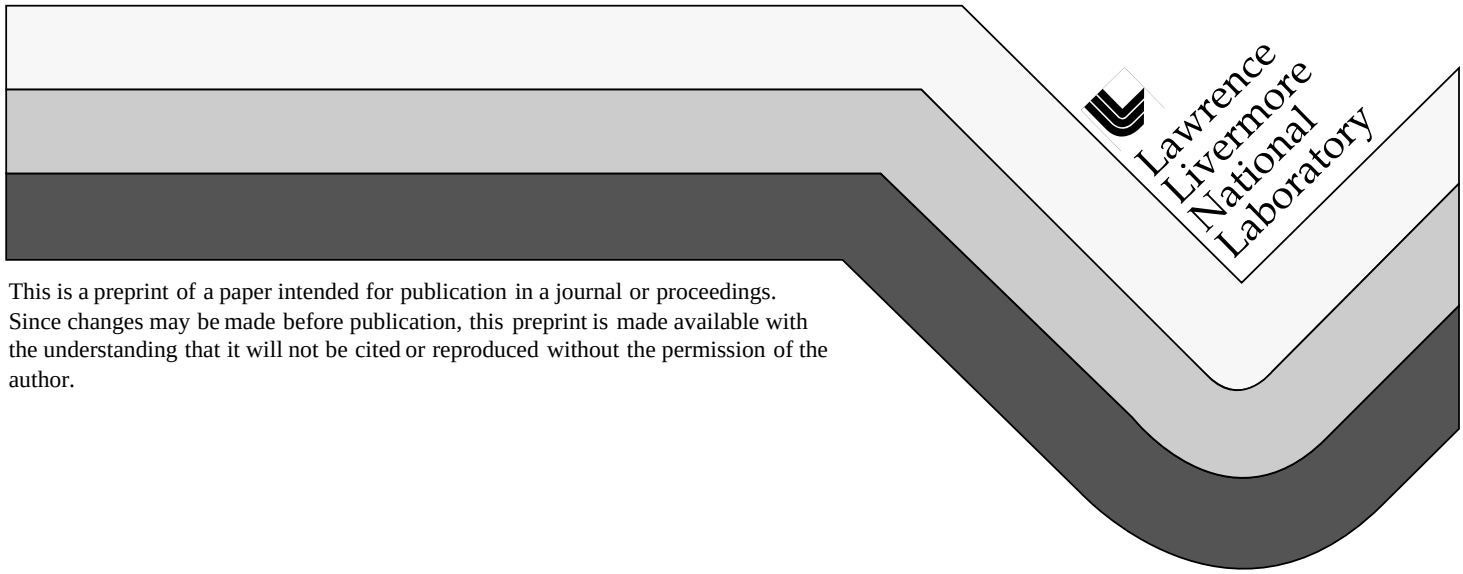
UCRL-JC-132902
PREPRINT

A Second-Order Method for Interface Reconstruction in Orthogonal Coordinate Systems

J. A. Greenough
D. T. Graves
P. Colella

This paper was prepared for submittal to the
1998 Nuclear Explosives Development Conference
Las Vegas, NV
October 25-30, 1998

December 23, 1998



A Second-Order Method for Interface Reconstruction in Orthogonal Coordinate Systems [1] (U)

J. A. Greenough
Lawrence Livermore National Laboratory
D. T. Graves, P. Colella
Lawrence Berkeley National Laboratory

We present a method in two-dimensions for reconstructing an interface from a distribution of volume fractions in a general orthogonal coordinate system. The method, in a cell by cell fashion, approximates the interface curve by a linear profile. The approach requires only local volume fraction information for the reconstruction. An integral formulation is used that accounts for the orthogonal coordinate system in a natural way. We use finite differences to approximate the slope of the required interface while retaining at worst second order accuracy for general interface orientations and an exact representation for coordinate system aligned ones. (U)

Keywords: interface reconstruction, multifluid hydrodynamics

Introduction

An approach for computing flows composed of thermodynamically distinct materials in Eulerian coordinates is based on a volume-of-fluid description of the system. In this type of method, each cell is described by mixture properties and individual phase properties. The individual phase properties include a volume fraction in each cell that is defined as the ratio of the volume of a cell occupied by a material to the total volume of the cell. From a fluid dynamical point of view, there is a set of equations that describes the dynamics of the effective mixture system, say the equations of gas dynamics, and additional ones that describe the motion of the volume fraction field, of equivalently the material interface, and a self-consistent set of equations for the evolution of the individual phase properties.

Numerically, this system of equations can be solved in the following steps:

- In single fluid regions (regions containing only one material), an appropriate numerical method for advancing in time the mixture equations is used, *e.g.* a higher-order Godunov method. Note that *effective* single fluid properties must be appropriately defined for the mixed cells.

- For cells containing more than one material, *i.e.* mixed cells, the multifluid equations must be solved (hereon referred to as the multifluid equations). This includes evolving the volume fraction field and the individual phase properties in a self-consistent fashion that retains global conservation.

The complete multifluid system of equations has been presented elsewhere (Colella, Glaz and Ferguson, 1998, Saltzman and Puckett, 1992, and Miller and Puckett, 1996) so will not be repeated

[1]Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

here for the sake of brevity and to maintain focus on the subject of the paper. Without going into the details of the multifluid update algorithm, this step requires the interface to be reconstructed cell by cell from the gridscale volume fraction distribution. As the location and orientation of the interface is recomputed as needed, we refer to it as a sub-gridscale feature of the flow. We have developed a new method for the reconstruction that easily generalizes to orthogonal coordinate systems and by using monotone limited finite differences, following Colella, Helmsen and Puckett (1997), it retains second-order accuracy and is faster and more efficient than other function minimization approaches (Pilliod and Puckett, 1995).

This paper will first establish the notation needed for describing the reconstruction method, then outline the steps of the reconstruction algorithm. We introduce the integral formulation that accounts for the general orthogonal coordinate system. The reduction of the local volume fraction distribution to a canonical orientation will be described next, followed by the calculation of the interface slope. We present two examples of calculating the slope of an interface, first for Cartesian coordinates and second for axisymmetric coordinates. Then we briefly describe how the reconstruction is coupled to an advection scheme for moving a material interface nondiffusively.

Terminology and Description of Problem

We consider an orthogonal curvilinear coordinate system in two dimensions consisting of independent variables (x^1, x^2), and with uniform grid spacing, $(dx^1, d\ x^2)$. We also consider a Cartesian coordinate system $(x\, y\ )$ and a mapping between the the two coordinate systems, $(x\, y\ ) \rightarrow (x^1, x^2)$, that is invertible and sufficiently smooth. We define scale factors, h^1 and h^2, given by

$$(h^i)^2 = (\frac{\partial x}{\partial x^i})^2 + (\frac{\partial y}{\partial x^i})^2, i \in \{1, 2\}. \tag{1}$$

Note that the scale factors in general are function of the variables (x^1, x^2). Analytically, a differential volume encompassed by differential lengths, dx^1 and dx^2, and is given by

$$dV = h^1 h^2 dx^1 dx^2. \tag{2}$$

For the case of cylindrical (axisymmetric) coordinates, where $1 = r$ and $2 = z$, we have

$$h^r = 1, h^z = 1, d\ V = 2\pi r dr dz. \tag{3}$$

For spherical coordinates, where $1 = r$ and $2 = \theta$, we have

$$h^r = 1, h^\theta = r sin\theta dV\ \ = 2\pi r^2 sin\theta dr d\theta. \tag{4}$$

Numerically we divide the spatial domain evenly into computational elements of size Δx^1 by Δx^2. The center of each cell is located at $((i+\frac{1}{2})\Delta x^1, (j+\frac{1}{2})\Delta x^2)$. We restrict attention to problems with only two fluids, which we identify with $\alpha = 1, 2$ and an associated volume fraction f^α in every cell. Note that this restriction only is important for the present algorithm. We have hybridized this method with a lower order method for treating cases with more that two fluids. If the volume of the computational cell is ΔV^c, this volume fraction is defined as

$$f^\alpha = \frac{V^\alpha}{\Delta V^c} \tag{5}$$

Note that the volume fractions satisfy the constraint $f^1 + f^2 = 1$.

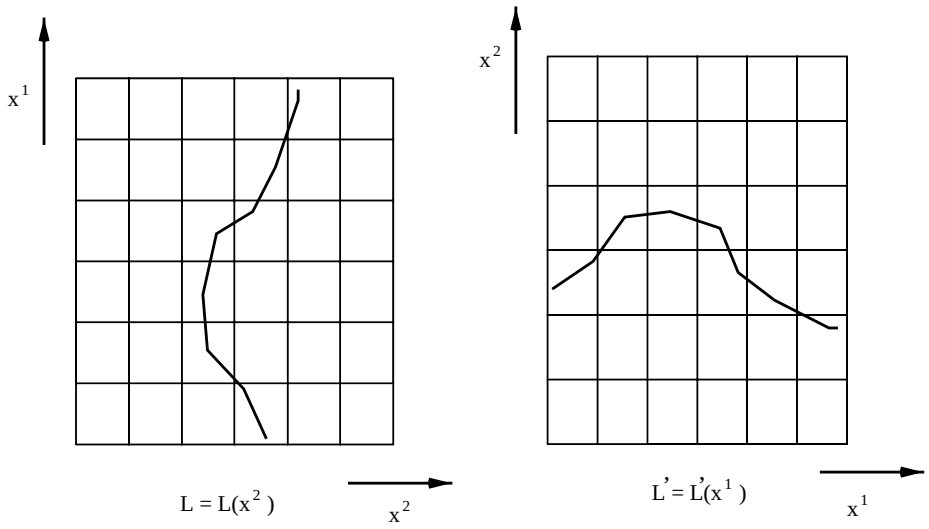


Figure 1: Illustration of the local orientation of the interface. The figure on the left shows the interface best described as a function of x^2, since the interface is locally closer to being horizontal. On the left, it is best described as a function of x^1, since the interface is locally closer to being vertical.

Canonical Interface Orientation

Given a line separating two fluids and a coordinate system (x^1, x^2), the description of an interface as a function of one of its independent variables is not uniquely defined. Say we arbitrarily define the interface location L to be a function of x^1 with $L = L(x^1)$. Equivalently, by a 90deg rotation of the coordinate system, we could obtain an interface location $\hat{L} = \hat{L}(x^2)$. This idea is simply illustrated in figure 1. In the case on the left, any description of the interface as a function of x^2 would be multiply defined but describing the interface as locally a function of x^1, as shown on the right gives a single valued function. Another reason for choosing the latter orientation is to have slopes that are well behaved insofar as they are bounded. In the configuration on the left, the slope is large, while on the right it is finite. This is the guide for choosing one orientation over another.

We use this concept to pick which local orientation is most suitable for the description of the interface. First we extract a 5x5 platter of volume fractions of the marked fluid, say fluid 1, surrounding the cell of interest. We then calculate which edge of the platter is "heaviest" with respect to fluid 1. That is, which edge has the greatest concentration of the marked fluid. Defining i and j to be the local (to the 5x5 platter) indices in the x^1 and x^2 directions, respectively, the

volume fractions are summed over each edge of the platter as

$$\begin{aligned} A_{bot} &= \sum_{i=1}^{5}\sum_{j=1}^{2} f_{i,j} \\ A_{top} &= \sum_{i=1}^{5}\sum_{j=4}^{5} f_{i,j} \\ A_{lef} &= \sum_{i=1}^{2}\sum_{j=1}^{5} f_{i,j} \\ A_{rig} &= \sum_{i=4}^{5}\sum_{j=1}^{5} f_{i,j} \end{aligned} \tag{6}$$

Define the heaviest edge to be that 5x5 grid edge as $A = max(A_k|k = bot,top,lef,rig\quad)$. If A_{top} or A_{bot} is found to be the greatest, the interface is said to be a function of x^1, otherwise the interface is a said to be a function of x^2.

Once the canonical orientation is selected, we can restrict the 5x5 platter to 3 wide by 5 tall. We retain the 5 tall so that we have accurate integrals that are given in the following sections.

Geometric Description of Interface

Without loss of generality, we assume that at a point the location of the interface can be described by the following graph:

$$\{(x^1, x^2) : x^2 = L(x^1)\} \tag{7}$$

Since we are modeling the interface as a linear function, within a cell the function L is of the form

$$L(x^1) = L_0 + L_1 x^1 \tag{8}$$

where L_0 and L_1 are constants.

In figure 2 we show the curve that we want to approximate with a linear function. Below the curve are full marked fluid cells, above we have empty marked fluid cells and the cells cut by the interface are mixed. It is in cell $(i,j\ )$ where we want to construct an approximation to the slope of the curve, $L = L(x^1)$. We designate the amount of marked fluid, in a restricted region (see figure 2), as the function, $Q(x^1)$, given explicitly as

$$Q(x_1) = \int_{x^{1,low}}^{x^1} \Big(\int_{\tau_{low}}^{L(\tau)} f^{marked}(\eta,\tau\ ) A_2(\eta,\tau\ ) d\eta \Big) d\tau \tag{9}$$

where

$$A_2 d\eta d\tau = dV, \tag{10}$$

The function, Q, contains the local coordinate system metric and the marked fluid volume fraction in the integrand as well as the interface $L(x^1)$ in the limits of integration. In order to recover the location of the interface, we must invert equation 9.

Slope Calculation

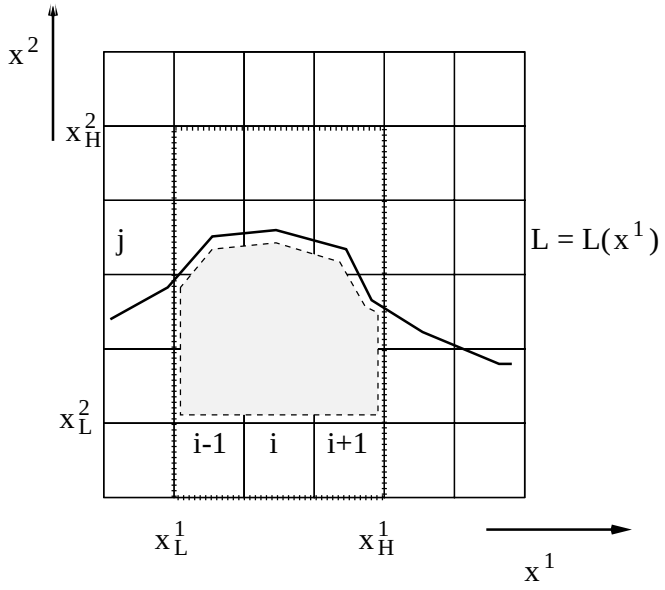


Figure 2: The volume of marked fluid in the shaded region is the area under the curve, $L(x^1)$. See narrative for orientation. The curve is taken as a function of x^1 and limit interest to $x_L^1 < x^1 < x_H^1$ and $x_L^2 < x^2 < L(x^1)$. The local 3 by 5 grid, about cell (i,j), is shown in the dashed online.

The previous section showed the formalism for representing the curve to be approximated. Within our local 3x5 platter of data, it is very simple to numerically calculate Q using 9:

$$Q_{i-3/2+m} = \sum_{k=i-1}^{i-1+m} \Big(\sum_{l=j-2}^{j+2} f_{k,l} \delta V_{k,l} \Big) \Big(\sum_{l=j-2}^{j+2} f_{k,l}^{marked} \delta V_{k,l} \Big) \tag{11}$$

where δV is the cell volume and $m = 1, 2, 3$. Notice that for $m = 1$, equation 11 is just the integral over the first column of the platter and $m = 2$ is the integral over all three columns of data. We further define $Q_{i-3/2} = 0$, with $m = 0$. This follows from equation 9 with the upper and lower τ limits of integration equal. In going from the continuous integral form to a discrete computation form using summation, the discrete Q exactly reproduces the integral result when integrating between cell edges.

So now we have 4 values of Q defined on cell edges. We can compute first derivatives $dQ/dx^1{}_{(i-1+m)}$, for $m = 0, 1, 2$, using the above values of Q.

The exact form of this derivative will be given in the examples to follow. In order to recover the slope of the linear profile, we use these three first derivatives to construct a limited monotonic approximation to the second derivative of Q using Van Leer style finite differences in cell (i,j) as required. These also will be given in the examples.

Locating the Line within the Cell

It remains to locate the interface within the cell. This is done so that the volumes delimited by the interface within the cell matche the volume fraction values in that cell. If we limit the slope so that $-1 \le L_1 \le 1$ and insist that $\Delta x^1 = x^2$ then only three possible line orientations are possible. This is shown in figure 3.

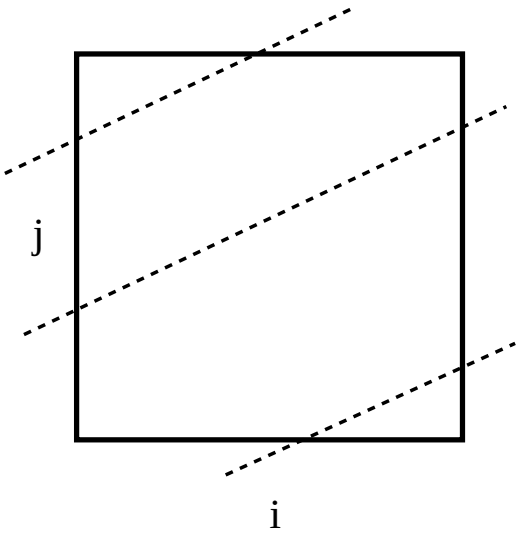


Figure 3: Given a slope of the line, three possible translations within the (i,j) cell are possible.

Given a slope, these cases differ by vertical translation of the line. So in practice, one proceeds through the cases until the line splits the cell in a way that matches the volume fractions. Note that for non-Cartesian geometries, the uppermost and lower most translation cannot be treated as the same case by reflection.

Example: Cartesian Coordinates

In the case of $x_1 = x$ and $x_2 = y$, equation 9 reduces to

$$Q(x) = \int_0^x L(x')dx' \tag{12}$$

(since the area function is independent of y, y_{low} is set to zero). So analytically, the height of the interface is given by

$$L(x) = \frac{dQ}{dx} \tag{13}$$

and discretized as follows

$$L_i = \frac{1}{\Delta x}(Q_{i+\frac{1}{2}} - Q_{i-\frac{1}{2}}) \tag{14}$$

Since all the coordinate metrics are unity in the case of Cartesian coordinates, the calculation of the height for the case of $x_1 = y$ and $x_2 = x$ is a simple permutation of x and y in the above formulae. The slope of the line is given as

$$\Delta L_i = sign(L_{i+1} - L_{i-1})Min(2|L_i - L_{i-1}|, 2|L_{i+1} - L_i|, 0.5|L_{i+1} - L_{i-1}|)/\Delta x^1 \tag{15}$$

where $sign(a)$ gives $+1$ if $a > 0$ and -1 if $a < 0$. This type of formula is known colloquially as "min-mod limiting". The three arguments of the Min function above can be identified as backward, forward and centered difference approximations, respectively.

Example: Axisymmetric Cylindrical Coordinates

Because non-trivial coordinate metrics are involved in axisymmetric cylindrical coordinates, the slope calculation becomes somewhat more difficult. In the case of $x_1 = r$ and $x_2 = z$, equation 9 reduces to

$$Q(r) = \int_0^r 2\pi L(r')r'dr' \tag{16}$$

(since the area function is independent of z, z_{low} is set to zero). So analytically, the height of the interface is given by

$$L(r) = \frac{1}{2\pi r}\frac{dQ}{dr} \tag{17}$$

and discretized as follows

$$L_i = \frac{1}{\Delta r}(Q_{i+\frac{1}{2}} - Q_{i-\frac{1}{2}}) \tag{18}$$

In the case of $x_1 = z$ and $x_2 = r$, equation 9 reduces to

$$Q(z) = \int_0^z \pi(L^2(r')' - R_{low}^2)dr' \tag{19}$$

which implies that (analytically) the height of the interface is given by

$$L(r) = (\frac{1}{\pi}\frac{dQ}{dz} + R_{low}^2)^{\frac{1}{2}} \tag{20}$$

We calculate the discrete height of the interface as follows

$$L_i = (\frac{1}{\Delta z}(Q_{i+\frac{1}{2}} - Q_{i-\frac{1}{2}} + R_{low}^2))^{\frac{1}{2}} \tag{21}$$

In both cases, once the interface height is calculated, the slope is computed following equation 15 for the center cell.

Coupling to Advection Scheme

In order to couple the reconstruction algorithm to an advection scheme for the volume fractions, we need to have velocities at the cell edges. Given these velocities and a time increment, Δt, we can define a total volume flux across the cell edge. This is shown schematically in figure 4. Then the problem is reduced to one of geometry where we must compute the volume of the quadrilaterals formed by overlaying the rectangle defining the total volume flux onto the quadrilaterals defining the volumes of the two fluids contained in the cell.

Results

We present results of the reconstruction method for a hydrodynamics problem in spherical geometry. The problem is that of a dense gas spherical shell embedded in a light gas background. The outer edge of the dense shell is pressurized (heated) so that a strong shock is driven into the shell towards the origin thereby forcing an implosion. The outer edge of the shell is driven outward where it eventually moves out of the computation domain. The initial configuration of the shell

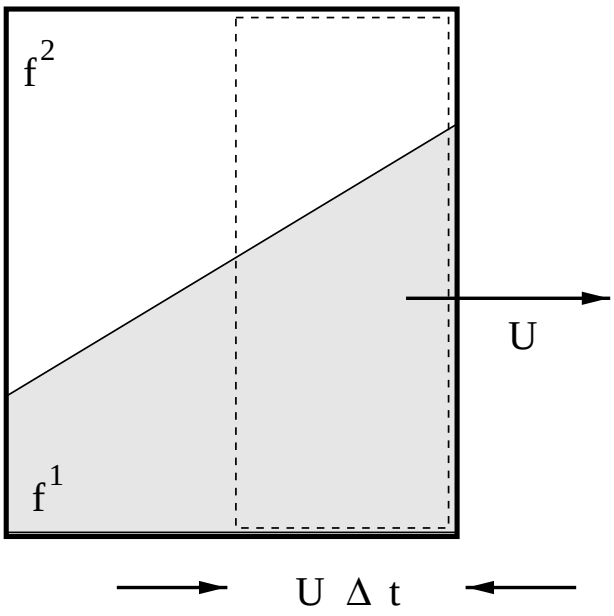


Figure 4: Illustration of advection of interface. The volume fluxed out of the cell during a timestep Δt is shown by the dashed rectangle. The quadrilateral volume of fluid 1 and fluid 2 with this rectangle are the volume fluxes of fluid 1 and fluid 2 during the timestep.

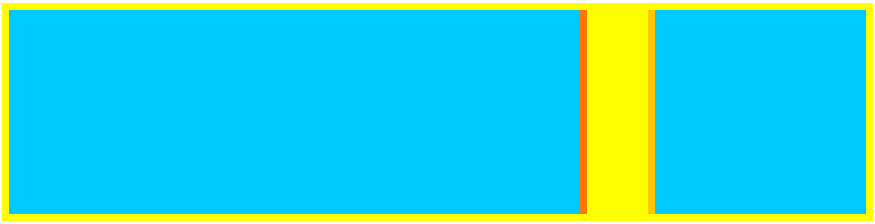


Figure 5: The initial configuration of the dense gas spherical shell shown in logical i and j coordinates. In this view, spherical shells appear as vertical lines. Yellow denotes full dense shell cells and blue denotes full light gas cells. The origin is the left edge of the computational domain.

volume fraction is shown in figure 5. The origin is to the left in the figure. Note that we display the problem in a logical i and j coordinate system. This shows spherical shells as vertical lines and will make it easy to see that the problem retains spherical symmetry exactly. At very late times, shown in figure 6, we see the outer shell edge has exited the computational domain and that inner edge is very close to the origin. At this time is has just started to reverse its direction of motion away from the origin. Note that spherical symmetry is exactly preserved.

References

Colella, P., Glaz, H. M., and Ferguson, R. E., "Multifluid Algorithms for Eulerian Finite Difference Methods," manuscript.

Puckett, E. G. and Saltzman, J. S., "A 3-D Adaptive Mesh Refinement Algorithm for Multimaterial Gas Dynamics," *Physica D*, **60**, 84–104 (1992).

Miller, G. H. and Puckett, E. G., "A Higher-Order Godunov Method for Multiple Condensed Phases," *J. Comp. Phys.*, **128**, 134–164 (1996).

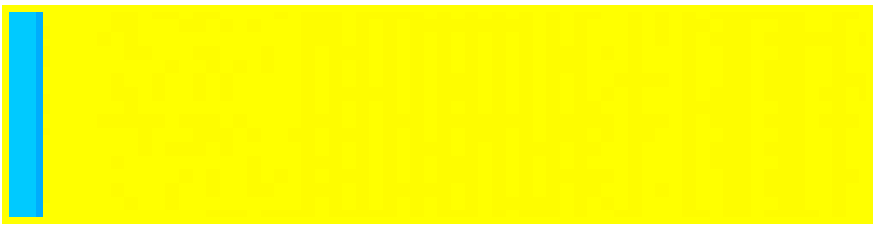


Figure 6: The late time cofiguration of the dense gas spherical shell shown in logical i and j coordinates. In this view, spherical shells appear as vertical lines. Yellow denotes full dense shell cells and blue denotes full light gas cells. The outer edge has exited the computational domain and the inner edge is just reversing its direction of motion away from the origin. The interface is still a spherical shell (vertical line).

Colella, P., Helmsen, J. and Puckett, E. G., ”Non-Convex Profile Evolution in Two Dimensions Using Volume of Fluids”, LBNL-40693, 1997.

Pilliod, J. E. and Puckett, E. G., ”Second-Order Volume-of-Fluid Algorithms for Tracking Material Interfaces,” in preparation, 1995.