Multimaterial Interface Reconstruction from the Moment Data

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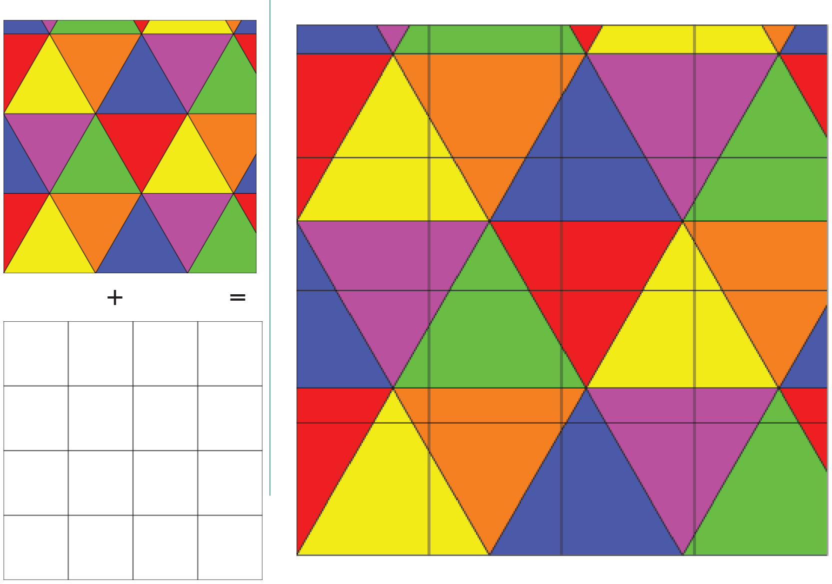
Volume-of-Fluid (VoF) methods [1] are widely used to approximate material interfaces in Eulerian fluid flow simulations. Instead of direct interface tracking, the VoF methods calculate the location of the interface at each time step from the solution data, namely from the cell-wise material volumes. This strategy faces no problem changing the topology of the interface dynamically; the choice of the cell-wise material volumes as an input for the interface reconstruction algorithm allows to preserve the volume of each material. Most VoF methods [2] use a single linear interface to divide two materials in a mixed cell; if the cell contains more than two materials, the two-material interface reconstruction algorithm is used repeatedly for extracting the materials from the mixture one by one. The VoF approach has apparent drawbacks: the resolution of the two-material interface reconstruction algorithm is 2 to 3 times lower than the resolution of the grid. There is no way to guess the order in which the materials should be separated from the multimaterial mixed cell, and, even if such an order is known *a priori* (is fixed), due to the limited resolution of the two-material algorithm, the multimaterial VoF reconstruction can be higher-than-first-order accurate only for the layered material structure, i.e., only if the true interfaces form no junction.



The new Moment-of-Fluid (MoF) technique effectively overcomes the limitations of the VoF approach by utilizing more data: in addition to the volumes, the cell-wise material centroids (the first moments) are used. In [3] we presented the two-material MoF algorithm, which locates the linear interface in a mixed cell by minimizing the defect of the first moment over all the cell partitions that preserve the material volumes. Now [4] we use the same governing principle to perform the polygonal partitioning of a multimaterial mixed cell.

A proper partitioning of the mixed cell with $M \geq 3$ materials is a challenging problem. We explore two different partitioning schemes. The basic one follows the multimaterial VoF strategy and separates the materials from a mixed cell one by one. There is an essential difference though: the MoF interface reconstruction does not require the user to specify the material order explicitly. The right order is determined automatically by trying all $M!$ possible material orders and finding the one that results in the minimal defect of the first moment. Another major improvement over the VoF, is that the MoF algorithm does not require the true interfaces to be nonintersecting to guarantee the second-order accurate approximation.

The search for the best partition above has combinatorial complexity in the number of materials: to get the answer, one has to try all $M!$ material orders. On the other hand, it is reasonable to expect only a limited number of the mixed cells in the whole computational grid to contain 3+ materials. Therefore, for a moderate M, the computational overhead, associated with the optimal order search, is not likely to be significant. Also, various material orders can be effectively tried in parallel.

The governing principle of the MoF reconstruction (minimization of the first moment defect) does not limit the choice of the partitioning scheme in any way; in order to achieve a lower defect of the first moment, one can expand the family of trial partitions at will. Thus, along with extracting materials from the mixture in series, we propose to use a more sophisticated partitioning scheme that separates the materials according to the "divide-and-conquer" principle: choose an arbitrary $\boldsymbol{m < M}$, separate the mixture of materials $\overline{\boldsymbol{1,m}}$ from $\overline{\boldsymbol{m + 1,M}}$, and then recursively apply this algorithm to each submixture containing 2+ materials. This procedure allows to generate $\boldsymbol{M!(M\text{-}1)!}$ trial *B-tree partitions* to choose from, which significantly increases the chances of finding an approximate partition that best fits the moment data. Such a partitioning scheme yields the MoF reconstruction of any B-tree partition with sufficiently smooth interfaces to be second-order accurate.

Although we explicitly address only the 2-D case, it is clear that all the partitioning and ordering strategies described are dimension-independent and are applicable in 3-D.

Unlike the VoF competitors, the Moment-of-Fluid interface reconstruction algorithm can partition multimaterial mixed cells in truly automatic manner; it is also capable of reconstructing complex interface junctions with second-order accuracy, which can hardly be achieved with the VoF methods.

For more information on MoF technique go to http://math.lanl.gov/vdyadechko/research, or contact Vadim Dyadechko at vdyadechko@lanl.gov.

[1] C.W. Hirt and B.D. Nichols, *J. Comp. Phys.* **39** (1), 201–225 (Jan. 1981).
[2] David J. Benson, *Appl. Mech. Rev.* **55** (2), 151–165 (Mar. 2002).
[3] V. Dyadechko and M. Shashkov, "Moment-of-Fluid Interface Reconstruction," Los Alamos National Laboratory report LA-UR-05-7571 (Oct. 2005).
[4] V. Dyadechko and M. Shashkov, "Multi-material Interface Reconstruction from the Moment Data," Los Alamos National Laboratory report LA-UR-06-5846 (Aug. 2006).

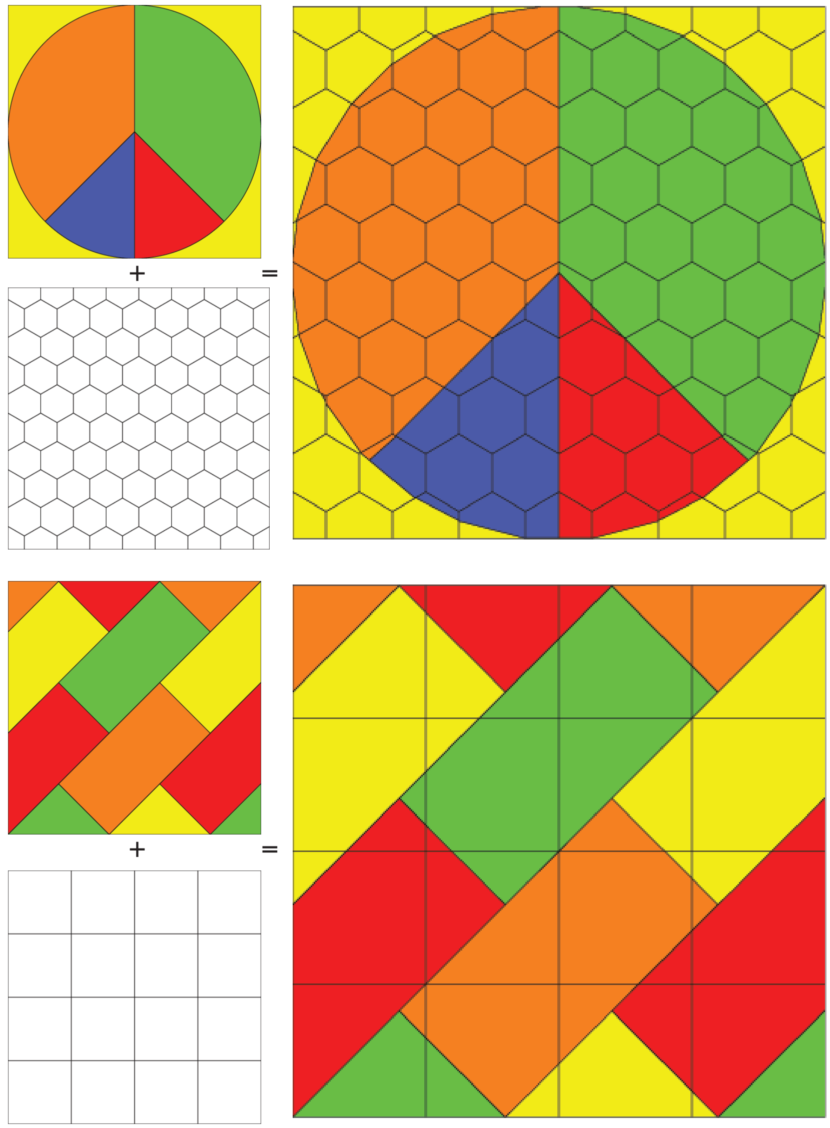


Fig. 1.
The figures show three examples of the multimaterial MoF reconstruction. For each case we show the true distribution of the material in the domain (different colors represent different materials) and the computational mesh. The input data for the MoF algorithm (cell-wise material moments) were calculated by intersecting the mesh cells with the true material shapes. We would like to emphasize the exceptional resolution of the method: even though the size of the material "tiles" in the first and the last configurations is comparable to the size of the mesh cells, the MoF algorithm can reconstruct them exactly.

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