Turbulent Mixing, Transport and Subgrid Models

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Two Phase Turbulent Mixing:
Unstable acceleration driven flow

- Goals of simulations
  - Macro Observable: overall growth rate of mixing region
  - Micro Observable: molecular mixing, for example chemical reaction rate
- Classical cases:
  - Rayleigh-Taylor and Richtmyer-Meshkov
    - Steady and impulsive acceleration
- Simulation challenge:
  - Sensitivity to fine scale details
    - algorithms, physics, initial conditions
  - Problems with experimental validation

Definitions for Turbulent Mixing

- An observable of the flow is
  - **SENSITIVE** if it shows dependence on numerical algorithms and/or on physical modeling (transport).
- **MACRO observables**: eg. of mixing zones
- **MICRO observables**: eg. chemical reaction rates

Explanation

- Macro observables describe the average mixing properties of the large scale flow

- Micro observables describe the atomic level mixing properties

Sensitive and Insensitive Observables

	Macro	Micro
Rayleigh-Taylor Steady acceleration	Sensitive	Sensitive
Richtmyer Meshkov Shock acceleration	Insensitive	Sensitive

RM has a highly unstable interface, in the absence of regularization, diverging as 1/delta x.

This divergent interface length or area causes sensitivity to atomic scale observables.

Chaotic Mixing: A challenge to the standard view

- Solutions are unstable on all length scales
- Under mesh refinement, new structures emerge
  - In this sense there is no convergence
  - Optimistically, we hope that the large scale structures converge and the new small scale ones that emerge under mesh refinement will not influence the large scale ones
  - Correct for insensitive variables only

Failure of the standard view

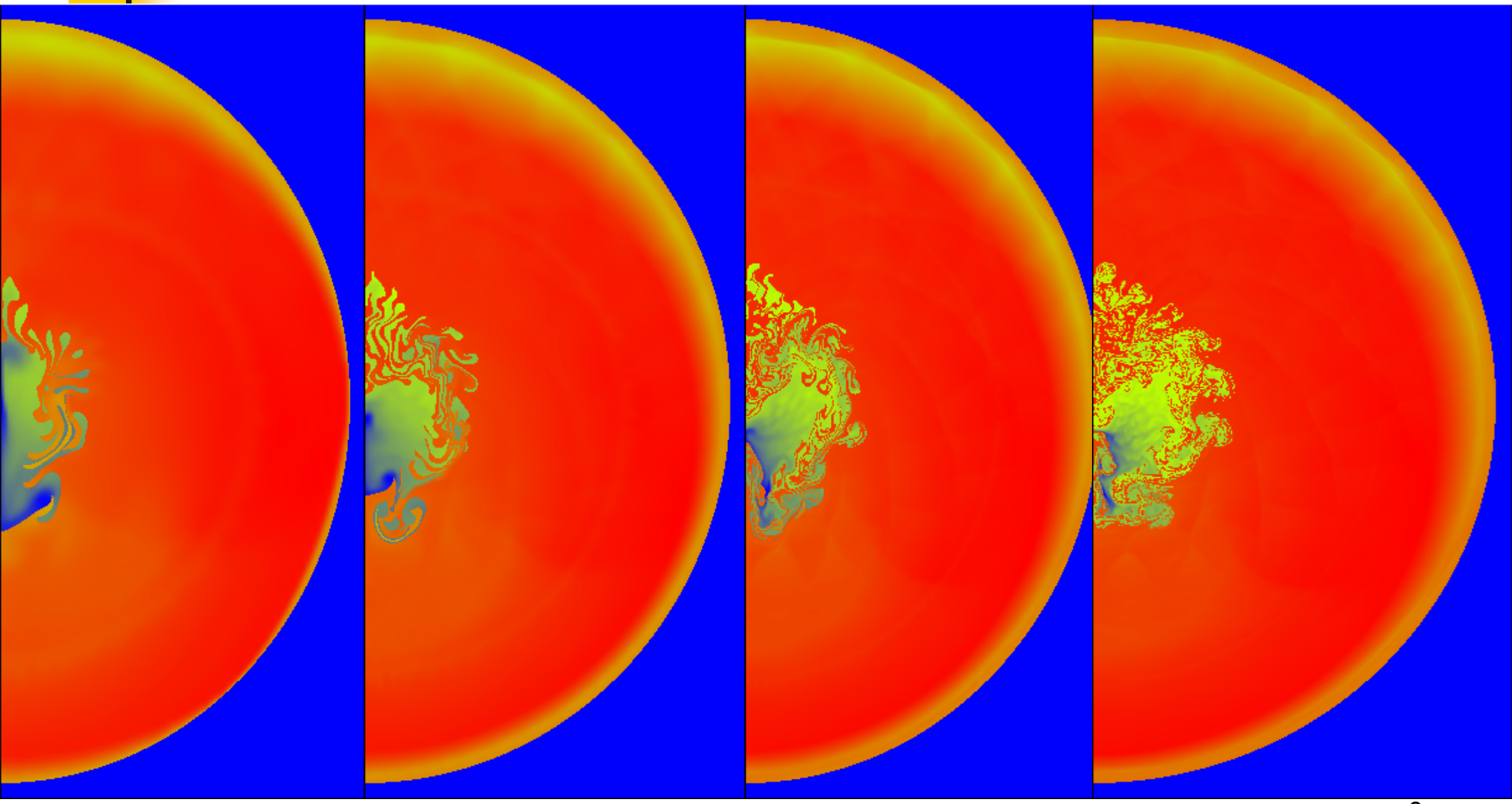
- Turbulent mixing and turbulent combustion
  - Atomic or molecular level mixing requires a new length scale (the molecules)
  - And a change in the laws of physics at these length scales or above.
  - Fluid transport: mass diffusion, viscosity, heat conduction:

$$U_t + \nabla F(U) = \nabla D \nabla U$$

Mesh convergence for RM flow

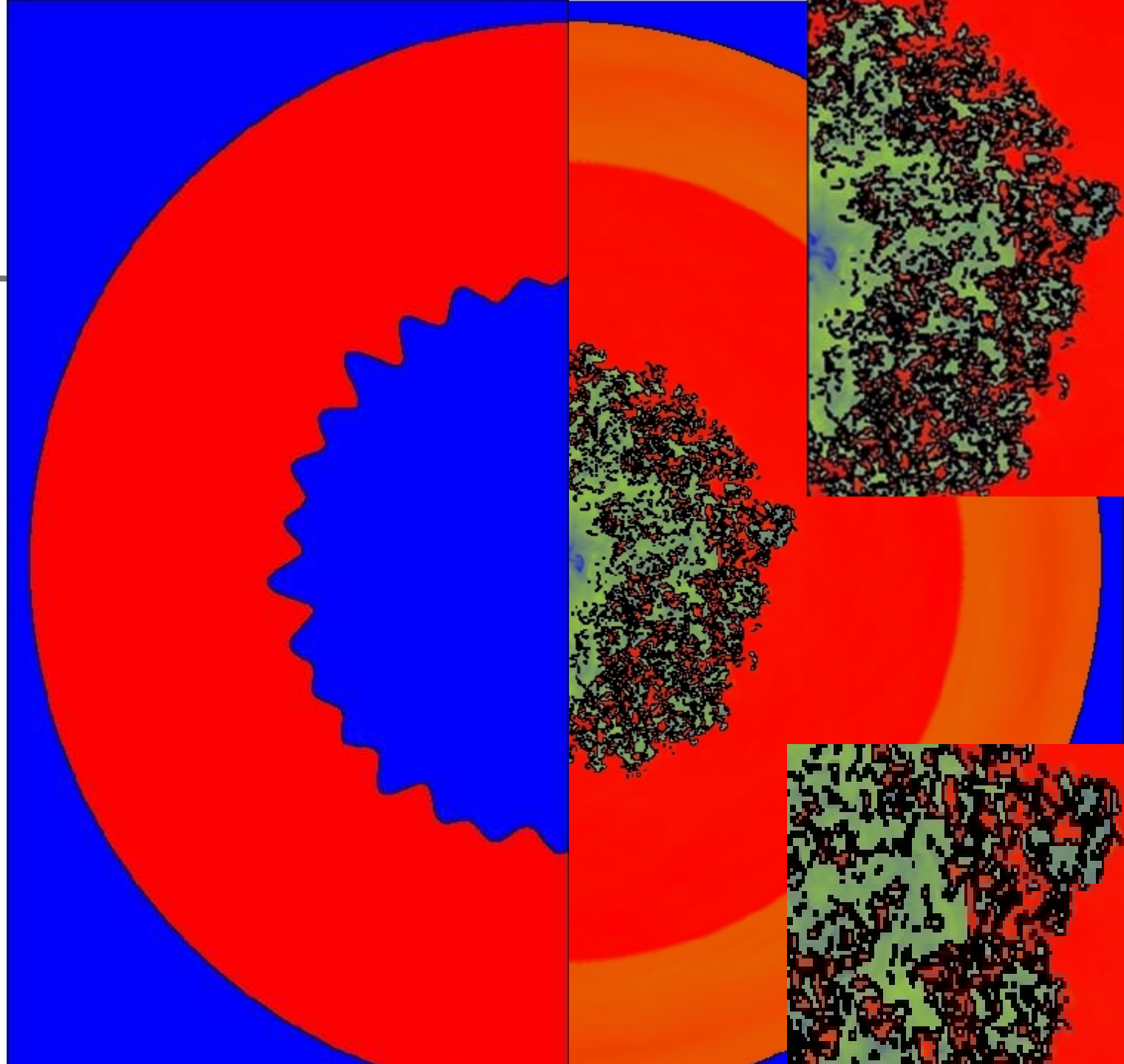
- A circular shock wave moves through a perturbed circular density discontinuity layer, reflects from the origin and moves outward
- Geometry motivated by inertial confinement fusion
- Macro observables converge
- Micro observables converge with physical transport, subgrid scale models and tracking

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

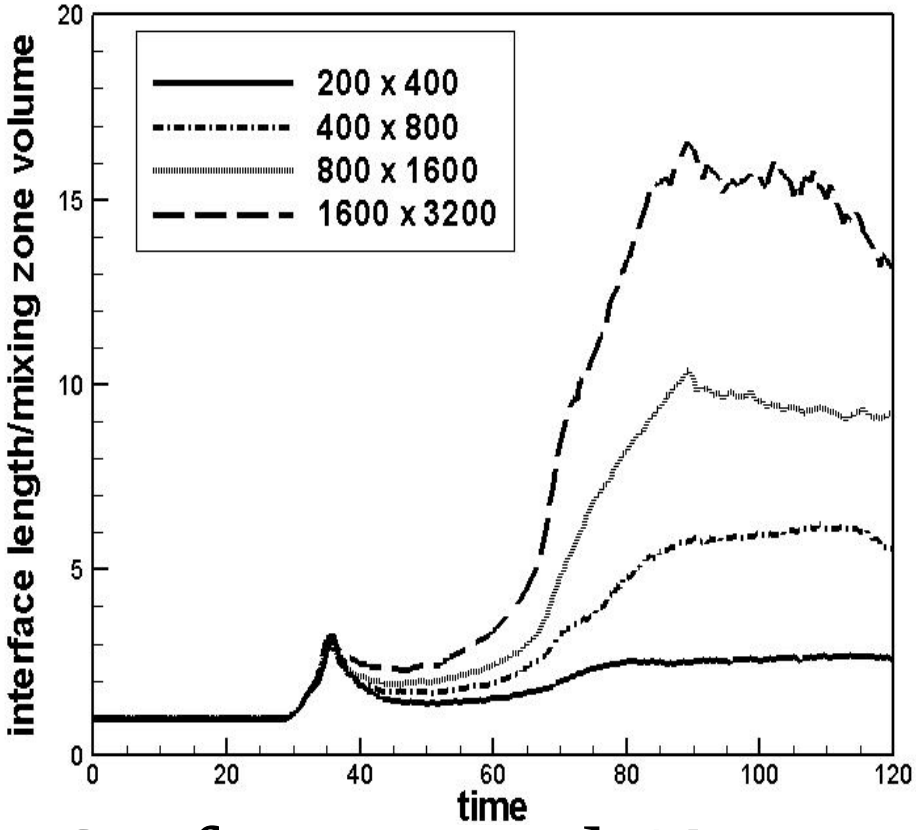


Circular RM instability

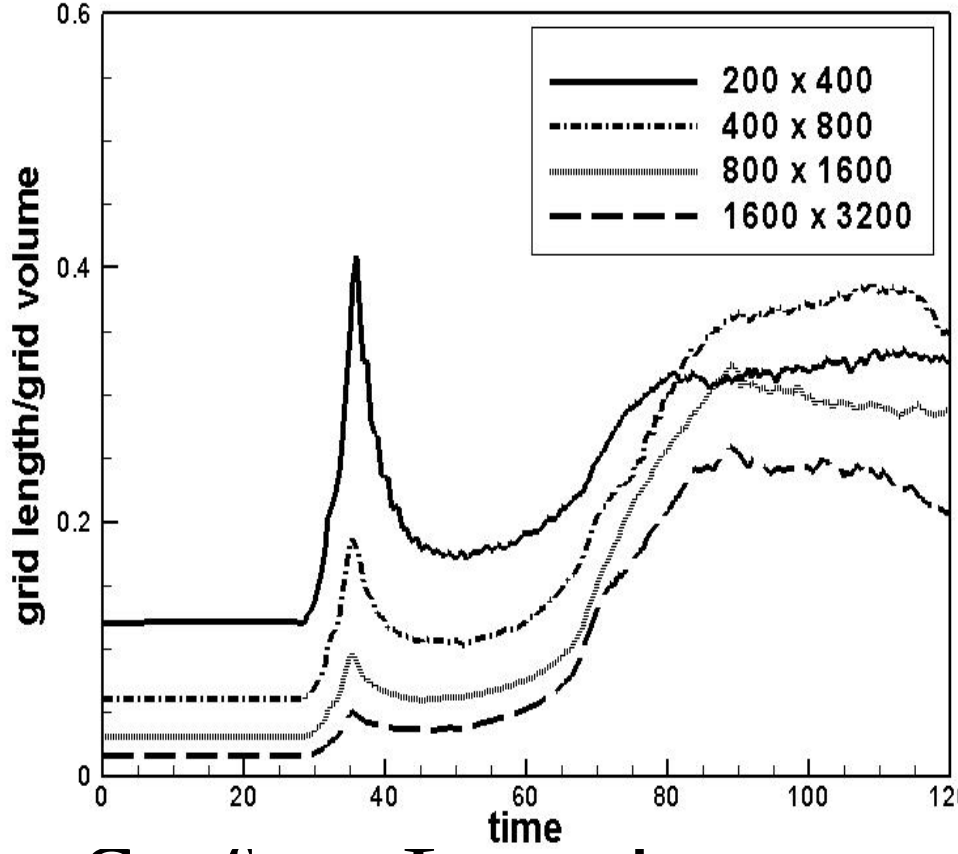
Initial (left) and after reshock (right) density plots. Upper and lower inserts show enlarged details of flow.



Chaotic dependence of interface length on mesh: Unregularized simulation



Surface Length/Area vs. time



$$\frac{\text{Surface Length}}{\text{Area}} \times \Delta x$$

Simplistic Error Analysis for Micro Observables in Chaotic Flow

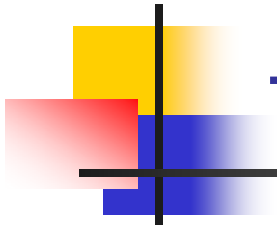
$$ERROR = C_1 \times \Delta x \times \text{Interface length (area)}$$

$$\text{Interface length (area)} = C_2 \times \Delta x^{-1}$$

$$ERROR = C_1 \times \Delta x \times C_2 \times \Delta x^{-1} = C_1 C_2 = O(1)$$

Error as results from numerical or physical modeling, e.g. numerical mass diffusion or ideal vs. physical transport coefficients

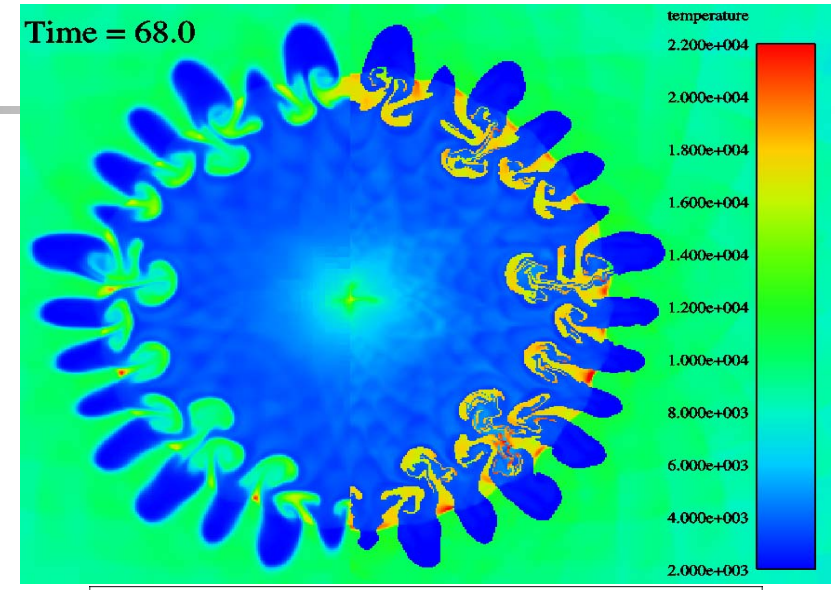
Comparison of FronTier and RAGE for 2D RM instability

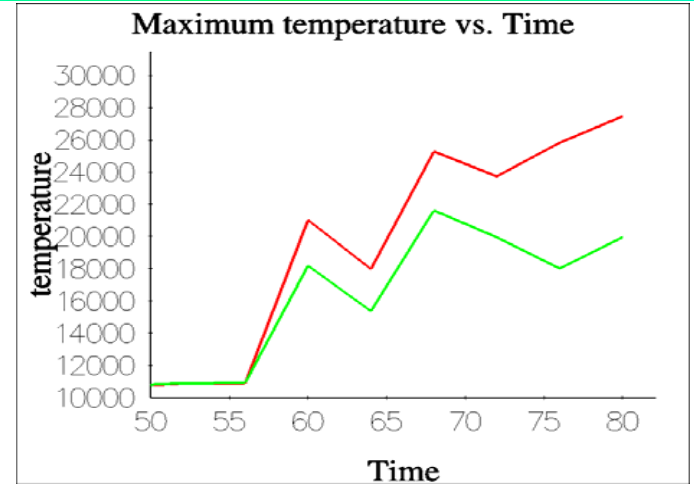


- T. Masser:
  - Macro variables not sensitive
  - Micro: Temperature is sensitive
- Stony Brook:
  - Macro variables: not sensitive
  - Interface length divergent
  - Micro: Mixture concentrations sensitive

Code comparison shows sensitivity for temperature: Difference of 50%

- Computation and analysis of T. Masser and J. Grove:
- 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.
- Mechanism responsible:
  - Thermal and Mass diffusion at the interface in RAGE.
- After reshock FronTier continues to have a significantly higher maximum temperature.
- Study led to upgrade for RAGE.





Rayleigh-Taylor Instabilities

- Alpha characterizes overall instability growth rate:

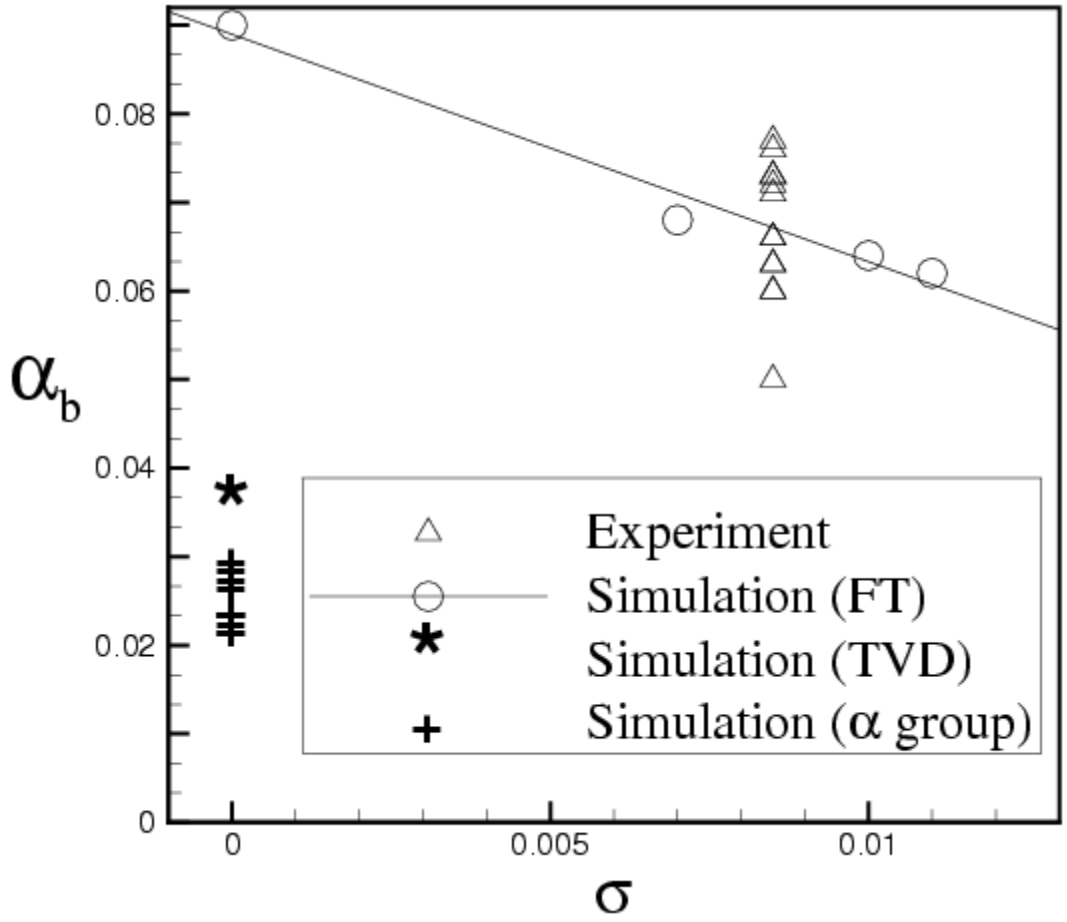
$$h_b = \alpha A g t^2$$

- Alpha is a sensitive variable
- Experiment: alpha = 0.055-0.07
- Simulation: three groups agree
  - Front Tracking: control numerical mass diffusion
  - Adler et al (particle methods):
  - Mueschke-Andrews-Schilling: control initial conditions
- Others disagree, with each other and with experiment, by factors of 1.5-3.

Comments on Role of Initial Conditions

- Andrews et al experiments:
  - Long wave length noise at about 75% of main (random high wave number) initial perturbation
- Youngs et al experiments:
  - Long wave length perturbations probably less than 10% of high wave number initial perturbation
  - Exceptions noted, with perhaps 20% strength
    - Even in these cases, alpha change is modest (10%)
- Conclusion:
  - Initial conditions only one piece of puzzle
  - Transport and surface tension another

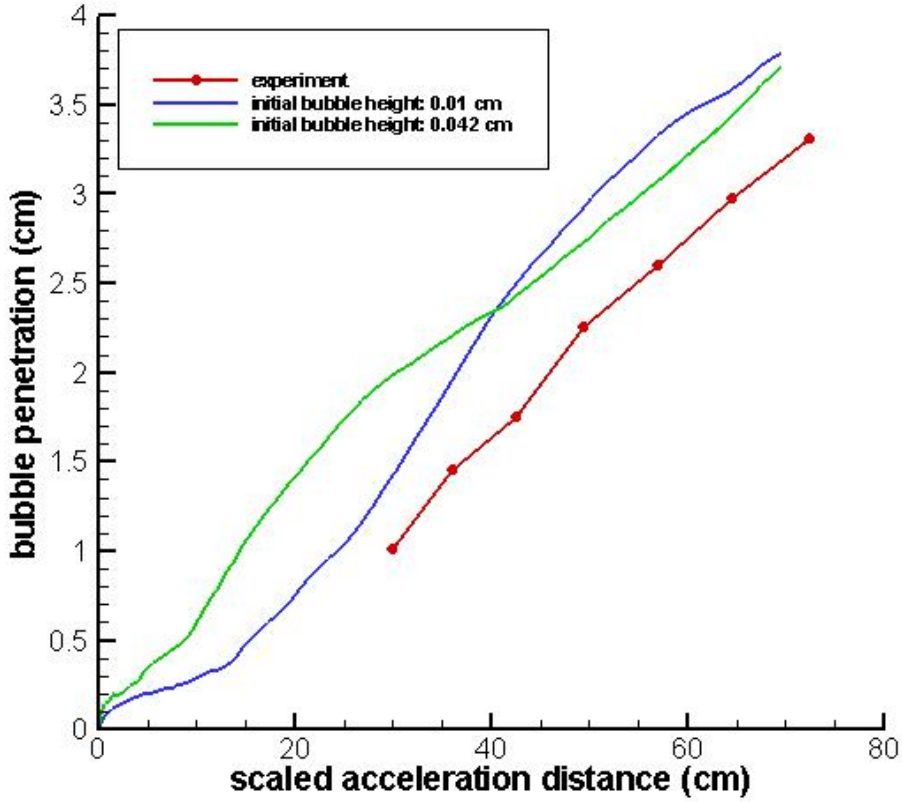
Comparison of simulations and experiment (Validation): For Rayleigh-Taylor unstable mixing



$\alpha =$ growth rate for mixing zone

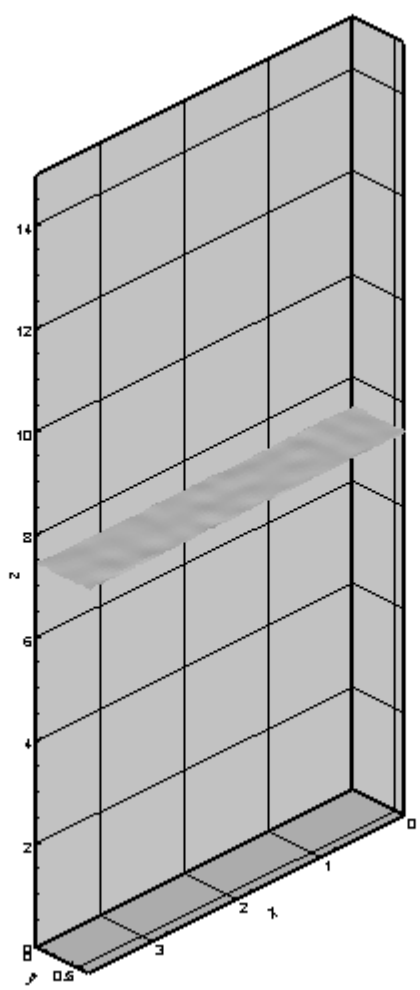
$\sigma =$ dimensionless surface tension

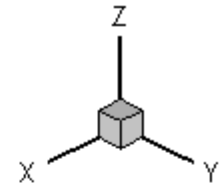
Simulation vs. Experiment
Miscible RT: Burrows, Smeeton, Youngs



Alpha = 0.061 (sim.) vs. 0.062 (exp.). Miscible RT with initial diffusion layer, mass diffusion and viscosity

12x2 modes, 8 cells/mode


14
12
10
8
Z
6
4
2
0
0.5
3
2
1
0


Z
X
Y

Molecular Scale Mixing Properties

- Molecular scale mixing properties are sensitive to physical modeling and to numerical methods unless fully resolved (direct numerical simulation = DNS)
- Correct simulation:
  - Use sub grid models (large eddy simulation = LES)
    - LES modify equations to compensate for physics occurring on small scales (below the grid size) but not present in the computation
  - Control numerical mass diffusion: use front tracking

Combine two classes of methods

- Capturing likes steep gradients, rapid time scales
  - Tracking is an extreme version of this idea
  - Often, no subgrid model and so not physically accurate for under resolved (LES) simulations
- Turbulence models like smooth solutions, slow time scales with significant levels of physical mass diffusion
  - Often, too many zones to transit through a concentration gradient
- Best of two ideas combined

Subgrid models for turbulence, etc.

- Typical equations have the form $U_t + \nabla F(U) = \varepsilon \Delta U$
- Averaged equations:

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

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

$$\overline{F(U)} \approx F(\overline{U}) + F_{SGS}(\overline{U})$$

F_{SGS} is the subgrid scale model and corrects for grid errors

Subgrid models for turbulent flow

$$F_{SGS}\left(\overline{U}\right) \equiv F\left(\overline{U}\right) - \overline{F\left(U\right)}$$

$$\overline{U}_t + F\left(\overline{U}\right) = \varepsilon\Delta U + \nabla F_{SGS}\left(\overline{U}\right)$$

$$F_{SGS}\left(\overline{U}\right) \approx \varepsilon_{\text{turbulent}} \nabla\overline{U} \quad \text{(key modeling step)}$$

$$\overline{U}_t + F\left(\overline{U}\right) = \left(\varepsilon + \varepsilon_{\text{turbulent}}\right)\Delta\overline{U}$$

Subgrid Scale Models (Moin et al.)

- No free (adjustable) parameters in the SGS terms
- Parameters are found dynamically from the simulation itself
- After computing at level Delta x, average solution onto coarser mesh. On coarse mesh, the SGS terms are computed two ways:
  - Directly as on the fine mesh with a formula
  - Indirectly, by averaging the closure terms onto the coarse grid.
  - Identity of two determinations for SGS terms becomes an equation for the coefficient, otherwise missing.
  - Assume: coefficient has a known relation to delta x and otherwise is determined by an asymptotic coefficient. Thus on a fine LES grid the coefficient is known by above algorithm.

Chemical reaction rate
No subgrid model

$$w = f_1 f_2 e^{T/T_{AC}}$$

T_{AC} = Activation Temperature

f_i = mass fraction of species i

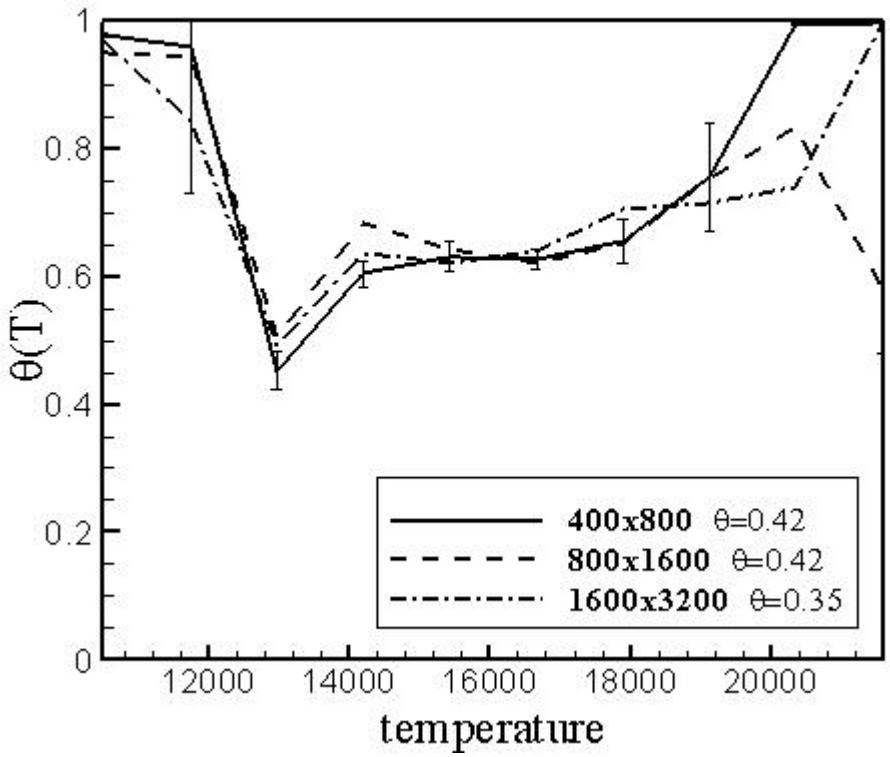
$$\theta_T = \frac{< f_1 f_2 >_T}{< f_1 >_T < f_2 >_T}; < \cdots >_T \text{ defined at fixed } T$$

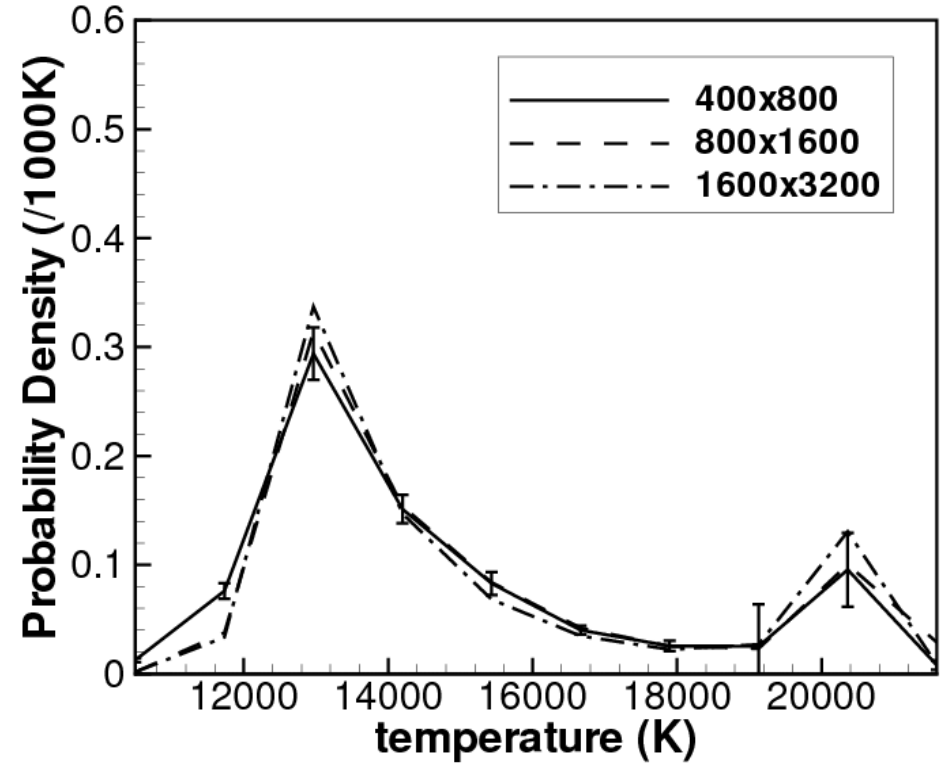
$d\nu(T)$ = probability distribution for T

$$< w >_T = < f_1 >_T < f_2 >_T \theta_T e^{T/T_{AC}} d\nu(T) = \text{ reaction rate}$$

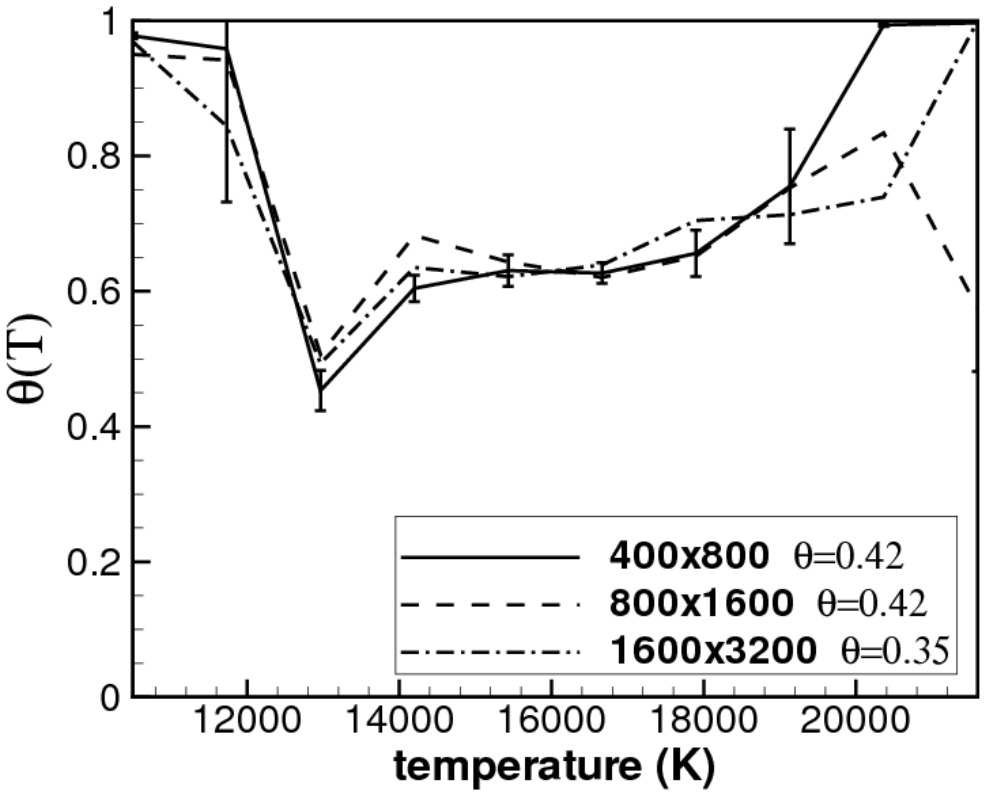
Re = 300. Theta(T) vs. T (left); Pdf for T (right)

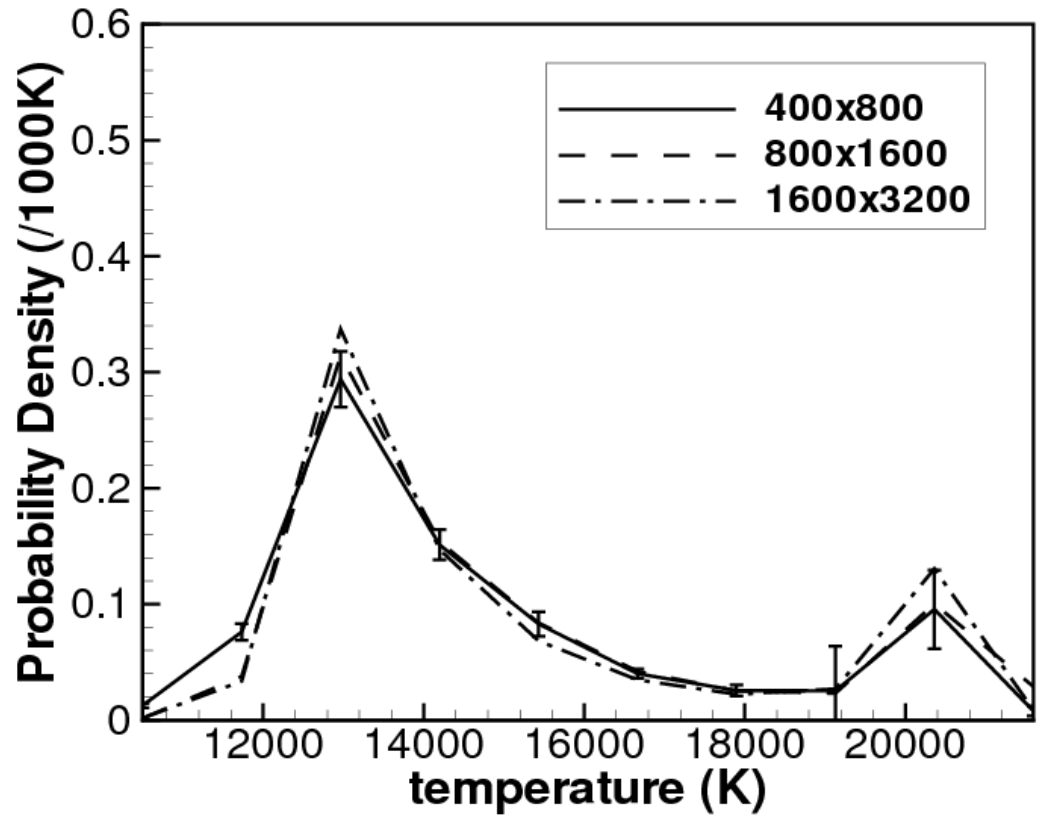
$$\theta = \frac{< f_1 f_2 >}{< f_1 >< f_2 >}$$



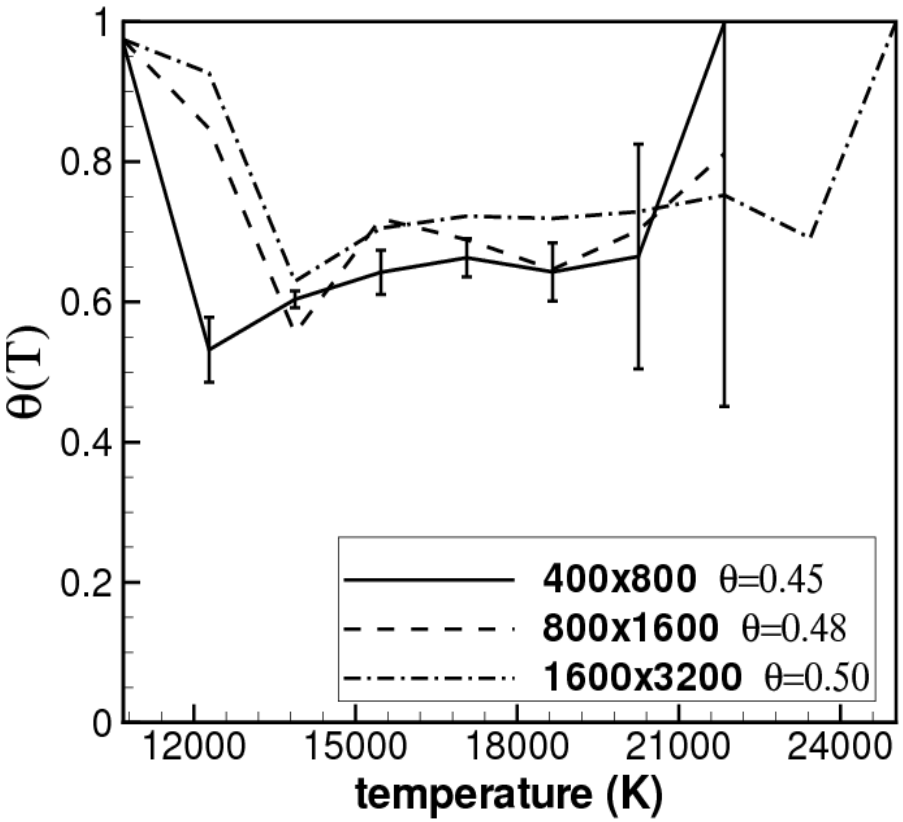


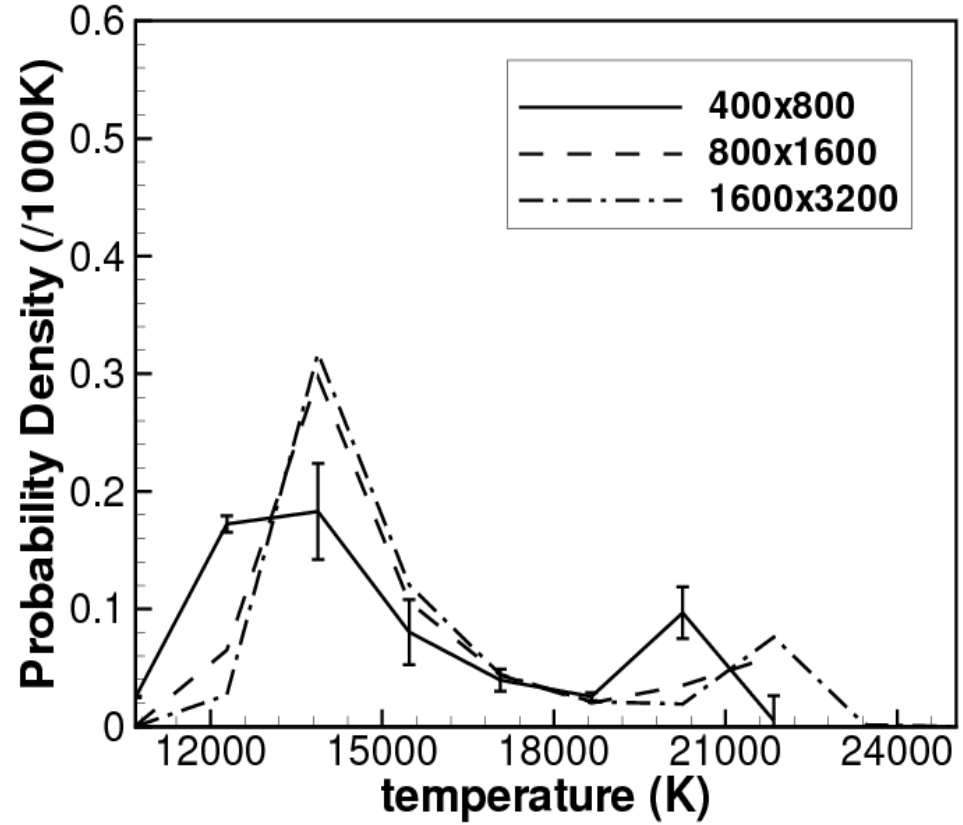
Re = 3000. Theta(T) vs. T (left); Pdf for T (right)





Re = 300k. Theta(T) vs. T (left); Pdf for T (right)





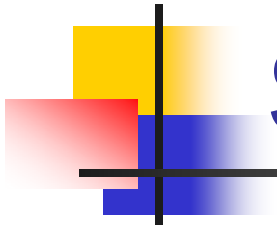
Convergence properties for reaction rate pdf for $w = \text{const.}\, f_1 f_2 \exp(T/T_{AC})$

Relative errors for pdf for reaction rate w, compare coarse to fine, medium to fine and relative fluctuations in coarse grid			
Re	c to f	m to f	fluct. c
300	0.48	0.23	0.24
3K	0.33	0.28	0.49
300K	0.31	0.15	0.25

Conclusion: numerical convergence of chemical reaction rates, using LES SGS models for high Schmidt number flows

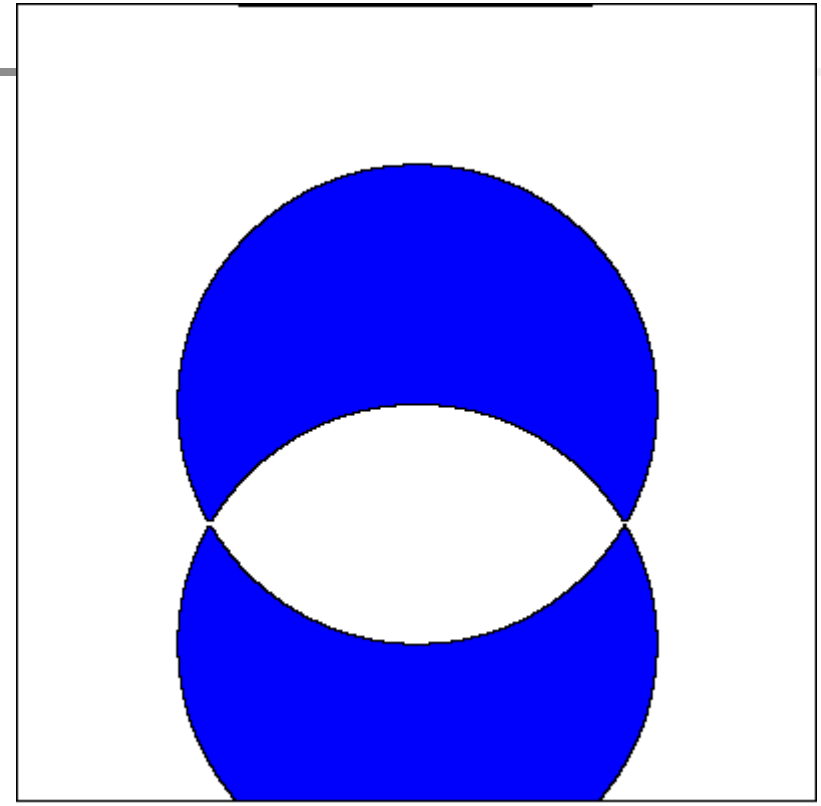
Convergence of w pdf

- Not just mean converges
- Moments to all order, ie full distribution converges



Summary

- Molecular level and even macro observables
  - Challenge to computational science
- Proposed resolution
  - Front tracking
    - Control numerical transport
  - Subgrid scale models
    - Convergent LES simulations
- Comparison of transport vs initial conditions



Thank You

Smiling Face: FronTier art simulation
Courtesy of Y. H. Zhao