Direct Numerical Simulations of Rayleigh-Taylor Instability

Daniel Livescu, Mark R. Petersen, Tie Wei, CCS-2

We have conducted high-resolution, high-Reynolds number DNS of the RT instability on the 0.5-Petaflops, 150-k compute cores BG/L Dawn supercomputer at LLNL. This includes a suite of simulations with Atwood numbers ranging from 0.04 to 0.9 and grid size of 1024^2 by 4032, and a high-resolution simulation of grid size 4096^2 by 4608 and Atwood number of 0.75, currently ongoing. After the layer width developed substantially, additional branched simulations were run under reverse gravity and zero gravity conditions. The simulations provide an extensive database to study RT turbulence, including mixing layer growth rates, turbulence and mixing asymmetries, self-similar behavior, and spectral characteristics. Individual terms of the moments transport equations are recorded to develop and validate turbulence closure models. Here we showcase preliminary results on the long-standing open question regarding the discrepancy between the experimentally and numerically measured mixing layer growth rates.

Rayleigh-Taylor instability (RTI), which is generated at the interface between a heavy and a light fluid subjected to a constant gravitational field in an unstable configuration, is of fundamental importance in a multitude of applications, ranging from fluidized beds, oceans and atmosphere, to inertial confinement fusion (ICF) and supernovae explosions [1-2]. Although this instability has been subjected to intense research over the last 50 years, early numerical studies have been restricted to coarse mesh calculations. On the other hand, it is experimentally notoriously difficult to accurately characterize the initial conditions and provide the detailed measurements needed for turbulence model development and validation. Thus, a large number of open questions remain unanswered about this instability, and even first-order global quantities, such as layer growth, are not completely understood and still give rise to intense debate [3]. Nevertheless, today's petascale computers allow fully resolved simulations of RTI at parameter ranges comparable to those attained in laboratory experiments, but providing, in carefully controlled initial and boundary conditions studies, much more information than the actual experiments. These extremely high-resolution simulations are enabling a look at the physics of turbulence and are testing turbulence models in unprecedented detail, hopefully contributing to a significant advance in our predicting capabilities.

To test various hypotheses related to the layer growth and elucidate the long-standing discrepancy between the experimentally and numerically measured growth rates, explore the turbulence and mixing characteristics, and provide data for model development and testing, we have performed fully resolved, very high resolution simulations of RTI with the CFDNS code [4]. These simulations, currently ongoing, are the largest fully resolved simulations of the RTI to date and cover the range of Atwood numbers, A=0.04–0.9, in order to study small departures from the Boussinesq approximation as well as large Atwood number effects, which are even less understood (Fig. 1). After the layer width developed substantially, additional branched simulations were run under reverse gravity and zero gravity conditions. This “gravity reversal” occurs in practical situations (e.g., ICF or pulsating stars), however there are no fully resolved simulations to date in this configuration.

While the bulk of these results are still being analyzed, we here showcase some preliminary results regarding the instability growth. The temporal evolution of the Rayleigh-Taylor (RT) layer width is an important question in applications, and one metric to gauge the efficacy of various models and numerical simulations. Although certain classes of initial conditions (e.g., if long wavelengths are present in the initial perturbation) may have a long-lasting influence on the growth rate, it is generally agreed that at long times, if the turbulence growth is unrestricted, the turbulent mixing layer grows quadratically in time:

$$h = \alpha A g t^2 + 2\sqrt{\alpha A g h_0}\, t + h_0$$

The quadratic growth has been known for a long time as a dimensionally consistent result confirmed by experimental data. This formula,

For more information contact Daniel Livescu at livescu@lanl.gov.

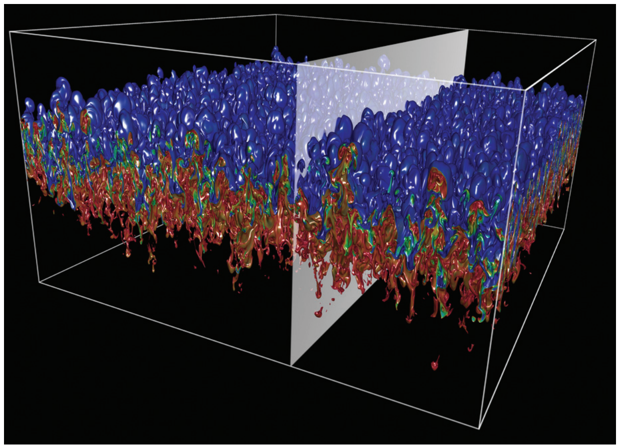

Fig. 1. Three-dimensional visualization of the density field showing the asymmetry of the Rayleigh-Taylor mixing layer, with the development of "bubbles" on the heavy fluid side and "spikes" on the light fluid side.

including various consistent ways for extracting the value of α, is further discussed in [3]. Nevertheless, the value of the growth rate, α, is still hotly debated and there is a large discrepancy between the values reported by numerical (non-direct numerical simulation [DNS]) simulations and many experiments, which constitutes a long-standing open question. To compound this open question, most numerical studies to date are under-resolved simulations relying on numerical errors to stabilize the Gibbs phenomenon. In addition, it is notoriously difficult, experimentally, to accurately characterize the initial conditions and provide the detailed measurements needed for turbulence model development and validation. The leading hypotheses for the discrepancy in the reported α values stem from these drawbacks—too large diffusion in the numerical simulations, and undesired perturbations corrupting the initial conditions in the experiments. In our fully resolved simulations we found little change in the value of α when varying the values of the molecular transport properties. Moreover, we have also performed simulations with various initial perturbation spectra. The preliminary analysis of these results points to two possible explanations for the higher growth rates measured in various experiments, and either one or both explanations can apply: (1) experimental set-up is too small and thus the measurements represent only the early time behavior, and/or (2) layer growth is affected by the lateral walls due to large wavelengths present in the initial perturbation spectrum. To exemplify, Fig. 1 presents results from several simulations with a top-hat initial perturbation spectrum and different spectrum widths and/or amplitudes. Even though the early time behavior may suggest different growth rates, the long time results show the same asymptotic value for α. While our results are preliminary, there are at least two experimental studies with carefully controlled initial conditions supporting the hypotheses above [5,6]. Nevertheless, both of these hypotheses represent serious obstacles in characterizing the practical behavior, due to the lack of generality of the early time evolution and of the interaction with the walls.

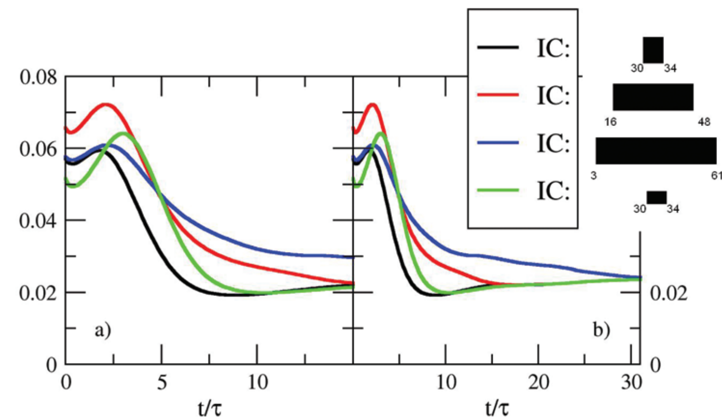

Fig. 2. Rayleigh-Taylor growth rate α from several simulations with A=0.04 and different initial perturbation spectra, shown in the legend. (a) Early time behavior may suggest different growth rates. (b) Long time results show the same asymptotic value.

[1] Livescu, D. and Ristorcelli, J.R., *J Fluid Mech* **605,** 145 (2008).
[2] Livescu, D., et al., *J Turbul* **10,** 1468 (2009).
[3] Livescu, D., et al., "New Phenomena in Variable-density Rayleigh-Taylor Turbulence," *Phys Scripta*, in press (2010).
[4] Livescu, D., et al., "CFDNS: A Computer Code for Direct Numerical Simulations of Fluid Turbulence," LA-CC-09-100 (2009).
[5] Carles, P., et al., *Phys Rev Lett* **96,** 104501 (2006).
[6] Olson, D.H. and Jacobs, J.W., *Phys Fluid* **21,** 034103 (2009).

Funding Acknowledgments
Science campaigns, LDRD DR 20090058