The Center for Astrophysical Thermonuclear Flashes

Computational Physics and Validation

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Outline

This talk:

- ☐ Overview of the CompPhys group [validation: talk Rosner]
- ☐ Rationale
- ☐ Astrophysics (applications)
- ☐ CompPhys (methods)
  - Algorithms
  - Assignments
  - Timeline
- ☐ Code (implementation), CS (execution), and Vis (analysis)

Greg Weirs:

- ☐ Increasing the flexibility of FLASH
- ☐ Role of the design process

Rationale for CompPhys

Provide a bridge between Astro and Code groups:

- Address requirements of the Astro group, relieving it from module development.
- Identify implementation requirements for the Code group.

In daily work…

- Focus on problems of the size of large physics module: key problems may never get done if distractions dominate research.
- Assess overall quality of the proposed numerical methods.
- Perform rigorous code verification.
- See validation as an ultimate test of the method.

FLASH Astrophysics Overview

All three problems require ***similar physics***…

…and all of them consist of ***two very different phases***:

- **Initial Conditions**
  - slow accretion, close to hydrostatic equilibrium
  - timescales entirely limited by sound speed
  - highly subsonic
- **Thermonuclear Runaway**
  - explosion or fast expansion driven by energy release
  - timescales usually limited by advection
  - subsonic or supersonic

We need to use ***two different classes of hydro solvers***, however….

The FLASH Code Now

- **Adaptive Mesh discretization** [poster Dwarkadas]

  based on PARAMESH, restricted to no refinement in time, fixed block sizes, quad/octtree data structure, parallel

- **PDE solvers** [poster Weirs]

hyperbolic	compressible explicit hydro including MHD, SRHD
elliptic	multipole for Poisson, multigrid for Helmholtz
ODE	explicit diffusion, viscosity, nuclear burning

- **Other components**

  realistic EOS

  multi-species (advection, reaction, possibly diffusion)

  particle advection

- **Specific characteristics**

  modular, flexible, extensible, portable [talk Siegel]

  tested, maintained, documented [talk Riley]

  CS- [talk Lusk, poster Dubey] and Math-supported [talk Dupont]

FLASH Astrophysics: Problems

FLASH Astrophysics: SN Ia

Computational target

a three-dimensional explosion, natural ignition, light curve.

- **Initial Conditions**

  highly subsonic and stratified, with angular momentum transport

  implicit

  hydrostatic equilibrium, convection, nuclear burning

- **Thermonuclear Runaway**

  supersonic, violent stellar explosion

  explicit

  detonation or deflagration (*flamelet* regime)

FLASH Astrophysics: Type I X-ray Burst

Computational target

a three-dimensional thermonuclear burst, fuel spreading.

- **Initial Conditions**
  - subsonic for surface layers, supersonic otherwise, H to He burning
  - strongly stratified, thin layer with shear and rotation (ocean modeling)
  - column (B~10^{12} G) or equatorial (B~10^{8} G) accretion, boundary layer
- **Thermonuclear Runaway**
  - inhomogeneous and transient, atmospheric winds, weak expansion
  - explicit
  - deflagration or detonation

FLASH Astrophysics: Classical Nova

Computational target

a three-dimensional nova model, common envelope phase.

- **Initial Conditions**
  - highly subsonic and stratified
  - implicit
  - hydrostatic equilibrium, convection, nuclear burning
- **Thermonuclear Runaway**
  - slow subsonic expansion
  - 2-D very different from 3-D
  - violent turbulent burning (*well-stirred* regime)

FLASH Computational Physics

FLASH CompPhys: Numerical Methods

❑ **low-Mach number flow solver**

[IC: SNIa, XRB, Nova]

front tracking

flame studies [SNIa], mixing problems with subgrid models [XRB, Nova]

directionally-unsplit compressible flow solver

necessary for front tracking, offers alternative to the existing solver

❑ **compressible implicit solver**

accretion flows and boundary layer simulations [IC: XRB]

(semi-implicit) relativistic MHD solver

column accretion and spreading [IC: XRB]

❑ **1-D non-LTE radiative transfer in moving media**

for postprocessing of multi-D hydro results [SNIa, Nova]

multi-D radiation transport

inexpensive, gray (minimum) / multi-group (at most) [XRB]

FLASH CompPhys: Proposed Solutions

- **low-Mach number flow solver** Poisson/Helmholtz solvers

  new hire: projection method, P. Colella current efforts P. Fischer, F. Rubini

- **front tracking**

  Natasha Vladimirova: CIP, passive scalar (NRL), level set (MPA)

- **directionally-unsplit compressible flow solver**

  T.P.: Godunov, CTU, P. Colella

- **compressible implicit solver** *hypre* package

  Greg Weirs: BIC (G. Patnaik), P. Woodward, W. Dai

- **(semi-implicit) relativistic MHD solver**

  Timur Linde: TVD, T. Gombosi, S. Komissarov, S. Falle

- **1-D non-LTE radiative transfer in moving media**

  Vikram Dwarkadas: collaborations [Avrett, Hauschildt, Hoeflich, Lundqvist, Pinto]

- **multi-D radiation transport** single-T flux-limited diffusion

  Alan Calder: Hayes & Norman scheme, J. Hayes/TSI, IBEAM

FLASH CompPhys: Implementation Timeline

low-Mach number flow solver	**2003/4**
front tracking	**2003/4**
directionally-unsplit compressible flow solver	**2003**
compressible implicit solver	**2004**
(semi-implicit) relativistic MHD solver	**2003**
1-D non-LTE radiative transfer in moving media	**2004**
multi-D radiation transport	**2004**

Implications for Other Groups

Implications for the Code Group

- **data structure**

  front tracking, multi-D radiation transport

- **driver**

  implicit solvers

- **communication**

  implicit solvers

- **elliptic solvers**

  low-Mach number flow solver

- **data interface**

  1-D non-LTE radiative transfer in moving media

Implications for the Computer Science Group

- **single processor performance**

  top-5 profiling, cache optimization

- **scalability studies** [poster A. Dubey]

  examine parallel performance in adaptive (FLASH) and uniform (community value) grid multi-physics calculations

- **parallel algorithms**

  identify opportunities for parallel execution

- **3-D visualization**

  ultimate method of data analysis, necessary for development; finishing current study and moving on to the next one

- **upcoming challenges: Flash Simulator**

  vector performance: expect substantial modifications

  to the computational kernels

Summary

- **Astro: self-consistent initial conditions**

  requires less intuition/speculation; replaces parameter studies
- **Astro: capturing the unresolvable**

  certain problems require front tracking + subgrid models
- **Code: high-level changes**

  current: flexible driver, next: additional data structures
- **CS: efficiency**

  scalability of integrated simulations (FLASH); uniform grid (community)
- **Vis: support multi-D data sets**

  faster data processing, closing current problem/starting a new one
- **CompPhys:**

  keep focus, interact with Astro/Code, seek help from CS/Vis, validate

Questions and Discussion