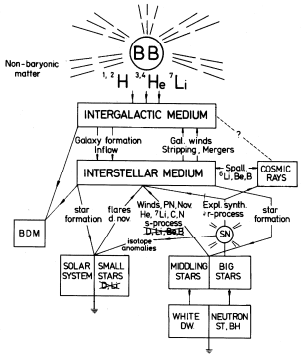
What are we trying to do: Understand how/why stars explode

Why is this interesting?

- The physics is intrinsically fascinating
  - (Nuclear) combustion under fully compressible, stratified conditions
  - Deflagration-detonation transition in “open” systems
  - Mixing at low and high Mach numbers
  - Sub-grid modeling for highly complex multi-physics systems
  - …
- The answers are a critical aspect of understanding the early history of our universe
  - “Chemical” evolution of stars and galaxies
  - Structure formation of the universe
  - Constraints on “dark energy”



How are we answering this question?

- By building a new generation *useable* computational tool: FLASH, taking advantage of
  - New computer architectures: portability/performance
  - New algorithmic developments (multi-grid, AMR, …): capabilities/performance
  - Extensive verification and validation - ties to new generations of lab experiments: believability

What was our history?

In December 1996, DOE/NNSA announced an “Academic Alliance” program in support of the Stockpile Stewardship Program and the associated Accelerated Scientific Computing Initiative

- Target was support of 5 Centers of Excellence, nominally @$5M/year for 5 years
- ~50 universities submitted preliminary proposals
- UofC submitted a proposal joint with Argonne/Mathematics & Computer Science: The “Flash Center”

Winners were announced in June 1997, with 5 winning institutions

- The Flash Center is “basic science”-oriented
- The 4 other Centers (at CalTech, Stanford, UofI/Urbana, and Univ. of Utah) are focused on a mix of basic science and engineering
- Funding started in Sept. 1997

Program was extended for additional 5 years in 2002

- All Centers won full extension, starting Oct. 2002

Where are we now, 6.5 years later?

Participants:

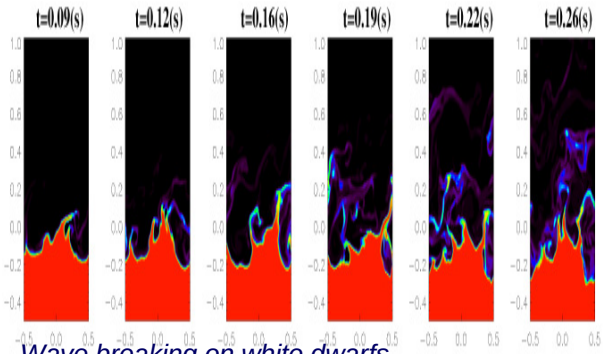
- 58 faculty, senior scientists, research associates, graduate students, computing staff, and 2 administrative staff
- Astronomy & Astrophysics, Computer Science, Enrico Fermi Institute, James Franck Institute, Mathematics, Physics; Argonne National Lab

Accomplishments:

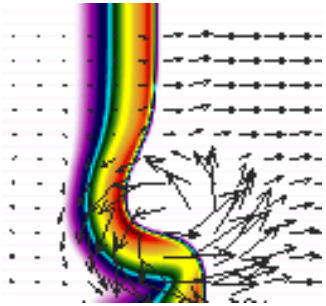
- **Computational science:**
  - **Widely-used community code for compressible reactive hydro, mhd/plasma physics, …**
- Astrophysics and physics:
  - Major new results for novae and supernovae
  - Major new results for combustion science and turbulent interface mixing
- Academic impacts at UofC:
  - Founding of Computations Institute & impetus towards hiring of new computational "applications" faculty: teaching a new computational science generation
  - Seeding of new large efforts in computational science: NSF ITR grants, NSF Physics Frontier Center
  - Close working relations with ANL

→ **Change of "culture"**

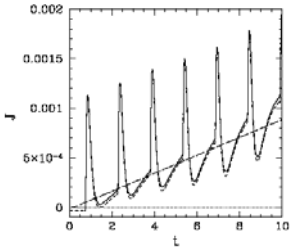
Where are we now, 6.5 years later?



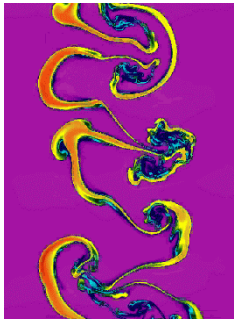
Wave breaking on white dwarfs



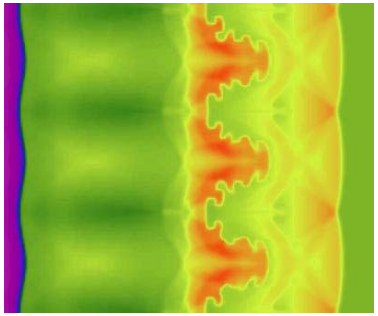
Flame-vortex interactions



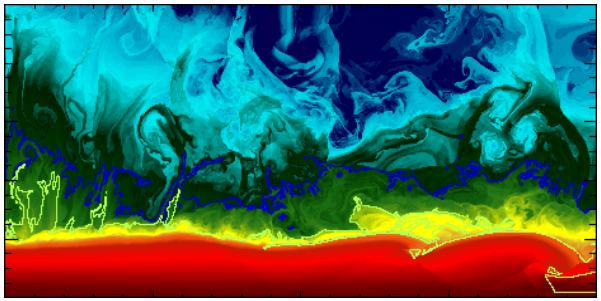
Magnetic reconnection (R. Fitzpatrick/UT Austin)



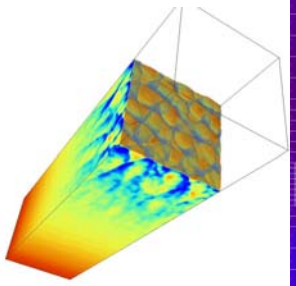
R-M instability



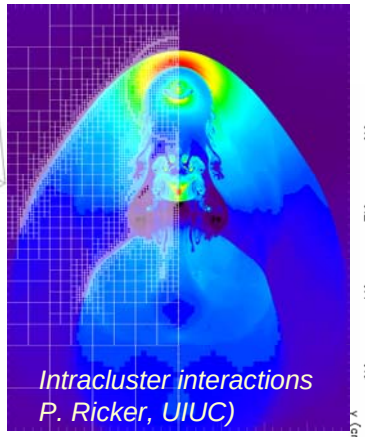
Laser-driven shock instabilities



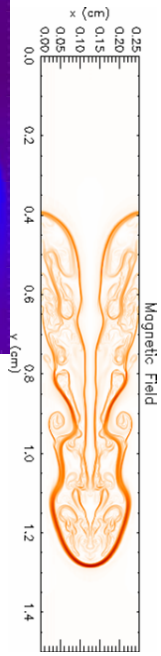
Helium burning on neutron stars

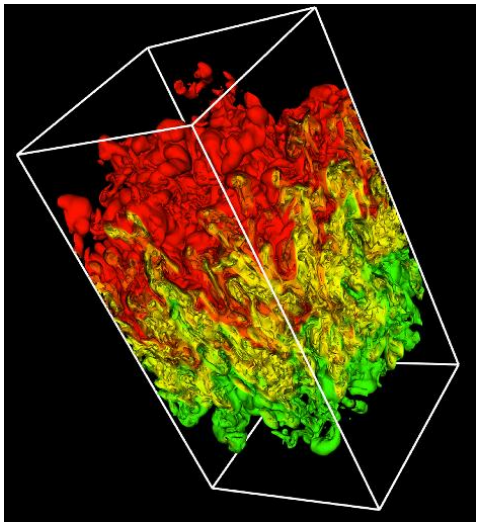


Cellular detonation

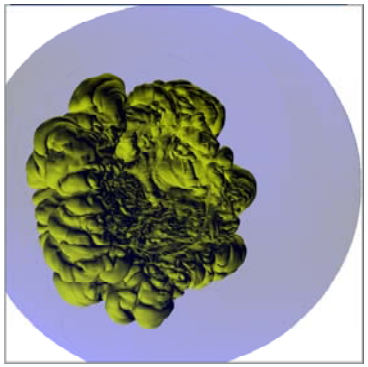


Intracluster interactions
P. Ricker, UIUC)

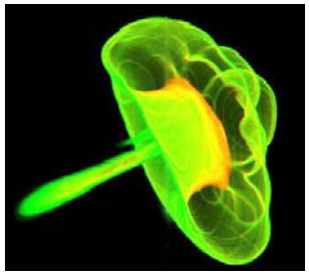




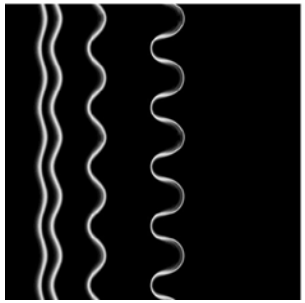
Magnetic and hydrodynamic Rayleigh-Taylor instabilities



Type Ia supernova:
off center ignition



White dwarf deflagration



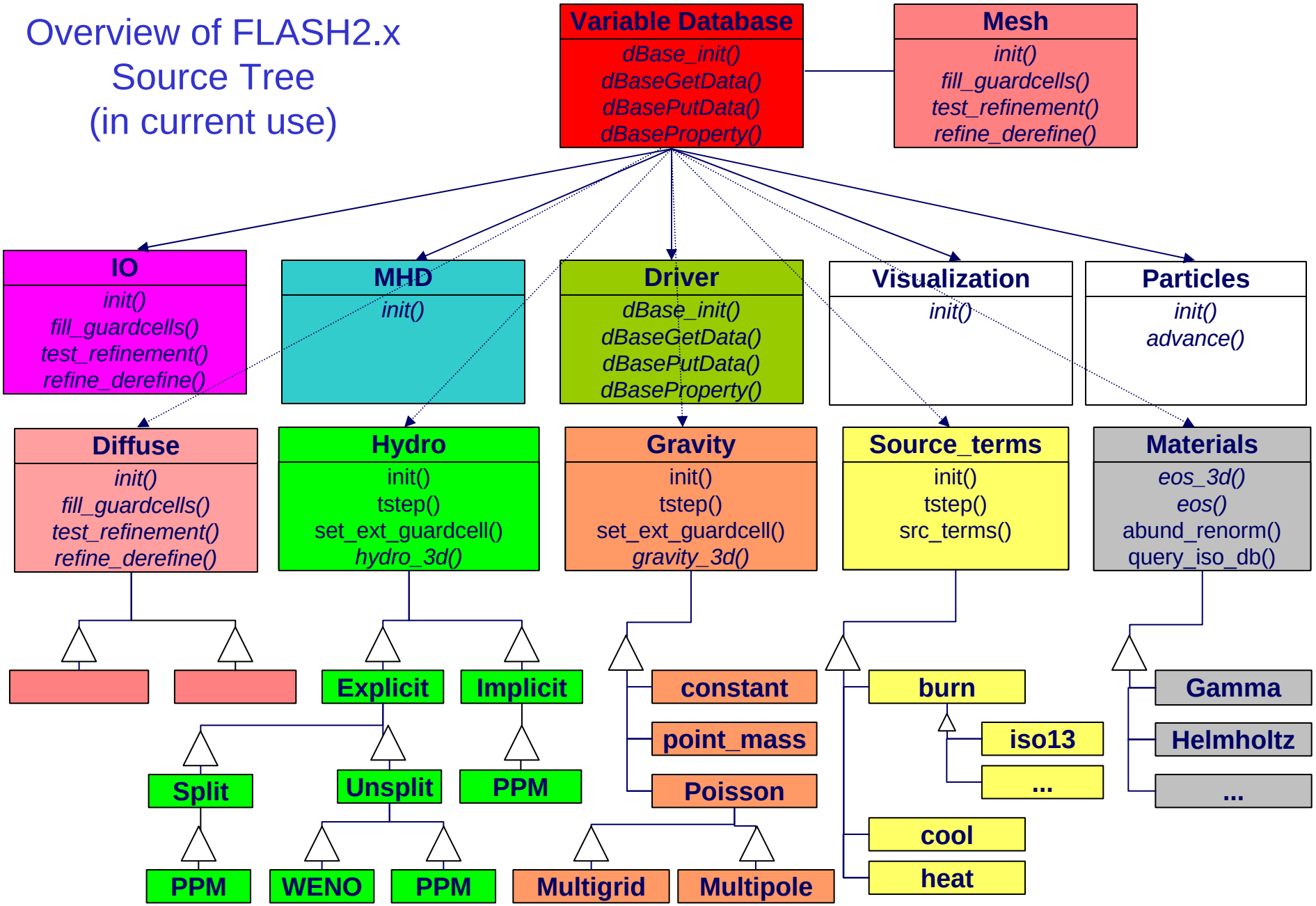
Landau-Darrieus instability

Some FLASH Details …

Physics Modules	Language (# lines of source)	Scaling/system; systems ported to	Birth year	Model
Explicit Euler/Navier-Stokes w/ AMR, combustion, EOS, ionization, gravity, resistive single-fluid mhd, relativistic single-fluid mhd, Hall mhd	F90/C/Python (500K)	6000 processors/ASCI Red; runs on all ASCI platforms, Cray X1, IBM BG/L, linux clusters	1998	MPI HDF/PNetCDF PVTK

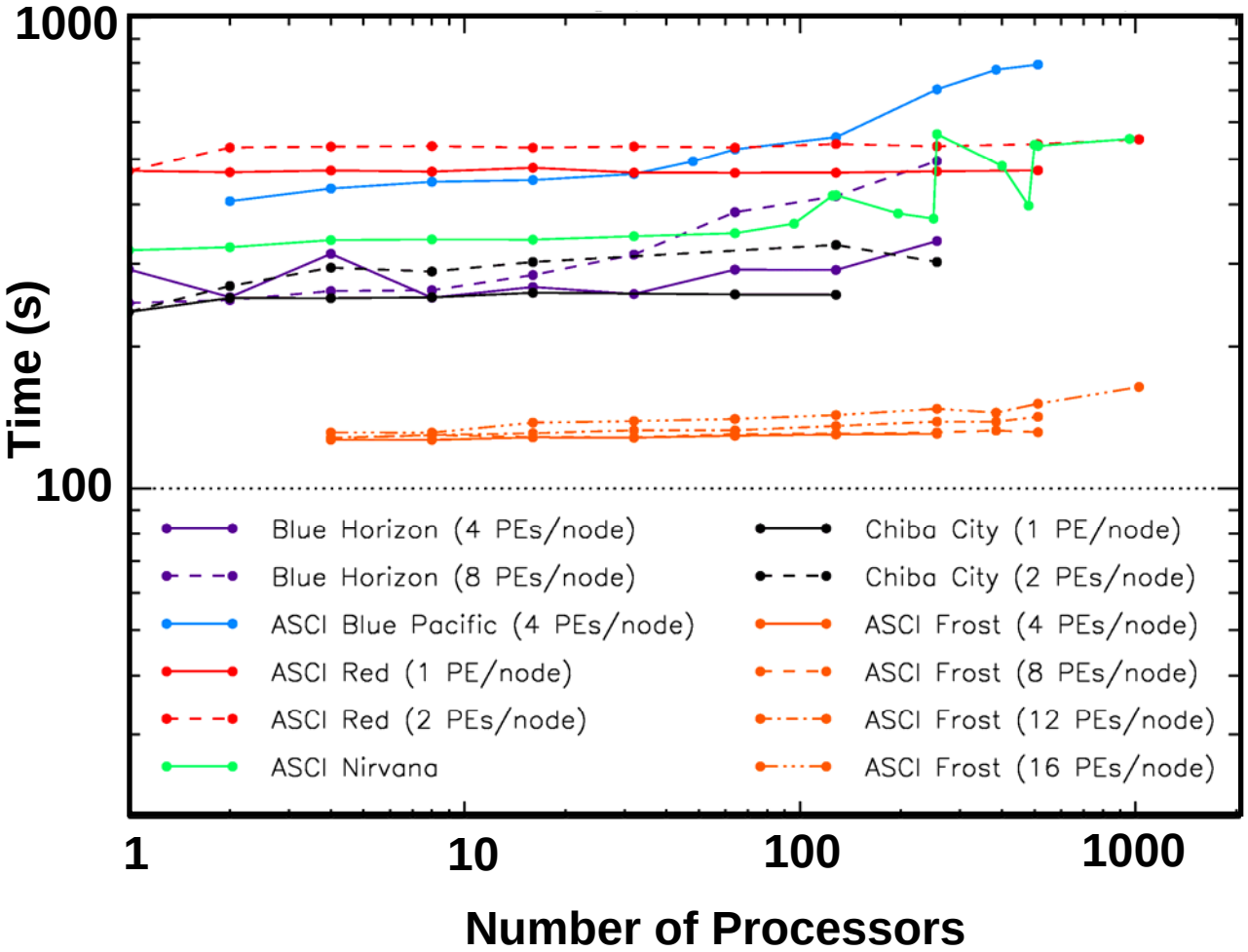
- Open source distribution model, not export-controlled
  - (some modules are restricted, however)
- In use world-wide, remote developers, …
- Code available at http://flash.uchicago.edu

Overview of FLASH2.x Source Tree (in current use)



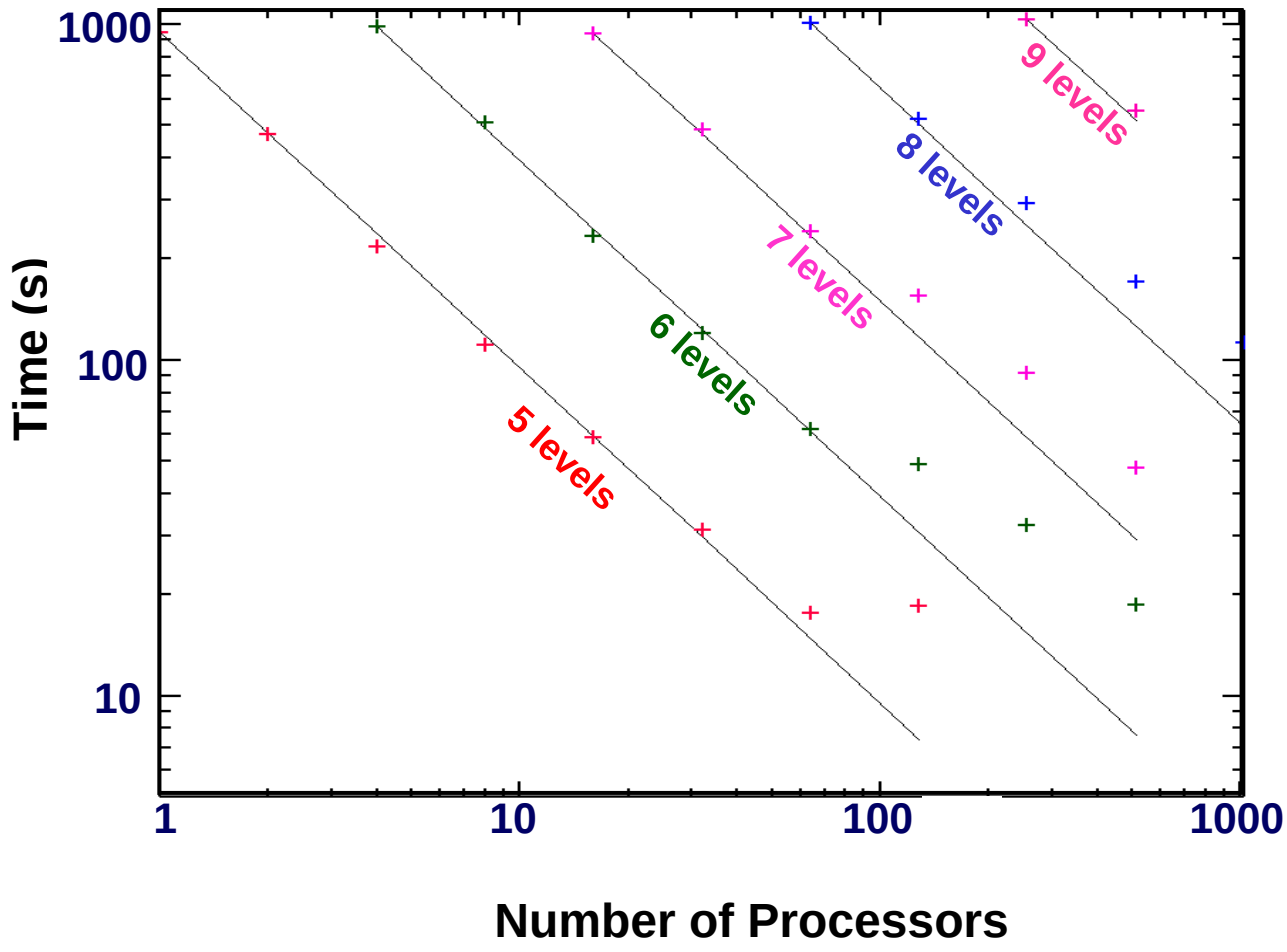
Flash hydro scales well and performs well, on “standard” MPP platforms

Constant work per processor

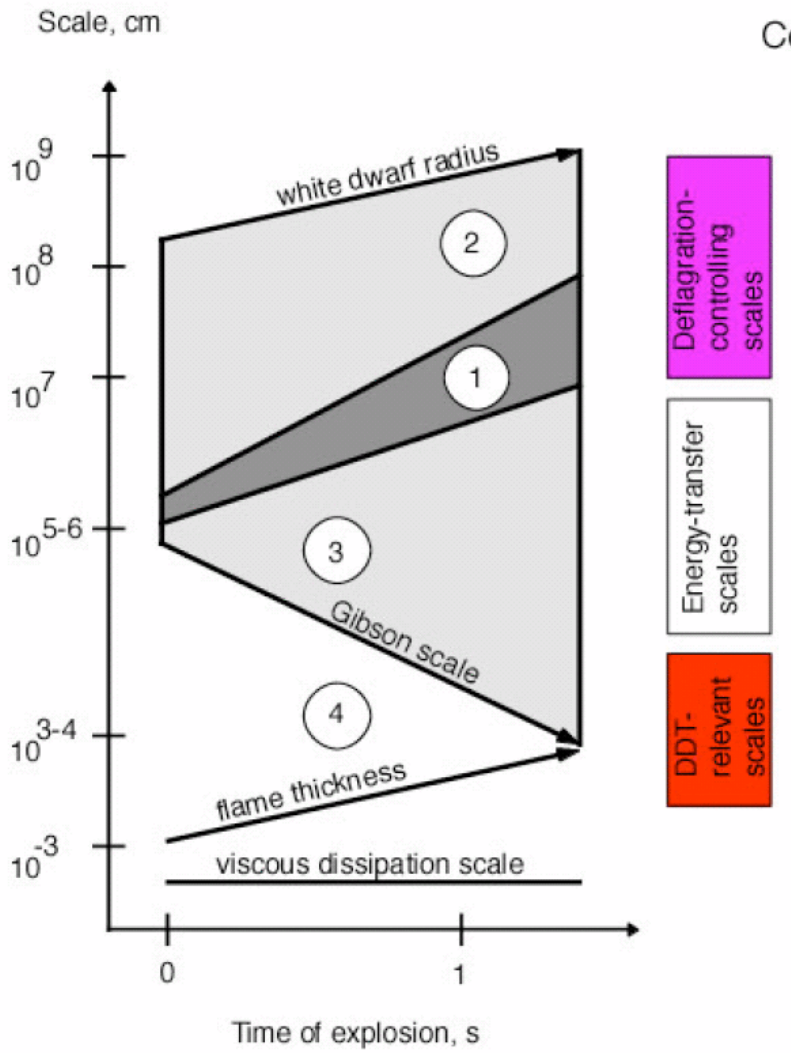


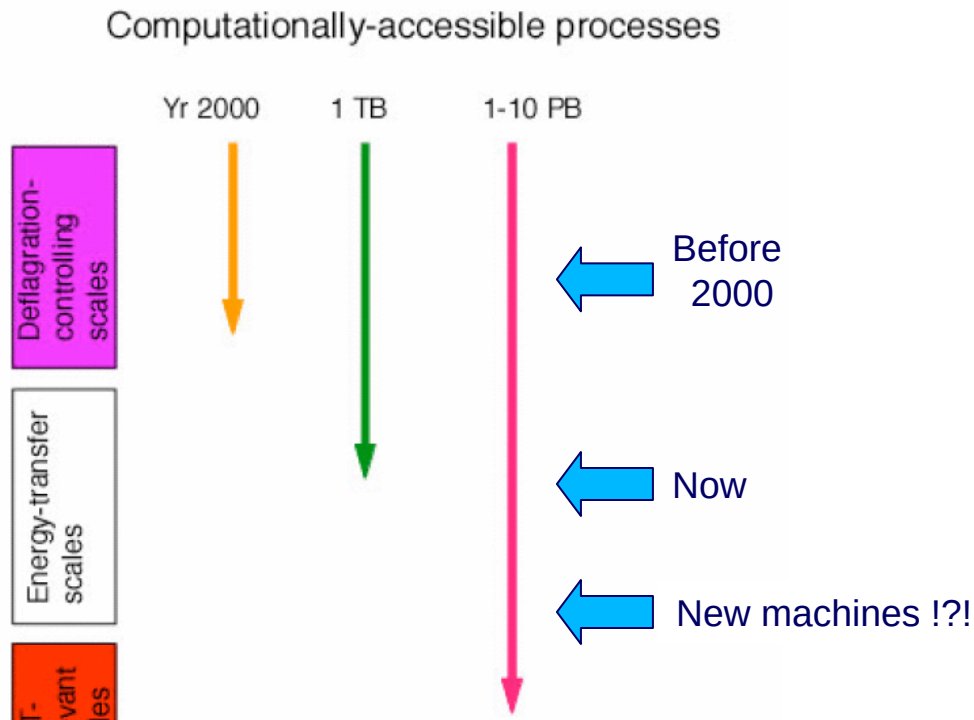
Scaling: Magnetic Rayleigh-Taylor

Blue Horizon



Where do we want to go?
Length scales in White Dwarf Deflagration





1. Turbulence is driven by Rayleigh-Taylor/flame instability
2. Turbulence is frozen by stellar 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 (i.e., remains smooth)

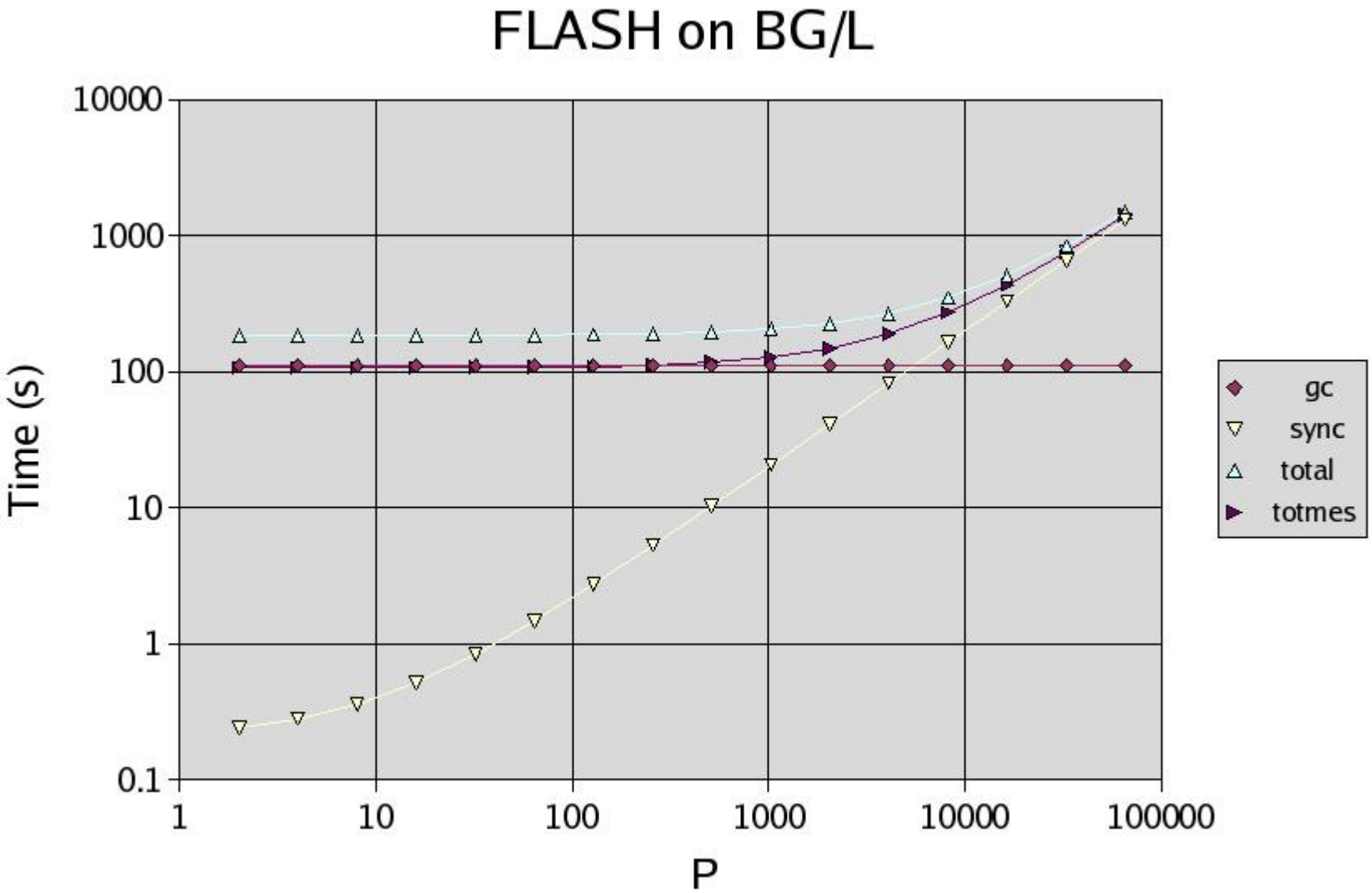
A glimpse of the future …

- Our major science challenges
  - Flame modeling (e.g., turbulent flame fronts)
  - Combining accurate solutions for very low and high Mach number mixing flows
- Our major code challenges
  - New machine architectures …
  - Memory …
  - Performance (multigrid, …)
  - Portability and maintainability …
  - Scalable visualization …

Looking to the future: Modeling FLASH

- Computational requirements obtained from
  - theoretical model
  - direct measurements on conventional systems
- Components of model:
  - Nearest Neighbor: ghost cell fills
    - Accurate statistical prediction of locality; Send/Recv
  - Global Communication: Redistribute blocks
    - Choose parameters
      - 10% refinement, every 10 timesteps; use to determine amount of communication
    - 2 Gathers, Send/Recv

(Crude) FLASH Performance Model Predictions



Early (crude …) FLASH results on BG/L

- FLASH ran unchanged on BG/L
  - No tuning as yet
  - No code re-writing (as yet!)
  - Got the right answer …

- Timing for weak scaling example (Sedov problem):

# P	total	evol	hydro	guard	flux	ref
32	212.342	211.072	149.215	30.423	10.155	8.652
64	212.397	211.105	149.239	30.432	10.138	8.663
128	212.393	211.107	149.271	30.412	10.140	8.649
256	212.470	211.147	149.259	30.417	10.138	8.659
512	212.436	211.103	149.262	30.328	10.165	8.684

- Early conclusions:
  - Network scales along with CPU count
  - A new level of performance predictability …

How did we get to this point?

- We knew what we ultimately wanted
  - Done Fully compressible reaction hydrodynamics (modest to high Mach #) [PPM, wENO, …]
  - Done Adaptive mesh [Paramesh], variety of geometries
  - Done Complex, varied EOS, variable composition
  - Done Diffusive heat transport (electrons, ions, [single group] photons; both explicit and implicit)
  - Done Self-gravity (multipole, multigrid)
  - Done Flame "subgrid" model
  - Done Single-fluid magnetohydrodynamics (mhd), nonrelativistic and relativistic [TVD]
  - Done Hall mhd, coupling to N-body code
  - x Small Mach number flows, rotation, …
- We started with something that already worked (solver: PPM, AMR: Paramesh)
  - Code group is protected from the onslaught of the physicists
  - We did not understand this at the beginning of our effort (!!)
- We built the code iteratively
  - Each new version has a desirable new feature
  - Each new version works, and is portable to all available platforms
    - Testing is automated; most features are tested nightly; results are posted on the web
  - We have a priori bounds on the allowed performance penalty of new features
  - We document everything as we go
- We evolved the right people

It was not easy … the science

- Stellar explosive nucleosynthesis is so complex that only computational solution is possible
  - Are numerically-derived solutions the correct solutions for “natural” systems?
  - Astrophysicists cannot do experiments!!
- Not all of the physics “ingredients” are well-understood
  - Combustion, fully nonlinear interface mixing, sub-grid modeling, …
- Making the world’s largest computers function effectively
  - Portability is a challenge: $\tau_{\text{machines}} << \tau_{\text{our software}}$
  - Systems software was/is unstable
    - $\tau_{\text{systems software}} << \tau_{\text{application software}}$
    - FLASH has become a systems software debugging tool …
  - Some CS is strongly oriented towards “demo” mode, and some CS couples strongly to the apps …
    - MPI works!
    - Algorithmic developments lag, e.g., we still need a fast multigrid solver for AMR on massively-parallel machines; portable parallel I/O is a work in progress; …

It was not easy … the sociology of academia

- Building a team turned out to be much harder than we expected
  - We had one very false start at the beginning …
    - Who is in charge?
  - Getting (astro)physicists, mathematicians, and computer scientists to work together effectively in an academic environment isn't trivial, given differences in
    - Language
    - Reward structure and working style
    - Intrinsic intellectual interests
- Working with NNSA is different from working with NASA, NSF, …
  - "Management" is an acquired skill …
- CS at UofC was not oriented to working with physical science "applications"
  - ANL was oriented towards working with apps
  - We "imported" ANL/CS to UofC …
- Code validation was an occasional diversion in astrophysics …
  - High energy density laboratory astrophysics is becoming a significant academic discipline!

What went right?

- We formed new scientific collaborations in areas where there were none before:
  - (astro)physics and CS: FLASH
  - (astro)physics and math: flame modeling
  - Astrophysics. CS, and experiments: validation
- Excellent rapport with DOE/NNSA program managers
  - Highly competent oversight and reviews
  - “tough love”
- We’ve made major progress, from CS to physics and astrophysics
  - FLASH is a useable, portable community code for a broad range of communities
  - We’ve made major breakthroughs in our understanding of novae and Type Ia supernovae

… and that leads us to

QUESTIONS AND DISCUSSION

QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.