# Recent Computational Simulations of Rayleigh-Taylor Mix Layer Growth with a Multi-fluid Model

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w/ acknowledgements to A.J.Scannapieco, Tim Clark, John Grove, Chuck Cranfill, et.al.

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# disclaimer

This is a partial sub-set of the viewgraphs presented at the 8th IWCTM.

The work on 'resolved scale' simulations is currently being prepared for publication, to be submitted to Physics of Fluids.

The work on 'sub-grid drift flux' simulations will be prepared for publication soon, to be submitted to a journal TBD.

# Recent computational simulations of Rayleigh-Taylor mix layer growth with a multi-fluid model.

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Abstract - LA-UR-01-2562

Recent results of computational simulations of the Rayleigh-Taylor mix layer are presented and discussed. Our previous work is summarized briefly comparing mix layer growth characteristics observed in different simulation modes including single fluid with initial density discontinuity, two-fluids with interface reconstruction and in a full multi-fluid dynamic approach. Recent comparisons under varying compressibility are presented showing negligible influence of compressibility on the mix layer growth rate. Using spectral analyses, perturbations intentionally introduced in the initial conditions are compared to long wave length perturbations introduced inadvertently in these initial conditions. The influence of these initial conditions on late time growth and growth rate are explored. The compressible multi-fluid model allows each fluid to have its own 'drift velocity' relative to the mass averaged fluid velocity. This can be applied in several ways within the mix layer to represent a real molecular mixing, a turbulent enhanced diffusive mixing, or an individual species 'sub-grid' convective drift flux. Examples of these in the Rayleigh-Taylor mix layer are discussed. Finally, we consider the combination of these factors which best matches the experimental results for mixing layer growth rates in incompressible experiments, and how these results may apply to compressible fluids.

# Introduction

- Goals:
  - simulate Rayleigh-Taylor mix layers accurately to predict atomic / molecular mixing (e.g., a reactive R-T mixing front) in macroscopic geometries.
  - use 'resolved simulations' to model mix layer growth and use drift flux (subgrid) simulations to model the mix layers atomically mixing components.
  - match experimental 'alpha' ($\alpha$), $h = \alpha A_t g t^2$ ← focus today
  - match refined experimental findings related to mixing front details.
- Central Issues
  - numerical mixing must be small enough to have a negligible effect on mix layer growth rates so that 'sub-grid' mixing can be represented realistically.
  - Hypothesis: the growth rate seen in computations, which have no subgrid mixing and small numerical diffusion, should equal or exceed the experimental value IF the experiment contains small scale dissipation which reduces the growth rate in the experiment.

# Summary of Relevant Work

- Experimental
  - wide range of experiments (mostly incompressible) show a mix layer growth rate which closely approximates the scaling, $h = \alpha A_t g t^2$
  - alpha bubble, $\alpha_b$ ~ 0.06-0.07 (earlier work, e.g., Youngs and Read et.al., ) - and ~ 0.05 (recent work, e.g., Dimonte, Schneider, et.al.)
- Computational
  - alpha bubble results range from ~ 0.03 - ~0.1
  - many 3-D methods (compressible or incompressible) trending towards low end, $\alpha_b$ ~ 0.03 ~ half experimental mean
  - front tracking w/ 2 distinct fluids ('Frontier code', Glimm, et.al.) at higher end, ~0.07-0.08
  - large variance in alpha just due to random seed in initial perturbation
    - (~ 0.05 +/- 20-50%, in 2-D compressible isothermal fluids, T. Clark, 2001)
  - 2-D results ~ 15% greater than 3-D results (Youngs, 1994).

# Summary of Our Methods

- Methods
  - 2-D multi-fluid Eulerian AMR formulation
  - compressible Euler equations in appropriate limit to recover incompressible approximation, supplemented with fluid volume fractions
  - ideal gas equation of state for each fluid
  - advection of fluid volume fractions in mixed cells at the interface
    - mixed cell treatment (Bowers and Wilson,1991)
    - interface reconstruction (D.Youngs, 1984, 1989)
  - high-order, monotonic Van Leer advection of fluid quantities
  - each fluid has its own density, internal energy and pressure in its fluid volume fraction within the 'mixed cells' (containing the interface)
  - in 'drift flux' representation of sub-grid mixing, each fluid has its own 'drift momenta' relative to the mass average which can be adjusted to represent realistic molecular diffusion or a range of assumed turbulent flux forms

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# Summary of Our Previous Results

- Previous Results
  - alpha bubble was found on a 128 x 128 grid with no sub-grid mix model, to be ~ 0.08 - 0.1, somewhat larger than experiments.
  - interface algorithm does not alter the growth rates significantly.
  - molecular mixing (by the drift flux) does not influence the mix layer growth rate but does create a unique distribution of molecularly mixed materials controlled primarily by the volume fraction of the lighter material.
  - drift flux mixing significantly above the molecular diffusion level reduces the mix layer growth rate (for the set-up in these results, a drift flux ~ 50 times greater matches experimental range ($\alpha_{bub}$~ 0.055)

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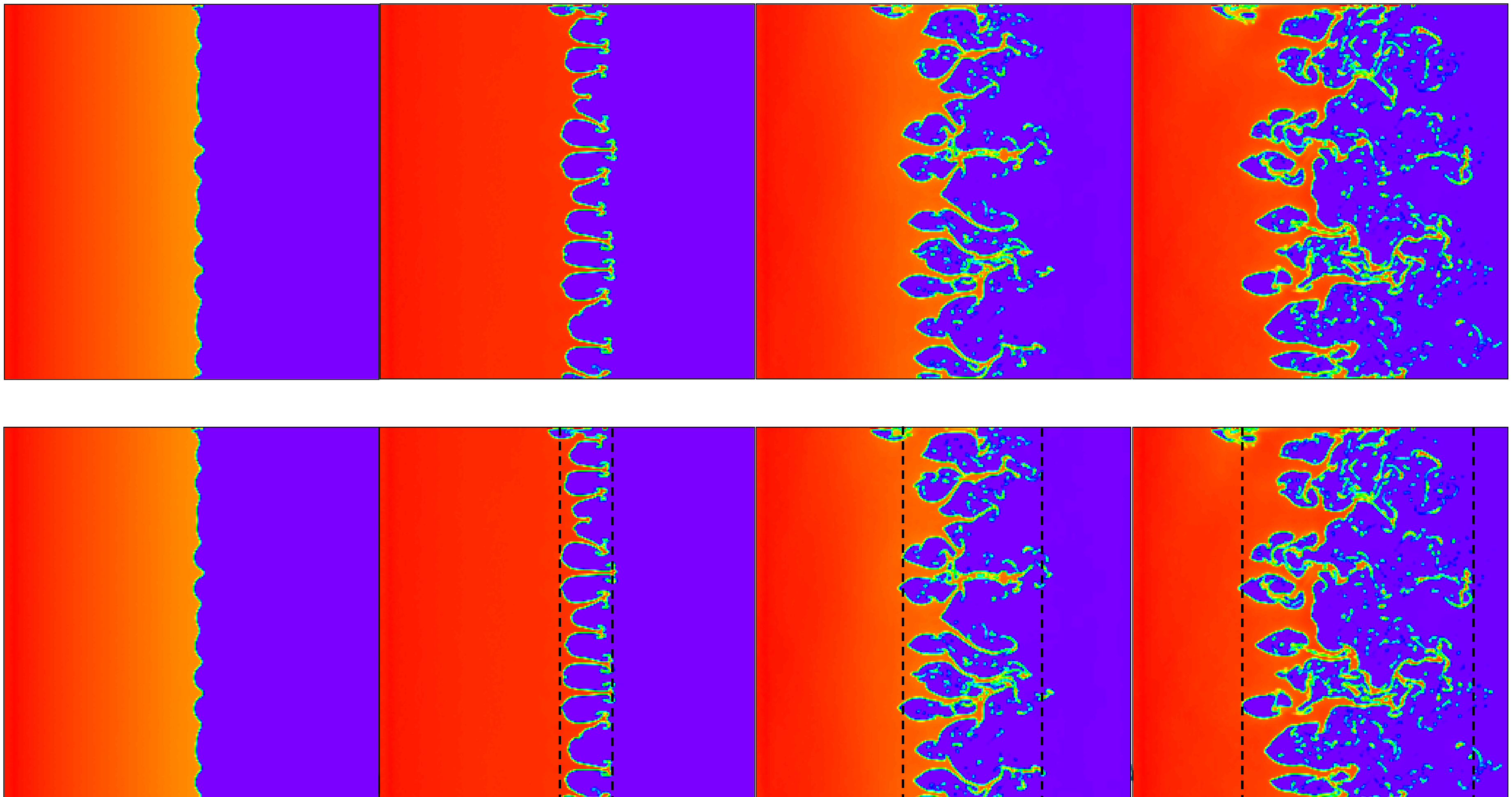
# Issues in Matching 'alpha' [and what our set-up uses]

- **Numerical**
  - grid resolution [$128^2$ or $256^2$ or $512^2$]
  - Interface treatment [mix cell volume fraction advection w/ Young's interface reconstruction]
  - Differencing schemes [high order monotonic Van Leer like scheme]
  - 2-D vs. 3-D [2-D only]
- **Initial Conditions**
  - initial perturbation magnitudes, [volume fractions, Vf, set to match interface perturbation]
    - perturbation on density [$\rho = \rho_1 Vf_1 + \rho_2(1.-Vf_1)$ ]
    - perturbation on internal energy [$\varepsilon = \varepsilon_1 Vf_1 + \varepsilon_2(1.-Vf_1)$ ]
  - wavelength spectrum, [30 modes, mode numbers 30 - 60, random phase, unit amplitude]
  - hydrostatic equilibrium by e(z), or ρ(z) [e(z), w/ $\rho = \rho_o$]
- **Physics**
  - compressible or incompressible formulation (w/ or w/o internal energy ) [compressible]
    - degree of compressibility [varied $Ma^2$ by 2 orders of magnitude]
  - fluid equations: Euler, viscid, internal or total energy [Euler using internal energy w/ optional multi-fluid drift flux for 'species momenta' relative to mass averaged single fluid velocity.]
  - Interface physics: surface tension, slip or traction, molecular diffusion, sub-grid mixing

# rt256bc4 den at t=20,40,60,80



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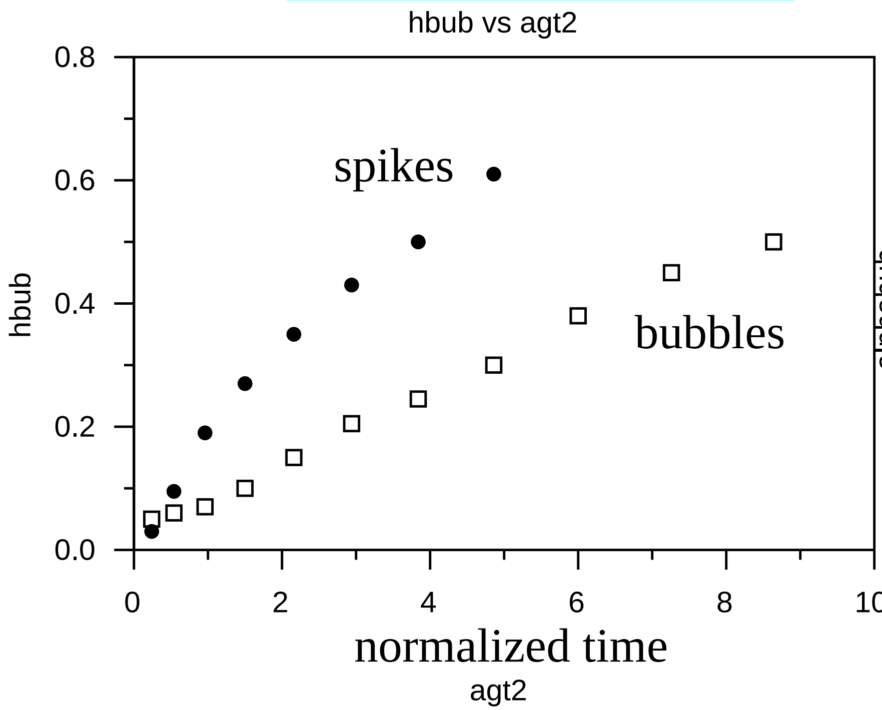
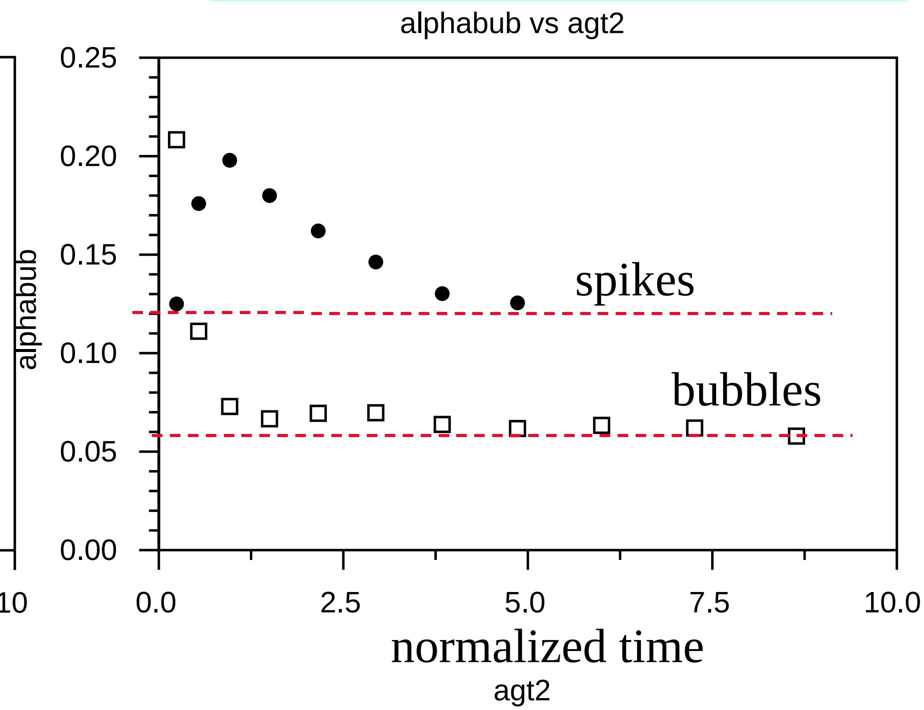
# RT mix width for 256 case

## mix layer width, h




## mix width growth coef, α



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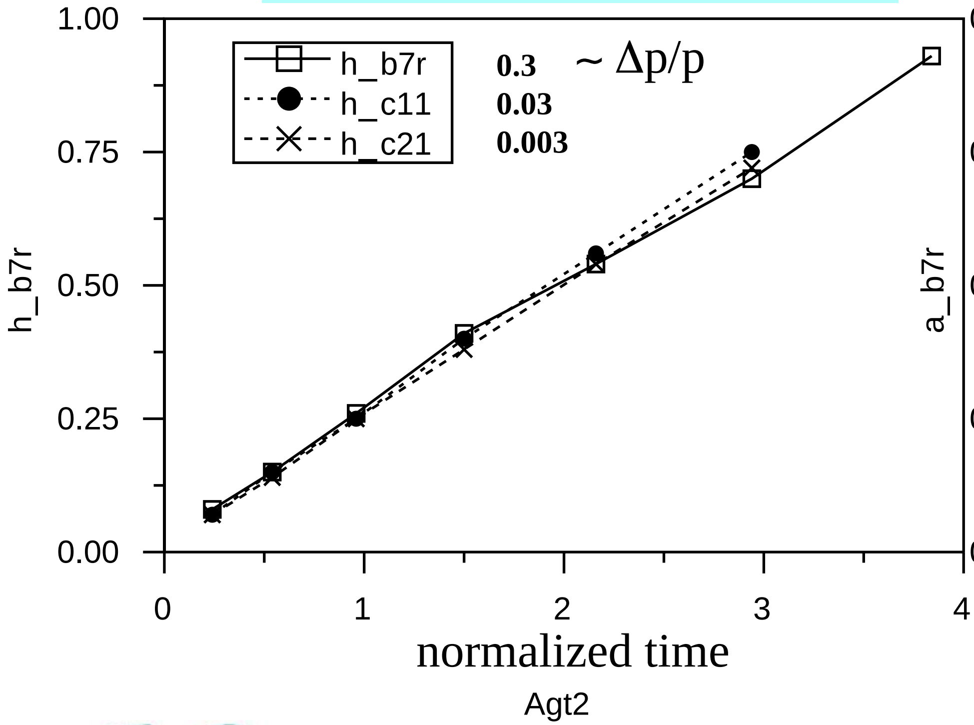
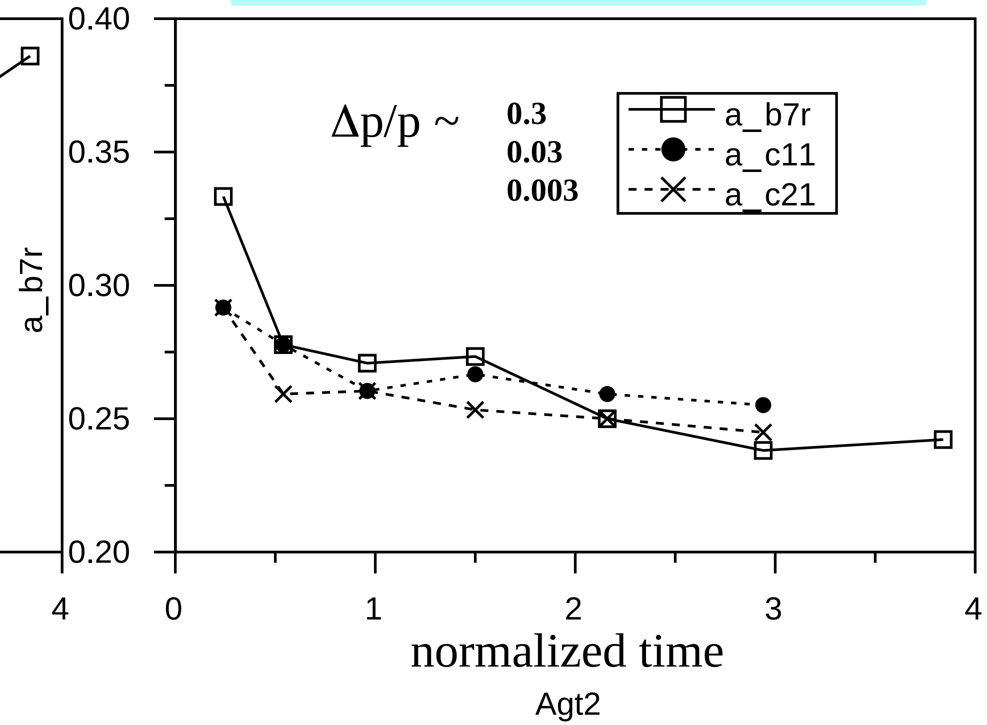
# RT mix width for varying compressibility

total mix layer width, h




mix width growth coef, α



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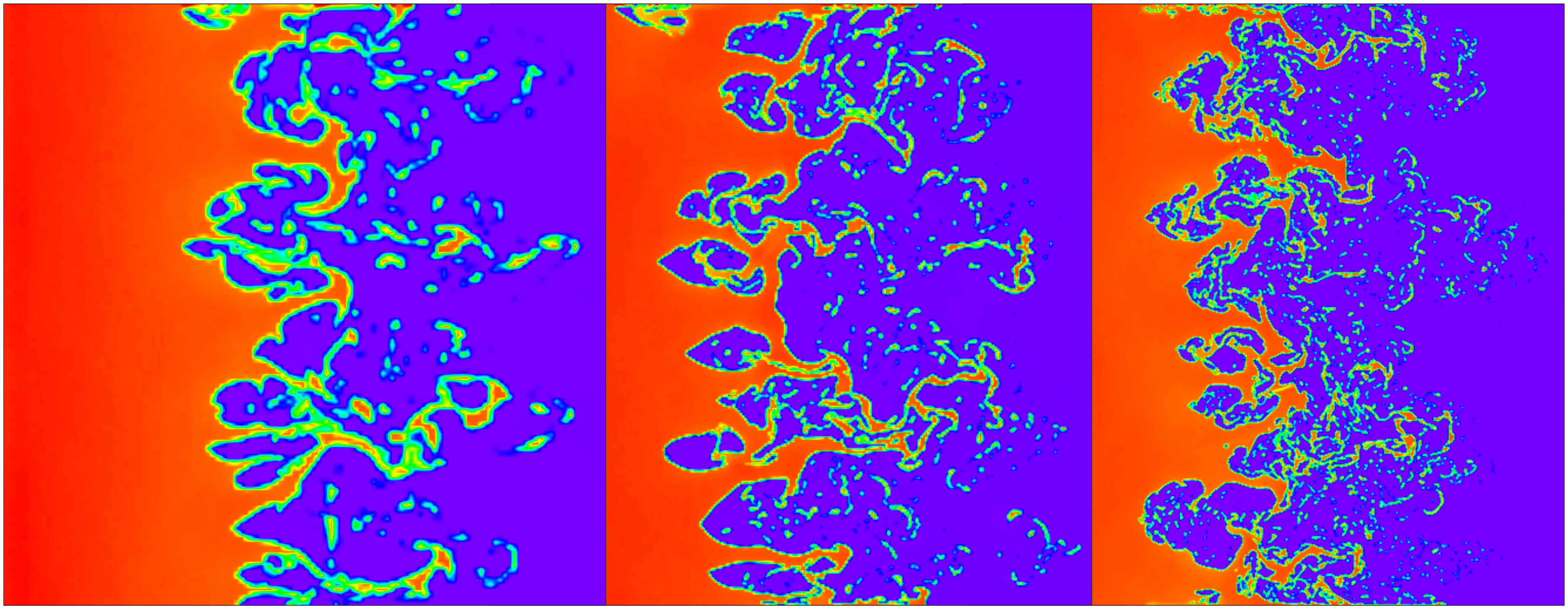
# BC4- Zint(IC) fixed

## grids $128^2$, $256^2$ & $512^2$ - each grid result on $512^2$



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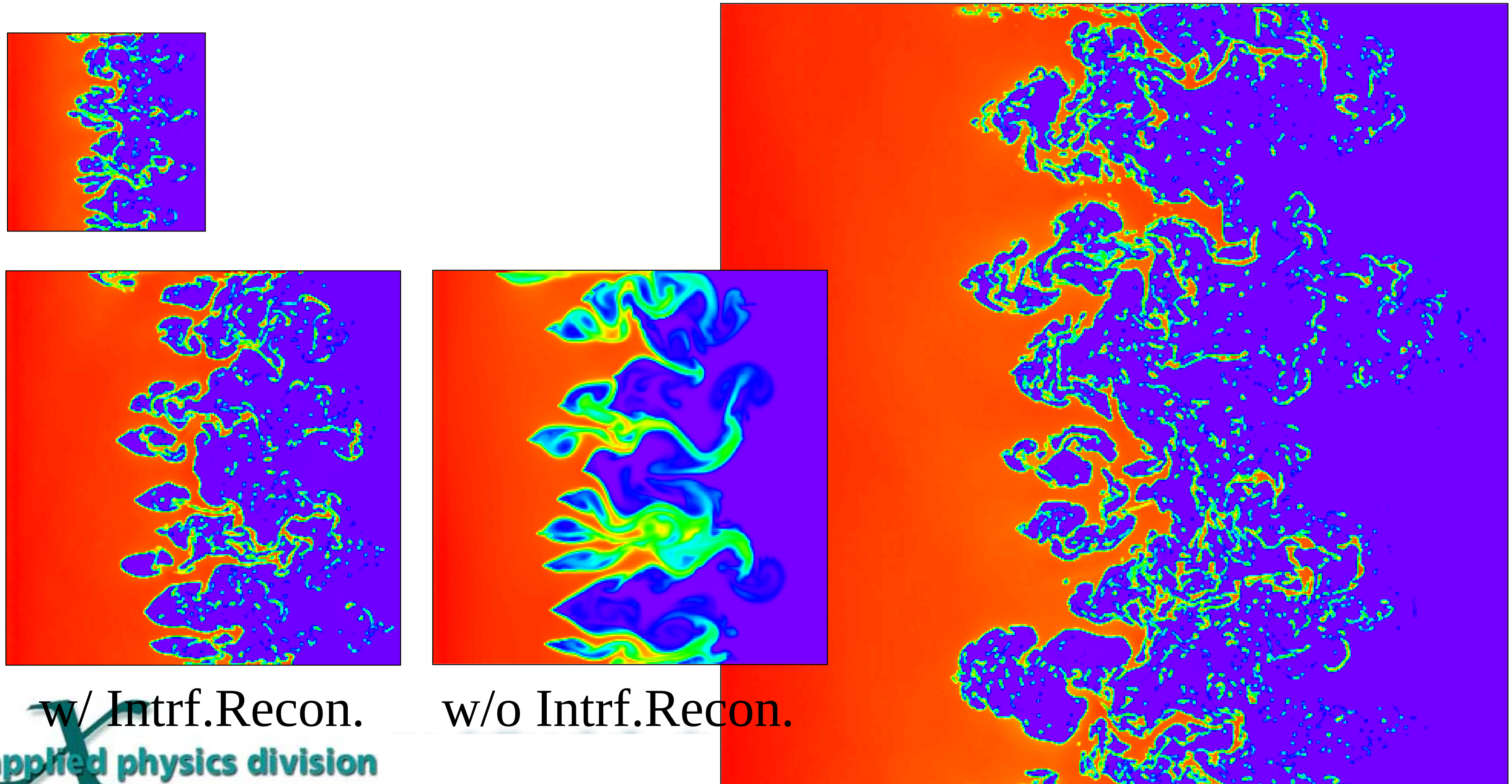
# BC4- Zint(IC) fixed

## grids $128^2$, $256^2$ & $512^2$ - actual grid results



w/ Intrf.Recon. w/o Intrf.Recon.

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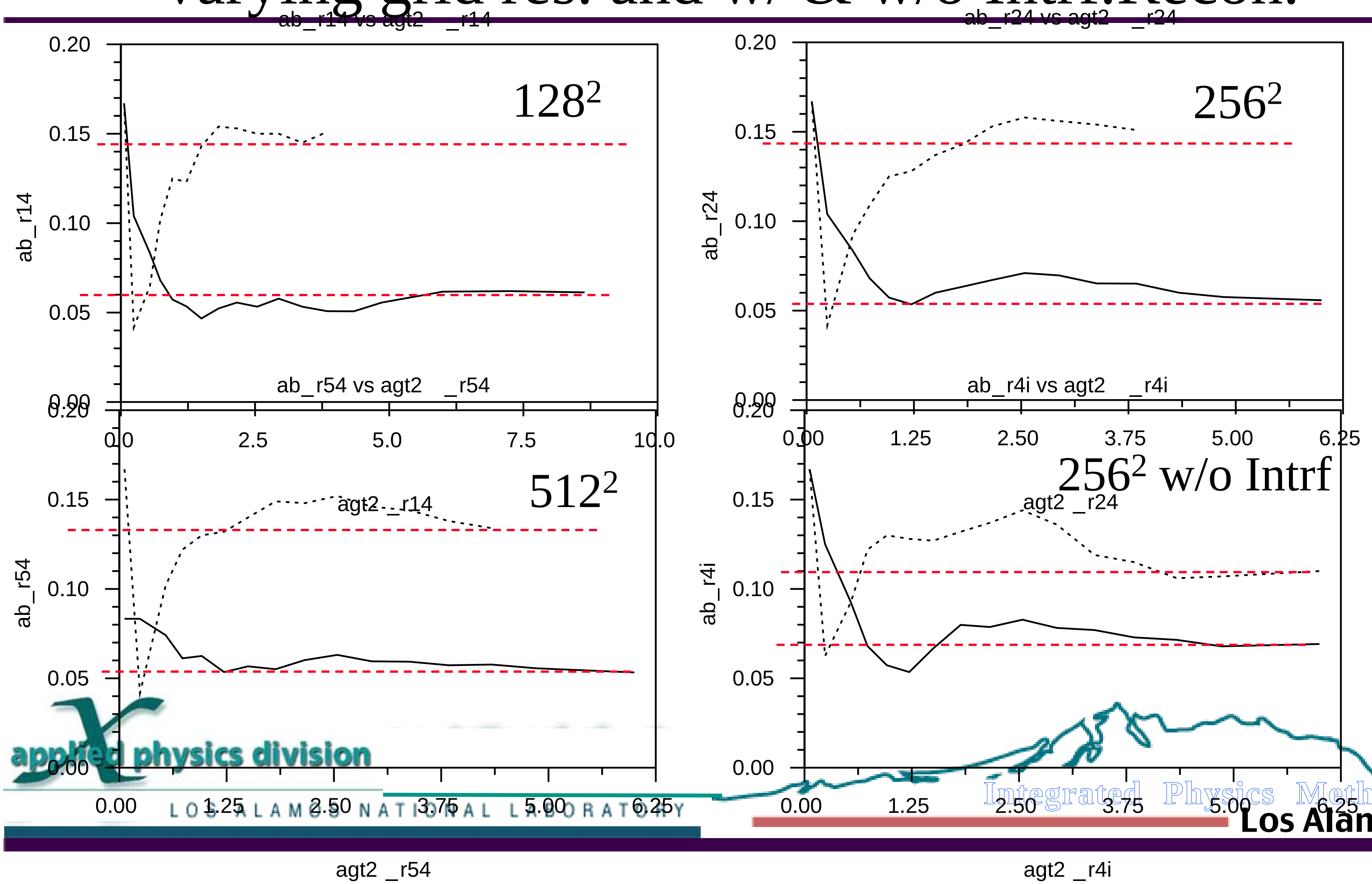
# Alpha (RT mix growth rate)
## BC4 -fixed Zint(IC) -
## varying grid res. and w/ & w/o Intrf.Recon.



# BC2- Vf(IC) fixed

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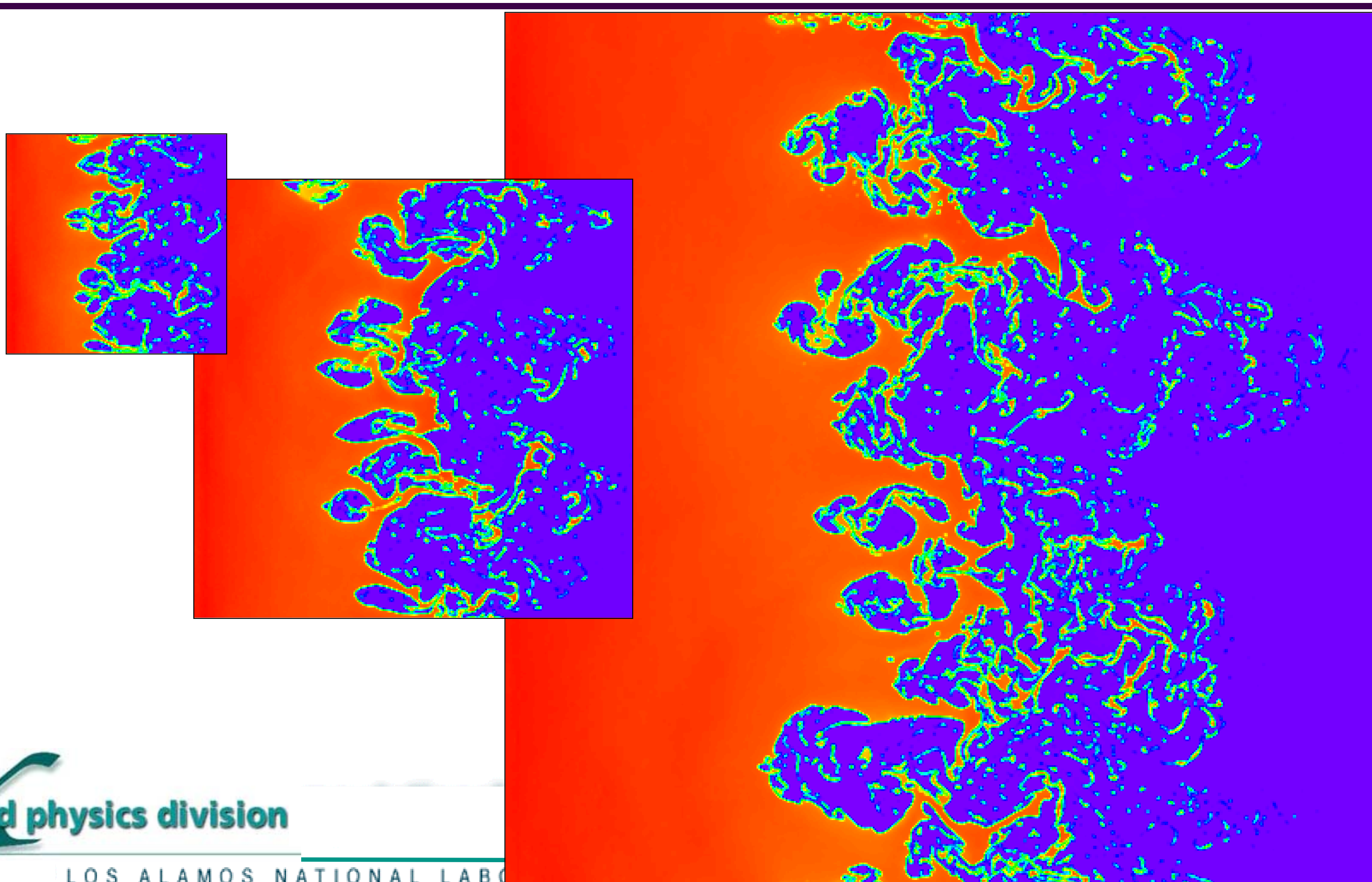
grids $128^2$, $256^2$, $512^2$ actual grid dimensions



applied physics division

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# Alpha (RT mix growth rate)
# BC2 -fixed $V_f$(IC) - varying grid res. and w/ & w/o Intrf.Recon.

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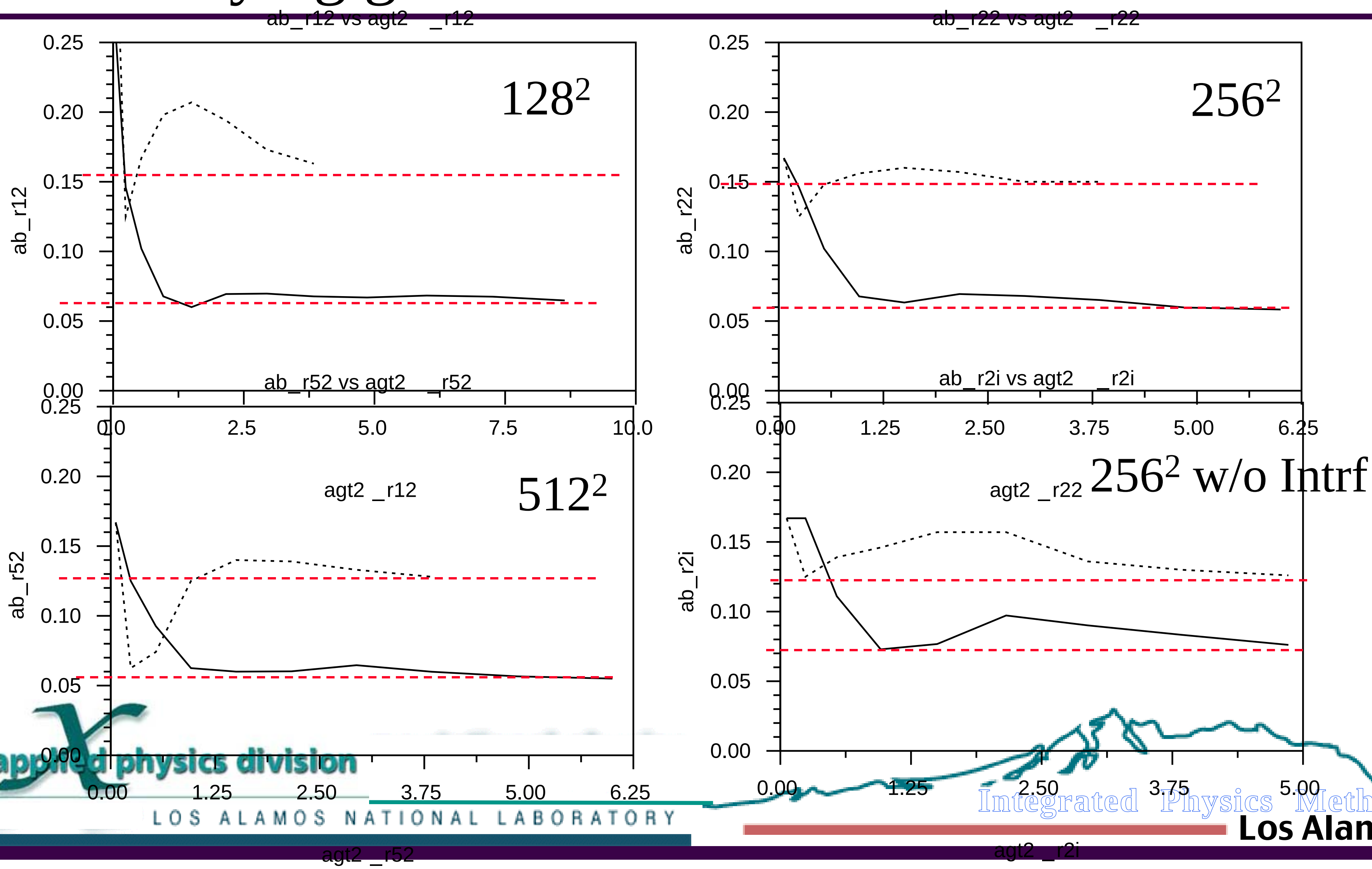

# BC2 (fixed VF(IC)) vs. BC4 (fixed Zint(IC))

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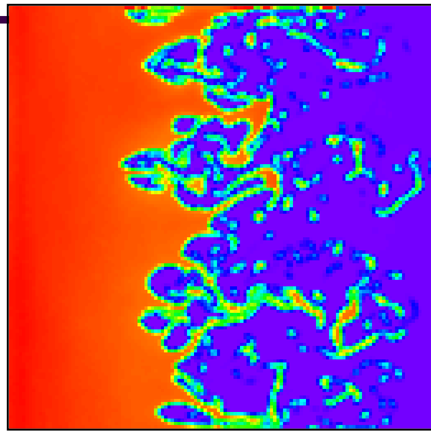
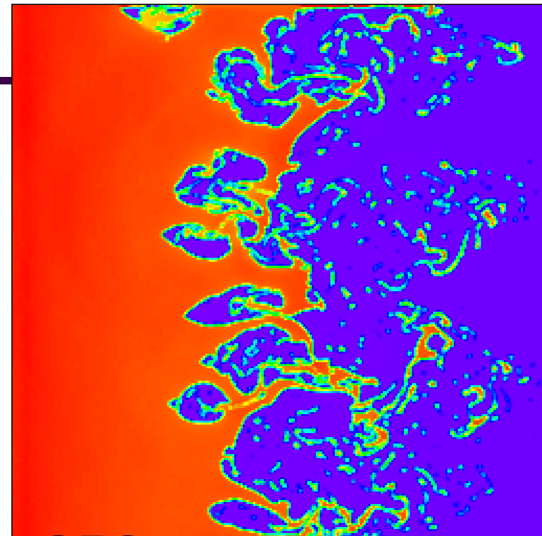
are the same structures seen across grid res. in either case?

BC2

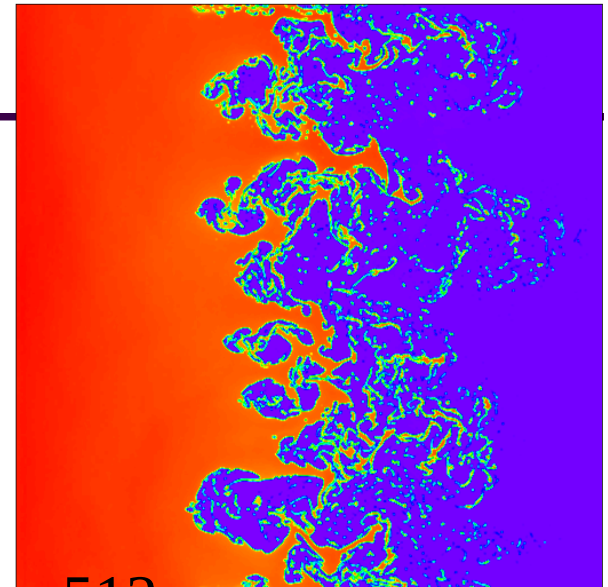
128



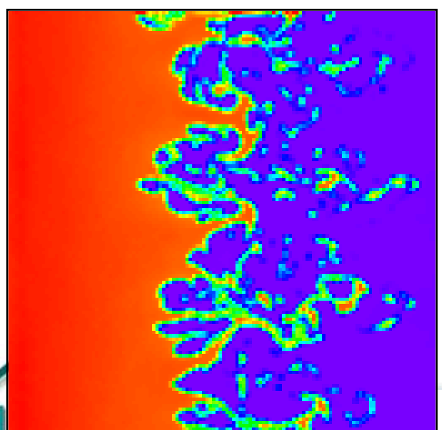
256

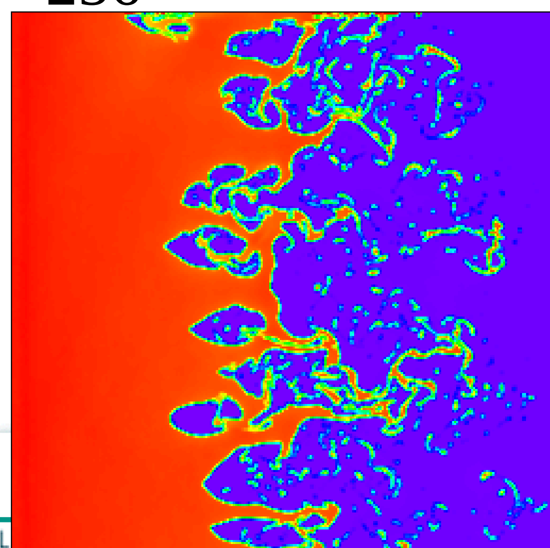


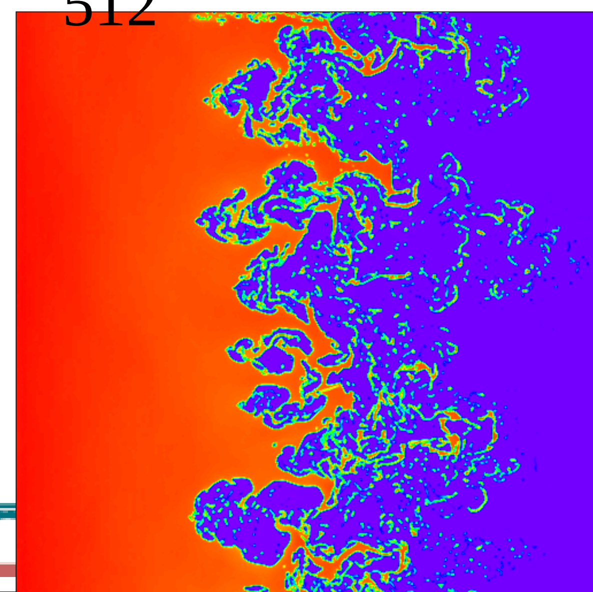
512



BC4







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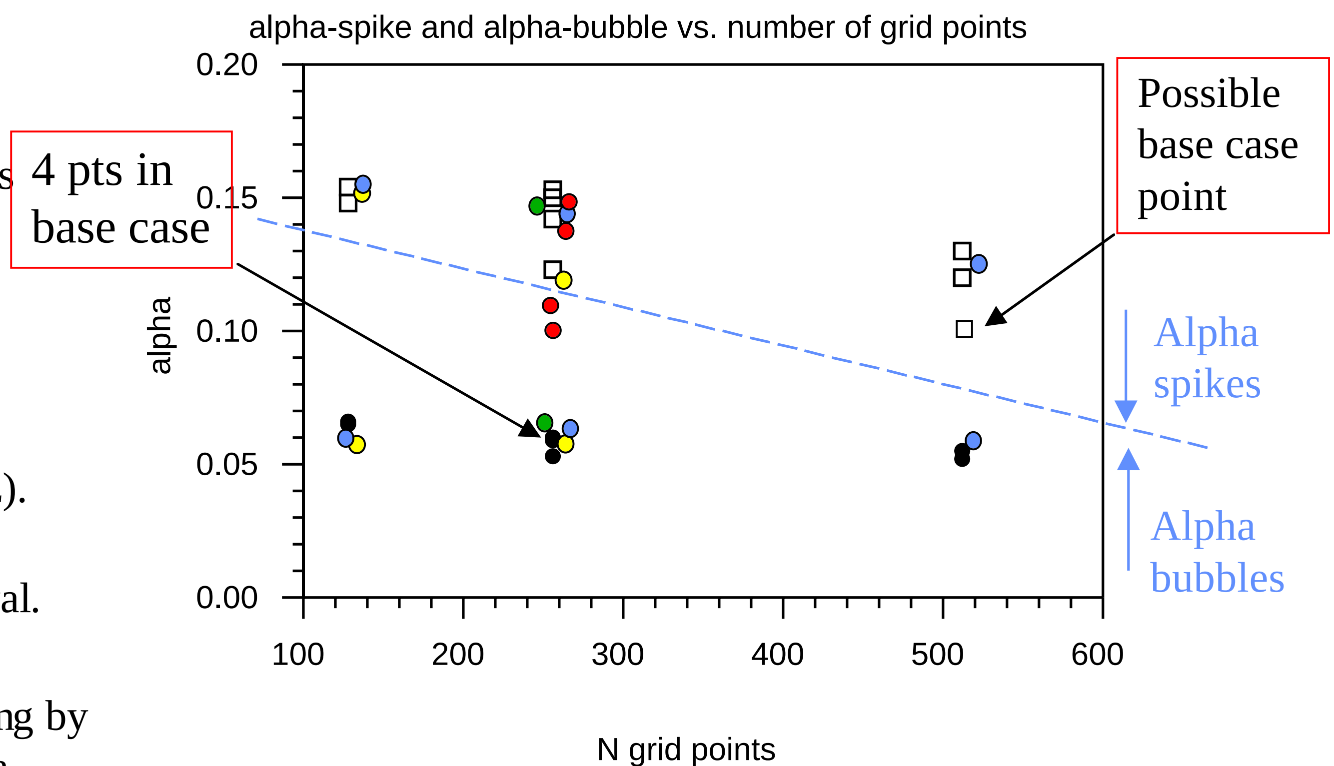
# RT resolved simulation cases alpha summary for At=0.8

- □ Base cases - spikes
- ● Base cases - bubbles
- ● (yellow) delta(IC)= delta(base case)/2 - bubble or spike
- ● (green) IC: $e = e_0$, $\rho = \rho(z)$.
- ● (red) x-ave contours eval.
- ● (blue) w/af- atomic mixing by drift flux momenta



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# Analytic model compared to fluid equations

Analytic model:

$$\frac{\partial h}{\partial t} = u$$

$$\frac{\partial u_i}{\partial t} + C_{Di}\frac{u_i^{\,2}}{(\delta_o + \alpha_o h_i)} = \beta_i Ag$$

Fluid model:

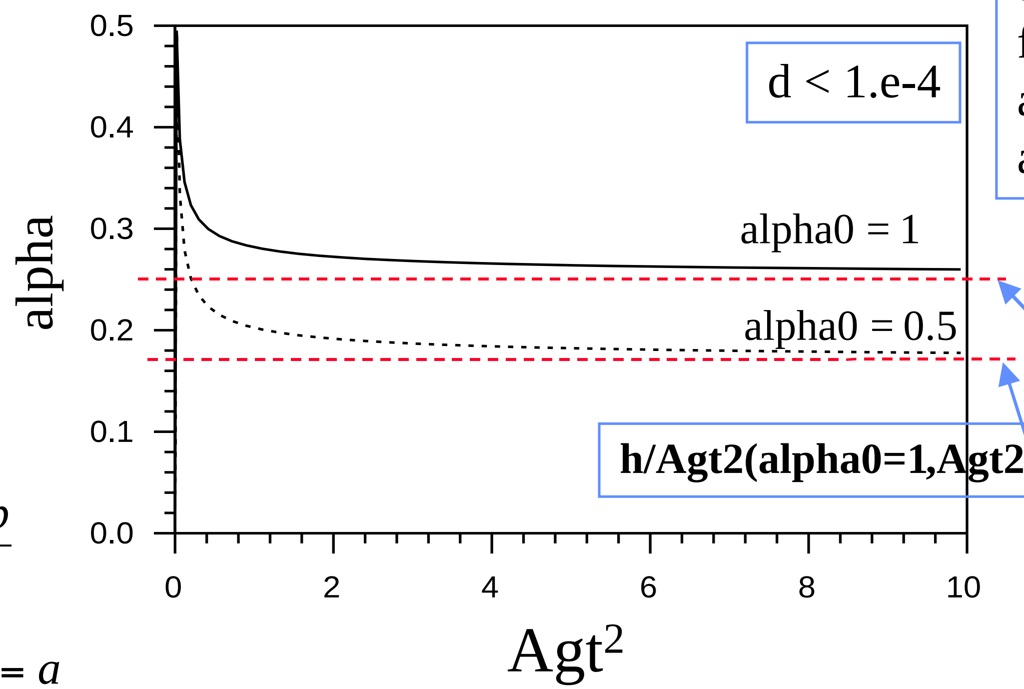
$$\frac{\partial h_m}{\partial t} \sim u_g$$

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = a \sim Ag - \frac{\nabla p}{\rho}$$

OR: $$\frac{\partial u}{\partial t} + \frac{\nabla u_s^2}{2} - u \times \omega = a$$

OR: $$\frac{\partial u}{\partial t} + \frac{u_x^2}{2L_x} + \frac{u_y^2}{2L_x} - u \times \omega \sim a$$

alpha result (h/Agt²)




alpha(tot)
for Dc=0.5
alpha0 = 1
alpha0=0.5

**h/Agt2(alpha0=1,Agt2>>100) -> 0.25**

**h/Agt2(alpha0=0.5,Agt2>>100) -> 0.17**

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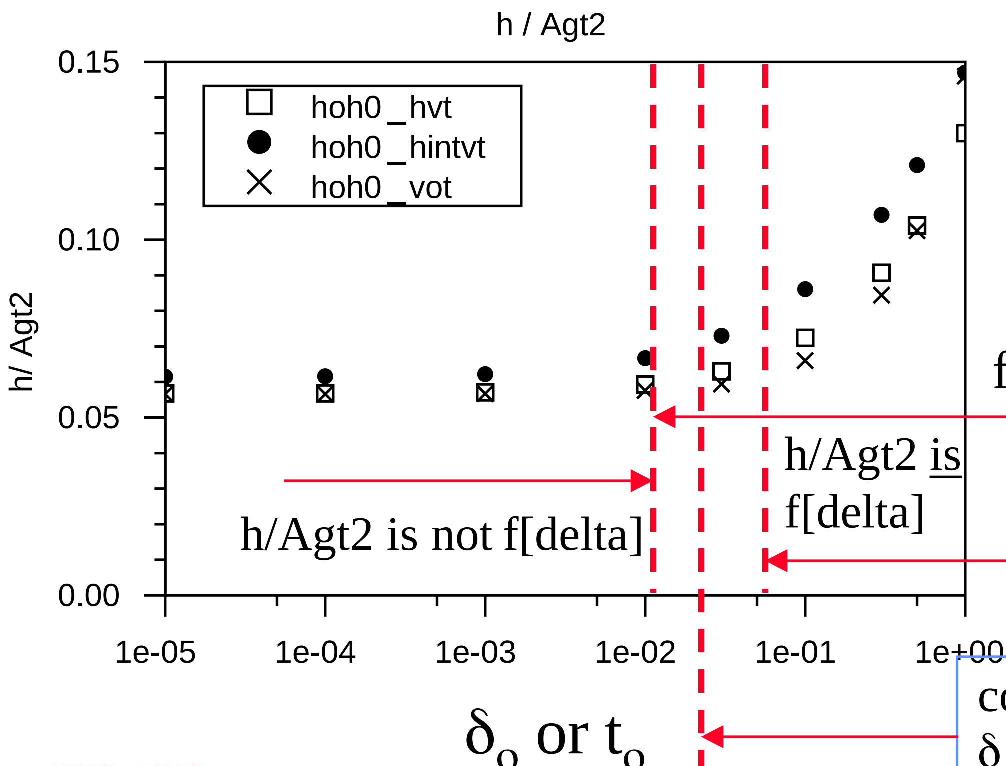
# h/Agt2 as f[delta0]

v determined as: hoh0_hintvt:

$$\frac{\partial v}{\partial t} + \frac{v^2}{(\delta_o + \alpha_c \int v\ dt)} = a \qquad \alpha_c = 0.12$$

Normalize $\delta_o$ to L = $Agt^2$

$\delta_o$ ~ variance of Vf(IC)




for comparison to comput. setup
$\delta_o$/L=1.e-2/5=0.002

comput on 128 grid:
$\delta_o$/L~var(Vf-IC)/L~0.7dx/70dx
or $\delta_o$/L(128)~1.e-2

comput on 256 grid:
$\delta_o$/L~var(Vf-IC)/L~0.7dx/140dx
or $\delta_o$/L(256)~0.5e-2

# RT spectral density for IC perturbation w/ modes k=30-60: $z_{int}(t=0) \sim Vf$

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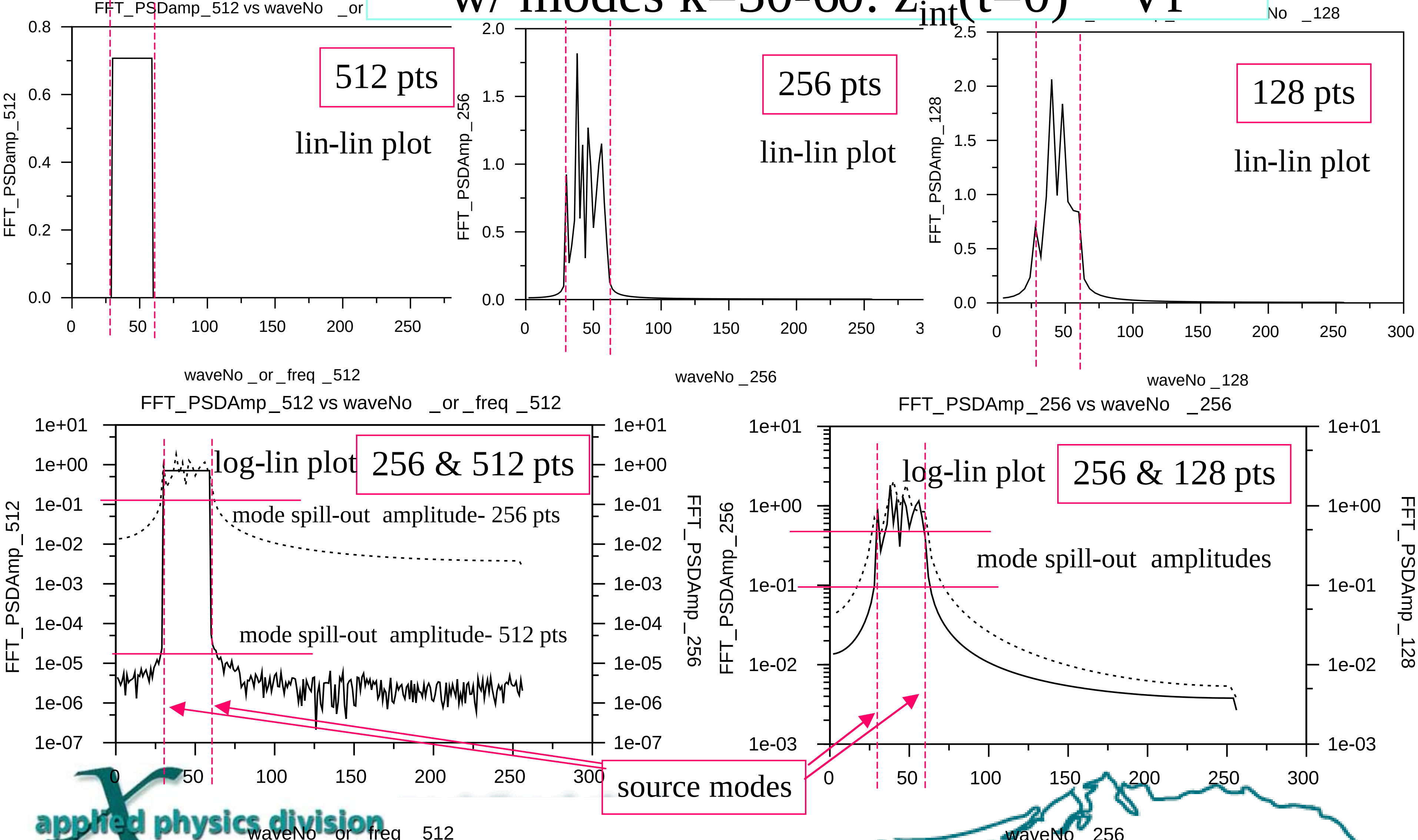

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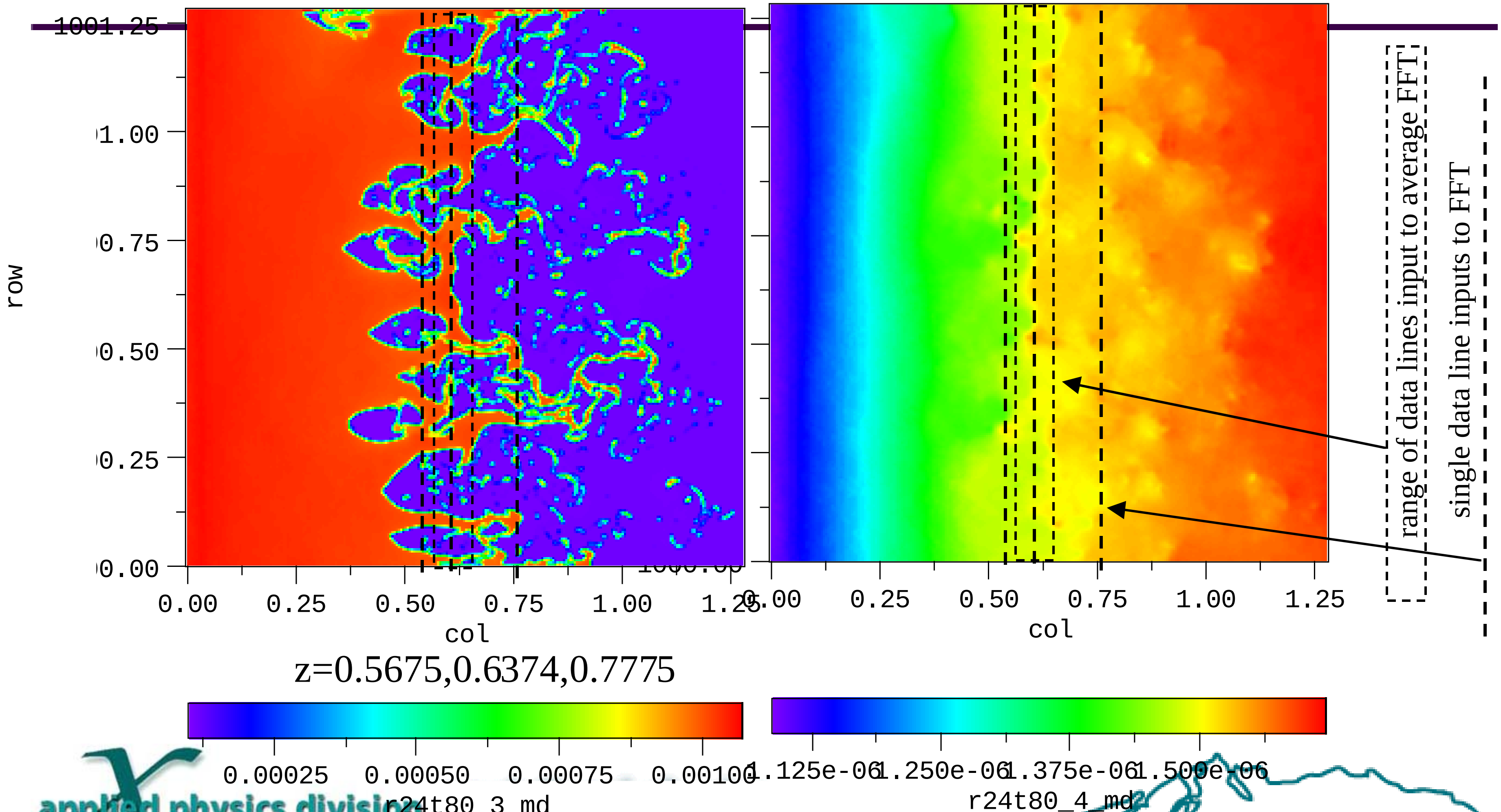
# locations for FFTs at t80



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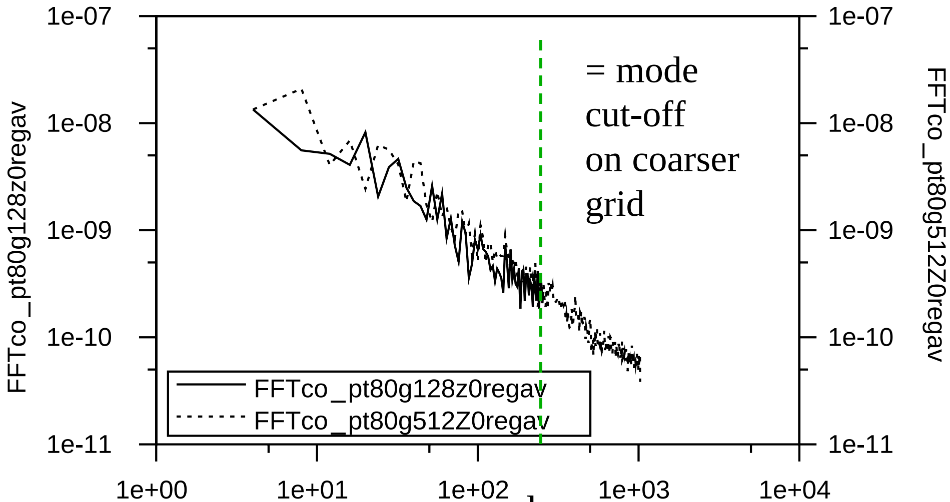
# FFTs p-t80 128 & 512

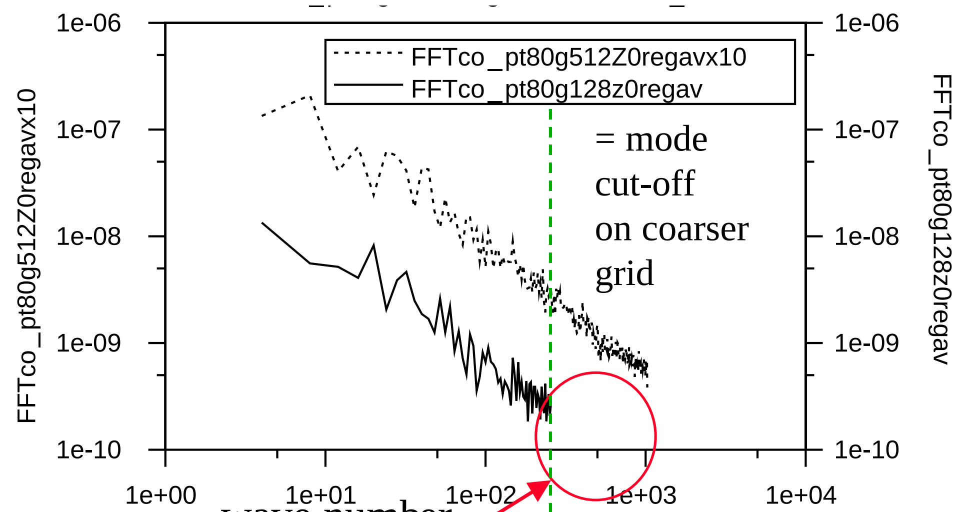
p spectra (left) w/ 10x shift on 512 grid (right) to compare

p-t80 128 & 512




wave number

p-t80 128 & 10x p-t80 512




wave number

Therefore, unresolved components on 128 grid appear to be irrelevant to small k, long wavelength mode growth**.

** alternative explanation: numerical errors on 128 grid and resolved high mode numbers on 512 grid both have the same effect on the small k, long wavelength mode growth***.

*** alternative alternate: the alternate is true and the effect in either case is ~ 0.

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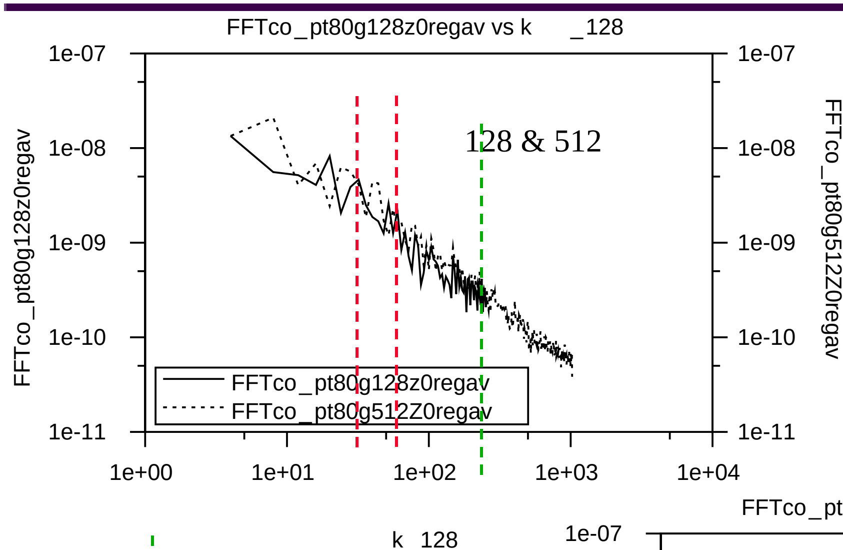
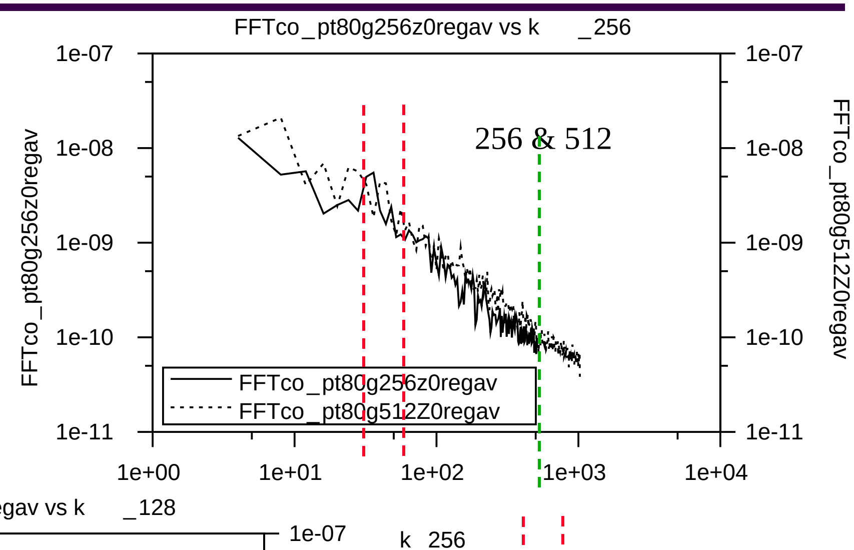
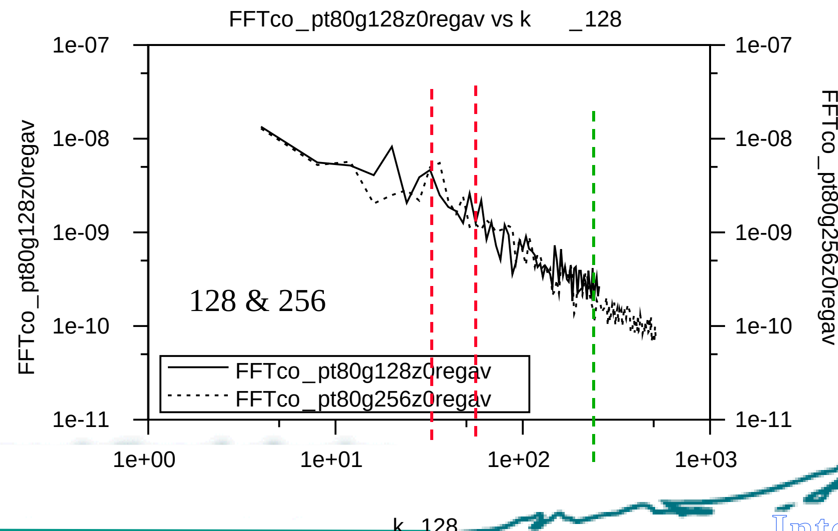
# FFTs p-t80, grids compared

## 128 & 512, 256 & 512, 128 & 256




= mode cut-off on coarser grid

= range of IC modes

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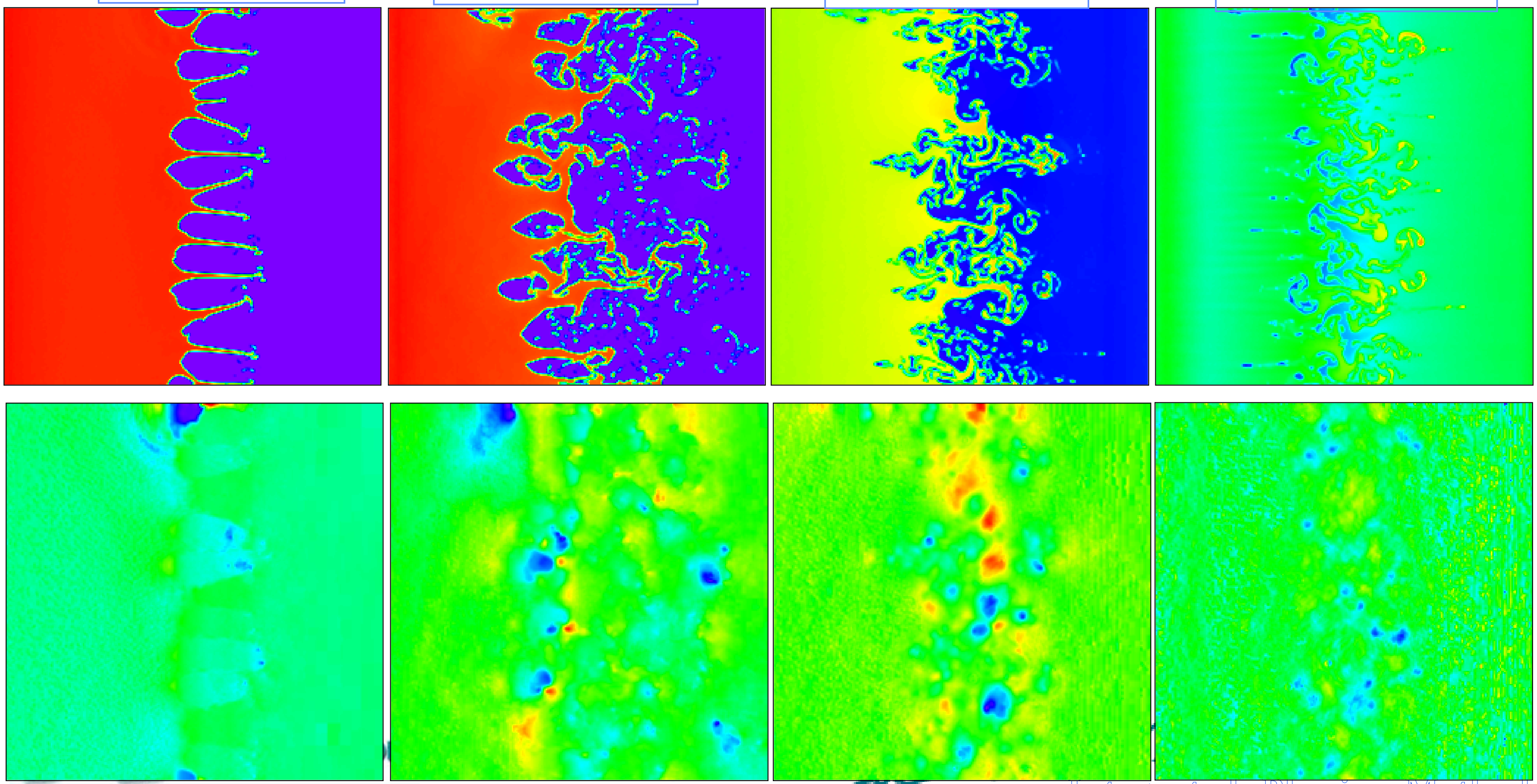
# RT mix at late time -varying Atw

| At = 0.96 | At = 0.8 | At = 0.33 | At = 0.048 |
|---|---|---|---|
| ρ1/ρ2 = 50 | ρ1/ρ2 = 9 | ρ1/ρ2 = 2 | ρ1/ρ2 = 1.1 |
| t = 60 (z = 2.6) | t = 80 (z = 3.84) | t = 120 (z = 3.6) | t = 320 (z = 3.66) |



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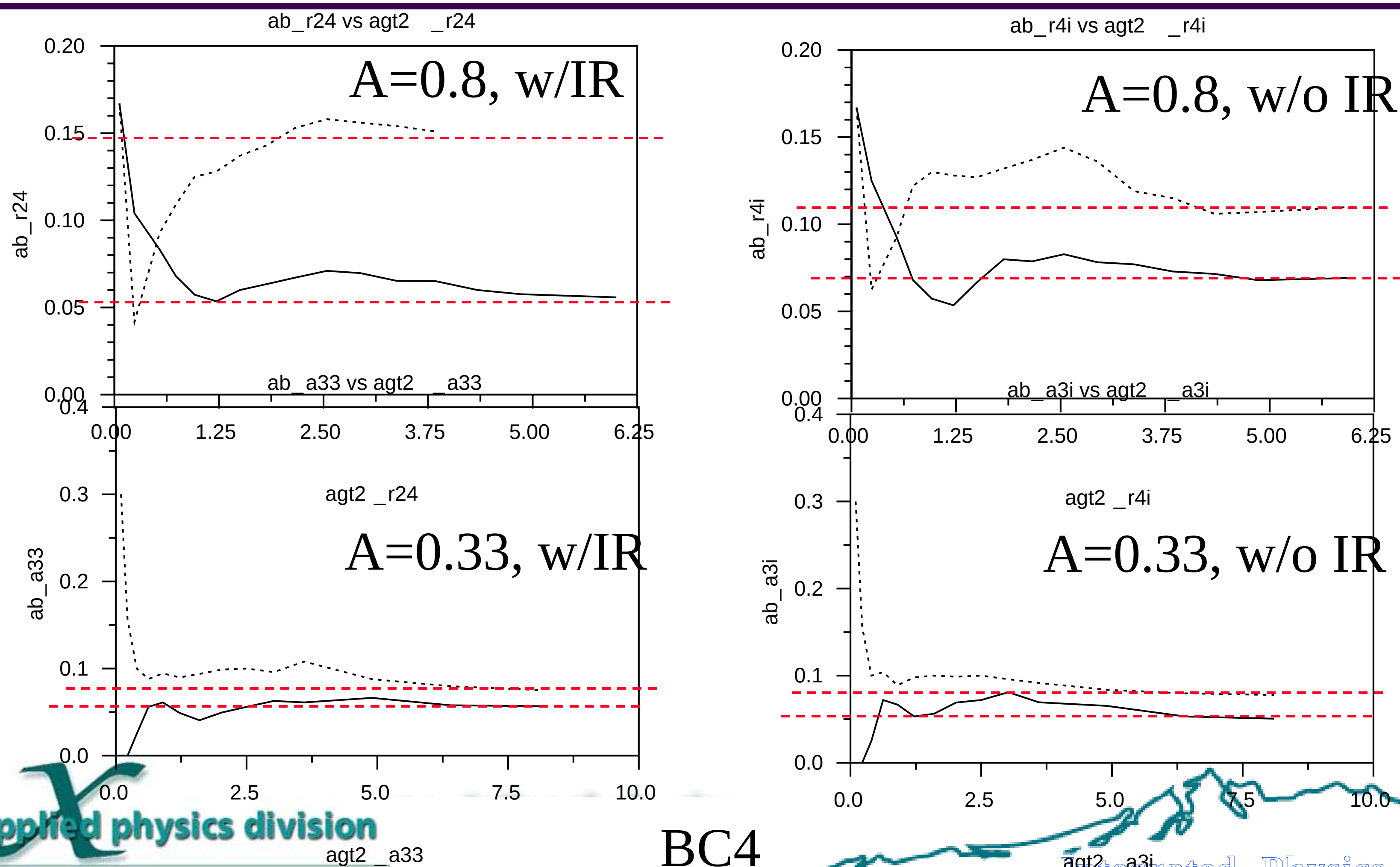
# Alpha (RT growth rate)
## for varying Atwood number and w/ & w/o Interface Recon.




BC4

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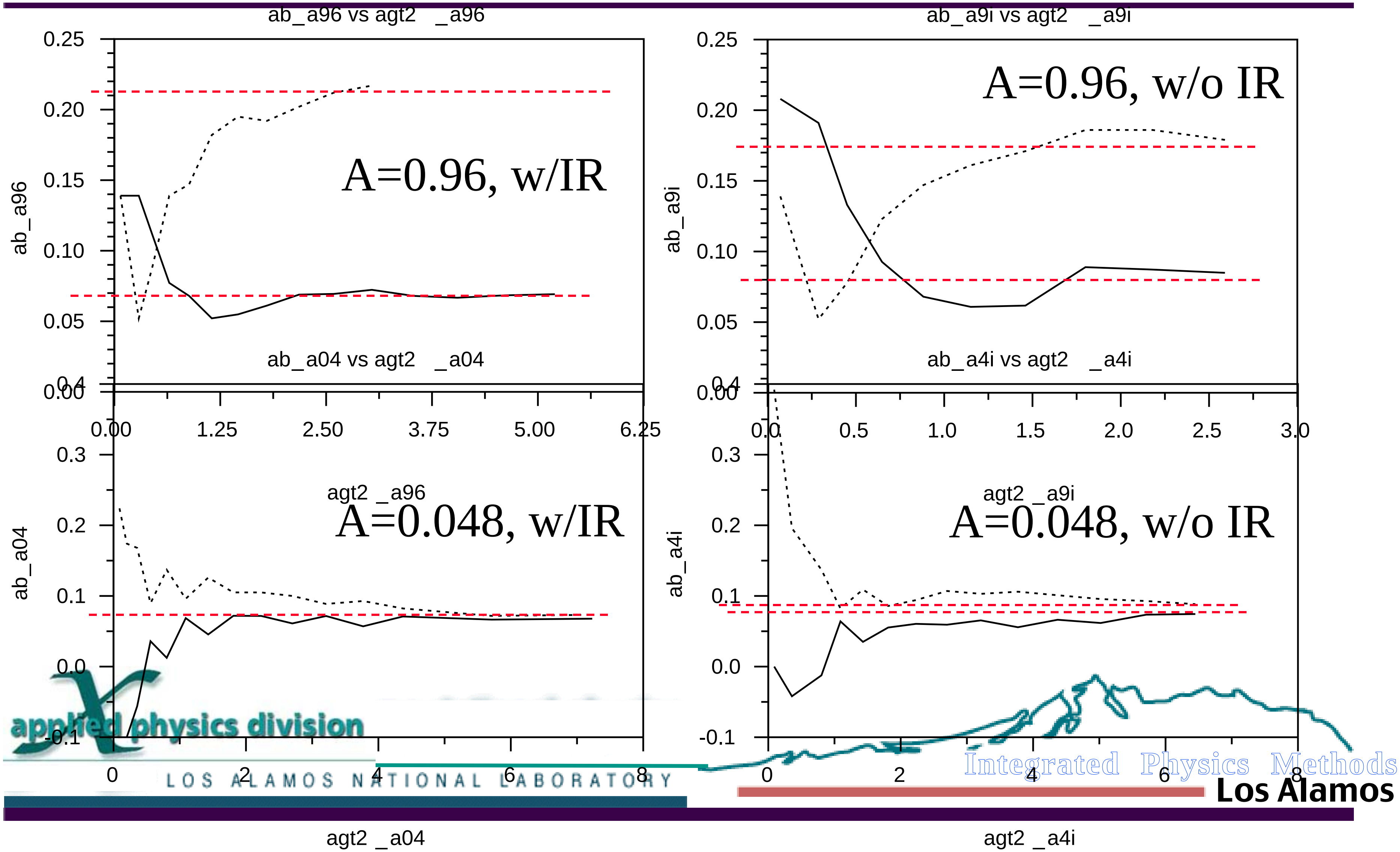
# Alpha (RT growth rate)

## for varying Atwood number and w/ & w/o Interface Recon.



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# Conclusions: R-T Mix Layer Growth

- **Results apply to 2-D multi-mode-IC simulations for At=0.8**
- **Grid convergence is good for alpha bubbles - less certain for alpha spikes.**
- **Alpha bubble computed here, ~ 0.05-0.065, agrees with experimental data.**
- **Discrepancy with other computations predicting lower alpha (~0.03)**
  - may be mostly due to treatment of internal energy discontinuity at interface and/or the internal energy in the long wavelength IC which contributes to growth rate through energy fluctuations.
  - a smaller difference (~15%) is expected between 2-D and 3-D.
  - It is shown to be unlikely that discrepancy is related to compressibility, hydrostatic equilibrium form, IC mode amplitudes or IC mode spectra details, or front evaluation methods..
- **Internal energy fluctuations dominate over density fluctuations where ($e_o/\rho_o$) is sufficiently small in the mix layer -**
  - this occurs in the heavier fluid even in limit as compressibility becomes 'negligible'.
  - $e_o$ is irrelevant in 'ideal' incompressible fluid, so only density fluctuations matter.
- **Transition from early time IC dominated regime to later time self-similar solutions is evident and agrees with analytic results.**
- **The resolved simulations appear to be adequately represented in the multi-fluid model so that we can now proceed to use the multi-fluid drift-flux model to represent the molecular mixing and/or sub-grid scale turbulent mixing within the Rayleigh-Taylor unstable mix layer.**