# SHOCK-INDUCED TURBULENT MIXING

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## EXECUTIVE SUMMARY:

This project aimed to perform high-fidelity simulations of shock-induced multi-material mixing in a simple yet realistic configuration. Shock-induced acceleration of an interface between two different fluids renders the interface unstable to Richtmyer–Meshkov (RM) instability. Initial perturbations of the interface grow rapidly due to spatially varying torque exerted by the shock on the interface. Interaction of the reflected shock with a distorted interface causes a rapid breakdown of the flow into a turbulent state, which further stirs up the interface and drives mixing.

Our simulations focused on the interaction of a normal shock wave with a planar fluid interface that is at an incline to the shock wave. RM instability and shock-driven mixing is of paramount importance in many modern engineering and scientific applications: hypersonic air-breathing engines to increase mixing of fuel and oxidizer, the physics of the collapse of supernovae, transition from deflagration to detonation due to shock-flame interaction, and energy generation through inertial confinement fusion.

## INTRODUCTION

The National Academy of Engineering has identified "Provide Energy from Fusion" as one of the grand challenges for engineering. Inertial confinement fusion (ICF) is a clean, sustainable source of energy and has the potential to play a huge role in addressing concerns about energy security and global climate change. The Richtmyer–Meshkov (RM) hydrodynamic instability that causes premature mixing of the capsule interface has been identified as a critical factor that limits the performance of ICF. Though the ICF problem is far more complex, predictive simulations of the hydrodynamics of shock-induced mixing is key to better design of ICF targets.

We focused on the RM instability due to a normal shock impinging on an inclined material interface (fig. 1). The simulations were coordinated with experiments at the Shock Tube & Advanced Mixing Laboratory at the Texas A&M University [4,5] and were the first to address critical issues of flow confinement by walls and resolve the effects of molecular mixing in shock-driven turbulent mixing. The proposed numerical algorithms (high-order spectrally optimized compact scheme and anisotropic solution-dependent artificial fluid properties for shock and interface capturing) and flow solver infrastructure (Miranda) are ideally suited for the problem. Conditions in the laboratory experiment were duplicated in the simulations. This will allow systematic validation of the computed results at large scales. Databases on RM-instability-driven turbulence at unprecedented spatial resolution will allow investigation of fundamental questions about turbulence physics in strongly driven transient flows and also support development of novel sub-scale closures for variable-density turbulence.

FIGURE 2: Overlay of z-vorticity and dilatation fields at t=1.5 ms. The vorticity drives the flow dynamics and the dilatation shows the shock structure that is responsible for the vorticity deposition.


## METHODS & RESULTS

Due to the nature of the problem, numerical simulations of the RM instability required algorithms that treat both turbulence and discontinuities in the form of shock waves and material interfaces accurately. This is a unique challenge that is not addressed by traditional algorithms for turbulence or shock and interface capturing since the latter often employ excessive numerical dissipation for stability whereas the former try to minimize the numerical dissipation that can damp out the small scales of turbulence. The conflicting requirements make this problem extremely challenging.

We addressed this problem by using a tenth-order spectrally optimized compact difference scheme [2] in conjunction with the localized artificial diffusivity (LAD) scheme [1,3] for shock and interface capturing. The high order and spectral accuracy of the compact difference scheme preserved a high fraction of the theoretically resolvable scales in the flow without dissipating them. The LAD scheme defaulted to one with very low dissipation in smooth regions of the flow and surgically introduced numerical dissipation near regions of shocks and interfaces.

Fig. 2 shows an overlay of vorticity (in brown and green) and dilatation (in red and blue). This image shows the vorticity deposited on the interface by the shock that drives the dynamics of the problem. Complex shock patterns in blue are also seen and cause inhibition of the instability growth rate. Fig. 3 shows the mass fraction of SF6 at a later time of turbulent mixing.

## WHY BLUE WATERS?

The large range of scales in flows involving the RM instability, from scales dictated by the geometry of the problem to the fine scales that govern molecular diffusion, makes this problem very demanding in terms of computational resources required. Even a simulation with one billion grid points does not adequately capture all the physical scales in the problem. Accurate depiction of all the flow features would require much higher spatial resolution. In addition, computational requirements cannot be lessened due to the lack of accurate lower-fidelity models like a subgrid-scale model for compressible multi-species wall-bounded flows. The availability of a petascale resource was critical to the success of this project.

HPC resources available under the next Track-1 system would allow us to complete more realistic simulations of the inclined interface RM mixing and with varying parameters, which would enable development of effective subgrid models for such flows in the future.

FIGURE 3 (BACKGROUND): Mass fraction of $SF_6$ at t=5.0 ms. The flow at this time is in a turbulent mixing regime that causes air and $SF_6$ to mix. Fully white is air and dark blue is $SF_6$. Shades in between represent mixed states.

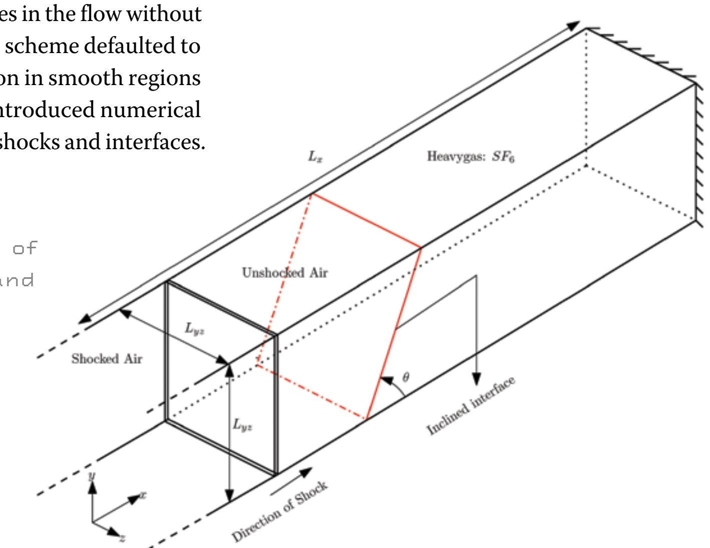


FIGURE 1: Schematic of the problem setup and initial conditions.