V & V forTurbulent Mixing

James Glimm[1,3]

With thanks to:

Baolian Cheng[2], John Grove[2], Xaolin Li[1], Roman Samulyak[3], David H. Sharp[2], Yan Yu[1], Yongmin Zhang[1]

and many present and former Stony Brook students:

Wurigen Bo[1], Jian Du[1,3], Bryan Fix1, Erwin George[7], Xicheng Jia[1], Hyeonseong Jin[6], T. Kaman[1], Dongyung Kim[1], Hyunsun Lee[1], Yuanhua Li[1], Hyun-Kyung Lim[1], Xinfeng Liu[8], Jinjie Liu[5], Thomas Masser[1,2], Nicolas Pestieau[1], Shuqiang Wang[1], Lingling Wu[1], Zhiliang Xu[4]

1. SUNY at Stony Brook
2. Los Alamos National Laboratory
3. Brookhaven National Laboratory
4. Notre Dame .
5. Arizona State University
6. Cheju National University, Korea
7. Warwick University, UK
8. University of California, Irvine

6 Current NNSA Staff Scientists from the Stony Brook Program

Is V&V a completed subject?

- Mechanical Engineers have issued a standard
  - Many good ideas
    - Verification first
      - Manufactured solutions
      - Convergence and order of convergence studies
      - Symmetries preserved?
    - Validation
      - Error bars for experiments and simulations
      - No tuning of code for validation comparisons
- Recent overview: Sandia SAND2007-0853 Verification and Validation Benchmarks W. Oberkampf and T. Trucano

ASME V&V 10-2006

Guide for Verification and Validation in Computational Solid Mechanics

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What is missing? All the difficult parts!

- Unstable flows
  - Mesh convergence in question
  - Problems with validation
- Multilevel problems
  - Propagation of errors through hierarchies of problem scale:
    - Unit problem to composite to full scale
    - Reduced descriptions of higher level composite and full scale problems
    - Averaged equations and closure
    - Subgrid models
    - Significant reduction in the number and quality of experiments and their instrumentation as the problem scale and realism increases
- Multiphysics problems
  - Nonlinear, multiscale problems
- Multiple time regimes
  - Propagation of errors; creation of errors

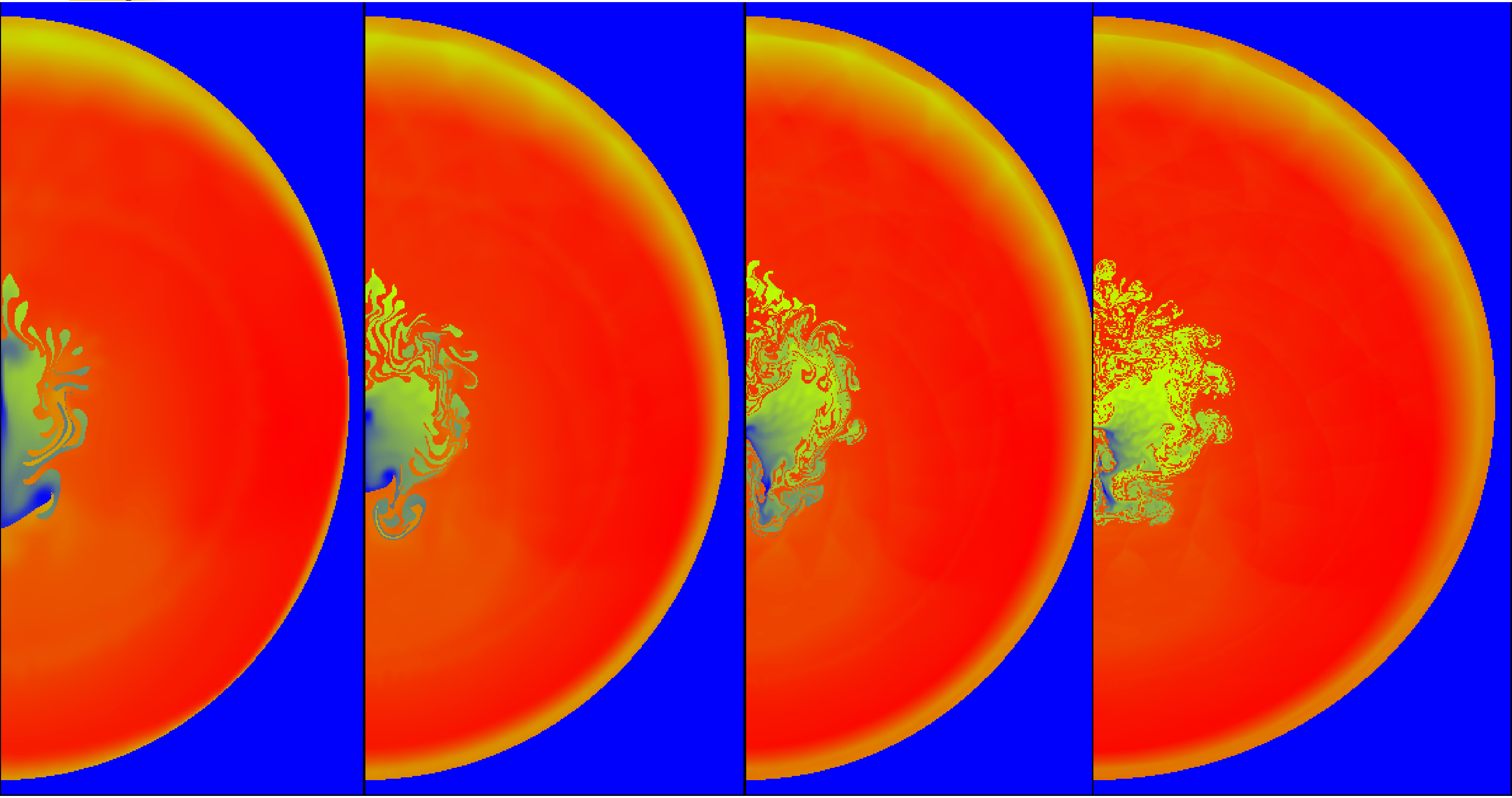
Outline of Presentation

- Unstable flows: Verification
  - Mesh convergence study
  - Comparison to Rage simulations
- Unstable flows: Validation
  - Rayleigh-Taylor: agreement among simulation, experiment, theory
- V & V for a two scale problem
  - Reduced description and averaged equations: comparison to DNS; comparison of closures

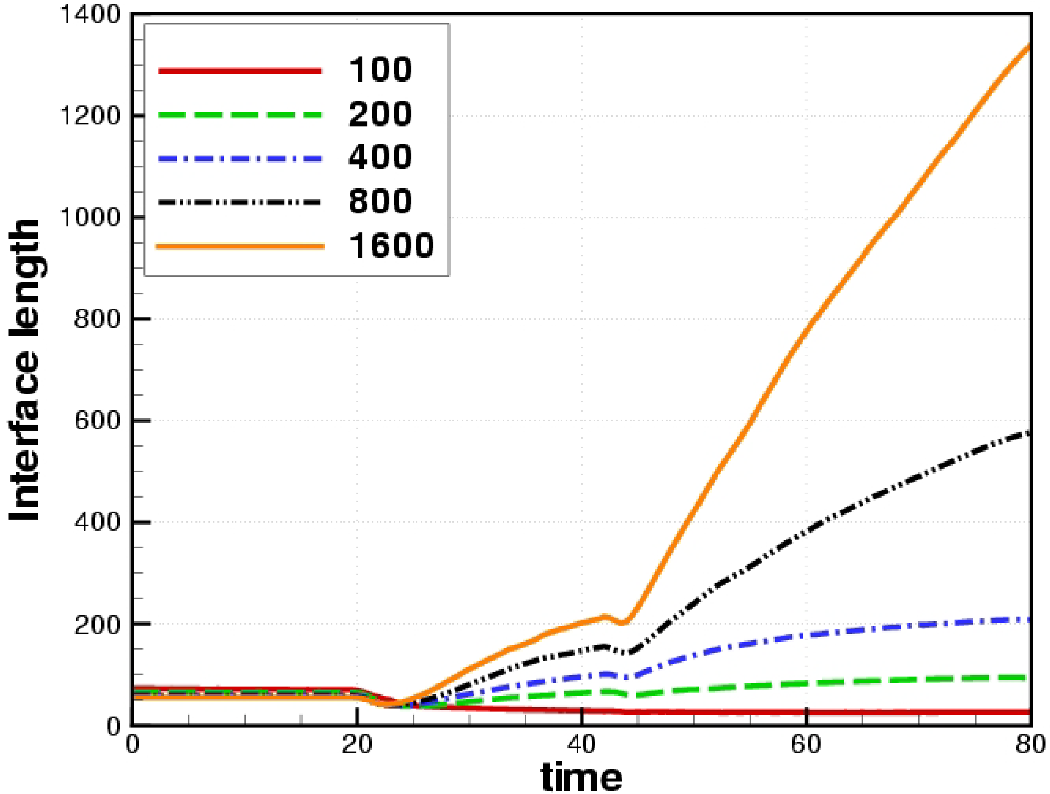
Verification

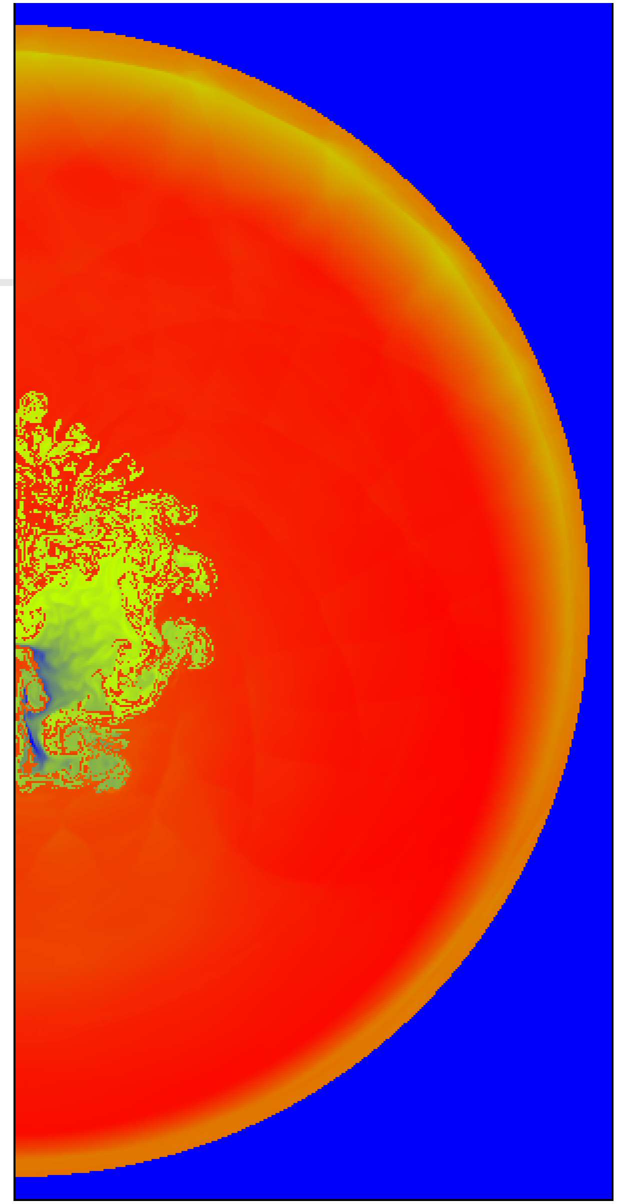
- Mesh convergence study for circular RM problem
  - Wave filters to locate shocks, mixing zone edges
  - Tracking to separate material within mixing zone
  - Comparison of like to like only
    - I.e.: twice shocked heavy fluid in mixing zone
  - Local average over symmetry variable (angle)
  - Result: many quantities converge

2D Chaotic Solutions: Shock implosion of perturbed interface with offset—4 grid levels



Interface length diverges under mesh refinement. Implications for convergence?





$$\text{ERROR} \propto \Delta x \times \text{ Interface length}$$

What does convergence mean?

- Look for reproducible quantities, in the spirit of an experimental scientist
  - Means, variances, statistical behavior
- Compare similar quantities, in the spirit of a statistician
  - Compare similar materials (heavy to heavy, light to light) and similar flow histories (shocked, mixed, etc.)
  - Convergence of flow regime interior boundaries as a separate question
- Formulate convergence for use in the context of needs of larger context
  - This point of view supports the previous bullets
- Achieve positive order of convergence for chaotic flow
  - Order depends on flow quantity and degree of averaging

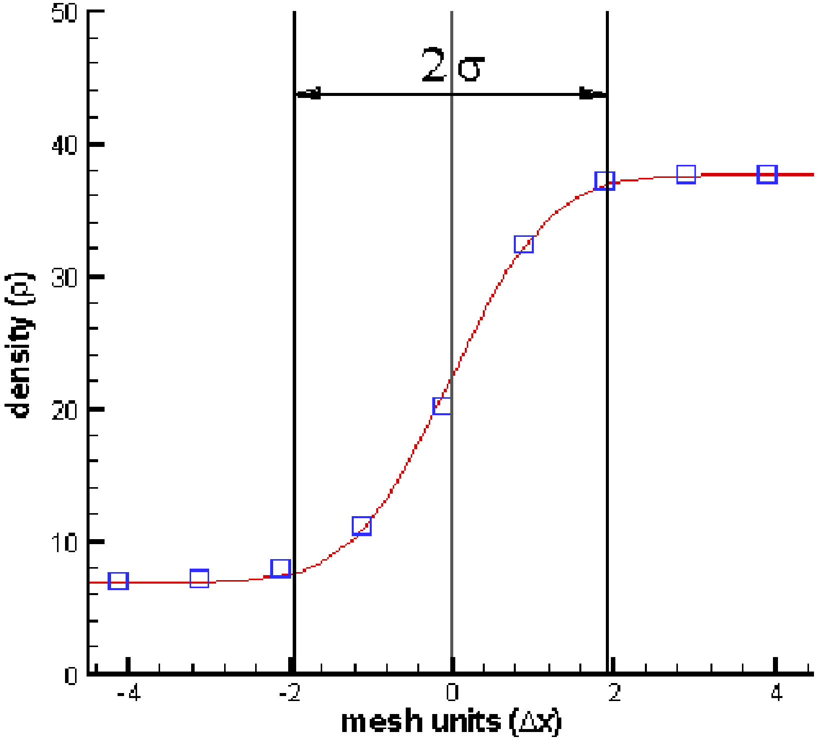
Wave Filter: To Decompose Flow History

- Filter starts with selection of an extended stencil and takes the extreme left and right states from the stencil
- From these states, a Riemann problem is constructed
- If there is a unique strong wave the analysis continues. Otherwise there is no wave or there are two or more waves interacting.
- This construction is applied at every space time point to assess possible presence of a wave

Wave Filter for Shocks and Contacts: Fit to an erfc

Solution states at mesh points within stencil range of filter are fit to an erfc, by least squares, to select best choice of mean (wave position) and STD (2STD = wave width)

Rarefactions: fit to ramp function



Error definition: means and variances

- Phase average and variance for pressure p and density ρ

$$\mu_{\Lambda_k} = \frac{< X_k \Lambda >}{< X_k >}$$

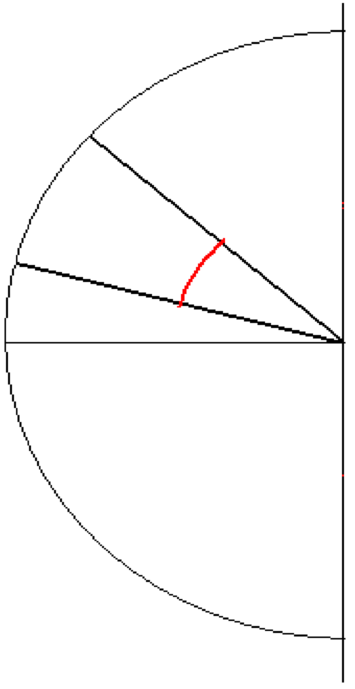
$$s^2_{\Lambda_k} = \frac{< X_k (\Lambda - \mu_{\Lambda_k})^2 >}{< X_k >}$$

where X_k is the phase indicator and Λ the averaged variable

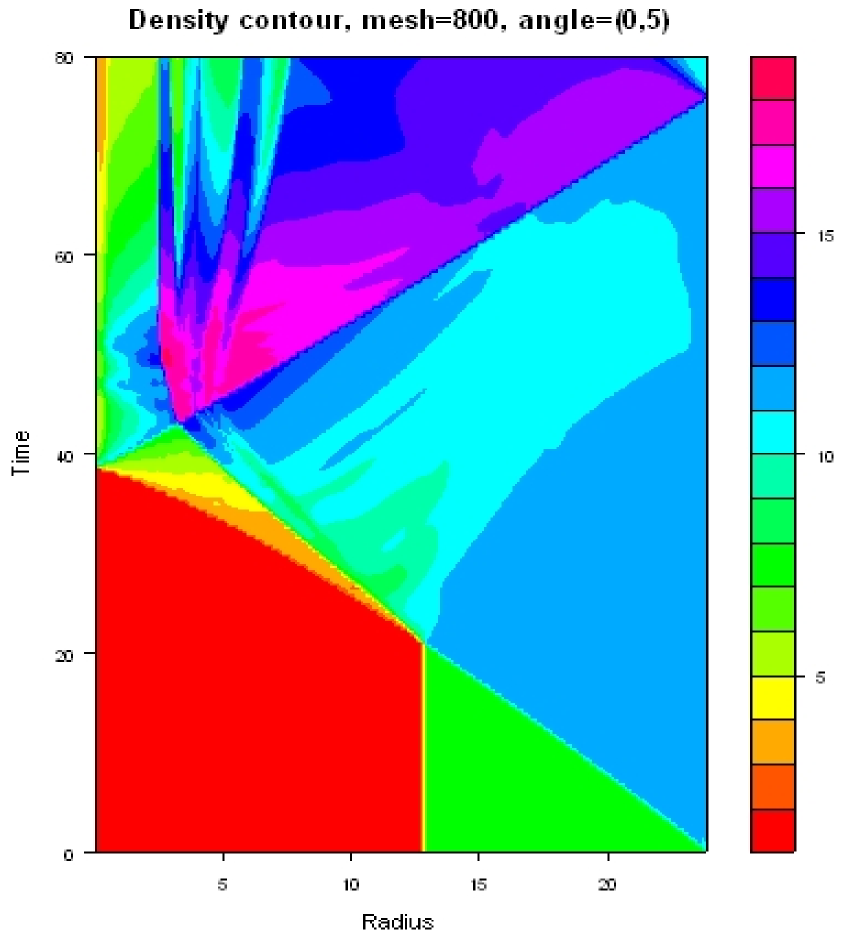
- Similarly, phase mass-weighted average for velocity v, internal energy e, total energy E and entropy s

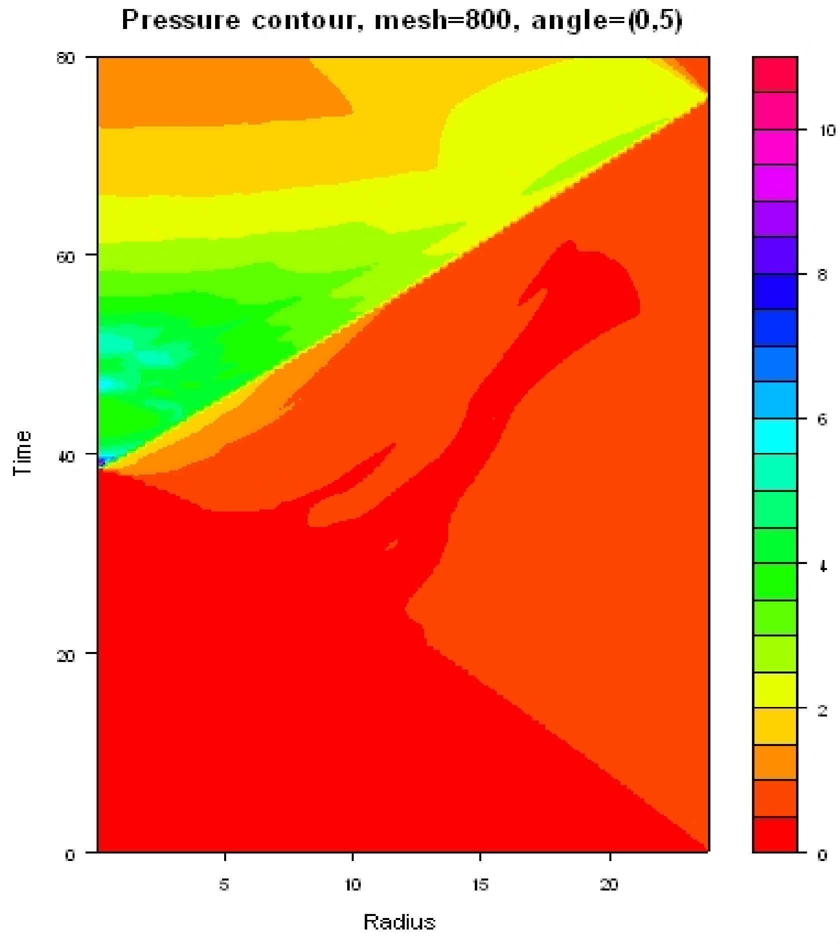
$$\mu_{\Lambda_k} = \frac{< X_k \rho \Lambda >}{< X_k \rho >}$$

$$s^2_{\Lambda_k} = \frac{< X_k \rho (\Lambda - \mu_{\Lambda_k})^2 >}{< X_k \rho >}$$

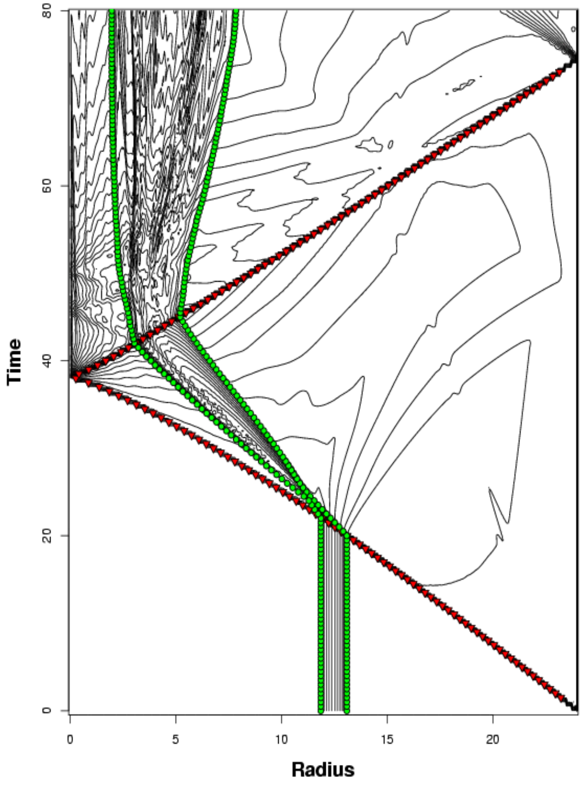


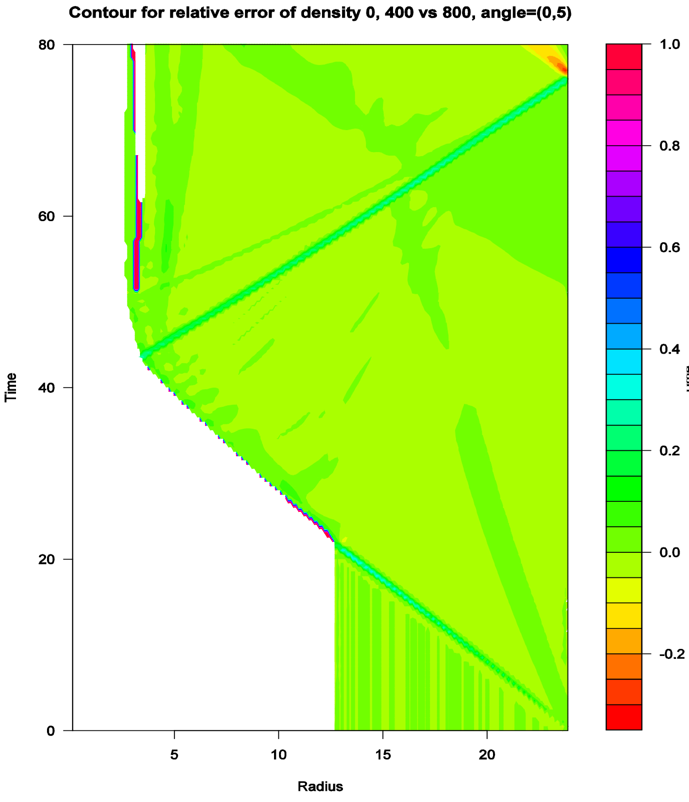
Average data over a 5 degree sector

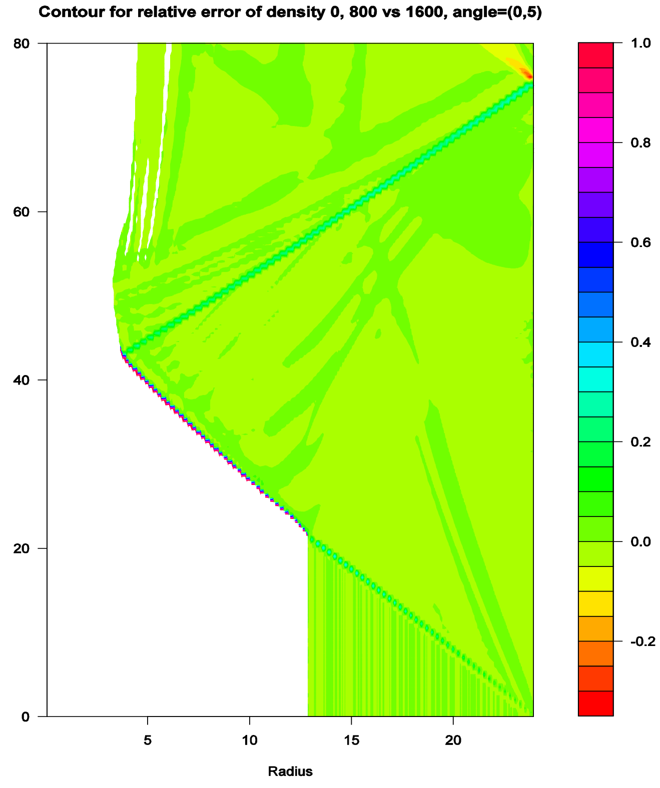




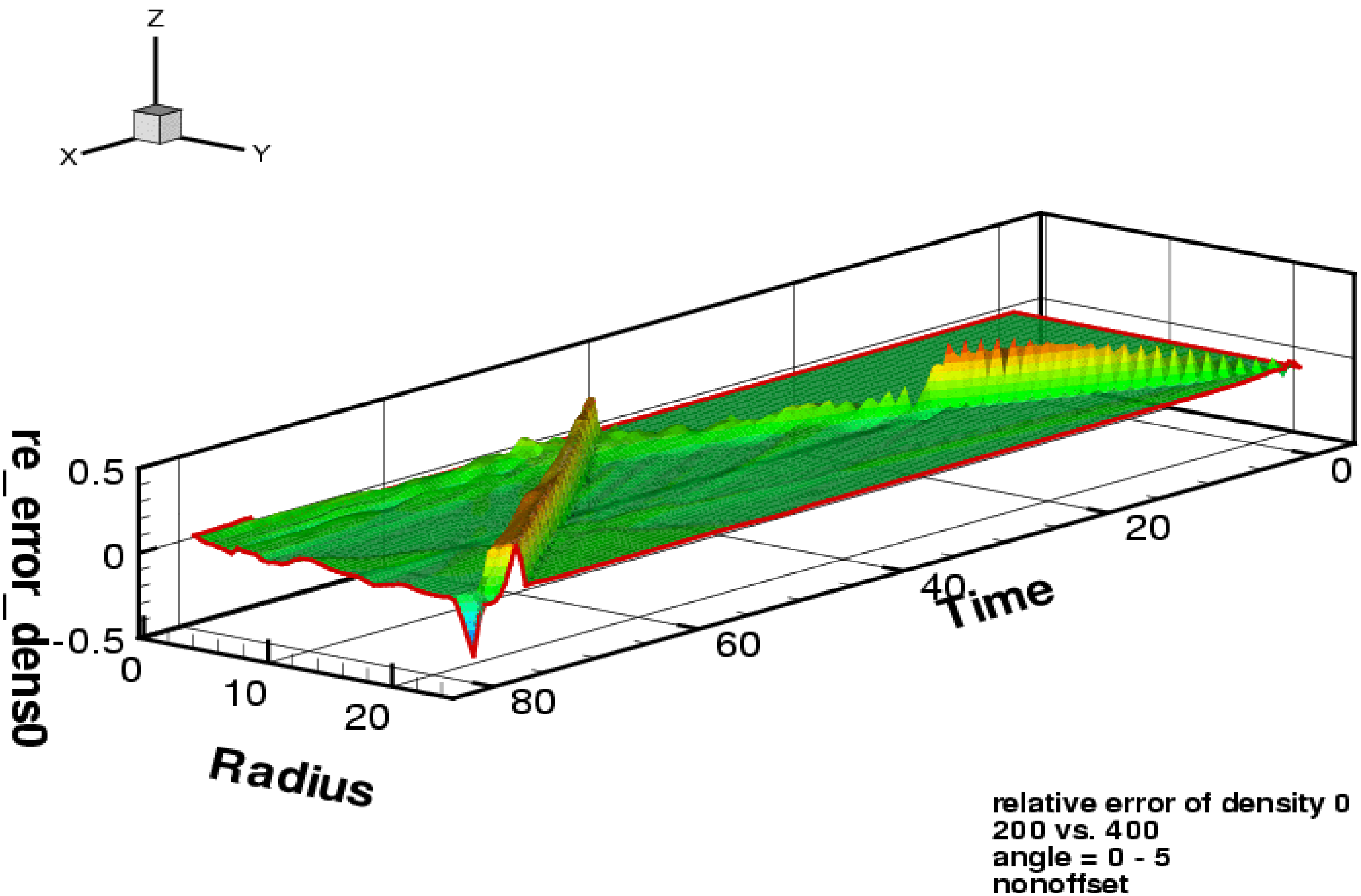
Error analysis: shocks, MZ edge positions and heavy fluid density converge 1st order





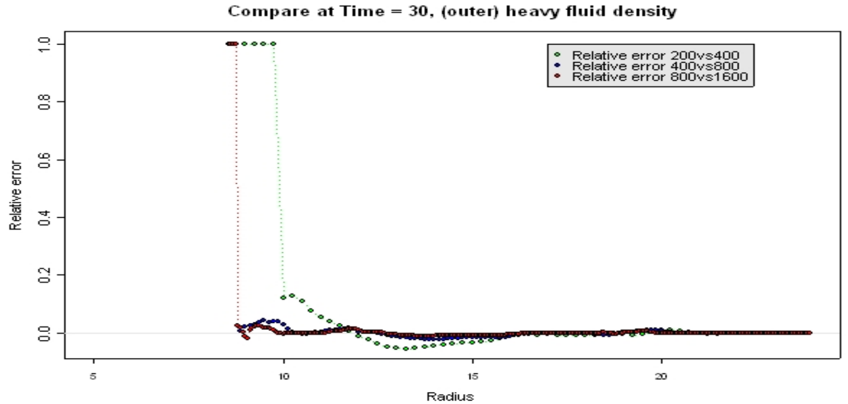


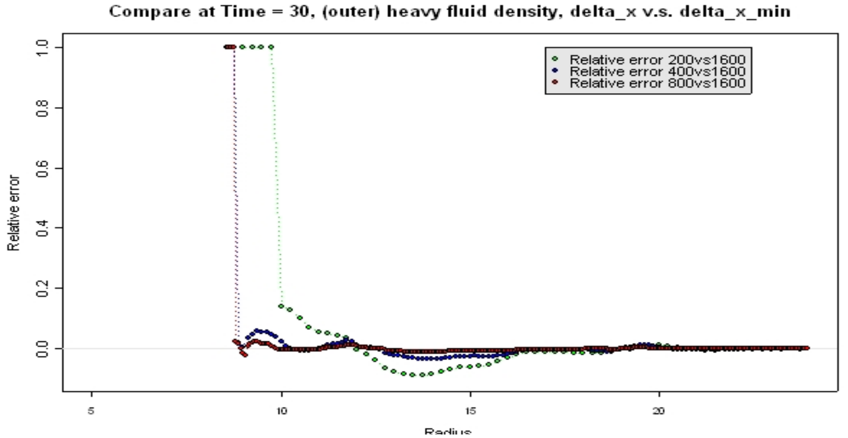
Heavy fluid density relative error. Compare 200x400 to 100x200 grids. Large ridges come from shock position errors.

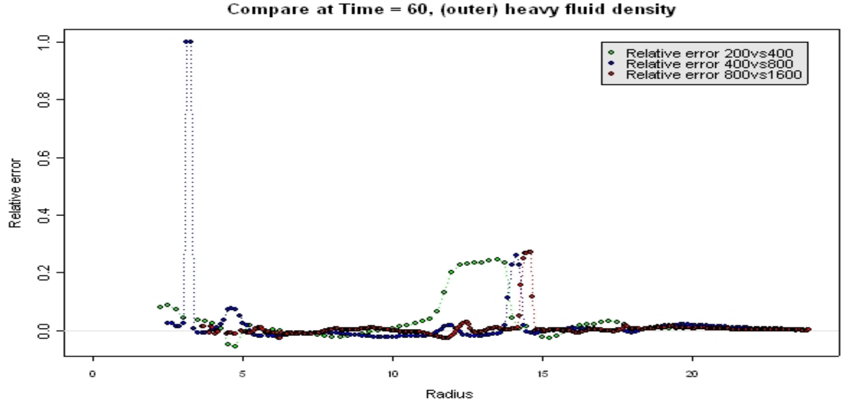


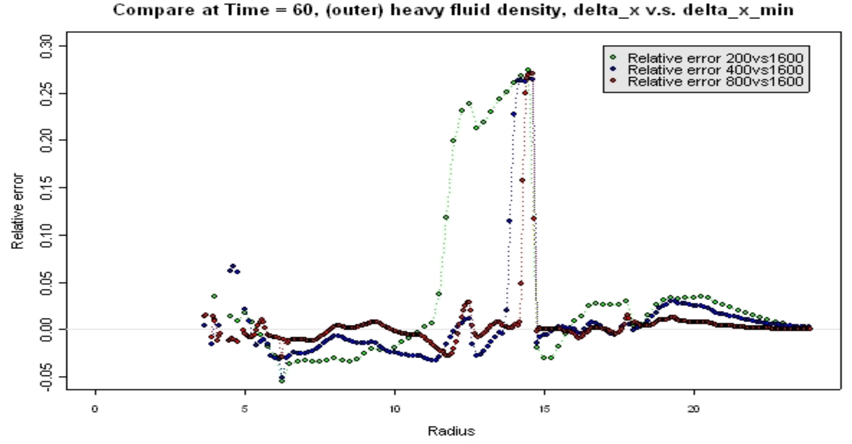
Solution and error are averaged over an angular sector of 5 degrees. Converging shock interacting with perturbed contact.

Error analysis: heavy fluid density error at four times





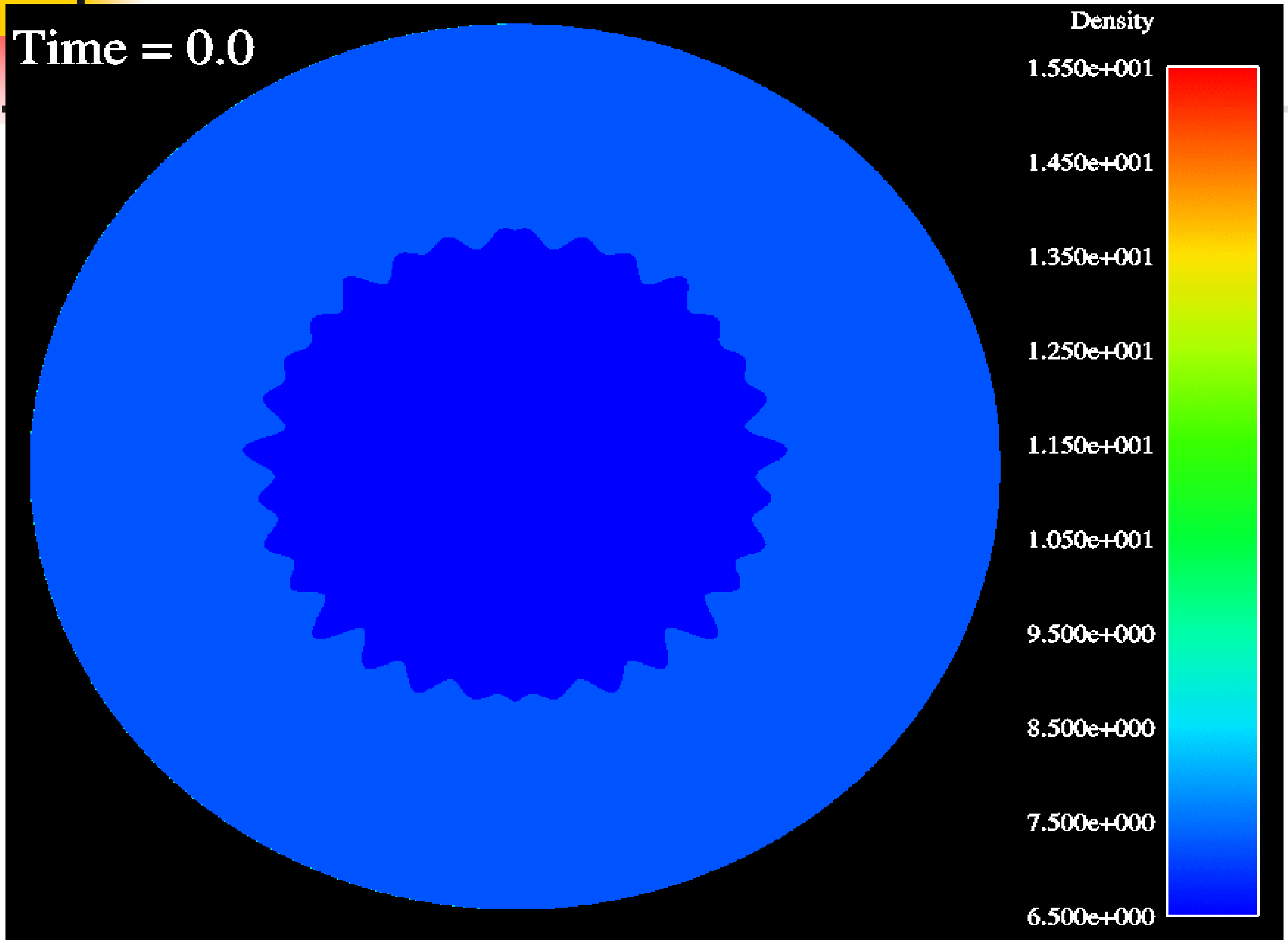




Comparison Study

- FronTier and Rage for same circular RM problem
- Rage work conducted at LANL by SB student Thomas Masser, supervised by John Grove
- Many quantities agree
- Peak temperatures differ by 50% and much greater (numerical) thermal diffusion in Rage
  - Physics in simulation has no heat conductivity

Rage vs. FronTier

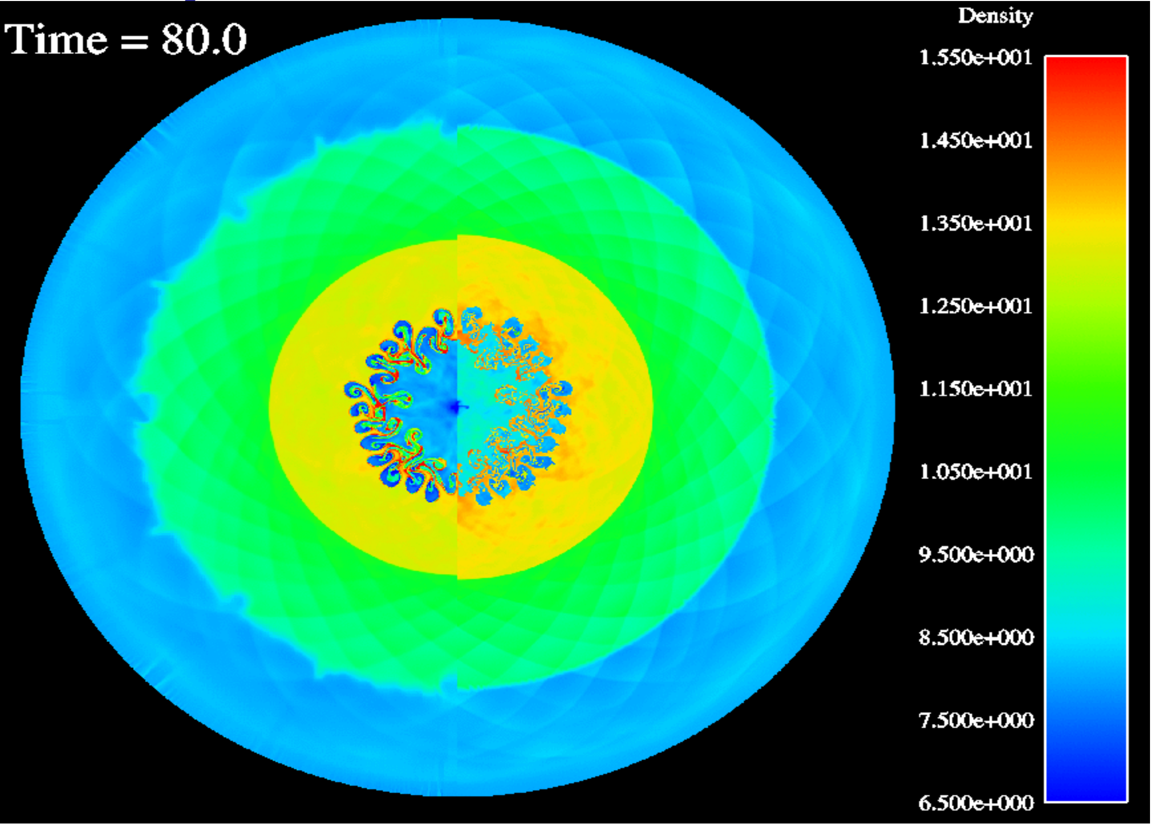


- Boundary values nearly identical
- Initial shock speeds comparable
- Discrepancies persist; e.g. high temperature fingers in FronTier
- Simulation by T.Masser and J. Grove, LANL

Time = µsec, P = Mbar, T = °Kelvin, v = cm/µsec, ρ = grams/cc

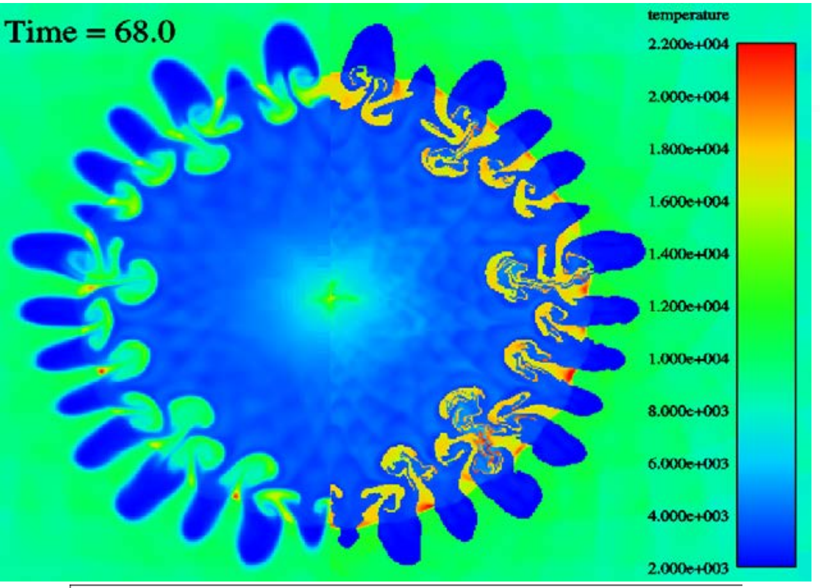
Front Tracking (FronTier) vs Untracked (RAGE) at Late Time

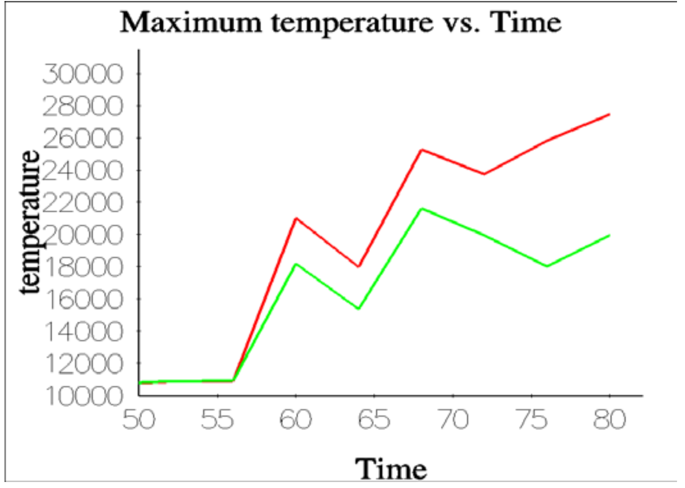
- Much more complex mixing structure in FronTier.
  - Interface smoothed by diffusion in RAGE
  - FronTier interface breaks up into droplets.
- Outgoing shock is ahead in FronTier.
- Mixing zone width is similar.
- Flow away from the interface is comparable.



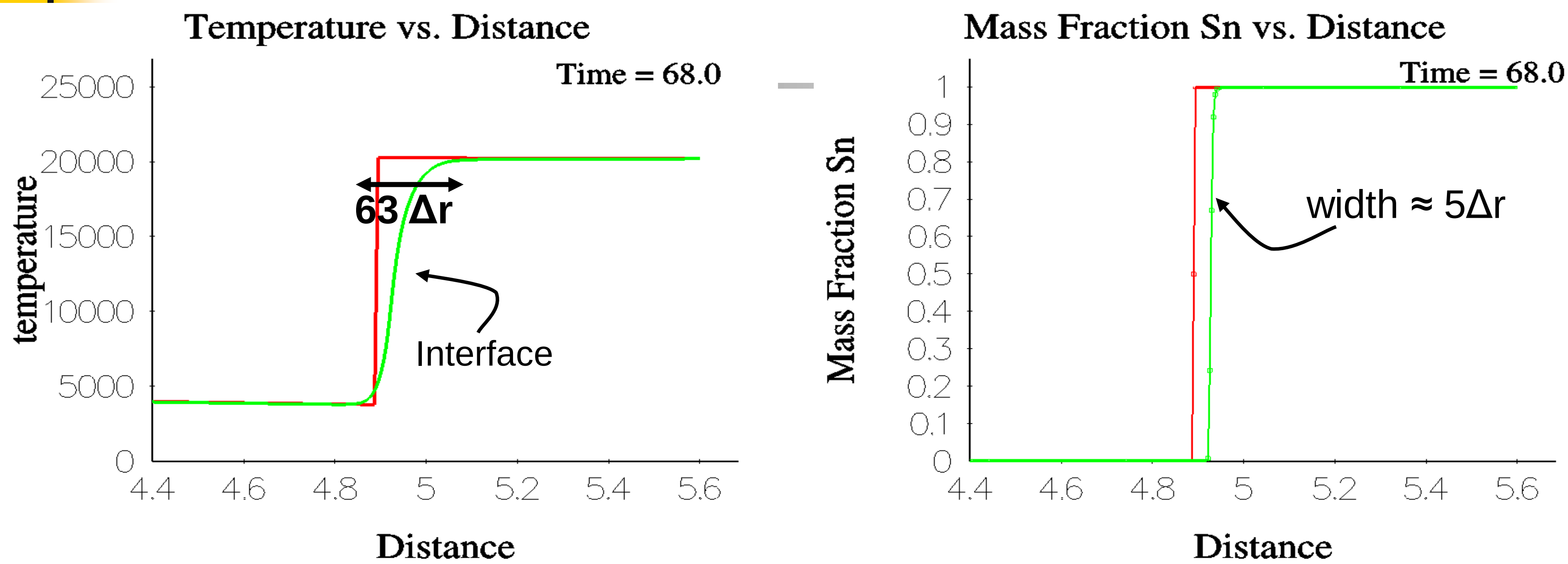
Major Temperature Differences at Reshock

- At reshock the fingers of tin are heated to a much higher temperature in the FronTier simulation than the corresponding fingers in the RAGE simulation.
- There are at least three possible mechanisms that might be responsible.
  - Velocity shear in FronTier missing in RAGE
  - Thermal and Mass diffusion at the interface in RAGE
  - Differences in the hyperbolic solver
- After reshock FronTier continues to have a significantly higher maximum temperature.





Thermal vs. Material Width of Contacts



After reshock

- Mass fraction width ≈ 5 zones
- Thermal width ≈ 63 zones at time 68 μsec
- Thermal width increases with each refraction

Verification: Conclusions

- Verification, for chaotic and unstable flows, depends on some level of averaging, to remove point to point statistical fluctuations
- Separation of convergence questions for wavefront locations and timing from variability in a “smooth” region between fronts yields a large decrease in variance
  - Software developed for this is easy to adopt
- Separation of distinct fluid components in a two phase flow also aids convergence (compare apples to apples)
- Addition of secondary physics will aid convergence
- Convergence was observed
- Interface length/area and nature of atomic level mixing needs further study
- Many open questions regarding influence of numerical artifacts and initial conditions

Validation: Rayleigh-Taylor mixing

- Systematic agreement of simulation with experiment and theory
  - Alpha, bubble width, bubble height fluctuations, theta, xi
  - Most relevant experiments included in agreement
    - Reed-Youngs, Smeeton-Youngs, Andrews experiments
    - Omitted:
      - Immiscible with surfactant (Dimonte and Smeeton-Youngs)
      - Initial diffusion layer (preliminary results)
  - Improved numerics (local grid based tracking) and physics (surface tension, diffusion, viscosity, etc.)

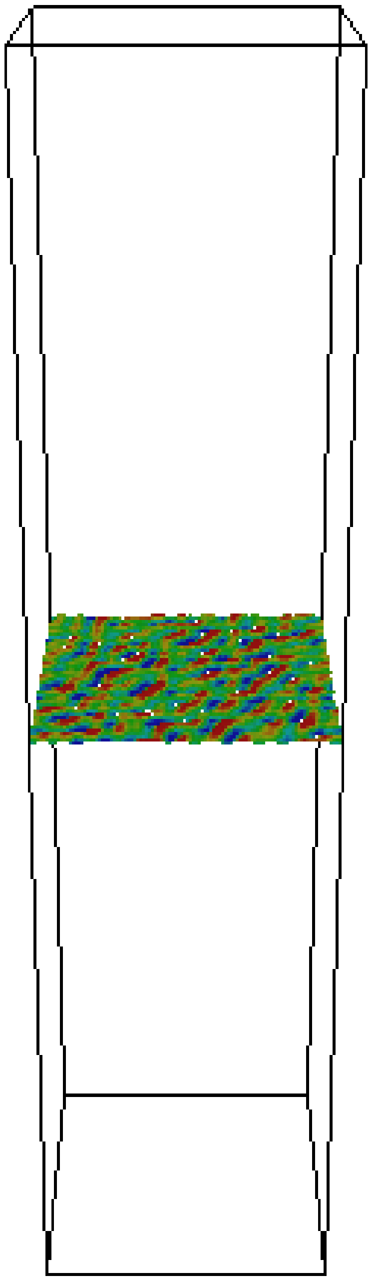
Validation: Comparison of Experiments and Simulations

Scale breaking physics	Alpha-experimental	Alpha-simulation	Experiments	Fluids
Surface tension	0.050-0.077	0.067	RY, SY	Liquid/liquid; liquid/gas
Surface tension with surfactant	0.050-0.061	????	SY,DS	Liquid/liquid
Mass diffusion	0.070	0.069	BA	Gas/gas
Initial mass diffusion	0.062	0.054*	SY	Liquid/liquid
Viscosity	0.070	0.069*	SA	Liquid/liquid
Compressibility		Up to 0.2	Lasers	plasmas

* Preliminary result

Rayleigh-Taylor simulation for weakly compressible fluids, immiscible fluids (with surface tension)

Color code represents height



Rayleigh Taylor Turbulent Mixing

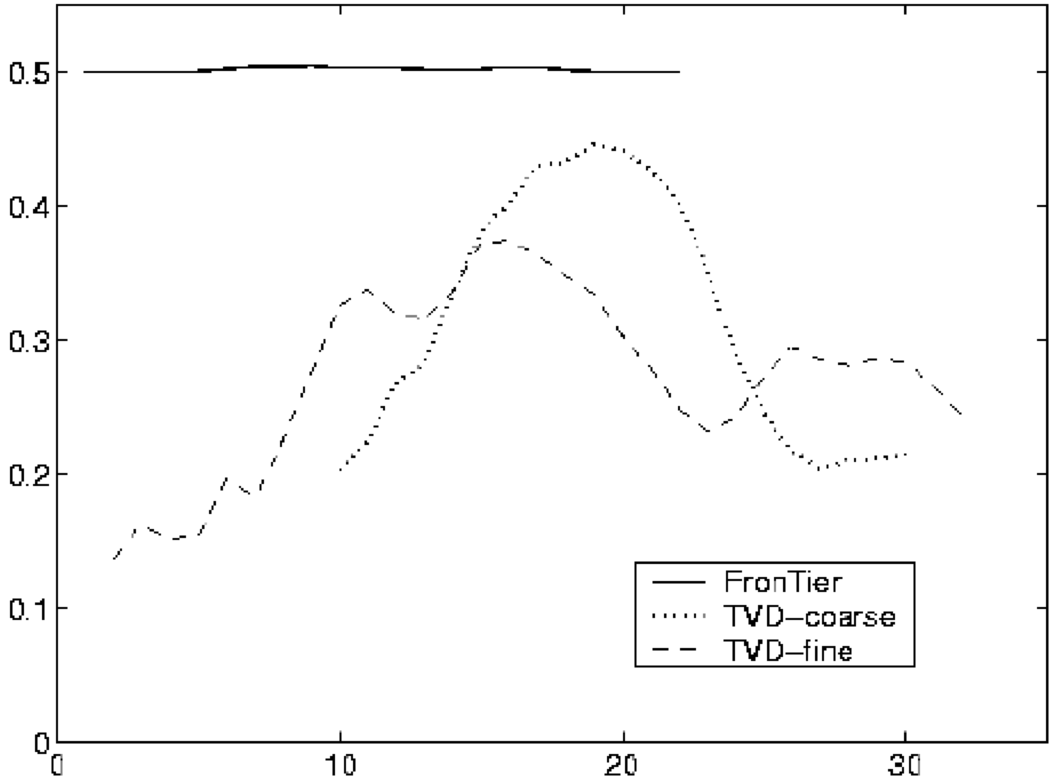
- Most computations underpredict mixing rates relative to experiments
- Cause appears to be numerical mass diffusion
- Theory (bubble merger models) agree with experiment and (our) simulations; mixing driven by bubble competition
- Role of initial conditions

Time Dependent Atwood Number

- Atwood number $$A = \frac{\rho_2 - \rho_1}{\rho_2 + \rho_1}$$
- For each z
  - Compute the maximum and minimum density
  - Form a space (height) and time dependent A(z,t) from min/max
  - A(z,t) depends on extreme density differences at fixed z,t
- Average A(z,t) over bubble region to get A(t)
- Untracked A(t) is about ½ nominal value due to mass diffusion; (incompressible) tracked A(t) is virtually constant
- If A(t) is used in definition of alpha, all low compressible simulations agree (with each other, with experiment, with theory)
- If A(t) is used in compressible simulations, all simulations are self similar, but self similar growth rate depends on compressibility
- *A(t) and alpha are sensitive to density EXTREMES; theta is sensitive to average density differences*

Time Dependent Atwood Numbers: Comparison of tracked and untracked simulations (untracked typical of alpha group simulations)

A(t)

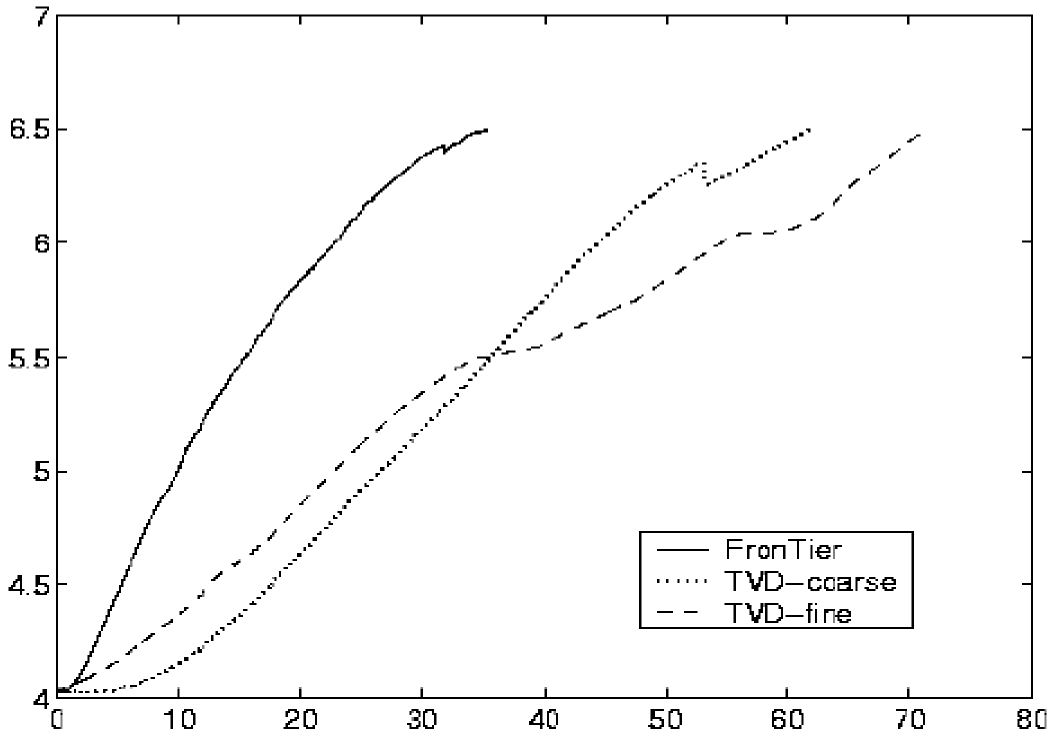


Time

FronTier and TVD Simulations without / with diffusion renormalization of time scales

Z

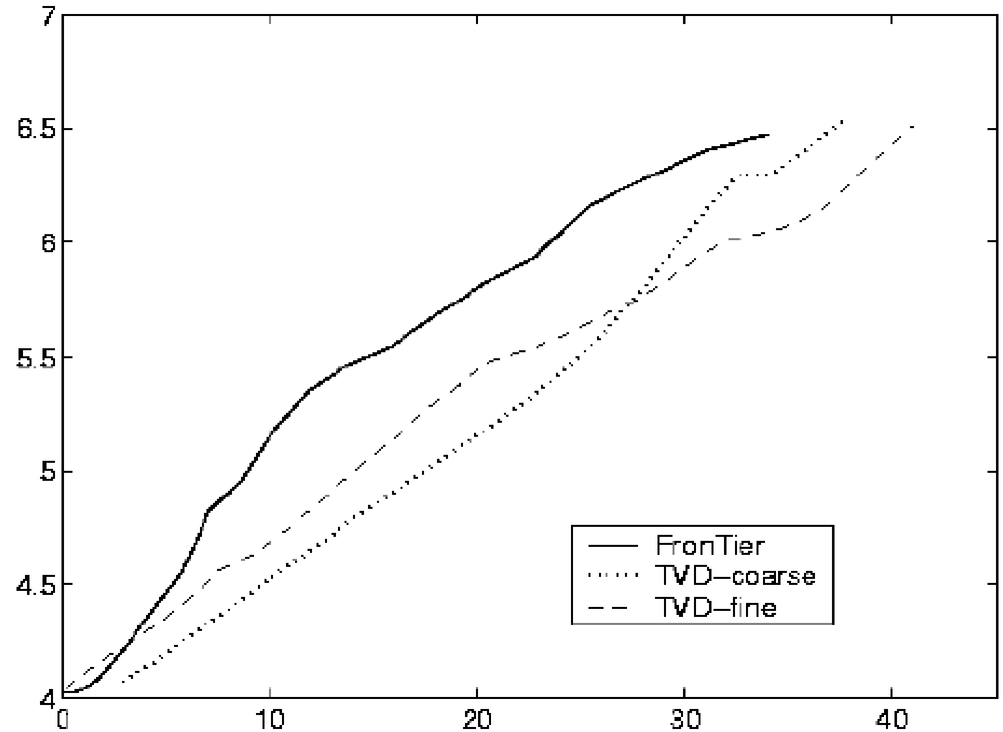
Alphas from theory, experiment, some simulations agree; most simulations disagree



$$Agt^2$$

Z

All alphas agree: theory, experiment, all simulations



$$2\iint gA(s)\,ds\,dt$$

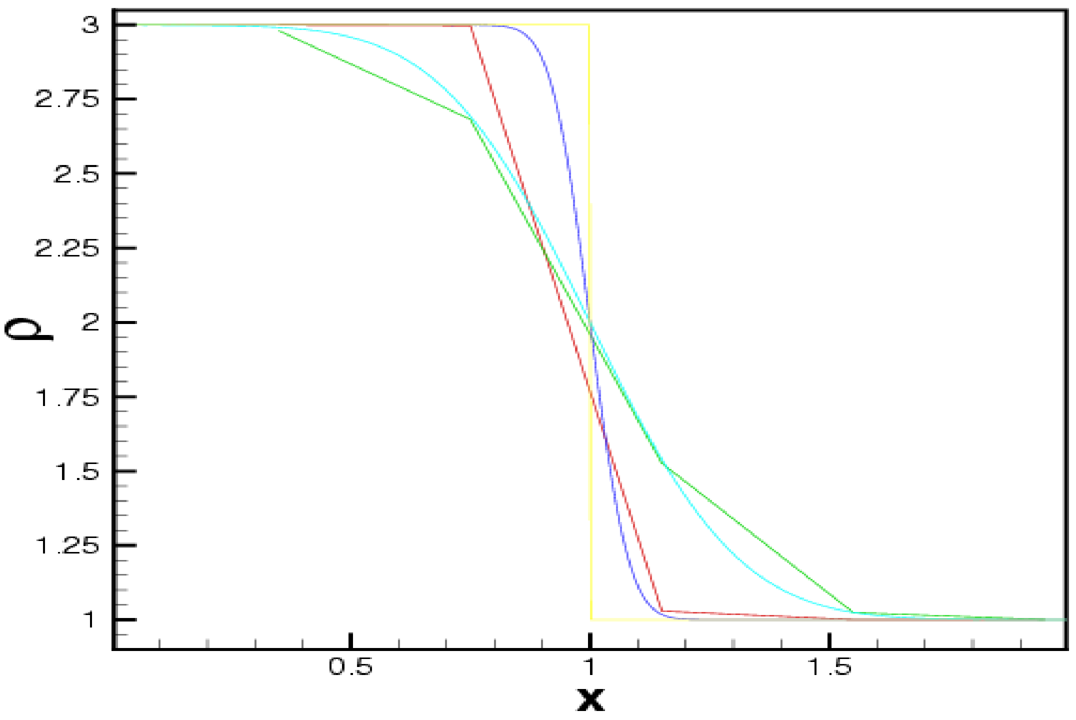
Physical Non-Ideal Effects

- Viscosity, mass diffusion, surface tension
- Compressibility
  - Solution depends on initial temperature stratification; assume isothermal. Initial density depends on height z, so that Atwood number is z dependent.
  - Possible increase of alpha by factor of 2 or more
  - Data interpretation using a time dependent Atwood number restores self similarity, but the mixing rate alpha increases with compressibility.

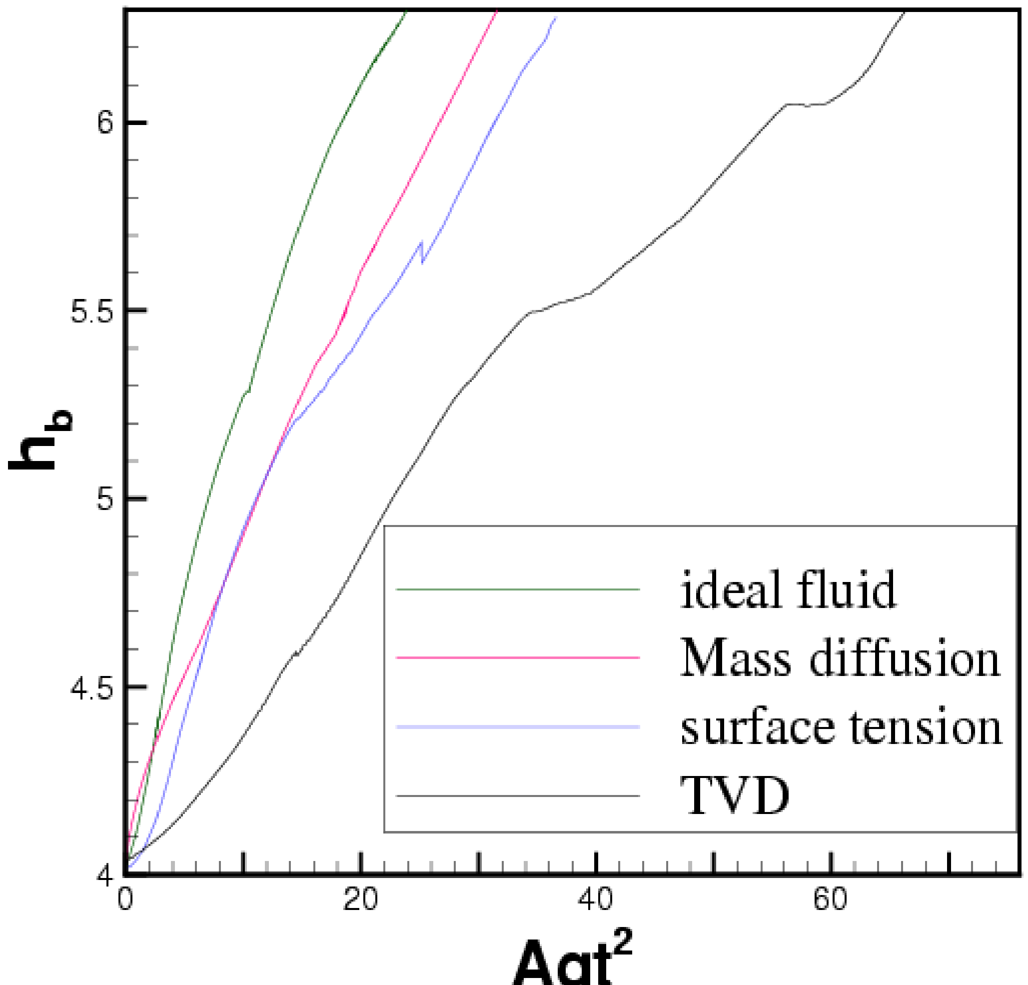
Subgrid model diffusion tracking compared to exact solution

Controlled diffusion (physical, not numerical diffusion).
Water and NaI solution.
Domain = 2 cm (5 cells);
200 and 1000 steps.
t = 10 and 150 ms.
Mixing zone = 0.2 cm and 0.8 cm = 0-2 cells.
Added to 3D code for RT mixing simulations.

Red (simulation) and Blue (exact), 200 steps
Green, two shades (simulation and exact), 1000 steps



Mixing rates h_b = bubble penetration vs. Agt^2. Ideal FronTier (green), surface tension (blue), mass diffusion (red), ideal TVD (purple)



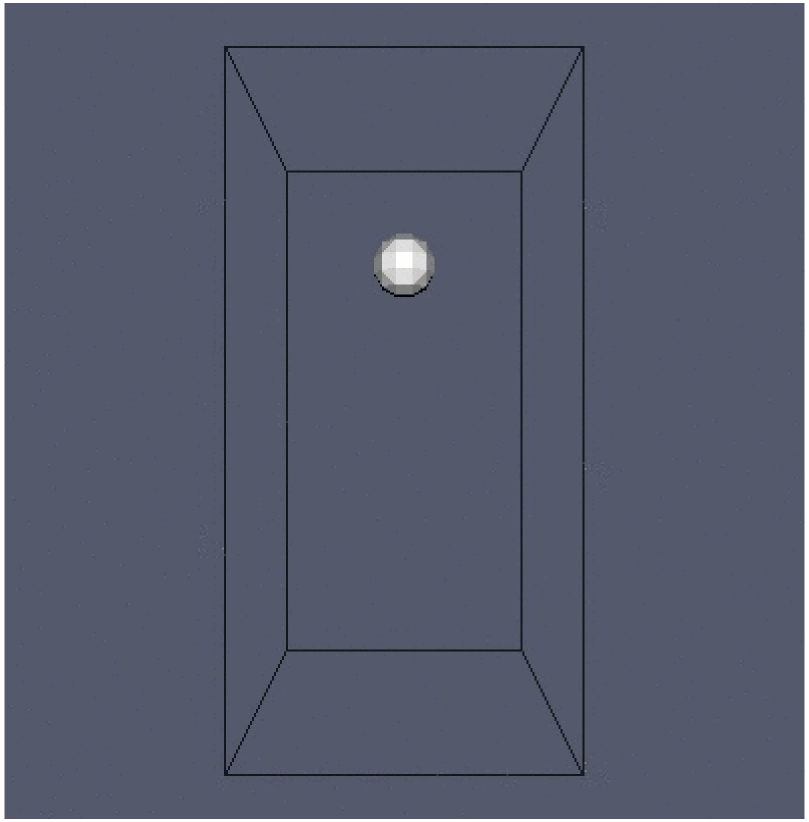
Comparison of Mixing Rates: Comparison, Simulation and Theory

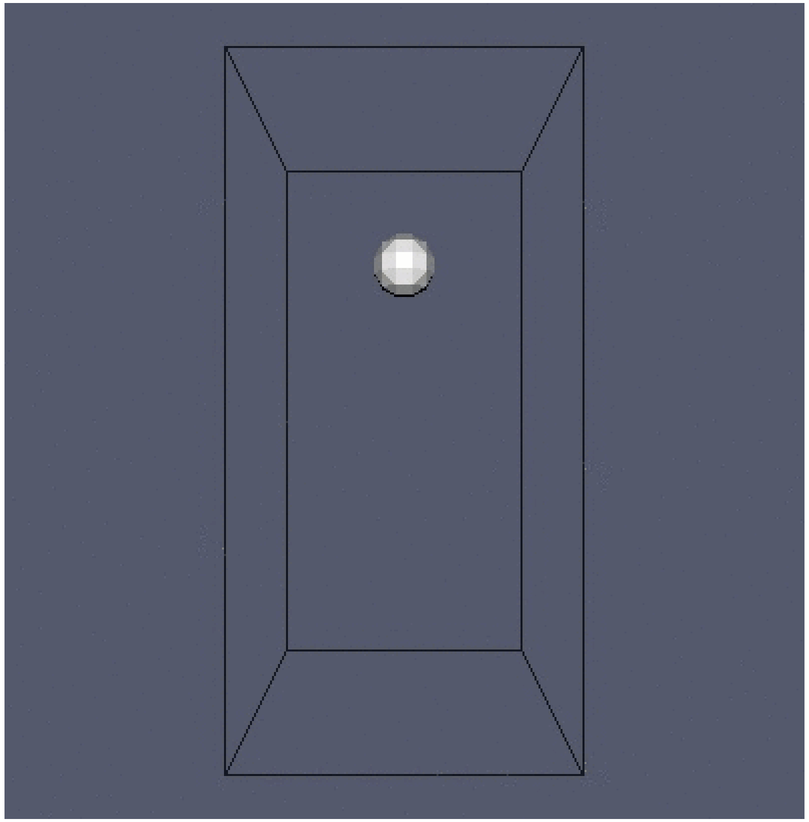
	Theory	Experiment	Simulation
height (alpha)	0.06	0.067	0.062
radius	0.01	0.01	0.01
height fluctuations		0.028	0.034
theta (average mixing rate--miscible)		0.8	0.8

Improved numerics

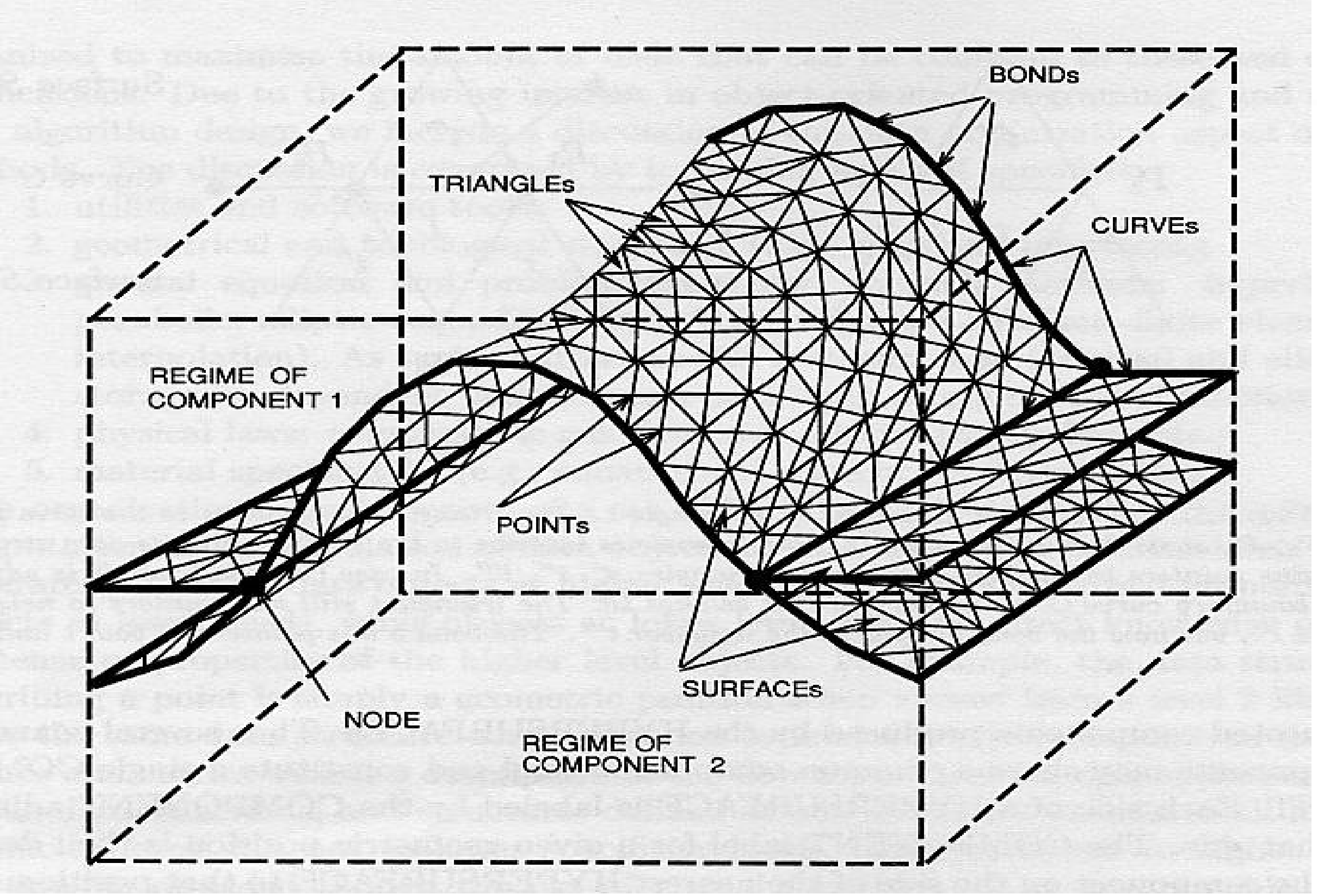
- Chaotic mixing flow is sensitive to numerical artifacts, which generally mimic physical artifacts
  - Mass diffusion, surface tension have both physical and numerical manifestions
  - Solutions appear to be sensitive to size of the physical/numerical mechanisms
  - For predictive simulation in a regime lacking controlled experiments, the only V&V plan is to eliminate the numerical artifacts and introduce the physical mechanisms
  - Front Tracking does both
    - Local grid based tracking: our current improved algorithm
    - Conservative tracking: under development

Fully Conservative Front Tracking: Droplet moving in air at about M = 1, Weber number = 4.71 (left); 471 (right)

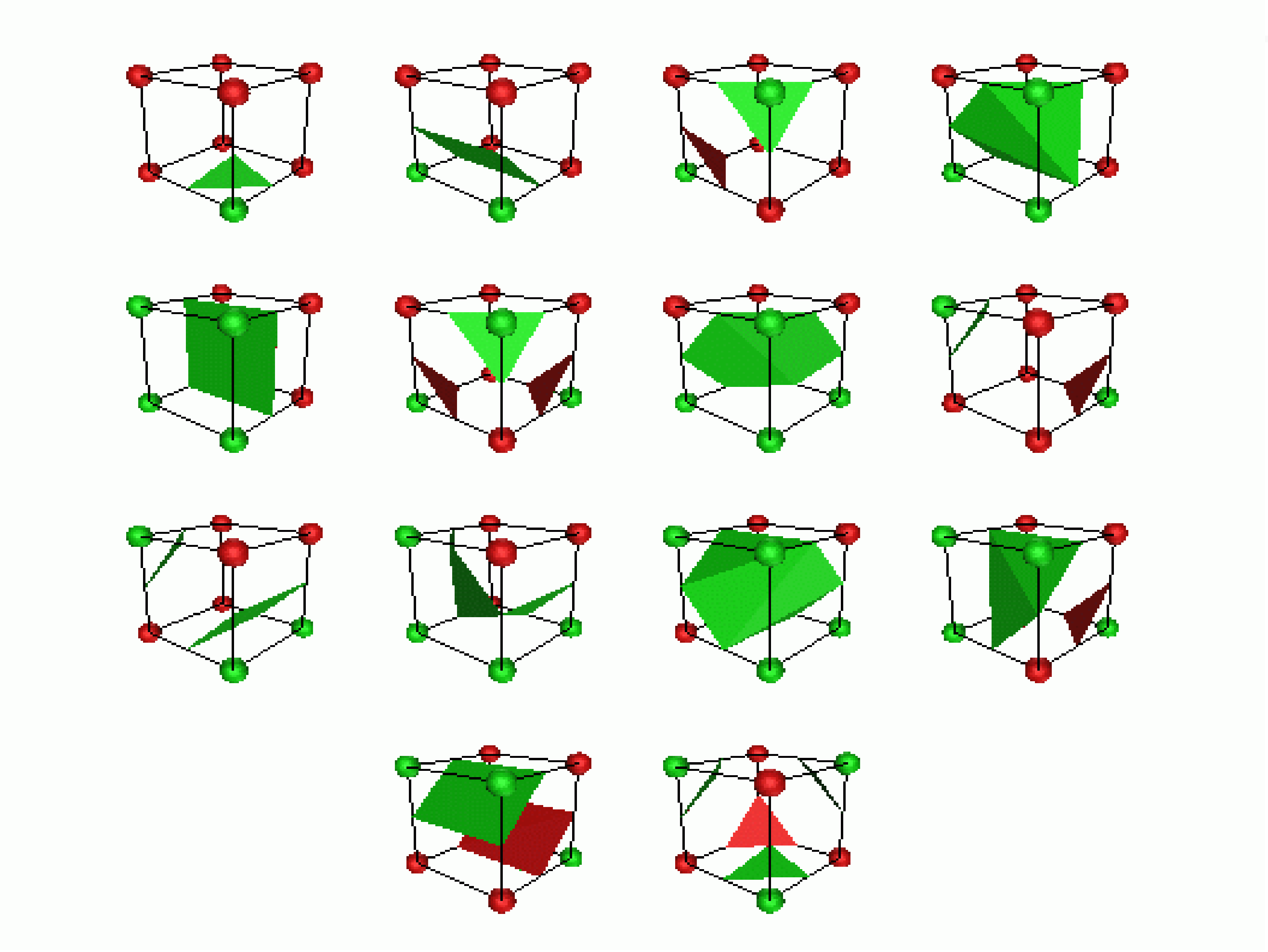




The 3D interface: Grid free



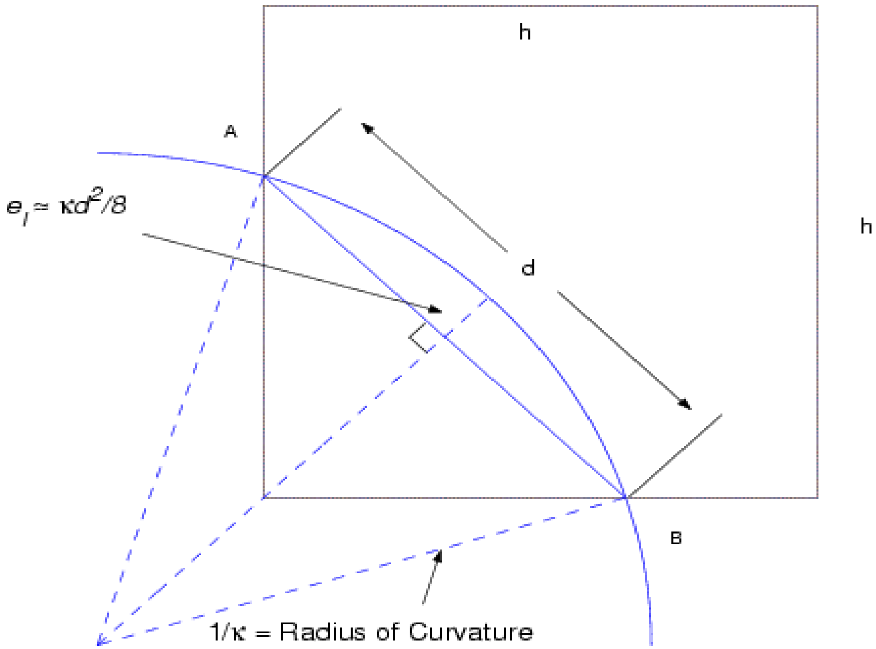
Grid-based interface reconstruction



Local Grid Based Tracking

- Grid Free: Front is lower dimensional manifold. Points move freely through a volume filling grid.
  - Accurate but not robust
- Grid Based: At each time step, front intersections with grid cell edges are determined, and in the interior of each cell the front is determined from these intersections.
  - Robust but not accurate
- Locally Grid Based: Use grid free locally in space/time only were needed to resolve bifurcations.
  - Accurate and robust

Grid based error analysis



$$\text{Error} = O(h^2) \approx \frac{\kappa d^2}{8} \text{ per step}$$

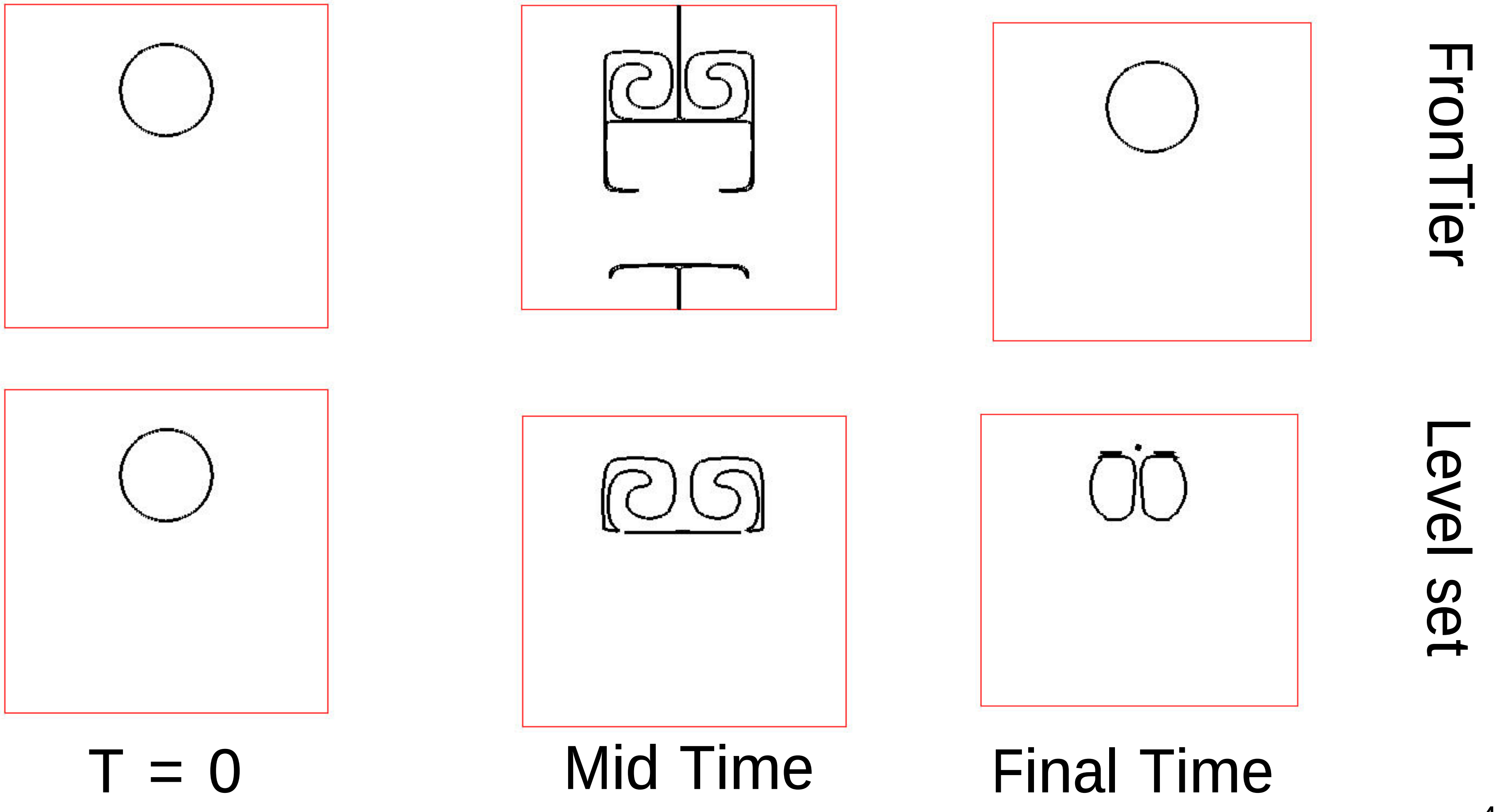
$$\sum \text{Error} \le \frac{h^2 \sum \kappa}{4} = O\left(\frac{h^2}{\Delta t}\right)$$

Error applies to all grid based capturing schemes, to level set methods and to grid based tracking. It is a type of numerical surface tension.

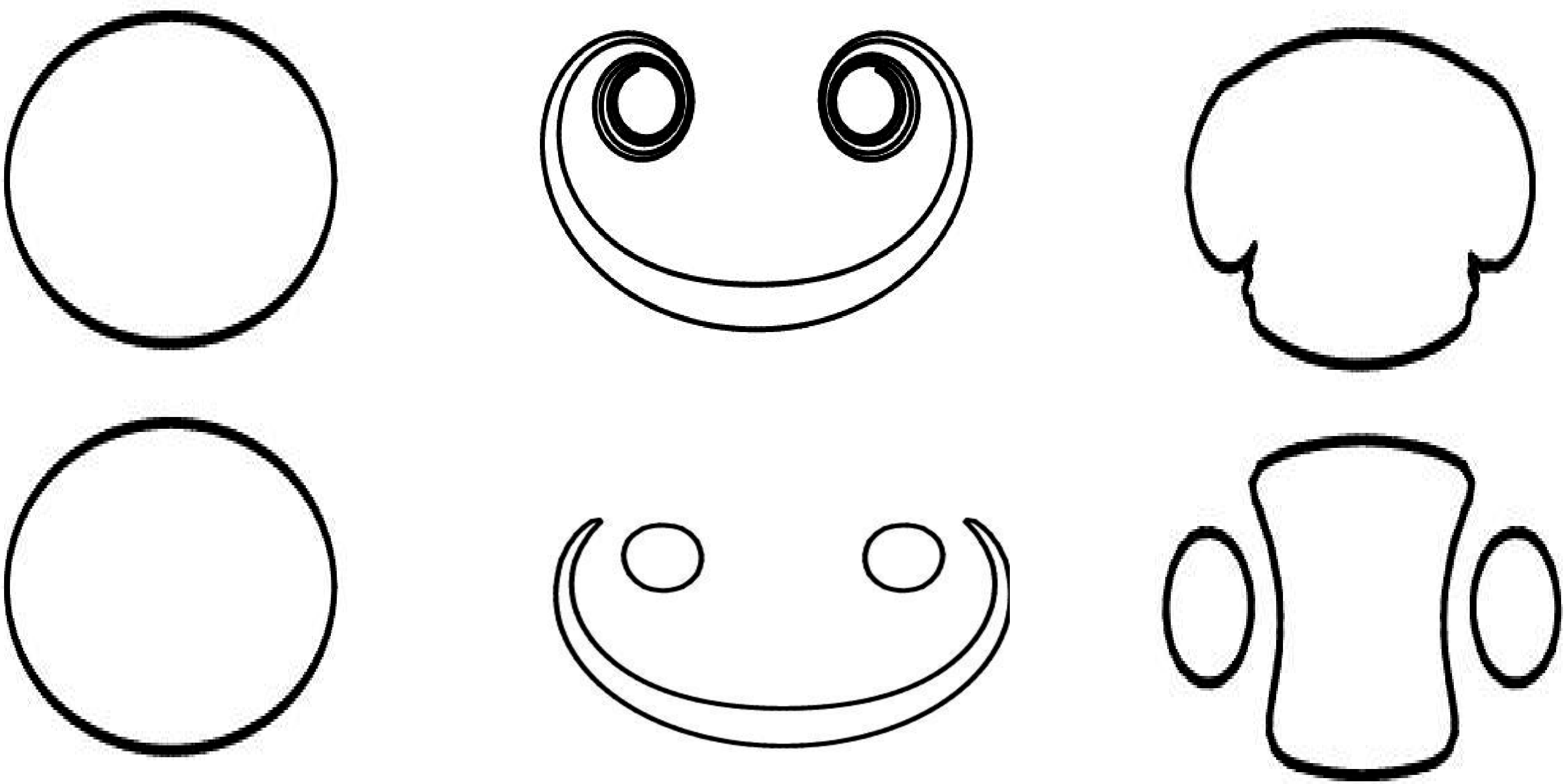
Systematic Comparison of Interface Methods

- Geometrical motion of simple shape in rotating or swirling velocity field and reverse motion back to original shape
  - Untracked methods (capturing) are worst
  - Level set: worst of tracked methods
  - Volume of fluid (SLIC/PLIC) is better
  - Particle methods (MAC) better but expensive and not practical
  - Front tracking is comparable to particle methods in accuracy

FrontTier (above)-Level Set (below) comparison: Multiple vortices and time reversal flow field



Swirling velocity field and reverse FronTier (top) and Level Set (bottom)



FronTier

Level Set

T = 0 Mid Time Final Time

Conclusions for Validation

- Validation has been achieved for a difficult chaotic mixing problem
  - Remaining open issues:
    - Role of initial conditions
    - Systematic study of the role of secondary physics
    - Further mesh refinement and later time, larger ensemble studies
    - Interface length/area and atomic level mixing properties
    - Simulation study comparisons should be extended

V&V for multilevel problems

- Bayesian framework for combining and propagating errors
  - Reduced order models: averaged equations, closure models, subgrid models
  - Probability model for errors of the reduced order models; probability model for experimental errors
    - Compare reduced order models to validated and verified DNS
    - Yields the Bayesian probability for discrepancy between simulation and experiment
      - Discrepancy = log probability of error = input to UQ analysis
      - Can be observed from numerical experiments (and physical ones)

Multilevel V&V

- Bayesian framework and uncertainty quantification
  - Many papers, by ourselves, by others
- Many useful tools from statistics
  - ANOVA, principal components, experimental design, sensitivity analysis (Adifor)
- Closure models and V&V for closure models

Averaged Equations

$$\overline{U_t} + \nabla \overline{F(U)} = 0$$

$$\overline{F(U)} \neq F(\overline{U})$$

$$\overline{F(U)} \approx F_{\text{ren}}(\overline{U})$$

Closure problem: find $F_{\text{ren}}(\overline{U})$

Complete two phase equations

$$\beta_k(z,t) \equiv \left\langle X_k(x,y,z,t) \right\rangle$$

$$\frac{\partial \beta_k}{\partial t} + v^* \frac{\partial \beta_k}{\partial z} = 0$$

$$\frac{\partial\left(\beta_k \rho_k\right)}{\partial t} + \frac{\partial\left(\beta_k \rho_k v_k\right)}{\partial z} = 0$$

$$\frac{\partial\left(\beta_k \rho_k v_k\right)}{\partial t} + \frac{\partial\left(\beta_k \rho_k v_k v_k\right)}{\partial z} = -\frac{\partial \beta_k p_k}{\partial z} + p^* \frac{\partial \beta_k}{\partial z} + \beta_k \rho_k g$$

$$\frac{\partial\left(\beta_k \rho_k E_k\right)}{\partial t} + \frac{\partial\left(\beta_k \rho_k v_k E_k\right)}{\partial z} = -\frac{\partial\left(\beta_k \rho_k v_k\right)}{\partial z} + \left(pv\right)^* \frac{\partial \beta_k}{\partial z}$$

Closure: v*, p*, (pv)*

- v* etc is a convex sum of the v's
- Coefficients are fractional linear in beta's
- Satisfies required conservation of mass, momentum and energy
- Entropy should not be preserved (even for smooth flows) as averaging is not isentropic, but entropy of averaging has a definite sign leading to an entropy inequality

Specification of closure

- Functional form of closure from theoretical analysis of equations

$$v^* = \mu_2^v v_1 + \mu_1^v v_2;\ \text{similar for } p^*$$

$$(pv)^* = p^* v^* + \text{similar multilinear expresion}$$

$$\mu_{\mathrm{j}}^{\mathrm{q}} = \frac{\beta_j}{\beta_j + d_j^q \beta_{j'}};\quad q = v, p, pv$$

- Parameters (d’s) in closure from analysis of DNS data

Closure, continued

- Most d's are insensitive and can be set to 1
- Only d^v is sensitive and only in RT case
  - d^v determined by ratio of mixing zone edge velocities V_1/V_2
  - Velocity ratio determined from buoyancy-drag model with excellent fit to experimental data
- Thus model has no free parameters (after fit to V_1/V_2 coming from validated simulation or from experimental data) or one free parameter without this fit

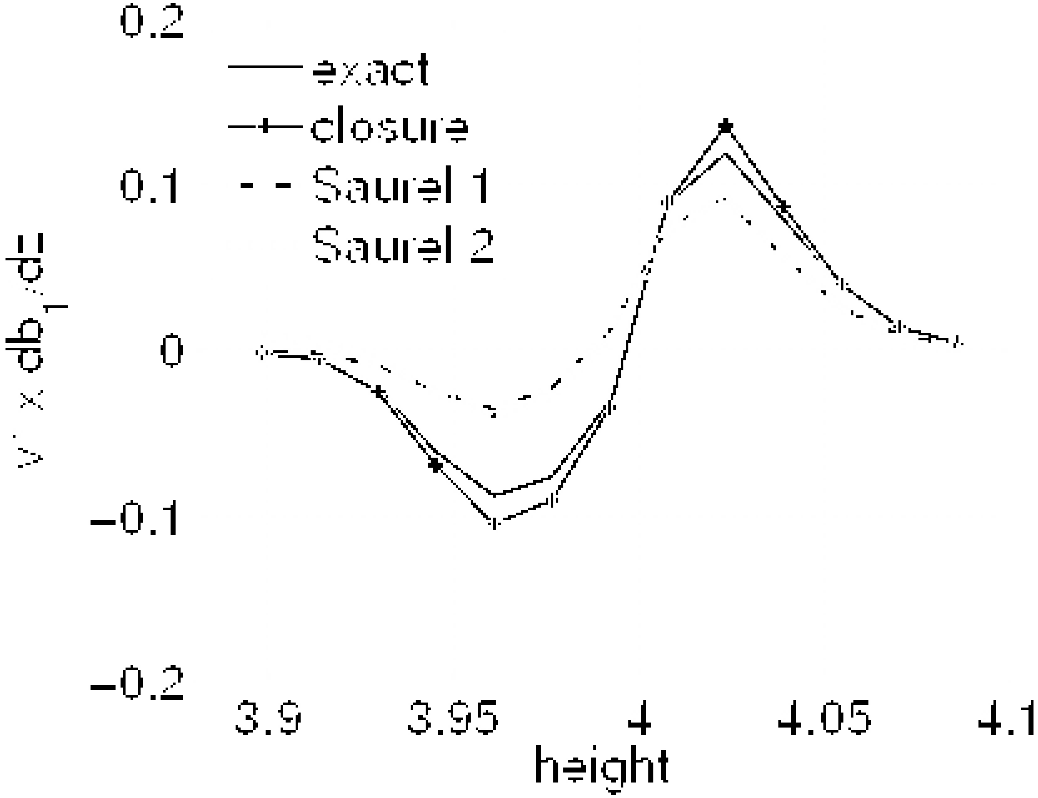
Example: study of v* and (pv)* closure

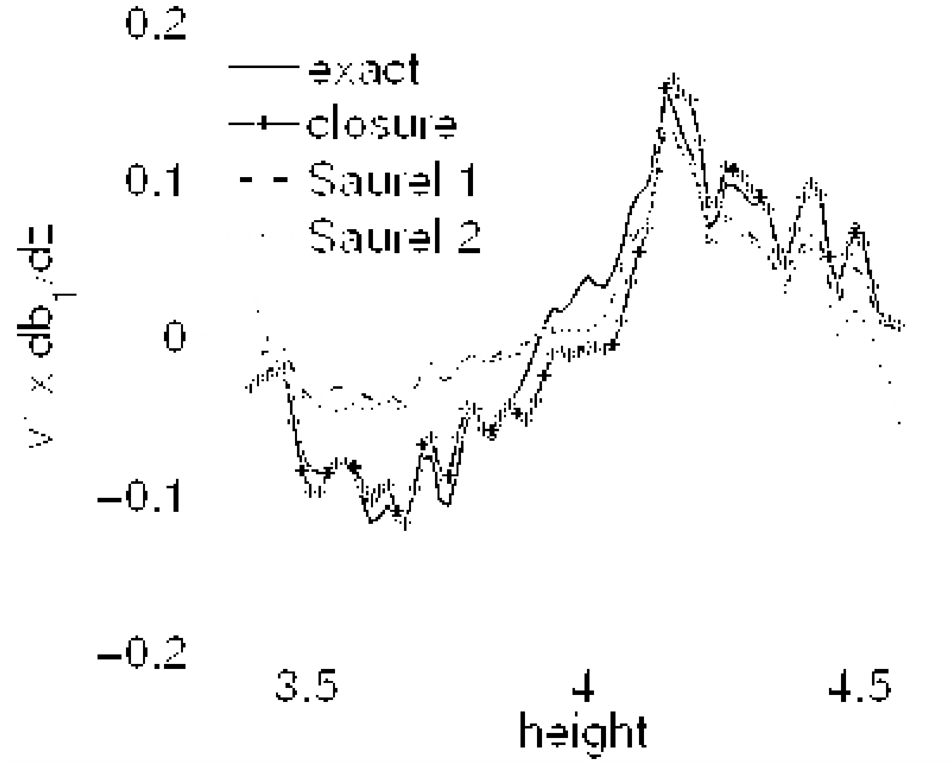
- **Three way comparison for <v_k grad X_k>**
- Direct data analysis from FronTier simulation
  - Simulation validated against laboratory experiments
- $v^* \dfrac{\partial \beta}{\partial z}$ Defined via closure hypothesis
- $v^* \dfrac{\partial \beta}{\partial z}$ Defined via closure hypothesis Following Abgrall-Saurel

Abgrall-Saurel closure

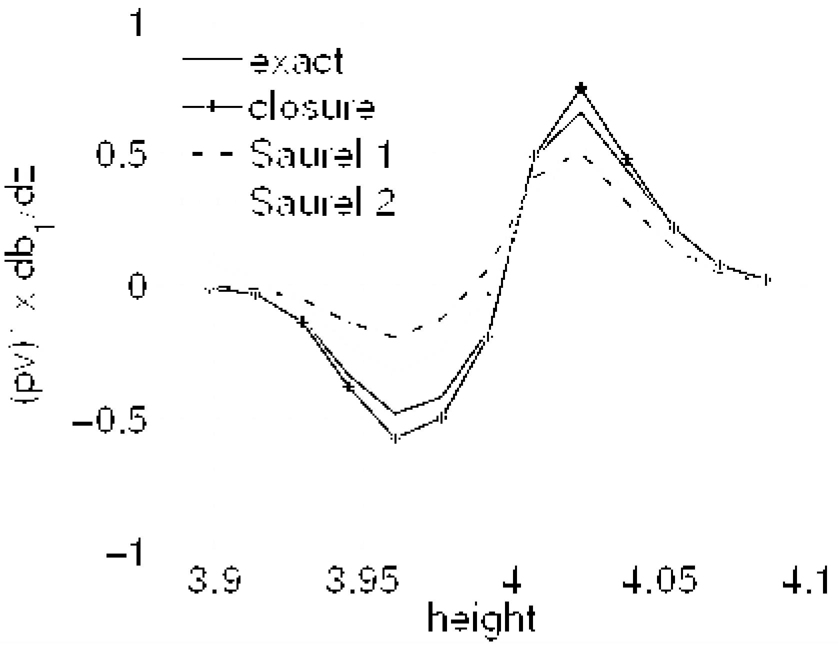
- Similar functional form
- Different definition of d^q
  - Motivated by analysis of model of subgrid physics
- Additional relaxation terms included
- Closure is less accurate than ours in comparison to validated RT and to verified RM data. Relaxation terms make comparison worse

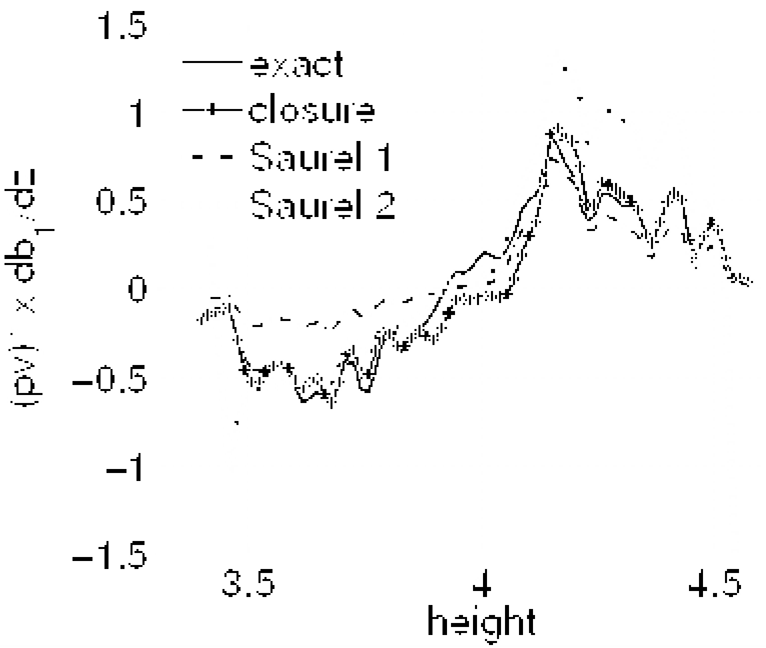
Validation and Comparison of Closures: v* comparison for RT data





(pv)* comparison for RT data Early (t = 4) and late (t = 9) times





Comparison of Closures

- Similar results for RM (circular implosion)
- Average error (v^*, p^*, $(pv)^*$):
  - Our closure: RT: 12%; RM: 9%
  - Saurel et al: RT: 51%; RM: 19%

Conclusions for Multiscale V&V

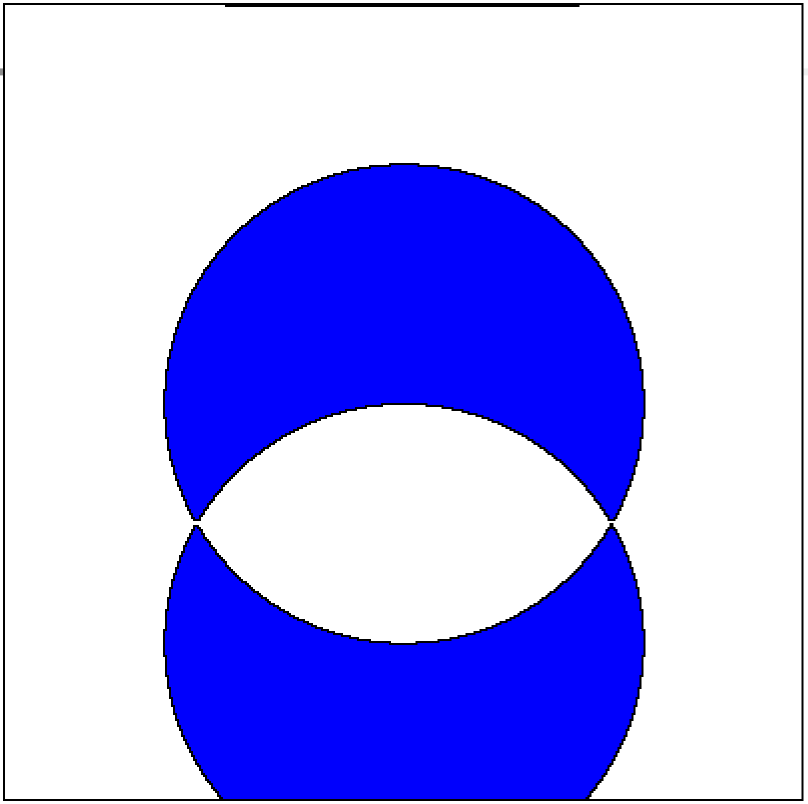
- Key issues:
  - Sparse data for composite or full scale problems
  - Difficulty in resolution and predictive simulations for composite and full scale problems
  - Difficulty in integrating predictions from unit problems to composite and full scale problems
- Reduced order models and closure: Illustrated for turbulent mixing
- Bayesian combination of errors: Frameworks exist

Related studies: FT for chaotic mixing flows, some with V&V

- Break up of diesel jet into spray
- Target studies for Muon Collider
- Pellet injection studies for ITER
- Oil reservoir/groundwater simulation studies

Conclusions: Turbulent mixing

- A framework and partial solution of the V&V problem for turbulent mixing has been presented
- Further work is needed
- Contributions of collaborators and of many colleagues working in this area is acknowledged



Thank You

Smiling Face: FronTier art simulation

Courtesy of Y. H. Zhao