Present and Future Requirements for m461:Stellar Explosions in Three Dimensions

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<u>1. m461: Stellar Explosions in Three</u> <u>Dimensions</u>

- Summarize your projects and expected scientific objectives through 2014
 - Modeling and simulations of transient phenomena in stellar astrophysics driven by either radiation or thermonuclear processes
 - Numerical solution of a coupled system of PDEs and ODEs
 - Tame nonlinearity!
- Our goal is to ...
 - Explain observed properties of exploding stellar objects
- Present focus is ...
 - Neutrino-driven core-collapse supernova explosions
- In the next 3 years we expect to ...
 - Link models to observations

Astronomy, Astrophysics, HEDP



Objects of Interest

- AGB stars
- O Classical Novae
- o X-ray Bursts
- Thermonuclear Supernovae (Type Ia)
- Core-collapse Supernovae (Type II & Ib/Ic)
- Hypernovae, collapsars, gamma-ray bursts

Astronomer's View



Astrophysicist's Natural Reaction





2. Current HPC Methods

(see slide notes)

- Algorithms used
 - Adaptive mesh discretization (4,096³ effective meshes)
 - Finite volume compressible hydrodynamics
 - Multigrid
 - Particle tracing (10⁶ particles)
- Codes
 - FLASH (MPI)
 - HOTB (OPenMP)
 - Nucnet (MPI or OpenMP)
- Quantities that affect the problem size or scale of the simulations (grid? particles? basis sets? Other?)
 - Grid
 - Time evolution

Modeler's View

A set of PDEs and ODEs

 $\partial_t \mathbf{U} + \nabla \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U})$ $\nabla^2 \Phi = 4\pi G \rho$

- PDEs of every possible type
- ODEs frequently stiff
- Complex equation of state (first closure relation)
- Multidimensional (4D...7D, more closure relations)
- Various discretization methods (finite volume solvers, multigrid, particles, subgrid, front tracking)
- o adaptive in space and time
- prone to produce demonstration runs
- o "unlimited" computing resources ("tree barking")

Transport

• A set of PDEs and ODEs

 $\partial_t \mathbf{U} + \nabla \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U})$ $\nabla^2 \Phi = 4\pi G\rho$

- PDEs of every possible type Ο
- **ODEs frequently stiff** Ο
- complex equation of state (first closure relation) Ο
- multidimensional (4D...7D, more closure relations) Ο
- various discretization methods (finite volume solvers, Ο multigrid, particles, subgrid, front tracking)
- adaptive in space and time
- prone to produce demonstration runs Ο
- "unlimited" computing resources ("tree barking")

Self-Gravity

• A set of PDEs and ODEs

 $\partial_t \mathbf{U} + \nabla \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U})$

 $\nabla^2 \Phi = 4\pi G\rho$

- PDEs of every possible type
- ODEs frequently stiff
- o complex equation of state (first closure relation)
- multidimensional (4D...7D, more closure relations)
- various discretization methods (finite volume solvers, multigrid, particles, subgrid, front tracking)
- o adaptive in space and time
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Nuclear Physics

• A set of PDEs and ODEs

 $\partial_t \mathbf{U} + \nabla \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U})$ $\nabla^2 \Phi = 4\pi G\rho$

- PDEs of every possible type
- ODEs frequently stiff
- **complex equation of state** (first closure relation)
- multidimensional (4D...7D, more closure relations)
- various discretization methods (finite volume solvers, multigrid, particles, subgrid, front tracking)
- o adaptive in space and time
- prone to produce demonstration runs
- o "unlimited" computing resources ("tree barking")

2. Current HPC Requirements

(see slide notes)

- Architectures currently used
 - Distributed memory (FLASH) or SMP (HOTB) CPU clusters
- Compute/memory load
 - 1,000 cores
 - 1 GB per core
 - 50,000 CPU hours per run (model)
 - 10⁶ CPU hours per year
 - 10-20 models
- Data read/written
 - 0.5/5 TB per model
 - 20 GB checkpoints
 - 0.5 TB per model moved out of NERSC, little moved in
- Necessary software, services or infrastructure
 - F90, C++, MPI, OpenMP, Python, VisIt, svn/git
- Known limitations/obstacles/bottlenecks
 - load imbalance
 - memory bandwidth
 - non-scalable data structures
- Hours requested/allocated/used in 2010
 - 1.0/2.5/2.0 million
- Additional info from the templates

Example #1: Binary WD Merger (DD)



Work done in collaboration with A. Gawryszczak (Copernicus Center, Warsaw). Computing cycles: DOE NERSC.

FLASH/WDM Parallel Performance



Example #2: Core-Collapse SN Explosions



Core-Collapse Shock Revival

- Massive stars
- Gravity bombs with energy extracted by neutrinos
- Accretion shock originally too weak
- Revived by neutrino heating of the post-shock matter, a.k.a. Standing Accretion Shock Instability



SASI in 3D



Spring 2010: Nordhaus & Burrows

- 3-D aids explosions compared to 2-D
- This is in essence an extension of what has been found by Janka & Mueller re 1-D to 2-D





Fall 2010: Janka & MPA group

○ Janka et al. fail to confirm Nordhaus & Burrows result



- This does not increase our confidence in numerical modeling!
- Increasing numerical resolution will NOT resolve the above discrepancy

The Challenge Continues

○ Theory incomplete ☺

○ Simulations unsuccessful ⊗

○ Experiments limited ⊗

Example #3: Postexplosion Mixing



Non-SN NP Examples



Thermonuclear runaways, but now in thin layers of material accreted by a degenerate star from a nondegenerate companion star (yes, most stars are binaries!)

- Degenerate star is a neutron star: X-ray burst
 - o strong gravity
 - o strongly degenerate matter
 - o ignition/propagation unknown
- Degenerate star is a white dwarf: Classical Nova
 - o weaker gravity
 - o moderately degenerate
 - o source of mixing (dredge up) unknown

NP Example: Classical Nova Runaway



Kercek et al. (1999)



NP Challenge: Hot CNO cycle



Next 5 Years

1. Hot CNO cycle in classical novae

- o T~300x10⁶K (or ~27 keV)
- o rho ~150 g/cc
- o 30% uncertainty for some of the reaction rates



2. ¹²C+¹²C ignition in binary WD (DD SN Ia)

- o T~2x10⁹K (~180 keV)
- \circ rho ~1x10⁶ g/cc
- o admixture of ⁴He

3. Parametrized core-collapse SN explosions

- o energetics
- o mixing and asymmetries
- o observable imprints of the SN engine

Next 10 Years

1. Paths to explosions

- o coupled physics (turbulence, mixing, diffusion)
- o long-term evolution
- o subgrid scale models

2. Paths in explosions

- o coupled physics (radiation-matter interactions)
- o nucleosynthesis in the neutrino-mediated plasmas
- o radiation sources
- Connecting scales (DNS -> LES)

3. Paths past explosions

- o long-term evolution
- o non-LTE physics
- o from discovery to predictions
- o sensitivities? adjoints?



Steinheimer et al. (2010)

3. HPC Usage and Methods for the Next 3-5 Years

(see slide notes)

- Upcoming changes to codes/methods/approaches to satisfy science goals
 - Approximate neutrino transport
 - Scalable nonlinear multigrid
- Changes to Compute/memory load
 - Compute x20
 - Memory x10
- Changes to Data read/written
 - Data x10
- Changes to necessary software, services or infrastructure
 - GPGPU tools?
- Anticipated limitations/obstacles/bottlenecks on 10K-1000K PE system.
 - Load imbalance (both due to discretization and physics)
 - Data locality
 - Scalability of global data structures
- Key point is to directly link upcoming NERSC requirements to science goals

Strategy for New Architectures

- How are you dealing with, or planning to deal with, many-core systems that have dozens or hundreds of computational cores per node?
 - MPI (OpenMP proved inefficient/less general)
- How are you dealing with, or planning to deal with, systems that have a traditional processor augmented by some sort of accelerator such as a GPU or FPGA or similar?
 - Planned
 - Preprocessor directives
 - Kernel extraction and analysis
 - Consider SC (CASTRO) or NSF (Athena) codes



Sutter (2009)

4. Summary

- What new science results might be afforded by improvements in NERSC computing hardware, software and services?
 - Physics-enhanced models (i.e. MHD)
 - Physics-coupling studies (in time, in space)
 - Model sensitivities
- Recommendations on NERSC architecture, system configuration and the associated service requirements needed for your science
 - Continue providing access to large memory per core systems
 - Actively support transition to limited memory per core architectures
 - Increase shared data space (NGFS, /project)
 - Provide users with control over scratch purging process
- NERSC generally acquires systems with roughly 10X performance every three years. What significant scientific progress could you achieve over the next 3 years with access to 50X NERSC resources?
 - Systematic studies of supernova explosion dependence on the progenitor structure
 - => Progenitor structure studies!
 - Model databases for sensitivity studies
- What "expanded HPC resources" are important for your project?
 - Data storage (both runtime and archival)
 - Data analysis and visualization
 - Remote connectivity (both for raw data transfers and interactive/X applications)
- General discussion