TeraScale Supernova Initiative

http://www.phy.ornl.gov/tsi/

Explosions of Massive Stars

12 Institution, 17 Investigator, 42 Person, Interdisciplinary Effort

⇒ ascertain the core collapse supernova mechanism(s)
⇒ understand supernova phenomenology
  ● element synthesis, neutrino and gravitational wave signatures, ...

Relevance:
⇒ Element Production
⇒ Cosmic Laboratories
⇒ Driving Application

[21 people from 24 institutions!]
Ties to DoE Facilities

- **RIA**
  better understanding nuclear physics of the r-process a primary justification for the construction of this facility

- **National Underground Science Laboratory**
  would be the site of a next generation supernova neutrino detection capability (1/2 Mton!; extra-Galactic!)

- **SNO**
  will play a pivotal role in future supernova neutrino detection and analysis

- **RHIC**
  understanding properties of high density nuclear matter critical to our understanding of stellar core bounce dynamics

... SNS ...
What will it take?
- Tera/Peta-Scale 3D, General Relativistic, Radiation Magnetohydrodynamics
- State of the Art Nuclear and Weak Interaction Physics

“Infrastructure” Needs: Transport
- Tera- and Peta-Scale Sparse Linear Systems of Equations

“Infrastructure” Needs: Hydrodynamics
- 1Gb/Write, 1-10 Tb/Variable/Simulation!
  - Manage?
  - Analyze?
  - Render?

“Infrastructure” Needs: Weak Interactions
- TeraScale Nuclear “Structure” Computation
Core Collapse Paradigm

Presupernova Structure
representative of a $15 M_\odot$ star

Core Collapse and Explosion

1.  
2.  
   
   neutrinos

   shock

3.  
6.  
7.  

Need Boltzmann Solution
Need Angular Distribution
Need Spectrum
“Gray” Schemes Inadequate
Spectrum Imposed
Limited Angular Information (Few Moments)
Parameterized (No First Principle Solution)
The bar is high! (10% effects can make or break explosions.)
Equations We Solve

**Dominant Computation:**
Nonlinear, integro-partial differential equations for the radiation distribution functions.

**Spherical Symmetry**
\[ f(r, \mu, E) \]

**Axisymmetry**
\[ f(r, \theta, \mu_1, \mu_2, E) \]

**No Symmetry**
\[ f(x, y, z, \mu_1, \mu_2, E) \]

**Example: Boltzmann transport equation for spherical symmetry.**

\[
\frac{1}{c} \frac{\partial F}{\partial t} + 4 \pi \mu_0 \frac{\partial (r \rho_0 F)}{\partial r} \\
+ \frac{1}{r} \frac{\partial ((1 - \mu_0^2)F)}{\partial \mu_0} \\
+ \frac{1}{c^2} [\frac{\partial \rho_0}{\partial t} + 3\mu \frac{\partial (\mu_0(1 - \mu_0^2)F)}{\partial \mu_0}] \\
+ \frac{1}{c^2} \mu_0^2 [\frac{\partial \rho_0}{\partial t} + 3\mu \frac{\partial (\mu_0(1 - \mu_0^2)F)}{\partial \mu_0}] \\
= \frac{j}{\rho_0} - \chi F \\
+ \frac{1}{c^2 \hbar^2} \frac{E_0^2}{d\mu_0} \int d\mu_0' R_{TS}(\mu_0, \mu_0', E_0, E_0) F(\mu_0', E_0) \\
- \frac{1}{c^2 \hbar^2} \frac{E_0^2}{d\mu_0} F(\mu_0, E_0) \int d\mu_0' R_{TS}(\mu_0, \mu_0', E_0, E_0) F(\mu_0', E_0) \\
+ \frac{1}{\hbar^2 c^2} (\frac{1}{\rho_0} - F(\mu_0, E_0)) \int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NS}(\mu_0, \mu_0', E_0', E_0) F(\mu_0', E_0') \\
- \frac{1}{\hbar^2 c^2} F(\mu_0, E_0) \int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NS}(\mu_0, \mu_0', E_0', E_0) (\frac{1}{\rho_0} - F(\mu_0, E_0))
\]

Scattering kernels input to Boltzmann equation. Memory bandwidth issues.

No Explosions! No Explosions!

New Microphysics? New Microphysics?

High-Density Stellar Core Thermodynamics Neutrino-Matter Interactions

New Macrophysics? (2D/3D Models) Fluid Instabilities, Rotation, Magnetic Fields

TSI will explore both!

⇒ No 2D/3D supernova models with realistic neutrino transport exist!
Supernova Simulation Timeline

- Year 1: Spherically Symmetric Models (3D)
- Year 2: Axisymmetric Models (5D)
- Year 3: No Imposed Symmetry (6D)
⇒ Size of inner core “piston” depends on total electron capture during collapse. Sets location of shock formation and initial shock energy.

⇒ Nuclear electron capture rates depend on “structure” of nuclei in stellar core.

- Solve very large eigenvalue problems.

One of the most beautiful aspects of this problem!
Carried out 1D collapse models with:
- Boltzmann neutrino transport.
- Ensemble of nuclei.
- State of the art electron capture rates.

For the first time, explored the ramifications of detailed electron capture rate computation on the dynamics of stellar core collapse.

Merger of nuclear physics and astrophysics at their respective frontiers.
Shock formation radii differ.
Preshock profiles differ.
Shock stall radii similar.
Postshock entropy, lepton profiles differ.
Will affect PNS instabilities.

Initially weaker shock, formed deeper, propagates out to same mass!
In its wake, leaves different core entropy, lepton gradients.
TeraScale Supernova Initiative
Scientific Discovery: Supernova Shock Wave Instability
(Blondin, Mezzacappa, and DeMarino (2002), The Astrophysical Journal, in press.)

The supernova shock wave may become unstable!

The instability may aid explosion and define the explosion's "shape." A prolate shape may explain the polarization of supernova light.

Instability-induced explosions ...
... are bipolar and shape preserving, ...
...
and oscillatory.

The instability results from a feedback loop:
Vorticity is introduced by the distorted shock, ...
... and pressure waves generated by this vorticity further distort the shock.
QuickTime™ and a
Compact Video decompressor
are needed to see this picture.
QuickTime™ and a Video decompressor are needed to see this picture.
“r-process” (rapid neutron capture)

Produces half the elements heavier than iron.
Believed to occur in neutrino-driven wind after explosion.
Believed to require neutron-rich conditions.
⇒ Difficult to produce.

An r-process can occur in proton-rich environments!
⇒ If nuclear reactions out of equilibrium.
Neutrino capture/scattering cross section measurements will help gauge theory for
- electron capture in stellar core collapse,
- r-process nucleosynthesis,
- and Terrestrial neutrino detection (Super-K, SNO, OMNIS).

3.2 \times 10^{15} \ \nu \ s / \ s

60 \ Hz \ Pulses

Supernova neutrino RMS energies between 10 and 25 MeV!
TSI will carry out multi-D stellar collapse simulations (Newtonian).
Gravitational wave signatures can be post-processed (in most cases).
Collaborate with PSU NSF PFC to include general relativity (Einstein equations) in TSI’s models.
**Implicit Time Differencing**

**Extremely Short Neutrino-Matter Coupling Time Scales**

**Neutrino-Matter Equilibration**

**Neutrino Transport Time Scales**

**Nonlinear Algebraic Equations**

**Linearize**

**Solve via Multi-D Newton-Raphson Method**

⇒ Large Sparse Linear Systems

**Transport Linear Systems (TOPS)**

\[
\frac{1}{c} \frac{\partial F}{\partial t} + 4\pi \mu_0 \frac{\partial (\rho^2 \mu_0 F)}{\partial \mu_0} \\
+ \frac{1}{\tau} \frac{\partial [1 - \mu_0^2 F]}{\partial \mu_0} \\
+ \frac{1}{\tau} \frac{\partial n\rho_0}{\partial t} + 3\nu \frac{\partial \mu_0 (1 - \mu_0^2 F)}{\partial \mu_0} \\
+ \frac{1}{\tau} \frac{\rho_0^2}{c} \frac{\partial n\rho_0}{\partial t} + \frac{3\nu}{\tau} \frac{\partial (E_0^3 F)}{\partial E_0}
\]

\[
= \frac{j}{\rho_0} - \chi F
\]

\[
+ \frac{1}{c\hbar^2 \epsilon^3} E_0^2 \int d\mu'_0 R_{TS}(\mu_0, \mu'_0, E_0) F(\mu'_0, E_0)
\]

\[
- \frac{1}{c\hbar^2 \epsilon^3} E_0^2 \int d\mu'_0 R_{TS}(\mu_0, \mu'_0, E_0)
\]

\[
+ \frac{1}{\hbar^2 \epsilon^3} \left(\frac{1}{\rho_0} - F(\mu_0, E_0)\right) \int dE_0 E_0^2 d\mu'_0 R^{\text{ret}}_{N,E,S}(\mu_0, \mu'_0, E_0, E_0) F(\mu'_0, E_0)
\]

\[
- \frac{1}{\hbar^2 \epsilon^3} F(\mu_0, E_0) \int dE_0 E_0^2 d\mu'_0 R^{\text{ret}}_{N,E,S}(\mu_0, \mu'_0, E_0, E_0)\left(\frac{1}{\rho_0} - F(\mu'_0, E_0)\right)
\]

**Progress:**

Sparse Approximate Inverses for 2D MGFLD (Saylor, Smolarski, Swesty; J. Comp. Phys.)

ADI-Like Preconditioner for Boltzmann Transport (D’Azevedo et al.; Precond 2001; SIAM)
Transport Developments (TSTT)

Alternative Transport Techniques

⇒ Discrete Ordinates (Currently Used)
⇒ Discontinuous Galerkin (Under Development)

Results from model “Milne” problem:

10X Faster, 10X Less Memory
de Almeida (2003)
Adaptive Quadratures (Direction Cosines) for Multidimensional Radiation Transport

- Greatest challenge to completing 3D Boltzmann simulations is memory.
- Minimize number of quadratures to minimize memory needs while maintaining physical resolution. (Also important for 1D/2D MGBT.)
- Distribute according to “generalized pathlength.”

Results for 1D Boltzmann Transport on “Milne” Problem (D’Azevedo):

- Extended Core
- Compact Core
Supernova Data

3D Hydrodynamics Run
- 5 Variables (Density, Entropy, Three Fluid Velocities)
- 1024 X 1024 X 1024 Cartesian Grid
- 1000 Time Steps

20 Terabyte Dataset

“The flea on the tail on the dog…”

Multidimensional Neutrino Data

\[ f(x, y, z, \mu_1, \mu_2, E) \]
\[ E_v(x, y, z, E) \]
\[ F_v(x, y, z, E) \]
\[ F_v'(x, y, z, E) \]
\[ E_v(x, y, z, E) \]

Composition
Query the composition of a fluid element.

Much of what we know about supernovae comes from light emitted from ejected atoms.
Driving developments in...

**Samatova et al. (2002)**

**Parvin et al. (2002)**

**Data Reduction**
- Order of magnitude reduction using PCA techniques.

**Data Analysis**
- Raw Data
- Dimensional Compression
  - PCA, ...

**Feature Extraction**
- Vortices, ...
- Feature-based visualization.

**Integration of Data Analysis and Visualization (ASPECT)**

**Agent Technology**

**Potok et al. (2002)**

- Raised many issues.

**Extensive efforts by SDM and LBL ...**
...and visualization (local, remote, collaborative)...

“Off-the-Shelf” Technologies
  ➔ EnSight
  ➔ TSB
  ➔ ParaView

Custom Visualization (VTK)
  ➔ Custom Representations
  ➔ Custom Functionality

Integrating visualization with
  ➔ data analysis (SDM collaboration),
  ➔ networking (collaboration with UTK/ORNL groups).
Working with Logistical Networking (UTK) and ORNL networking groups to significantly improve our data transfer rates between TSI “nodes” for local, remote, and collaborative visualization.

End-user tools create files from blocks (redundant) stored on depots.

Multiple streams combine to give high throughput.

Use LoRS as file service for HRM?

Move data between depots with full available bandwidth.
Assess Code Performance on Parallel Platforms
Identify Code Optimizations to Increase Performance

TSI Code Suite
- **Hydrodynamics:**
  - VH-1 (PPM)
  - ZEPHYR (Finite Difference)
- **Neutrino Transport:**
  - AGILE-BOLTZTRAN: 1D General Relativistic Adaptive Mesh Hydrodynamics with 1D Boltzmann Transport
  - V2D: 2D MGFLD Transport Code
  - V3D: 3D MGFLD Transport Code (Under Development)
  - 2D/3D Boltzmann Code (Under Development)

Instrument Codes with Performance Tools: SvPablo, Tau

Instrumentation helped improve tools!
**TSI Code Suite**

- **Hydrodynamics:**
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  - V2D: 2D MGFLD Transport Code
  - V3D: 3D MGFLD Transport Code (Under Development)
  - 2D/3D MGVET Code (Under Development)
  - 2D/3D Boltzmann Code (Under Development)

### Verification and Validation

- **Verification (Two Approaches, Same Equations)**
  - Comparing 2 discretizations of 1D MGBT.
  - *(Liebendoerfer, Rampp, Janka, and Mezzacappa (2003))*
  - Multifrequency crooked pipe.
  - ...

- **Validation (3 Approaches)**
  - Comparing 1D MGFLD and 1D MGBT.
  - *(Liebendoerfer et al. (2002))*
Selected as a testbed application for the ORNL Cray X1 evaluation.

Participated in U.S.-Japan Computational Science Roundtable (Strayer, Mezzacappa).

- Submitted a proposal for U.S.-Japan collaboration on supernova dynamics on the Earth Simulator.

Percentage of Peak
(Single: Single Processor)

<table>
<thead>
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<th></th>
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<th>Cheetah</th>
<th>Seaborg</th>
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<tr>
<td>AB NES</td>
<td>24% (Single)</td>
<td>12% (Single)</td>
<td>46% (Single)</td>
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<td>AB</td>
<td>9% (Single)</td>
<td>5% (Single)</td>
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<tr>
<td>V2D</td>
<td>18% (1024)</td>
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<tr>
<td>GENASIS</td>
<td>30% (Single)</td>
<td>15% (Single)</td>
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**AB NES**: Scattering kernel (R) module from AGILE-BOLTZTRAN (AB) code.

**AB**: 1D, multiangle, multifrequency, Boltzmann code.

**V2D**: 2D, multifrequency, flux-limited diffusion code.

**GENASIS**: 2D, multiangle, multifrequency, Boltzmann code.

- Radiation solve only, no scattering kernels.

**2 Biggest Pieces:**
- Computing kernels.
- Solving Boltzmann equation.
We (community) have exploding models, but no realistic exploding models.

No realistic 2D/3D models.

**Fundamental Ingredients in a Supernova Model**
- Neutrinos - Must have multifrequency, accurate neutrino transport.
- Fluid Instabilities - Must include neutrino transport. Depends on microphysics! SAS Instability!
- Rotation
- Magnetic Fields
- General Relativity

**Precision** (microphysics and macrophysics) modeling is a must. Anything else is exploratory.

Even if explosions are obtained in a model with a subset of the above ingredients, modeling efforts must push forward until all are included. Any one of these can qualitatively alter the outcome and conclusions.

**Staged Approach**
- **Layer the Microphysics**
- **Layer the Macrophysics**
- **Layer the Dimensionality**
  - Understand and “control” the nonlinearities and their interactions.
  - Only way to ascertain the explosion mechanism and understand supernova phenomenology with any confidence.

We (TSI) expect significant progress this year:
- Beginning to merge states of the art in microphysics and macrophysics.
- First 2D models with 2D, multifrequency neutrino transport.
In its first year of operation:

- TSI has achieved scientific discovery!
- Interdisciplinary collaboration has enabled this discovery!
- Progress has been made in many science enabling areas.
- Effort has grown to involve 121 researchers and 24 institutions!

The SciDAC model is working!

At 18% of peak on 1024 processors,
- 1/2 year wallclock per 1/2 supernova second for 2D, multifrequency flux-limited diffusion.
- What about 2D Boltzmann transport?
- What about 3D?

Would like a factor of at least 5 improvement in throughput.
- New algorithms.
- New architecture (X1)?

We need to invest now.
- Invest in algorithm, code, infrastructure, and scientific development now
  for science we want in 5-10 years.
- Next generation mission data will require interpretation.
- New experimental facilities will require motivation and guidance.
- Machines will reach PetaFlop speeds by 2009-2010.