Very High Resolution Simulation of Compressible Turbulence on the IBM-SP System

Winner of 1999 Gordon Bell Award for Performance

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Turbulence is around us everywhere

- **Smoke of a fire**
- **Abrupt wind changes**
- **Flow of a stream**
- **Behavior of stars and galaxies**
- **Flow inside a jet engine**
- **Flow over an airfoil**

- **Whenever disparate fluids are in contact and subjected to a force, there is the possibility of turbulent mixing**

Turbulence is characterized by ...

- **Wide range of length scales**
- **Rapid mixing**
- **Unpredictability**

- **Extent and nature of mixing affects surface area to volume ratio, hence reactivity of the mixture**

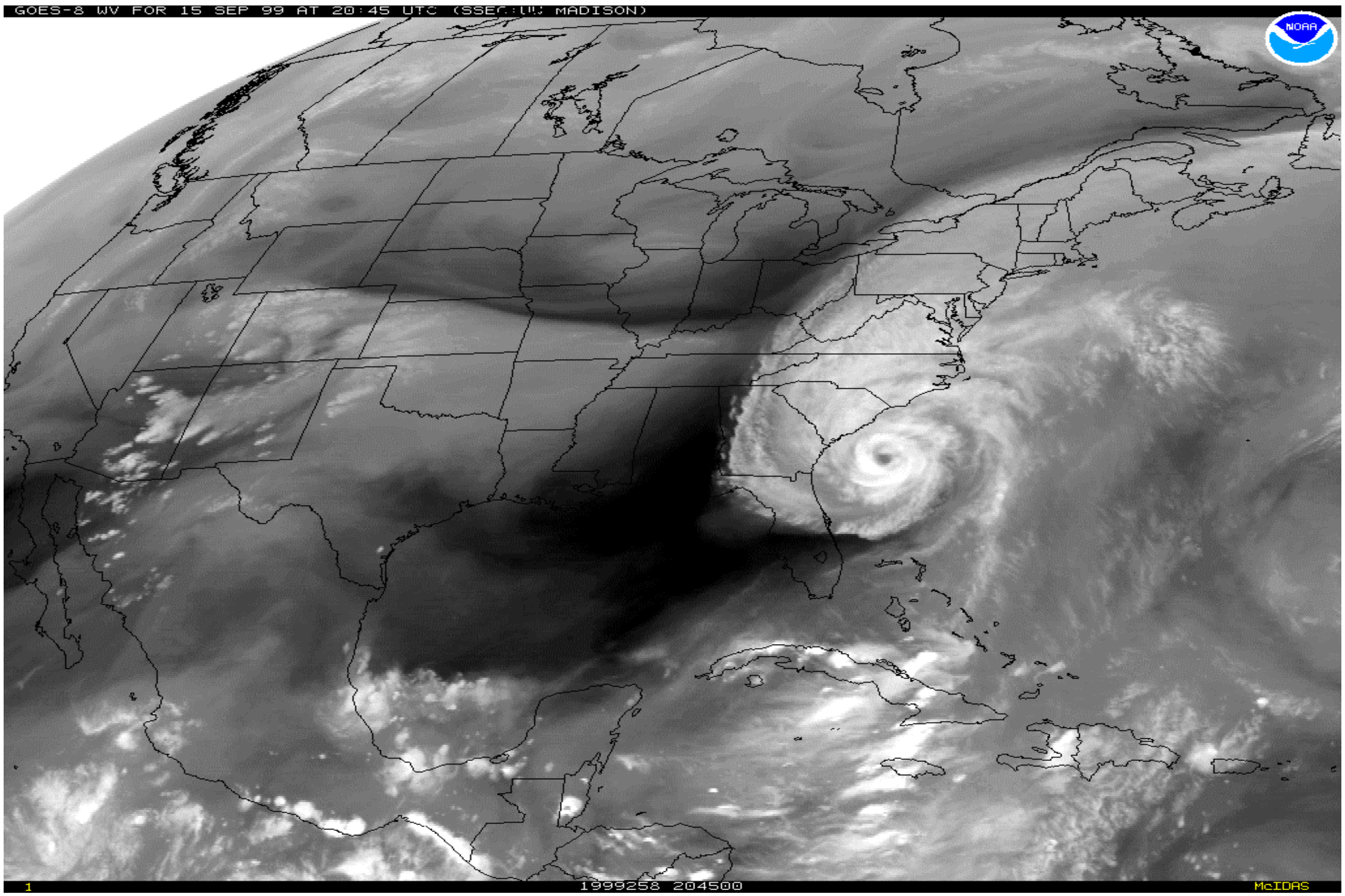
Simulating turbulence is challenging

- Wide range of length scales requires high resolution

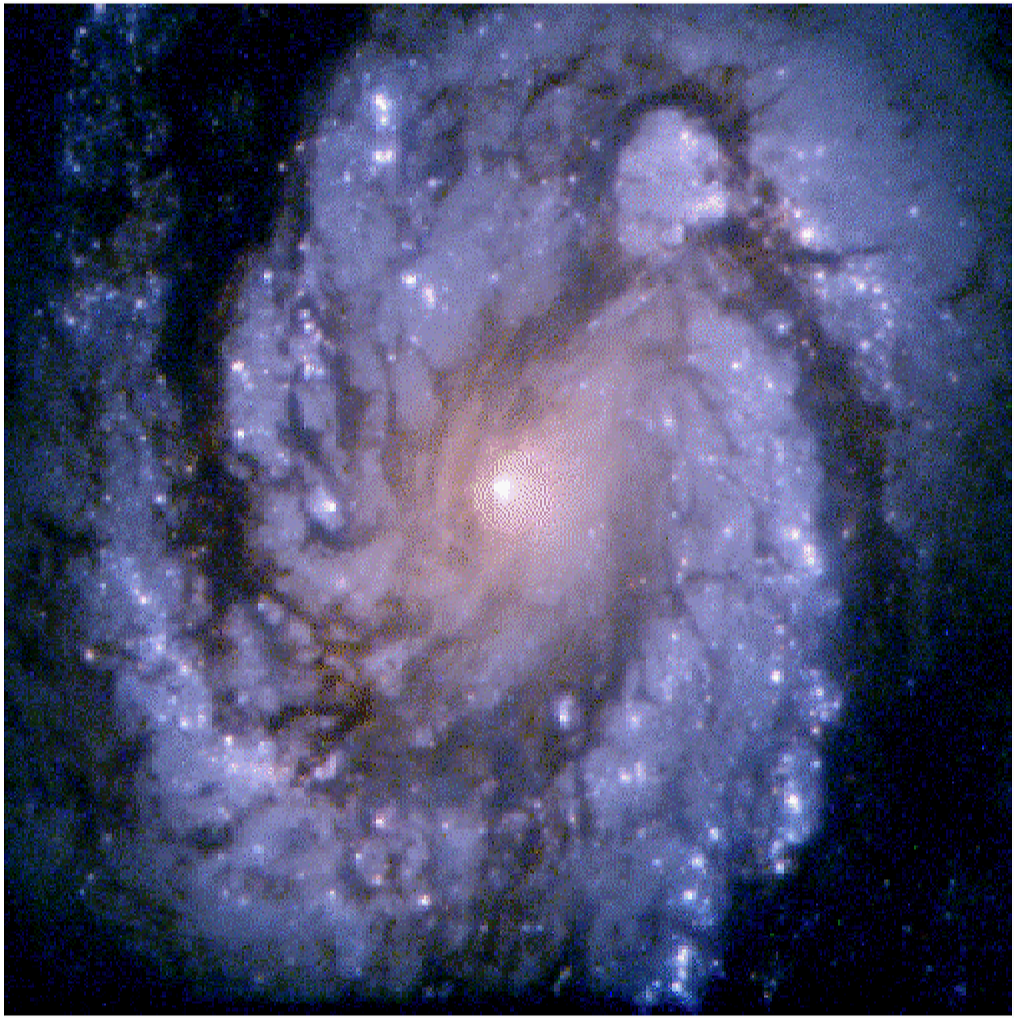
- 3-D flows fundamentally different from those in 2-D
  - conservation of enstrophy in 2-D

- At high compressibility, need to preserve shocks

Hurricane Floyd viewed from GOES satellite (courtesy U. Wisconsin and NOAA)

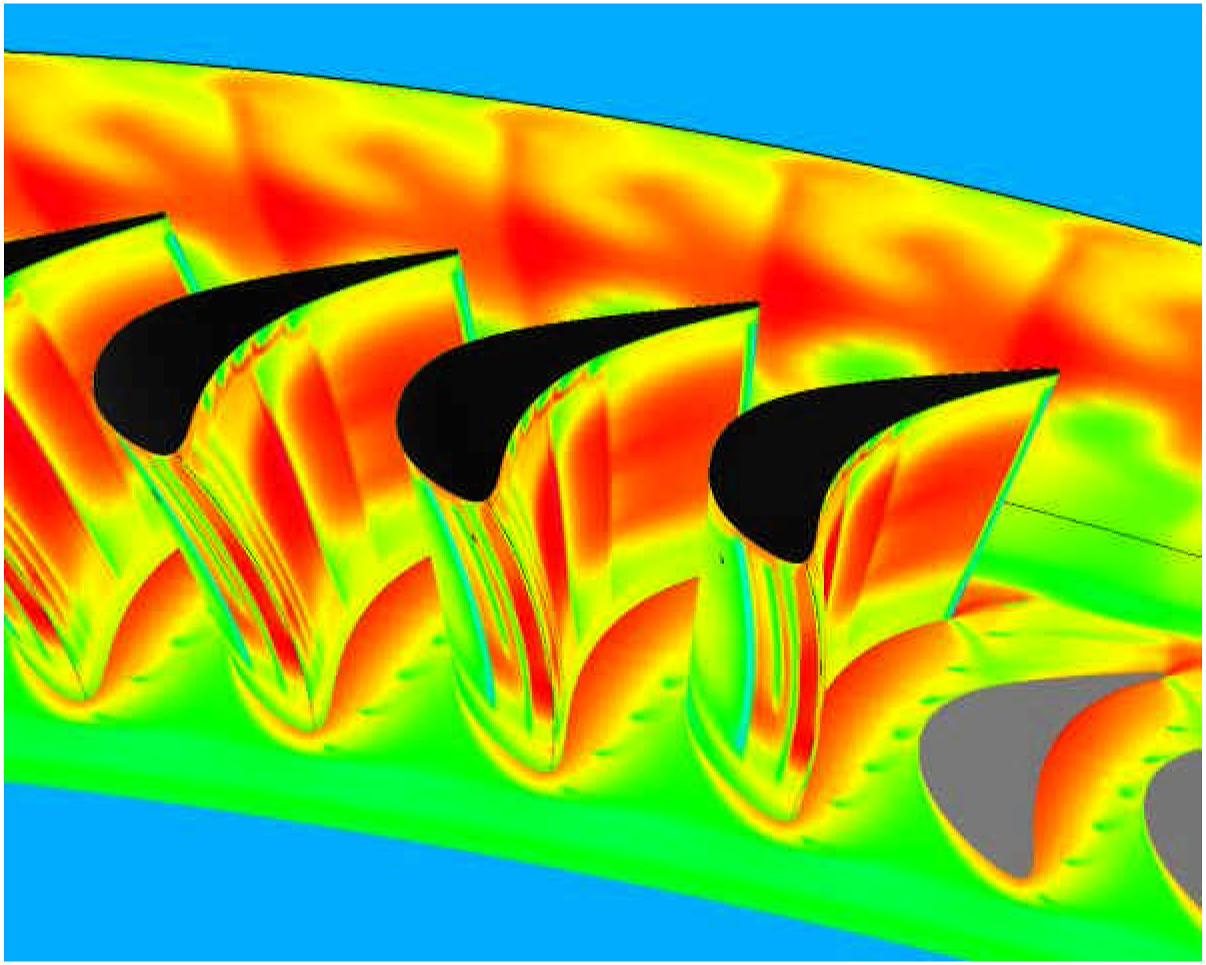


M100 Galactic nucleus (courtesy Space Telescope Science Inst. and NASA)

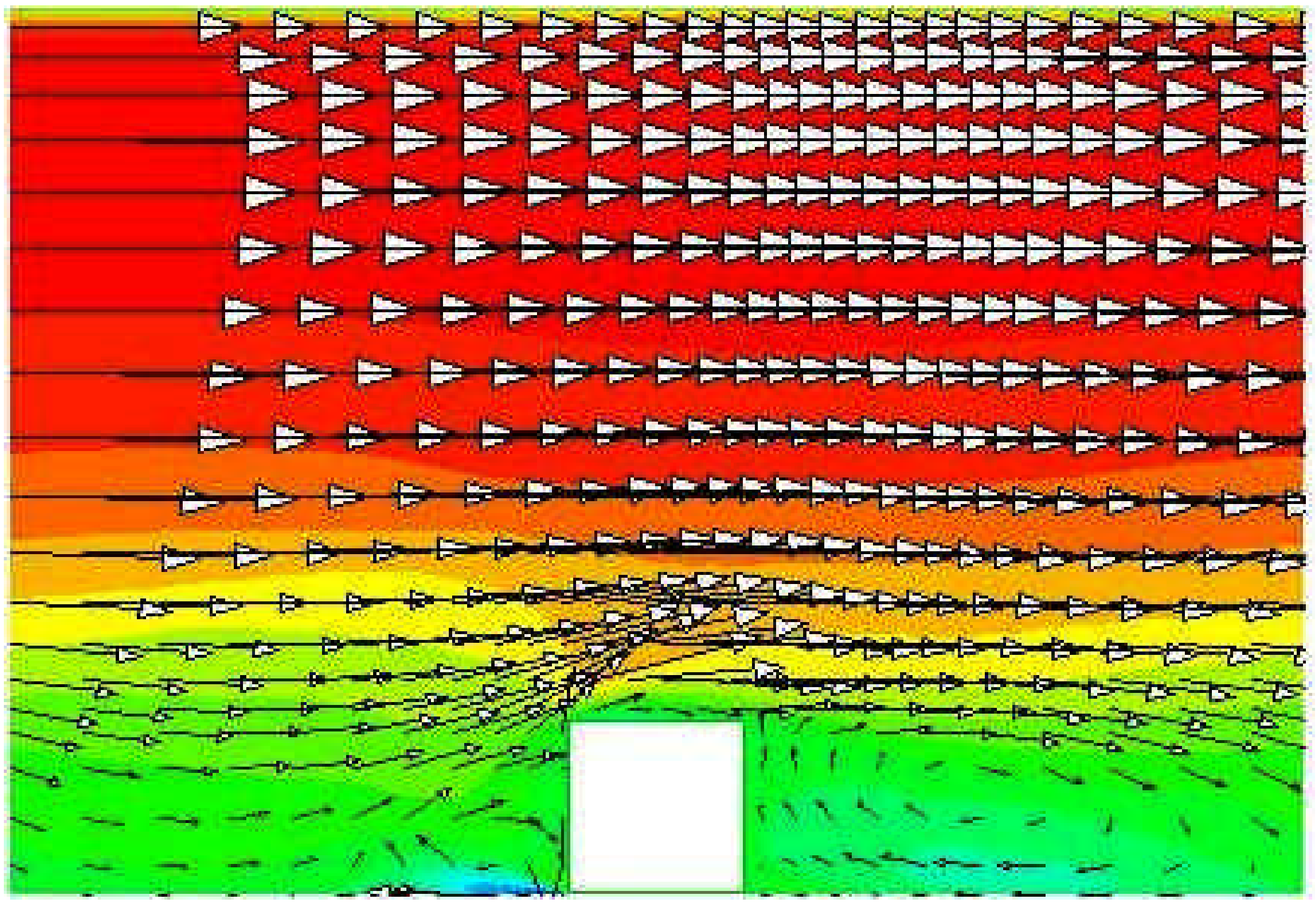


Surface temperature in turbine rotor

(courtesy S.V. Subramanian, ASE Technologies, Inc.; and NASA)

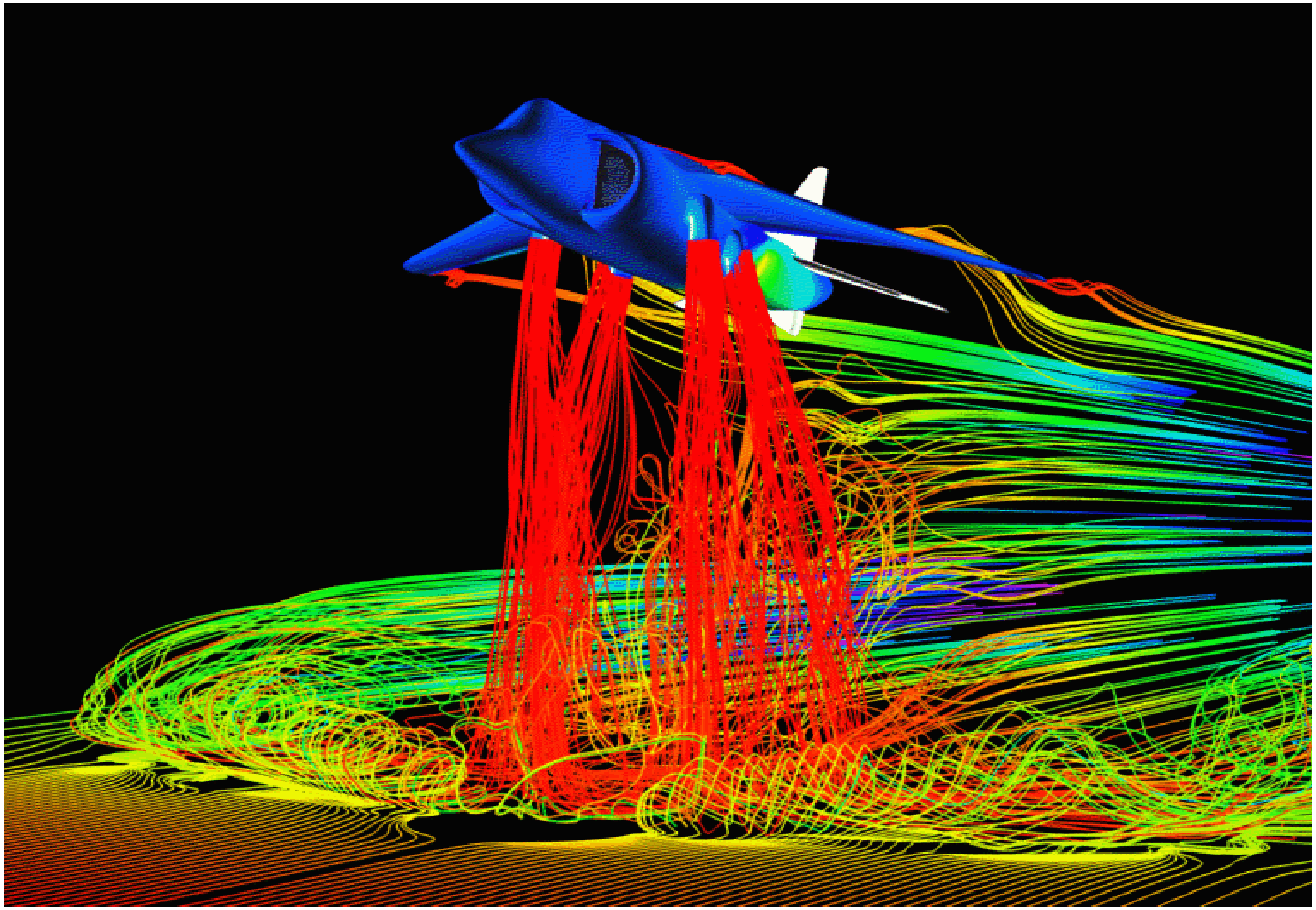


Flow in ribbed channel (courtesy R.H. Pletcher, Iowa State Univ.; and NASA)

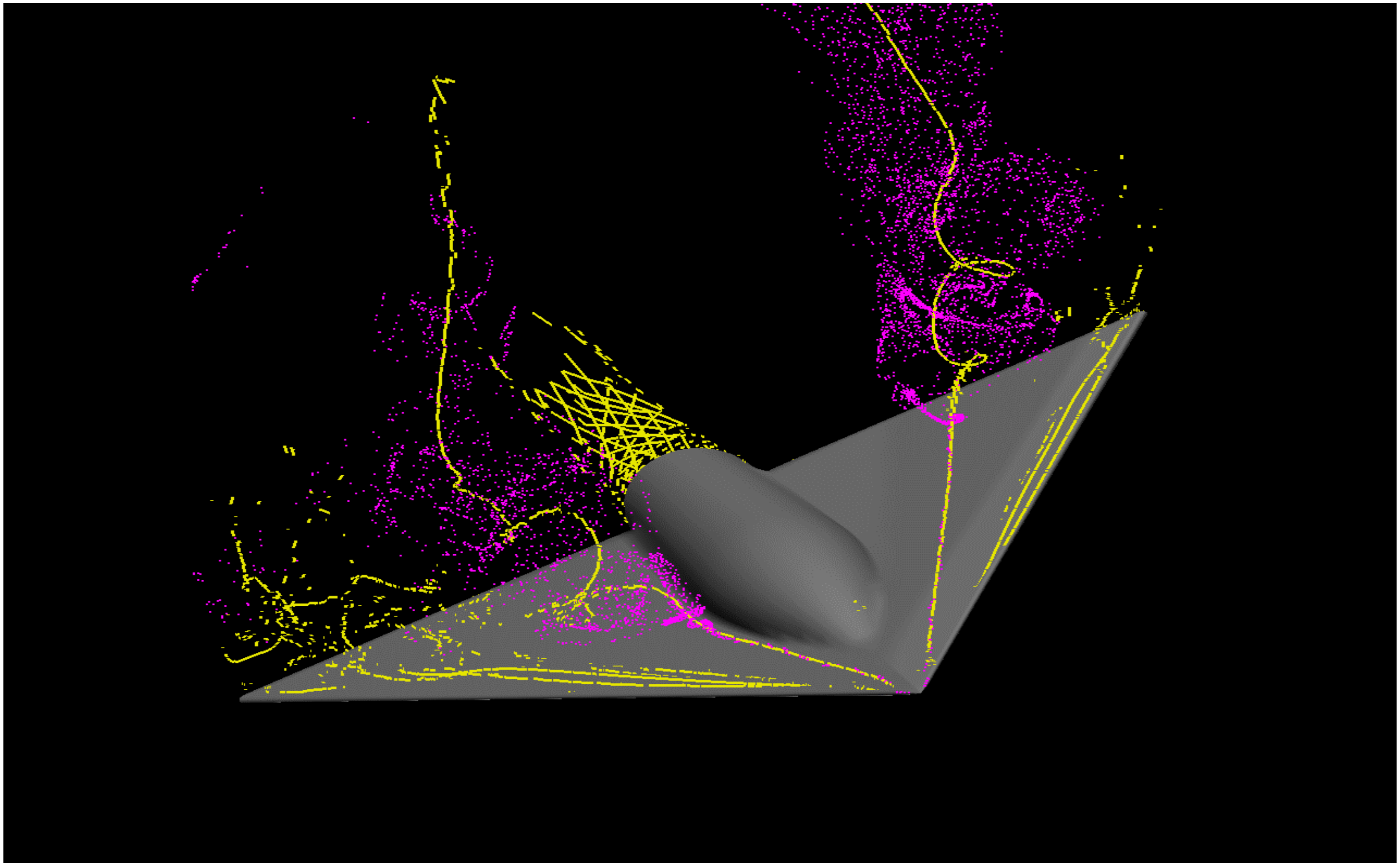


Streaklines near nozzle of harrier aircraft

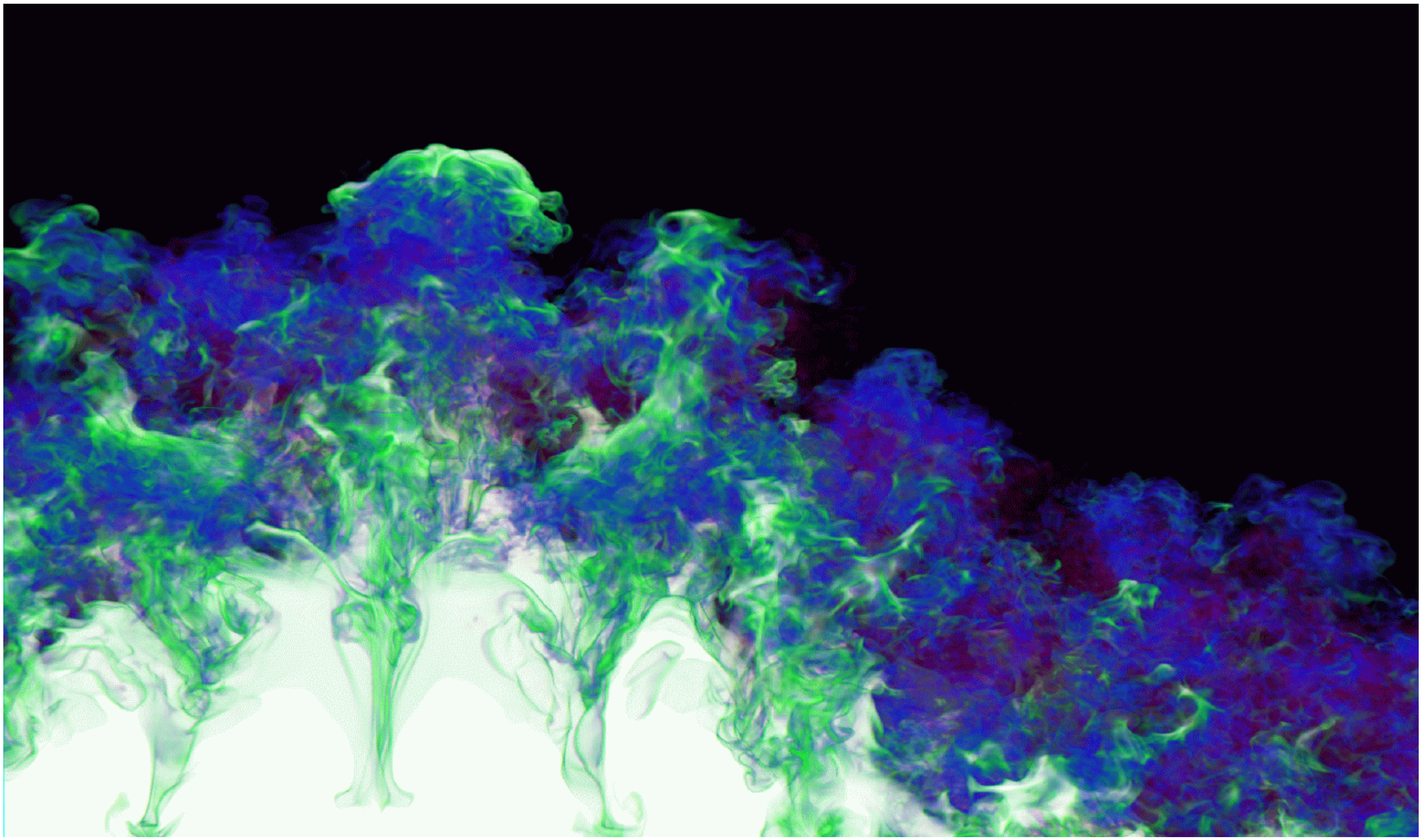
(courtesy W. VanDalsem, NASA Ames)



Vortex cores about a Delta wing (courtesy N. Chaderjian, NASA)



Simulation of Richtmyer-Meshkov instability



Areas to be discussed

- The simplified Piecewise Parabolic Method (sPPM) - algorithm and code
- IBM machine configuration
- Proof-of-principle tests
- Richtmyer-Meshkov instability
- Execution and performance of R-M simulation
- Postprocessing and interpretation of scientific data
- Summary and conclusions

We use the simplified Piecewise Parabolic Method (sPPM)

- sPPM is a higher-order accurate Godunov method originated by Colella and Woodward
  - Lagrangian followed by remap (Eulerian)
  - directionally split
- Solves Euler equations (no physical dissipation)
- Fortran 77
- Three-dimensional domain decomposition
- Posix threads plus MPI
- Effective cache utilization
- Overlap communication and computation
- 32-bit arithmetic

The IBM system was assembled in Poughkeepsie, New York

The IBM SST machine at LLNL

- ASCI Blue-Pacific system
- Three 488-node sectors
- Sectors connected by six HPGN switches
- Each node has four 332-MHz PowerPC 604e processors and 1.5 - 2.5 Gbytes local memory
- Peak performance is 3.9 TeraOp/s
- There are 62.5 Tbytes of RAID storage

The ASCI Blue-Pacific system has three 488-node sectors

LLNL's initial IBM ASCI system, with 512 processors, executed a 13-million-zone Rayleigh-Taylor simulation in 1996

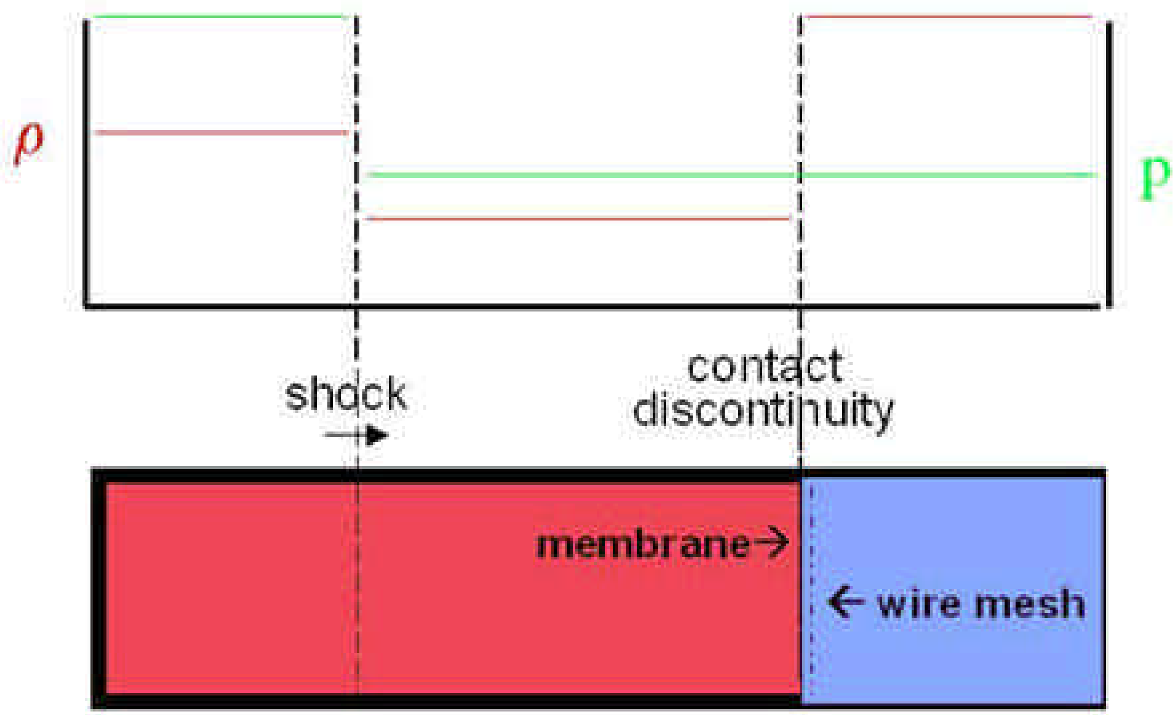
Proof-of-principle tests

- Standard sPPM benchmark case
  - over 24 billion zones
  - utilized 5832 processors (9 x 9 x 18 decomp.)
  - executed for over an hour at sustained 1.05 Tflop/s (32-bit) (counted flops using execution trace tool)
  - 90% on-node parallel efficiency
  - 95% inter-node parallel efficiency
  - nearly 100% communication overlap for large grid
  - overall parallel efficiency of 85%

Proof-of-principle tests, cont.

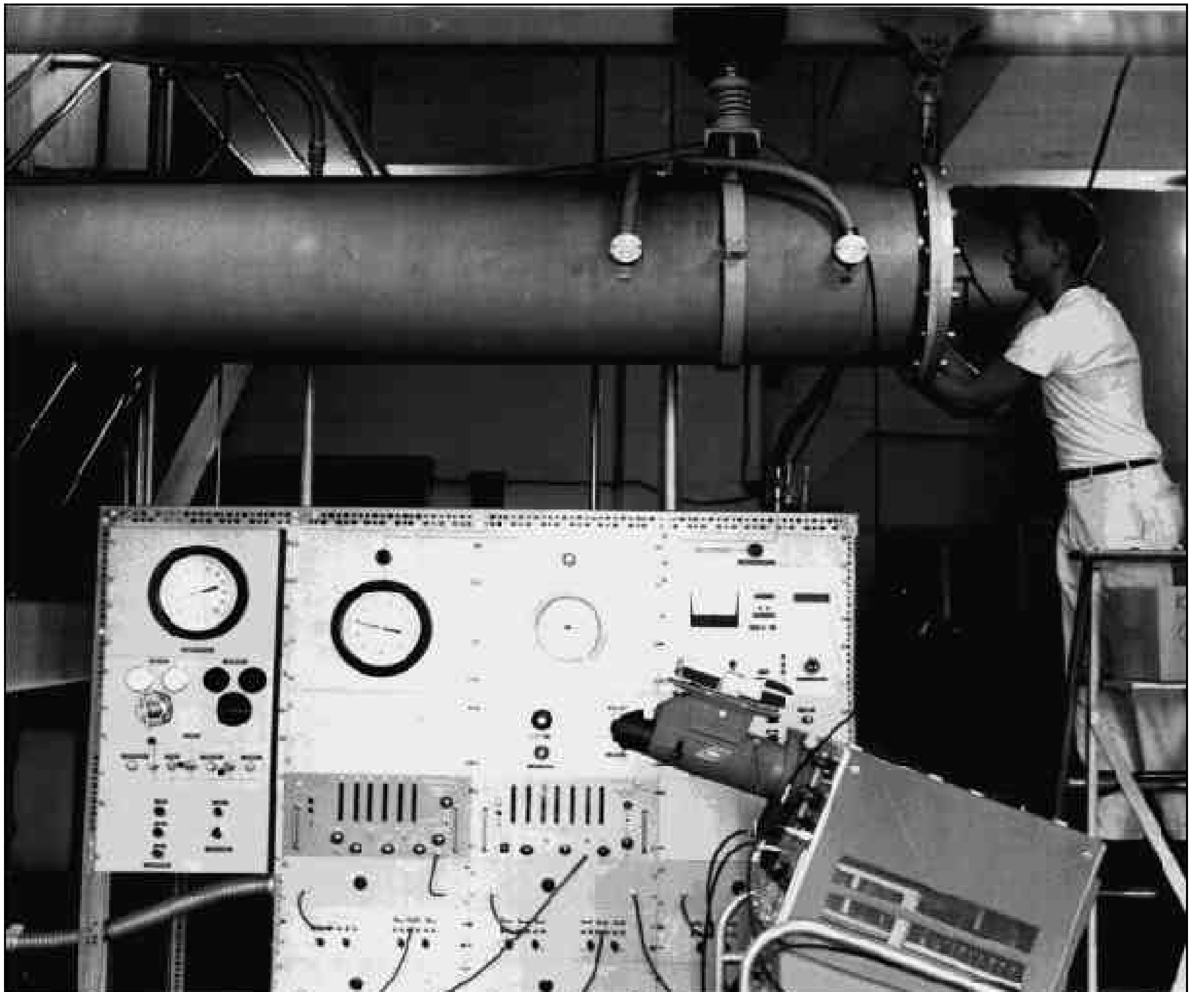
- **Modified kernel**
  - **fewer operations/temporaries, loop reconstruction, MASS library**
  - **achieved 1.18 Tflop/s (2 timesteps)**
  - **achieved 50% reduction in wall time**
- **Large problem**
  - **70.8 billion zones fit in memory**
  - **used unmodified kernel and original driver**
  - **achieved 0.88 Tflop/s**

Richtmyer-Meshkov mixing occurs when shock intersects contact discontinuity

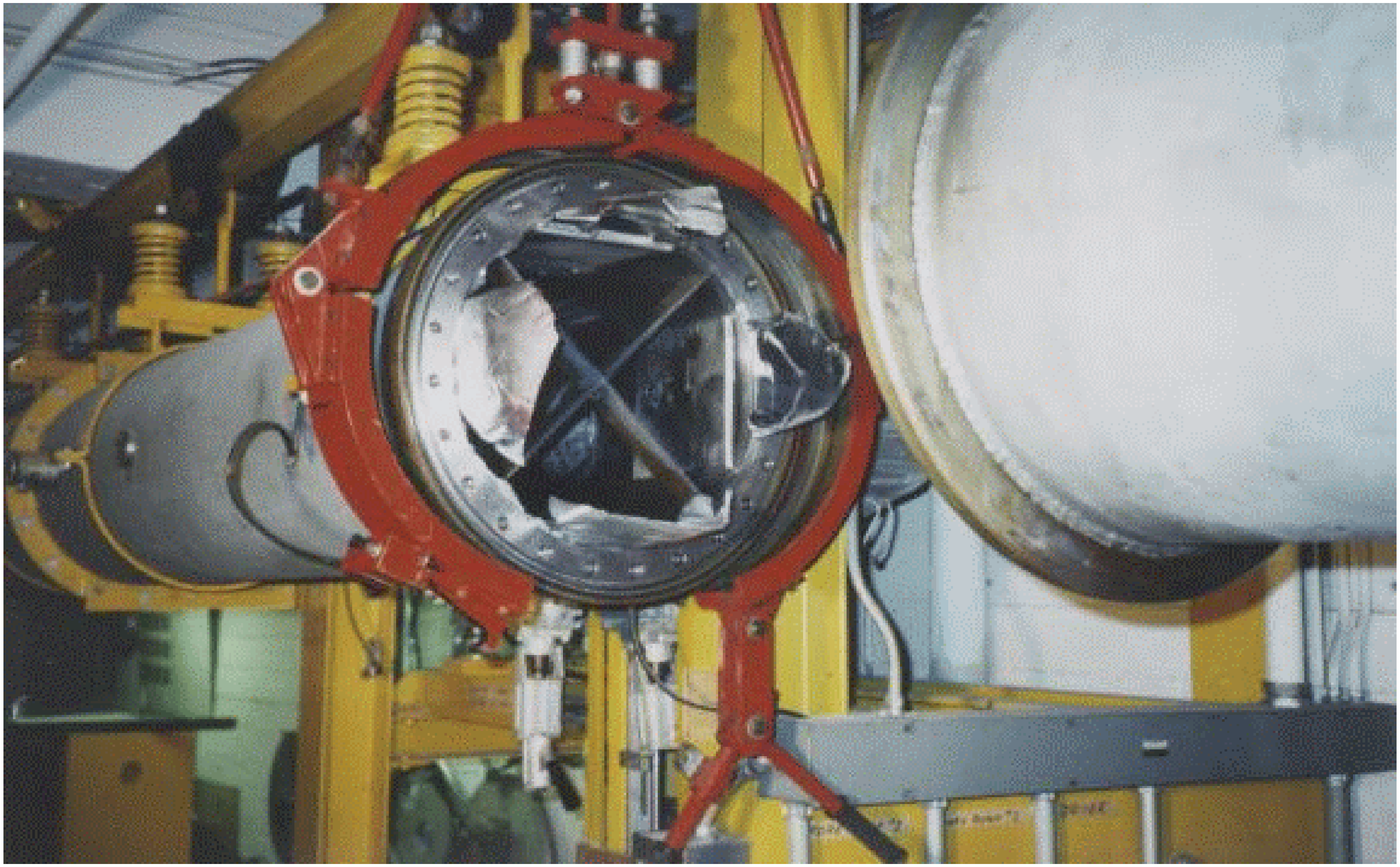


(schematic diagram of shock tube)

Caltech shock tube, vintage 1961 (courtesy of the Archives, California Institute of Technology)



Caltech 17” shock tube, present day



Shock tube experiment of Vetter & Sturtevant (Caltech)

- Two gases separated by membrane pushed against wire mesh
  - for this simulation, assume single γ=1.3 gas
- Mach 1.5 shock impinges from left
- Two-scale perturbation of contact discontinuity location
  - long wavelength - distortion of mesh
  - short wavelength - mesh spacing

Richtmyer-Meshkov simulation executed on IBM SST machine at LLNL

- **Executed on 2048 x 2048 x 1920 grid**
- **Used 960 computational nodes (virtually 2 complete sectors), arranged in 8 x 8 x 15 domain decomposition**
- **Problem duration of 27,000 timesteps, corresponding to 9 transverse sound crossing times**
- **Simulation took 173 hours of machine time, spread over 226 hours of wall time**
- **Over 3 Tbytes of graphics data, spread over 275,000 files, was produced**

- ***Sustained throughput of around 0.6 Tflop/s (32-bit)***

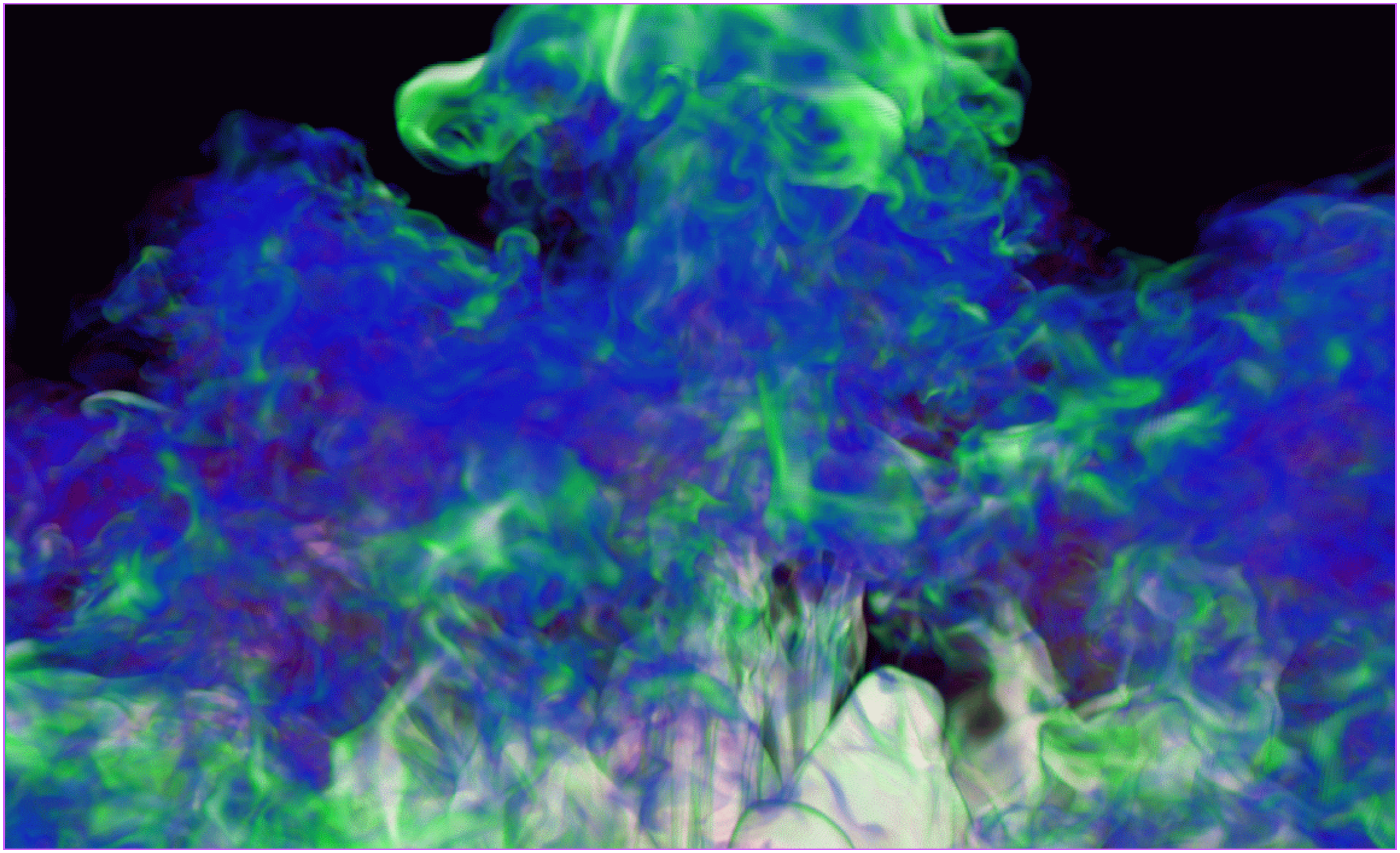
Scientific simulation performed well

- Sustained throughput was around 0.6 Tflop/s (32-bit)
- Throughput (flops per second) per computational node slightly lower than in 1.18 Tflop/s proof-of-principle test
  - further improved kernel had lower flop rate, but shorter time to solution
  - smaller local grid yielded poorer overlap of communication
  - system daemons were left operating

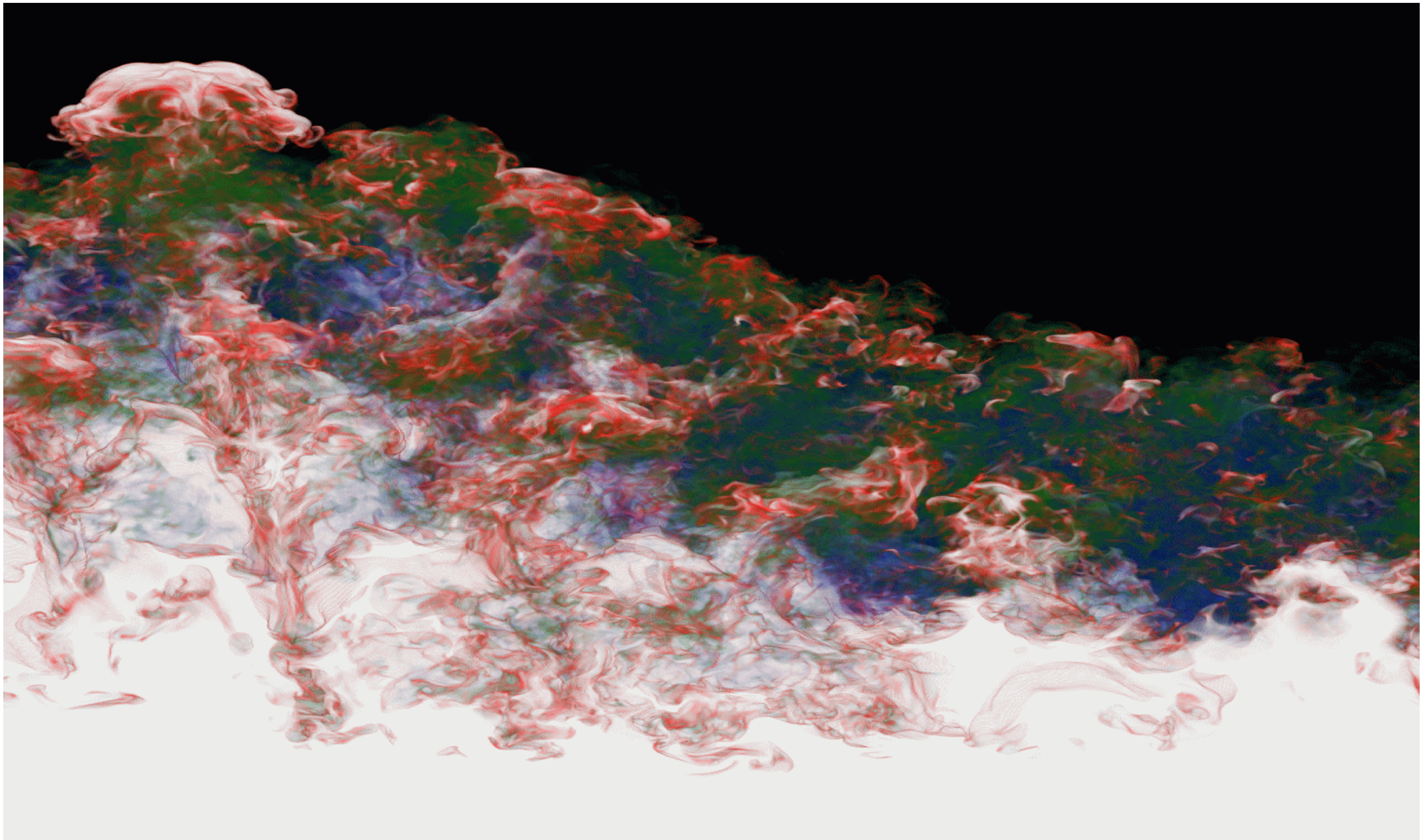
Volume rendering

- Uses brick-of-byte (BOB) files
  - one byte of information per grid point
  - byte value represents physical quantity, subject to user-specified transformation
- U. Minnesota volume renderer HVR
  - SGI Infinite Reality engine using high-capacity RAIDed disks
  - texture hardware, parallel processing
- Volume renderings in this presentation display entropy

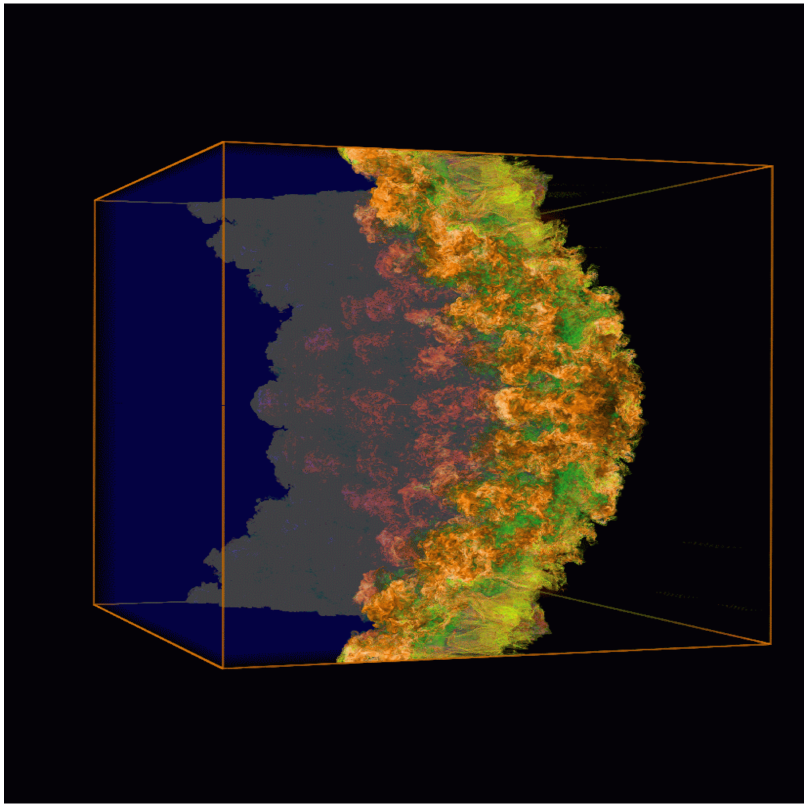
Simulation of Richtmyer-Mevhkov instability

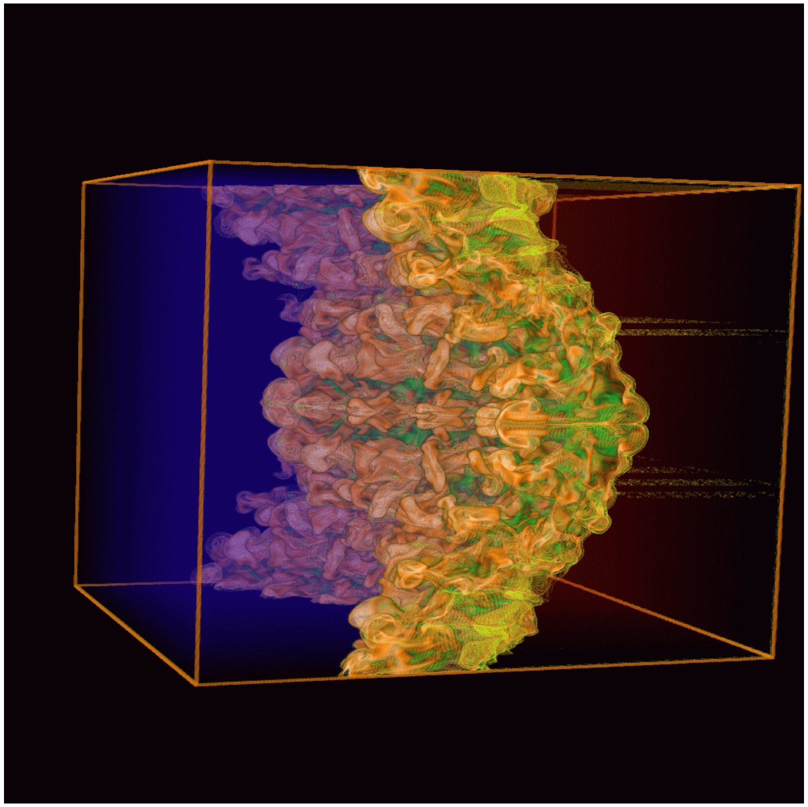


Simulation of Richtmyer-Meshkov instability

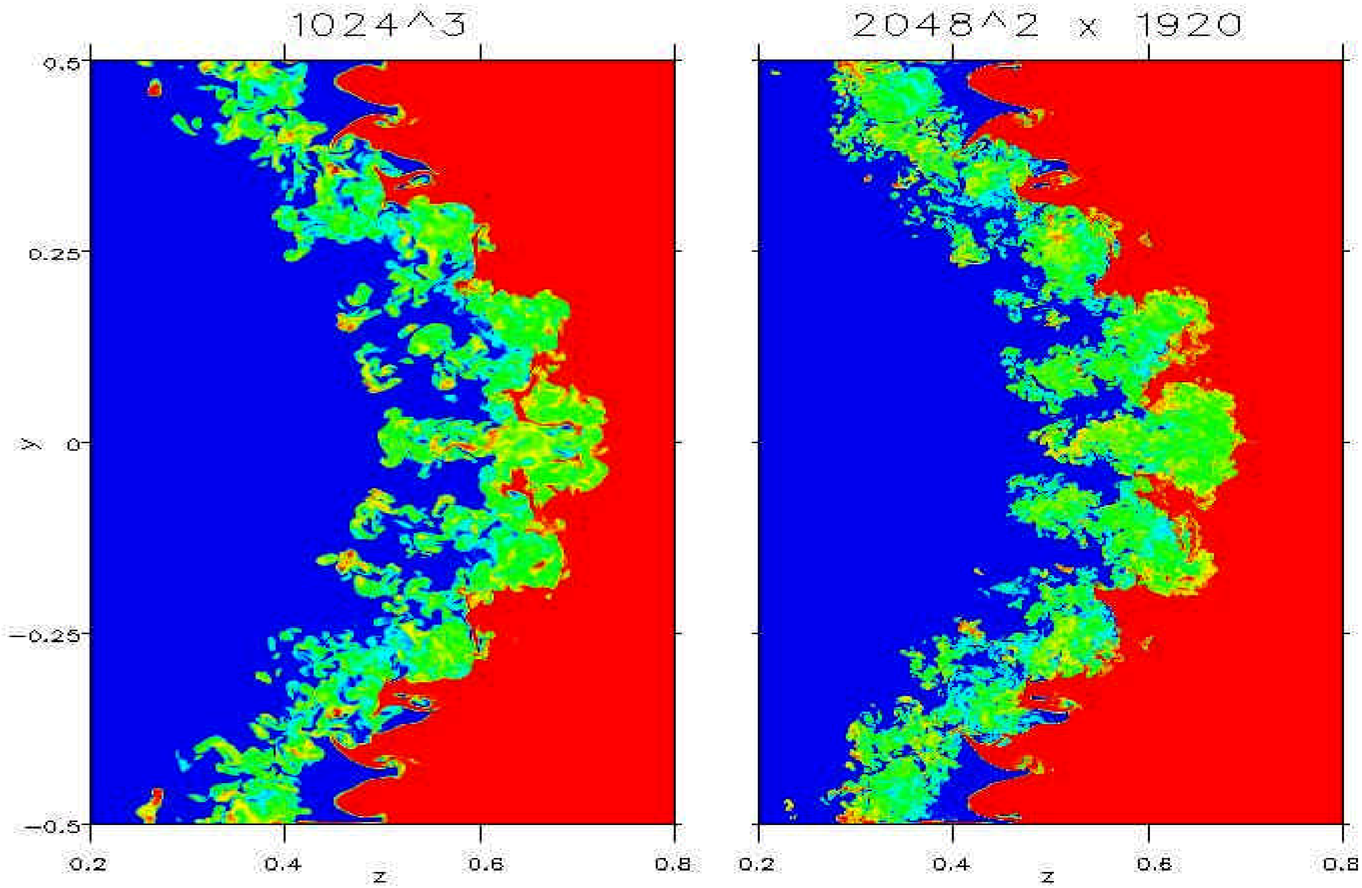


Volume renderings of high- and low-resolution simulations

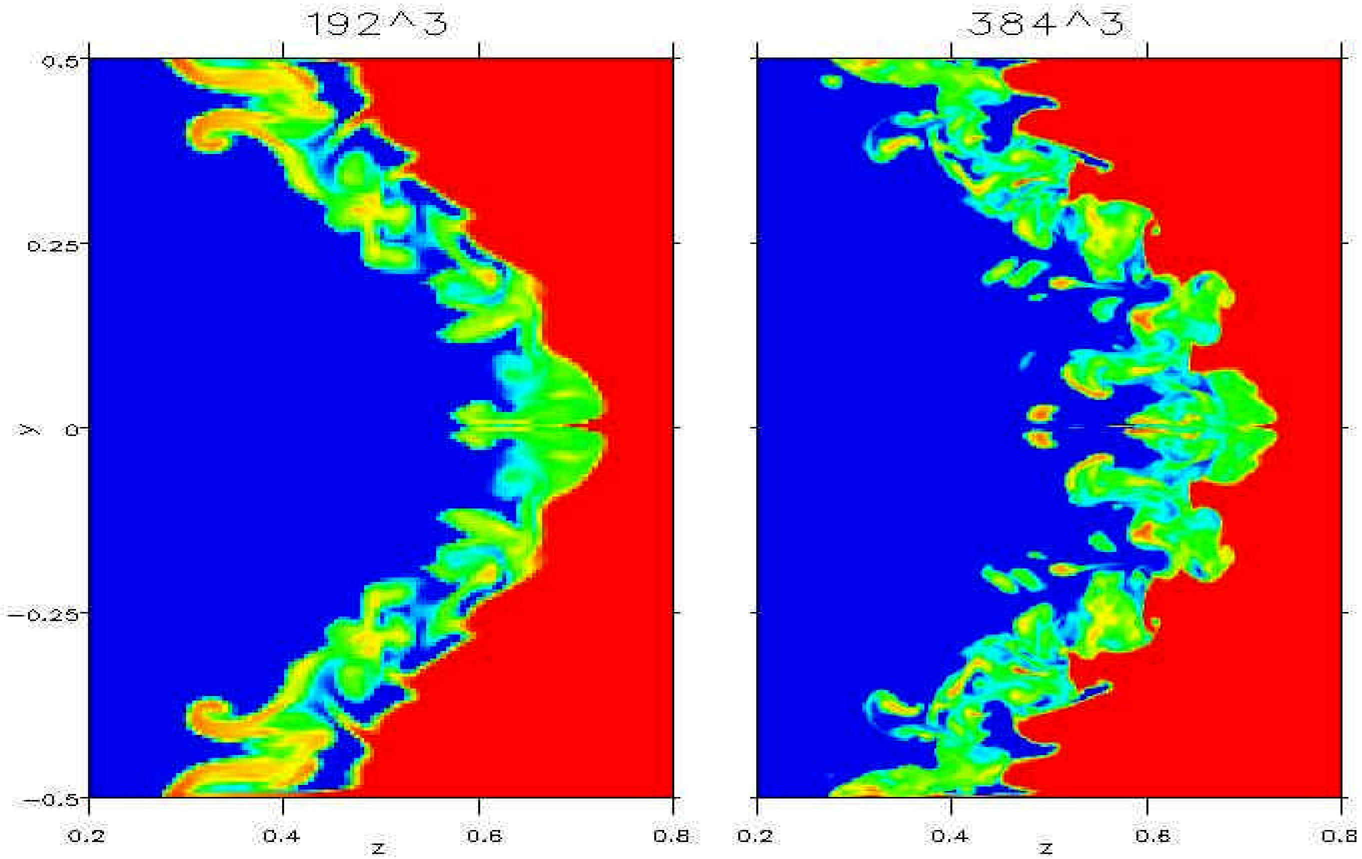




Higher-resolution cases show fine-scale structure



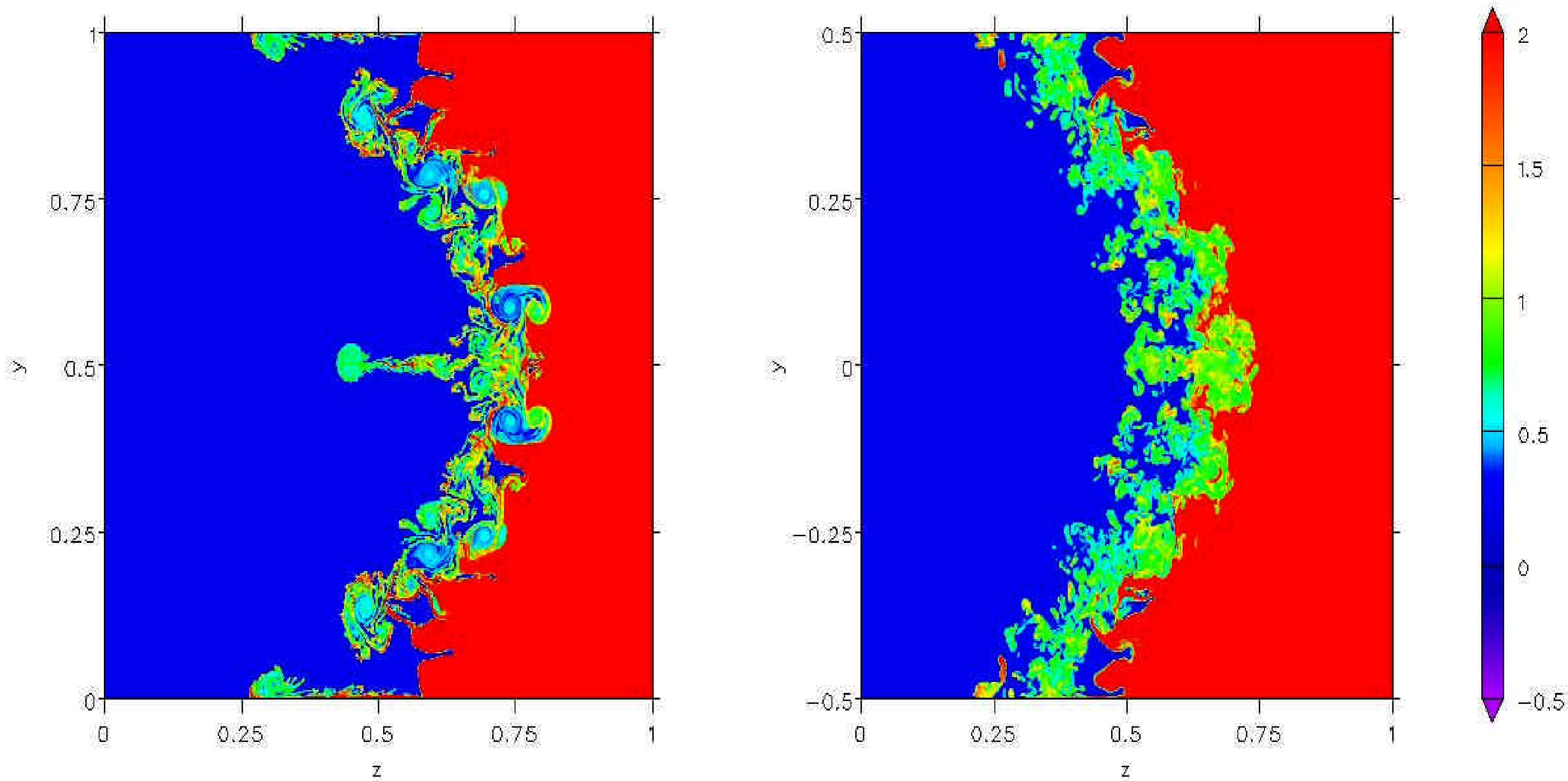
Lower-resolution cases show large-scale structures



Transition to turbulence

- Coarser resolution cases show large-scale structure
- Finer resolution cases show fine-scale structure
- Transition between 384 x 384 x 384 and 1024 x 1024 x 1024
  - consistent with conjecture of Dimotakis (Caltech)
  - needed high resolution to observe and verify this transition

3-D and 2-D simulations show different character



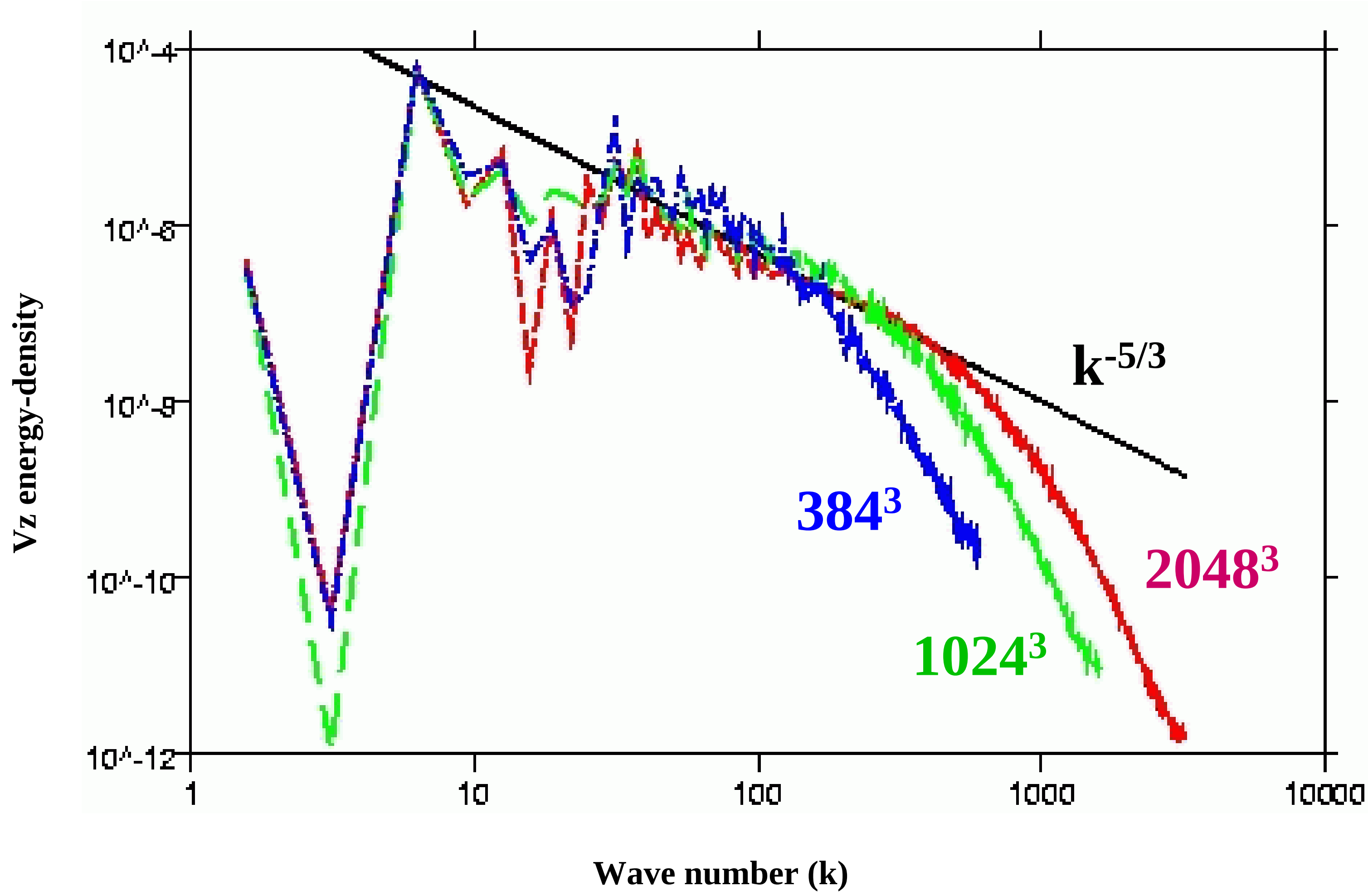
Solution exhibits different character in three dimensions

- 3-D dynamics
  - forward cascade
  - fine structures
- 2-D dynamics
  - inverse cascade
  - extended structures
- For reactive fluids, predicted reaction rates would vary significantly with respect to dimensionality and resolution

Generalized postprocessing

- Uses compressed dump files
  - two bytes of information per gridpoint
  - dynamical variables represented, subject to linear transformation
- a3d postprocessor from U. Minnesota
  - calculates combinations of algebraic, differential, or integral forms on raw data
  - produces histograms, cuts through data,...

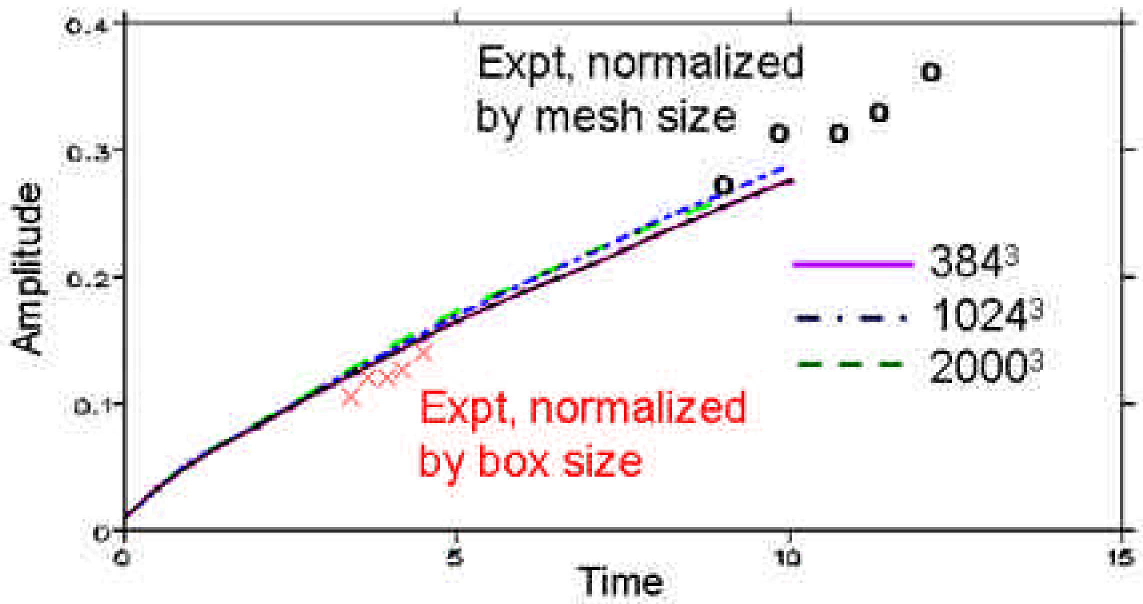
Spectral results show convergence and meaningful inertial range



Existence of inertial range

- **High-resolution case shows inertial range for wave numbers ranging from 30 to 300**
  - **numerical dissipation decreases with resolution**
- **Convergence trend (with respect to resolution) indicates that this inertial range is meaningful**
- **Dimotakis conjectures that existence of this inertial range allows transition from large-scale structures to fully-developed turbulence with increasing (in this case, numerical) Reynolds number**

Mixing layer extent converges and agrees with experiment



We succeeded in a very ambitious calculation that

- **until now was not feasible**
- **used order of magnitude more grid points than previous fluid turbulence simulations**
- **achieved 0.6 Tflop/s (32-bit) on 960 computational nodes**

Running in 3-D and at high resolution enabled...

- Simulation of development of fine scale structures from interactions of long- and short-wavelength phenomena
- Elucidation of differences between 2-D and 3-D turbulence
- Exploration of conjecture regarding transition from unstable flow to fully developed turbulence with increasing Reynolds number
- Ascertainment of convergence of computed solution with respect to mesh resolution

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