

Multimaterial Interface Reconstruction Using Particles and Power Diagrams

Rao V. Garimella, Samuel P. Schofield, Raphael Loubere, T-7; Marianne M. Francois, CCS-2

We have developed a new method for volume-conservative reconstruction of multimaterial interfaces in flow simulations. The method reconstructs piecewise-linear interfaces using only the material volume fractions in cells of a computational mesh, and therefore, belongs to the Piecewise Linear Interface Construction (PLIC) class of interface reconstruction methods [1].

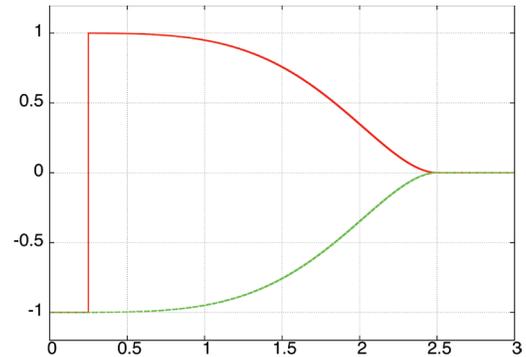
Fig. 1. Velocities of two particles of the same material (red) and different materials (green) as a function of particle separation.

The distinguishing feature of our method is that the reconstructed interface in cells with three or more materials has the same topology, independent of the order in which materials are specified. This is different from other PLIC methods, which generate substantially different reconstructions for different material orderings.

Order-independent reconstruction of the interface with the right topology reduces errors such as bits of material breaking off from the bulk of the material and helps to capture the complex physics at multimaterial junctions more accurately.

The technique we have developed reconstructs interfaces in multimaterial cells using particle attraction and repulsion to locate the materials in the cells, and a weighted Voronoi diagram called a Power Diagram [2] to partition the cell into subcells of pure materials.

Initially, particles of different material types are placed randomly in mixed cells containing three or more materials and all neighboring cells (pure or mixed). An attraction-repulsion model that defines particle velocities as a function of particle separation is initiated between the particles. (See Fig. 1.) In the model, particles of the same materials attract each other, in general, and particles of different types repel. When two particles of the same type get too close



to each other, however, they repel each other. When any two particles move too far apart, there is no interaction between them. Using this model, particles are then allowed to migrate to their final positions. The system is stabilized using a simulated annealing type rescaling of particle velocities. The centroids of the clustered particles in their final position determine the location of the different materials in the cell.

The partitioning of the cell into subcells of different materials is done by a Power Diagram of the centroids of the materials. Power diagrams are a partitioning of space that bear a close resemblance to simple Voronoi diagrams. In a power diagram, the *power* of a point, x , with respect to a site, X_i , with weight w_i , is defined as $(\|x - X_i\|^2 - w_i^2)$. The *power region* of a site X_i is the locus of points whose power with respect to X_i is lesser than their power with respect to any other site X_j .

The weights of the sites in each cell control the relative areas of their associated polygons. Therefore, if each site in the cell represents the centroid of a material, then the material volume fractions in the cell can be controlled by adjusting the weights. The weights required to exactly match the material volume fraction in any cell are computed by solving the following system of equations:

$$F(w_1, w_2, \dots, w_n) - V = 0$$

A scalar equation in the system represents the discrepancy between the actual volume fraction and the specified volume fraction of a particular material. There are as many equations in the system as there are clusters of particles. Note that there may be more equations than the number of materials since particles of a material may cluster into two or more groups.

We have implemented this method for interface reconstruction in structured and unstructured meshes, and have seen that the method works quite well in capturing the topology of such interfaces. We show some results here to illustrate the capabilities of this method.

In Fig. 2, we illustrate the performance of the particle model. On the left, the initial configuration of particles in a 4 x 4 structured grid is shown. The exact interface in this mesh is shown as a dark diagonal line. The final position of the particles is shown on the right. It can be seen from this figure that the method moves the particles to the positions we expect them to be in.

Figure 3 compares the performance of a traditional Volume of Fluid (VoF) method and the current method in the reconstruction of a three-material T-junction interface. The reconstruction with the PLIC method is perfect when the correct order of materials is chosen (top left), but not very good when a different order is used (top right). On the other hand, our method creates the right interface topology whatever the material ordering (bottom).

Future work in this research includes smoothing of the interfaces, better particle models to capture details such as filaments, and incorporation of clustering algorithms to detect multiple groups of particles of the same type in a cell.

For more information contact Rao V. Garimella at rao@lanl.gov.

- [1] W.J. Rider and D.B. Kothe, *J. Comp. Phys.* **141**, 112–152 (1998).
- [2] F. Aurenhammer, *SIAM J. Comput.* **16** (1), 78–96 (1987).

Funding Acknowledgements

NNSA’s Advanced Simulation and Computing (ASC) Program.

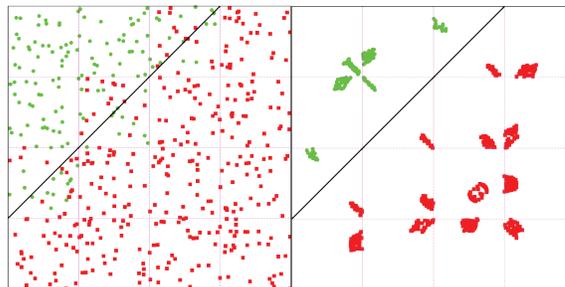


Fig. 2. Left—initial distribution of particles in a mesh; Right—final distribution of particles after application of the particle model. The dark line shows the exact interface from which the input volume fractions were computed.

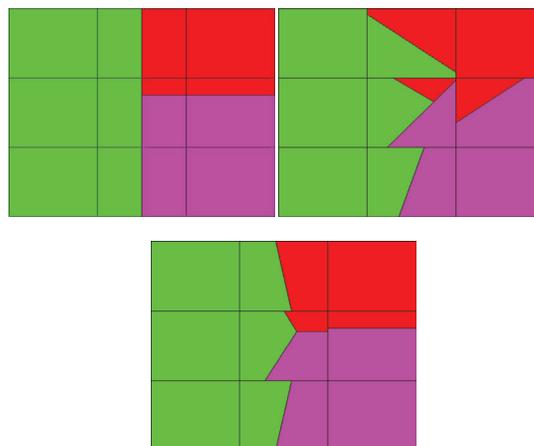


Fig. 3. Three-material reconstruction by a traditional PLIC method with the right ordering of materials (top left), PLIC reconstruction with a different ordering of materials (top right), and reconstruction using our order-independent algorithm (bottom).