Computational Physics & Validation

Tomek Plewa

Hua Pan, Timur Linde, Greg Weirs, Dahai Yu

Todd Dupont

Outline

FLASH Center Overview

Center-specific activities

- V&V in astrophysics
- V&V in the Center
  - Verification of new computational modules
    low Mach number flow solver, level set
  - Validation
    shock-cylinder experiment

Summary

- Improving computational machinery, aiding experiment design, lower overall costs
- Changing culture in astrophysics/computational sciences

The FLASH Center

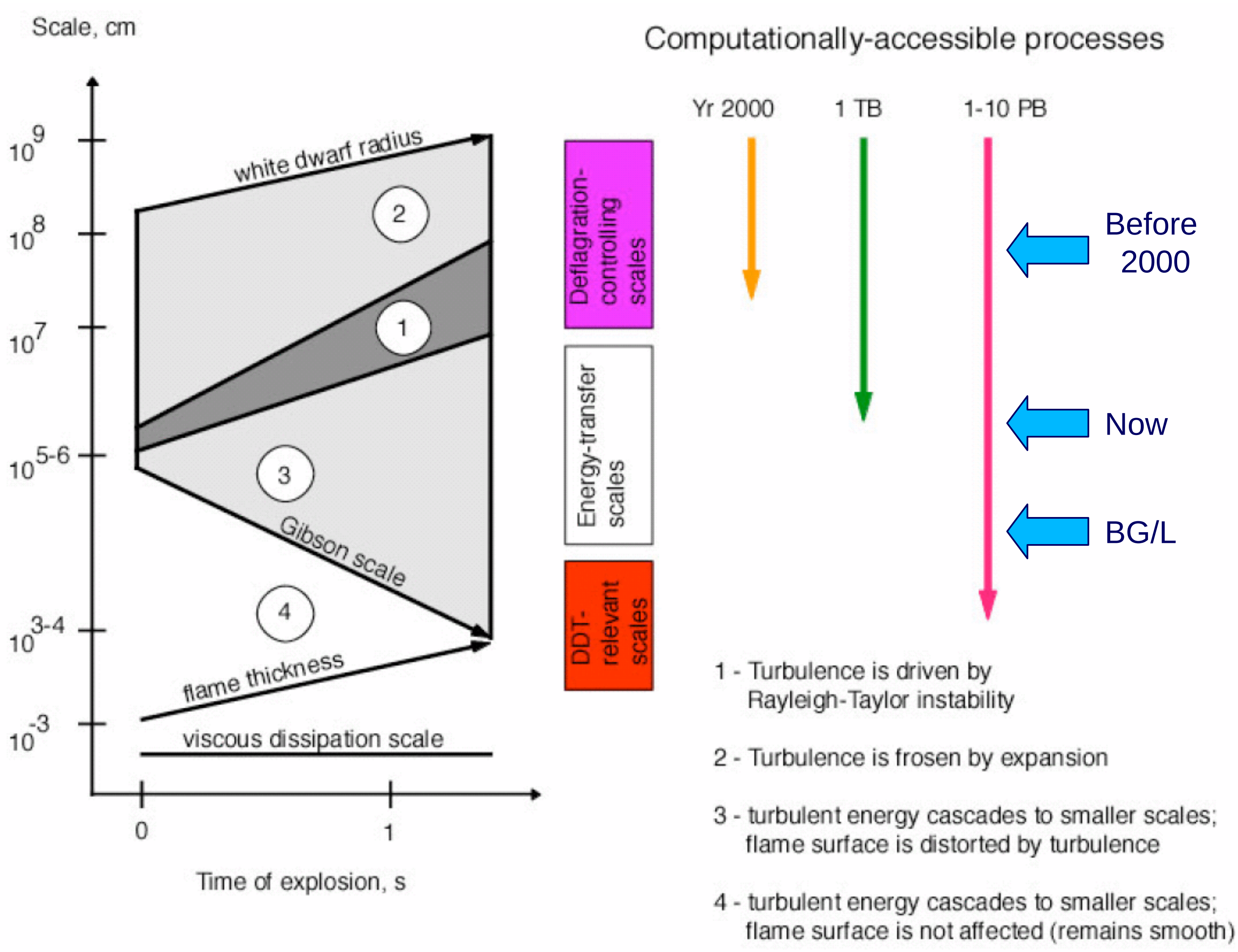
Target Applications

- Compact accreting stars (white dwarf, neutron star)
- Reactive hydrodynamics (DNS or subgrid model)
- Initial conditions close to hydrostatic equilibrium (self-gravity)
- Complex EOS (dense nuclear matter)

Example: Type Ia Supernova

- Massive white dwarf
- Subgrid model for nuclear flame
- Self-gravity
- Degenerate EOS

Length scales in White Dwarf Deflagration



What do we mean by V&V ???

A process aimed at creating simulation-based confidence.

Verification: solving equations right

- Analytic results used for comparison
- In a way more technical, formal
- Implementation verification (code); solution verification (appl)

Validation: solving right equations

- Experimental results used for comparison
- Strongly physics-oriented

V&V in Astrophysics

- Verification ranging from simple analytic problems to code-code comparison.
- No direct access to experiments: use scaling laws
- Absolutely **NO** culture of validation!

THE ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES, 143:201–229, 2002 November

ON VALIDATING AN ASTROPHYSICAL SIMULATION CODE

A. C. CALDER,[1,2] B. FRYXELL,[1,3] T. PLEWA,[1,2,4] R. ROSNER,[1,2,3] L. J. DURSI,[1,2] V. G. WEIRS,[1,2] T. DUPONT,[1,5] H. F. ROBEY,[6] J. O. KANE,[6] B. A. REMINGTON,[6] R. P. DRAKE,[7] G. DIMONTE,[6] M. ZINGALE,[1,8] F. X. TIMMES,[1,2] K. OLSON,[1,9] P. RICKER,[1,2] P. MACNEICE,[9] AND H. M. TUFO[1,5]
Received 2001 August 3; accepted 2002 June 12

ABSTRACT

We present a case study of validating an astrophysical simulation code. Our study focuses on validating FLASH, a parallel, adaptive-mesh hydrodynamics code for studying the compressible, reactive flows found in many astrophysical environments. We describe the astrophysics problems of interest and the challenges associated with simulating these problems. We describe methodology and discuss solutions to difficulties encountered in verification and validation. We describe verification tests regularly administered to the code, present the results of new verification tests, and outline a method for testing general equations of state. We present the results of two validation tests in which we compared simulations to experimental data. The first is of a laser-driven shock propagating through a multilayer target, a configuration subject to both Rayleigh-Taylor and Richtmyer-Meshkov instabilities. The second test is a classic Rayleigh-Taylor instability, where a heavy fluid is supported against the force of gravity by a light fluid. Our simulations of the multilayer target experiments showed good agreement with the experimental results, but our simulations of the Rayleigh-Taylor instability did not agree well with the experimental results. We discuss our findings and present results of additional simulations undertaken to further investigate the Rayleigh-Taylor instability.

Subject headings: hydrodynamics — instabilities — methods: numerical — shock waves

VERIFICATION AND VALIDATION

VALIDATING ASTROPHYSICAL SIMULATION CODES

Astrophysical simulations model phenomena that can't be fully reproduced terrestrially. Validation then requires carefully devising feasible experiments with the relevant physics. The authors describe validating simulations against experiments that probe fluid instabilities, nuclear burning, and radiation transport, and then discuss insights from—and the limitations of—these tests.

Much of the contemporary research in astrophysics necessarily involves the development of models and simulation technology to help us understand the complex phenomenon underlying astrophysical events. As with any modeling approach, numerical models and simulation codes developed for astrophysical applications must be thoroughly verified and validated to demonstrate their accuracy and assess their credibility. Although verification and validation (V&V) is maturing as a discipline due to its importance in fields such as computational fluid dynamics (CFD), until recently it has received scant attention in the astrophysical literature.

In astrophysics, validation is a challenging problem because many of the conditions of interest can't be reproduced in terrestrial laboratories. In addition, astrophysical settings such as the interiors of stars are not directly observable. Even if this were not a problem, most astrophysical events happen at extreme distances, making observation difficult if not impossible. The complexity of astrophysical events also makes validating an astrophysical simulation code difficult. Astrophysical events typically involve many complex interacting physical processes, all of which must be included in a realistic model. Direct numerical simulations (for example, resolving all of a problem's scales of interest) are often beyond the capabilities of current computers, requiring the development of approximate methods and descriptions of the physical processes on scales smaller than the simulation can track (subgrid models).

Validation requires identifying the physical

1521-9615/04/$20.00 © 2004 IEEE
Copublished by the IEEE CS and the AIP

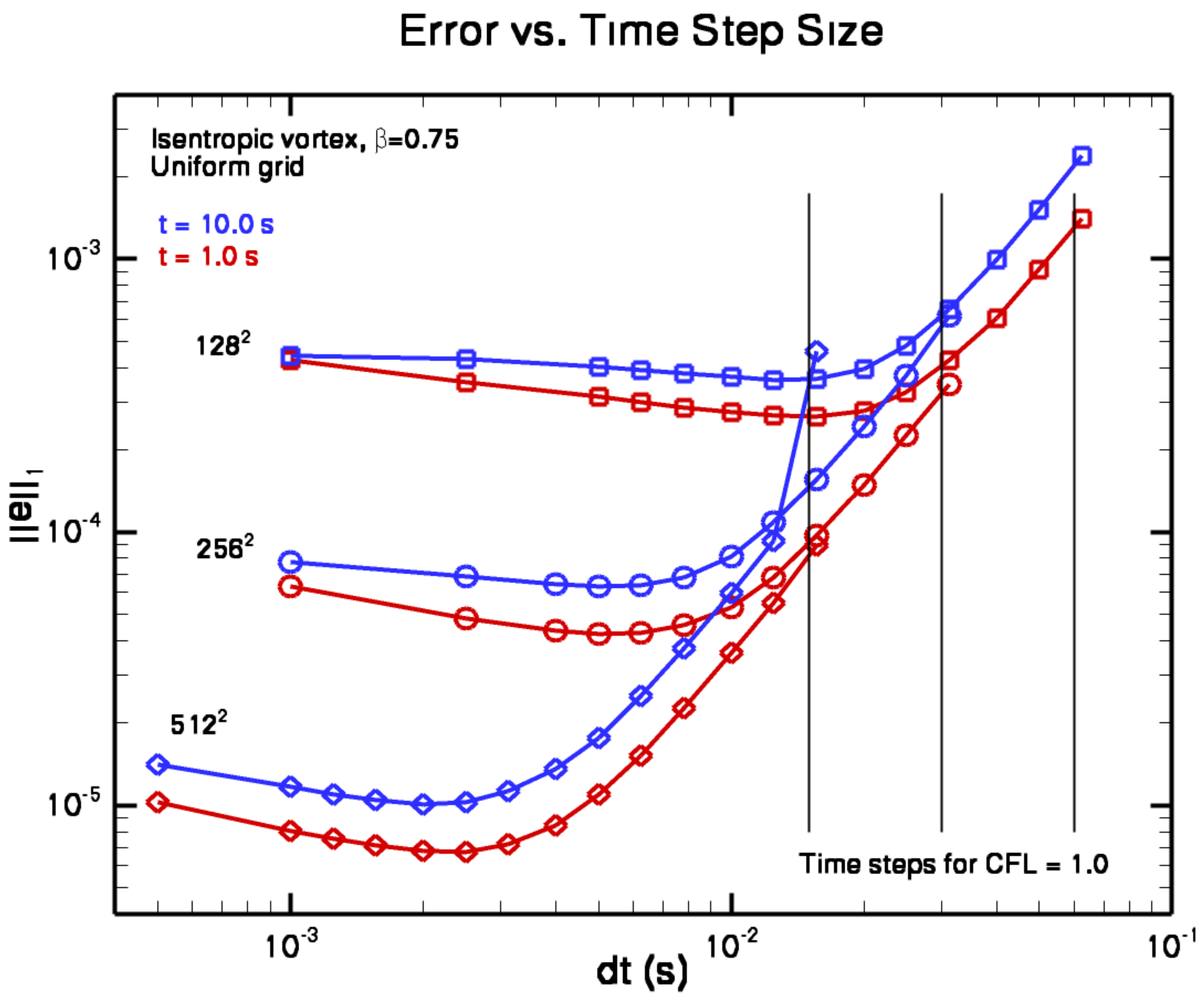
ALAN CALDER, JONATHAN DURSI, BRUCE FRYXELL, TOMEK PLEWA, GREG WEIRS, AND TODD DUPONT
University of Chicago
HARRY ROBEY, JAVE KANE, AND BRUCE REMINGTON
Lawrence Livermore National Laboratory
FRANK TIMMES AND GUY DIMONTE
Los Alamos National Laboratory
JOHN HAYES
University of California, San Diego
MIKE ZINGALE
University of California, Santa Cruz
PAUL DRAKE
University of Michigan
PAUL RICKER
University of Illinois
JIM STONE
Princeton University
KEVIN OLSON
NASA Goddard Space Flight Center

Verification of Computational Modules

Verification exploits elementary tests with known analytic solutions or "converged" numerical solutions (the latter is not strict but practical).

- FLASH Examples
  - Assessing time-accuracy of compressible flow solver
  - Evolution of the level set function
  - Convergence rates for low Mach number flow solver

Verification of Compressible Flow Solver

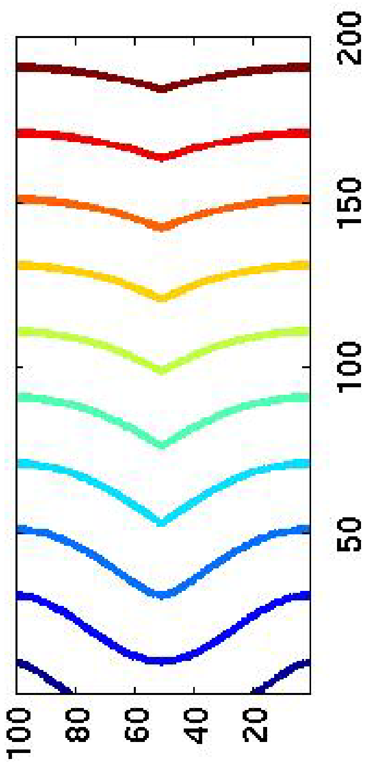


Verification of Prototype Level Set Module

poster

smooth front

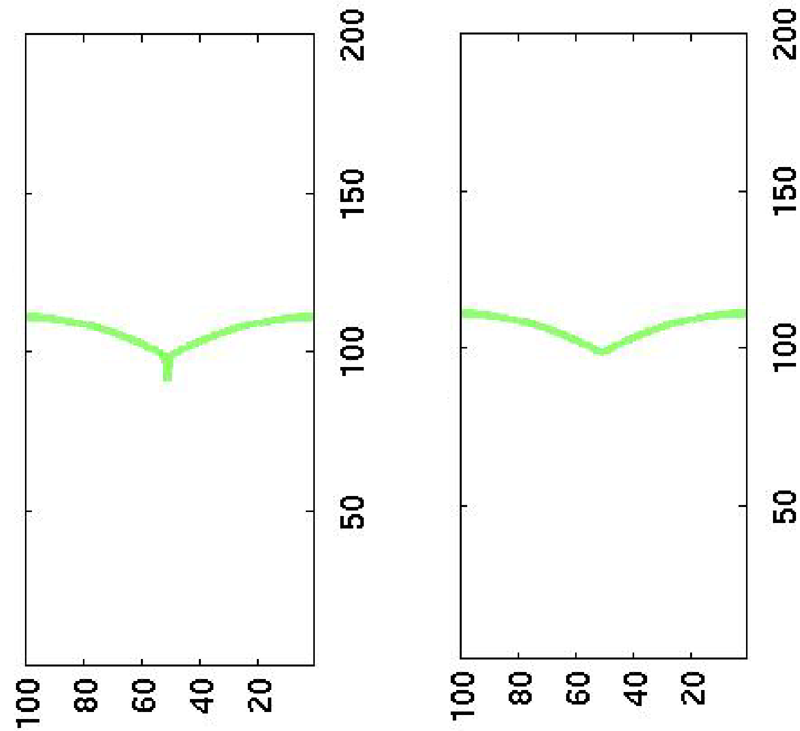
cusp formation



t=80

simple upwind

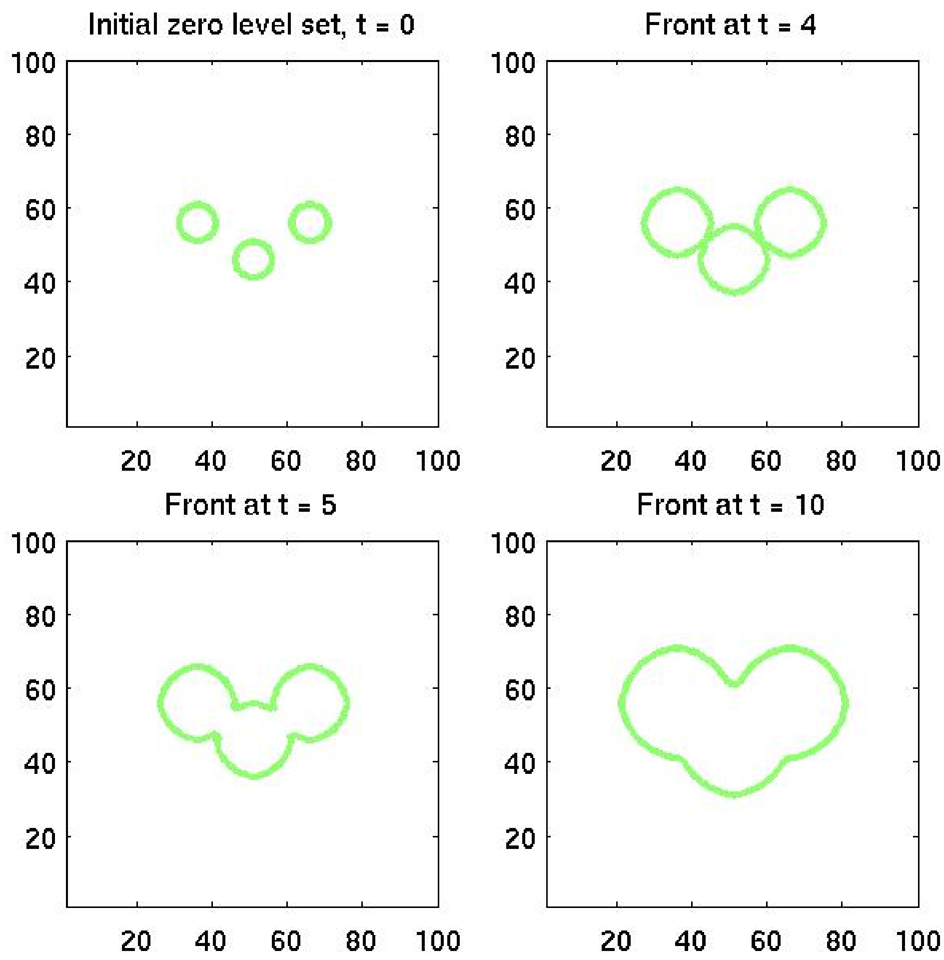
improved upwind



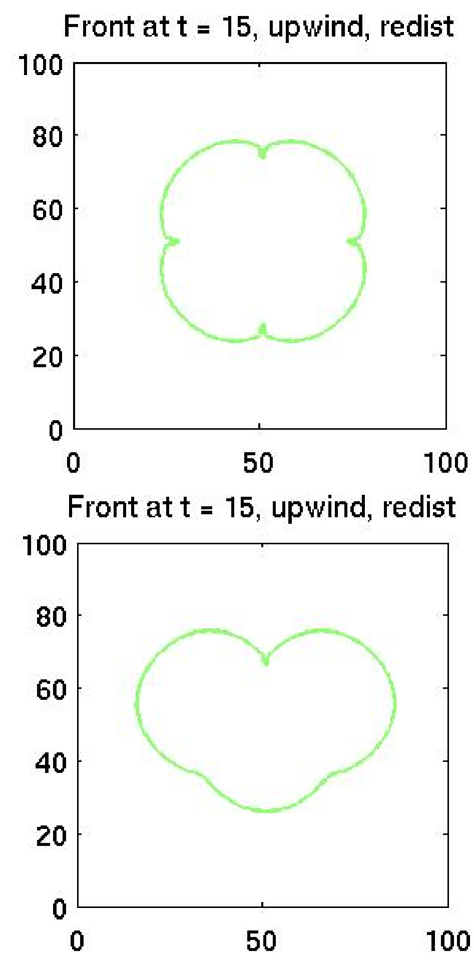
Verification of Prototype Level Set Module

poster

Improved Upwind



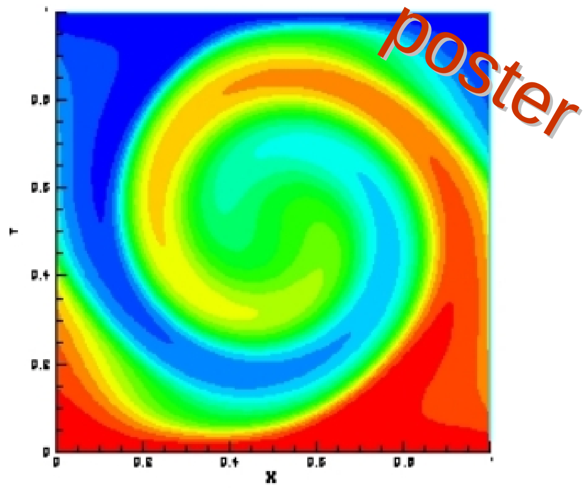
Original Upwind

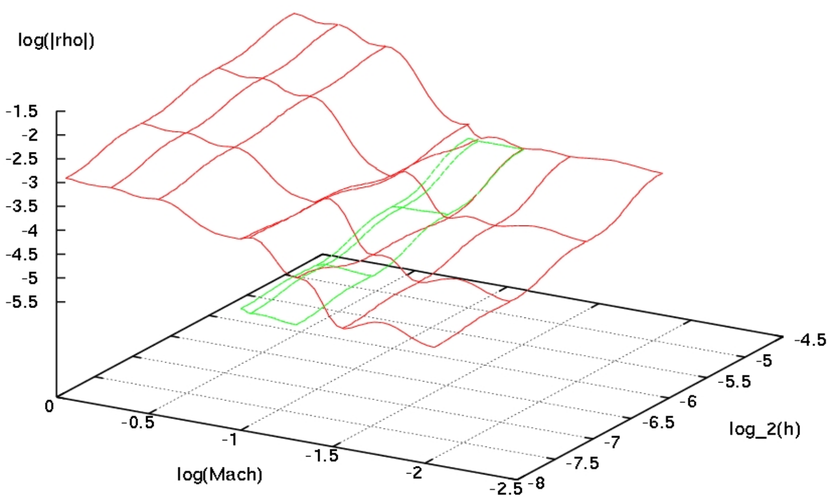


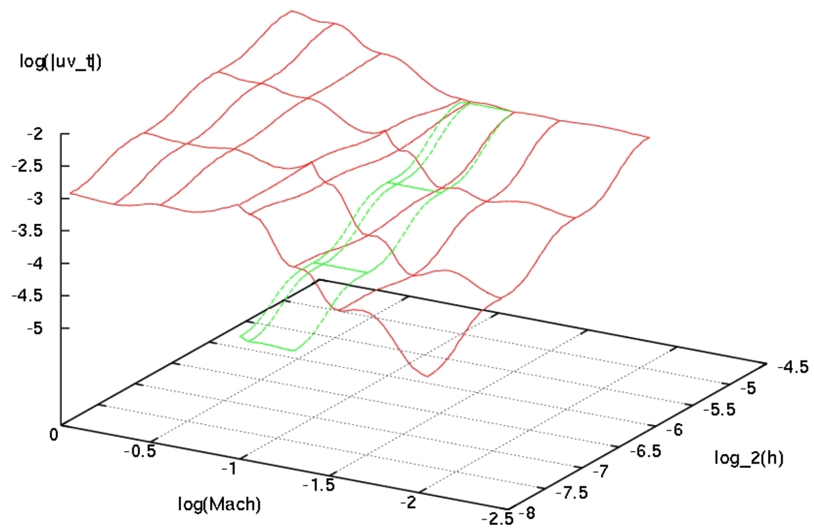
Verification of Prototype Low Mach Number Flow Solver

- Motivation
  gravity waves, nova pre-TNR, WD pre-ignition

- Low speed projection method (Colella and Pao,1999)
  - Based on projection method for incompressible flows
  - Valid for subsonic or weakly compressible flow
  - Velocity field decomposition
    Incompressible part: explicit solver
    Acoustic part: implicit solver



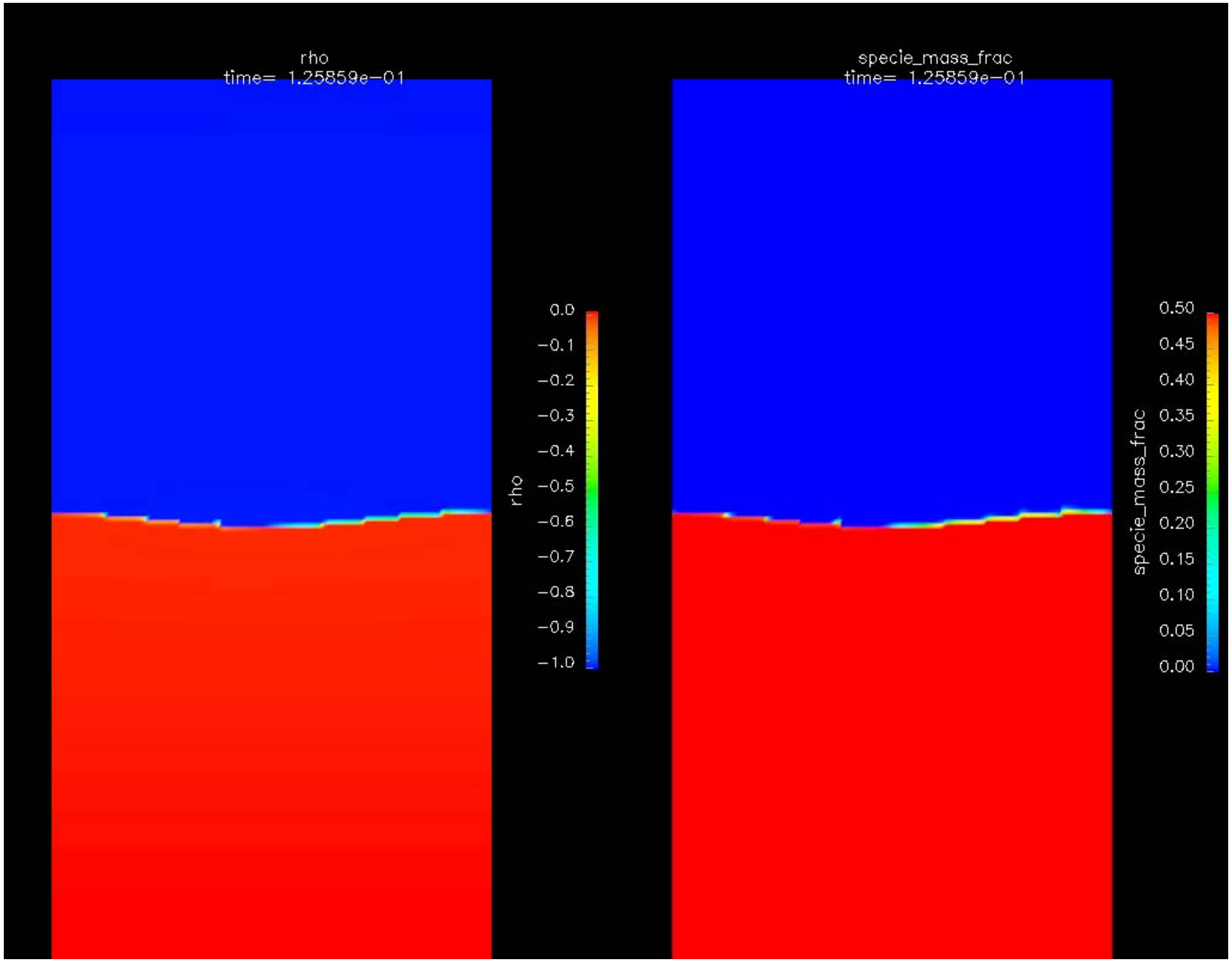




Verification of Prototype Low Mach Number Flow Solver

Gravity wave breaking towards nova mixing studies

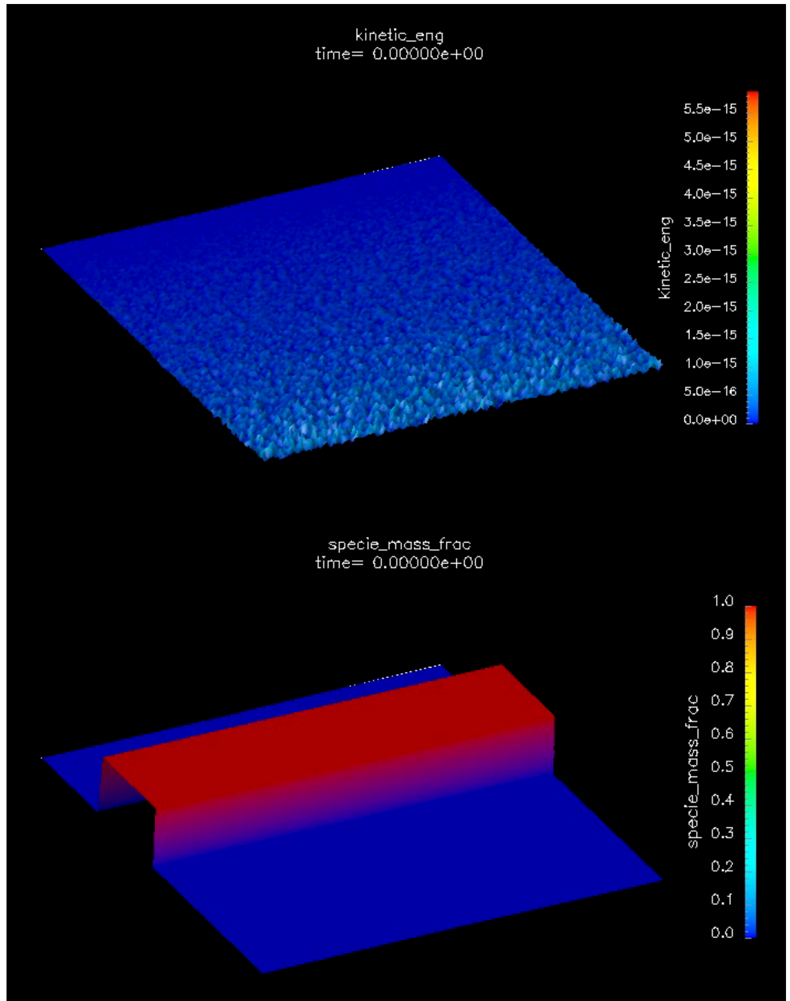
poster



Verification of Prototype Low Mach Number Flow Solver

Penetrative convection towards white dwarf core convection

poster



Past Validation of Computational Modules

- Access to experiments: collaborations with LANL (shock-tube) and LLNL (high-energy density laser) experiments.
- Initial program: alpha-group collaboration on RTI (Labs & AWE)

PHYSICS OF FLUIDS VOLUME 16, NUMBER 5 MAY 2004

A comparative study of the turbulent Rayleigh–Taylor instability using high-resolution three-dimensional numerical simulations: The Alpha-Group collaboration

Guy Dimonte
Los Alamos National Laboratory, Los Alamos, New Mexico 87545

D. L. Youngs
Atomic Weapons Establishment, Aldermaston, Reading, Berkshire RG7 4PR, United Kingdom

A. Dimits, S. Weber, and M. Marinak
Lawrence Livermore National Laboratory, Livermore, California 94551

S. Wunsch
Sandia National Laboratories, Livermore, California 94551

C. Garasi and A. Robinson
Sandia National Laboratories, Albuquerque, New Mexico 87185-0819

M. J. Andrews and P. Ramaprabhu
Texas A & M University, College Station, Texas 77843-3123

A. C. Calder, B. Fryxell, J. Biello, and L. Dursi
University of Chicago, Chicago, Illinois 60637

P. MacNeice and K. Olson
NASA Goddard Space Flight Center, Greenbelt, Maryland 20771

P. Ricker, R. Rosner, F. Timmes, H. Tufo, Y.-N. Young, and M. Zingale
University of Chicago, Chicago, Illinois 60637

(Received 2 May 2003; accepted 29 January 2004; published online 8 April 2004)

Past Validation of Computational Modules

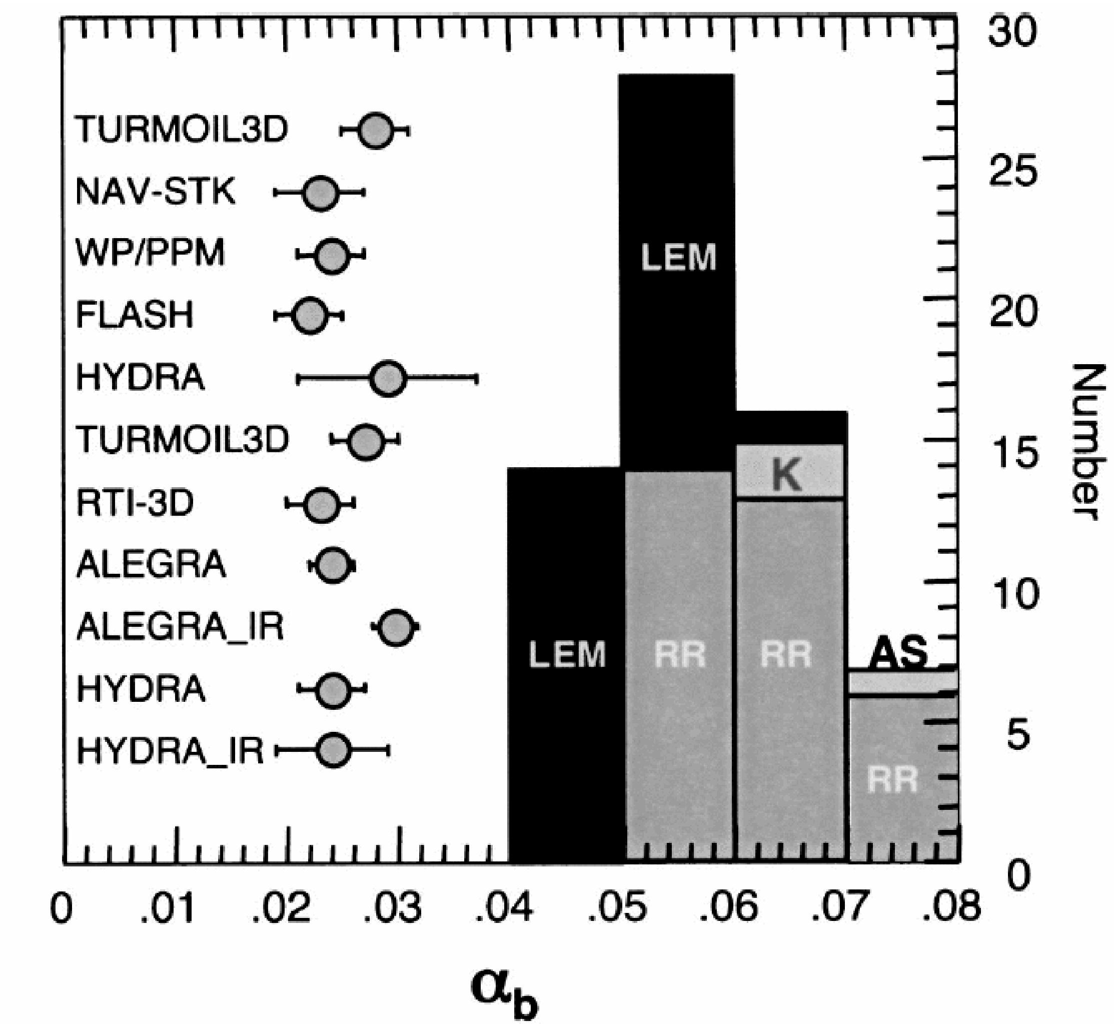
- Initial program: alpha-group collaboration on RTI (Labs & AWE)

TABLE I. Code types and names.

Institution	Code	Method	Zoning	IR
AWE	TURMOIL3D	Eulerian	256×256×512	No
			128×128×256	No
U. Chicago	FLASH	P-P-M	256×256×512	No
LLNL	WP/PPM	P-P-M	256×256×512	No
LLNL	NAV/STK	N-S	256×256×512	No
Texas A & M	RTI-3D	Eulerian	128×128×256	No
LLNL	HYDRA	ALE	256×256×512	No
			128×128×256	Yes and No
Sandia NL	ALEGRA	ALE	128×128×256	Yes and No

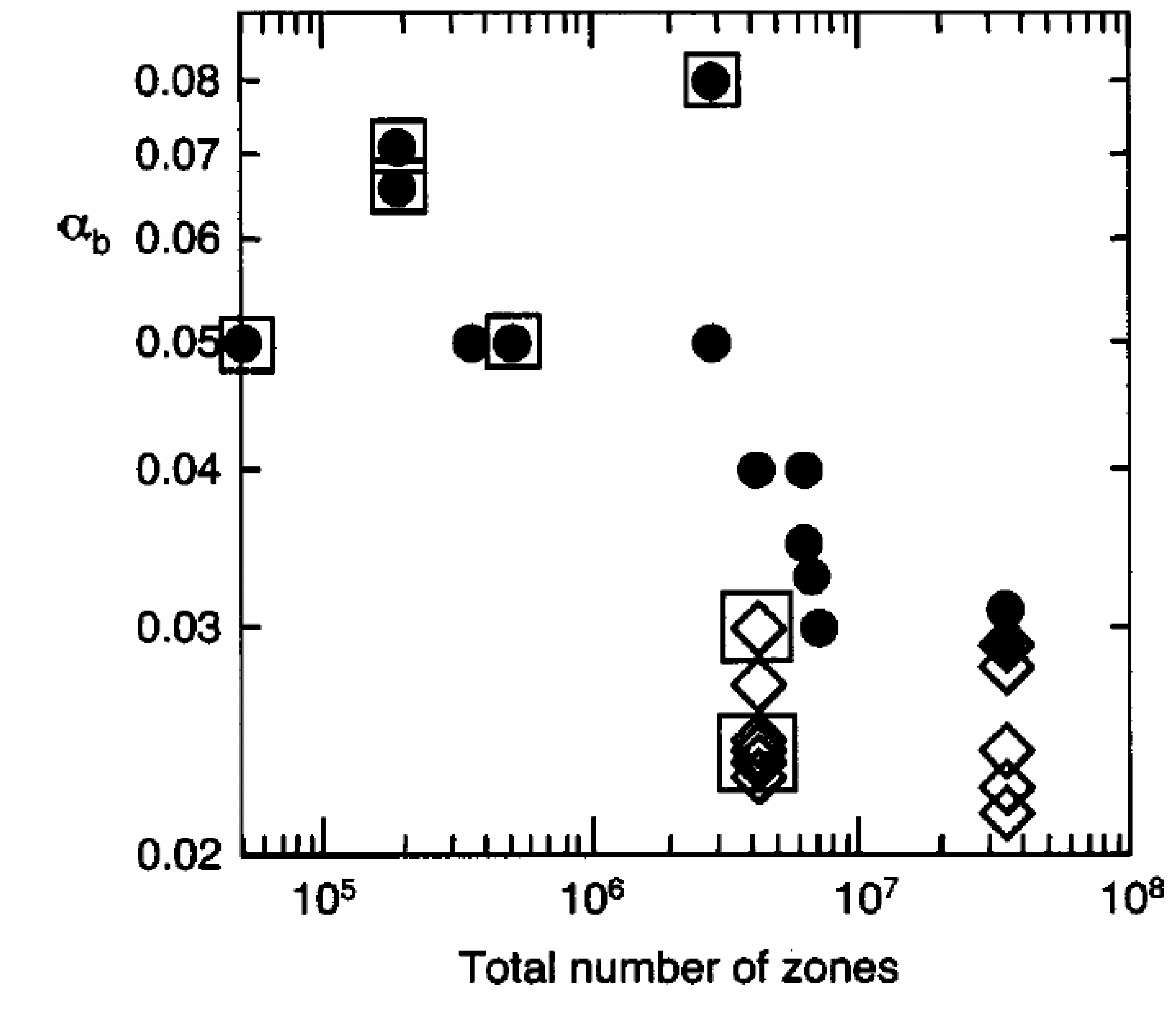
Past Validation of Computational Modules

- Initial program: alpha-group collaboration on RTI (Labs & AWE)



Past Validation of Computational Modules

- Initial program: alpha-group collaboration on RTI (Labs & AWE)



Past Validation of Computational Modules

similarity ratio of $D_b/h_b \sim 0.54 \pm 0.07\, \rho_h/\Sigma\rho$. The first NS (Refs. 23, 25, 31, 35, 36, 38, 39) conducted in two dimensions (2D) without front-tracking (FT) obtained $\alpha_b \sim 0.035-0.05$. Larger values of α_b were expected in 3D since single modes grow faster (larger Fr) than in 2D. Instead, the highest resolution 3D simulations[35,38–42] obtained $\alpha_b \sim 0.03$. Simulations with FT obtained larger values $\alpha_b \sim 0.05-0.08$ in both 2D (Refs. 32, 33, 48) and 3D (Refs. 14, 17, 43, 44), and this was associated with the reduction in numerical diffusion. However, Glimm *et al.*[32] also reported that α_b decreased to as small as 0.038 late in time as the bubble "connectivity" (entrainment) increased. When entrainment was reduced in the LEM (Ref. 30) by increasing the surface tension 50-fold, α_b increased by 20%. Unfortunately, this also imposed long wavelength initial perturbations and these can also increase α_b.[21,22,31,34,40,49] Although these various results can be confusing, they do suggest that entrainment and the initial conditions can affect the value of α_b.

- Conclusion: possibly an unresolved component in the ICs

Experiment Analysis Techniques (Basic Physics)

Can we find a set of initial conditions that would result in a certain, possibly observed, state a at a later time?

Andrei Draganescu (currently at SNL)

- Nonlinear problems involving several unknown parameters

  Example: experimental uncertainties (the initial conditions)

- Mathematical representation: PDE-constrained optimization problem

- Main result: for a model problem (linear parabolic equations) determining initial conditions is relatively cheap

- Next step: designing a structure to combine automatic differentiation and this form of multigrid.

Current Validation of Computational Modules

- Access to experiments: collaborations with LANL (shock-tube) and LLNL (high-energy density laser) experiments
- Current program: shock-tube shock-cylinder experiment (LANL)
- Presentations at the AMR Chicago workshop and HEDLA (posters), and La Jolla V&V workshop and IWPCTM9 (talks); working towards the refereed journal publication

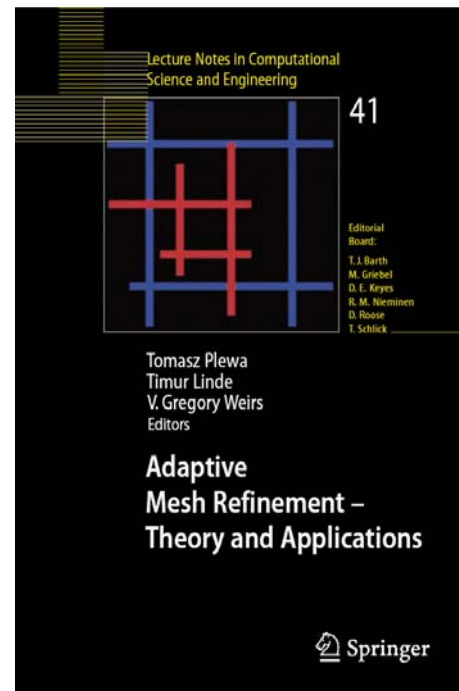
Simulation of Vortex–Dominated Flows Using the FLASH Code

Vikram Dwarkadas,[1] Tomek Plewa,[1] Greg Weirs,[1] Chris Tomkins,[2] and Mark Marr-Lyon[2]

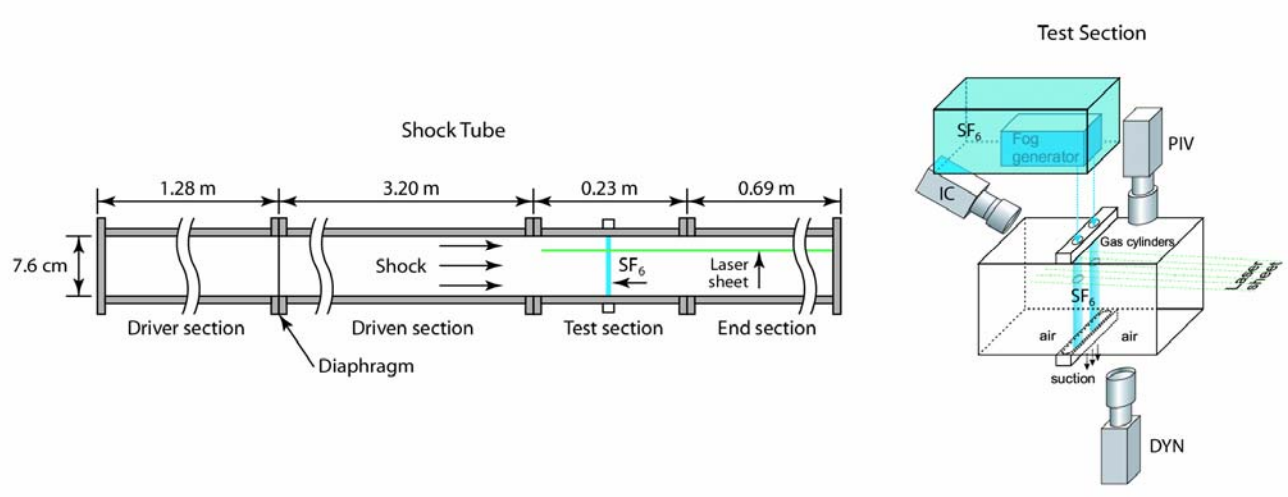
[1] ASCI FLASH Center, University of Chicago vikram@flash.uchicago.edu, tomek@flash.uchicago.edu, weirs@flash.uchicago.edu
[2] Los Alamos National Laboratory ctomkins@lanl.gov, mmarr@lanl.gov

1 Abstract

We compare the results of two–dimensional simulations to experimental data obtained at Los Alamos National Laboratory in order to validate the FLASH code. FLASH is a multi–physics, block–structured adaptive mesh refinement code for studying compressible, reactive flows in various astrophysical environments. The experiment involves the lateral interaction between a planar Ma=1.2 shock wave with a cylinder of gaseous sulfur hexafluoride (SF_6) in air.



Case Study: LANL Shock-Cylinder Experiment



- A column of sulfur hexafluoride (SF_6) falls through the air-filled test section; $M_{SF6} \sim 5\ M_{air}$
- A Mach 1.2 shock traverses the cylinder and continues down the tunnel
- Indirect SF_6 visualization, by visible-light scattering water/glycol “fog”
- Direct SF_6 visualization, by Rayleigh-scattering off SF_6 molecules
- Particle Image Velocimetry (PIV) with fog
- One image per experiment; time sequence can be constructed because of repeatability

Flowfield Development

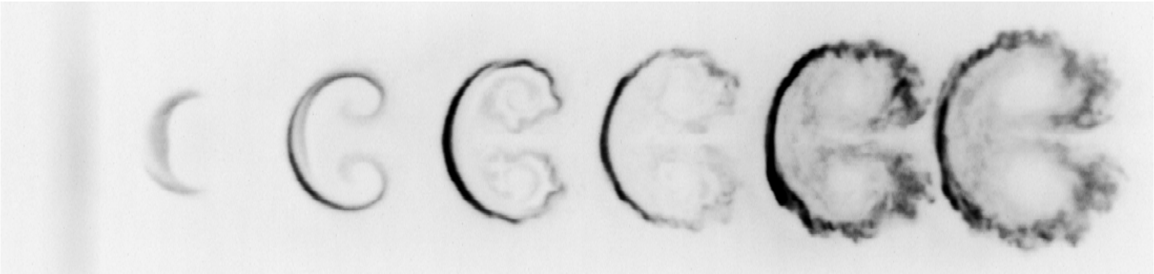
Phase I: shock-interaction

- Misalignment of pressure and density gradients results in baroclinic vorticity deposition at the interface as the shock traverses the cylinder
- Compressible, wave dominated
- Fast, < 50 μs

Phase II: instability growth

- A counter-rotating vortex pair forms, and secondary instabilities (Kelvin-Helmholtz) develop on the interface
- Weakly compressible, dominated by viscosity, instabilities, vortex dynamics
- Slow, ~800 μs
- *Highly sensitive to conditions established in Phase I*

Flowfield Development



- Experimental time series, water/glycol fog visualization of SF_6 mole fraction.
- Images correspond to 50, 190, 330, 470, 610, and 750 μs after shock impact
- Composite image does not preserve time-distance relationship

Past Focus

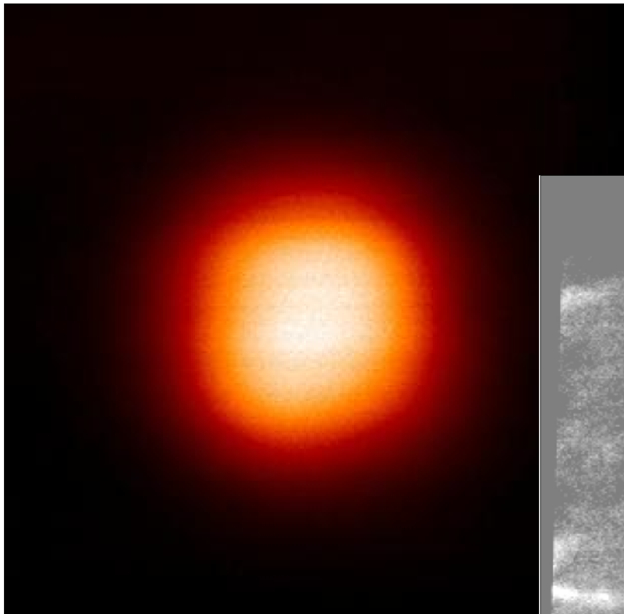
Aspects considered in depth:

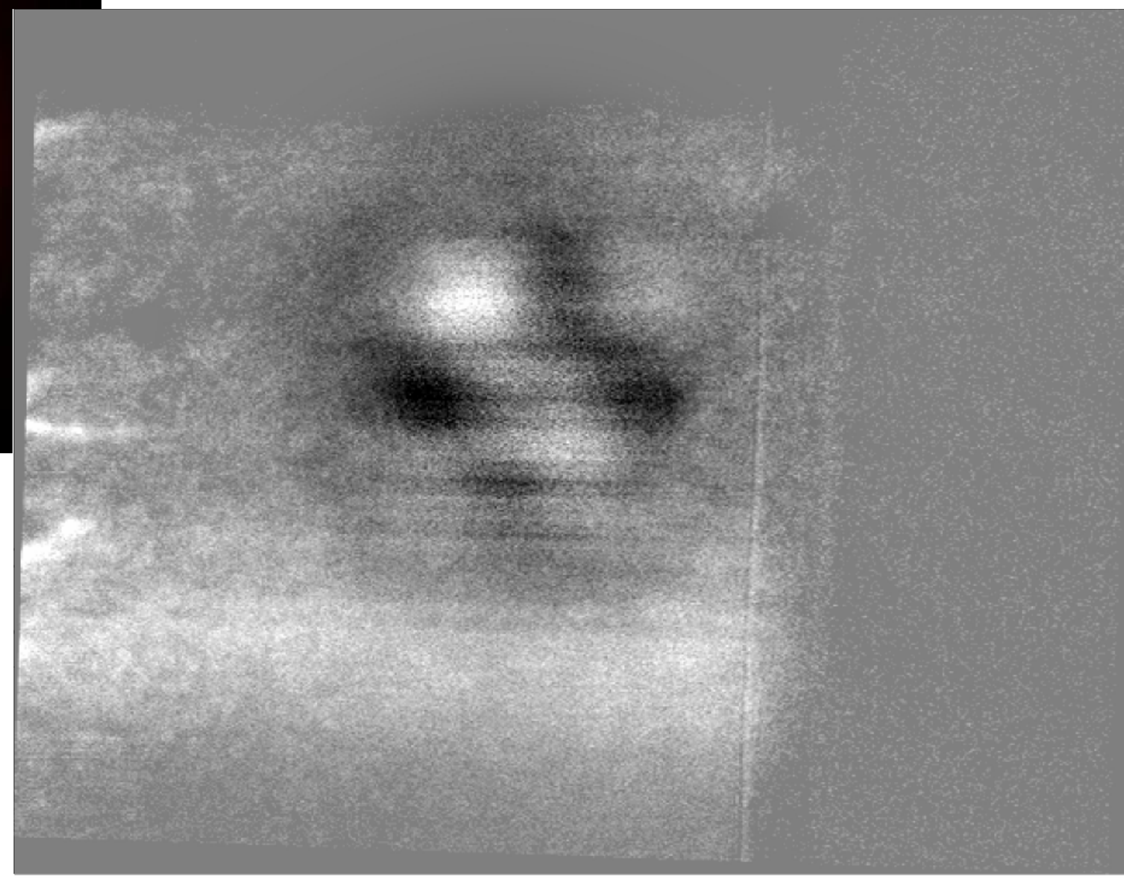
- Initial conditions
- Sensitivity to simulation parameters:
  - Resolution (numerical viscosity)
  - Adaptive Mesh Refinement (AMR)
  - Courant number
  - Mesh refinement criteria
- Velocity fields
- Double cylinder configuration
- Speculative 3-D calculation

Other possible aspects:

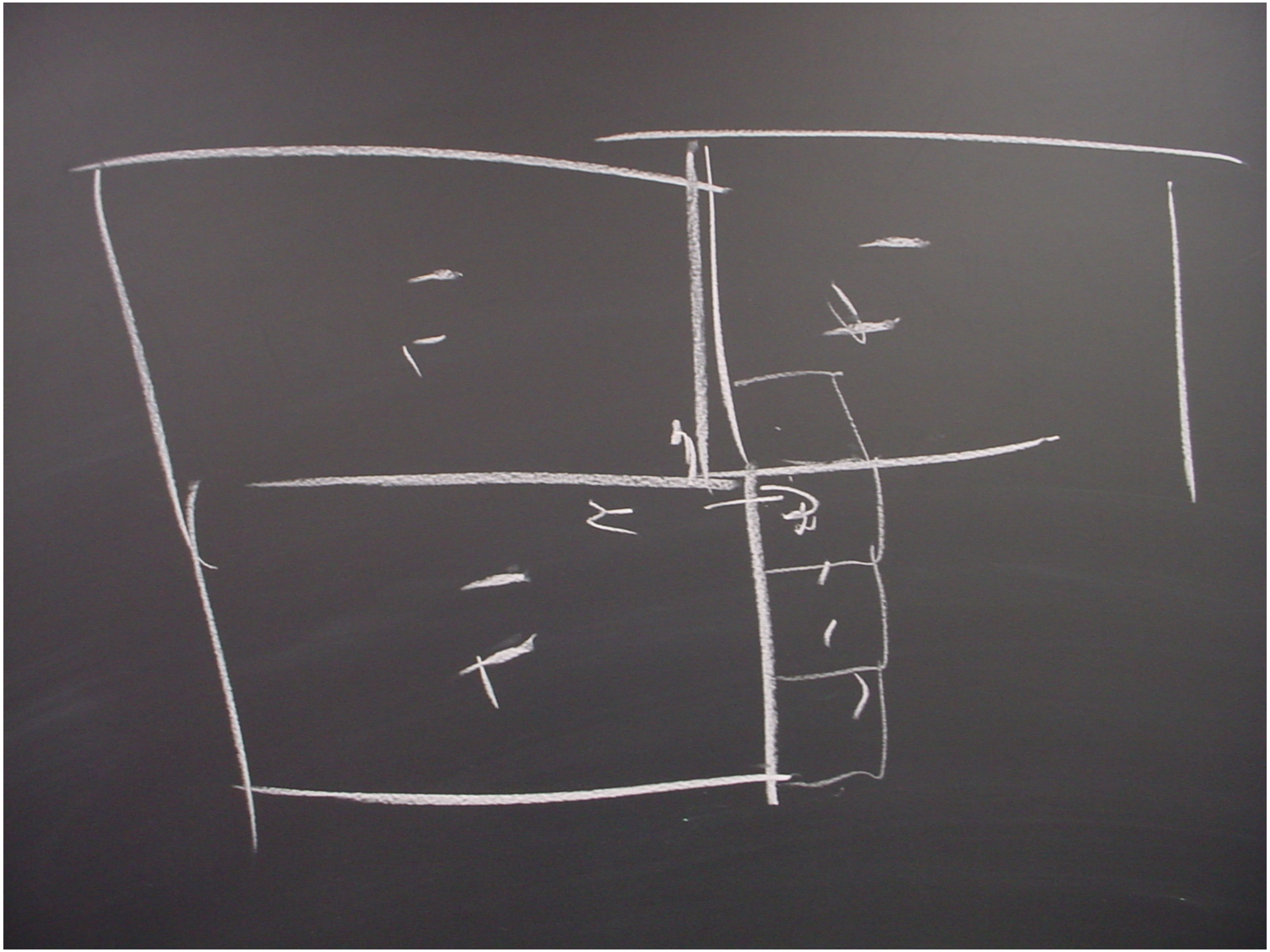
- Shock strength
- Equation of state

Initial Conditions: Cylinder Cross-section

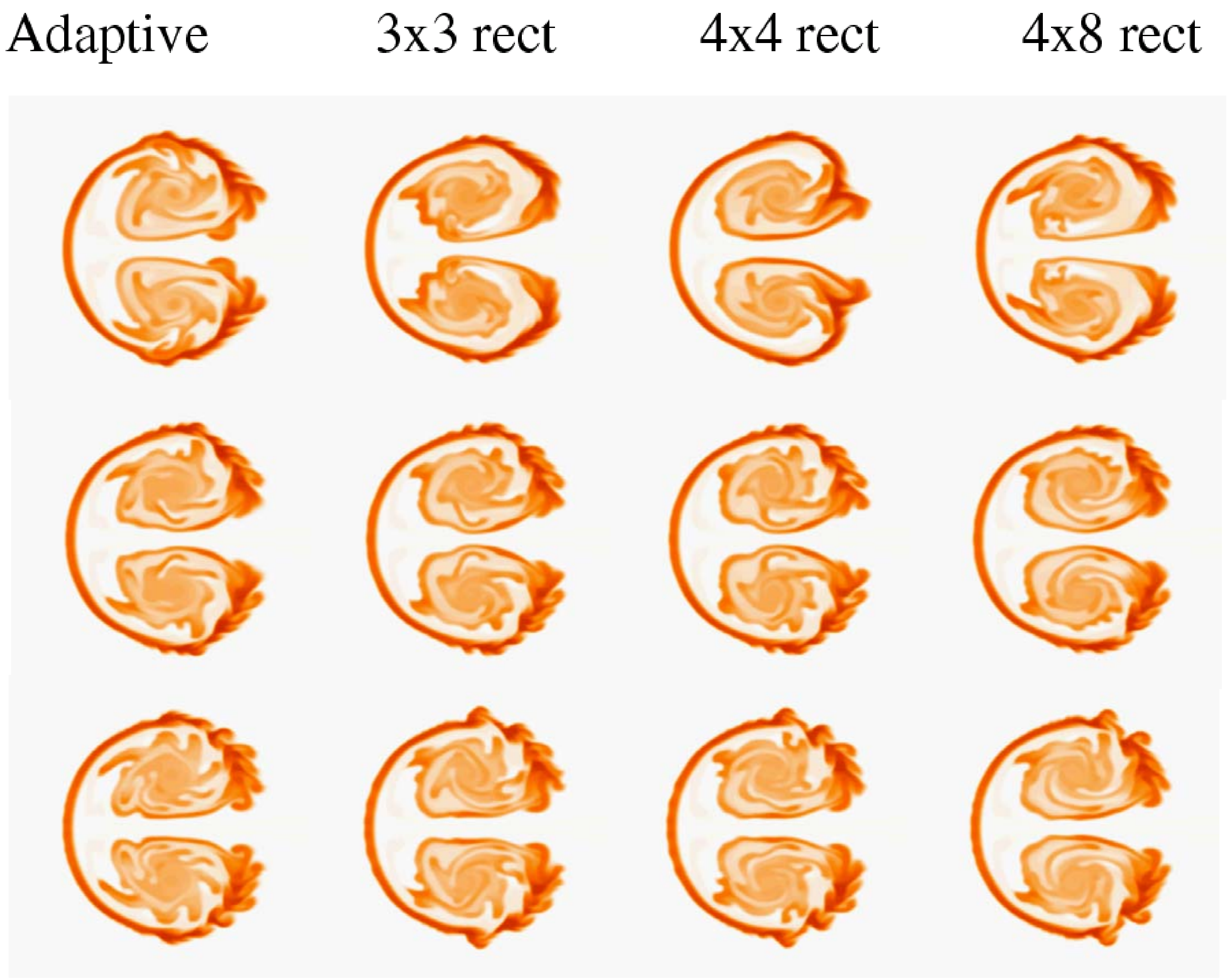




FLASH Code is the AMR code



CFL dependency

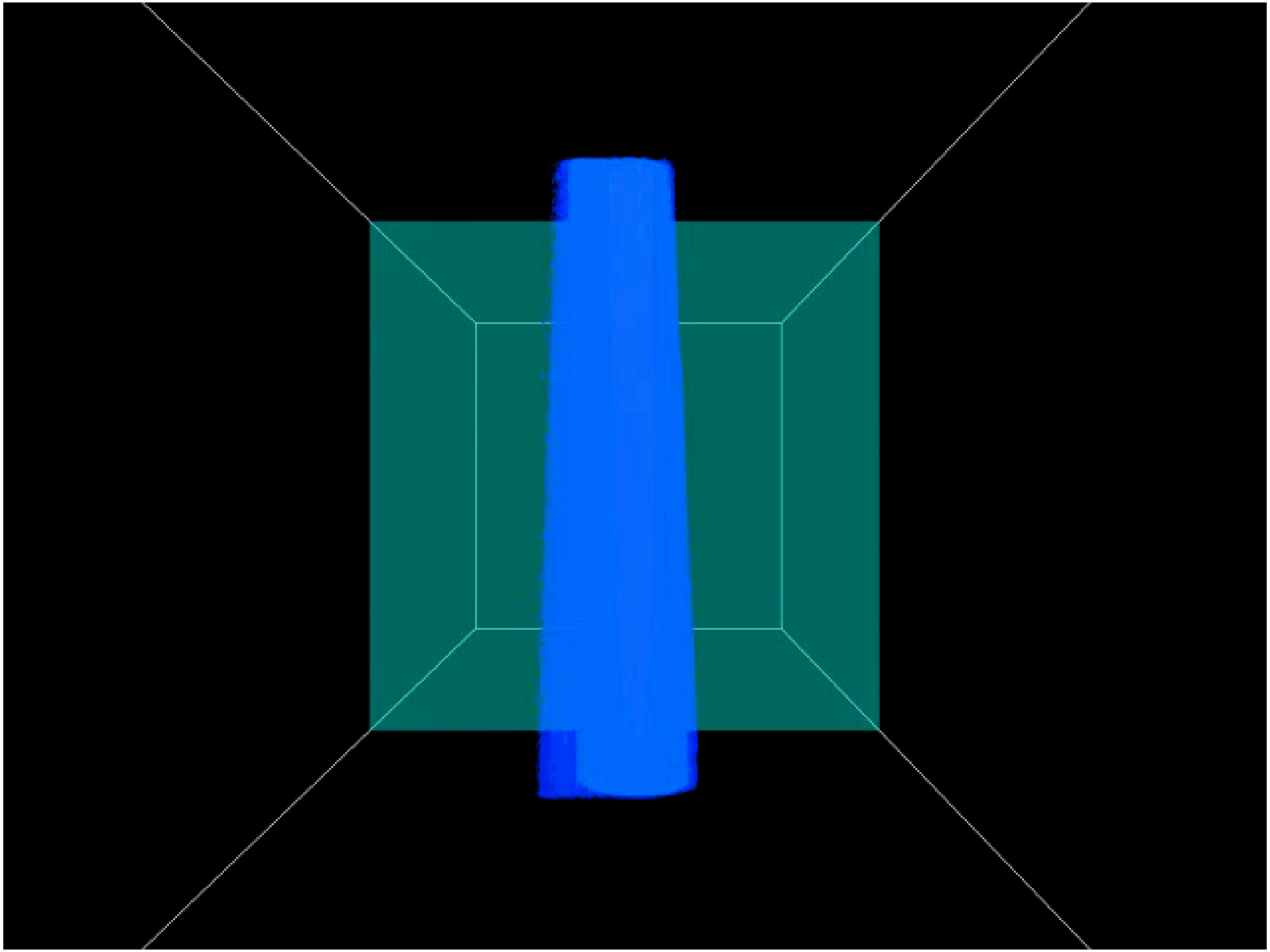


CFL=0.8

CFL=0.4

CFL=0.2

3-D Shock-Cylinder Interaction (speculative)

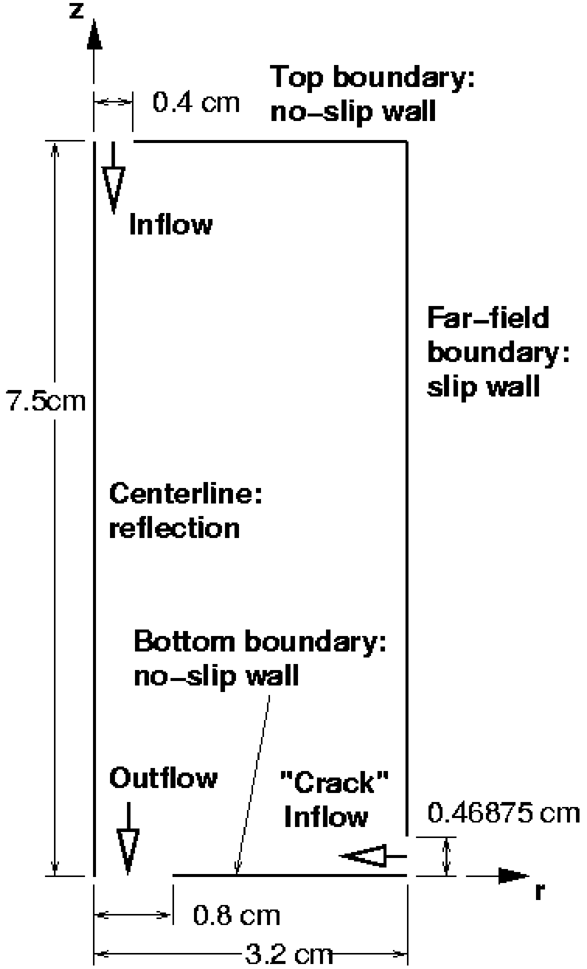


Current Focus

- Initial conditions
- Better metrics
- Three-dimensional effects

Simulations of Initial Conditions

- Axisymmetric code (Todd Dupont)
- Motivation: Determine X_{SF6}
- Motivation: Initialize three-dimensional flowfield
- Solve (single) species and momentum equations and elliptic equation for pressure
- Convection, gravity, constant viscosity, constant binary diffusion, variable density, isothermal
- Run until steady state is achieved



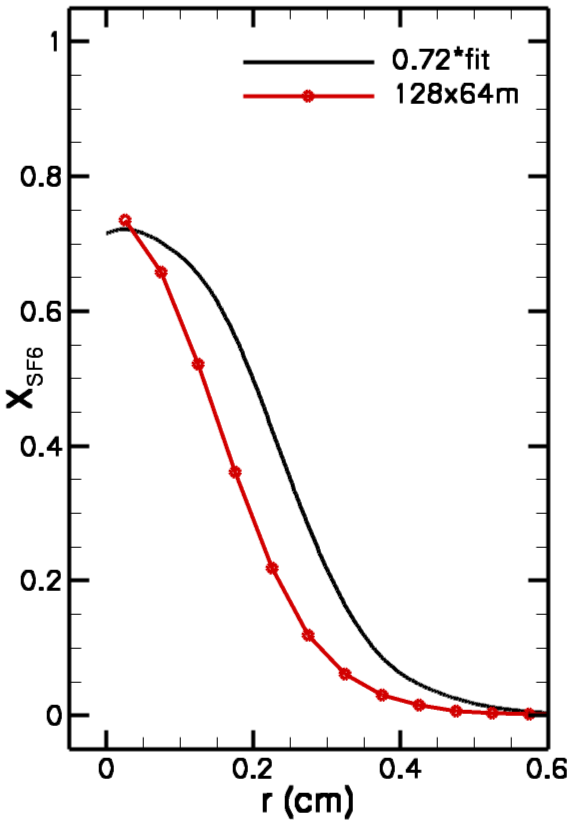
Simulations of Initial Conditions

- Axisymmetric code input parameters:
  Inlet velocity (parabolic profile)
  LANL estimate: 10 cm/s
  Inlet mass fraction of SF_6
  LANL estimate: 1.0
  Simulation Parameters
  dimensions of domain
  resolution

- Code output:
  SF_6 mole fraction profile
  Fit to experimental image
  X_{SF6} in the image plane
  LANL estimate: 0.8

Inlet Y_{SF6} = 1.0
Inlet v_z = 10.0 cm/s

poster



Gravity-Diffusion Competition

poster

- Inlet velocity too low

  the profile is too narrow (closer to the centerline than the experimental data): gravitational acceleration of SF_6 leads to necking

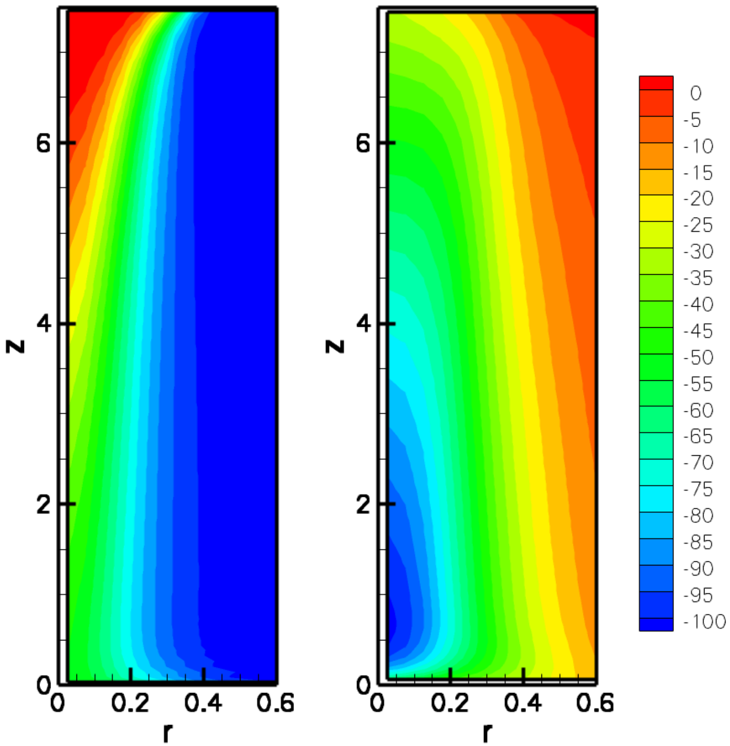
- Inlet velocity too high

  the profile is too steep: diffusion does not have enough time to act

- The inlet mass fraction affects the gravitational acceleration and the output X_{SF6}

SF_6 mole fraction

v_z



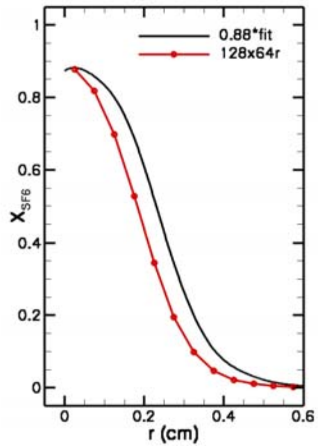
Inlet v_z = 15.0 cm/s

Inlet Y_{SF6} = 1.0

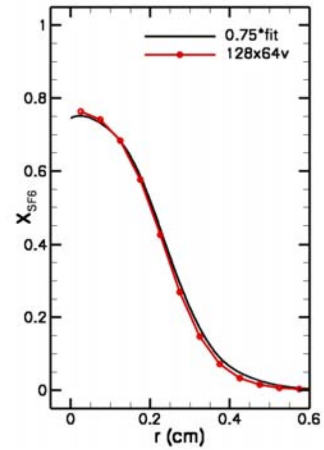
Simulations of Initial Conditions

poster

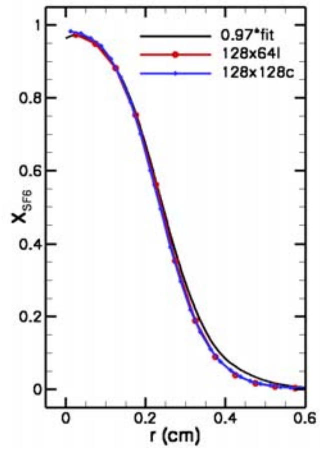
Inlet Y_{SF6} = 1.0
Inlet v_z = 15.0 cm/s



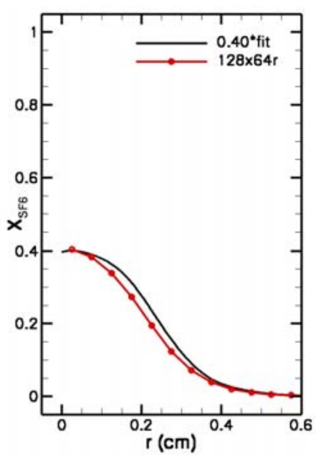
Inlet Y_{SF6} = 0.95
Inlet v_z = 22.50 cm/s



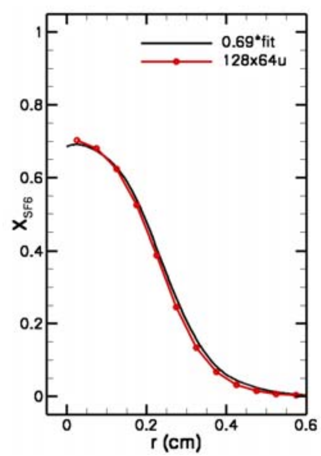
Inlet Y_{SF6} = 1.0
Inlet v_z = 25.0 cm/s



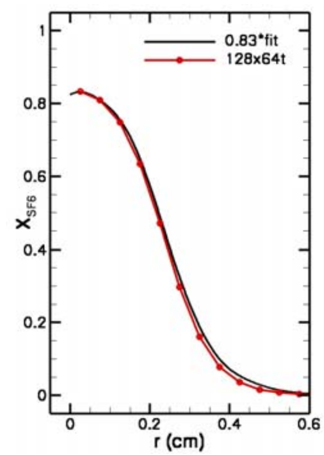
Inlet Y_{SF6} = 0.8
Inlet v_z = 15.0 cm/s



Inlet Y_{SF6} = 0.9315
Inlet v_z = 21.85 cm/s

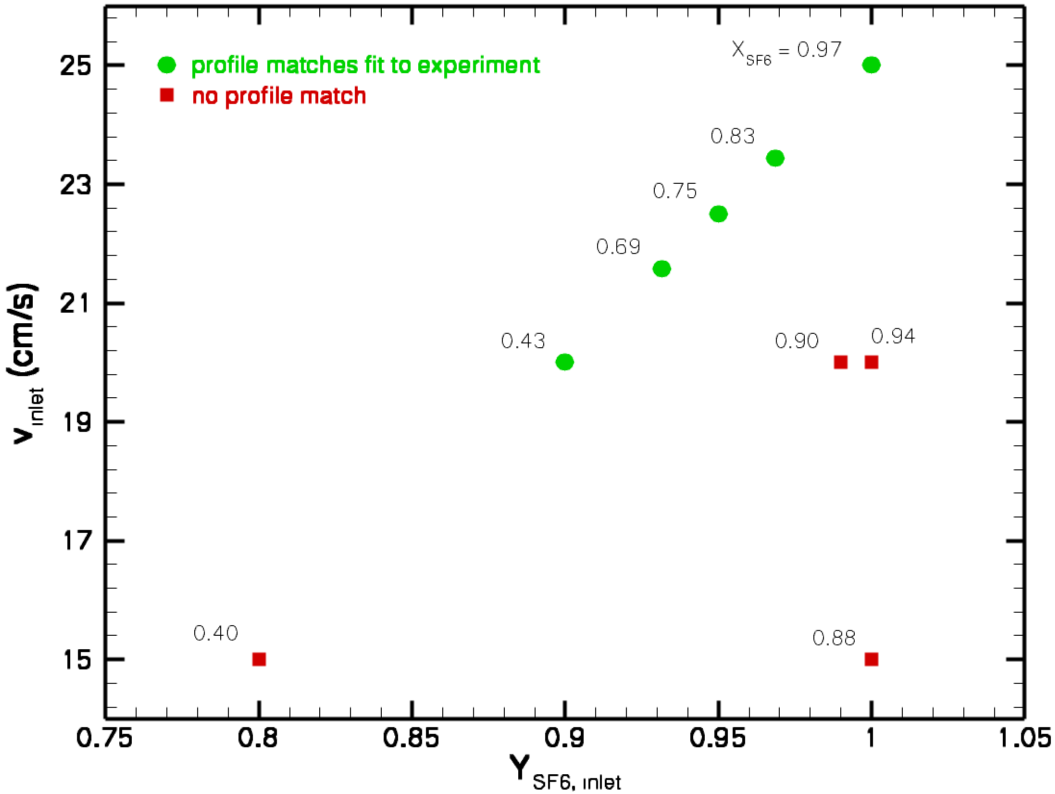


Inlet Y_{SF6} = 0.9685
Inlet v_z = 23.43 cm/s



Simulations of Initial Conditions

poster



- It's not so easy to determine the initial conditions!
- Profile "matches" collapse on a line on the plane: one parameter family
- Should quantify error in matching experimental fit

Looking for Better Metrics

- While visual comparisons were ok to start with, we need a better basis for comparison to experimental data.

  A new metric should be:

  Quantitative

  Well-defined

  Physically meaningful

Possible Metrics

Some possibilities

- Self-induced vortex velocity
- Circulation

Circulation and self-induced vortex velocity both measure the vorticity deposited during the shock interaction.

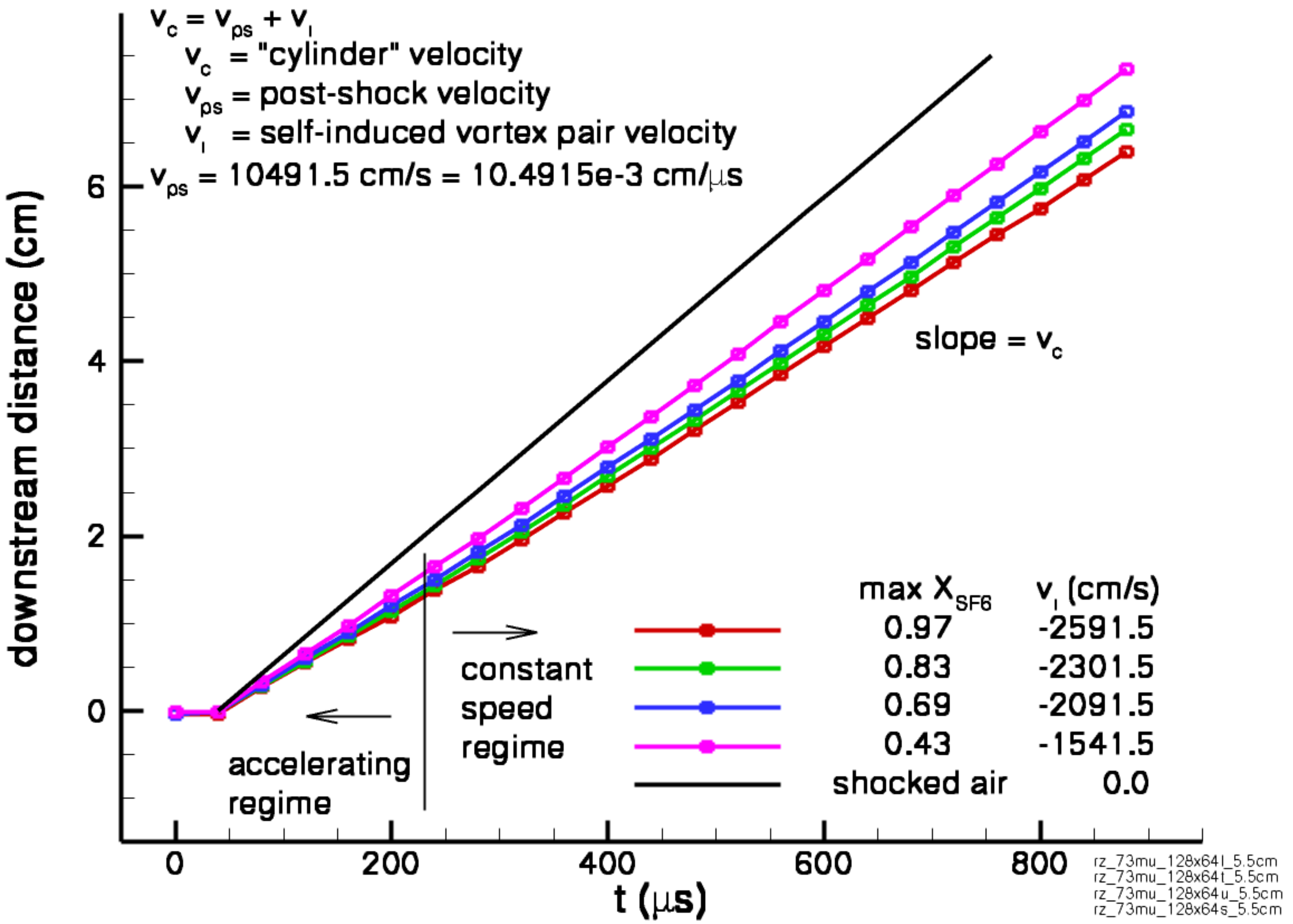
Properties

- Insensitive to small scale structure
- Insensitive to numerical (and physical) viscosity

Application

- A way to probe the initial composition gradients (X_{SF6}), a necessary step before studying evolution on small scales (secondary instabilities, turbulence, diffusion)

Induced Velocity vs. Initial Composition



Circulation

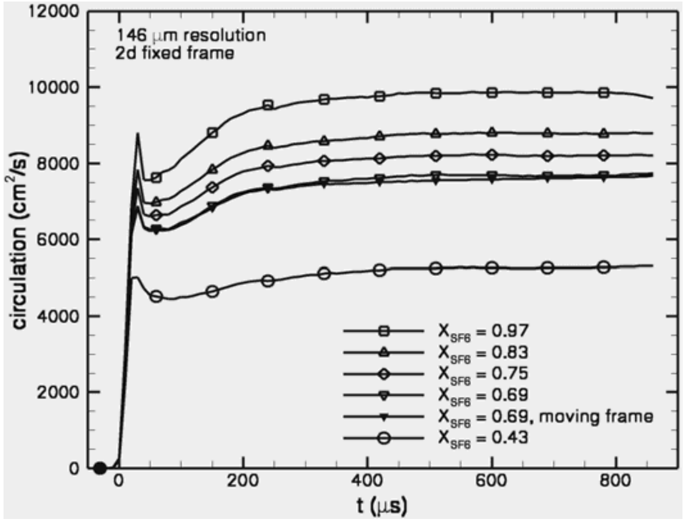
Circulation is the integral of vorticity:

$$\Gamma = \iint \overline{\omega} \cdot dA$$

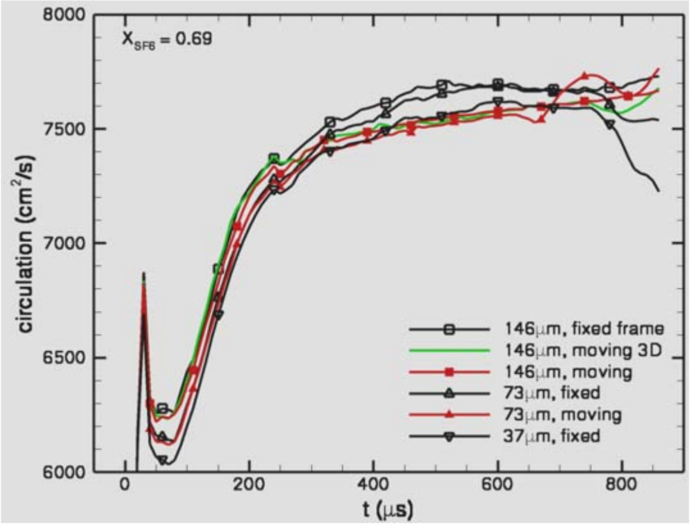
- We consider only the z-component of vorticity
- We integrate over the lower-y half of the domain (lower half in the spanwise dimension)

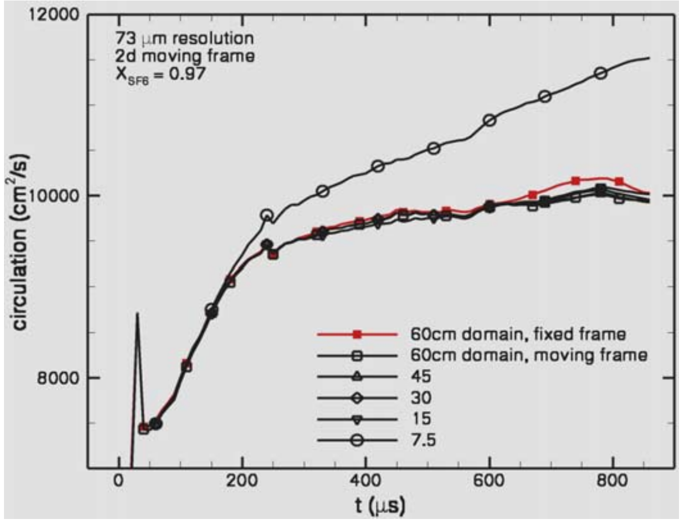
Circulation Sensitivity

Initial SF_6 Mole Fraction



Resolution, Ref. Frame





Domain Size

3-D Simulations

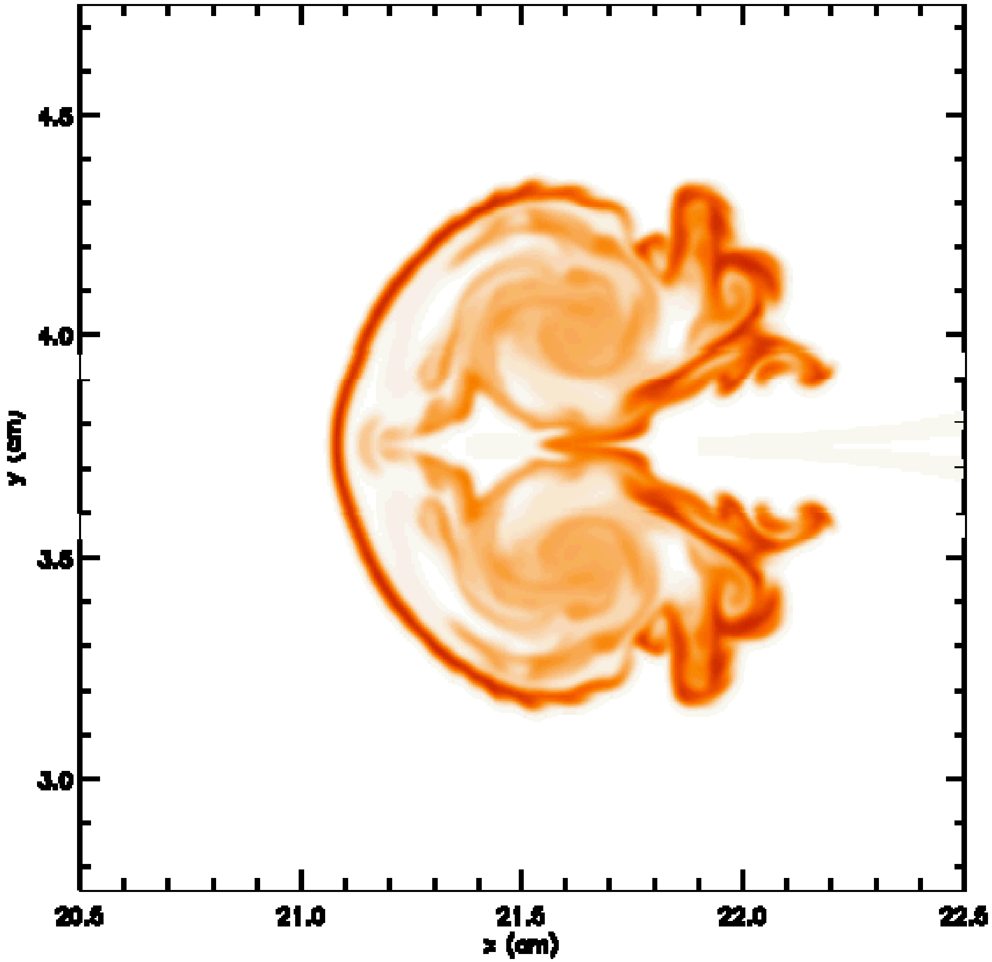
Are three-dimensional effects important?

- SF_6 and air diffuse as the SF_6 flows through the tunnel, leading to vertically varying composition, and thus density, gradients
- Instability growth and small scale structure are generally three-dimensional

We are just beginning to analyze 3D simulations.

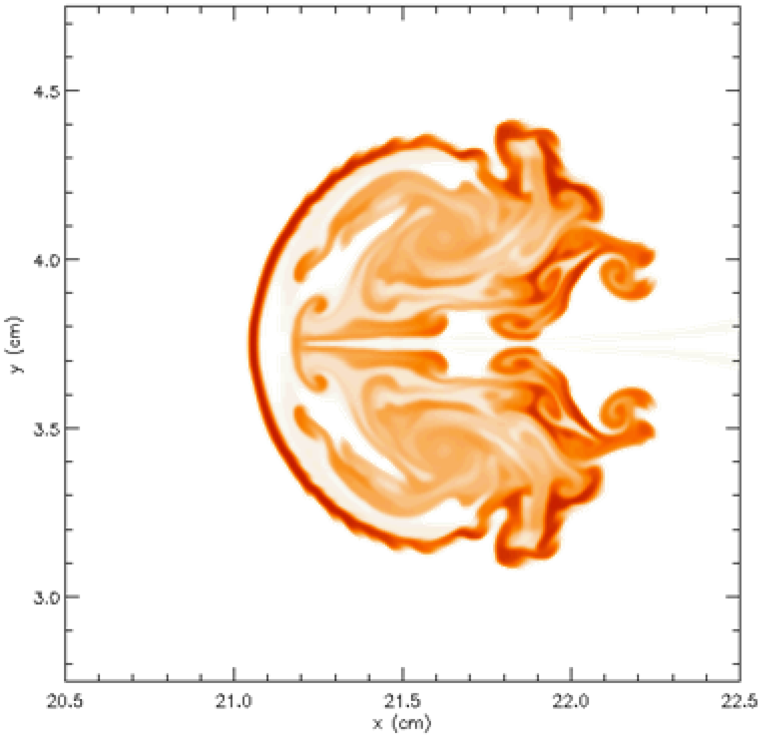
We have left the validation program proper – no experimental data.

2-D vs. 3-D Flow Morphology

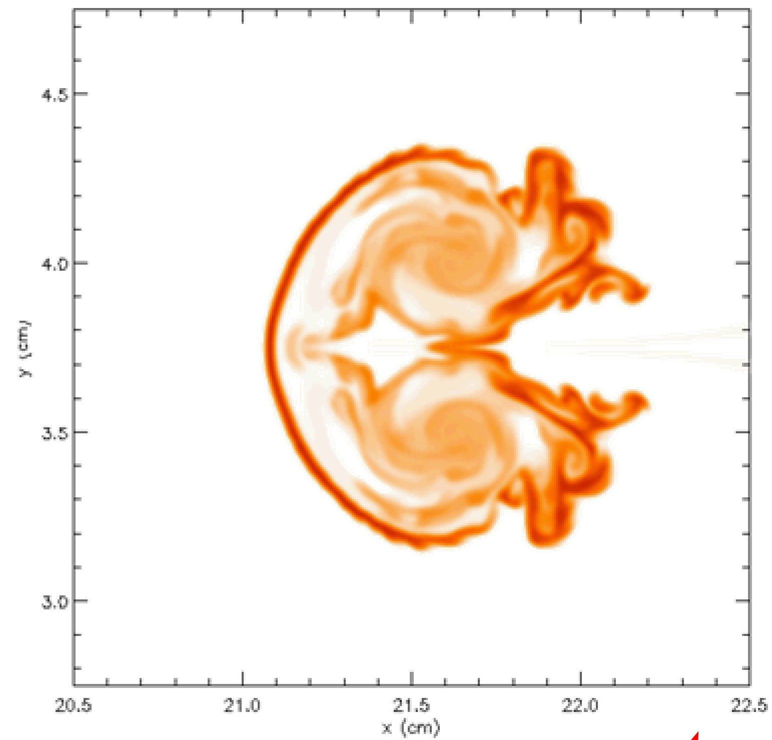


3-D

2-D vs. 3-D Flow Morphology



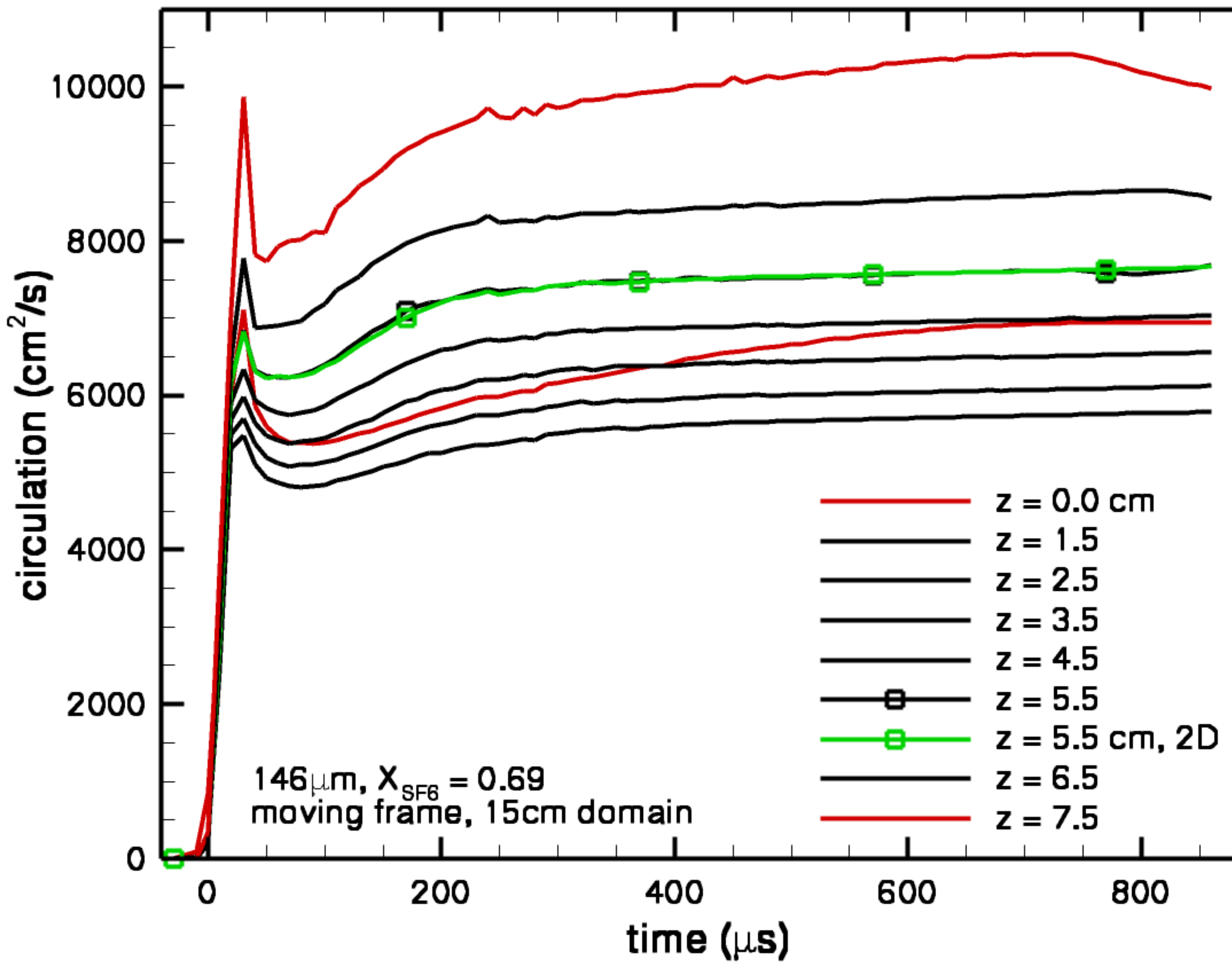
2-D, t = 750 μs



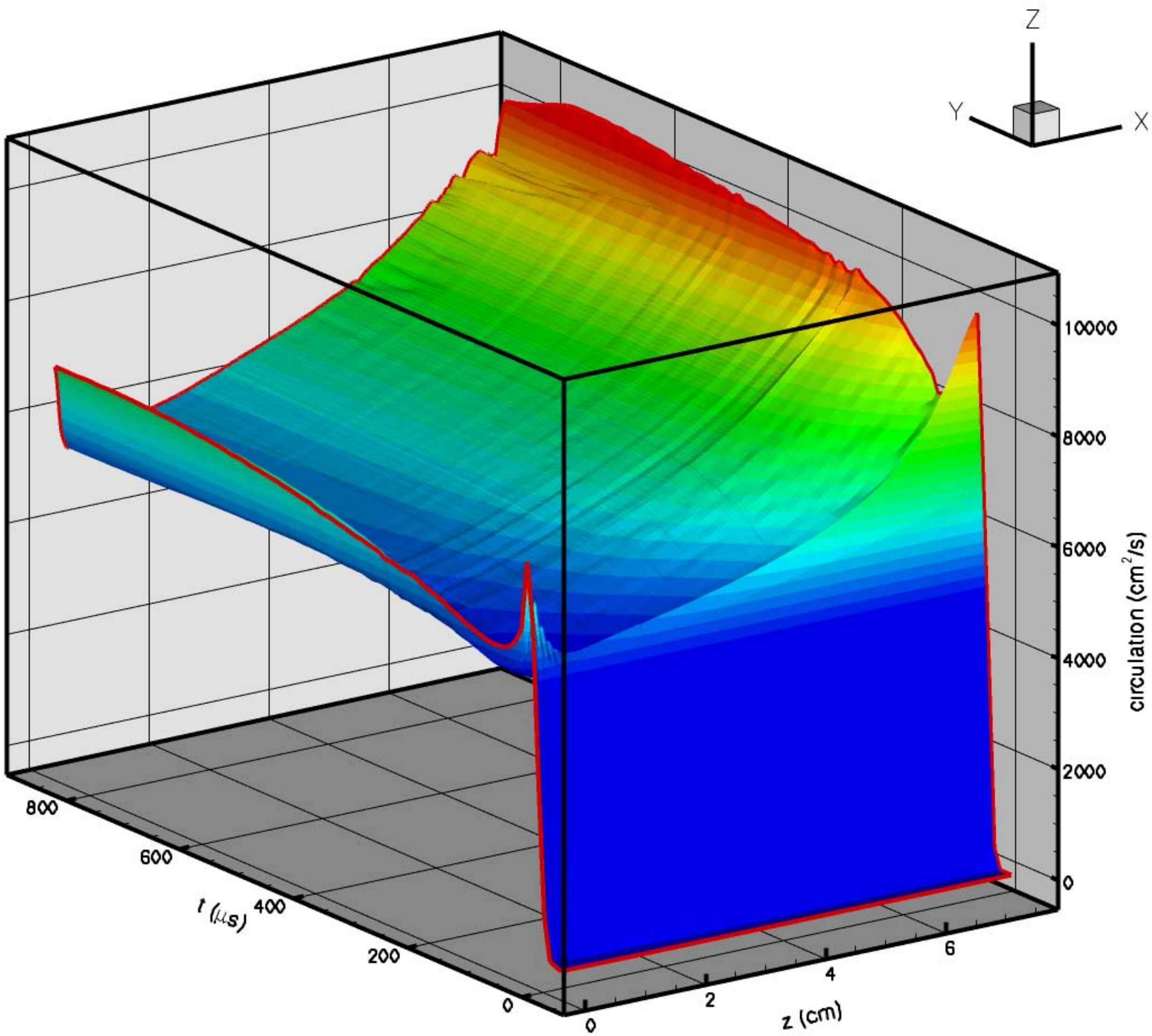
3-D, t = 750 μs

…simulation demonstrates that nature is…

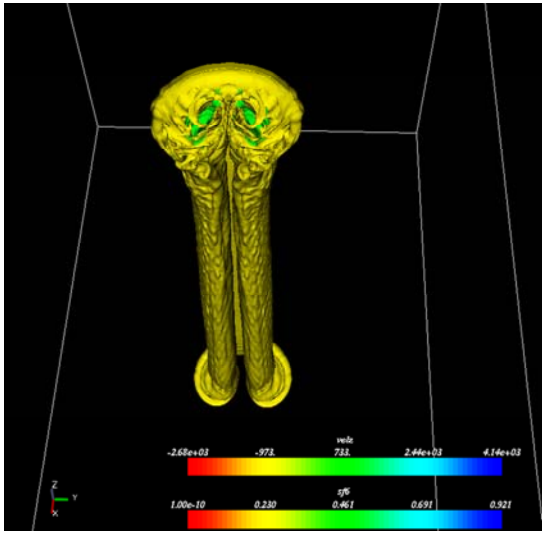
3-D Simulation: Circulation



3-D Simulation: Circulation



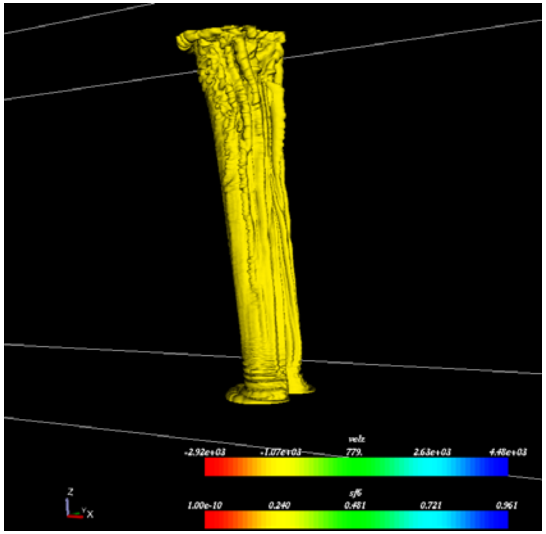
3-D Simulation: Flow Visualization



$X_{SF6} = 0.69$

$t = 750\ \mu s$

Mild structures are visible on the back of the cylinder



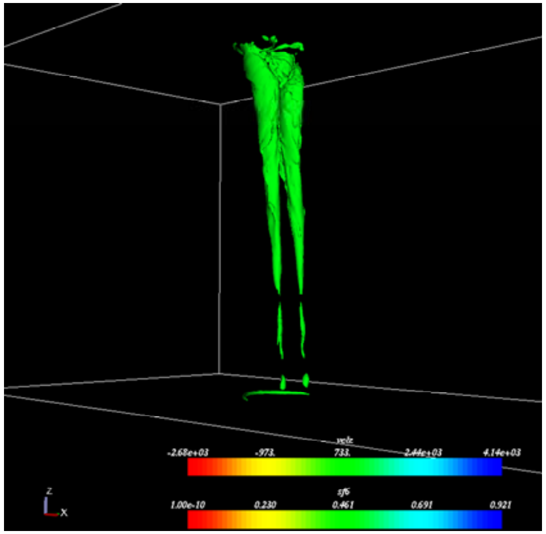
$X_{SF6} = 0.97$

$t = 750\ \mu s$

More structure is visible near the top wall than the bottom

The top of the cylinder has a higher self-induced velocity, resulting in a slight tilt

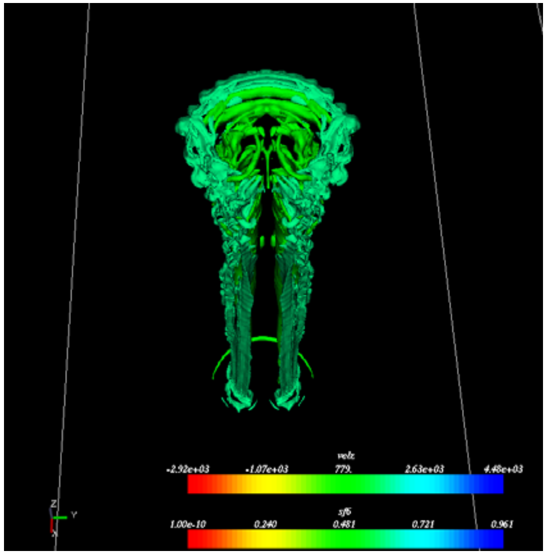
3-D Simulation: Flow Visualization



X_{SF6} = 0.69
t = 750 μs

Note vertical tubes of positive z-velocity, associated with the two primary vortex cores

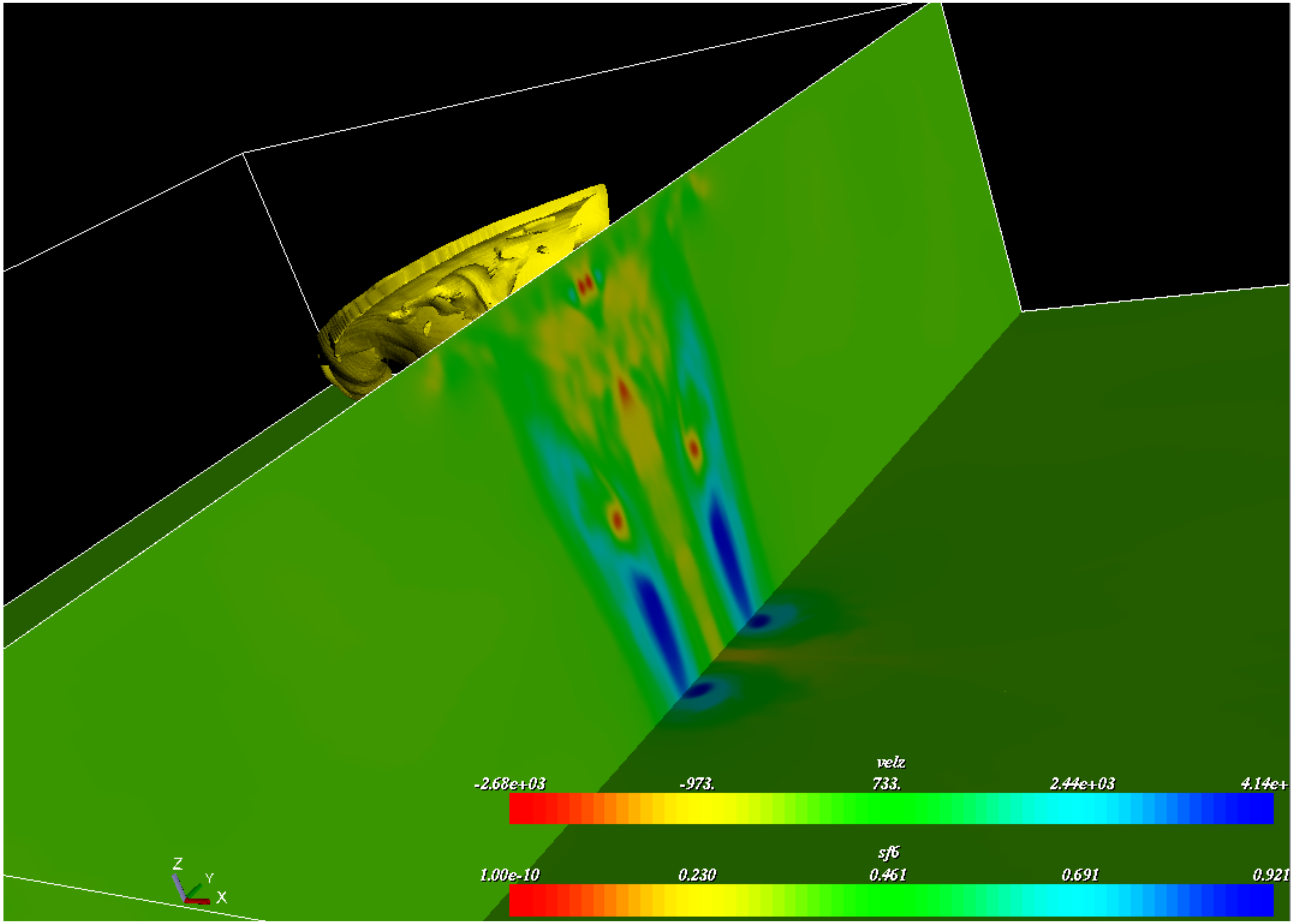
Spreading as the top wall is approached indicates acceleration



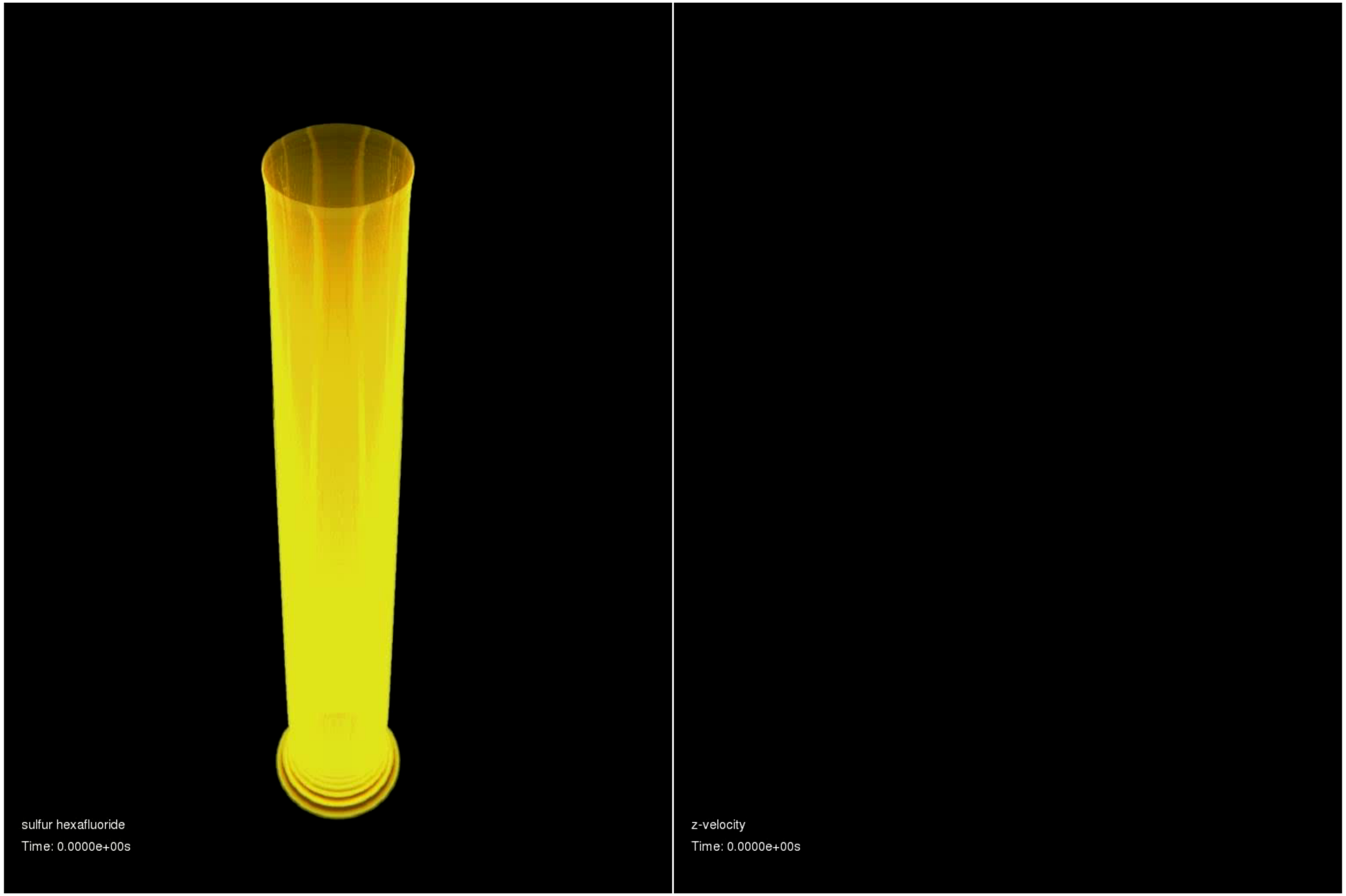
X_{SF6} = 0.97
t = 750 μs

Note vertical tubes of positive z-velocity, associated with the two primary vortex cores

3-D Simulation: Flow Visualization



3-D Simulation: Flow Visualization



LANL Experiment Summary

- Early validation for the shock-cylinder interaction was ***qualitative*** and focused on the influence of simulation parameters
- Led to a discovery of time-dependent ***error component*** in the AMR-aided simulations allowing for possible code improvement
- Attracted interest of experimentalists, modifications of the experimental setup ***expected: feedback loop***
- Work in progress:
  - Initial conditions metrics, 3-D effects
  - Draft paper (especially that Greg is soon departing to SNL)

Summary: Astrophysicist's View on V&V

- Astrophysics is observationally driven
- In 99% astrophysics is about "touching beyond"
- Predictive capabilities are often essential for success
- Promotion of V&V ideas in astrophysics is important
- The Center is not exception in this regard

Summary: Lessons Learned

- V&V is a **chain of procedures** that has to be strictly followed (Astro)
- Importance of finding **good validation experiment**
- Experiments not considered as **good validation experiments** today may become useful in the future
- The most scientifically attractive experiments are not necessarily **good validation experiments**
- Close interaction with experimentalists, understanding of experimental parameters
- Making next iteration: modifying experiments based on the simulation results, feedback loop

V&V Tools

- SQA: automated tools, coding standards, design procedures (Code)
- Lack of established general framework for verification
- Lack of tools aiding data analysis in validation

Future Plans

Science

- Reach ***next level physics*** in the current experiment (multi-physics)
  - Optimize the existing experiment based on simulation results
  - Expand diagnostic capabilities
  - Aid in designing new experiment

Interactions

- Continue ***promoting V&V*** in astrophysics and other computational sciences
- Strengthen V&V as a ***science communication platform*** with the Labs
  - HED may be the most effective way of achieving that in a long-term, but our work with LANL is the best studied case
  - direct access to experiments, use of predictive power of the simulation tools, aiding in experiment design, lower overall costs