FLASH Center Verification & Validation
Overview

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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
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

Time of explosion, s

Scale, cm

10^9
10^8
10^7
10^5-6
10^3-4
10^{-3}

white dwarf radius
Gibson scale
flame thickness
viscous dissipation scale

DDT-relevant scales
Energy-transfer scales
Deflagration-controlling scales

Yr 2000
1 TB
1-10 PB

Before 2000
Now
BG/L

1 - Turbulence is driven by Rayleigh-Taylor instability
2 - Turbulence is frozen by expansion
3 - turbulent energy cascades to smaller scales; flame surface is distorted by turbulence
4 - turbulent energy cascades to smaller scales; flame surface is not affected (remains smooth)
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!

ON VALIDATING AN ASTROPHYSICAL SIMULATION CODE

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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

Error vs. Time Step Size

Isentropic vortex, $\beta=0.75$
Uniform grid

$t = 10.0 \text{ s}$
$t = 1.0 \text{ s}$

$128^2$

$256^2$

$512^2$

$10^{-3}$ $10^{-2}$ $10^{-1}$

The ASC/Alliances Center for Astrophysical Thermonuclear Flashes
The University of Chicago
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)

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

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Validation and Computational Modules

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

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<th>$\alpha_b$</th>
<th>0.09</th>
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<th>0.07</th>
<th>0.06</th>
<th>0.05</th>
<th>0.04</th>
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Similarity ratio of $D_b/h_b \sim 0.54 \pm 0.07 \rho_b/\Sigma \rho$. 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 $\alpha_b$ 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 $\alpha_b$ 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, $\alpha_b$ increased by 20%. Unfortunately, this also imposed long wavelength initial perturbations and these can also increase $\alpha_b$. $^{21,22,31,34,40,49}$ Although these various results can be confusing, they do suggest that entrainment and the initial conditions can affect the value of $\alpha_b$.
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

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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 a 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

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The University of Chicago
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

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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.