FLASH Center Verification & Validation Overview

Tomek Plewa

Computational Physics and Validation Group

V&V DOE Workshop

LaJolla, July 2004

Advanced Simulation and Computing (ASC)
Academic Strategic Alliances Program (ASAP) Center
at The University of Chicago

Outline

FLASH Center Overview

Center-specific activities

- V&V in astrophysics
- V&V and computational methods
  - Case study: shock-cylinder interaction
    - Are 2-D experiments truly two-dimensional?
    - AMR and vortex-dominated flows
    - New message from Courant, Friedrichs, & Lewy
- SQA in code development

Summary

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

The FLASH Center

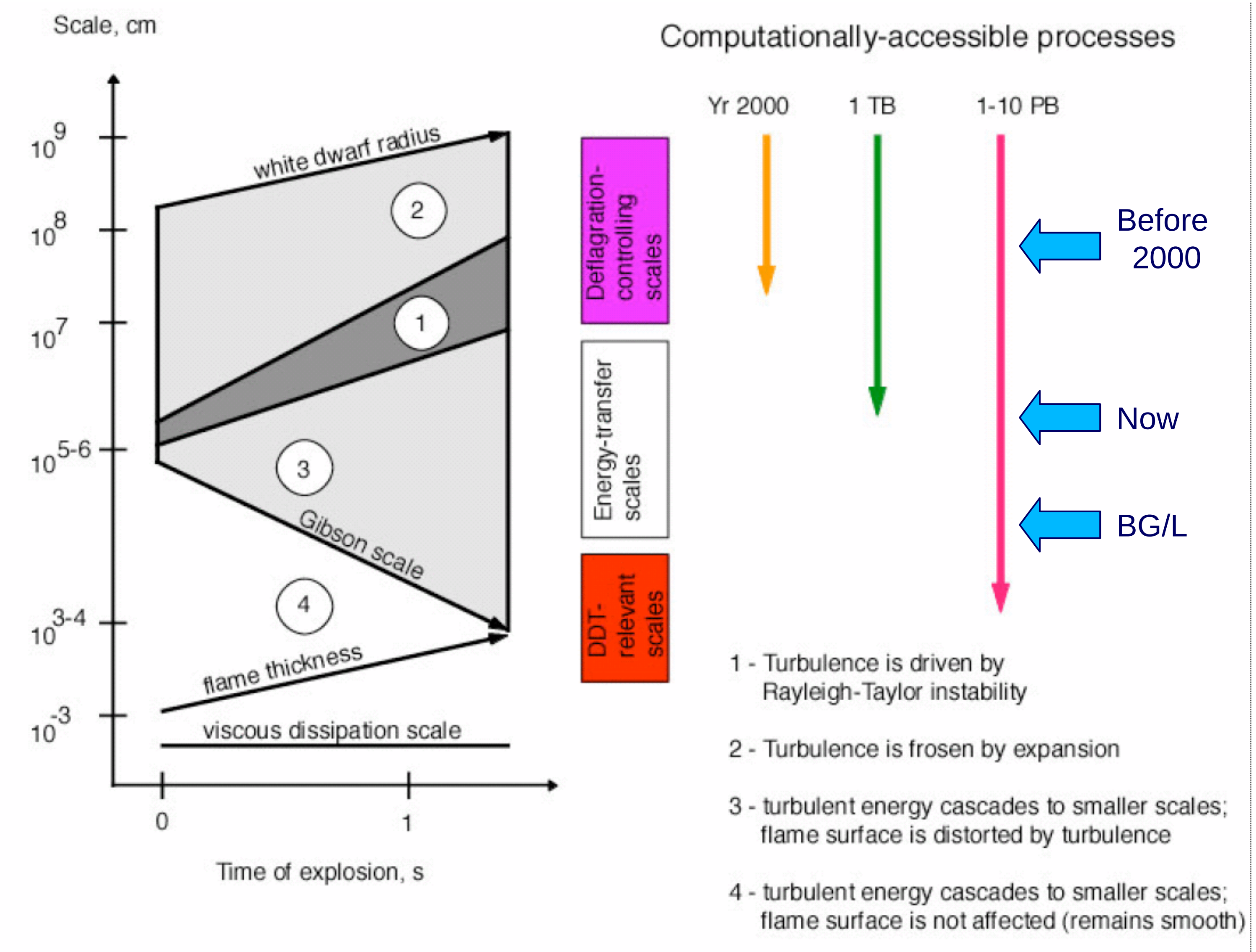
Target Applications

- 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



V&V and 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

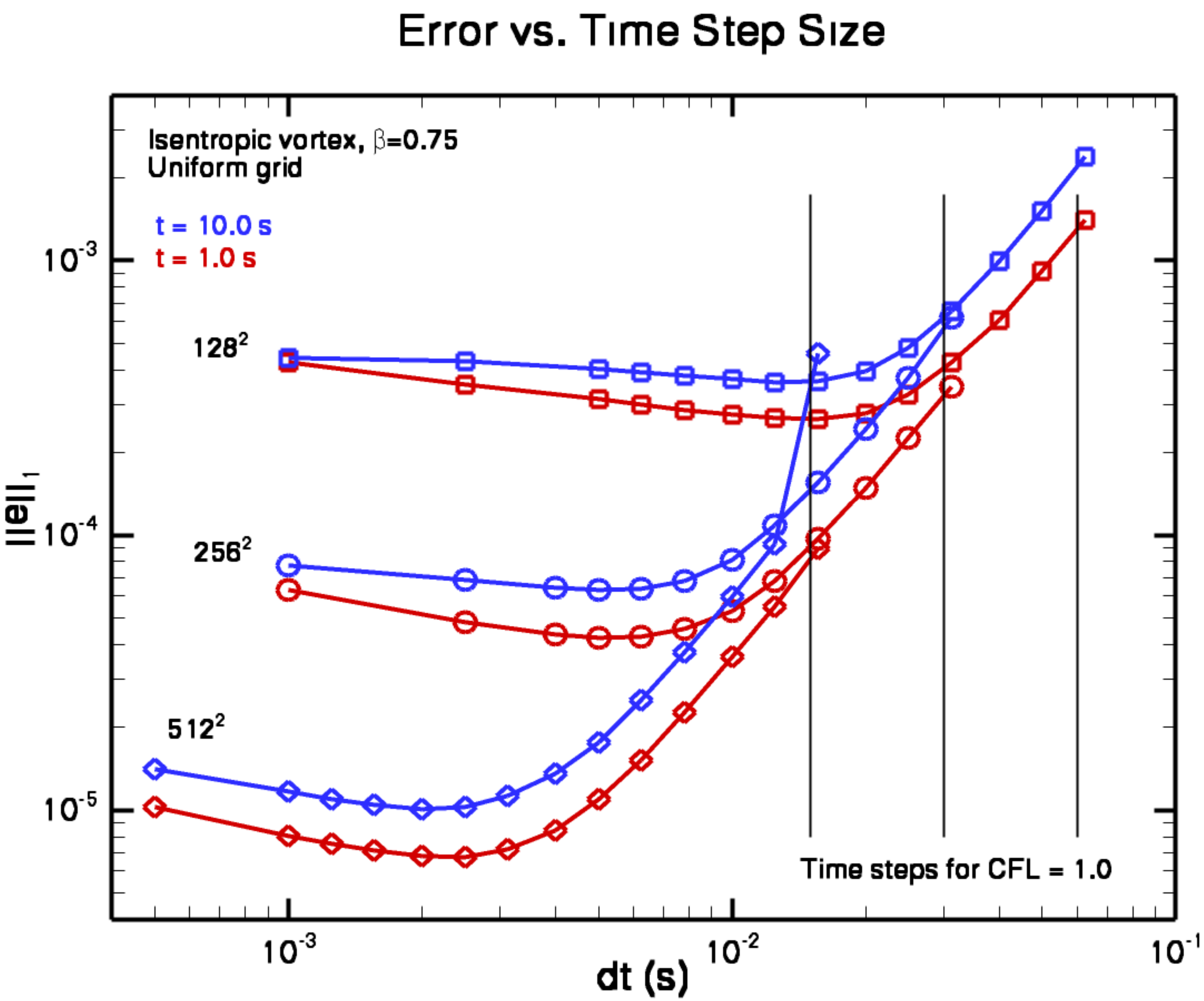
We present a case study of validating an astrophysical simulation code. Our study focuses on validating FLASH, a parallel, adaptive-mesh hydrodynamics code for studying the compressible, reactive flows found in many astrophysical environments. We describe the astrophysics problems of interest and the 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 of Computational Modules

- Verification exploits elementary tests with known analytic solutions or “converged” numerical solutions (not strict but practical).
- Example: advection-diffusion-reaction subgrid model for evolution of the nuclear flame.
- Example: reactive hydrodynamics with tracer particles (for calculation of nucleosynthetic yields).
- Example: assessing time-accuracy
  - Smooth advection problem with known analytic solution
  - Solve with different fixed time steps
  - Calculate error

Verification of Computational Modules



Validation and 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

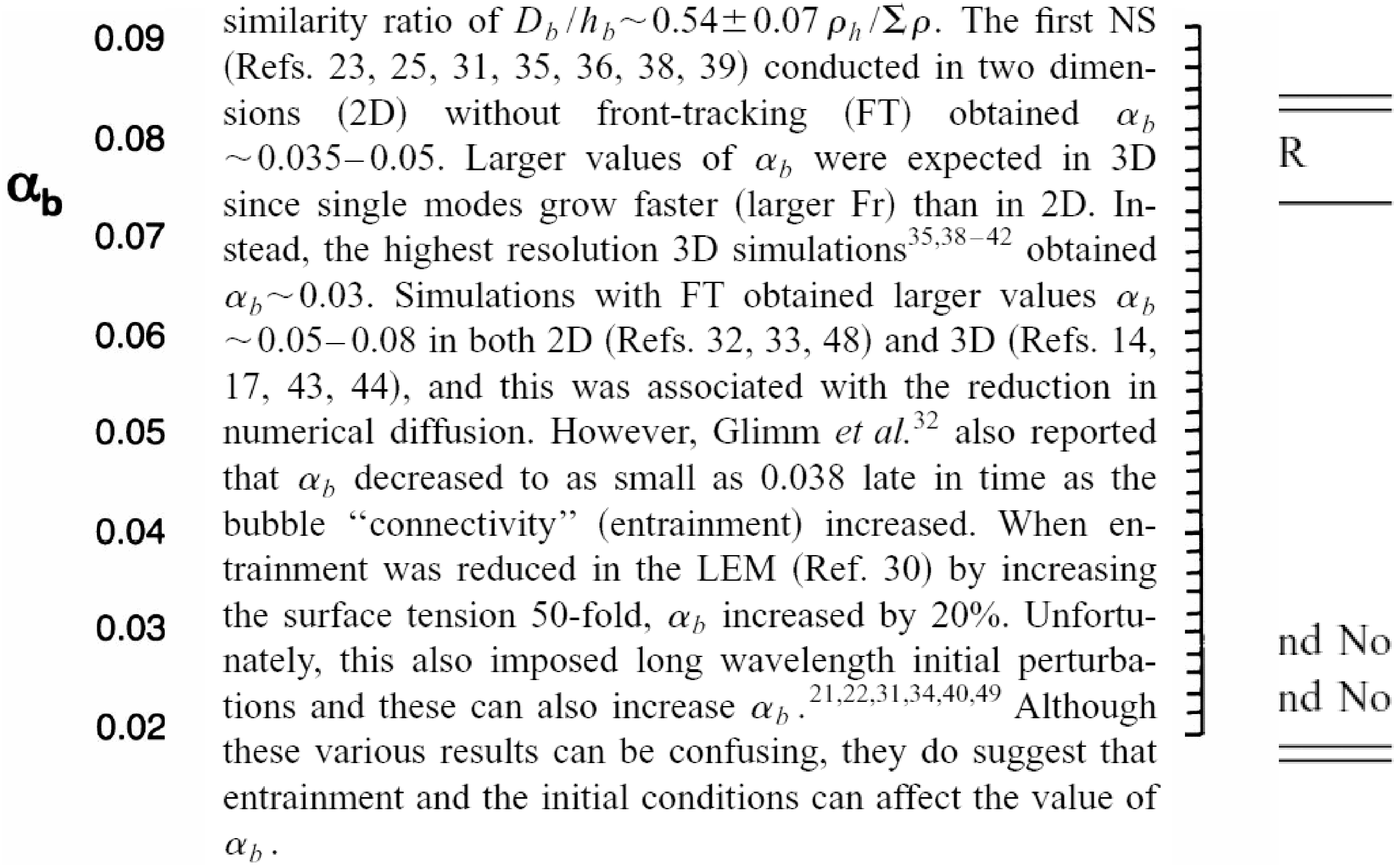
A. C. Calder, B. Fryxell, J. Biello, and L. Dursi
University of Chicago, Chicago, Illinois 60637

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)

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



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.

Validation and 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)

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]

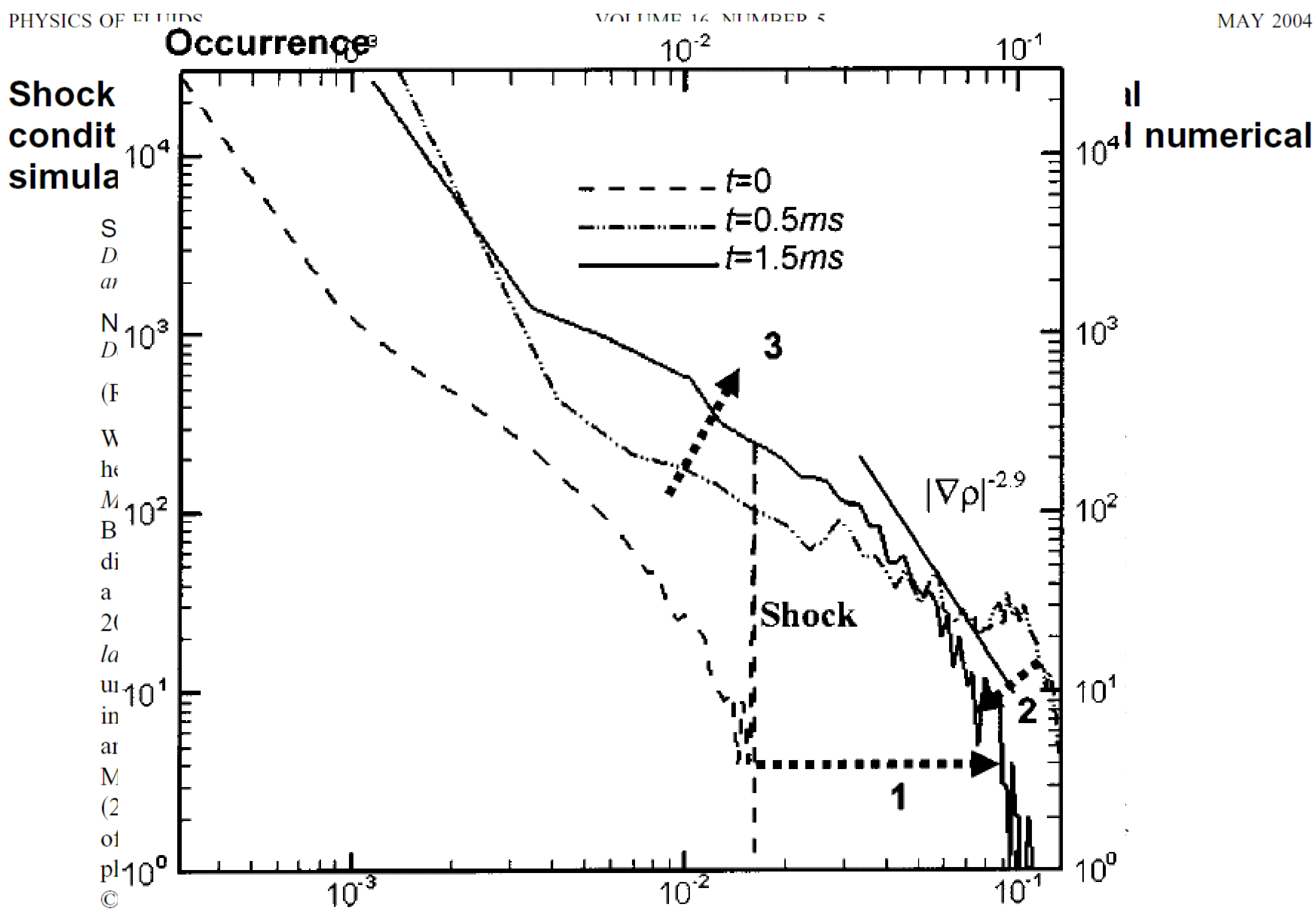
[1] ASCI FLASH Center, University of Chicago vikram@flash.uchicago.edu, tomek@flash.uchicago.edu, weirs@flash.uchicago.edu
[2] Los Alamos National Laboratory ctomkins@lanl.gov, mmarr@lanl.gov

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 envi-

Validation and Computational Modules

- FLASH is community program, freely (with usual restrictions) available for research
- External contribution: shock-cylinder experiment (Jacobs, LANL)



Experiment Analysis Techniques

Andrei Draganescu (moving to SNL later this year)

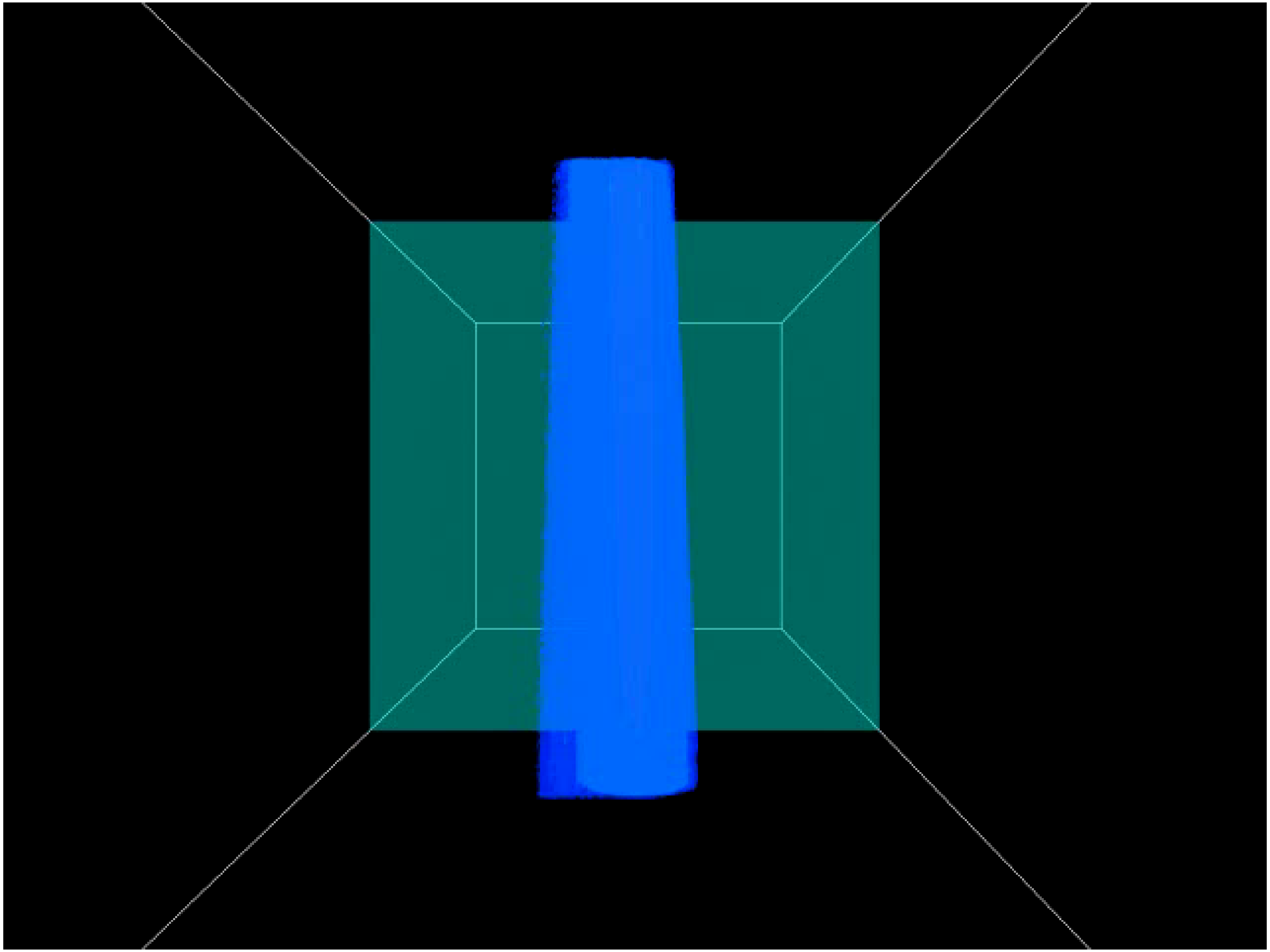
- Consider experimental uncertainties (the initial conditions)
- Consider a dirty bomb scenario (pollution pattern)
- Weather prediction might be another example

- Nonlinear problems involving several unknown parameters
- Mathematical representation: stochastic PDEs, optimal control

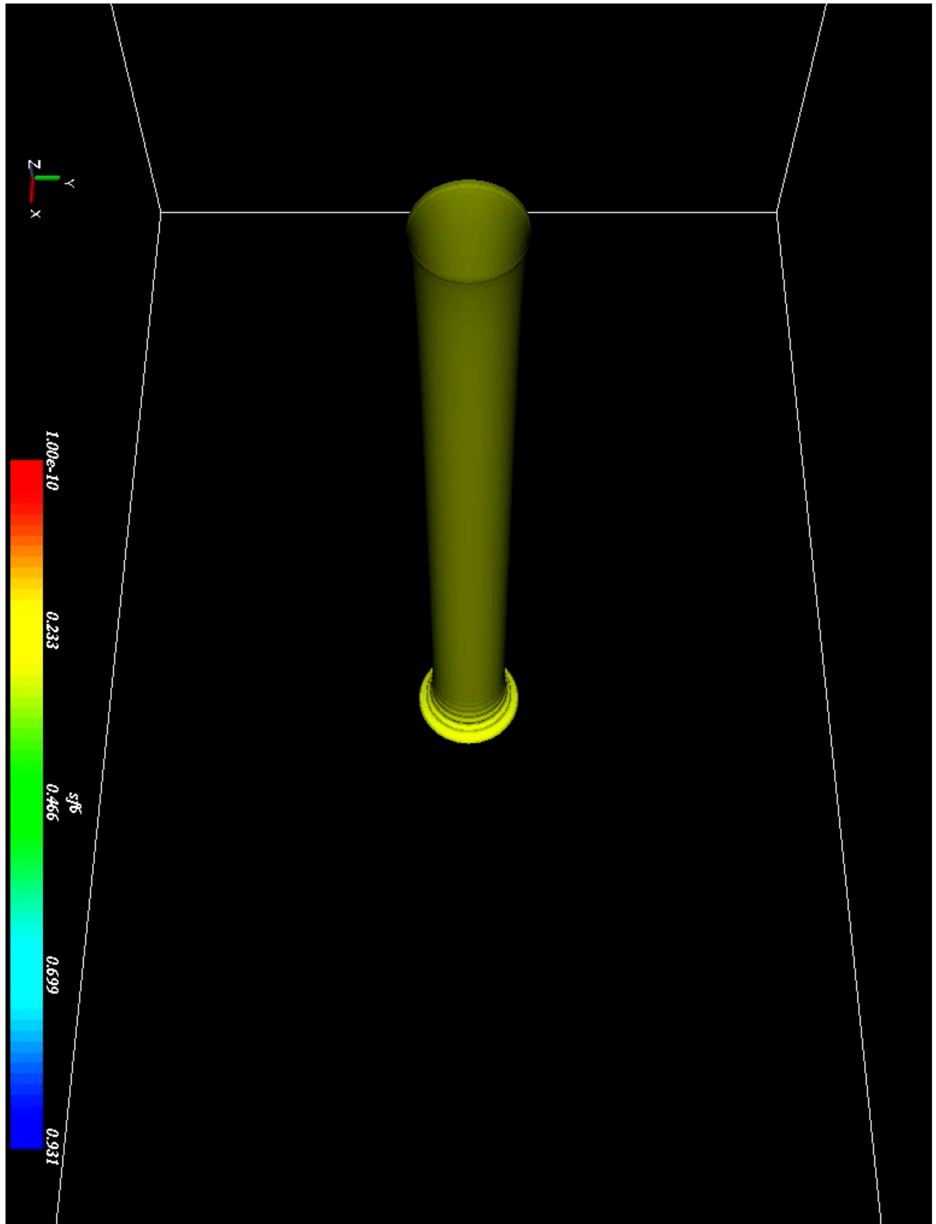
- Use automatic differentiation in the optimization process
- Use multigrid to couple different scales in the problem

- Main result: function computation cost is not the limiting factor
- Main difficulty: lack of tools suitable for automatic differentiation

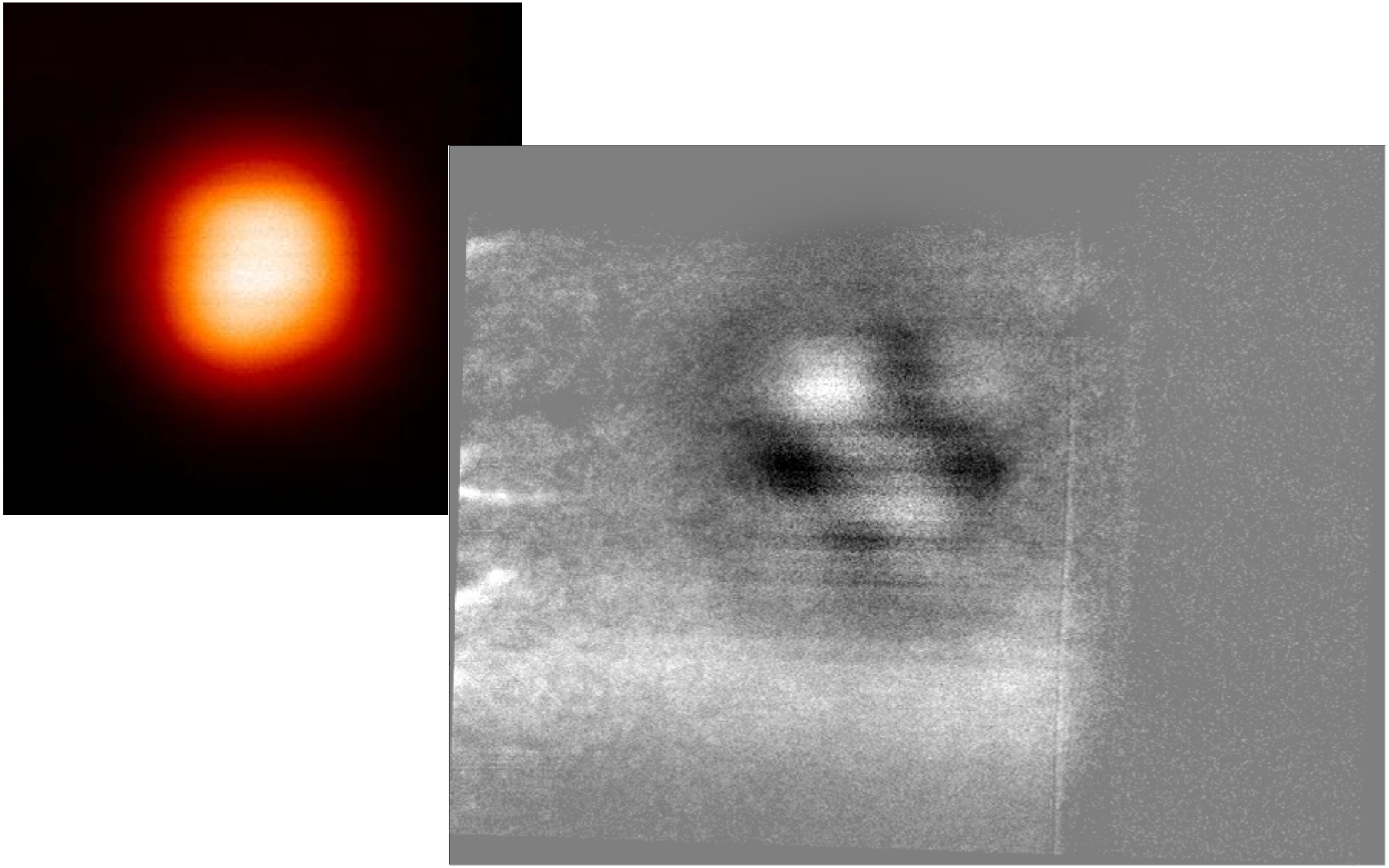
Case Study: Shock-Cylinder Interaction (speculative)



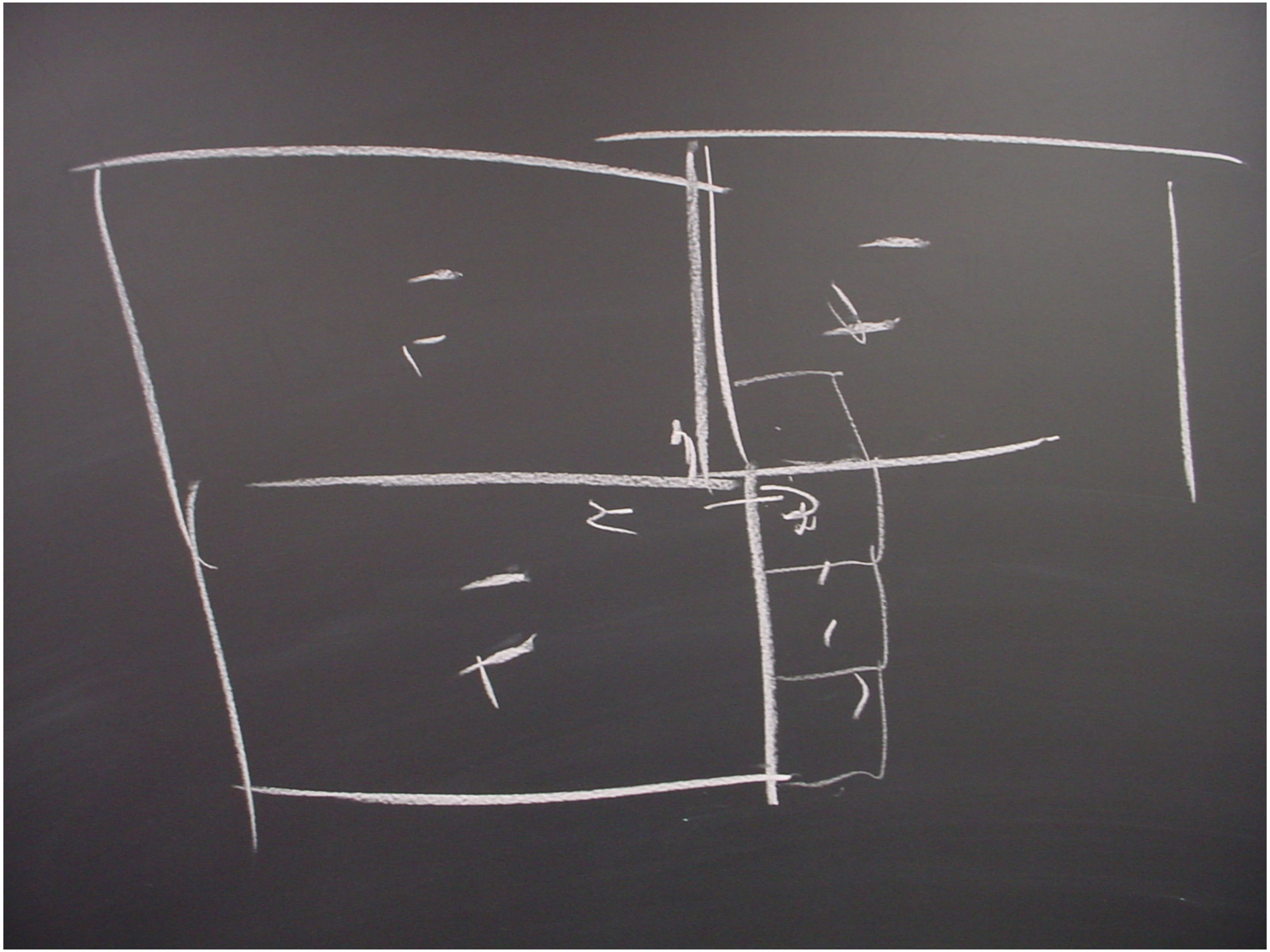
Case Study: Shock-Cylinder Interaction (realistic)



Initial Conditions: Cylinder Cross-section



FLASH Code is the AMR code

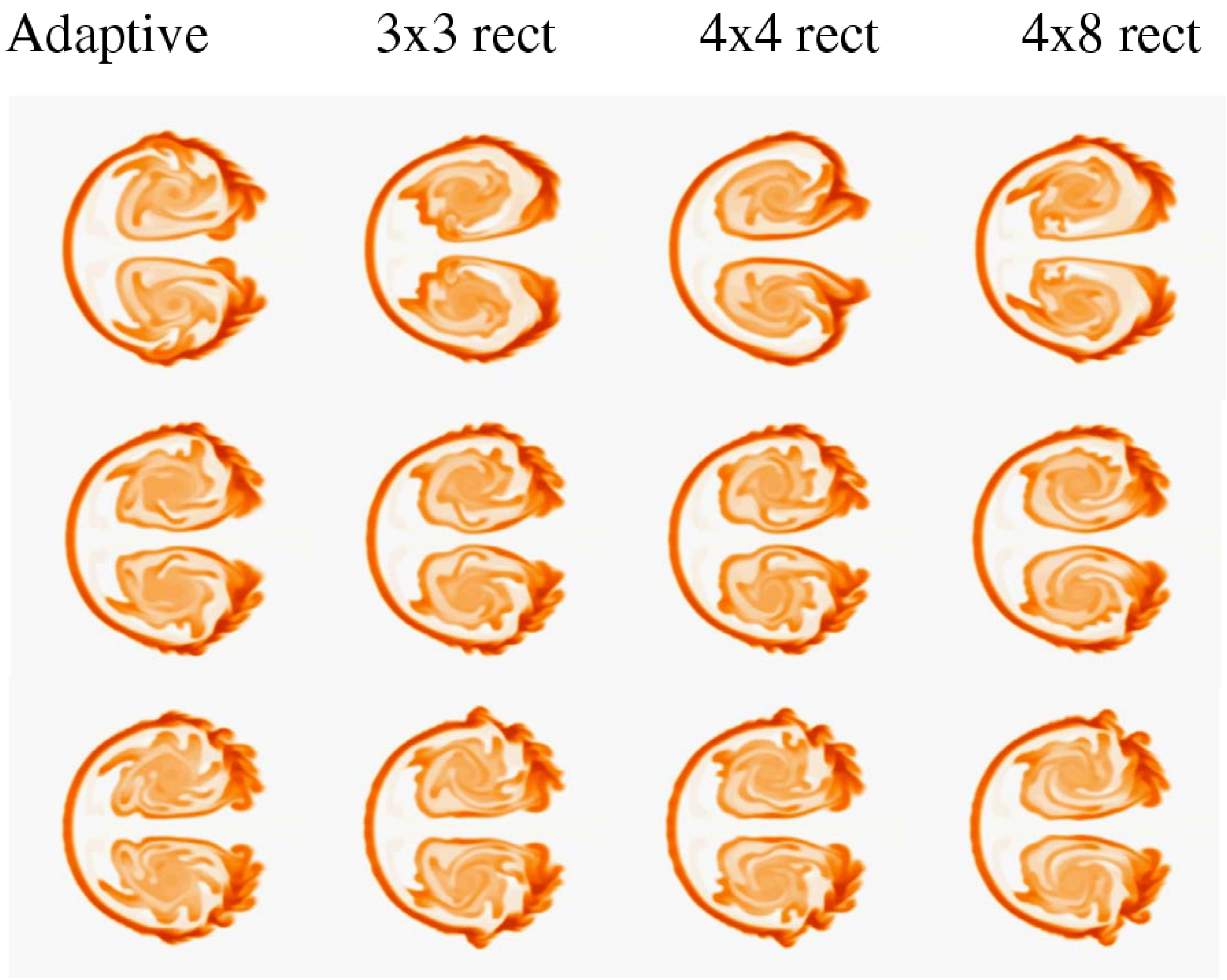


CFL dependency

CFL=0.8

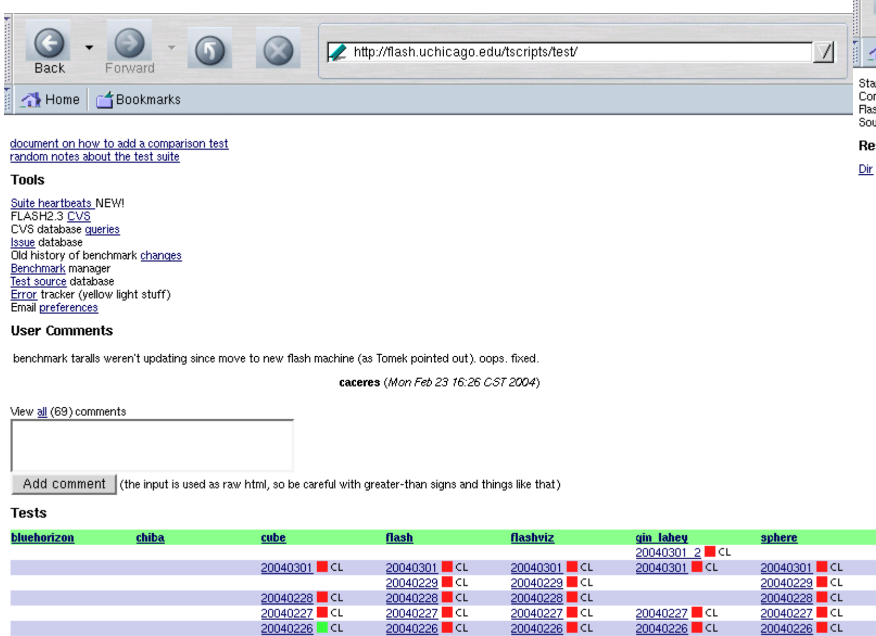
CFL=0.4

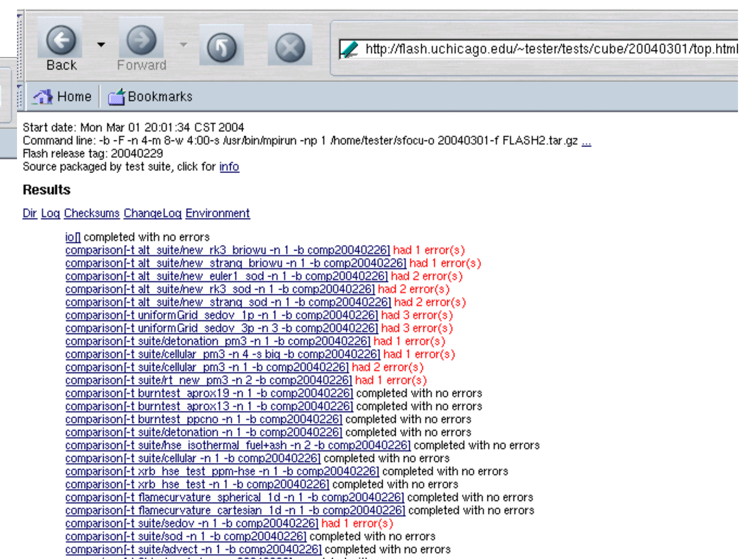
CFL=0.2



Software Quality Assurance

- Pure sciences rarely offer formal education or training: hands-on approach.
- SQA begins with code design: follow standards, design guidelines, specifications, etc. (FLASH2 -> FLASH3)
- Has to be a daily practice, encouraged/enforced by use of automated monitoring tools (FLASH test suite).





Lessons Learned

- 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

- V&V is a chain of procedures that has to be strictly followed
- It is important to find a **good validation** experiment
- Understanding of experiment is crucial
- 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

- Development asks for automated tools, maintenance demands them
- Lack of general framework for verification: Not possible? Not appreciated enough? Nothing to compare with: share your tools!

Future Plans

- Reach *next level physics* in the current experiment (multi-physics)
- Expand diagnostic capabilities
- Aid in optimization of the existing and design of new experiments
- Make a big circle: come back to HED (need diverse regimes, resources limited)
- Provide community service: continue promoting V&V in astrophysics and related fields

Summary

- V&V is an essential component of the Center's work.
- The Center introduced V&V methodology to astrophysics, promotes and truly builds V&V-related consciousness among astrophysicists and computational scientists.
- Interaction with the National Laboratories, especially DP Labs, is crucial for the V&V effort (direct access to experiments, use of predictive power of the simulation tools, aiding in experiment design, minimize overall costs).
- Elements of Software Quality Assurance are present in everyday's work, supported by specialized, developed in-house software and guided by design rules and custom programming standards. More should be done.