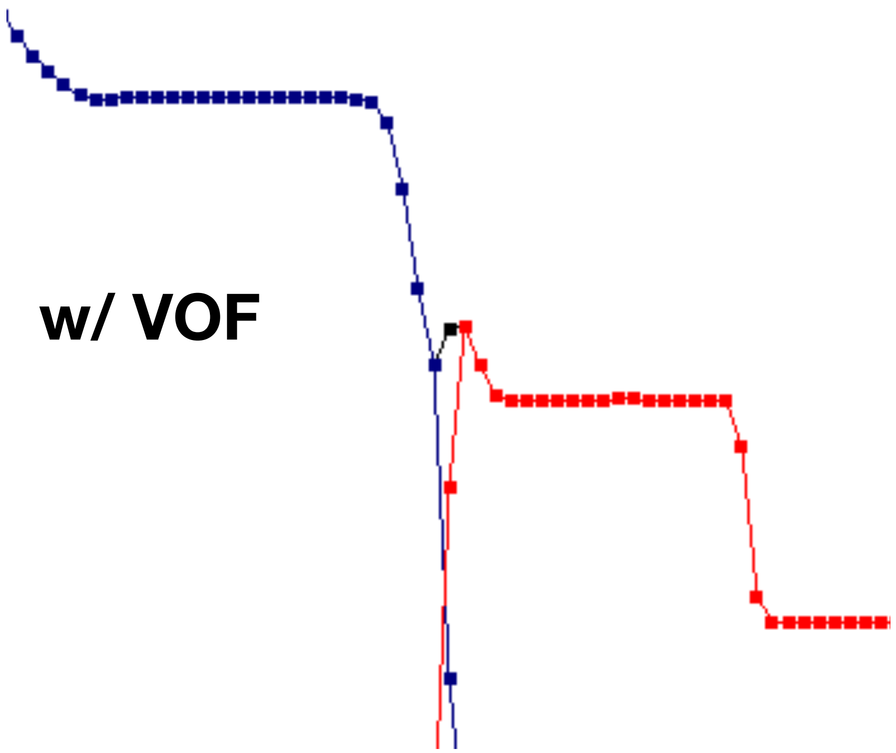
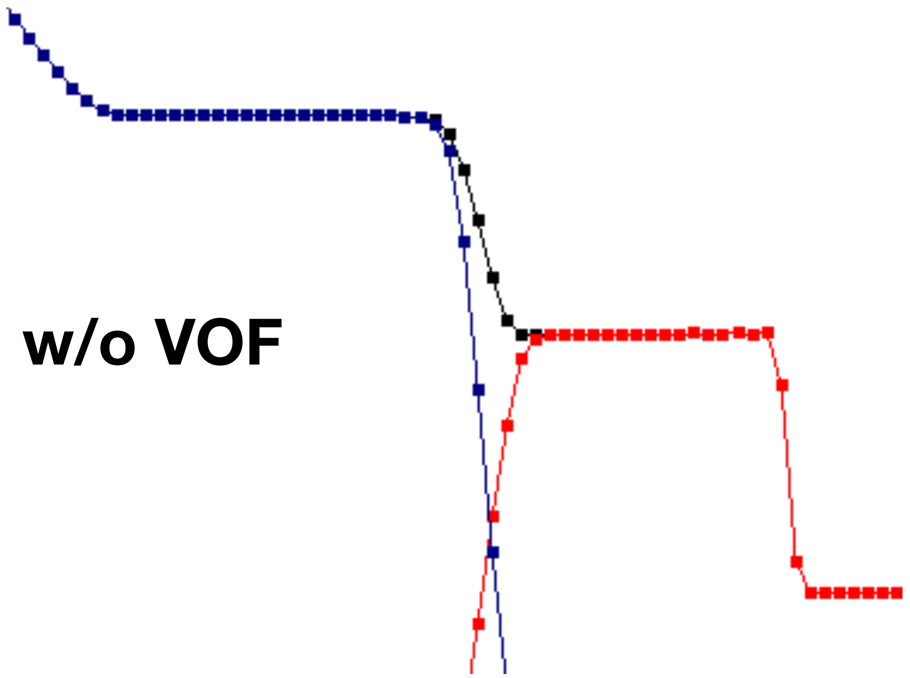
Implementation of a 2D Unsplit Volume of Fluid (VOF) Interface-capturing Method for Multifluid Compressible Flows in the FLASH Code





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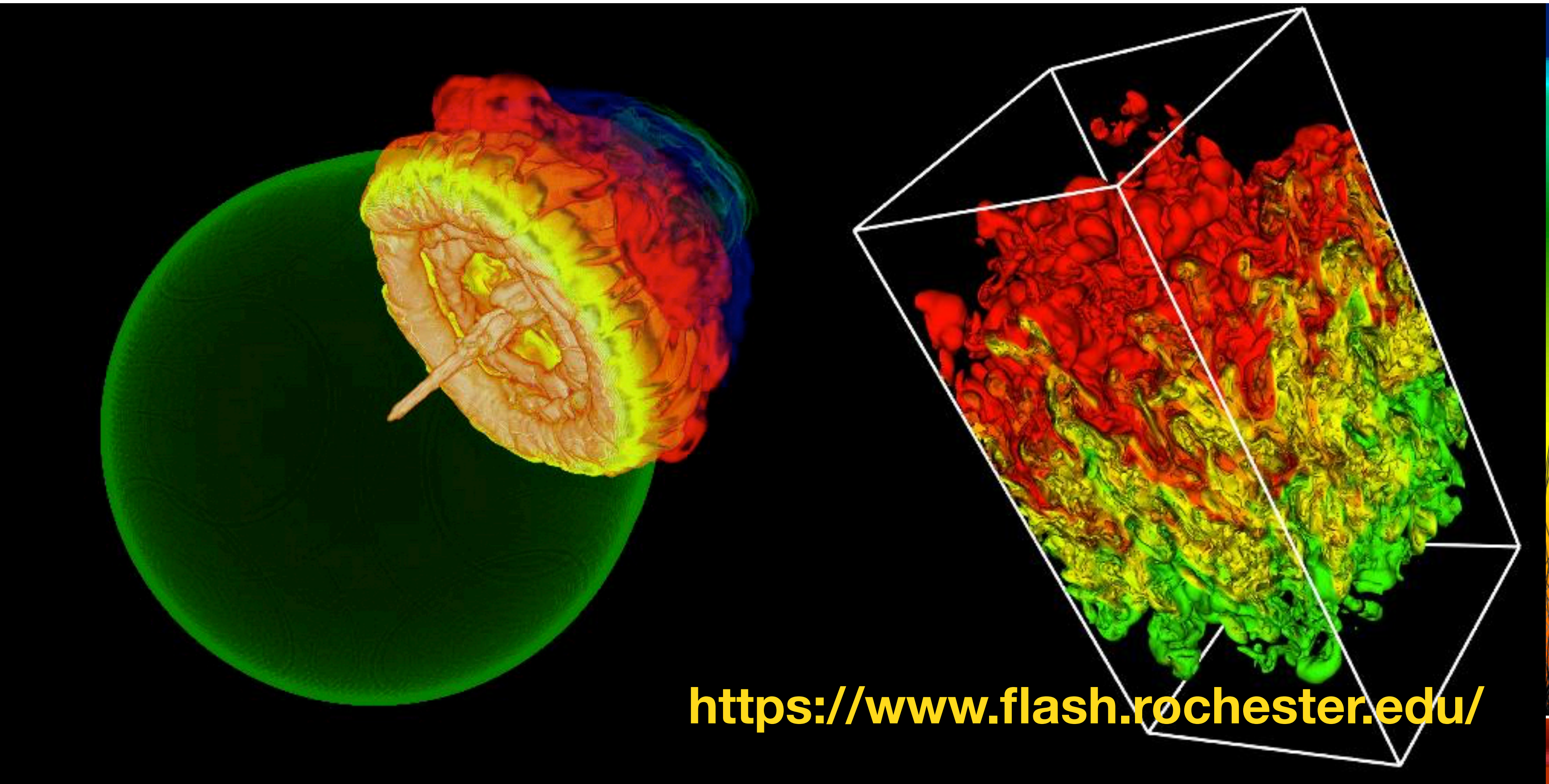
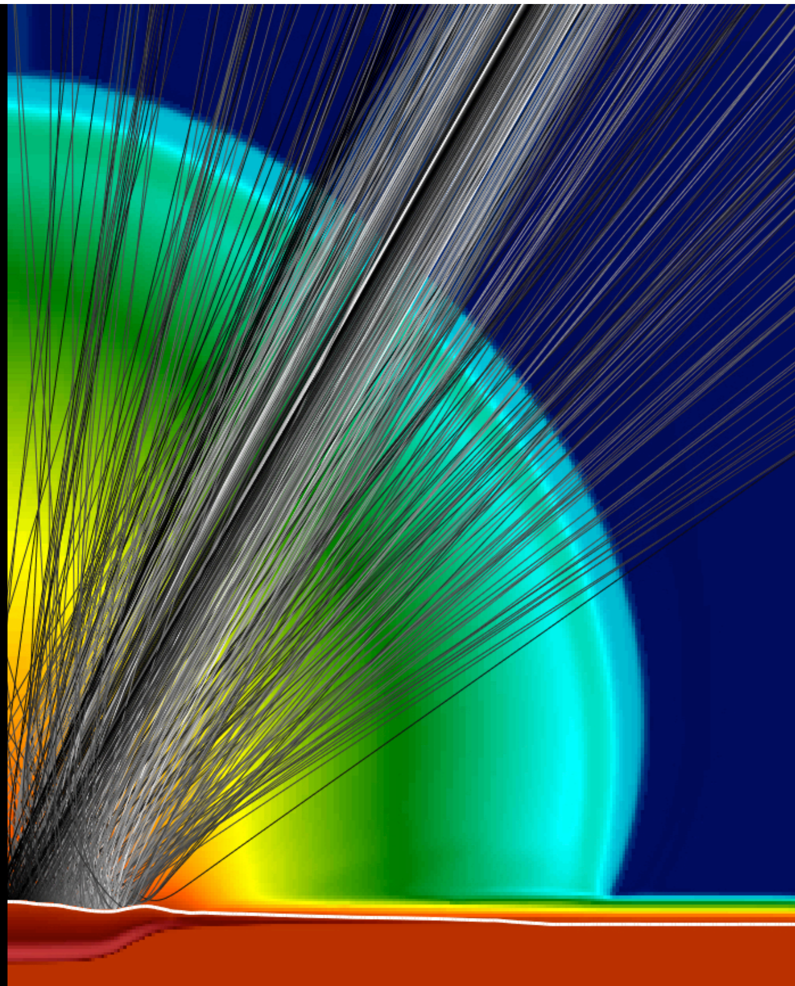
The FLASH code

- FLASH is a publicly available, high performance computing (HPC), adaptive mesh refinement (AMR), finite-volume, hydro and MHD code with extended physics capabilities. Supported primarily by the U.S. DOE NNSA.
- FLASH is professionally managed software in continuous development for 20 years: coding standards; version control; daily automated regression testing; extensive documentation; user support; integration of extensive code contributions from external users.

> 3,500 users world wide

>1,200 papers published with FLASH





Summary

- Added capability of Flash's hydrodynamics solver to capture interfaces in compressible multi fluid flow using VOF
- Verification on 1D two-fluid Riemann problems shows that Flash is able to correctly predict shock speeds while maintaining material interfaces
- PLIC reconstruction of interfaces enables VOF advection in two dimensions
- Integration with the unspilt hydrodynamics solver in Flash requires corrections for volumes advected through cell corners

Volume-of-Fluid

- Computational fluid dynamics (CFD) typically treated as an algebraic problem

$$U_i^{n+1} = U_i^n - \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} \frac{1}{\Delta x}(\hat{f}_{i+1/2} - \hat{f}_{i-1/2})dt$$

- Tracking material interfaces is inherently a geometric problem
- The volume-of-fluid (VOF) method attempts to bridge the two
  - Evolve volume fraction of component fluids (interface capturing)
  - Reconstruct material interfaces from volume fractions

Multifluid Hydro

(i) Single Velocity for all component fluids

(ii) Material interfaces remain in pressure equilibrium

- Pure cells neighboring pure cells w/ same type treated like single fluid hydro

- Mixed cells and cells with potential to become mixed get interface reconstruction & volume advection

[1] W. J. Rider and D. B. Kothe, "Reconstructing Volume Tracking," *Journal of Computational Physics*, vol. 141, no. 2, pp. 112–152, Apr. 1998, doi: 10.1006/jcph.1998.5906.

[2] G. H. Miller and E. G. Puckett, "A High-Order Godunov Method for Multiple Condensed Phases," *Journal of Computational Physics*, vol. 128, no. 1, pp. 134–164, Oct. 1996, doi: 10.1006/jcph.1996.0200.

[3] E. G. Puckett and J. S. Saltzman, "A 3D adaptive mesh refinement algorithm for multimaterial gas dynamics," *Physica D: Nonlinear Phenomena*, vol. 60, no. 1–4, pp. 84–93, Nov. 1992, doi: 10.1016/0167-2789(92)90228-F.

Solution Update

$$\partial_t(f^\alpha) + \nabla \cdot (\mathbf{u} f^\alpha) = \frac{f^\alpha \Gamma}{\Gamma^\alpha} \nabla \cdot \mathbf{u}$$

- "advected" volume fractions are updated ignoring RHS

- $\nabla \cdot \mathbf{u}$ is inferred by enforcing sum of volume fractions to be one

$$f^{\alpha,adv} = f^{\alpha,n} - \frac{1}{V_i}\left(V^{\alpha,adv}_{i+1/2} - V^{\alpha,adv}_{i-1/2}\right)$$

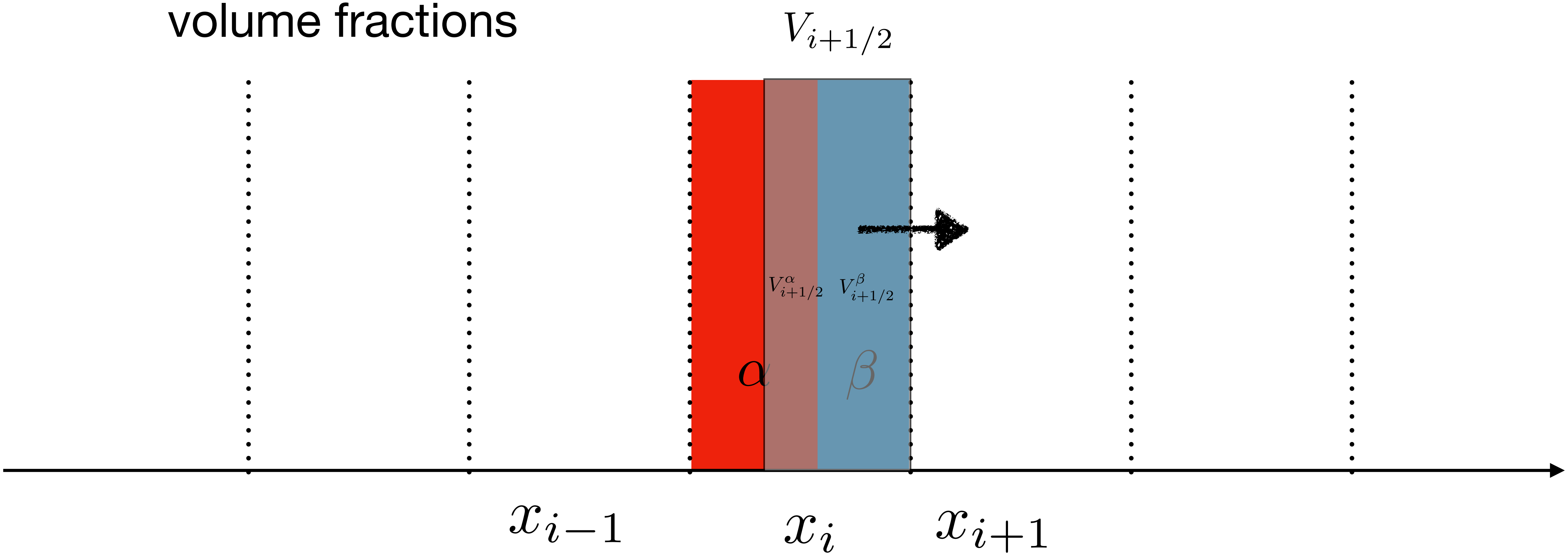
$$\nabla \cdot \mathbf{u}_i \approx 1 - \sum_\alpha f^{\alpha,adv}$$

- Γ^α also needs to be advected with the volume

$$\Gamma^\alpha \equiv \frac{\rho^\alpha c_\alpha^2}{P^\alpha} \qquad \Gamma = \left(\sum_\alpha \frac{f^\alpha}{\Gamma^\alpha}\right)^{-1}$$

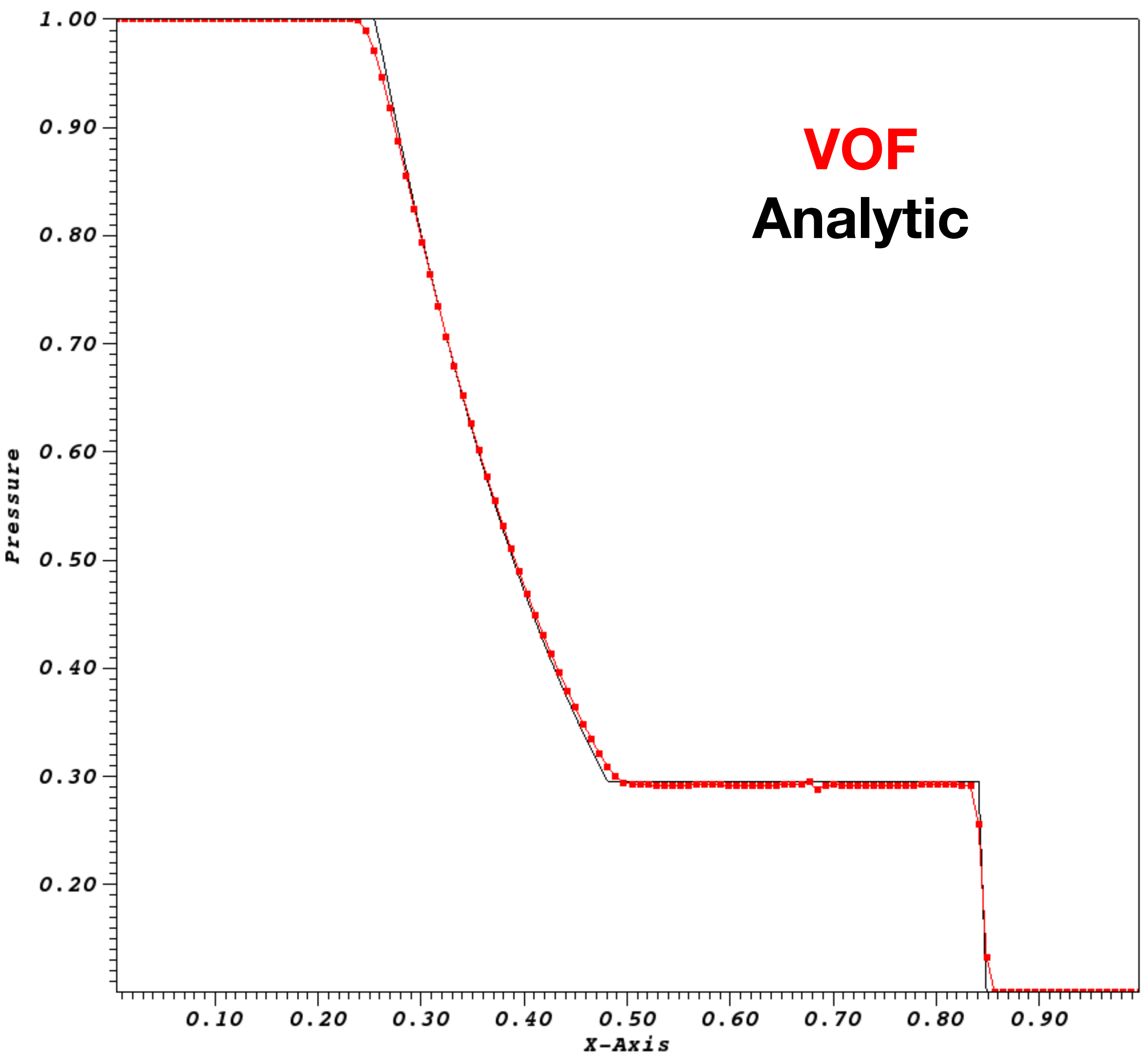
Advected Volumes

- Single-fluid hydro update gives a volume flux through cell interfaces
- VOF cuts advected volume with an interface to give flux of component volume fractions
- In 2D interfaces need to be reconstructed from neighboring volume fractions



1D Implementation in FLASH

- Sod shock tube with a jump in gamma
  - 1.5|1.4
  - Shock Speeds match analytic solution to 1D two-fluid Riemann problem
  - Mixing at material interface contained to a few cells



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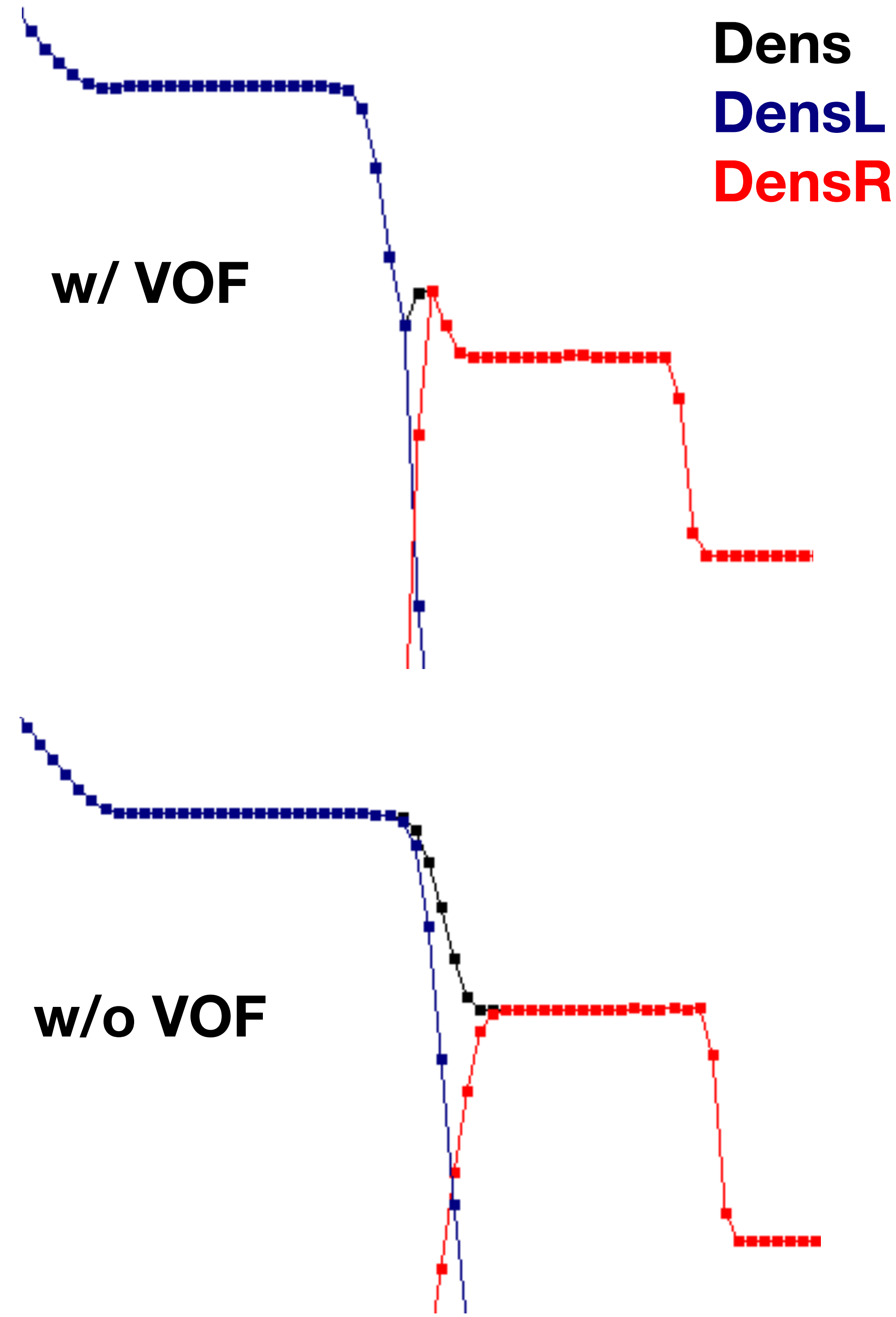
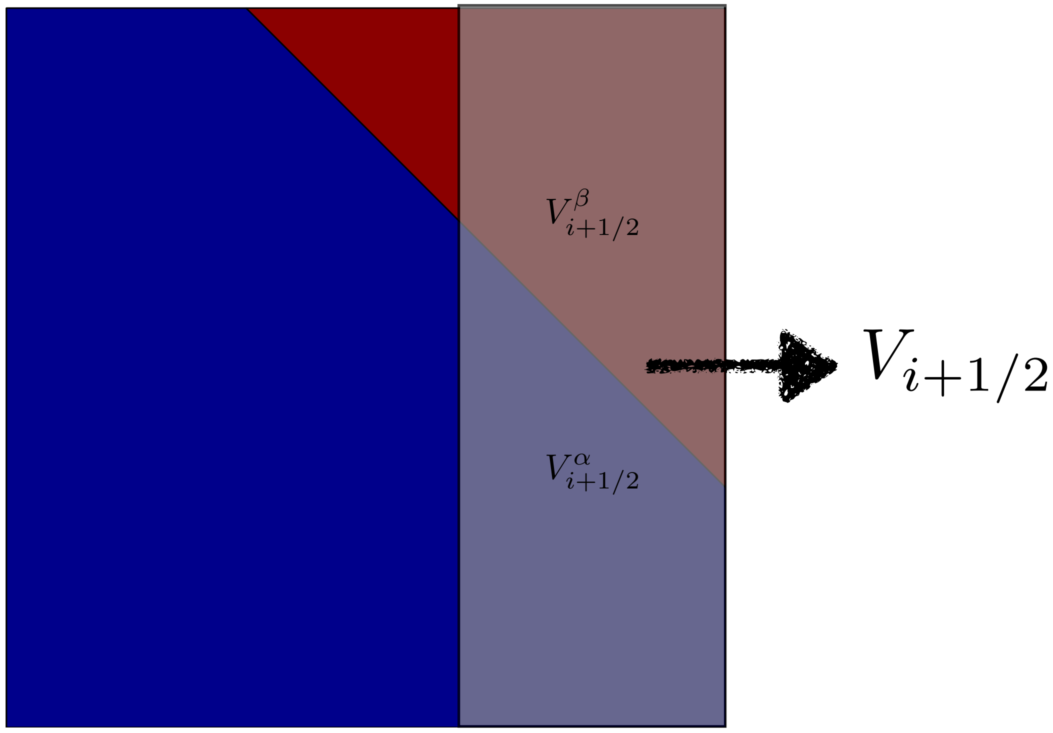


Piecewise Linear Interface Calculation (PLIC)

$$\mathbf{n} \cdot \mathbf{x} + \rho = 0$$

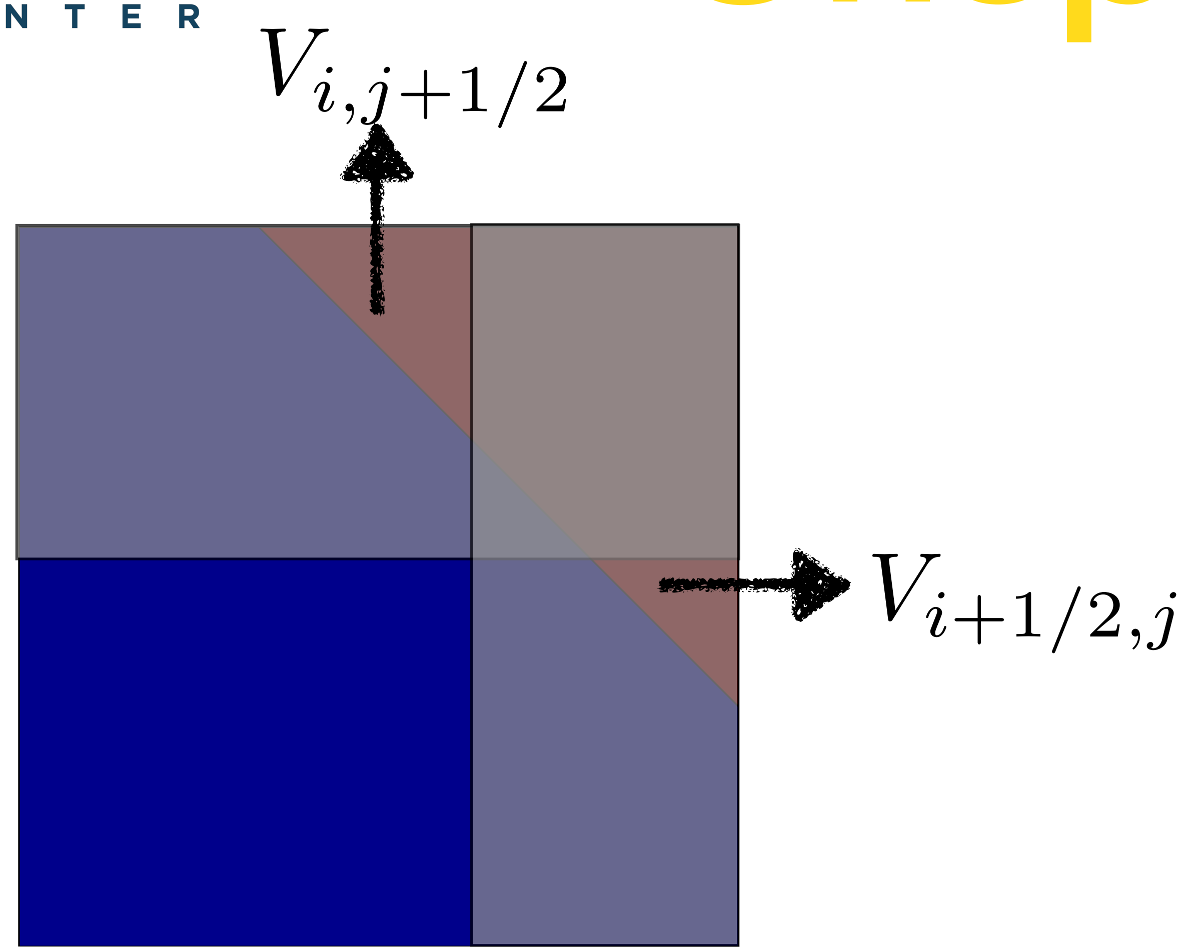


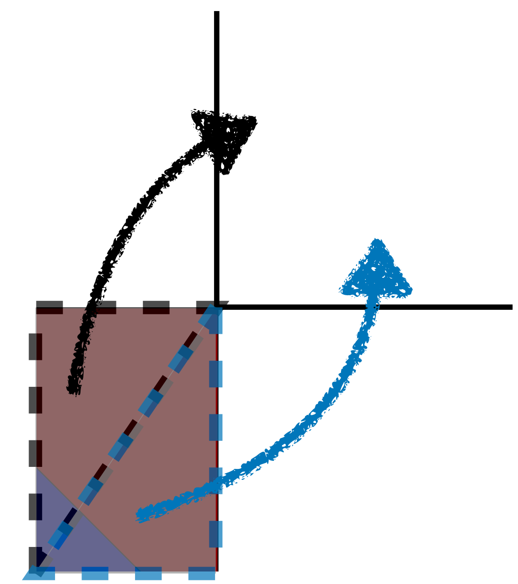
- Interface normal reconstructed as gradient of volume fraction
- Line constant fit to cell's volume fraction

[1] W. J. Rider and D. B. Kothe, "Reconstructing Volume Tracking," *Journal of Computational Physics*, vol. 141, no. 2, pp. 112–152, Apr. 1998, doi: 10.1006/jcph.1998.5906.

[2] D. Youngs, "An interface tracking method for a 3D Eulerian hydrodynamics code," Jan. 1984.

Unsplit VOF

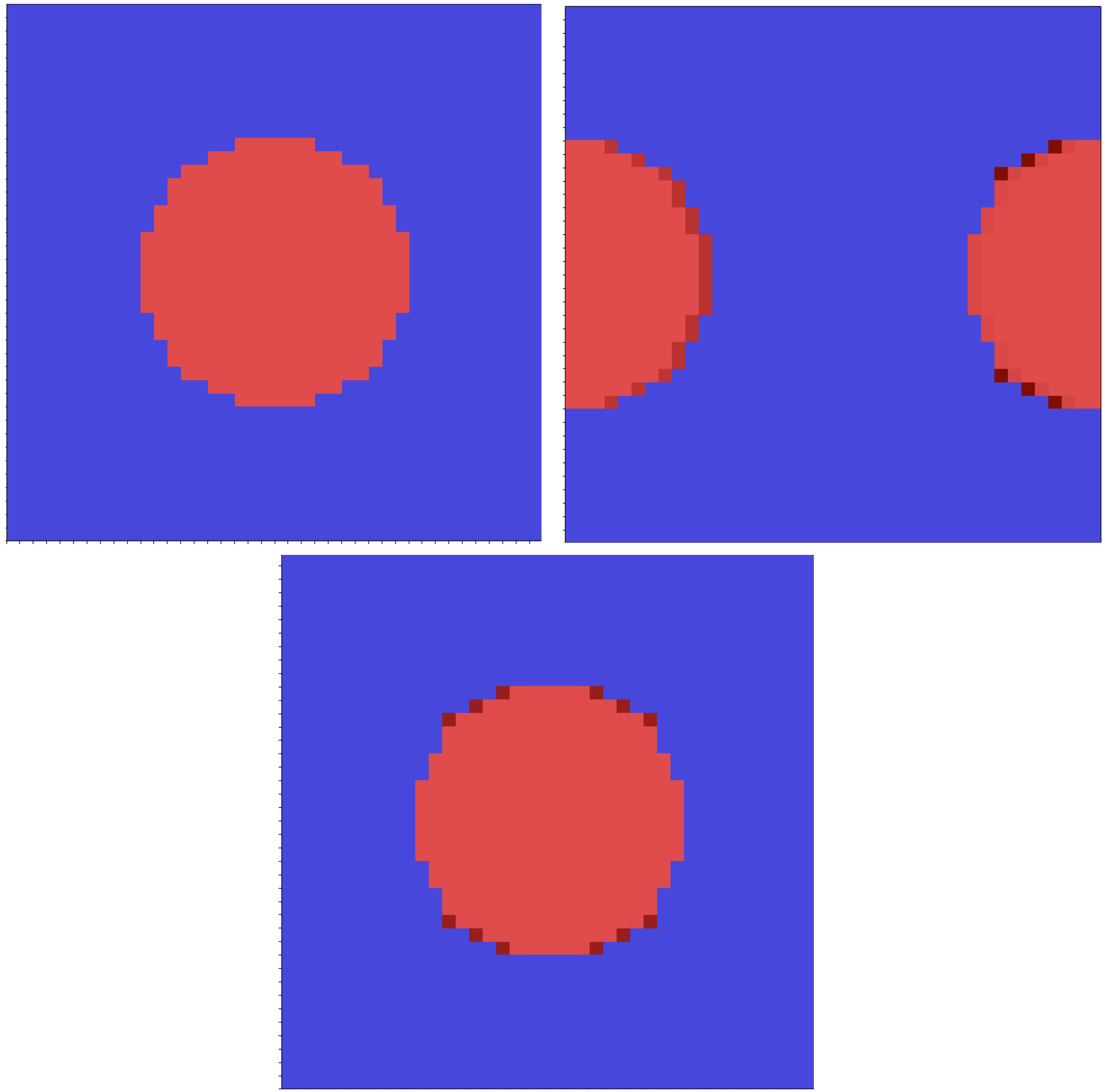




- Unsplit hydro updates using x & y fluxes simultaneously
- Corner volume fluxes need to be reassigned to neighboring faces

[1]
W. J. Rider and D. B. Kothe, "Reconstructing Volume Tracking," *Journal of Computational Physics*, vol. 141, no. 2, pp. 112–152, Apr. 1998, doi: 10.1006/jcph.1998.5906.

2D Advection



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Compressible Multifluid Hydro

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla P = 0$$

$$\partial_t (\rho E) + \nabla \cdot (\mathbf{u}(\rho E + P)) = 0$$

- Each component has

$$\Gamma^\alpha \equiv \frac{\rho^\alpha c_\alpha^2}{P^\alpha}$$

- Also for equivalent single fluid

$$\Gamma = \sum_\alpha \left(\frac{f^\alpha}{\Gamma^\alpha} \right)^{-1}$$

Solution Update

- Momentum is updated w/ single fluid fluxes
- Component density and energies are updated using single fluid fluxes weighed according to the ratio of advected volumes at the interface

$$\mathbf{F}^{\rho^\alpha}_{i+1/2}\frac{V^\alpha_{i+1/2}}{V_{i+1/2}}\mathbf{F}^{\rho}_{i+1/2}$$

Pressure Relaxation

- After update component pressures may not be in equilibrium with single fluid pressure

$$P^\alpha \neq P$$

- Adjust volume fractions, densities & energies to get to an average pressure: $P = \frac{\sum_\alpha f^\alpha / \Gamma^\alpha}{\sum_\alpha \frac{f^\alpha}{P^\alpha \Gamma^\alpha}}$

$$f^\alpha = \frac{f^\alpha}{\alpha}(1 \quad \frac{P}{P^\alpha})$$

$$f^\alpha \qquad f^\alpha + \quad f^\alpha$$

$$\rho^\alpha \qquad \frac{f^\alpha \rho^\alpha}{f^\alpha + \quad f^\alpha}$$

$$f^\alpha \rho^\alpha E^\alpha \qquad f^\alpha \rho^\alpha E^\alpha \qquad P \quad f^\alpha$$

2D Advection