Molecular mixing as a consequence of stirring by turbulence is an important process in many practical applications. If the microscopic densities of the fluids participating in the mixing are very different, we refer to such flows as variable density (VD) flows in contrast to the Boussinesq approximation in which the densities are close. In VD flows, the velocity field is no longer solenoidal, even if the fluids participating in the flow are incompressible. VD mixing is encountered in atmospheric and ocean flows, astrophysical flows, combustion and many flows of chemical engineering interest. 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. density gradient points opposite to the body force), 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 (RT) instability and is of fundamental importance in a multitude of applications, from fluidized beds, oceans and atmosphere, to ICF and supernovae explosions. Due to RT instability, any perturbation with a wavelength larger than the cutoff due to surface tension (for the immiscible case) or mass diffusion (for the miscible case) will grow. As the perturbation grows, smaller and larger eddies are generated by nonlinear interactions and eventually the flow becomes turbulent.

In many cases, the density ratio between the two fluids is large (e.g. air interpenetrating helium has a density ratio of 7), yet most studies to date address the low density ratio case and no Direct Numerical Simulations have been performed for Atwood number, A > 0.5 (corresponding to a density ratio of 3), where 0<A<1. Previous results at Atwood numbers up to 0.5 [1,2,3] indicate that mixing becomes qualitatively different at high density ratios (the variable density case) compared to the case when the densities of the two fluids are commensurate (the Boussinesq approximation). Thus, in an idealized triply periodic configuration, [1] pure heavy fluid mixes more slowly than pure light fluid: an initially symmetric double delta density PDF is rapidly skewed. The density PDF skewness generation mechanism, $< \nabla \cdot \nabla \rho \rho \rho >$, can be shown to be determined, [3] through changes in the magnitude of the density gradient, by the eigenvalues of the strain rate tensor and the relative alignment between the density gradient and the eigenvectors of the strain rate tensor. Both the eigenvalues and relative alignment are different in the pure heavy and light fluid regions. In the heavy fluid regions, the eigenvalues of the strain rate tensor have lower values, as the larger inertia of the heavy fluid leads to lower deformation rates of the fluid blobs. Larger inertia of the heavy fluid also leads to decreased alignment with the local flow. Thus, the local structure of the flow changes in response to the inertia of the fluid particles. Consequently, the inertia of the heavy fluid reduces the rate at which it is broken up by stirring, decreasing the local surface area of the pure heavy fluid blobs, which is related to the magnitude of the density gradient. The net result is that the magnitude of the density gradient is lower in the pure heavy fluid regions, along with the rate of molecular mixing, and the density PDF becomes skewed.

For the RT configuration at large density differences, this suggests that molecular mixing proceeds differently on the two sides of the RT layer. Experiments to date have not investigated this possibility. One consequence for the Rayleigh-Taylor case (as found from a 3072^3 simulation at A=0.5) [4] is that the penetration distance of the pure heavy fluid is larger than that of the pure light fluid. [2,3] The mixing asymmetry is likely also the cause of the bubble-spike anomaly (higher growth rate on the spike side compared to the bubble side), which was observed experimentally, but never explained.
As the Atwood number is increased above 0.5, the consequence of the mixing asymmetry becomes more obvious: the two edges of the mixing layer develop into “spikes” on the light fluid side and “bubbles” on the heavy fluid side. This can be clearly seen in Fig. 1, which shows the density field from a 2304x4096^2 Rayleigh-Taylor simulation at A=0.75, the largest fully resolved instability simulation to date. The simulation was performed on the ASC Dawn supercomputer, at Lawrence Livermore National Laboratory, during the open science runs. Most of the simulation was run on the full Dawn machine (147,456 processors). Currently, the simulation is being extended to 4608x4096^2.

Three-dimensional visualization of such large data sets also imposes enormous challenges and novel techniques were developed for this. Thus, Fig. 1 was generated using a parallel, hardware-accelerated analytical ray casting algorithm.

Fig. 1. (a) Three-dimensional visualization of the density field showing the asymmetry of the Rayleigh-Taylor mixing layer, with the development of “bubble” on the heavy fluid side (a) and “spikes” on the light fluid side (b).