Computational Physics and Validation

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Site Review
Chicago, October 16, 2003

Outline

Group in the Center

Projects

- Flame model
- Validation
- Initial models
- Implicit hydrodynamics
- Magnetohydrodynamics
- AMR workshop

Summary

- Issues
- Future plans
- Accomplishments

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CompPhys Group in the Center

Astrophysics

- supporting Type Ia supernova modeling
  - construction of initial models in hydrostatic equilibrium
  - nuclear flame model

Basic Physics

- validation
- stiff problems

Code

- multigrid (Poisson and Helmholtz) solvers
- multipole Poisson solvers
- code architecture proposals

CS

- Argonne FLASH numerics workshops (12/02 and 06/03)
- desktop visualization

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CompPhys Projects

Primary Group focus:

- flame capturing (Vladimirova, Weirs, Robinson, Plewa)

  advection-diffusion-reaction, thick flame model [after A. Khokhlov]
- validation (Dwarkadas, Plewa, Weirs)

  [with C. Tomkins, B. Benjamin, LANL]

Major projects:

- hydrostatic initial models (Plewa)
- implicit hydro solver (Weirs)

  BIC [after G. Patnaik]
- MHD solvers (Linde)

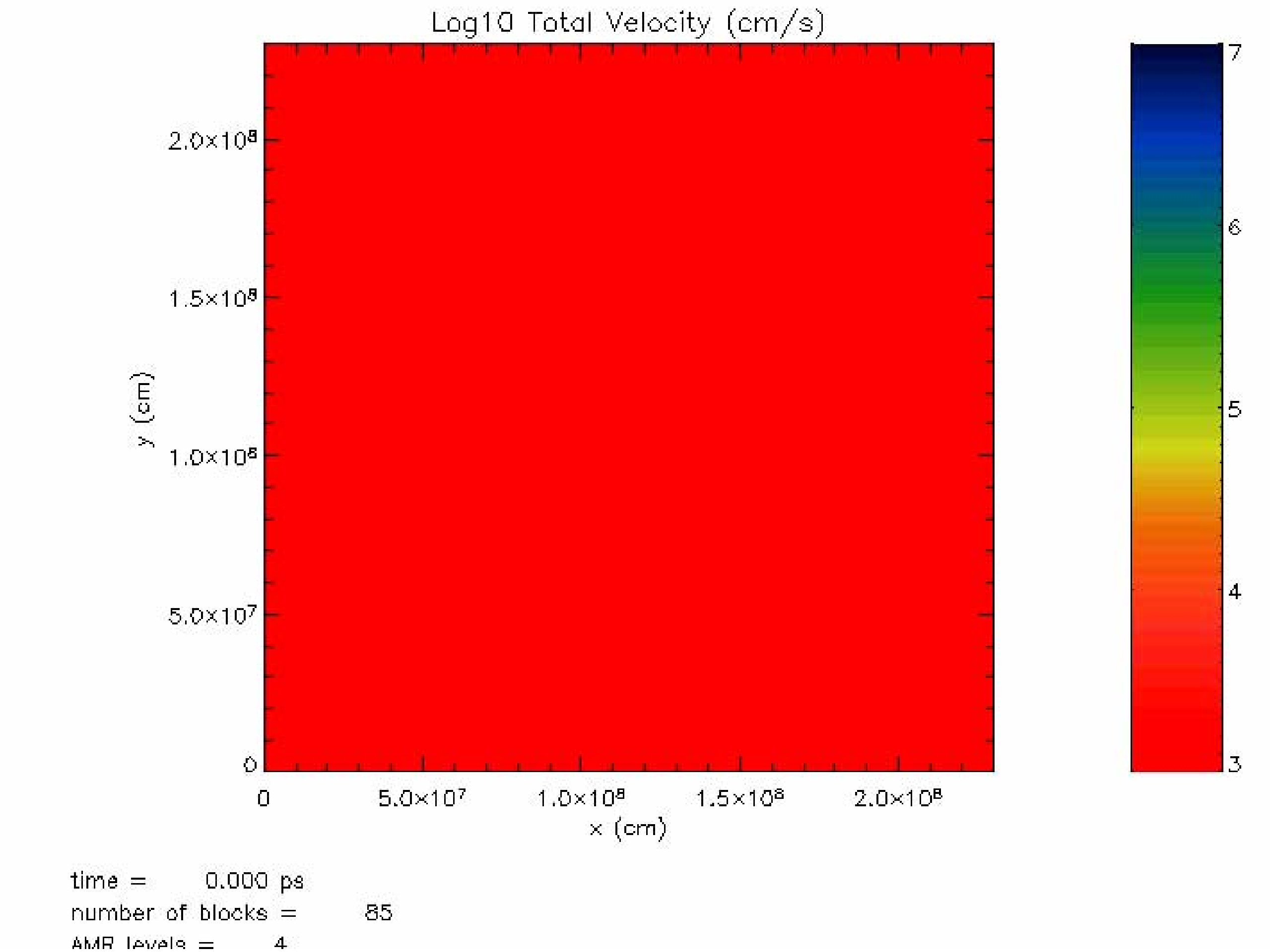
  [with K. Germaschewski, after T. Gombosi, S. Komissarov, S. Falle]
- AMR workshop (Plewa, Linde, Weirs)

  3 days-long meeting, 100 participants (about 20% from the Labs)

Initial models for Type Ia simulations

- No evolutionary stellar models produced in-house. Available models obtained from different external researchers.
- Models are obtained for objects in state very close to hydrostatic equilibrium, and have to be mapped to FLASH.
- Mapping process usually breaks delicate state of equilibrium due to differences in
    - discretization (lagrangian vs. eulerian, resolution),
    - physics (either assumptions or numerical model).

Initial models for Type Ia simulations



Low Mach Number Method

Motivation

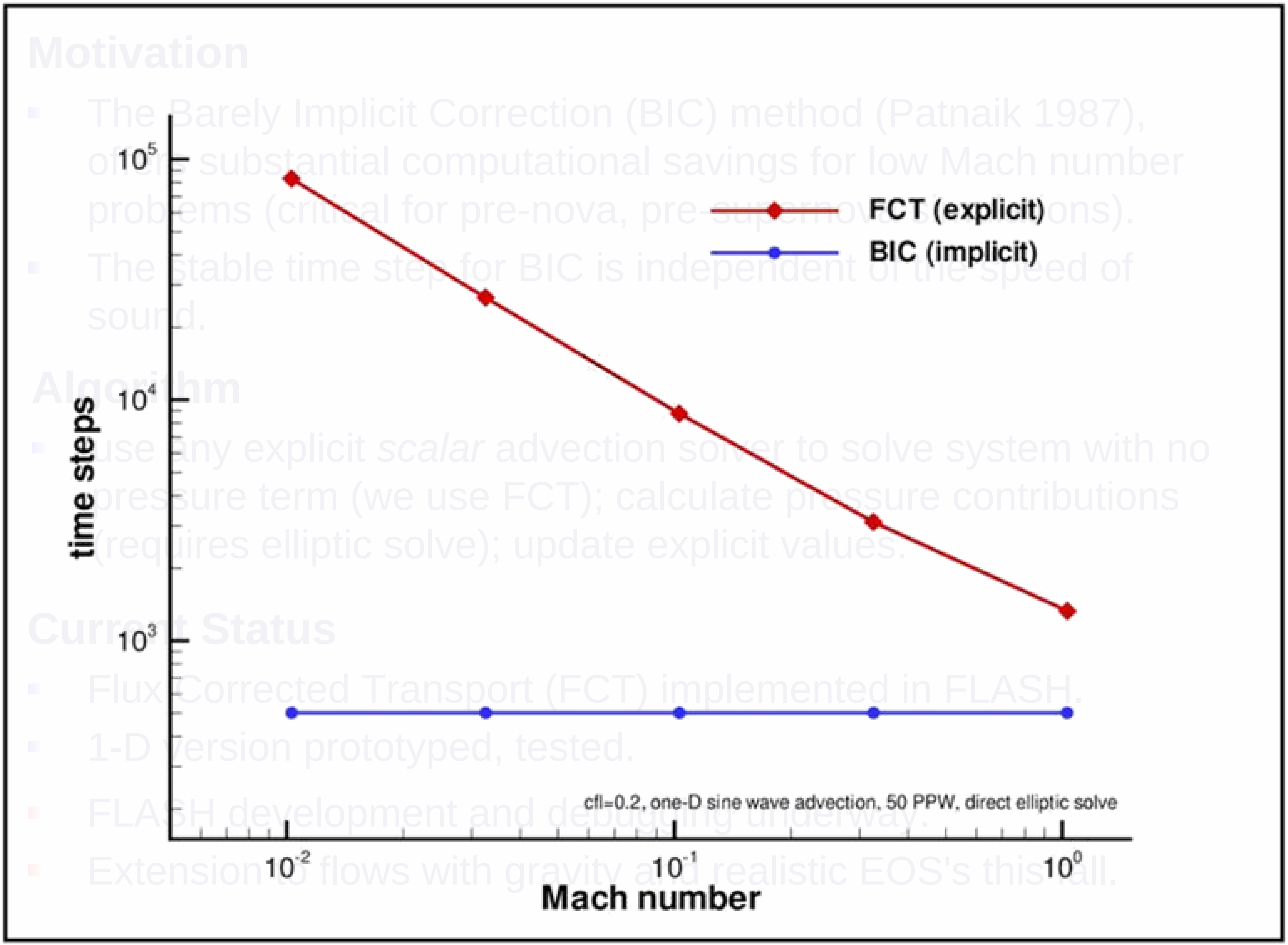
- The Barely Implicit Correction (BIC) method (Patnaik 1987), offers substantial computational savings for low Mach number problems (critical for pre-nova, pre-supernova simulations).
- The stable time step for BIC is independent of the speed of sound.

Algorithm

- use any explicit *scalar* advection solver to solve system with no pressure term (we use FCT); calculate pressure contributions (requires elliptic solve); update explicit values.

Current Status

- Flux Corrected Transport (FCT) implemented in FLASH.
- 1-D version prototyped, tested.
- FLASH development and debugging underway.
- Extension to flows with gravity and realistic EOS's this fall.



Advances in Hall and Relativistic MHD

Motivation

- essential for studying accretion processes
- crucial for mass loading of the stellar magnetosphere
- critical to understanding generic plasma phenomena

Hall MHD

- external contribution by Kai Germaschewski (CMRS)
- 2-D cartesian, two-fluid model integrated with FLASH
- explicit 3-D model in FLASH; need an implicit model

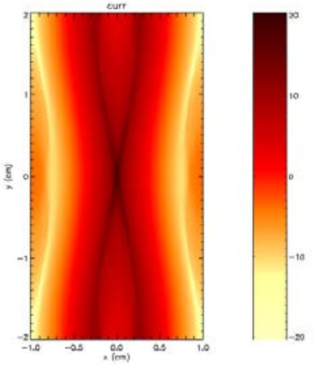
Relativistic MHD

- implemented the first version in FLASH
- working on improvements in the first version

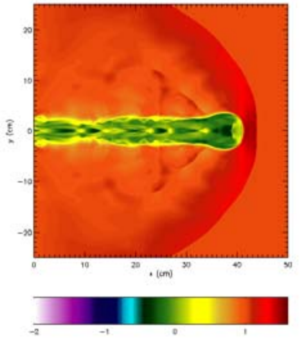
MHD in non-cartesian geometries

- extended MHD to cylindrical coordinates (C. Zanni)
- extension to spherical coordinates

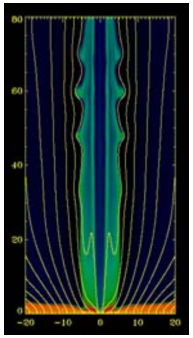
Magnetic reconnection
In a two-fluid plasma



Light relativistic MHD jet



Jet launching by accretion disk



AMR Workshop

Overview

- Hosted by the Flash Center on September 3-5, 2003.
- About 100 participants (18 participants from Labs,13 countries).
- 26 oral presentations including 12 invited talks.
- Kept us (Tomek, Carrie, Mila, Timur, Greg, Brad) quite busy at times!

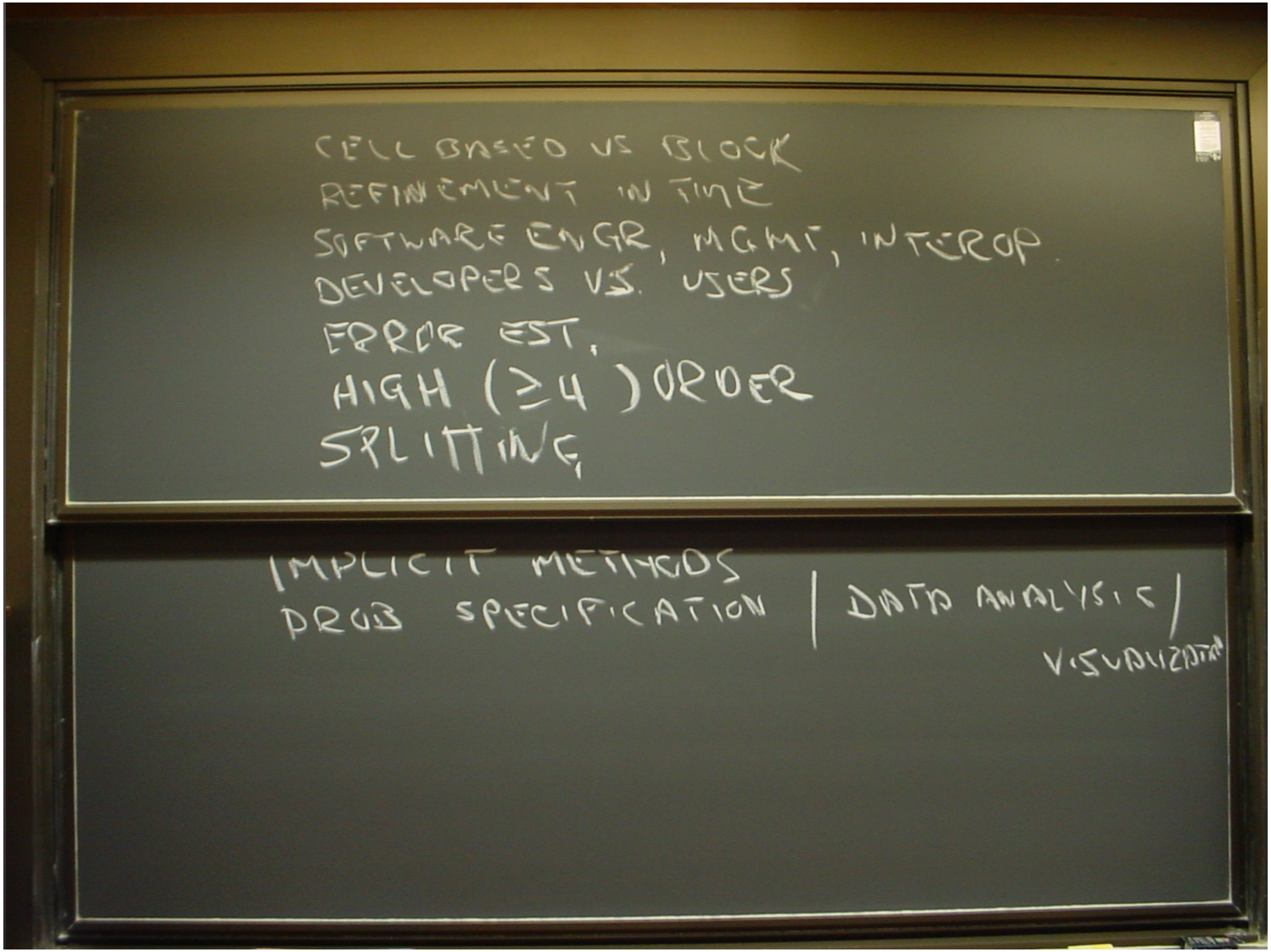
Scientific value

- exchange ideas, share expertise, discuss current problems
- hands-on-code participation in the benchmark session
- publication of the proceedings (Timur, Tomek, Greg)

Community value

- bring people together, including a number of younger colleagues
- strengthen existing and establish new collaborations
- propose holding meetings on more regular basis

AMR Workshop



CELL BASED VS BLOCK
REFINEMENT IN TIME
SOFTWARE ENGR, MGMT, INTEROP.
DEVELOPERS VS. USERS
ERROR EST.
HIGH (≥4) ORDER
SPLITTING
IMPLICIT METHODS
PROB SPECIFICATION | DATA ANALYSIS / VISUALIZATION

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Flame Capturing – Formulation

- **Advection-Diffusion-Reaction model (Khokhlov)**

$$\begin{aligned} \phi_t + \mathbf{v} \cdot \nabla\phi &= \kappa \nabla^2 \phi + R(\phi) \\ \dot{q} &= q \left[R(\phi) + \kappa \nabla^2 \phi \right] \end{aligned}$$

ϕ – tracer, or reaction progress variable, $0 < \phi < 1$,

κ – tracer diffusivity,

R – tracer reaction rate,

q – heat release, erg/g,

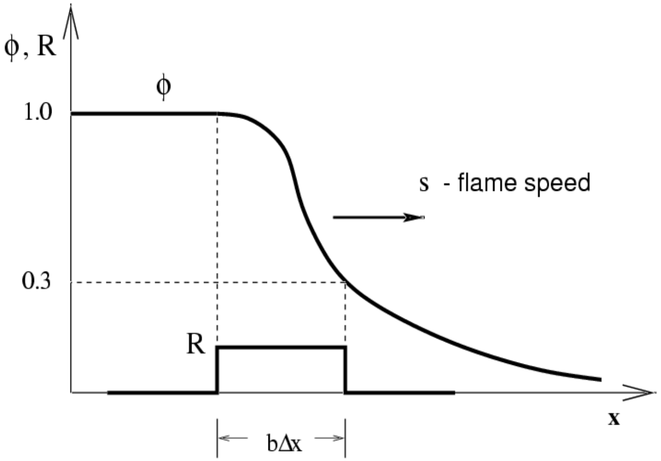
s – laminar flame speed, $s = s(\kappa, R)$

l – laminar flame thickness, $l = l(\kappa, R)$

Khokhlov reaction rate:

$R = const$ for $0.3 < \phi < 1$,

$R = 0$ elsewhere.



Flame Capturing – Coupling Options

A. The tracer ϕ is advected by PPM:

$$\frac{\partial \phi}{\partial t} + \nabla(\mathbf{v}\phi) = \kappa \nabla^2 \phi + R$$

B. The tracer ϕ is advected by external module:

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = \kappa \nabla^2 \phi + R$$

C. The tracer ϕ is advected by PPM, with external compressibility fix:

$$\frac{\partial \phi}{\partial t} + \nabla(\mathbf{v}\phi) = \kappa \nabla^2 \phi + R + \phi \nabla \mathbf{v}$$

D. The product $\rho\phi$ is advected by PPM:

$$\frac{\partial (\rho\phi)}{\partial t} + \nabla(\mathbf{v}\rho\phi) = \rho\left(\kappa \nabla^2 \phi + R\right)$$

Flame Capturing – Complete Set of Equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0, \\
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) &= -\nabla P + \mathbf{f}, \\
\frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + P)\mathbf{v}] &= \mathbf{v} \cdot \mathbf{f} + q\rho\dot{\Phi}, \\
\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \phi \mathbf{v}) &= \rho\dot{\Phi}, \\
\dot{\Phi} &= \kappa \nabla^2 \phi + R(\phi), \\
\rho E &= \rho e + \frac{\rho \mathbf{v} \mathbf{v}}{2}, \\
e &= e(\rho, P)
\end{aligned}
$$

Flame Capturing - Verification

Initial conditions

- gamma-law gas, equally spaced grid
- laminar flame (velocity, diffusion coefficient, energy release)
- analytic background hydro state

Parameters

- resolution (number of cells per reaction zone)
- density jump across the front (Atwood number)
- background flow velocity (translational invariance)

Typical metrics

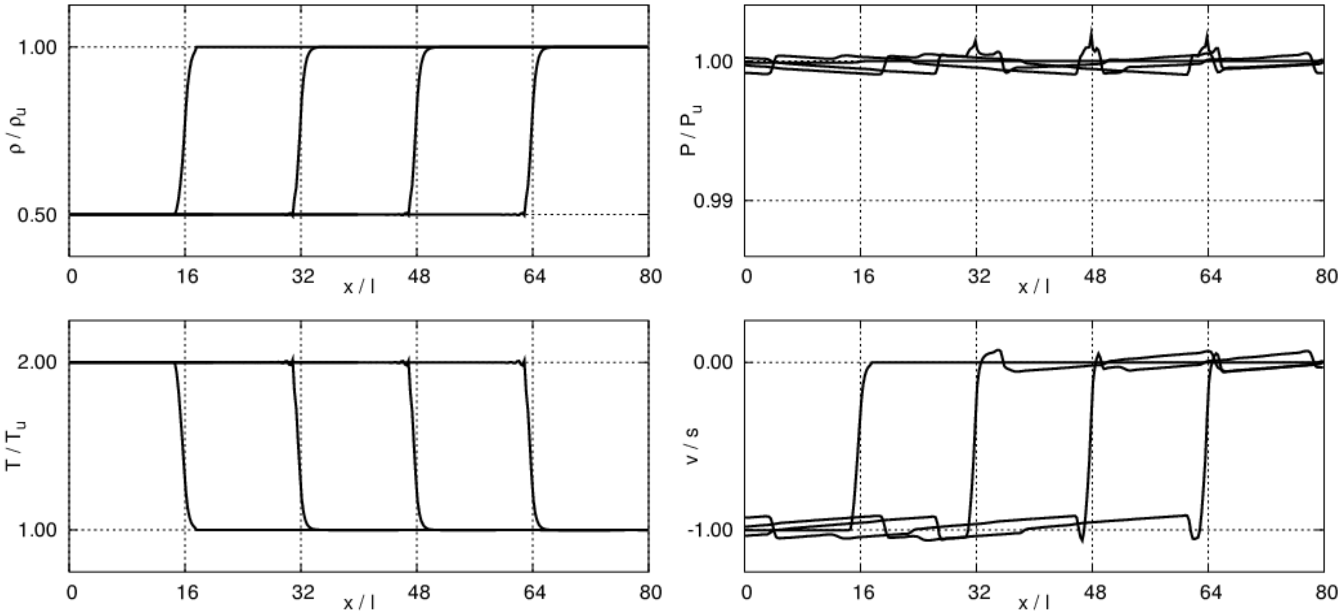
- total energy release
- flame speed

Flame Capturing – Verification I

Compressibility effects (important during late stages)

- Factor of 2 density jump, 4 points across reaction zone.
- Flame propagates from left to right, solutions shown at four times (dashed lines – location assuming incompressible case).

compressible



- “Incompressible” flame speed too small by ~30%.

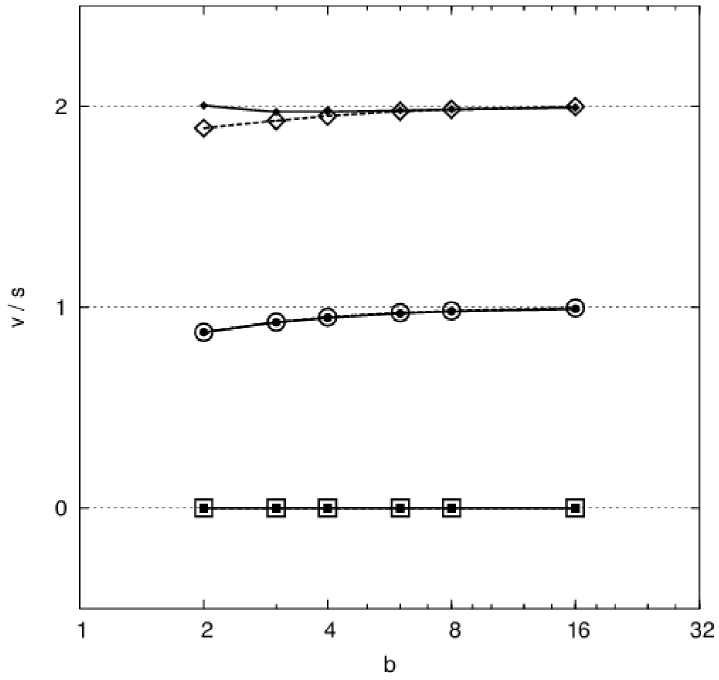
Flame Capturing – Verification II

Flame speed test

Computed traveling wave speed as a function of resolution for different advection velocities (squares: v = -s, circles: v = 0, diamonds: v = +s).

Solid line corresponds to isochoric fluid, dashed line corresponds to the fluid with factor of 2 density jump.

compressible



Flame Capturing – Verification III

Other completed tests

- realistic stellar EOS's;
- variable flame speed (laminar, turbulent);
- 1/2/3-D cartesian, 2-D cylindrical, and 1-D spherical.

Flame Capturing – Summary

Current status

- We have developed a working knowledge of the model and its domain of validity.
- Model is fully implemented in FLASH and is being used in production simulations.

Coming improvements

- Extension to spatially variable stellar composition (will make our implementation unique).
- Two-stage, $^{12}C+^{12}C$ and NQSE/NSE, energy release.

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Validation – LANL experiments overview

- `flash.uchicago.edu/˜vikram/validation/index.html`

- **Shock-cylinders interaction experiments (Bob Benjamin, LANL)**

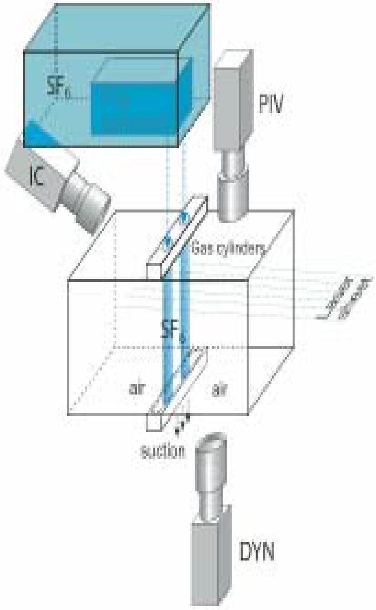
  Version of the standard shock-cylinder problem (several groups, more recently Zoldi & Benjamin, Rider & Greenough).

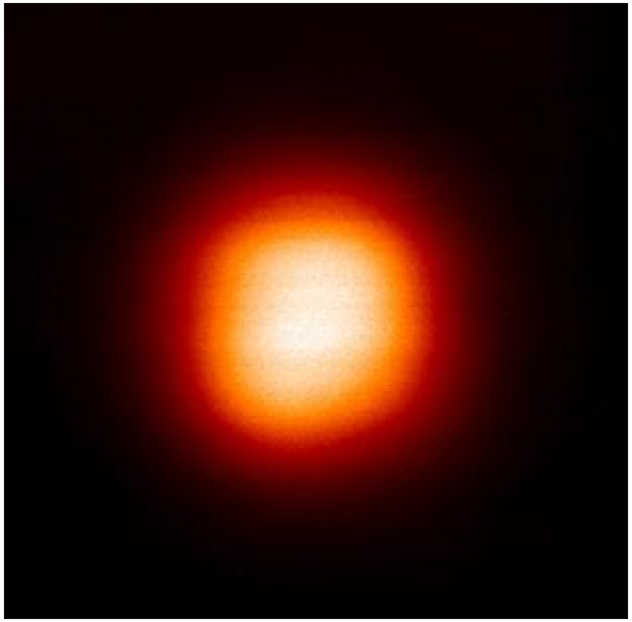
- **Begin with a single cylinder (compare with work of Zoldi)**…
- role of hydro scheme (resolution, features)
- uncertainties in data (e.g. initial conditions – maximum concentration, 3-dimensional effects)

- **…continue into two cylinder problem (unexplored territory).**
- new dynamics: individual/collective/mutual character
- look into possible 3-dimensional effects
- attempt to model complete experimental system

Validation – Experimental setup

LANL experiment test section.





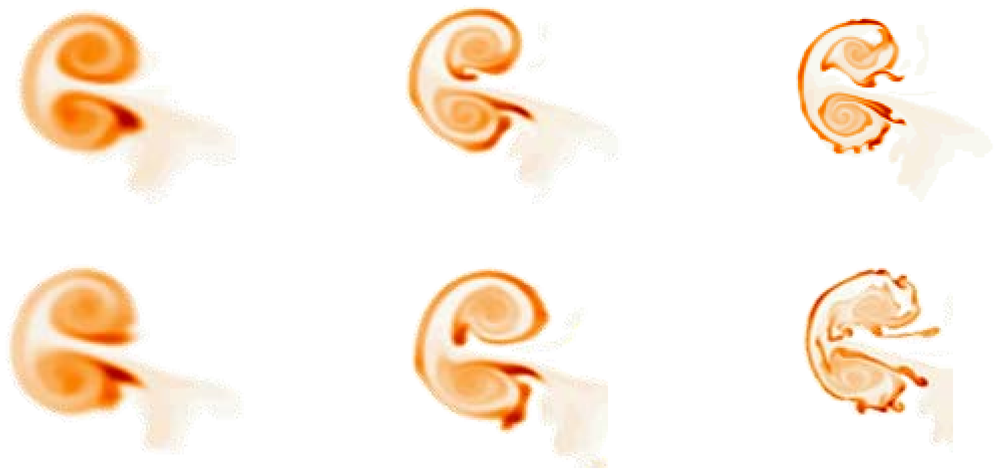
Initial conditions for single cylinder experiment.

Validation – single cylinder experiment

6 Level | 7 level | 8 Level

Conc: 0.6

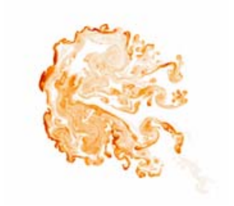
Conc: 0.8



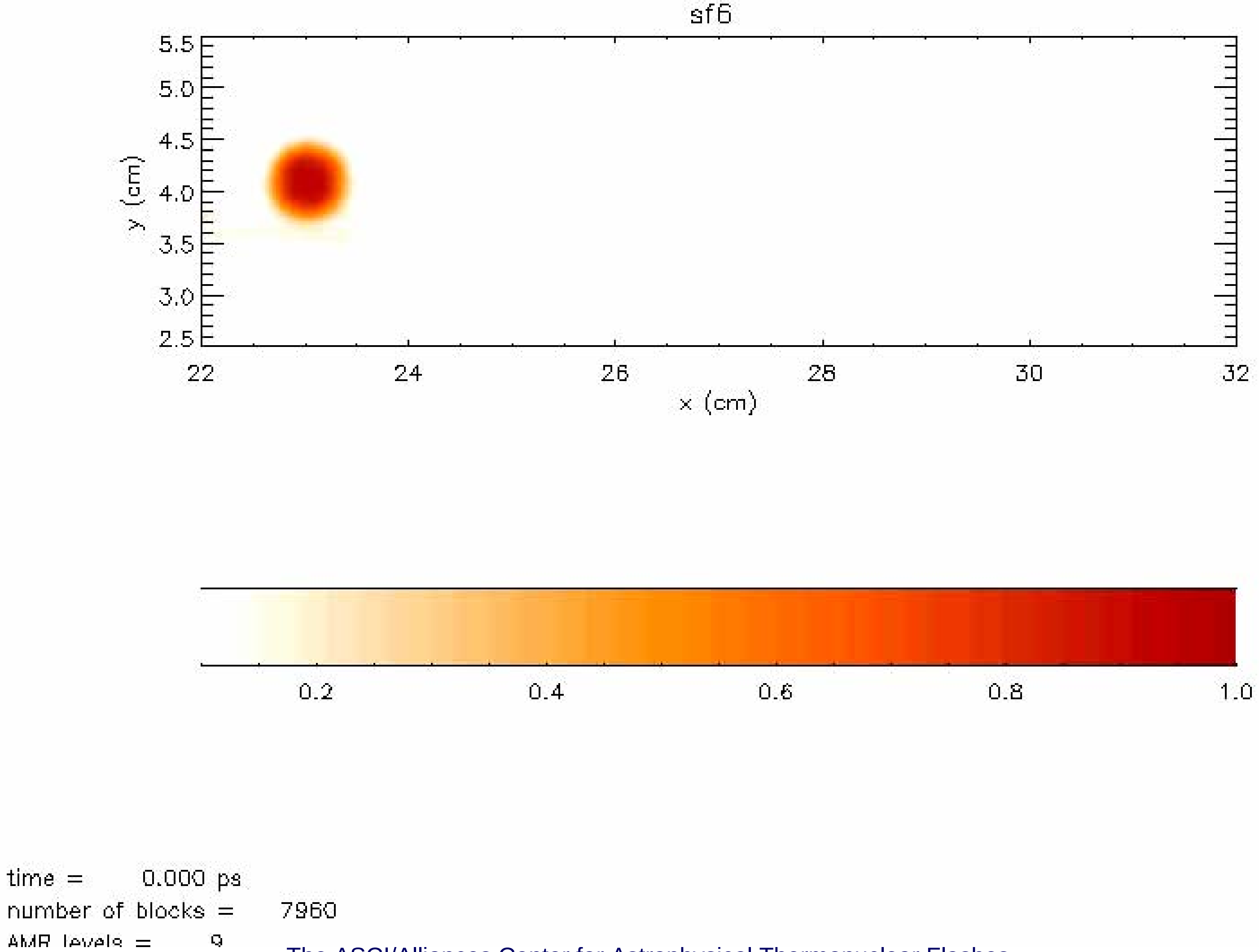
Conclusions

1) primary instability leads to formation of two vortex cores
2) amount of structure increases with maximum concentration (steeper gradients)
3) secondary instabilities clearly visible in models with higher resolution

10 Level

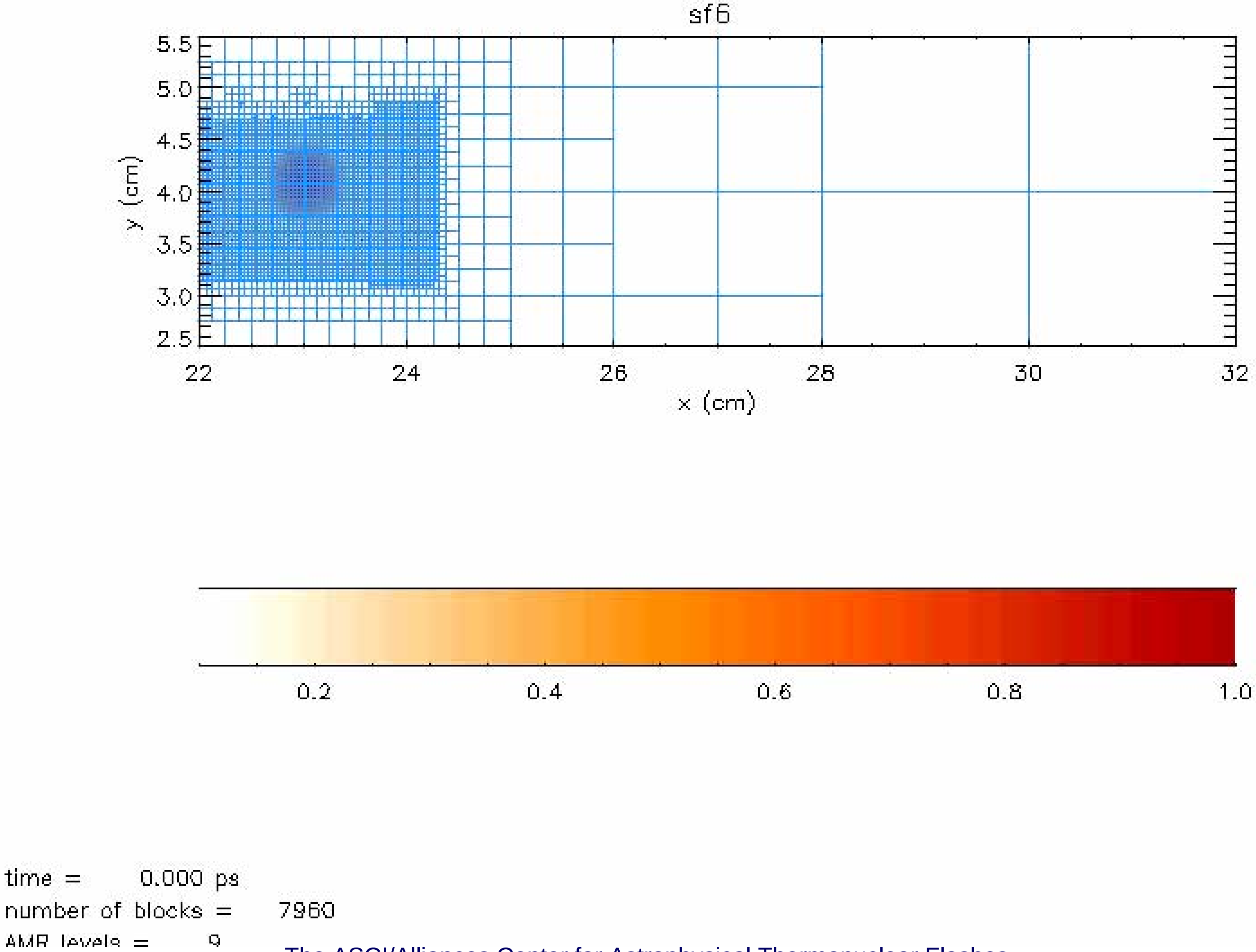


Validation – single cylinder, overall evolution



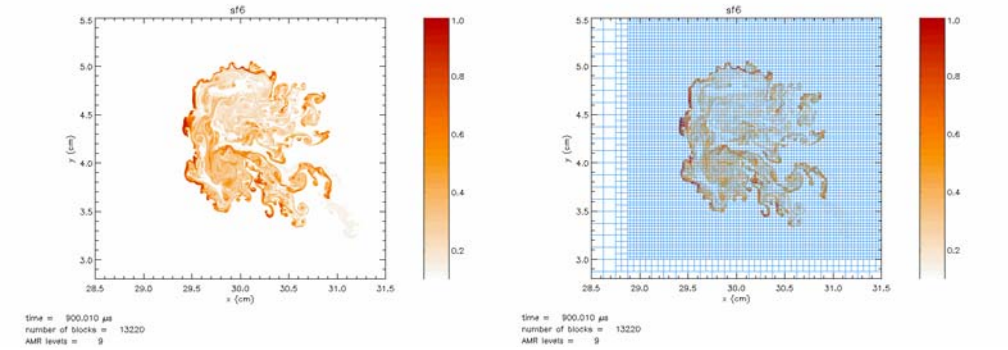
time = 0.000 ps
number of blocks = 7960
AMR levels = 9

Validation – single cylinder, grid adaptivity

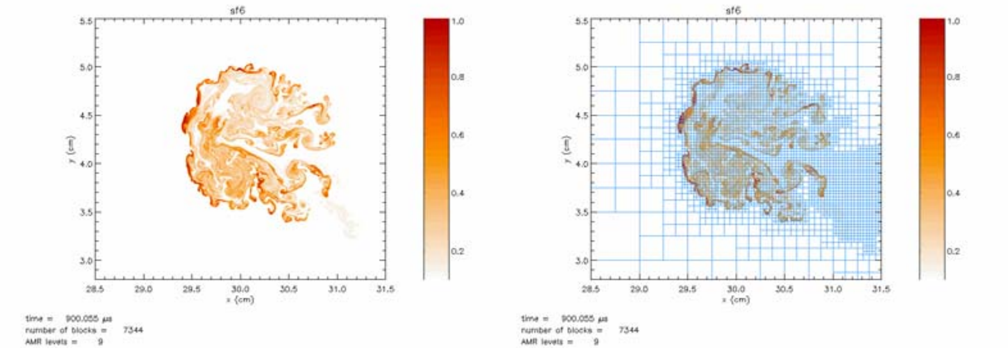


Validation – flow-mesh interaction

Locally uniform grid



Fully adaptive solution



- With adopted refinement criteria adaptive solution is nearly similar to uniform grid solution, but offers a speed-up by a factor of 60.

Validation - double cylinder

t=0 t=330 μs t=760 μs

Case A S/D=1.2

Experiment

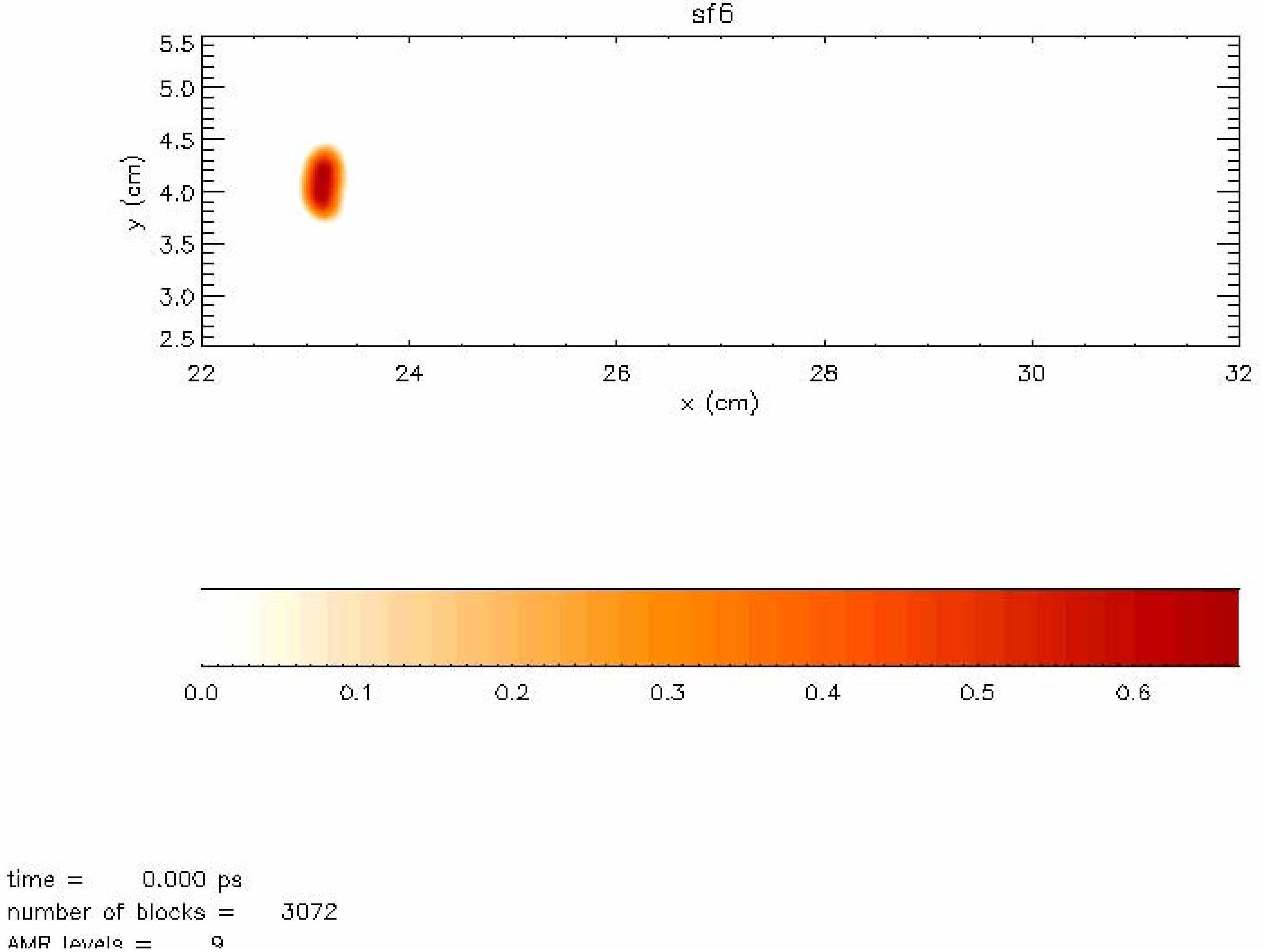
Simulation

Case C S/D=2.0

Conclusions

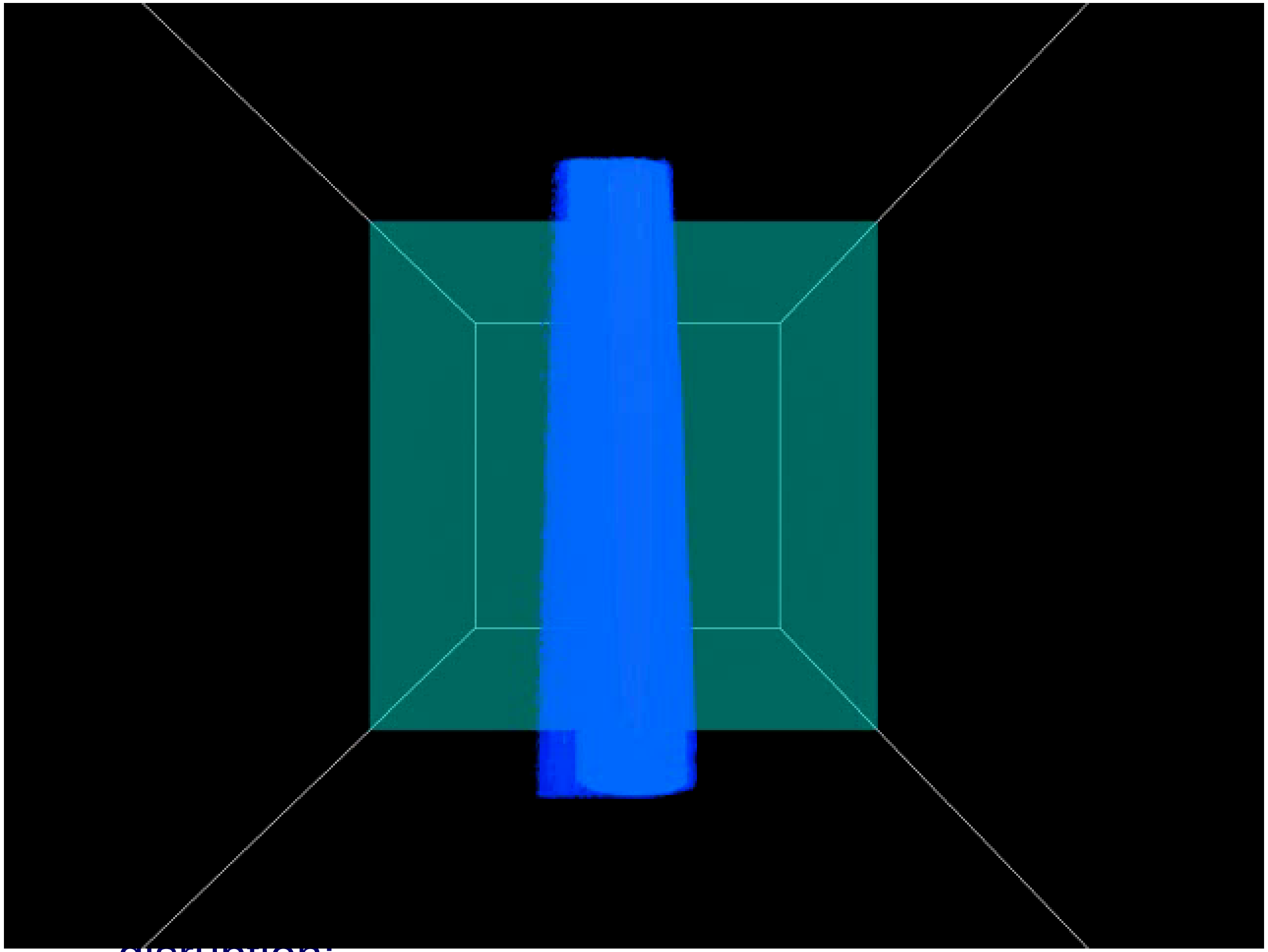
- amount of small structure depends on concentration (as in one cylinder);
- evolution changes character depending on distance between the cylinders;
- mutual drifting occurs for intermediate cylinder separations;
- amount of cylinder rotation depends on concentration;
- our simulations appear to reproduce the smaller separations much better.

Validation - double cylinder



time = 0.000 ps
number of blocks = 3072
AMR levels = 9

Validation – 3D aspects

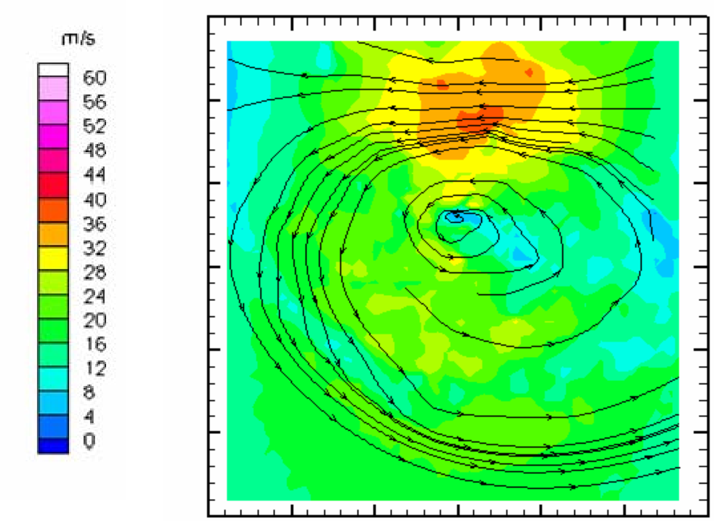


disruption;

- drag depends on concentration (see below);
- 3-D effects are likely to dominate secondary instability.

Validation – single cylinder, velocity field

Experiment



Simulation

- General agreement is good, although the simulation predicts much higher velocities usually than are seen in the experiment. This has also been noted by other researchers working in this area.

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Issues

Computing resources

- *Problem*: available resources inadequate to achieve computational goals in timely fashion.
- *Reason*: most group members are foreign nationals (applied 6 weeks ago and still waiting); the field is relatively small – chances to hire U.S. citizens are small.
- *Solution*: situation remained the same for a year. Trying to gain access to supercomputer installations beyond ASCI OCFs (computing grants at PSC, applications to INCITE/NERSC, MCR cluster; Weirs using QSC, lobbying for enabling FLASH on QSC).

Other issues

- Archival data storage largely insufficient.
- 3-D visualization software needs further improvements.

Future

Group focus

- Detailed explosive nucleosynthesis (+6 months)

  together with Astro & Code groups
- Implicit flow solvers (+6 months)

  Weirs, Pan [collaboration with G. Patnaik, P. Colella]
- Validation

  Weirs, Plewa, Dwarkadas [collaboration with H. Robey, B. Remington, LLNL]

Major projects

- Models with rotation (+1 year)

  Plewa + Astro [collaboration with N. Langer]
- Radiative transfer in moving media (>1 year)

  Vikram Dwarkadas + new hire [collaboration with P. Hoeflich]
- Multi-D radiation transport

  depending on applications/manpower (magnetized boundary layer?)

Accomplishments

Computational modules

- flame capturing model (minor improvements still possible)
- MHD and relativistic MHD modules
- implicit hydro module

Validation

- shock-cylinders interaction, 2- and 3-D simulations, flow-grid interaction, the role of initial conditions, primary instability correctly captured, velocities appear too large but we may have an explanation for that
- extend validation to laser experiments at LLNL

Inter-group interactions

- code framework definition
- initial models, flame models
- visualization

Community service

- The Chicago Workshop on Adaptive Mesh Refinement Methods

Discussion