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Solution Verification and Analysis of xRAGE Modeling of the Rayleigh-Taylor Instability

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Abstract

- xRAGE is used to produce multiple model outputs of the Rayleigh-Taylor instability with varying mesh properties to determine a relationship between mesh properties, potential error, and instability length scales.
- We present both qualitative and quantitative analyses to assess numerical errors associated with the model, focusing on the convergence rates of both global and local numerical error metrics and the relationship between convergence rate and physical features of various length scales.
- Emphasis is placed on the early and transitional time regimes of the instability, as late time behavior becomes turbulent and various metrics used for analysis begin to diverge between simulations.

Introduction

- xRAGE is an Eulerian hydrocode that uses a spatially fixed mesh with Adaptive Mesh Refinement (AMR).
- Each simulation is conducted over a 2 dimensional, constant-size square domain with an area of 25 cm^2.
- For each simulation run 3 parameters are allowed to vary: i) the number of largest cells that fit horizontally and vertically (referred to as imxset), ii) the size of the largest cell, and iii) the size of the smallest cell.
- These simulations are meant to mimic the experiment conducted by Waddell et al (2001).
- The heavy fluid is a nearly saturated calcium nitrate/water solution, while the light fluid is a 70% isopropyl alcohol/water solution.

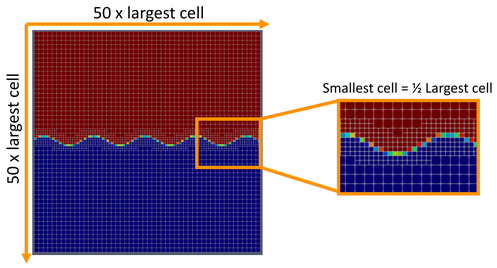

Figure 1: Diagram of AMR cells for square domain. The cells along the interface between the solutions are the most refined, since this is an area of interest.

Model Runs: General Study

- For the general study, the level of adaptive mesh refinement is set to 1.
- The number of cells vertically and horizontally (assuming all cells are the size of the largest cell) changes between each run.
- To accommodate a constant domain, the largest cell and smallest cell sizes must also change.
- A table of all simulations conducted for this study is presented below:

Number of Cells	Largest Cell	Smallest Cell	Levels of Refinement
50	0.5000	0.2500	1
100	0.2500	0.1250	1
150	0.1667	0.0833	1
200	0.1250	0.0625	1
250	0.1000	0.0500	1
300	0.0833	0.0417	1
400	0.0625	0.0313	1
500	0.0500	0.0250	1
600	0.0416	0.0208	1
700	0.0357	0.0179	1
800	0.0313	0.0156	1
900	0.0277	0.0139	1

Table 1

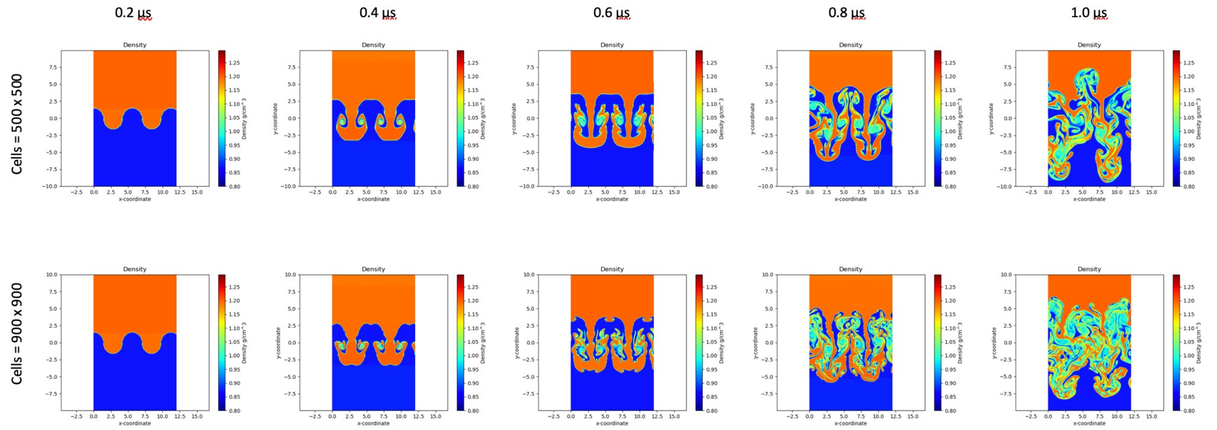

Figure 2: Density field snapshots for two different model runs. Top row corresponds to 500 cells horizontally and vertically, while the bottom row corresponds to 900 cells horizontally and vertically. Each column corresponds to a simulation time between 0.2 microseconds and 1.0 microseconds.

Density Fields

- Qualitatively, from figure 2, the simulations match closely up to about t = 0.8 μs.
- To examine this quantitatively, equation (1) is used to calculate the differences between the most 'exact' density field (900 x 900) and the predicted density field (in the case of figure 3, a 500 x 500 run):

$$D_{sq} = (exact_t(x,y) - predicted_t(x,y))^2 \qquad (1)$$

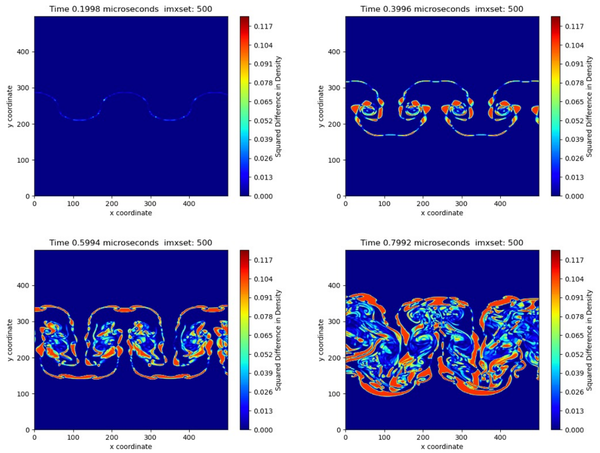

Figure 3: Squared difference in density fields between a 900 x 900 grid and a 500 x 500 grid each with one level of refinement at various simulation times. Calculated using equation (1).

- From figure 3, as time increases, areas of large differences arise.
- At t ~ 0.8 μs, coherent regions of red structures form, highlighting large areas of differing densities between the two simulations.
- If equation (1) is collapsed spatially, an L2 error can be calculated to yield a single point for each imxset value at a specified time (presented in figure 4):

$$L2 = \sum_{y=0}^{500}\sum_{x=0}^{500}(exact_t(x,y) - predicted_t(x,y))^2 \qquad (2)$$

- Note on summations: since each simulation uses a geometrically different mesh, the output of each run is interpolated over a uniform 500 x 500 grid so that they can be directly compared.

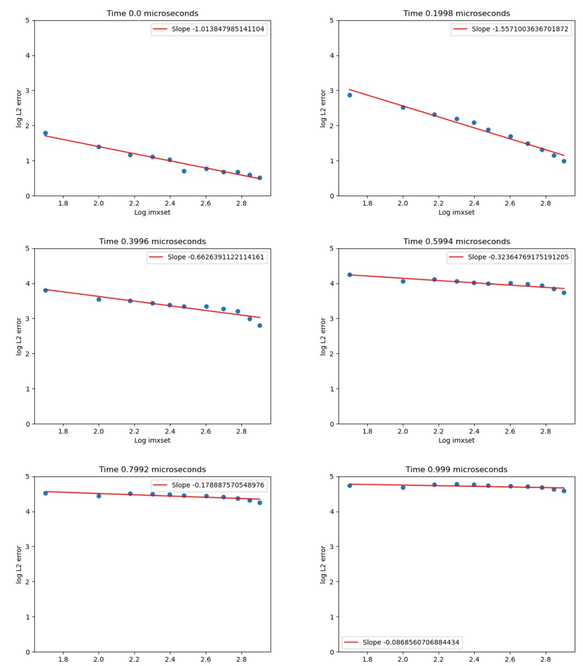

Figure 4: Converging trends for density field errors of varying imxset values. At early times the slope is about -1.0.

- The theoretical order of convergence for xRAGE is $\mathcal{O}\sim 1$, so we are finding the expected behavior at early times.
- This decays quickly after some amount of simulation time.
- Likely due to unresolved small-scale features as the instability begins to transition to a more non-linear/turbulent regime.

Model Runs: Adaptive Mesh Refinement Study

This study is intended to act as a check on the AMR scheme. Several runs are conducted to mimic the results from the imxset = 600 case with one level of refinement as presented in the general study (table 1).

Number of Cells	Largest Cell	Smallest Cell	Levels of Refinement
150	1.67E-1	2.08E-2	3
300	8.33E-2	2.08E-2	2
600	4.17E-2	2.08E-2	1
1200	2.08E-2	2.08E-2	0

Table 2

- Equation (1) was used to determine the degree of similarity between each AMR simulation from table 2 and the 600 x 600 case from table 1.
- From figures 5 and 6, it was determined that simulations with smaller imxset values, but more levels of refinement are comparable to simulations with a large imxset value and fewer levels of refinement.

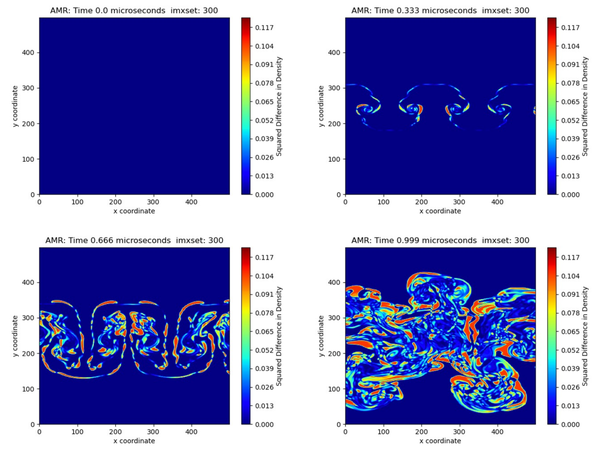

Figure 5: Squared difference in density fields between a 600 x 600 grid with one level of refinement and a 300 x 300 grid with 2 levels of refinement at various simulation times. Values were calculated using equation (1).

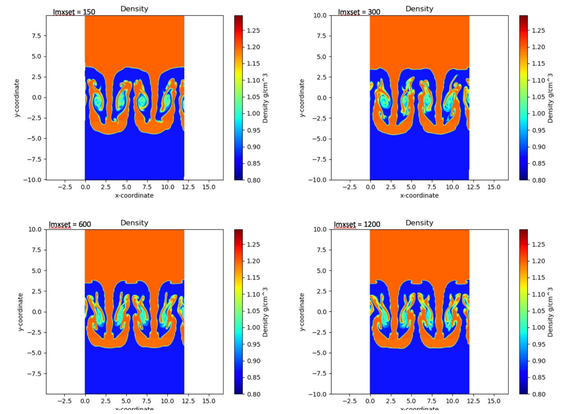

Figure 6: Density field snapshots at time = 0.63 microseconds for all AMR simulations in accordance with table (2).

Findings and Future Work

- Higher resolution is not always better – may resolve unphysical features.
- Simulations with smaller imxset values, but more levels of refinement are comparable to simulations with a large imxset value and fewer levels of refinement.
- Future Work: Investigate the convergence of different length-scales.

References

1. Grove, John W. "Eulerian Applications Project - xRage Introduction and Overview." Los Alamos National Laboratory, (2019).
2. Waddell, J. T, C. E Niederhaus, and J. W Jacobs. "Experimental Study of Rayleigh–Taylor Instability: Low Atwood Number Liquid Systems with Single-mode Initial Perturbations." Physics of Fluids (1994) 13.5 (2001): 1263-273. Web.
3. Wilkinson, J. P, and J. W Jacobs. "Experimental Study of the Single-mode Three-dimensional Rayleigh-Taylor Instability." *Physics of Fluids (1994)* 19.12 (2007): 124102. Web.