Towards peta-scale shock/turbulence computations

Dr. Eric Johnsen[1], Dr. Johan Larsson[1], Britton Olson[1], Prof. Sanjiva K. Lele[1] (PI), Prof. Parviz Moin[1], Dr. Andrew W. Cook[2]
[1] Stanford University, [2] Lawrence Livermore National Laboratory

Motivation

In a wide range of fluid flows, interactions between the following items lead to complex phenomena whose basic physics are not well understood:

- High Reynolds-number turbulence,
- Strong shocks,
- Interfaces and density variations.

Examples include supernovae explosions, scramjet combustion, ICF, detonations, shock wave lithotripsy.

Objectives

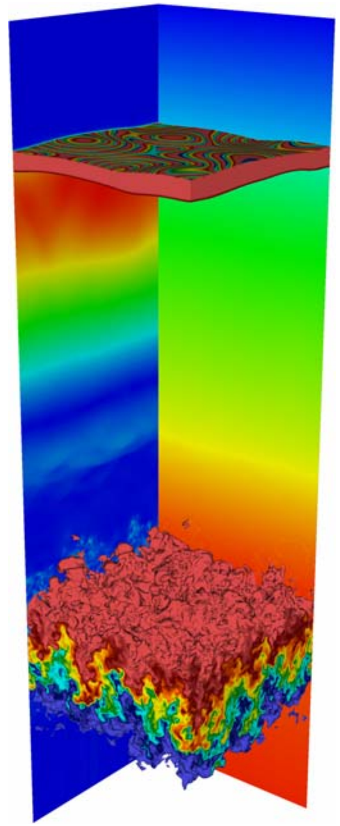
The goals of the present work are to:

1. Develop the best possible numerical algorithms capable of simulating turbulent flows with shocks,
2. Implement these algorithms on massively-parallel architectures,
3. Provide a scientific understanding of shock-turbulence interactions and multi-material mixing in complex flows.

Numerical methods

Several codes based on different algorithms have been developed and compared in the present study:

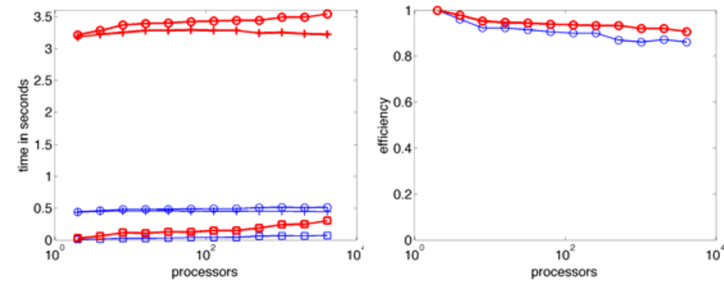
- *Hybrid*:
  - Shock-capturing (WENO) near discontinuities,
  - High-order accurate central differences in smooth regions,
  - Discontinuity sensor.
- *Miranda*:
  - High-order accurate compact schemes,
  - Artificial diffusivities to regularize the solution.
- *ADPDIS3D*:
  - High-order non-dissipative base scheme,
  - Adaptive multistep filter.
- Shock-fitting:
  - Track shock and apply jump conditions across it,
  - High-order finite difference approximations in smooth regions.



3D Compressible Rayleigh-Taylor instability (256x256x1024) with Xe (top) and Ne (bottom) using *Miranda*. Local Mach number (left panel), density on a log scale (right panel), Xe mass fraction in mixing region (lower iso-volume), temperature of the resulting shock wave (upper iso-volume).

Large scale computations
(*Hybrid* code)

- Programming language: C++,
- Parallelization: domain decomposition
  - Intra-node communication: MPI,
- Weak scaling efficiency above 91% for realistic grids when going from 2 to 4096 processors
  - NERSC Franklin machine,
- Collaborations with other SciDAC projects:
  - PERI: code profiling to optimize the computational efficiency,
  - VACET: visualizations with *VisIt*.

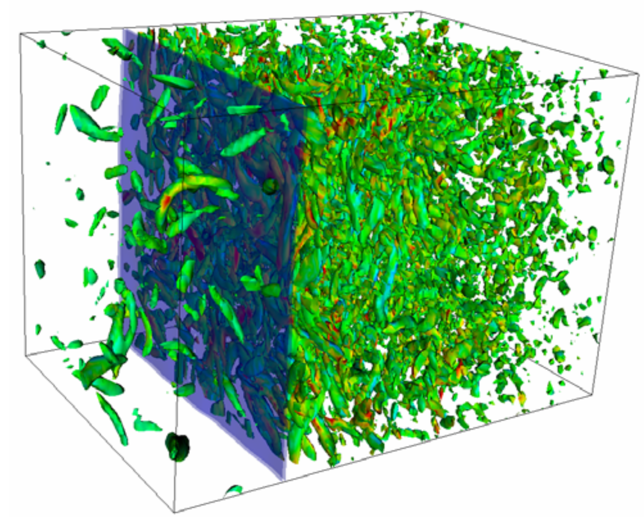


Left: time (seconds) for full time step (circle), all communication (squares), and deduced compute time (plus); right: weak scaling efficiency. 32^3 (red) and 64^3 (blue) points per processor are used.

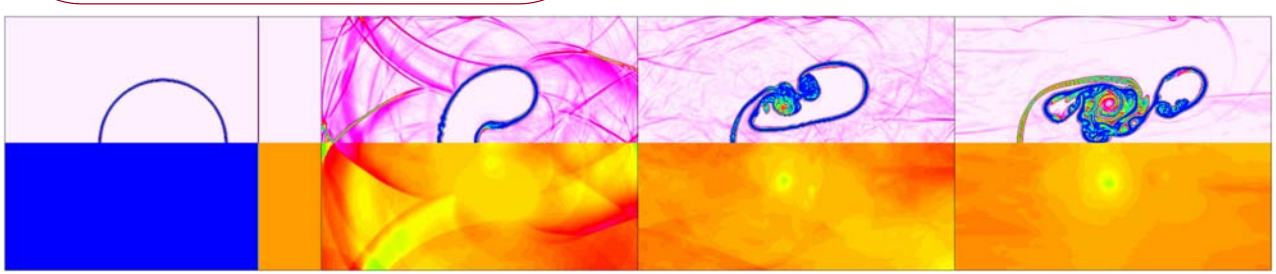
Shock-turbulence interaction

Isotropic turbulence passing through a normal shock wave:

- Hybrid method:
  - Shock-capturing near the shock,
  - Low dissipation elsewhere,
- Transverse vorticity amplified by shock compression,
- Inviscid adjustment towards equilibrium behind the shock,
- Dependence of the instantaneous shock structure on the problem parameters,
- Low-Reynolds number effects and under-resolution in current results
  - Need for higher-resolution simulations.



3D shock/turbulence interaction (296x64x64) with M=2, M_t=0.15, Re_λ=60 (shock: transparent isosurfaces of compression; vortex cores: isosurfaces of the 2nd invariant of the velocity gradient tensor, colored by vorticity magnitude).



Mach 1.22 shock in air impacting a He cylinder (400x160) using a quasi-conservative multifluid scheme (top: numerical Schlieren; bottom: pressure).

Multi-material flows

- Interfacial instabilities: Richtmyer-Meshkov, compressible Rayleigh-Taylor,
- Quasi-conservative scheme: stable and robust treatment of interfaces and shocks,
- Importance of vorticity generation:
  - At large scales: leads to the deformation of certain flow structures,
  - At small scales: drives the turbulent mixing.

Acknowledgements

This work is supported by the DoE Scientific Discovery through Advanced Computing (SciDAC). This SciDAC project consists of a collaboration with Dr. W. Cabot (LLNL), Dr. A. Cook (LLNL), Dr. B. Sjogreen (LLNL), Dr. H. Yee (NASA AMES), and Prof X. Zhong (UCLA).

SciDAC 08 Conference
Seattle, WA, July 13-17, 2008