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ALE Simulations of Turbulent Rayleigh-Taylor Instability in 2-D and 3-D

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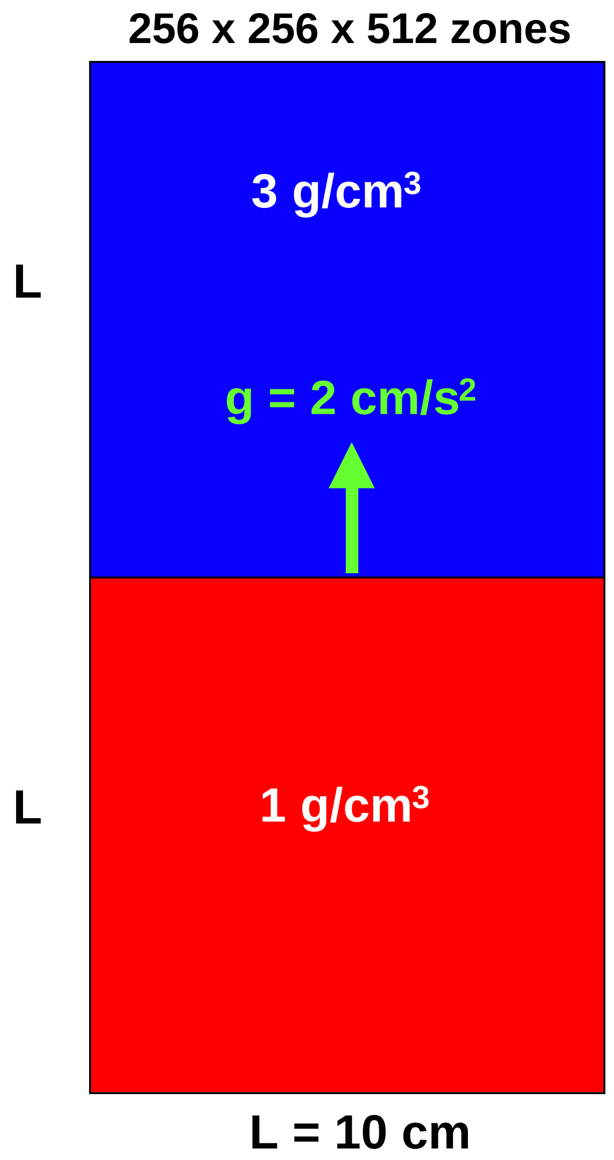
We have simulated the "α - group" turbulent Rayleigh-Taylor problem in 2-D and 3-D with the ALE code, Hydra

- Weakly compressible RT with a random initial surface spectrum restricted to short wavelength modes (4-8 zones/λ)
- Hydra is a 3-D parallel ALE code with interface reconstruction
- Zoning convergence is suspect
  - Simulated linear growth rates for the seed modes are as low as 15% of the correct classical value
  - In 3-D, modes with *k* aligned with the mesh grow faster than others
- We use a initial surface comprised of cosine modes to avoid aliasing due to reflection span-wise boundary conditions
- 2-D simulations show weak dependence on zoning up to 1024$\times$2048
- 3-D simulations with interface reconstruction predict $\alpha_b \sim 0.03$-0.055, $\alpha_s \sim 0.06$
- Simulations without interface reconstruction show only slightly lower penetration but much more small-scale mixing

Initial configuration & adiabatic equilibrium

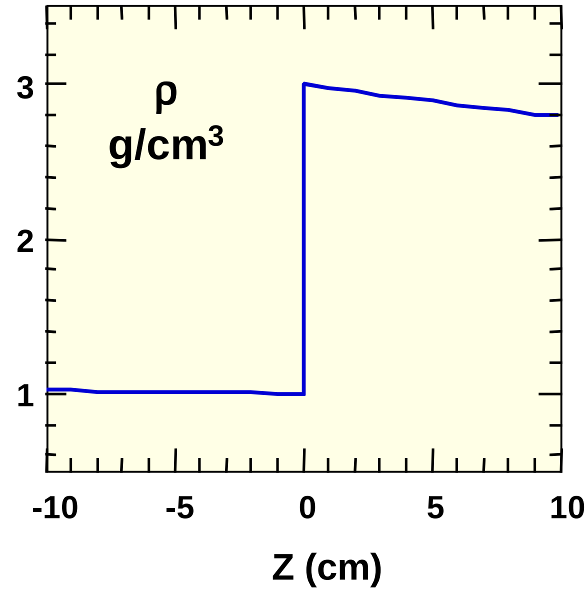


$$\frac{dP}{dz} = -\rho g$$

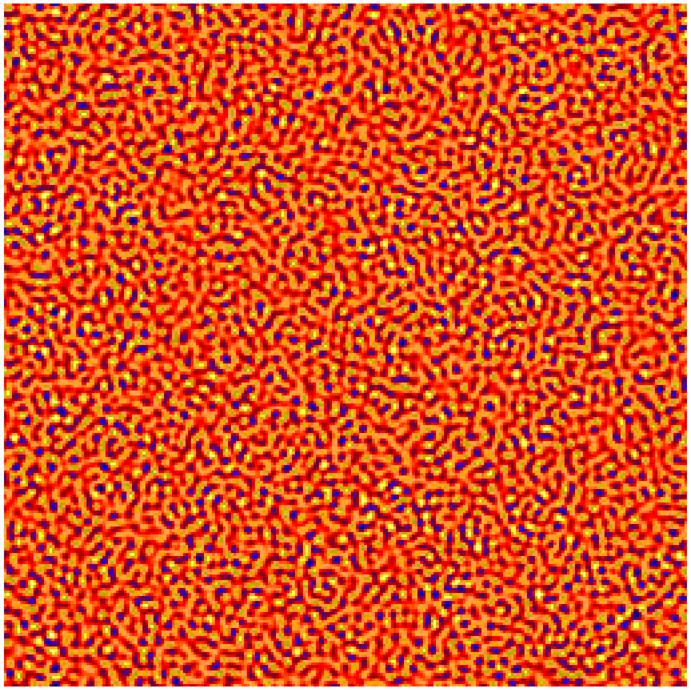
$$P = P_o\left(\frac{\rho}{\rho_o}\right)^{\gamma}$$

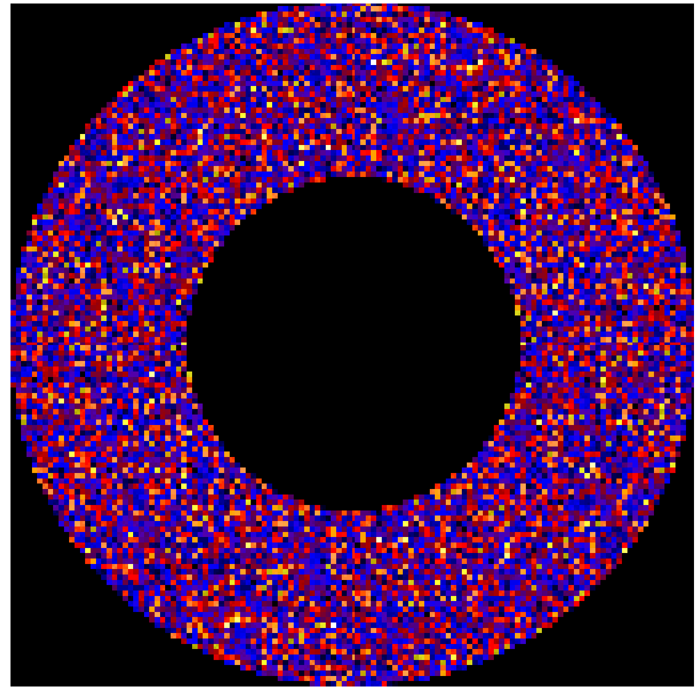
$$\rho = \rho_o\left(1 - \frac{\gamma - 1}{\gamma}\frac{\rho_o g z}{P_o}\right)^{\frac{1}{\gamma - 1}}$$

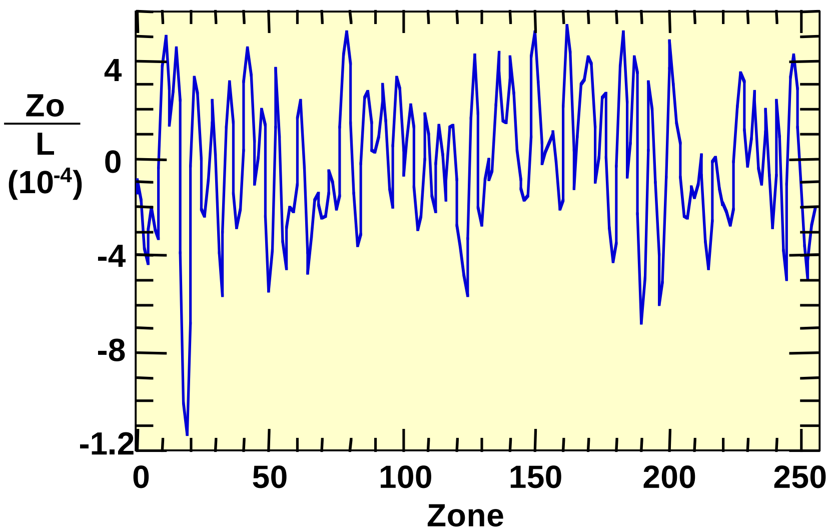
$\gamma = 5/3$, $P_o = 500$ dyne/cm^2

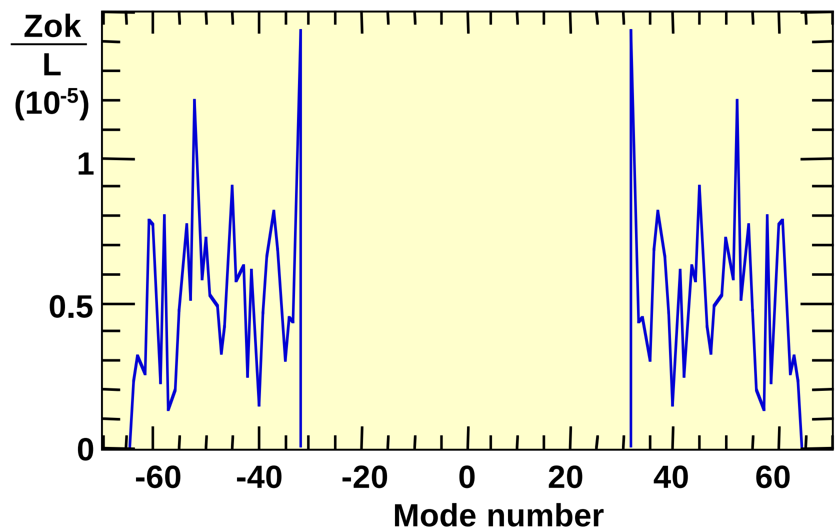


Initial conditions (David Youngs) are random & distributed in wavenumber shell (modes 32-64) close to Nyquist limit

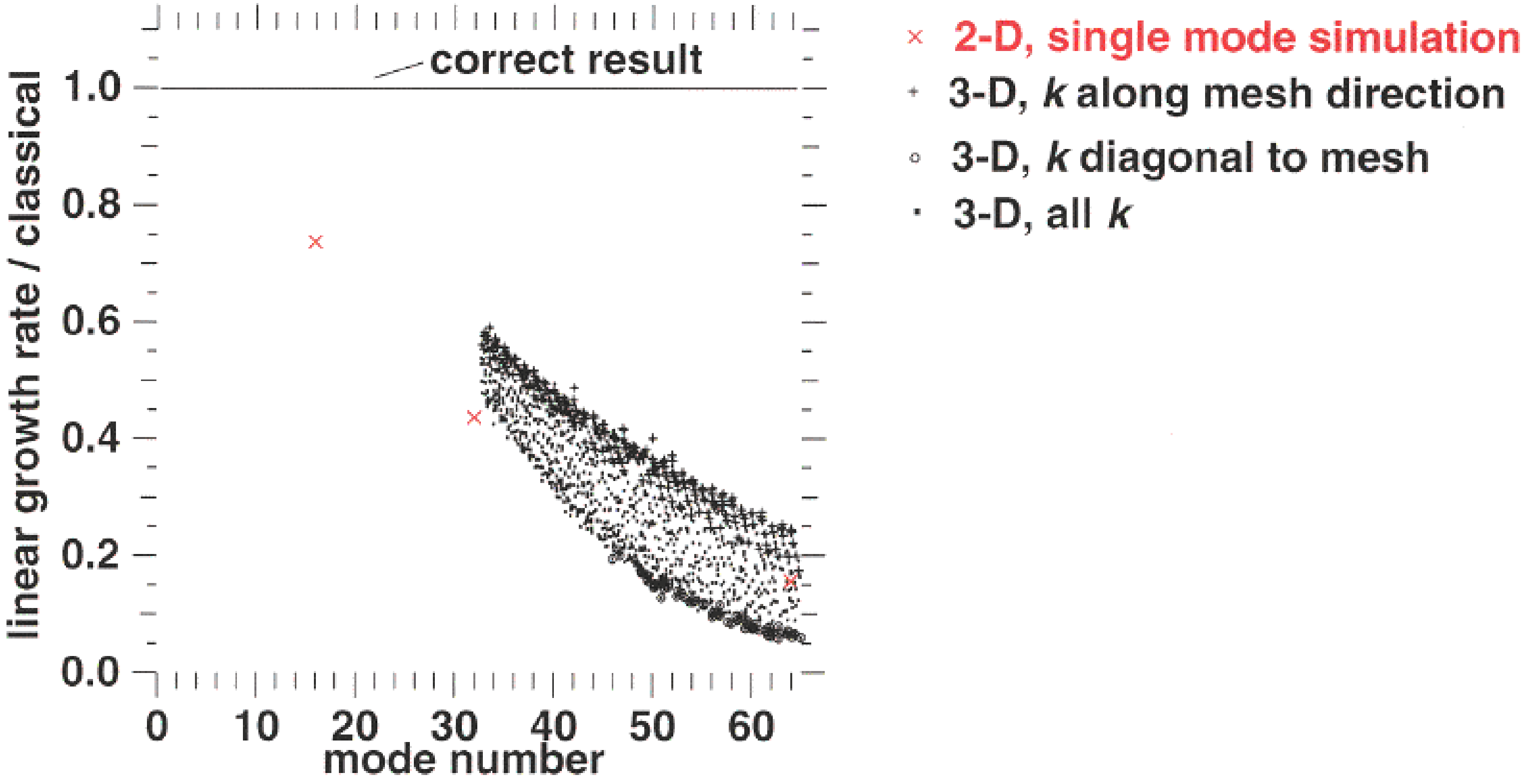








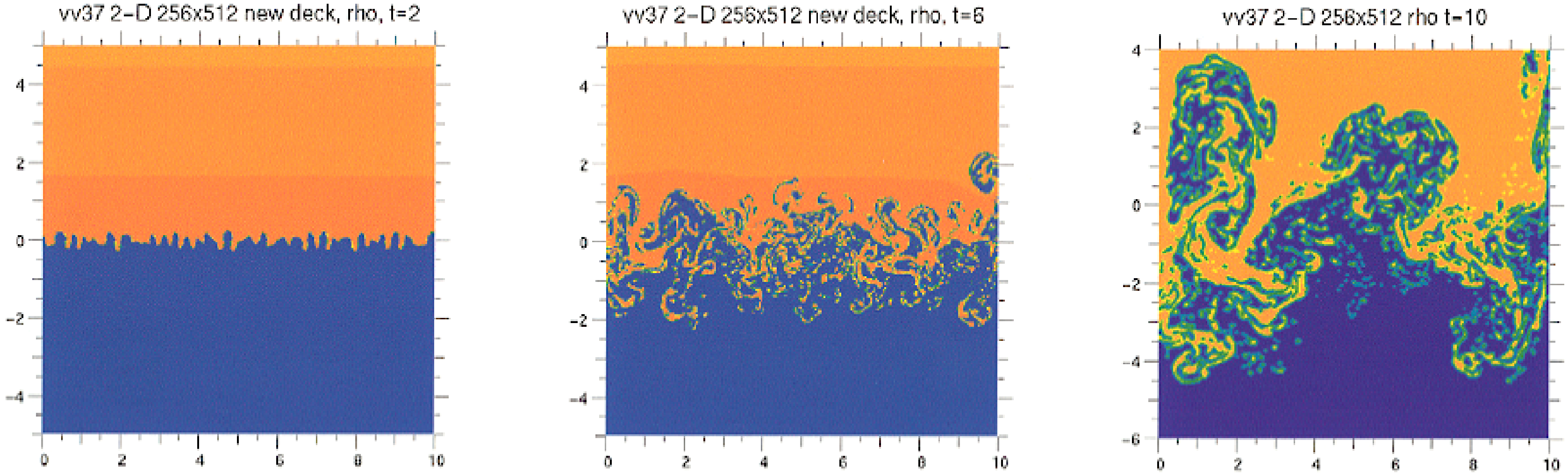
Simulated linear growth rates of seed modes are far below classical due to under-resolution



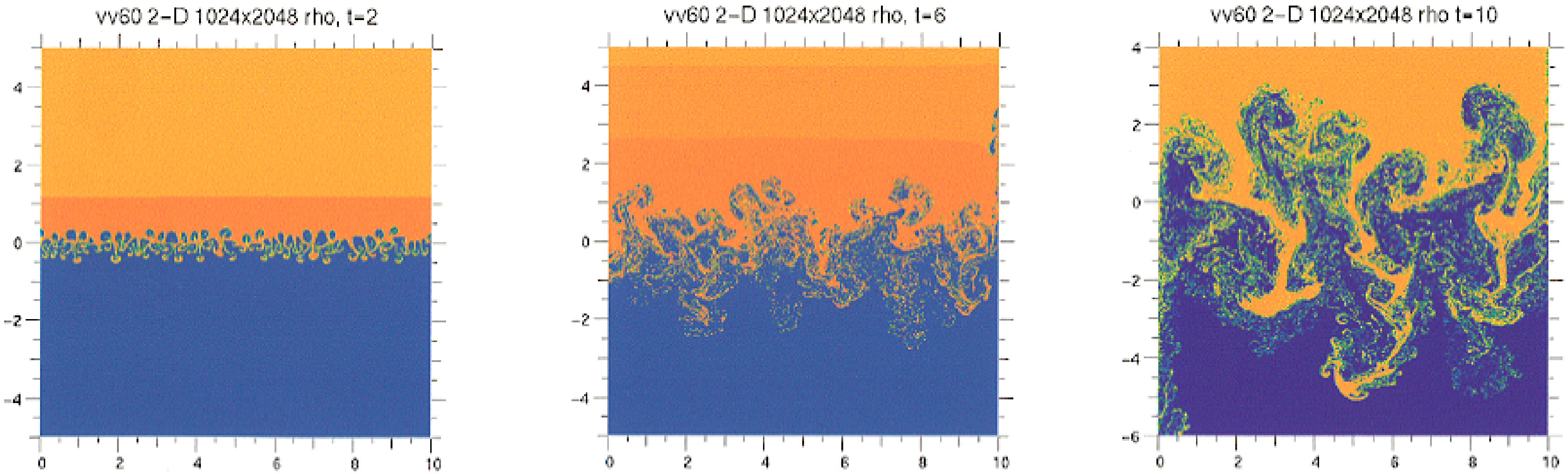
- If the simulation were converged, all modes would grow at the classical rate
- Also note that the simulated growth rate depends upon the orientation of the wave vector, *k,* to the mesh

In 2-D, the mix *extent* at late times does not change much with zoning refinement

2-D 256×512 (1x)

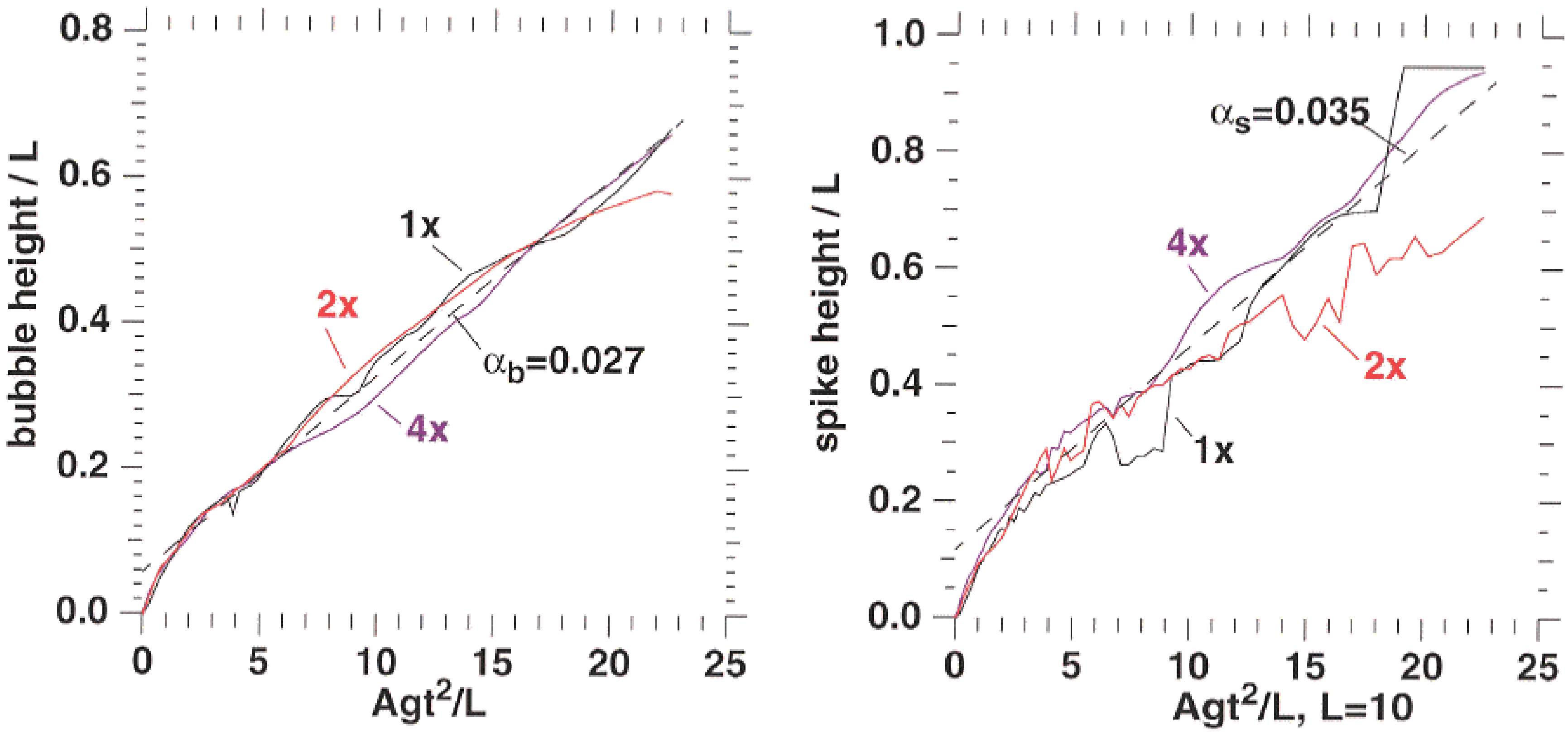


2-D 1024×2048 (4x)



- **The seed modes are clearly under-resolved with nominal zoning**

Zoning refinement beyond the nominal resolution does not significantly affect the mix extent in 2-D runs

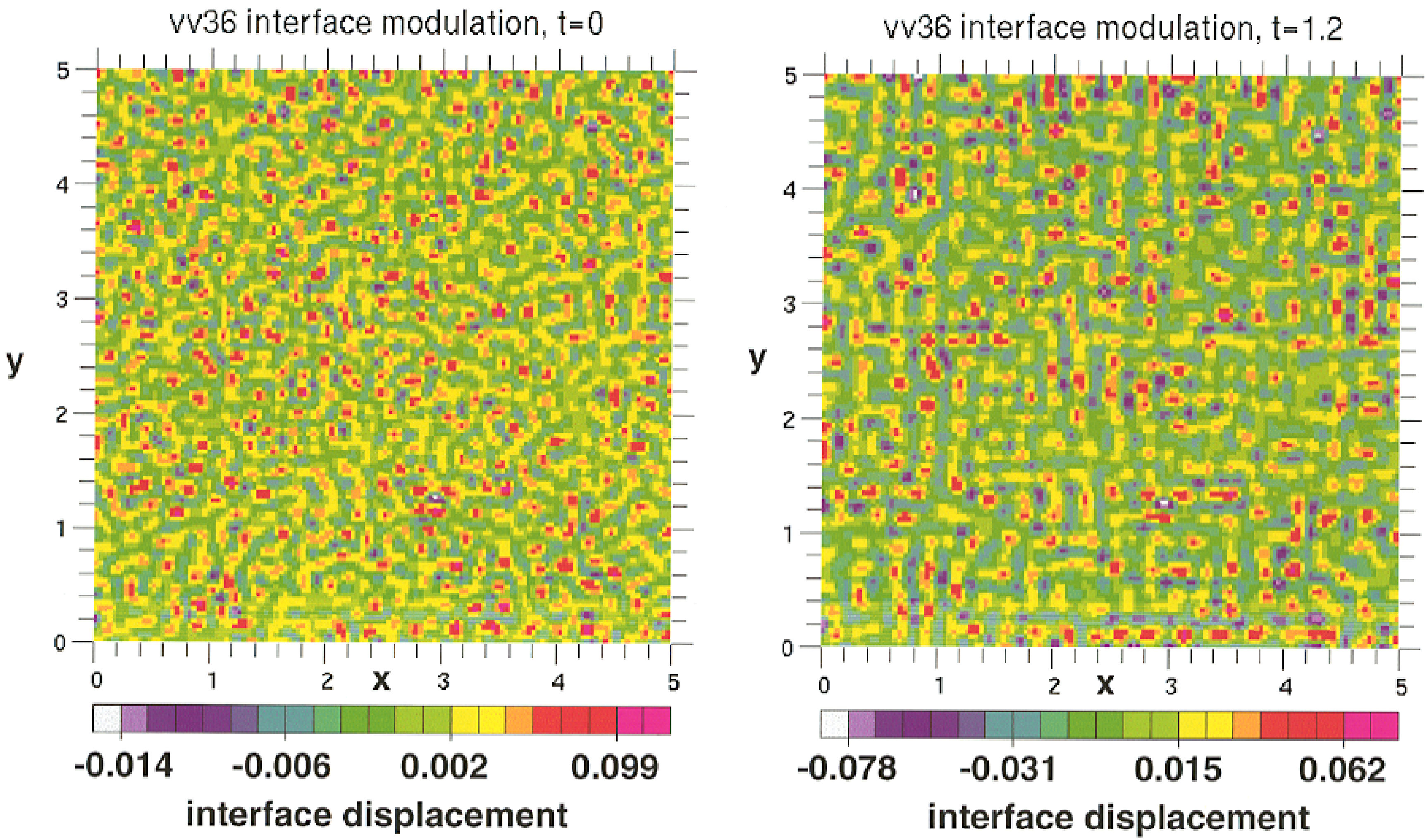


- 1x - nominal 256×512, 2x - 512×1024, 4x - 1024×2048
- Bubble and spike limits are taken at 1% volume fraction within 2 < x < 8
- The small number of large bubbles or spikes at later times introduces uncertainty due to selection statistics

We have performed $128^2 \times 512$ 3-D simulations in one quadrant of the nominal α problem

- We use 1/4 of the specified initial interface, a 5x5 cm square
- The zone size, initial amplitude, initial wavelengths, and g are preserved from the nominal problem (not scaled by L)
- This preserves three of the four dimensionless length ratios of the problem
  - λ_0/l
  - a_0/l
  - $P/(\rho g \lambda_0)$
  - L/l not preserved
  - l - zone size, a_0 - initial amplitude, L - box size
- Results are expected to be nearly the same as for the full problem until the mix extent becomes comparable to the box width
  - This will occur earlier in time by a factor $\sim 2^{1/2}$ than for the full problem
- We have recently completed the full size $256^2 \times 512$ problem without interface reconstruction

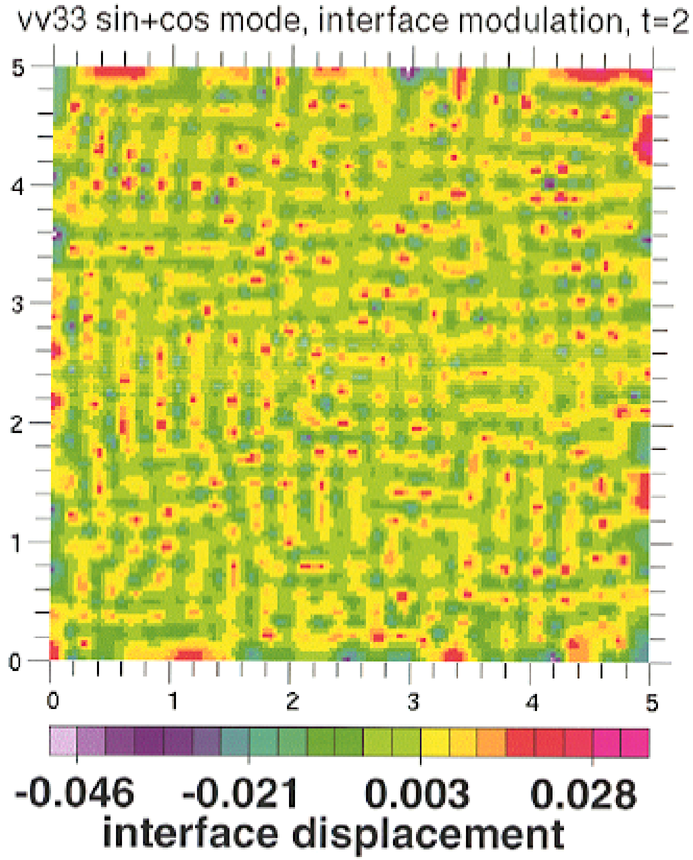
Under-resolution of the initial perturbations results in mesh imprinting - a numerical artifact



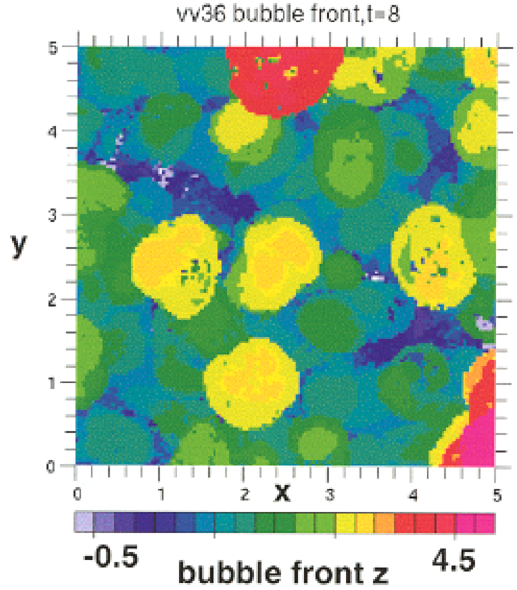
- The random isotropic initial surface evolves into a "checker board" pattern because of more rapid linear growth of modes aligned with the mesh

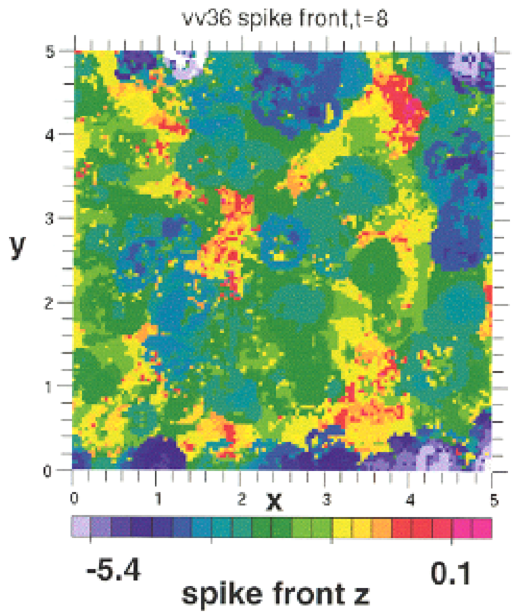
The surface finish definition including sine and cosine modes should not be used with reflection boundary conditions

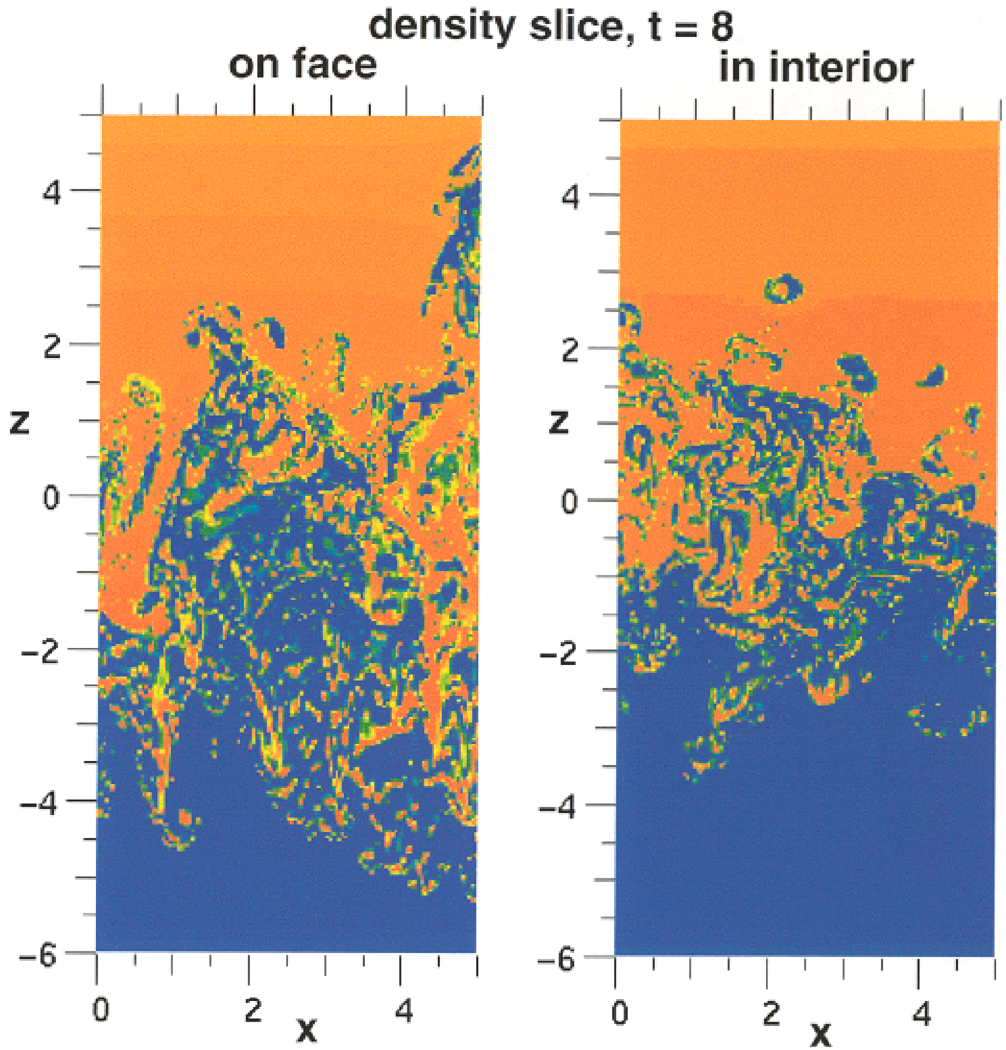
- Reflection boundary conditions support a spectrum consisting of integer and half-integer cosine modes
- Sine modes in the original surface definition are aliased into half-integer cosine modes. A "sine" mode with reflection bc has a cusp ot the boundary resulting in excessive growth near the boundary even in the linear phase
- Therefore, we used a surface finish obtained from Youngs containing only cosine modes, but which looks very similar to the original surface



Spurious enhanced penetration at faces and corners is probable a consequence of reflection boundary conditions





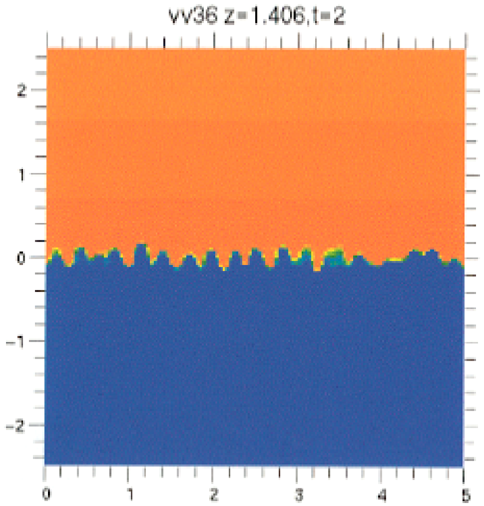


- This may result from higher symmetry of the flow at edges and corners

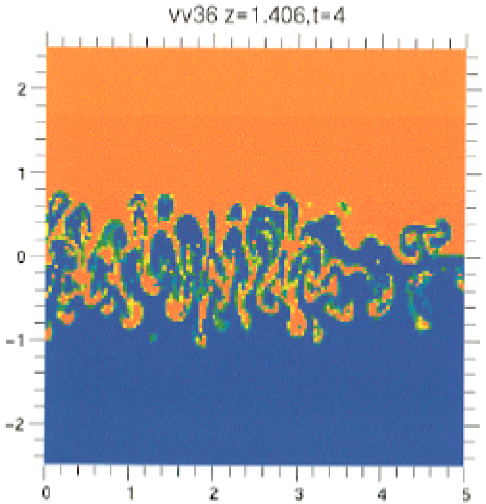
- **Data analysis excludes volume near boundaries to minimize the influence of this effect**

The simulation with interface reconstruction shows breakup into many small drops at late times

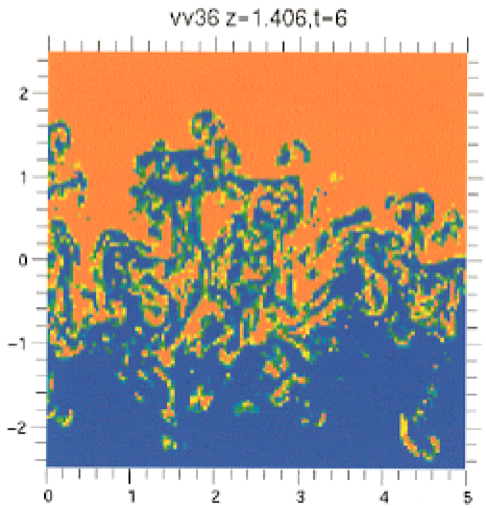
- Sequence of density cuts of 3-D 1282x512 simulation in the interior (away from a face)



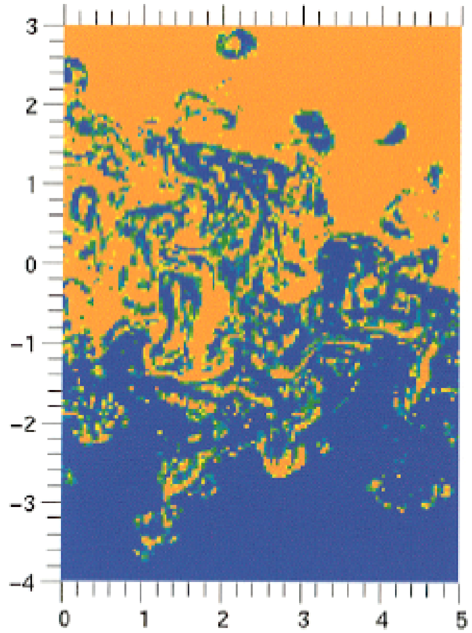
t = 2



t = 4



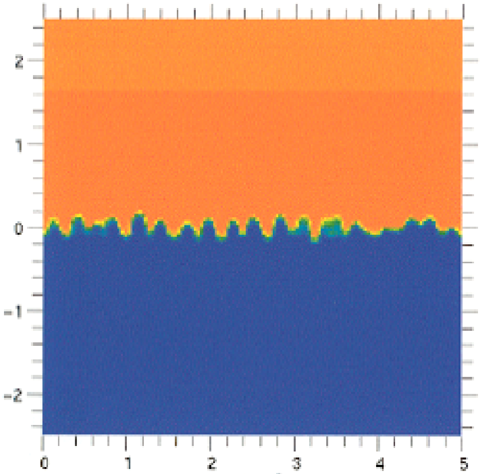
t = 6



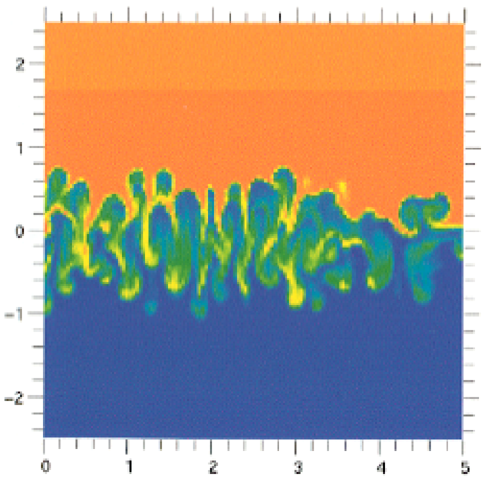
t = 8

Simulations without interface reconstruction predict a mix extent only slightly lower, but show much more small scale mixing

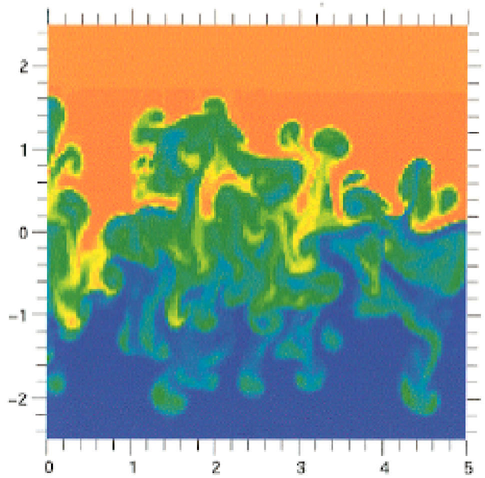
density cuts in 3-D $128^2 \times 512$ simulation without interface reconstruction



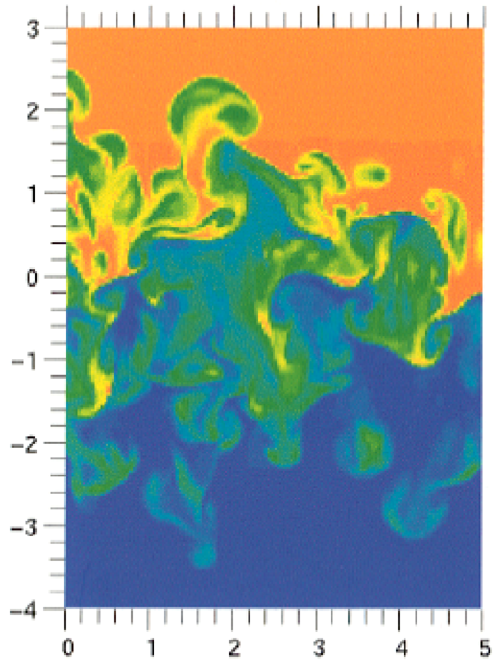
t = 2



t = 4



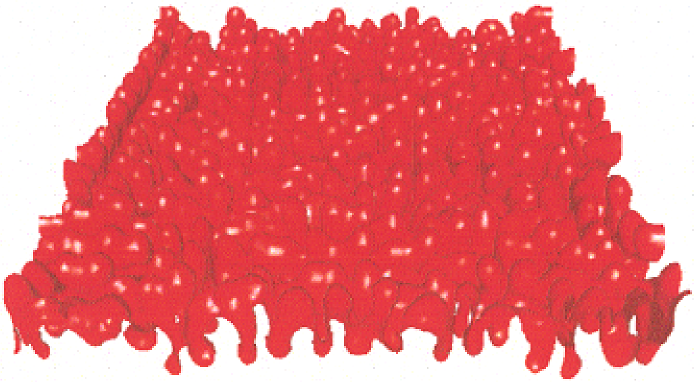
t = 6



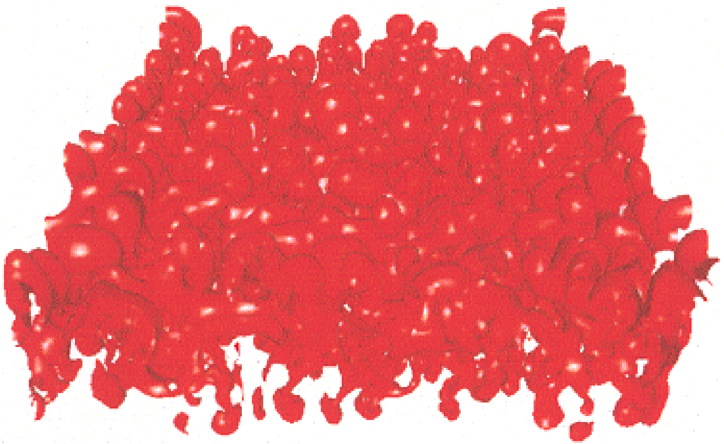
t = 8

The 3-D simulation shows the expected transition to turbulence, followed by bubble merger

visualization of interface, identified as $\rho = 2$ contour



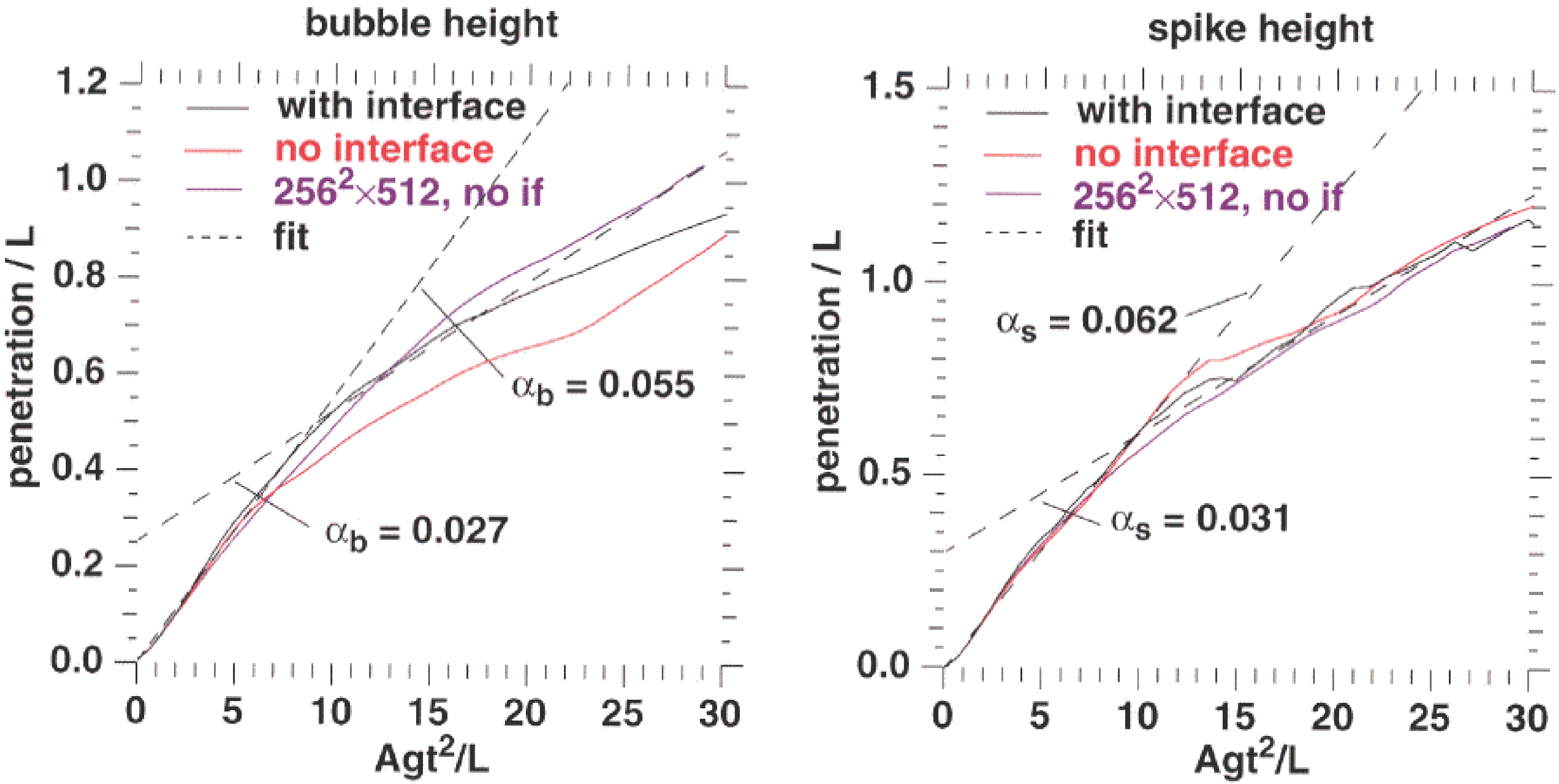
t = 2



t = 4

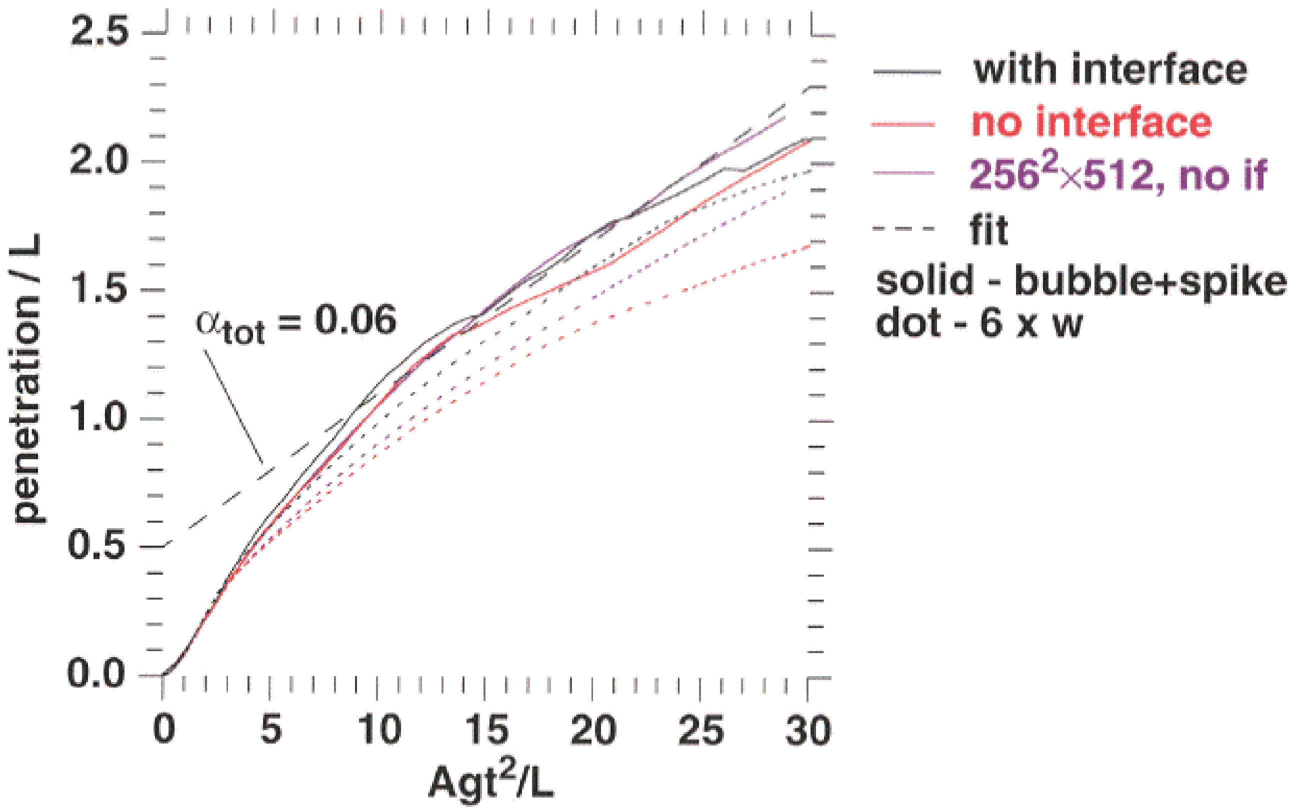
t = 6

It is not apparent that the mix extent ever reaches an asymptotic t^2 growth



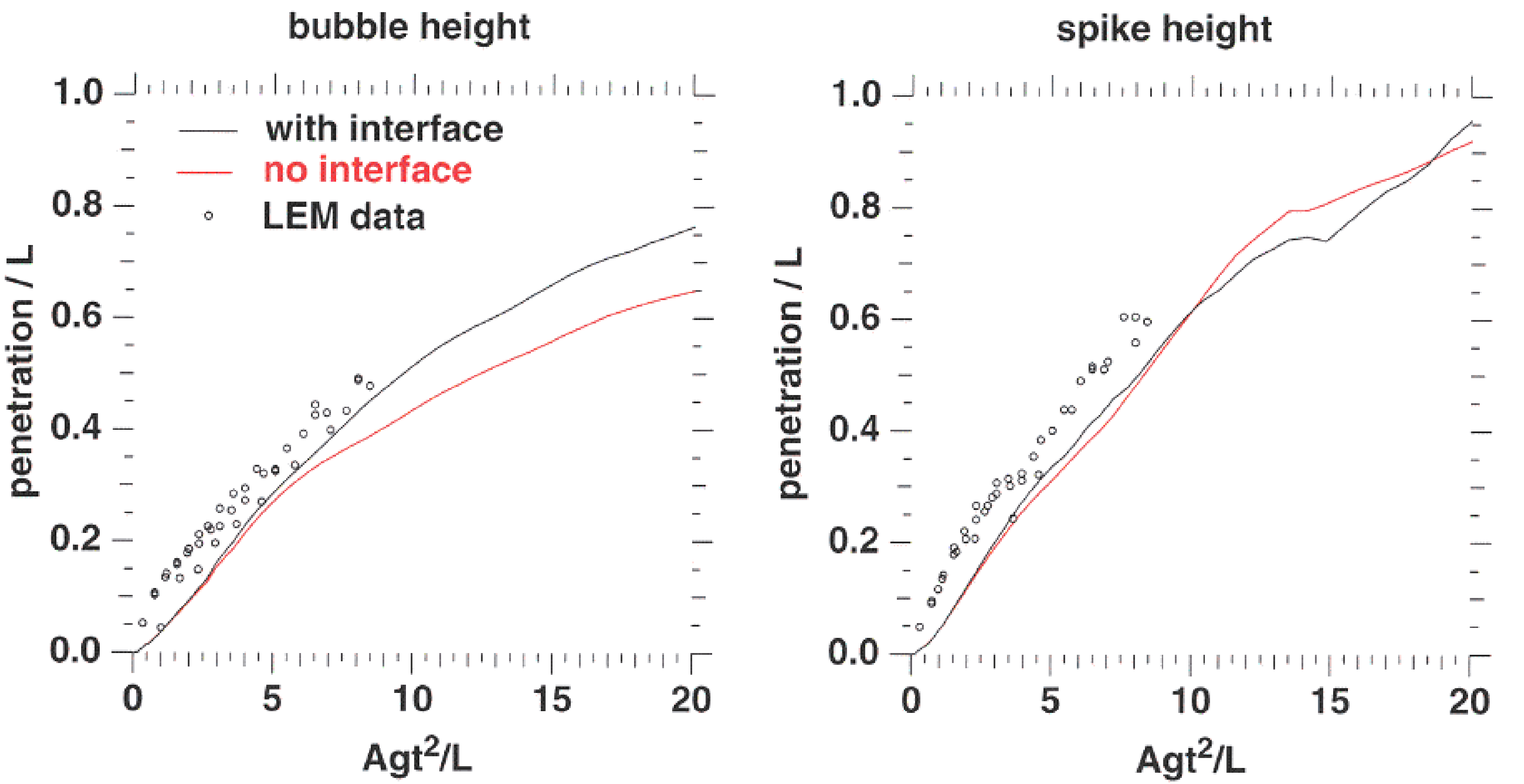
- "fit" lines are drawn by eye
- Interface reconstruction gives only modestly higher growth, only on the bubble side
- All cases show the slope, α, decreasing with time
- On the bubble side, the full scale problem retains a higher growth rate later in time as it can grow bigger bubbles (all curves are scaled as L=5)
- The growth of the spikes does not change with problem size

The total mix width and integral width measure also exhibit decreasing slope with time

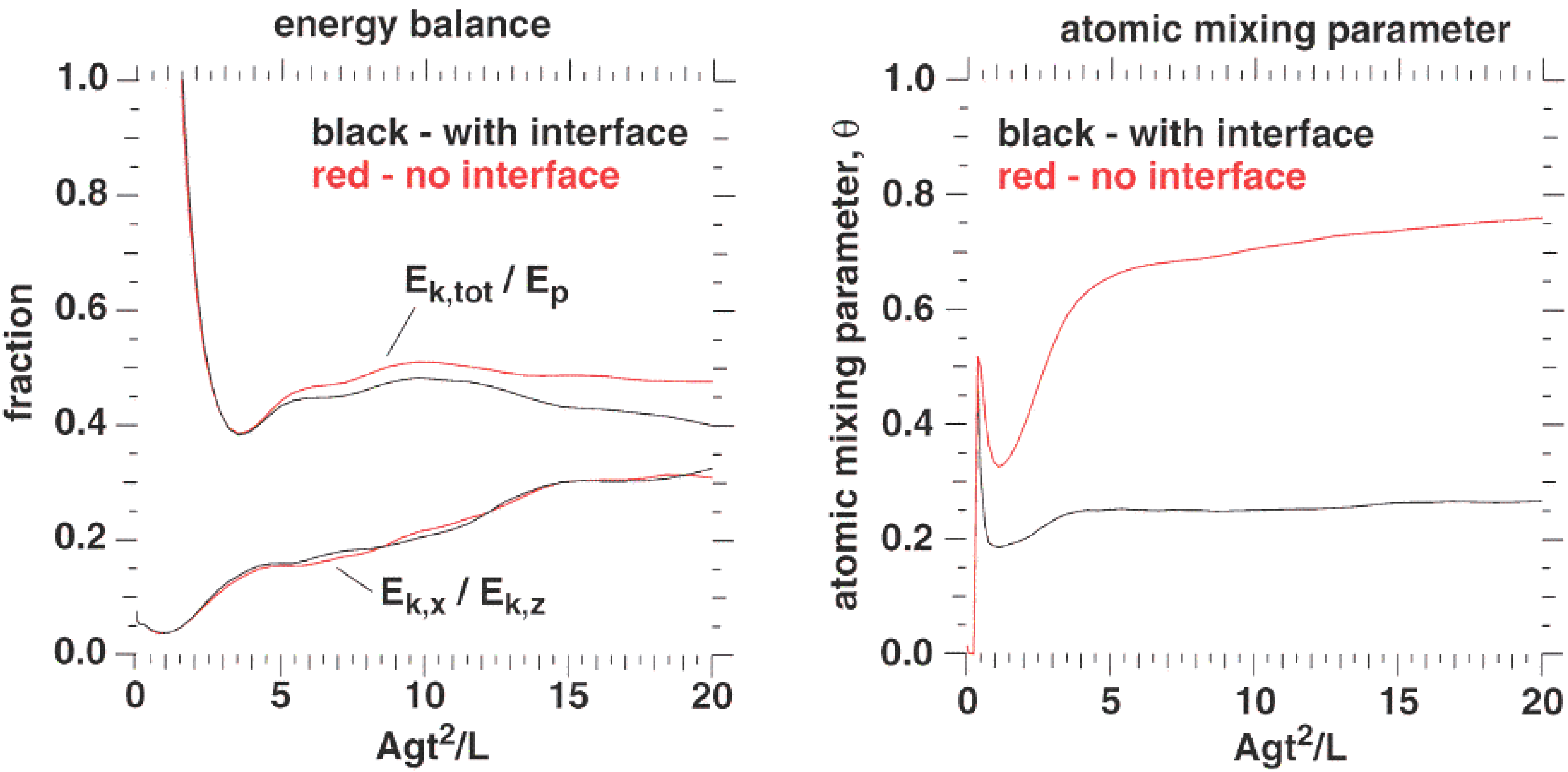


- w - Andrews and Spalding integral width
- The full scale and one quadrant simulations nearly overlay when scaled with the *same L* (5 here) as the initial amplitude and wavelength were not scaled with L
- We believe that the box size affects the growth only by limiting the size of the largest bubbles late in time, which is a *breakdown* of self-similarity rather than a feature of the scaling

Simulations lie below the LEM data when scaled by the box size; however, the slope is about right

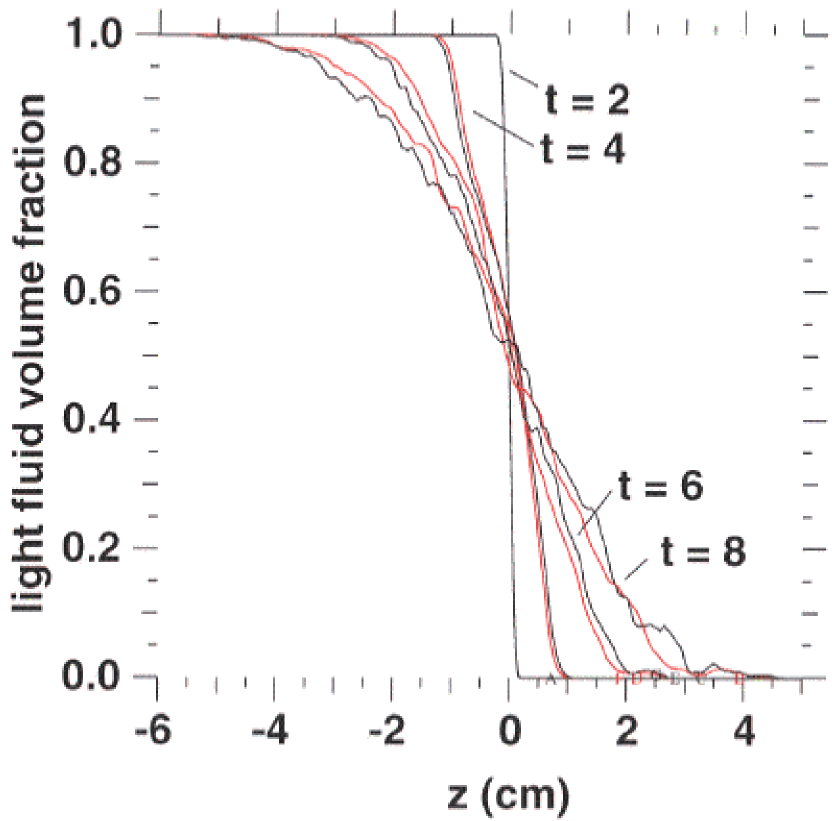


The simulation without interface reconstruction gives atomic mixing ~0.7, but similar dissipation to the run with tracking



- E_p - potential energy drop, dissipated energy, $E_{k,z}$ kinetic energy in streamwise direction, $E_{k,x}$ kinetic energy in one spanwise direction, $E_{k,tot}$ - total kinetic energy
- The atomic mixing parameter for the interface reconstruction run is an upper limit because post-processing does not account for the interface reconstruction and treats zones through which the interface passes as mixed

Volume fraction histograms are also very similar with or without interface reconstruction



black - with interface reconstruction

red - no interface

Conclusions

- Under-resolution of the initial perturbations introduces numerical artifacts, but it is uncertain if the simulated mix extent is compromised
  - 2-D runs show no significant change in mix extent with zoning refinement
- Interface reconstruction has only a modest effect on mixing extent
  - However, internal structure of the mixing zone is affected
- These runs do not appear to specify a definite value of α
  - 3-D simulations of one quadrant of the nominal α problem show monotonically decreasing α with increasing time
  - α_b drops from ~0.055 at early times to ~0.03 later in time
  - α_b remains high longer for the full scale problem
  - α_s ~ 0.06 at early times; also appears to drop later in time
- Simulations lie below the LEM bubble, spike penetration data
  - slope of spike penetration and early time slope of bubble penetration are close to measured slopes of penetration vs. t^2