Recent Progress in FLASH: High-Energy-Density Physics Applications

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The Physics of Intracluster Medium: Theory & Computation
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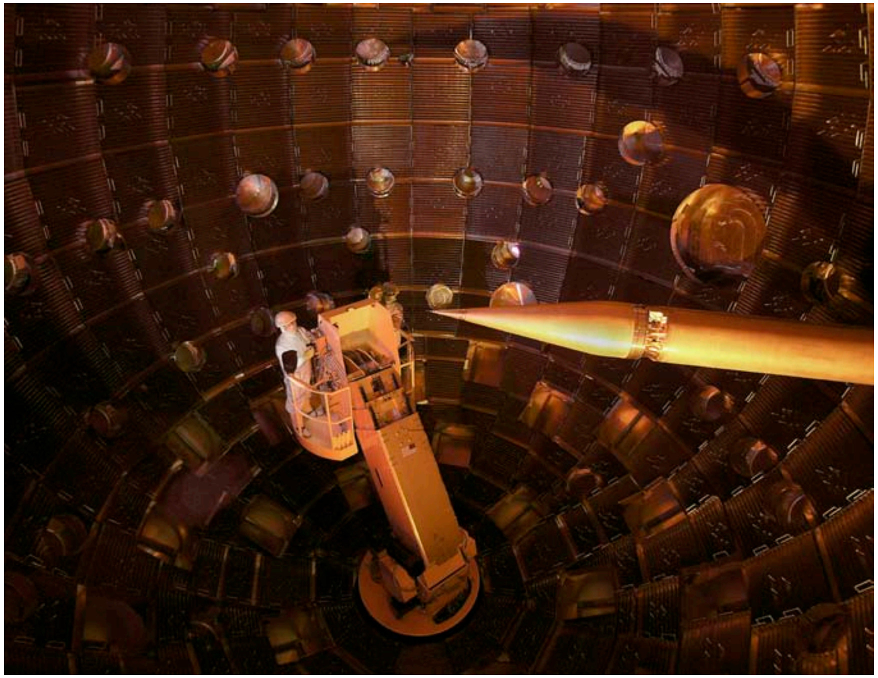
An Advanced Simulation & Computing (ASC)
Academic Strategic Alliances Program (ASAP) Center
at The University of Chicago

National Ignition Facility at LLNL



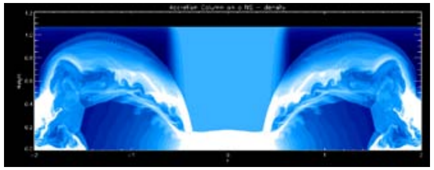
Outline of Talk

- What is the FLASH code?
- New capabilities to FLASH as an open toolset for High-Energy-Density physics (HEDP)
- HEDP capabilities in Unsplit Staggered Mesh Magnetohydrodynamics solver
  - Two time-stepping schemes:
    - A new fully implicit Jacobian-Free Newton-Krylov type solver
    - An explicit Super-Time-Stepping (STS)
  - Anisotropic Spitzer-Braginskii heat conductivity model
  - Magnetic field generation: The Biermann battery effects

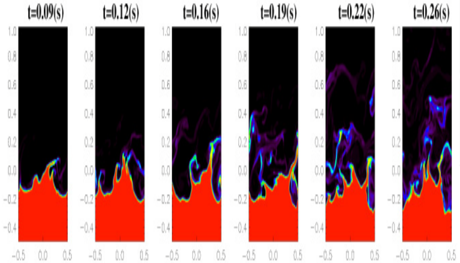
What is FLASH?

- FLASH is a publicly available astrophysical community code
  - Highly compressible multi-physics reactive flow solver
  - Component-based, fully modular, extensible open science code
  - Adaptive mesh refinement, massively parallel, runs on laptops, scales well on large HPC machines (e.g., BG/L, Intrepid BG/P, Jaguar XT5)
  - Riemann solvers for hydro, magneto-hydrodynamics, relativistic hydrodynamics; gravity, nuclear burning, source terms, material properties; equations of state
  - Have been professionally developed and managed for more than a decade
  - More than 1700 downloads, 600 users, 340 research papers
  - Funded through the DOE-supported ASC/Alliance Academic Strategic Alliance Program to the Center for Astrophysics Thermonuclear Flashes at the U of Chicago
  - Fryxell et al. (2000); Dubey et al. (2009)

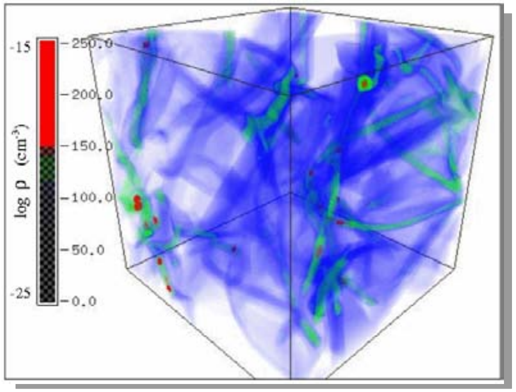
FLASH Capabilities Span a Broad Range…



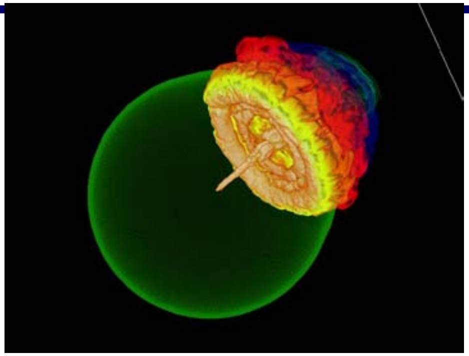
Shortly: Relativistic accretion onto NS



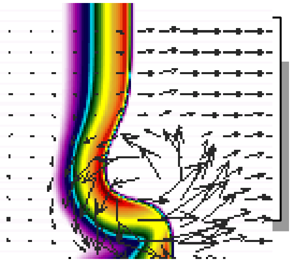
Wave breaking on white dwarfs



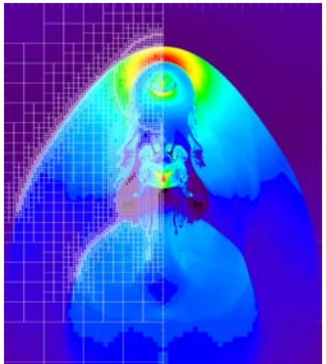
Gravitational collapse/Jeans instability



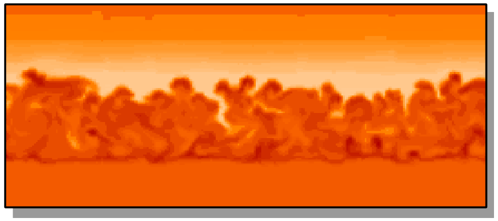
Type Ia Supernova



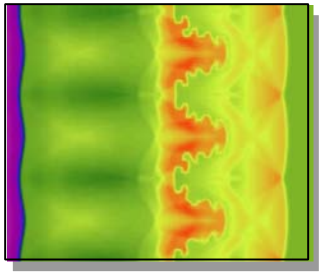
Flame-vortex interactions



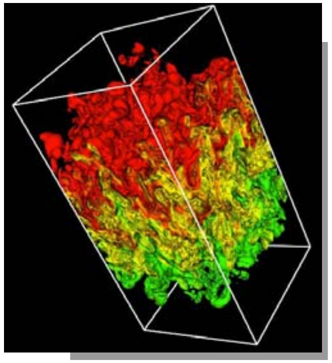
Intracluster interactions



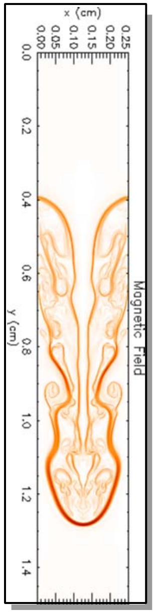
Nova outbursts on white dwarfs



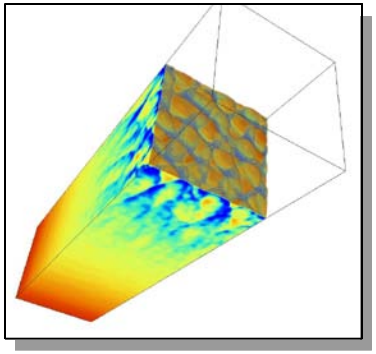
Laser-driven shock instabilities



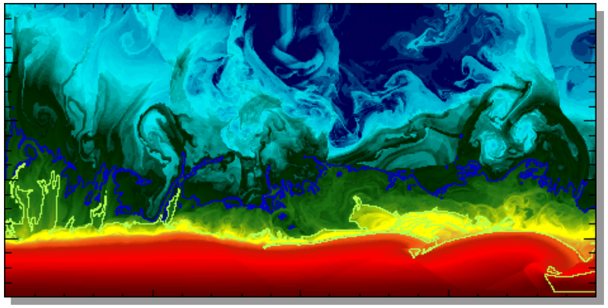
Rayleigh-Taylor instability



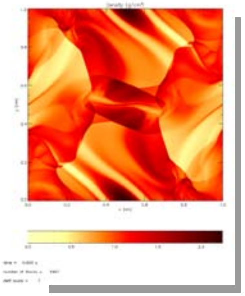
Magnetic Rayleigh-Taylor



Cellular detonation



Helium burning on neutron stars



Orzag/Tang MHD vortex

Richtmyer-Meshkov instability

The FLASH Code Contributors

- Active Contributors:
  - Anshu Dubey, Chris Daley, Shravan Gopal, Carlo Graziani, Dongwook Lee, Paul Rich, Klaus Weide, Gouhua Xia, Paul Ricker, Cal Jordan, John ZuHone, Kevin Olson, Marcos Vanella

- Past Major Contributors:
  - Bruce Fryxell, Katie Antypas, Alan Calder, Jonathan Dursi, Robert Fisher, Dean Townsley, Timur Linde, Andrea Mignone, Tomek Plewa, Lynn Reid, Katherine Riley, Andrew Siegel, Dan Sheeler, Frank Timmes, Natalia Vladimirova, Greg Weirs, Mike Zingale

High-Energy-Density Physics (HEDP) in FLASH

- ☐ Wide range of physical conditions, nonlinear phenomena
  - ☐ In HEDP, pressure ~ 1Mbar, high temperature, low density
  - ☐ Air at density of 1mg/cm^3, pressure ~ 1Mbar is reached at a temperature above 10 keV ~ 100 million K

- ☐ Omega Laser Facility at U of Rochester, Z-pinch machine at SNL, NIF at LLNL
  - ☐ Experimental data span orders of magnitude in temperature & density, length scales from the microscopic to macroscopic
  - ☐ Crucial to have 3D, multi-scale, multi-physics computer simulations on HPC platforms to design and understand HEDP

- ☐ Advanced Simulation and Computing (ASC) Program in DOE NNSA and Office of Advanced Scientific Computing Research (ASCR) in DOE Office of Science are funding the Flash Center to add capabilities to FLASH to make it an open toolset for the academic community

Adding HEDP Capabilities in FLASH

- ❑ Three-temperature (3T) treatment of radiation-hydrodynamics
- ❑ Laser energy deposition using ray tracing
- ❑ Time-stepping schemes: JFNK implicit and STS explicit
- ❑ Spitzer-Braginskii type heat conductivity
  - ❑ Isotropic & anisotropic in the presence of magnetic fields
- ❑ Magnetic field generation: Biermann battery term for MHD

Unsplit Staggered Mesh MHD Solver

- Shock-capturing high-order Godunov Riemann solver (Lee & Deane, JCP, 2009)
  - Finite volume method
  - Adaptive mesh refinement, uniform grid
  - First order Godunov, 2nd order MUSCL-Hancock, 3rd order PPM, 5th Order WENO scheme
  - Approximate Riemann solvers: Roe, HLL, HLLC, HLLD, Marquina, modified Marquina, Local Lax-Friedrichs
  - Divergence of magnetic fields is numerically controlled on a staggered grid, using a constrained transport (CT) method (Evans & Hawley, 1998)
  - Wide ranges of plasma flows $10^{-6} \leq \beta(\equiv p/B_p) \leq 10^6$
  - Extremely large Courant stability limit (CFL ~ 1 for 3D)
  - TVD slope limiters for preserving non-linear monotonicity in discontinuous solutions
    - Monotonicity preserving upwind PPM slope limiter for MHD (Lee, presented at Astronum 2010 meeting, in preparation)

Diffusive Time Scale

- Fact:

$$\Delta t_{\text{Diffusion}} \approx \Delta x^2;\;\; \Delta t_{\text{Advection}} \approx \Delta x$$

- Diffusive time scale dominates as refinement levels increase
- Two approaches:
  - Jacobian-Free Newton Krylov implicit solver (e.g., Knoll and Keys 2004; Toth et al. 2006)
  - Super-Time-Stepping (explicit) (Alexiades et al., 1994)

Implicit Solver in FLASH3

- NSF Grant award (PHY-0903997) for fiscal years 2009 – 2011, $400K
  - Drs. Fausto Cattaneo and Dongwook Lee

- Jacobian-Free Newton-Krylov implicit scheme (e.g., Knoll and Keys 2004; Toth et al. 2006)
  - 2nd or higher order accurate in space and time to solve $Ax = b$
  - GMRES iteration to seek solutions in Krylov subspace
  - Hybrid method of using both Explicit/Implicit blocks in a computational domain
  - Requires load balancing between two different explicit/implicit types of blocks

- Schwarz-type preconditioner
  - Preconditioner to accelerate convergence rates for iterative solution
  - Schwarz-type preconditioner minimizes the need for off-processor data
  - Efficient approach in FLASH's block-structured AMR

- The implicit solver will extend FLASH's capability to overcome small diffusive time scales in both astrophysical and HEDP applications

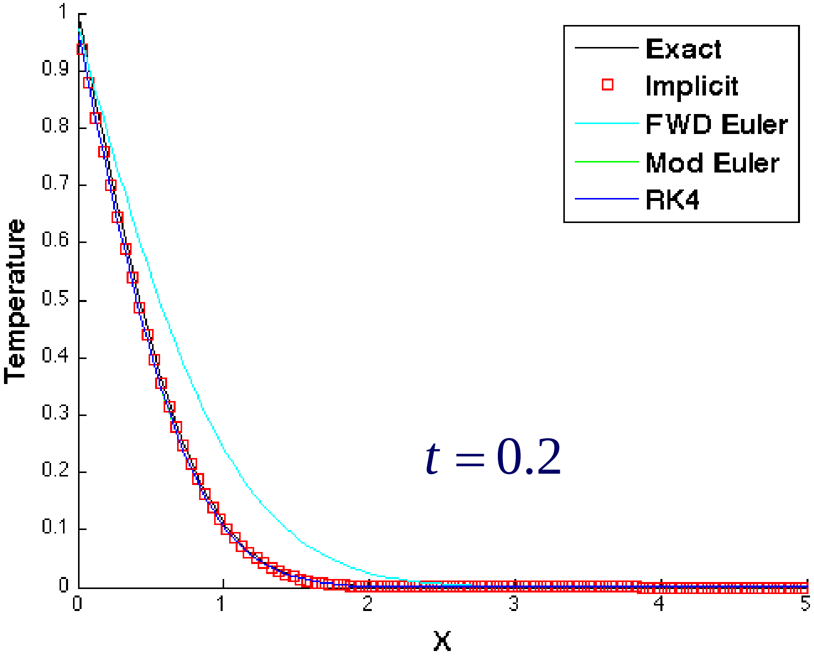
Model 1D heat equation

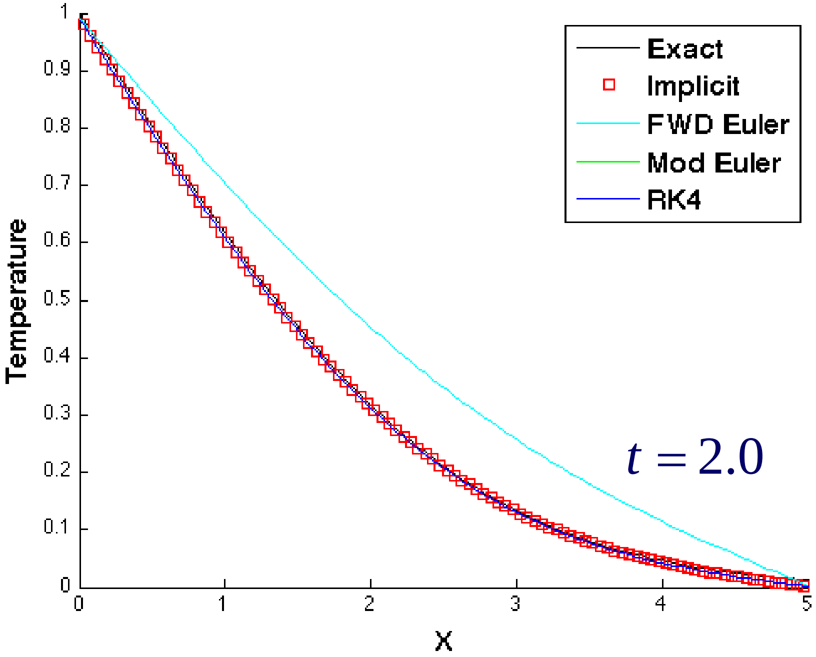
- A model 1D heat equation solved on a serial uniform grid using a JFNK fully implicit solver

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$$

$$\mathrm{IC}: \; T(x=0, t=0) = 1; \; T(x>0, t=0) = 0$$

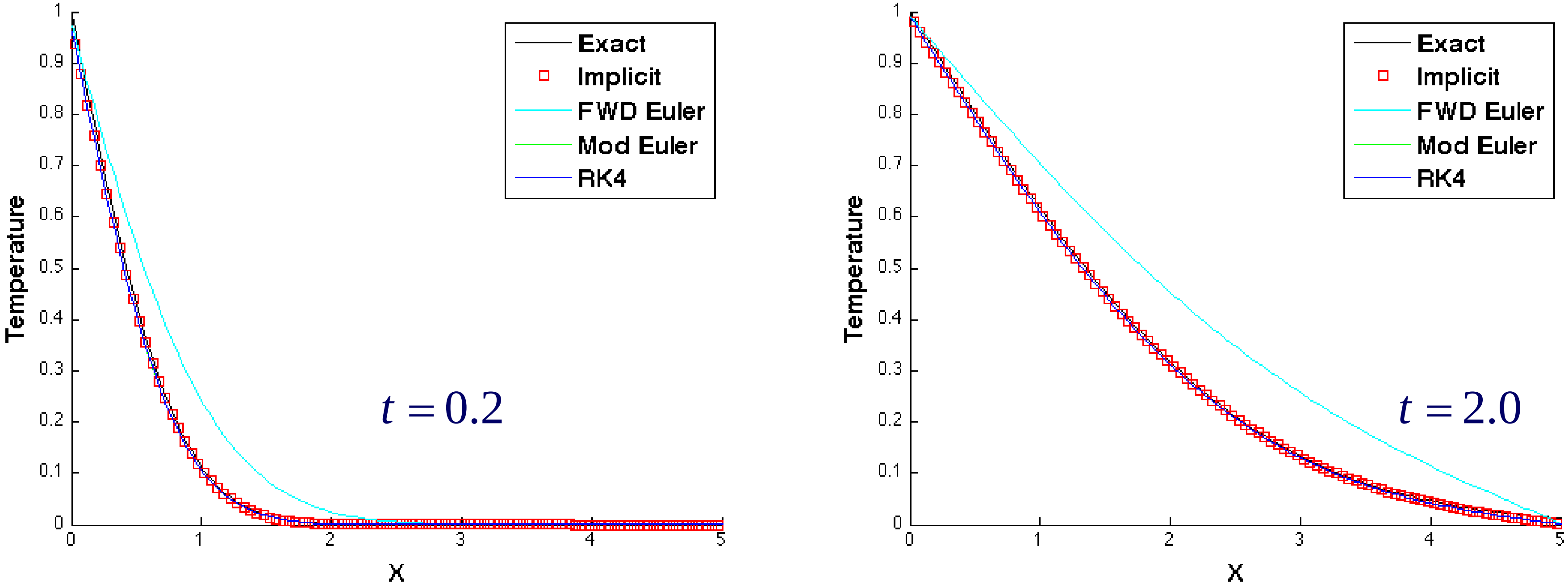
$$\mathrm{BC}: T(x=0, t>0) = 1; \; T(x=5, t>0) = 0$$





Model 1D heat equation

- A model 1D heat equation solved on a serial uniform grid using a JFNK fully implicit solver
- Explicit CFL = 0.9 (~1800 time steps); implicit CFL=10.0 (~160 time steps)



Super-Time-Stepping Algorithm

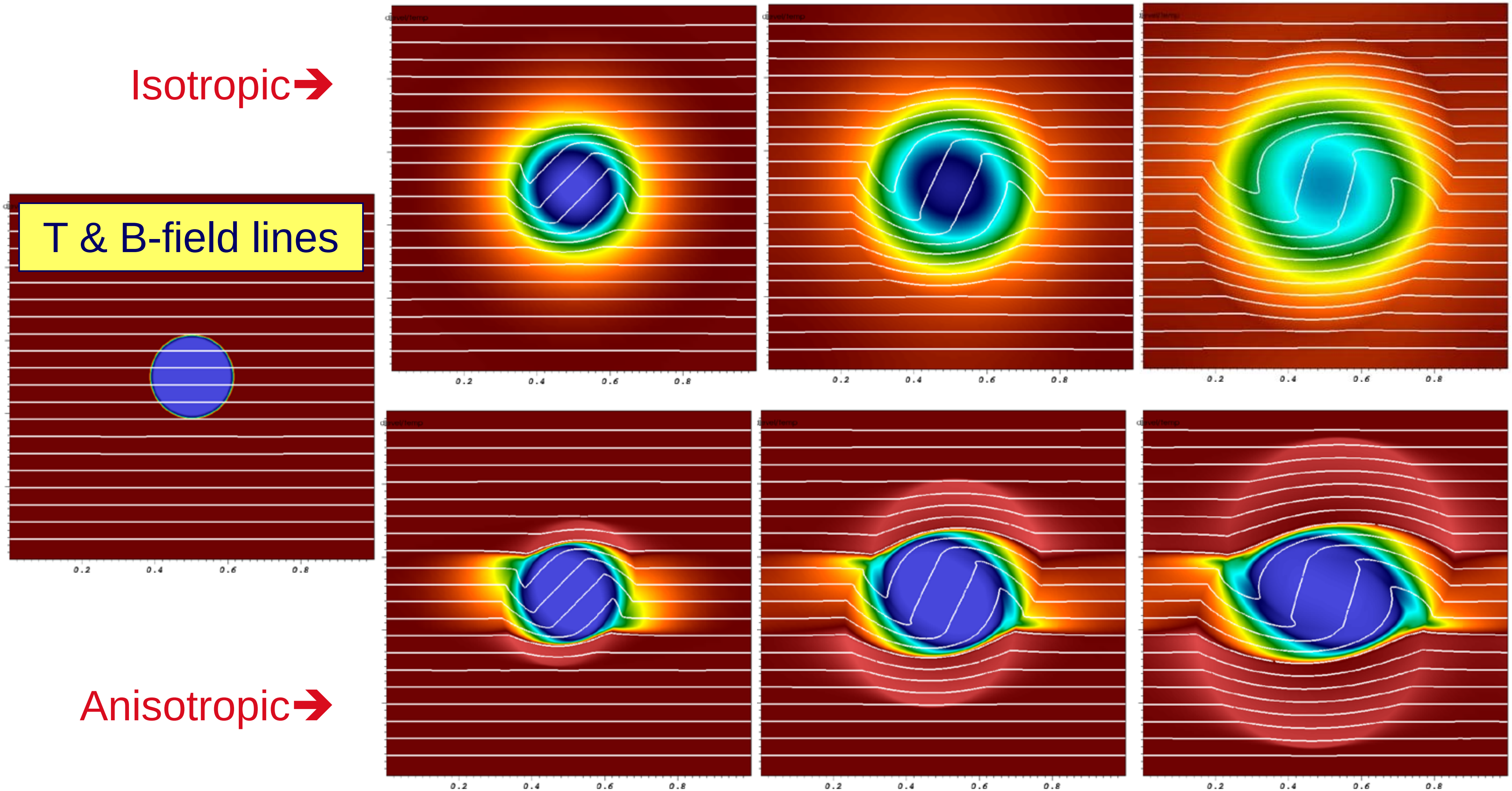
- An explicit time stepping algorithm by Alexiades et al., 1994
    - Increase time step dt by using modified orthogonal Chebychev polynomial
    - Stability and Optimality property in Chebychev polynomial of degree N
    - Maximize duration of $\Delta t_{STS} = \sum_{i=1}^{N_{STS}} \tau_i$, subdivided into small N_{STS} sub-time steps τ_i
    - Impose stability restriction only at the end of sub-time steps $\tau_i,\ i = 1,\ldots,N$

- Originally for parabolic (diffusion) system

- Extended to hyperbolic (advection) system, and combined hyperbolic-parabolic (advection-diffusion) system in FLASH3
    - ~30% increase in performance for hyperbolic system
    - An order of magnitude increase in time steps in parabolic system

Isotropic vs. Anisotropic Heat conduction

- ❑ MHD Rotor test with $\chi_c = 5\times10^7$ for a cold plasma regime



Isotropic➔

T & B-field lines

Anisotropic➔

- ❑ For hot plasmas, a full Spitzer conductivity can be used

Spitzer Thermal Conductivity

- Thermal Conductivity following the formulation of Spitzer, 1962:

$$\nabla \cdot Q \text{ source term for conservation of energy}$$

$$Q = \sigma \nabla T$$

$$\sigma\left(X_i, \rho, T\right) = \kappa T^{5/2}$$

$$\kappa = 9.2 \times 10^{-7}$$

- Provides a valid approximation of electrical conductivity for hot, dilute magnetized plasma
    - Simple isotropic conductivity in FLASH2
    - A new anisotropic conductivity
    - Collaboration with Ruszkowski et al.
        - Cosmological cluster formation simulations with anisotropic thermal conduction and radiative cooling
    - Transport of heat along magnetic field lines

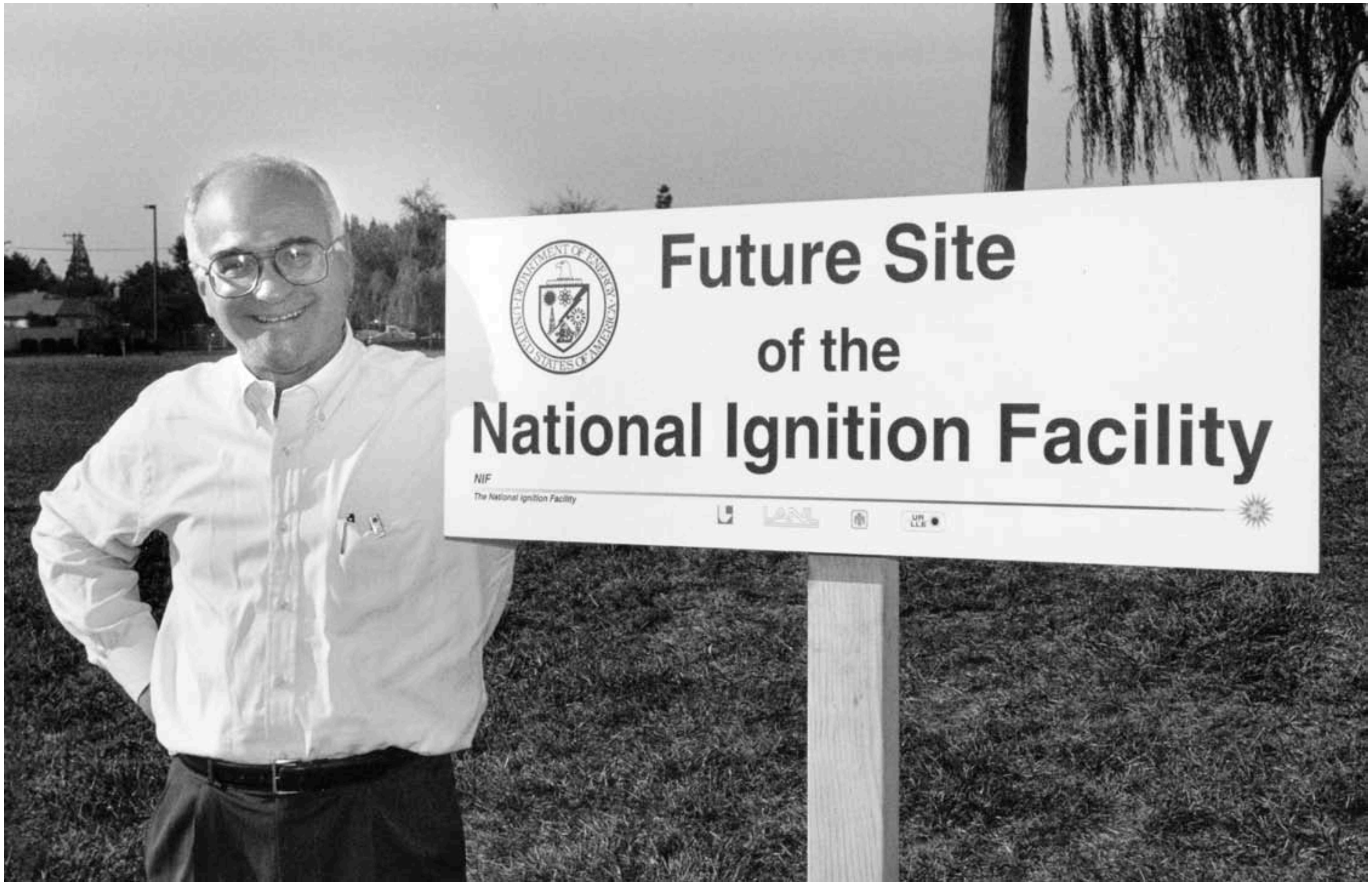
The Biermann Battery Effects

- Cosmic magnetic fields are ubiquitous, but their origins remain unclear
- Biermann bettery term is important in recreating cosmic conditions within the lab and in computations
- Magnetic fields are important because they modify transport process, accelerate particles and exert body forces
- Battery term can play an important role in seeding magnetic fields in HEDP simulations

$$\frac{\partial \mathrm{B}}{\partial t} = \nabla \times \mathrm{v} \times \mathrm{B} - c\frac{\nabla n_e \times \nabla p_e}{n_e^2 e}$$

- In FLASH’s single-fluid radiation-hydro model with 3T, a simple battery approximation is available (Kulsrud 2004; Xu 2008) assuming:
  - Charge neutrality, LTE, a constant degree of ionization in space
  - For more complicated HEDP described by non-LTE, two-fluid model is required

Back then we were… 1990’s



Here we are in 2010!

FLASH, an open toolset for the academic HEDP community