Direct Numerical Simulations of Rayleigh-Taylor Instability with 0.04 ≤ A ≤ 0.9

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We have concluded our high-resolution, high-Reynolds-number Direct Numerical Simulations (DNS) of the Rayleigh-Taylor instability (RTI) on the 0.5-petaflop/s, 150-k compute cores BG/L Dawn supercomputer at LLNL. This represents a large set of simulations that include a suite of runs with Atwood numbers ranging from 0.04 to 0.9 and a multitude of initial conditions on a grid size of 1024^2 by 4608, as well as a high resolution run of grid size 4096^2 by 4032 and Atwood number of 0.75. After the layer width had developed substantially, additional branched simulations were run under reverse gravity and zero gravity conditions. The simulations provide an extensive database for the study of RTI turbulence and its dependence on the initial conditions, including mixing layer growth rates, turbulence and mixing asymmetries, self-similar behavior, and spectral characteristics. Individual terms of the moments transport equations have been recorded to develop and validate turbulence closure models. Here, we showcase the preliminary analysis of the data in connection with the growth of the layer and the turbulence problem.

Molecular mixing in response to stirring by turbulence is an important process in many practical applications. When the microscopic densities of the fluids participating in the mixing are very different, these flows have been referred to as variable density (VD) flows, in contrast to the Boussinesq approximation in which the densities are commensurate [1]. Fundamental turbulence studies as well as specific engineering models for such VD flows are scarce [2,3]. Many of these flows are driven by acceleration (e.g., gravity in geophysical and astrophysical flows) which, because the density is not uniform, leads to large differential fluid accelerations. If the acceleration is constant and the fluid configuration is unstable (i.e., the density gradient points opposite to the acceleration), a fluid instability is generated in which small perturbations of the initial interface between the two fluids grow, interact nonlinearly, and lead to turbulence. This instability is known as the Rayleigh-Taylor instability (RTI) and is of fundamental importance in a multitude of applications, from fluidized beds, oceans and atmosphere, to inertial, magnetic, or gravitational confinement fusion, and to astrophysics.

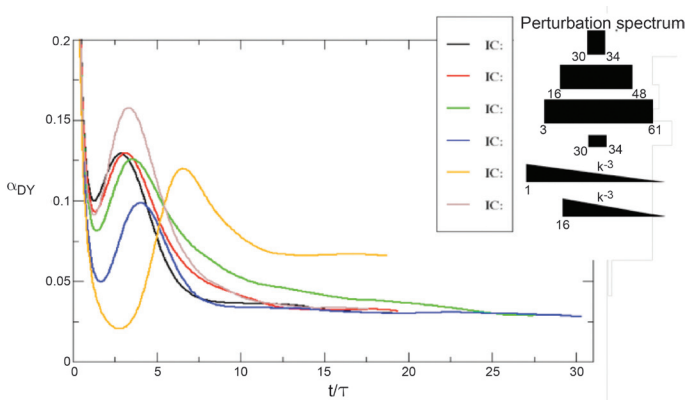

Fig. 1. Rayleigh-Taylor bubble growth rate α from several simulations with A=0.04 and different initial perturbation spectra, shown in the legend. DNS with appropriate perturbation spectrum can reproduce the higher growth rates seen in the experiments.

Although this instability has been subjected to intense research over the last 50 years (e.g., over 100 RTI-related papers are published every year in peer-reviewed journals), early numerical studies have been restricted to coarse mesh calculations. On the other hand, it is notoriously difficult, experimentally, 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 [4,5]. 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 condition studies, much more information than the actual experiments [2]. These extremely high-resolution simulations are enabling a look at the physics of turbulence and testing turbulence models in unprecedented detail, hopefully contributing to a significant advance in our predicting capabilities.

To examine the turbulence and mixing properties, provide data for model development and testing, and explore the influence of the initial conditions, we have performed fully resolved, very-high-resolution simulations of Rayleigh-Taylor instability with the CFDNS code [6]. These simulations are the largest fully resolved simulations of the RTI to date and cover the range of Atwood numbers A=0.04 to 0.9 in order to study small departures from the Boussinesq approximation

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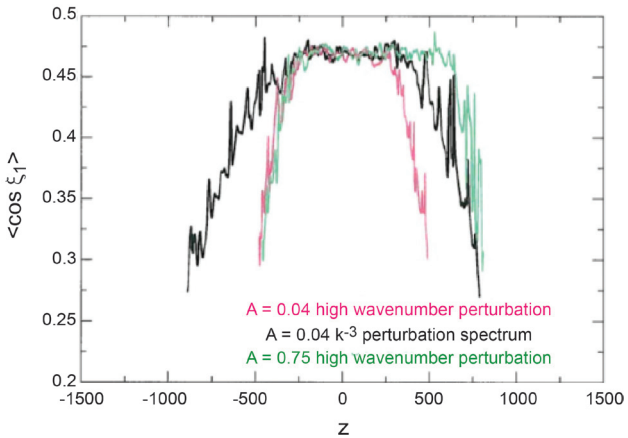

Fig. 2. The variation across the layer of the mean cosine of the angle between the vorticity vector and the most extensional eigenvector of the strain rate tensor. The interior turbulent regions do not depend on the initial conditions for a given A and the vorticity alignment is similar to other canonical turbulent flow. The edge regions have clear non-turbulent behavior and their extent depends on the initial conditions.

as well as large Atwood number effects, which are far less understood. Thus, most previous studies address the low-to-moderate A and no DNS have been reported, prior to the present set, for A>0.5. At high A, the velocity field is no longer solenoidal even when the two fluids are incompressible. The development of the instability and the mixing itself are fundamentally different at high and low A [1,5]. After the layer width had developed substantially, additional branched simulations were run under reverse gravity and zero gravity conditions. This "gravity reversal" occurs in practical situations (e.g., inertial confinement fusion [ICF] or pulsating stars), however there are no fully resolved simulations to date in this configuration.

Our preliminary analysis of the data has shed new light on the long-standing open question regarding the discrepancy between the numerically and experimentally computed mixing layer growth rates [7]. Thus, the results point to two possible explanations for the higher growth rates measured in various experiments (either one or both explanations can apply): 1) experimental set-up too small and thus the measurements represent only the early time behavior, and/or 2) layer growth affected by the lateral walls due to large wavelengths present in the initial perturbation spectrum. These hypotheses are also supported by two recent experimental studies with carefully controlled initial conditions [8,9]. An important finding resulting from our extensive dataset is that we were able to identify classes of initial conditions which can lead to faster-mixing layer growths, comparable to the experimental values.

In general, higher self-similar growth rates are obtained if the initial perturbation spectrum contains significant low-wave-number content, such as a spectrum of the type k^{-3} starting at k=1. In this case, the instability is laterally confined (the horizontal scales cannot grow larger) and the growth mechanism is different than mergers of bubbles and spikes, as previously thought to characterize RTI layer growth. In fact, the behavior near the edges of the dominant bubble/spike is very similar to what we discovered in a previous study occurs in single-mode RTI at late times [10]. In this case, the vortexes generated on the sides of the bubble/spike self-propagate towards the edges of the layer and the induced velocity due to these vortexes helps the instability growth. This mechanism occurs for the other classes of initial conditions as well, however the vortical motions are influenced by the vortices in the nearby bubbles/spikes and the induced velocities are much weaker. Nevertheless, even for these cases, the merger growth mechanism is still less important for the overall growth. Further investigation of the edge regions has also shown, for the first time, that the mixing layer consists of a fully turbulent inner region and a turbulent/non-turbulent interface near the edges. The turbulent region becomes independent of the initial conditions for a given A, while the turbulent/non-turbulent interface retains the memory of the initial conditions and can grow at different rates for various classes of initial conditions. This shows that the mixing layer width measure in use today needs to be updated and establishes a minimum growth rate for the overall layer width, as that given by the inner turbulent region.

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Funding Acknowledgments
Weapons Program, Science Campaign 4