

**LA-UR-16-26997**

Approved for public release; distribution is unlimited.

**Title:** Nested Dissection Interface Reconstruction in Pececillo

**Author(s):** Jibben, Zechariah Joel  
Carlson, Neil N.  
Francois, Marianne M.

**Intended for:** Report

**Issued:** 2016-09-13

---

**Disclaimer:**

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

## Nested Dissection Interface Reconstruction in Pececillo

Z. Jibben, [zjibben@lanl.gov](mailto:zjibben@lanl.gov)  
N. Carlson, [nnc@lanl.gov](mailto:nnc@lanl.gov)  
M. Francois, [mmfran@lanl.gov](mailto:mmfran@lanl.gov)

A nested dissection method for interface reconstruction in a volume tracking framework has been implemented in Pececillo, a mini-app for Truchas, which is the ASC code for casting and additive manufacturing. This method provides a significant improvement over the traditional onion-skin method, which does not appropriately handle T-shaped multimaterial intersections and dynamic contact lines present in additive manufacturing simulations. The resulting implementation lays the groundwork for further research in contact angle estimates and surface tension calculations.

### Background and Motivation

Pececillo is a mini-app that represents the casting and additive manufacturing processes found in the production code Truchas. It is being used to investigate improved algorithm and code designs for current and future architectures prior to their deployment in Truchas.

The traditional onion-skin method [4] currently implemented in Truchas reconstructs the phase interface between multiple immiscible media modeled with the volume of fluid method by summing volume fractions in material order to calculate normal vectors, which are used to calculate the interface position across the cell. For T-junctions this leads to the unphysical situation where reconstructed interfaces overlap, creating a zone occupied by multiple materials.

### Description

The nested dissection method [2] addresses this issue by instead sequentially removing zones behind a reconstructed phase-interface from the

computational cell, and locating later interfaces on the remaining polyhedron. This produces a collection of polyhedra which describe the material geometry in a cell which can then be used for calculating material fluxes.

The interface normal vector is estimated from the normalized gradient of the volume fraction,

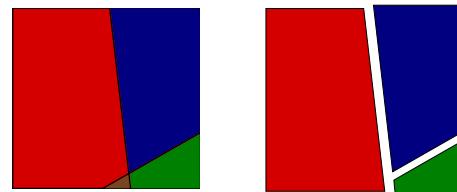
$$\hat{\mathbf{n}}_{m,i} = \frac{\nabla \mathcal{F}_{m,i}}{|\nabla \mathcal{F}_{m,i}|}. \quad (1)$$

The phase interface location is then found using Brent's iterative method to solve for the plane constant  $\rho$  in

$$V(\hat{\mathbf{n}}_{m,i}, \rho) - \mathcal{F}_{m,i} V_i = 0 \quad (2)$$

where  $V_i$  is the cell volume and  $V(\hat{\mathbf{n}}_{m,i}, \rho)$  is the volume of the region of the polyhedron clipped by the phase interface [3] described by the equation of a plane

$$\mathbf{x} \cdot \hat{\mathbf{n}}_{m,i} - \rho = 0. \quad (3)$$



Onion Skin (left), Nested Dissection (right)

### Anticipated Impact

The nested dissection method is expected to greatly increase the accuracy of dynamic contact line tracking, and lays the groundwork necessary for research in prescribing dynamic contact angles. The resulting code will be adapted for implementation in Truchas, improving its additive manufacturing simulation capability.

### Path Forward

Scalable methods for calculating surface tension and contact angles are now being investigated in Pececillo using the improved interface reconstruction now available. Other interface reconstruction improvements, such as a direct analytic approach [1] and a material-order-independent method [5], present considerable advantages and may also be implemented.

# Nested Dissection Interface Reconstruction in Pececillo

---

## Acknowledgements

Los Alamos Report LA-UR-XX-XXXX. This work was sponsored by the Advanced Simulation and Computing Program's (ASC) Telluride Project, and carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

## References

- [1] S. Diot and M. M. Francois. An interface reconstruction method based on an analytical formula for 3d arbitrary convex cells. *J. Comput. Phys.*, 305:63–74, 2016.
- [2] V. Dyadechko and M. Shashkov. Reconstruction of multi-material interfaces from moment data. *J. Comput. Phys.*, 227:5361–5384, 2008.
- [3] J. E. Hopcroft and P. J. Kahn. A paradigm for robust geometric algorithms. *Algorithmica*, 7:339–380, 1992.
- [4] W. J. Rider and D. B. Kothe. Reconstructing volume tracking. *J. Comput. Phys.*, 141:112–152, 1998.
- [5] S. P. Schofield, R. V. Garimella, M. M. Francois, and R. Loubère. A second-order accurate material-order-independent interface reconstruction technique for multi-material flow simulations. *J. Comput. Phys.*, 228:731–745, 2009.