TeraScale Supernova Initiative

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

Scientific Discovery through Advanced Computing

Office of Science
U.S. Department of Energy

March 24, 2000

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:

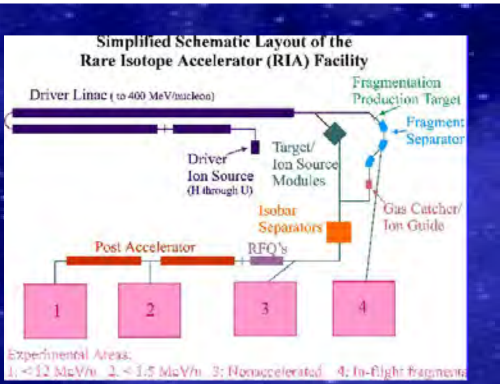
- ⇨Element Production
- ⇨Cosmic Laboratories
- ⇨Driving Application

121 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

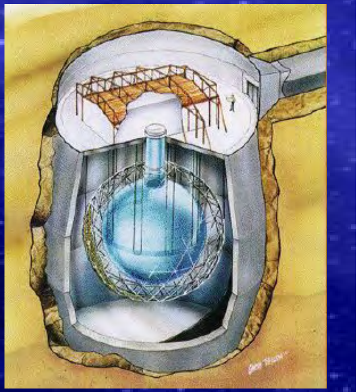


- National Underground Science Laboratory

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

- SNO

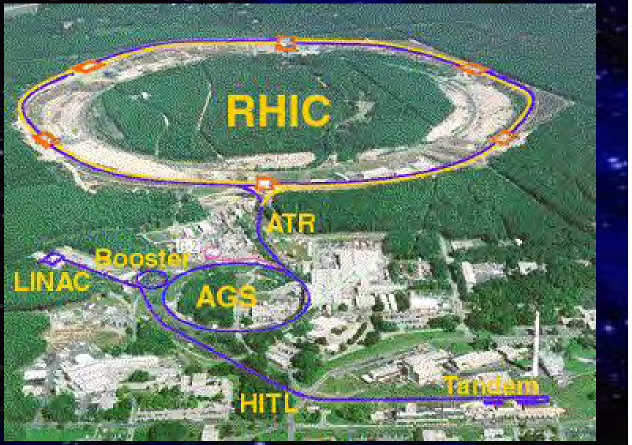
  will play a pivotal role in future supernova neutrino detection and analysis



- RHIC

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

… SNS …



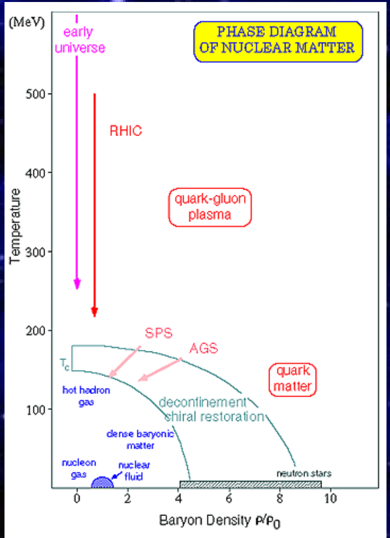


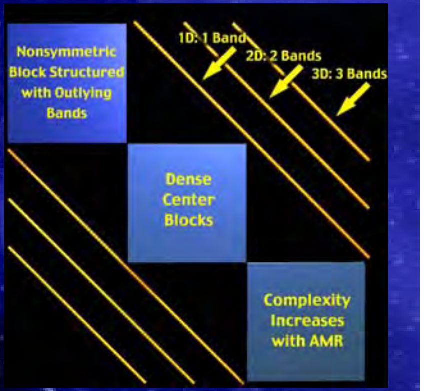
Figure III.1: Phase diagram of nuclear matter.

What will it take?

- Tera/Peta-Scale 3D, General Relativistic, Radiation Magnetohydrodynamics
- State of the Art Nuclear and Weak Interaction Physics

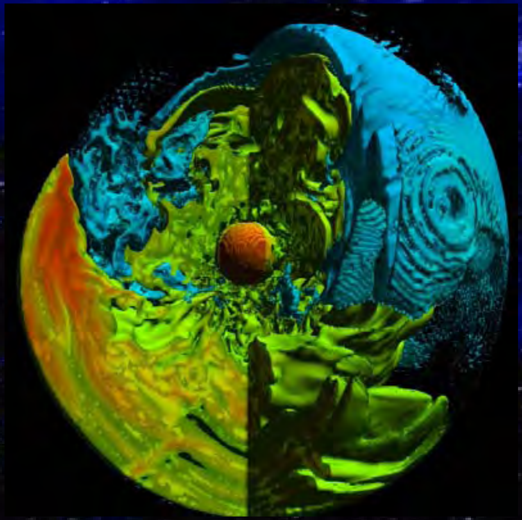
"Infrastructure" Needs: Transport

- Tera- and Peta-Scale Sparse Linear Systems of Equations



"Infrastructure" Needs: Hydrodynamics

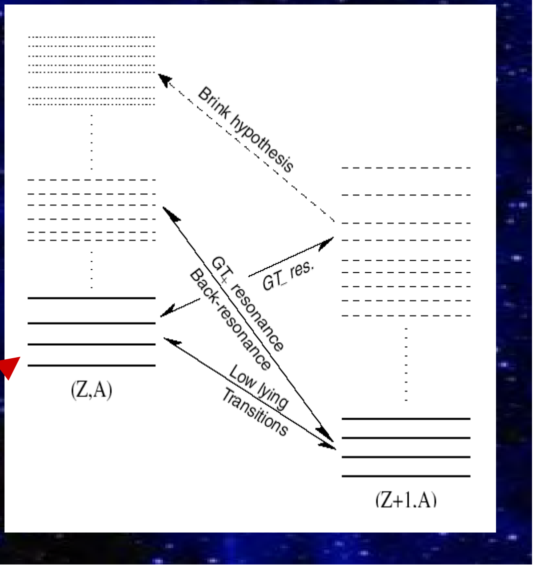
- 1Gb/Write, 1-10 Tb/Variable/Simulation!
    - ➲ Manage?
    - ➲ Analyze?
    - ➲ Render?



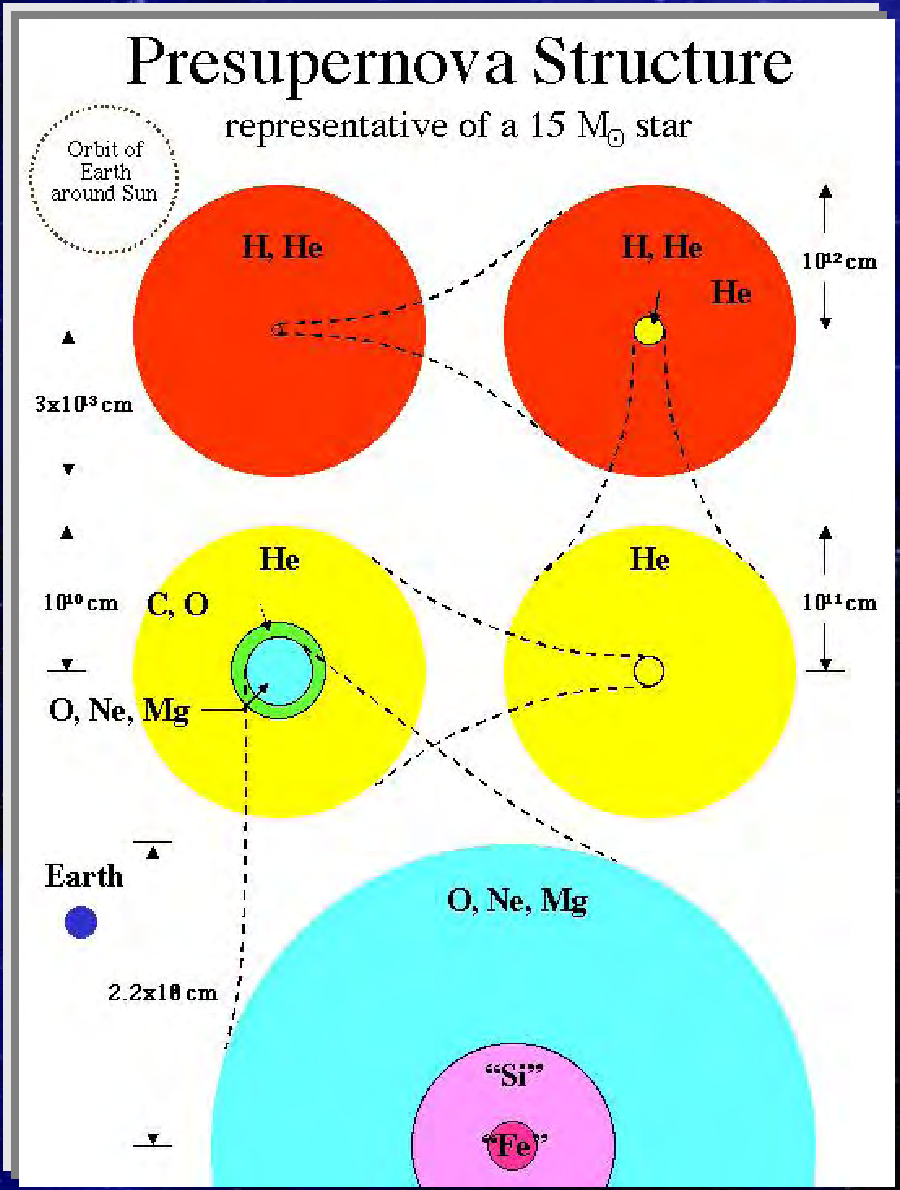
"Infrastructure" Needs: Weak Interactions

- TeraScale Nuclear "Structure" Computation

Nuclear Levels

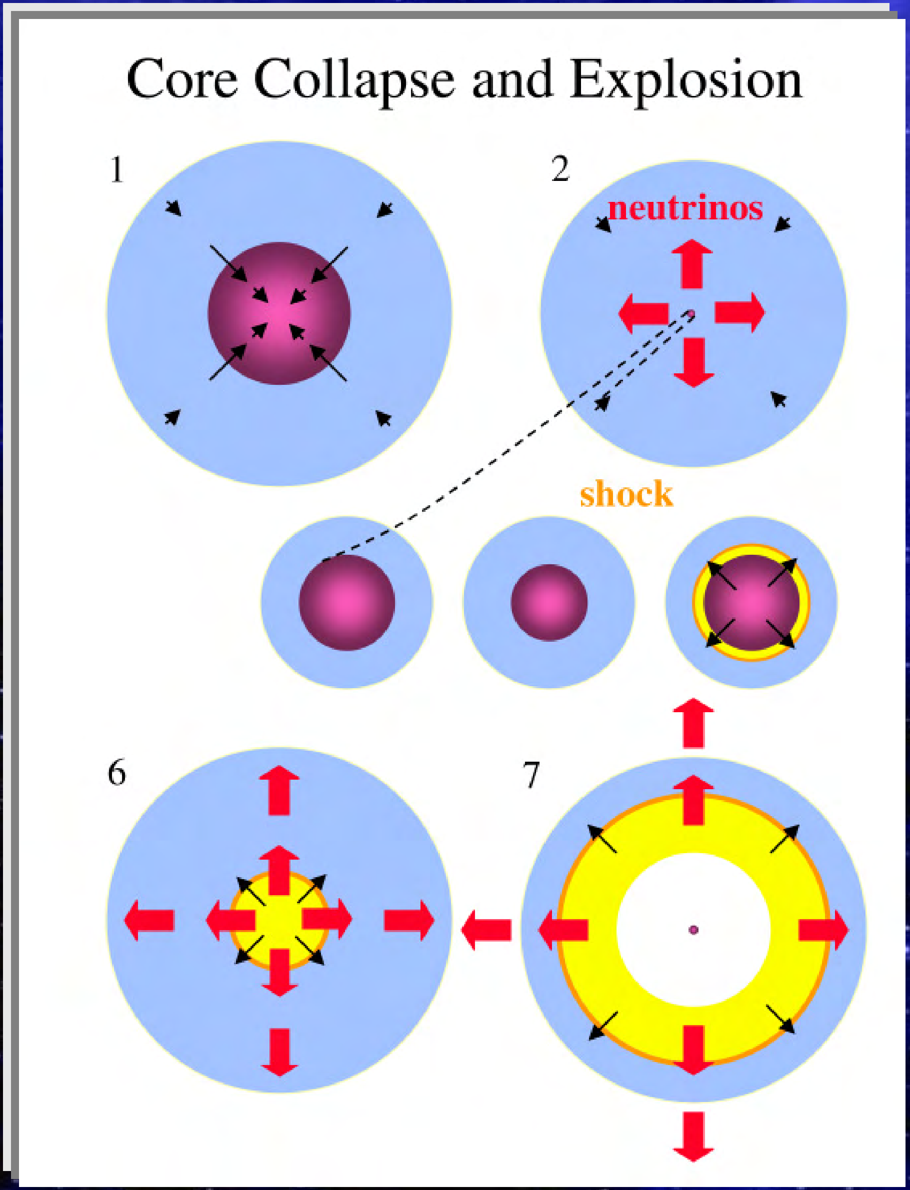


Core Collapse Paradigm



Presupernova Structure

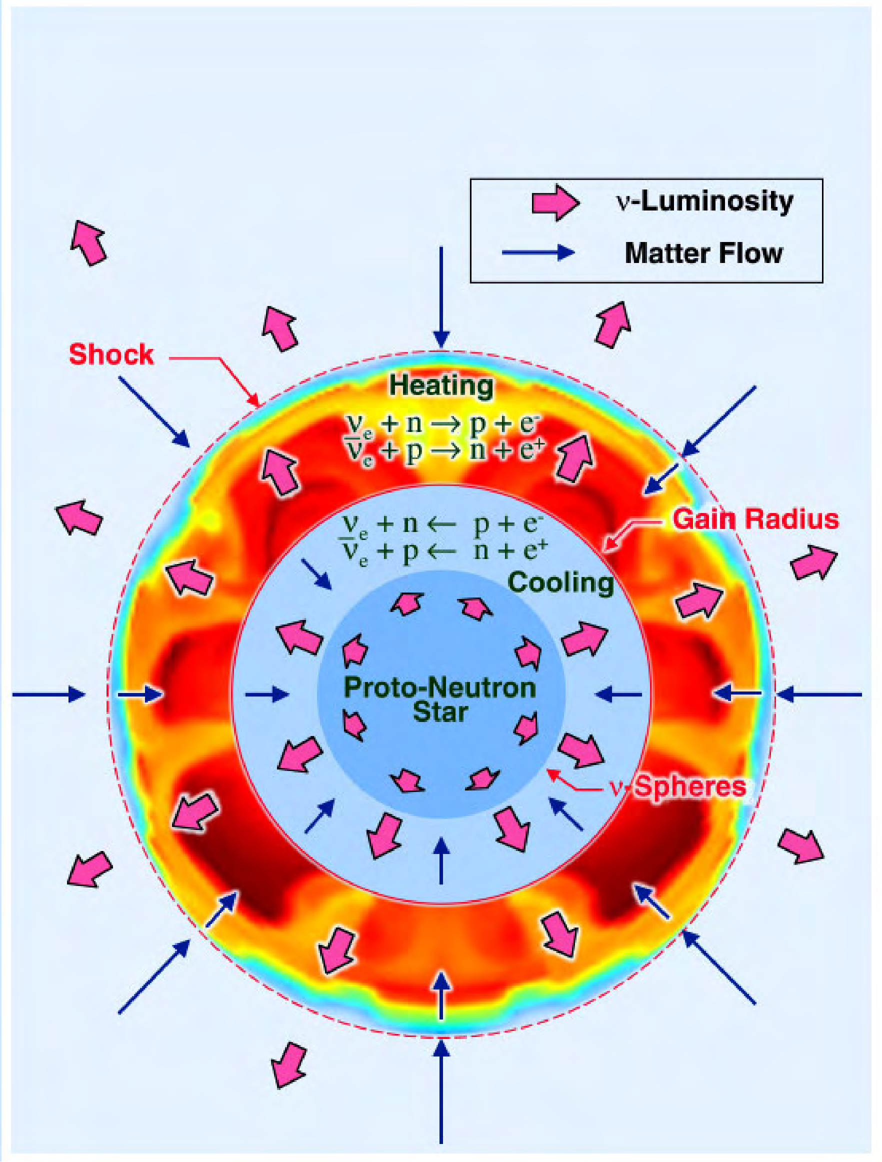
representative of a 15 $M_\odot$ star

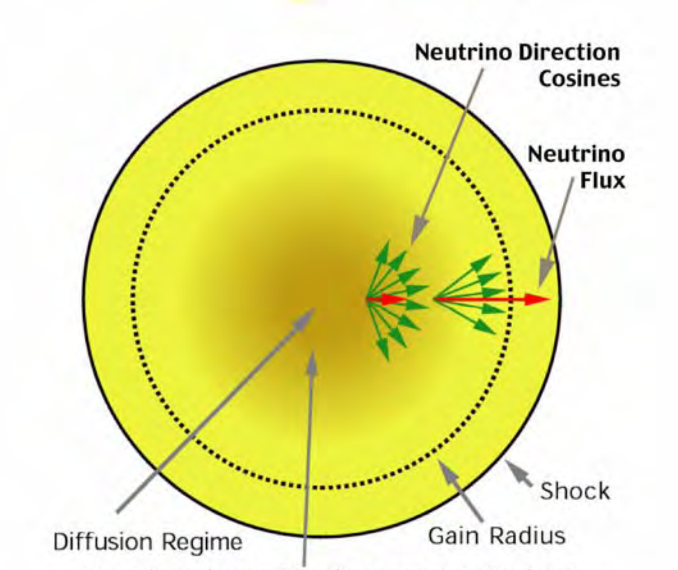


Core Collapse and Explosion

Anatomy of a Supernova

Convection





$$\dot{\epsilon} = \frac{X_n}{\lambda_0^a}\frac{L_{\nu_c}}{4\pi r^2}\langle E_{\nu_c}^2\rangle\langle\frac{1}{\mathcal{F}}\rangle + \frac{X_p}{\bar{\lambda}_0^a}\frac{L_{\bar{\nu}_c}}{4\pi r^2}\langle E_{\bar{\nu}_c}^2\rangle\langle\frac{1}{\bar{\mathcal{F}}}\rangle$$

- ➲ *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	$f(r,\mu,E)$	$R(r,\mu,E,\mu',E')$
Axisymmetry	$f(r,\theta,\mu_1,\mu_2,E)$	$R(r,\theta,\mu_1,\mu_2,E,\mu_1',\mu_2',E')$
No Symmetry	$f(x,y,z,\mu_1,\mu_2,E)$	$R(x,y,z,\mu_1,\mu_2,E,\mu_1',\mu_2',E')$

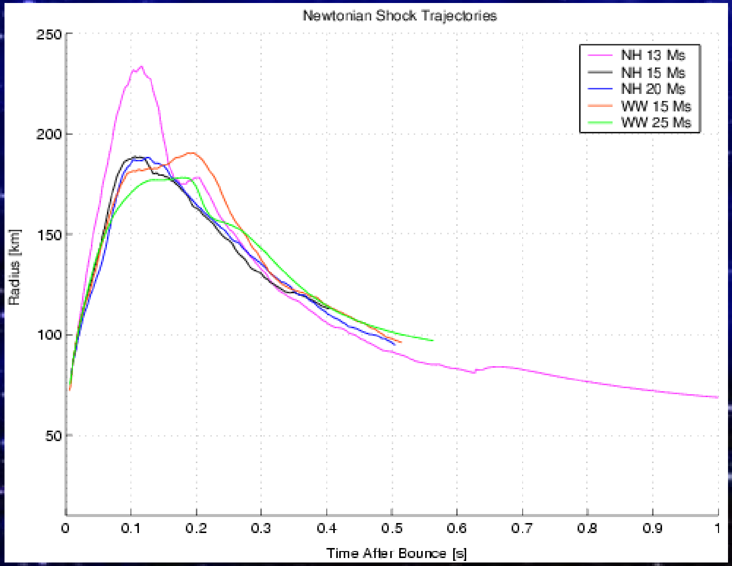
Example: Boltzmann transport equation for spherical symmetry.

$$
\begin{aligned}
\frac{1}{c}\frac{\partial F}{\partial t} &+ 4\pi\mu_0\frac{\partial(r^2\rho_0 F)}{\partial m} \\
&+ \frac{1}{r}\frac{\partial[(1-\mu_0^2)F]}{\partial\mu_0} \\
&+ \frac{1}{c}\left(\frac{\partial ln\rho_0}{\partial t}+\frac{3v}{r}\right)\frac{\partial[\mu_0(1-\mu_0^2)F]}{\partial\mu_0} \\
&+ \frac{1}{c}\left[\mu_0^2\left(\frac{\partial ln\rho_0}{\partial t}+\frac{3v}{r}\right)-\frac{v}{r}\right]\frac{1}{E_0^2}\frac{\partial(E_0^3F)}{\partial E_0} \\
&= \frac{j}{\rho_0}-\tilde{\chi}F \\
&+ \frac{1}{c}\frac{1}{h^3c^3}E_0^2\int d\mu_0' R_{IS}(\mu_0,\mu_0',E_0)F(\mu_0',E_0) \\
&- \frac{1}{c}\frac{1}{h^3c^3}E_0^2F\int d\mu_0' R_{IS}(\mu_0,\mu_0',E_0) \\
&+ \frac{1}{h^3c^4}\left(\frac{1}{\rho_0}-F(\mu_0,E_0)\right)\int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NES}^{in}(\mu_0,\mu_0',E_0,E_0')F(\mu_0',E_0') \\
&- \frac{1}{h^3c^4}F(\mu_0,E_0)\int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NES}^{out}(\mu_0,\mu_0',E_0,E_0')\left(\frac{1}{\rho_0}-F(\mu_0',E_0')\right)
\end{aligned}
$$

Scattering kernels input to
Boltzmann equation.
Memory bandwidth issues.

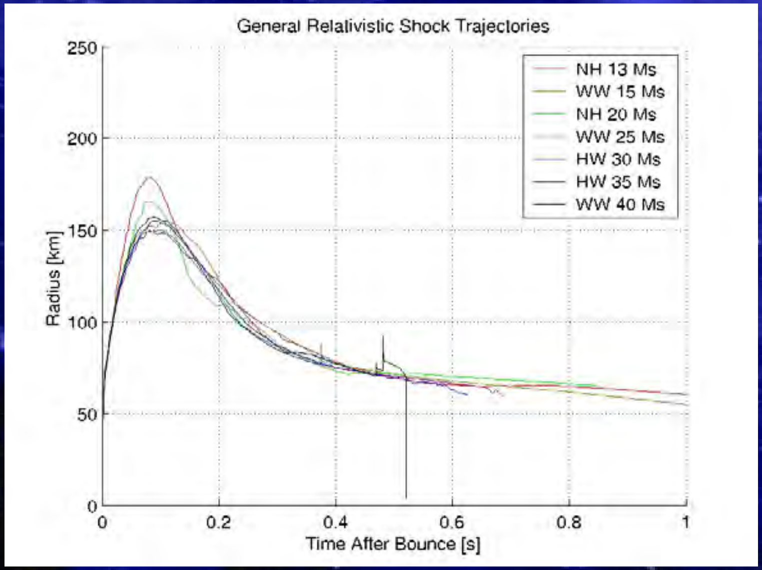
Completed: Spherical Models with Boltzmann Transport

Newtonian



Messer et al. (2002)

General Relativistic



Liebendoerfer et al. (2002)

No Explosions!

TSI will explore both!

New Microphysics?

High-Density Stellar Core Thermodynamics

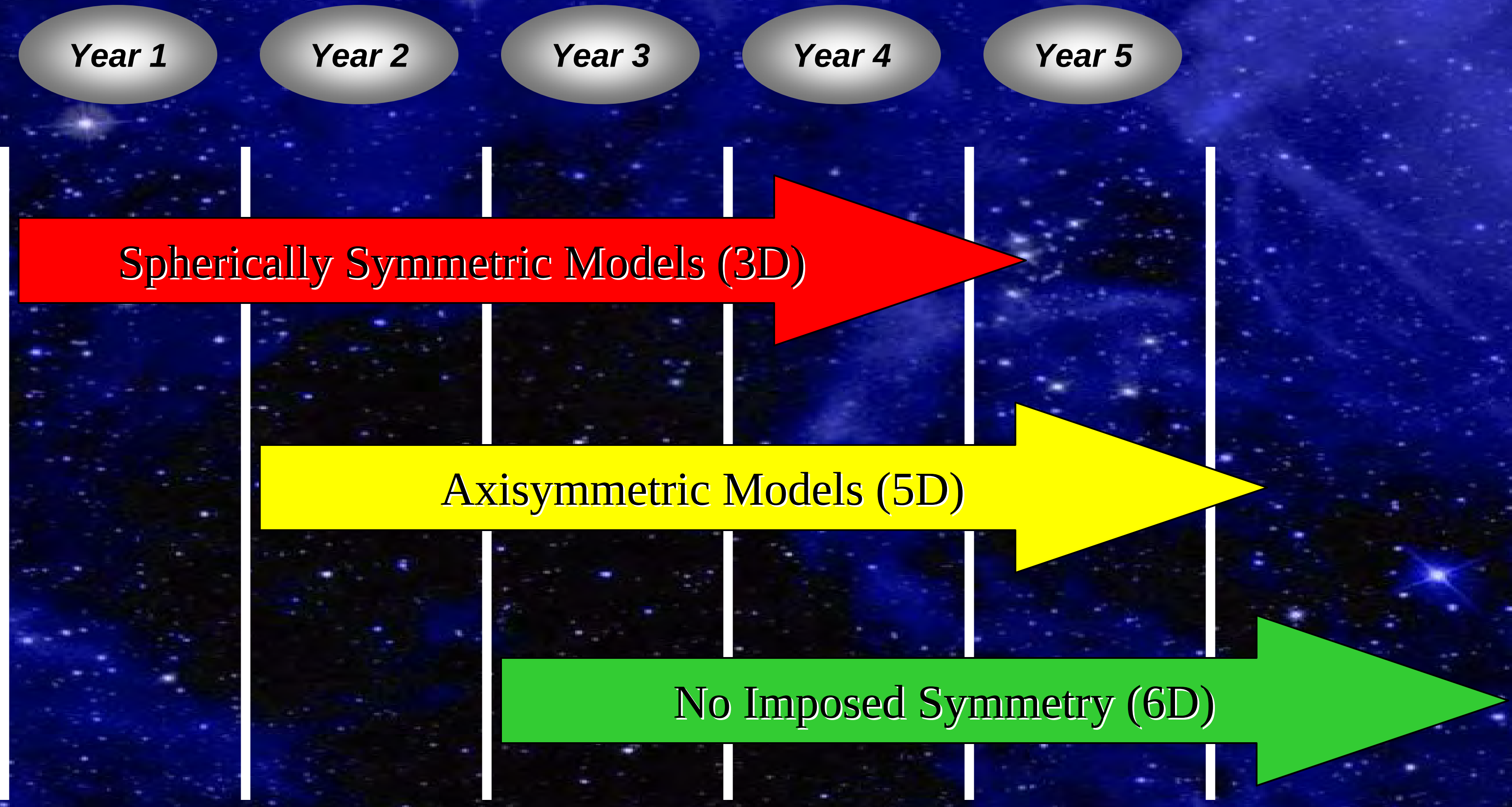
Neutrino-Matter Interactions

New Macrophysics? (2D/3D Models)

Fluid Instabilities, Rotation, Magnetic Fields

⇨*No 2D/3D supernova models with realistic neutrino transport exist!*

Supernova Simulation Timeline



Year 1

Year 2

Year 3

Year 4

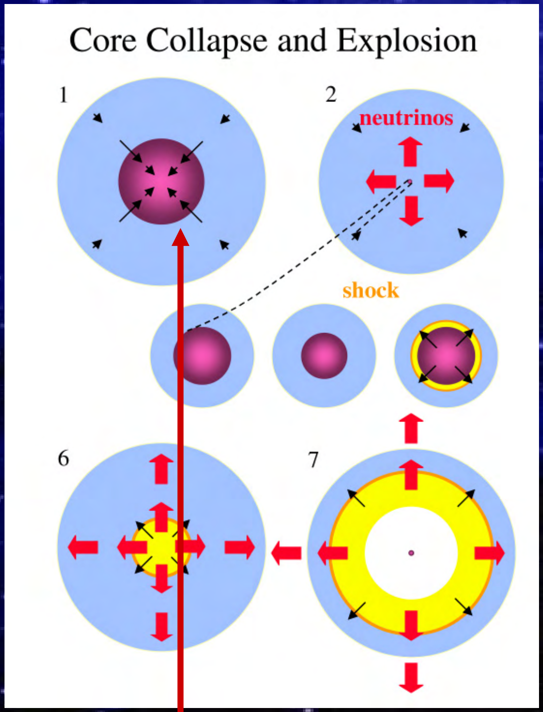
Year 5

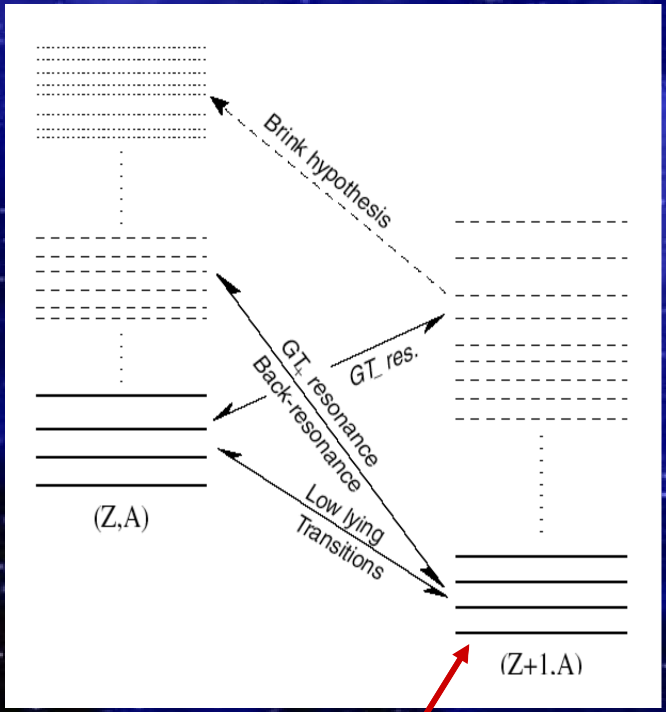
Spherically Symmetric Models (3D)

Axisymmetric Models (5D)

No Imposed Symmetry (6D)

When Micro and Macro Worlds Meet...





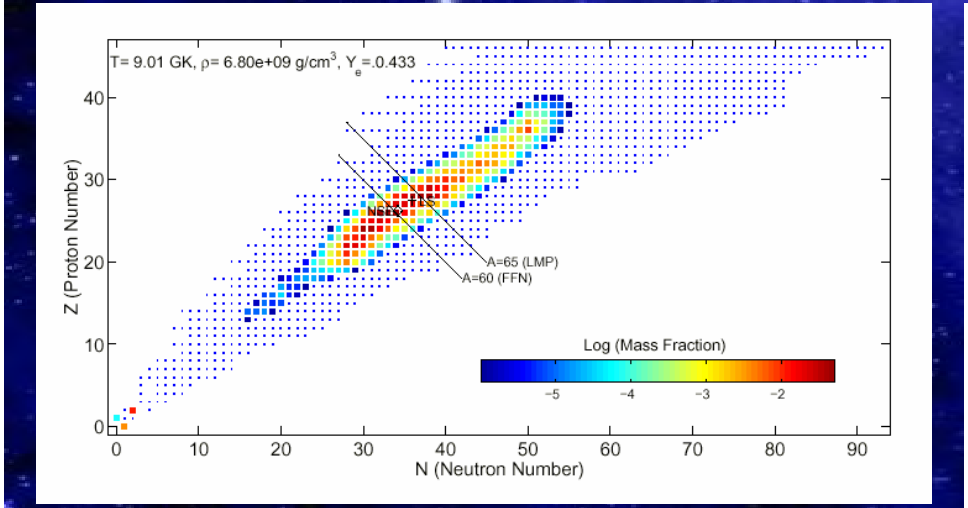
⇨Size of inner core “piston” depends on total electron capture during collapse.
Sets location of shock formation and initial shock energy.

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

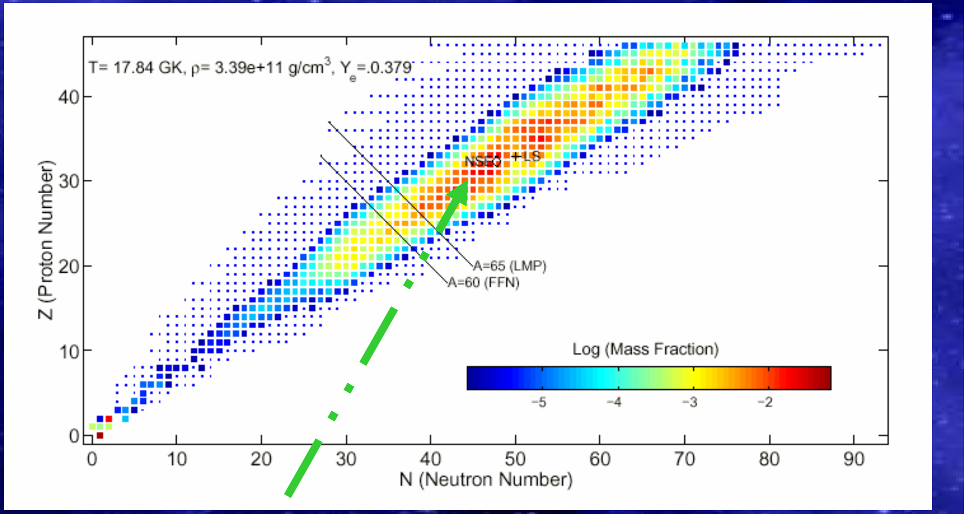
- Solve very large eigenvalue problems.

One of the most beautiful aspects of this problem!

Near onset of collapse...



Near neutrino trapping...



Hix et al. (2003)

Use SMMC/RPA hybrid model (Dean/Langanke) until shell models reach requisite A.

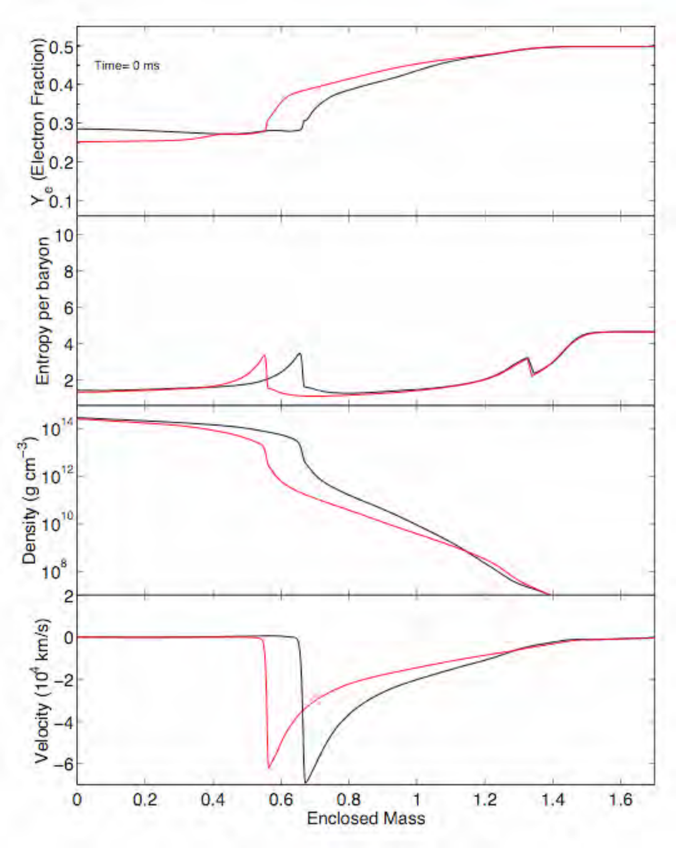
Carried out 1D collapse models with:

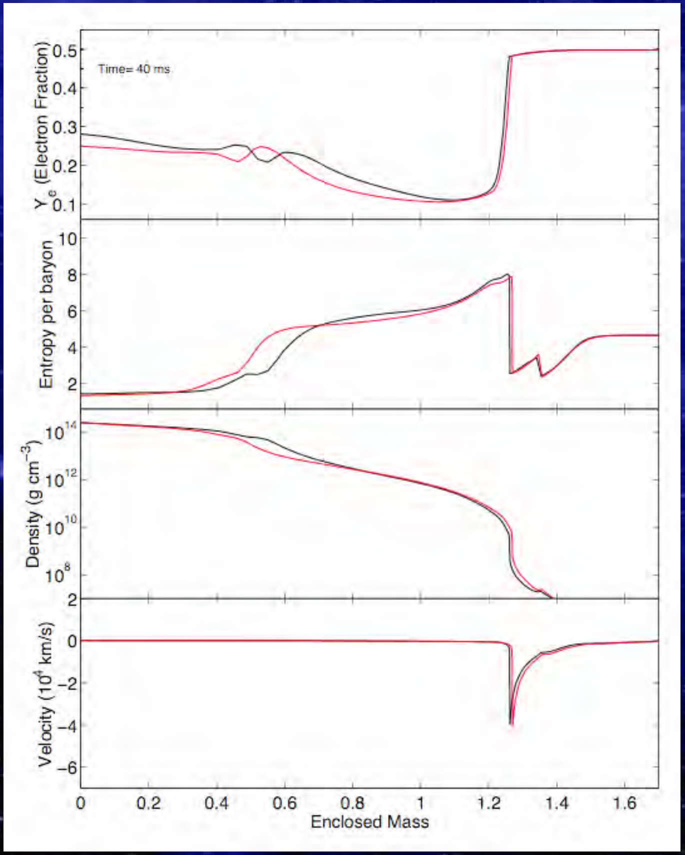
- Boltzmann neutrino transport.
- Ensemble of nuclei.
- State of the art electron capture rates.

→ ***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.

Langanke et al. (2003), Hix et al. 2003
Physical Review Letters (submitted)





- ⇨ *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

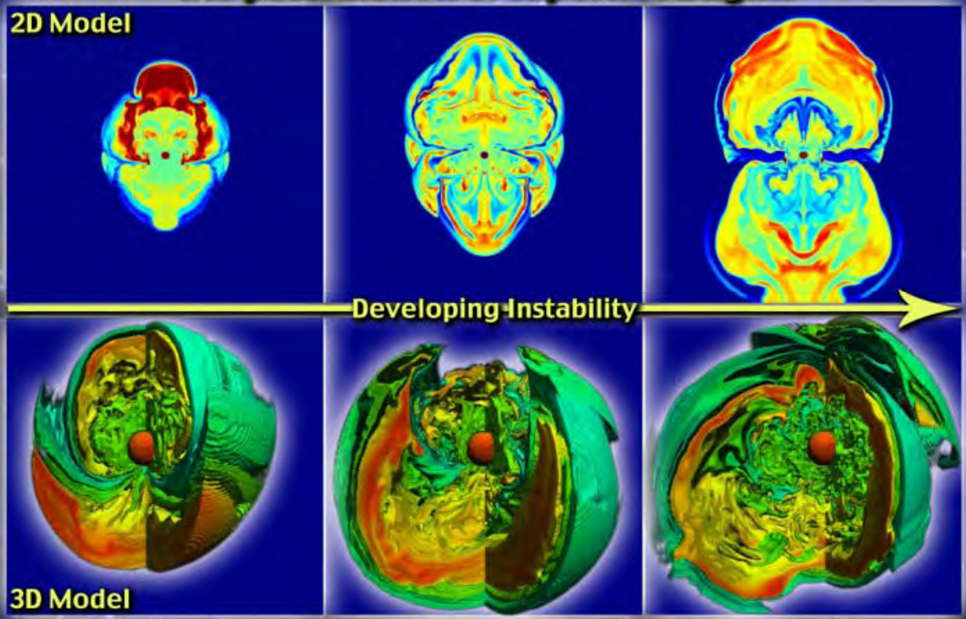
Scientific Discovery: Supernova Shock Wave Instability

(Blondin, Mezzacappa, and DeMarino (2002), The Astrophysical Journal, in press.)

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

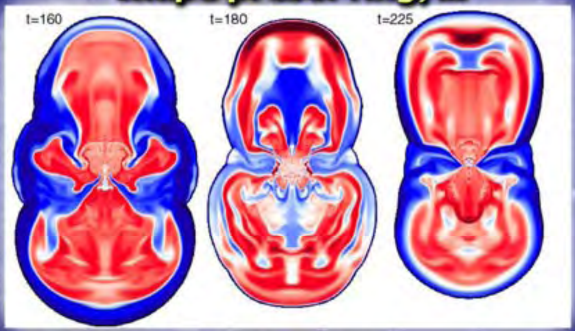
The supernova shock wave may become unstable!

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

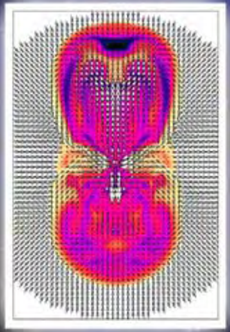


Instability–induced explosions ...

... are bipolar and shape preserving, ...

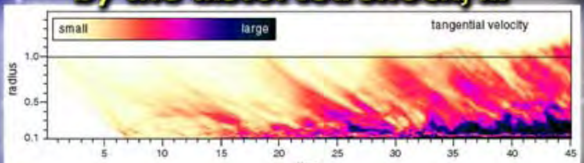


... and oscillatory.

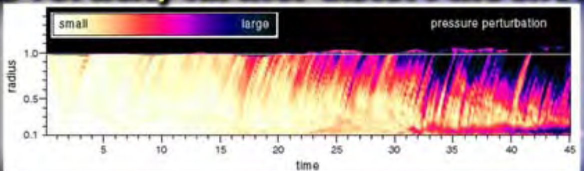


The instability results from a feedback loop:

vorticity is introduced by the distorted shock, ...



... and pressure waves generated by this vorticity further distort the shock.



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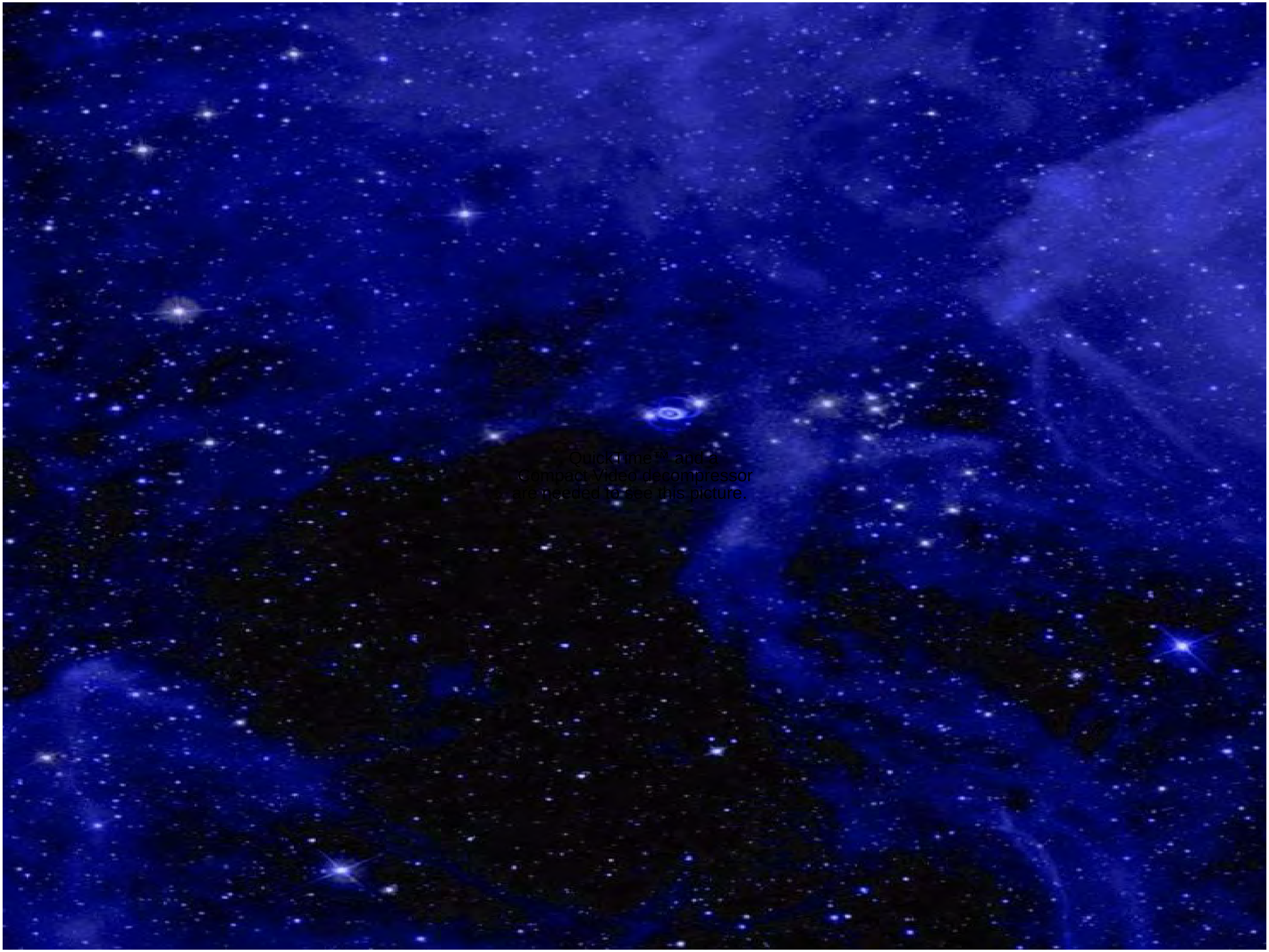
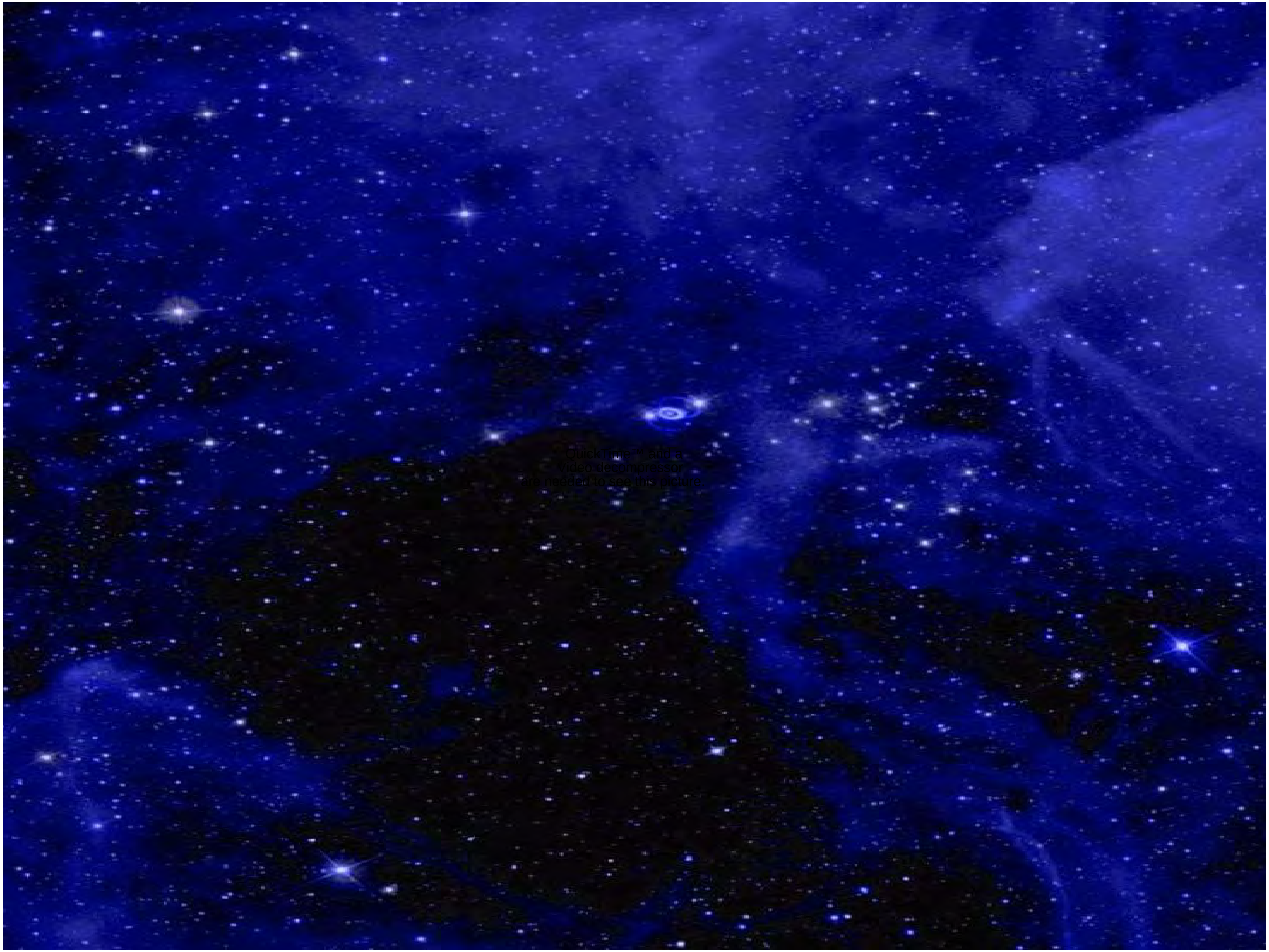


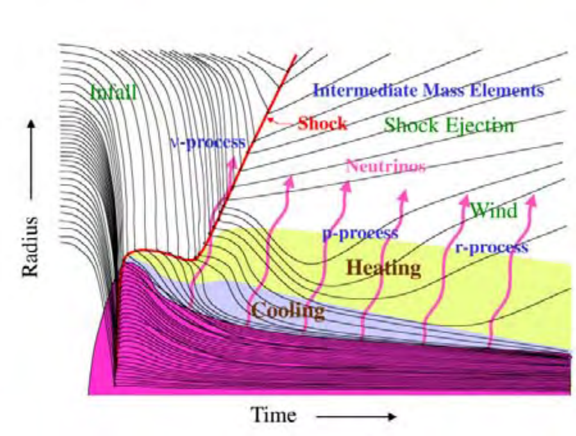
QuickTime™ and a
Compact Video decompressor
are needed to see this picture.

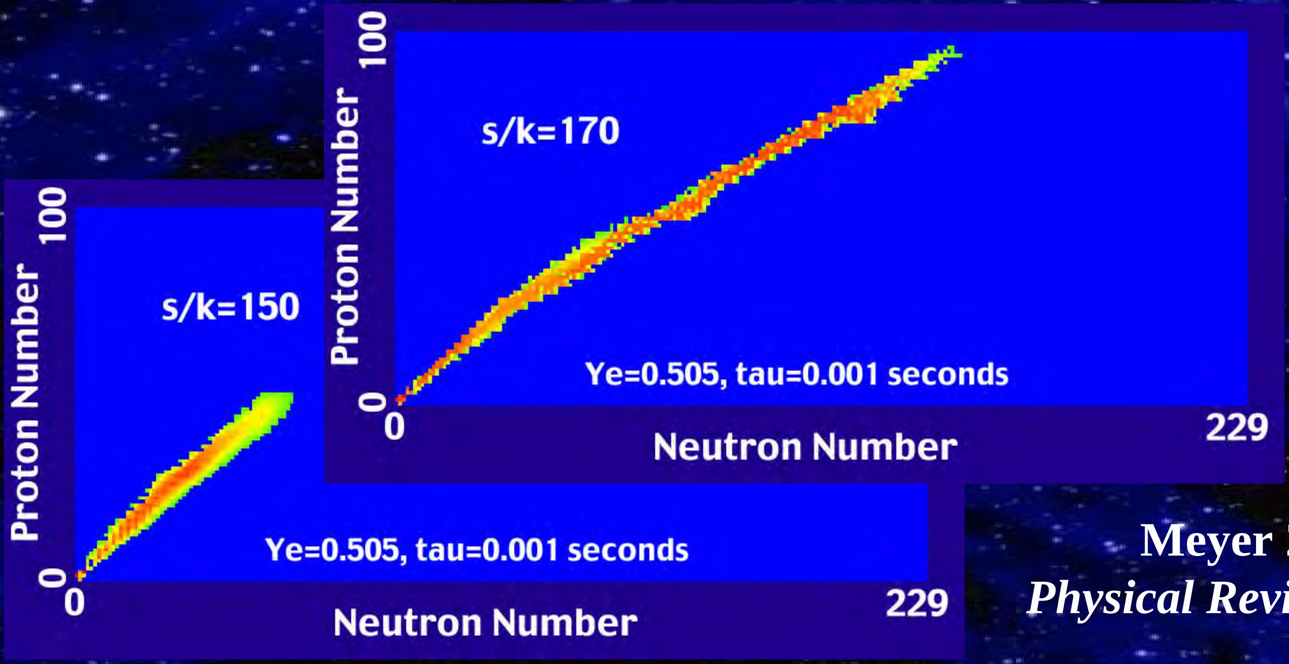


QuickTime™ and a
Video decompressor
are needed to see this picture.

“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.



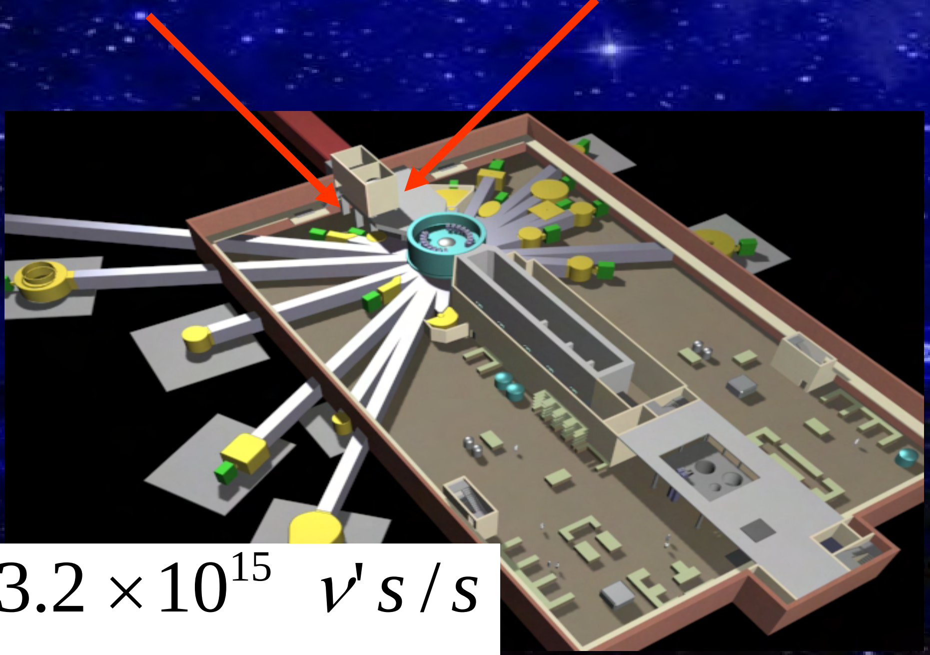


Meyer 2003
Physical Review Letters

An r-process can occur in proton-rich environments!
⇨If nuclear reactions out of equilibrium.

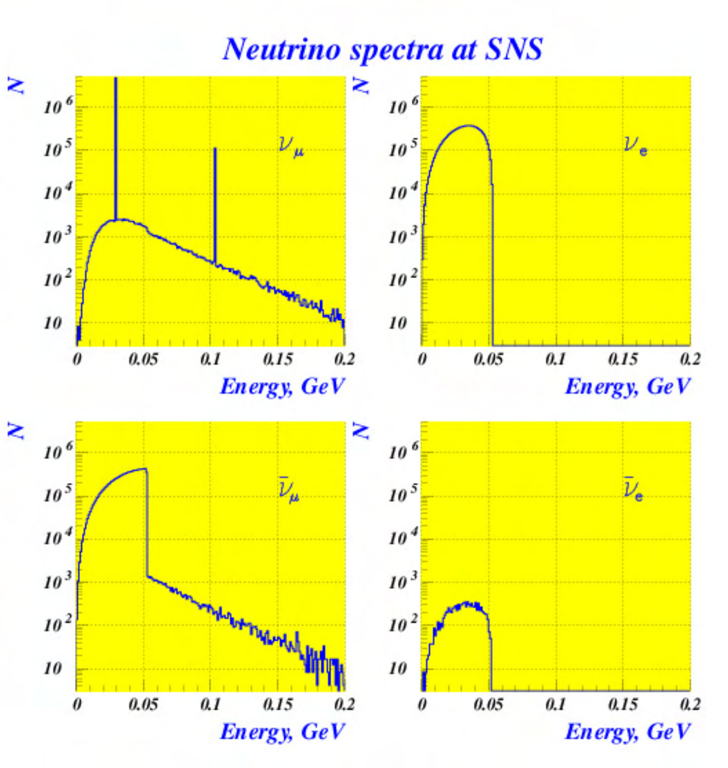
Neutrino-Nucleus Cross Section Measurements at the SNS

Possible Neutrino Detector Locations



$$3.2 \times 10^{15} \quad \nu' s / s$$

$$60 \;\; Hz \;\; Pulses$$



Supernova neutrino RMS energies between 10 and 25 MeV!

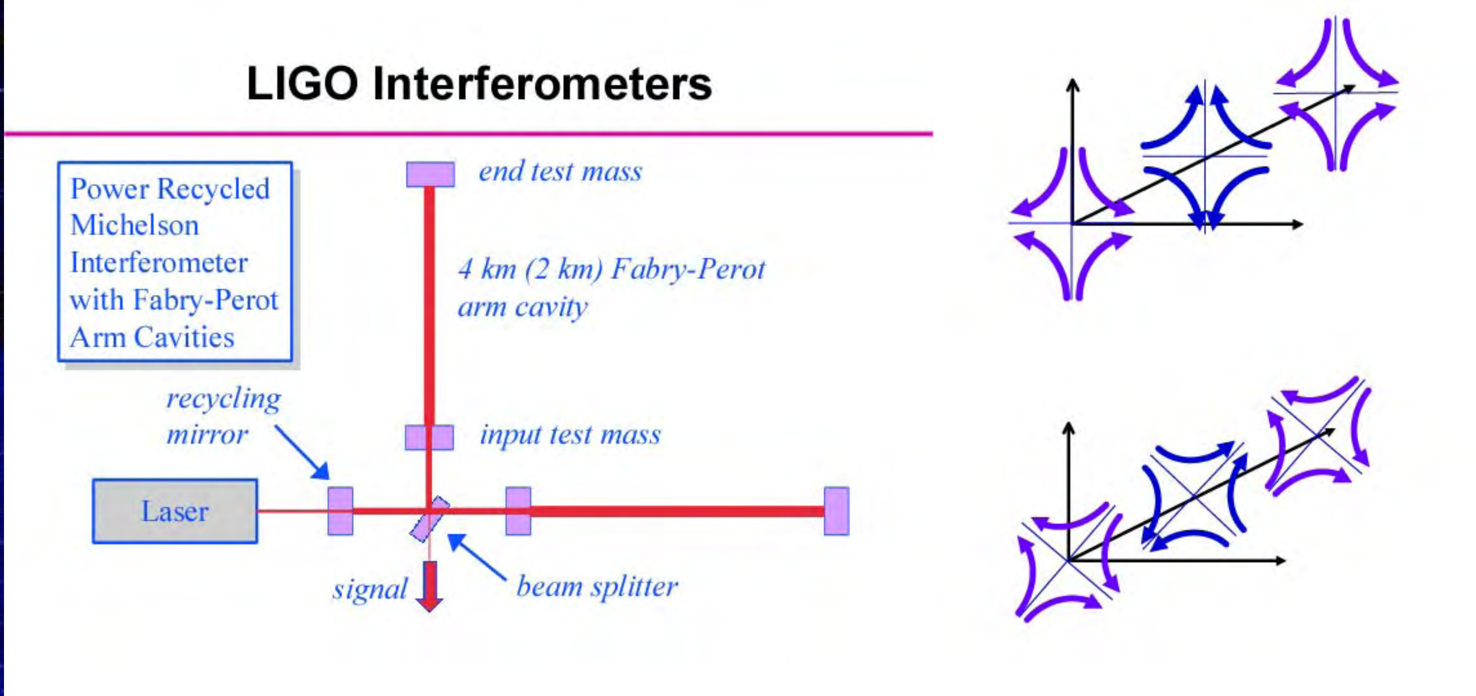
Neutrino capture/scattering cross section measurements will help gauge theory for

- ⇨*electron capture in stellar core collapse,*
- ⇨*r-process nucleosynthesis,*
- ⇨*and Terrestrial neutrino detection (Super-K, SNO, OMNIS).*

Gravitational Waves

DoE-NSF Partnership

- 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.



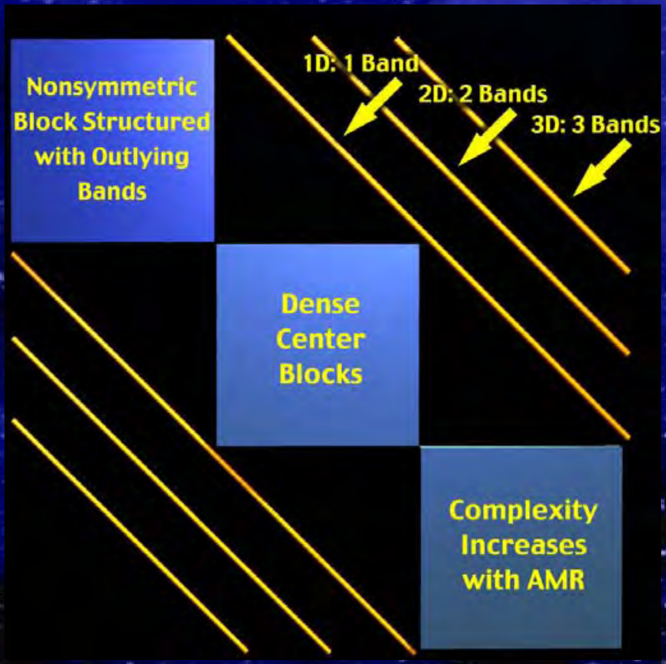
Transport Linear Systems (TOPS)

$$
\begin{aligned}
\frac{1}{c}\frac{\partial F}{\partial t} &+ 4\pi\mu_0\frac{\partial(r^2\rho_0 F)}{\partial m} \\
&+ \frac{1}{r}\frac{\partial[(1-\mu_0^2)F]}{\partial\mu_0} \\
&+ \frac{1}{c}(\frac{\partial ln\rho_0}{\partial t}+\frac{3v}{r})\frac{\partial[\mu_0(1-\mu_0^2)F]}{\partial\mu_0} \\
&+ \frac{1}{c}[\mu_0^2(\frac{\partial ln\rho_0}{\partial t}+\frac{3v}{r})-\frac{v}{r}]\frac{1}{E_0^2}\frac{\partial(E_0^3F)}{\partial E_0} \\
&= \frac{j}{\rho_0}-\tilde{\chi}F \\
&+ \frac{1}{c}\frac{1}{h^3c^3}E_0^2\int d\mu_0' R_{IS}(\mu_0,\mu_0',E_0)F(\mu_0',E_0) \\
&- \frac{1}{c}\frac{1}{h^3c^3}E_0^2F\int d\mu_0' R_{IS}(\mu_0,\mu_0',E_0) \\
&+ \frac{1}{h^3c^4}(\frac{1}{\rho_0}-F(\mu_0,E_0))\int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NES}^{in}(\mu_0,\mu_0',E_0,E_0')F(\mu_0',E_0') \\
&- \frac{1}{h^3c^4}F(\mu_0,E_0)\int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NES}^{out}(\mu_0,\mu_0',E_0,E_0')(\frac{1}{\rho_0}-F(\mu_0',E_0'))
\end{aligned}
$$

Boltzmann
<u>Equation</u>
nonlinear
integro-PDE

Nonlinear Algebraic Equations

- ✸ *Linearize*
- ✸ *Solve via Multi-D Newton-Raphson Method*
  - ⇨ *Large Sparse Linear Systems*



Implicit Time Differencing

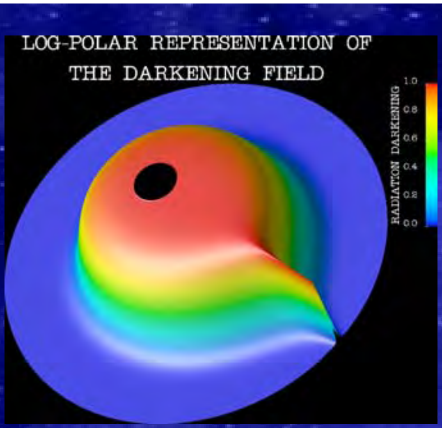
- ✸ *Extremely Short Neutrino-Matter Coupling Time Scales*
- ✸ *Neutrino-Matter Equilibration*
- ✸ *Neutrino Transport Time Scales*

<u>Progress:</u>

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)

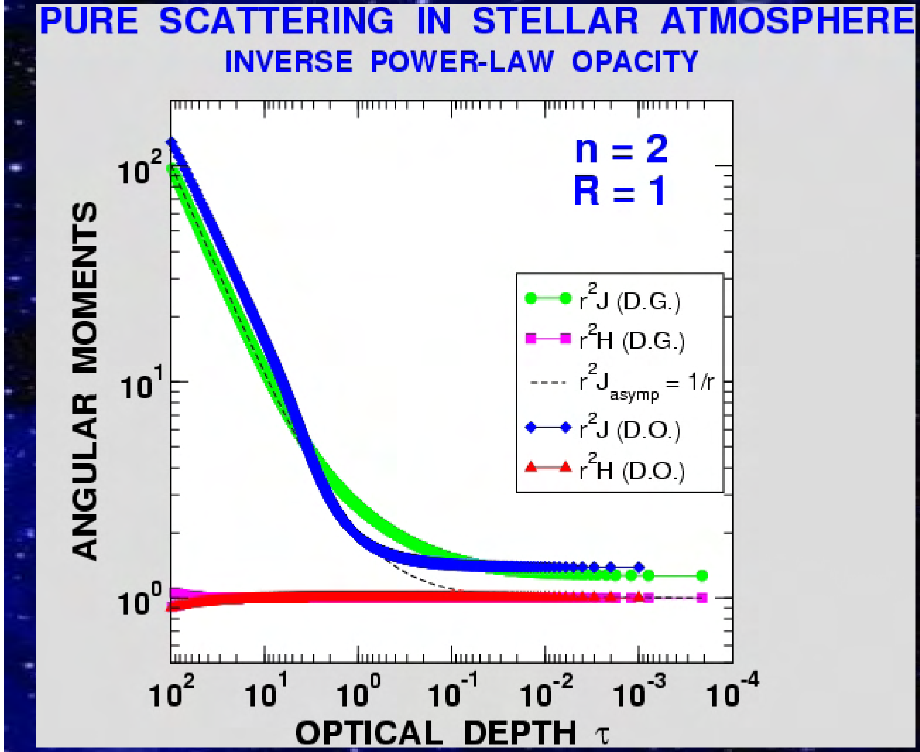
Transport Developments (TSTT)

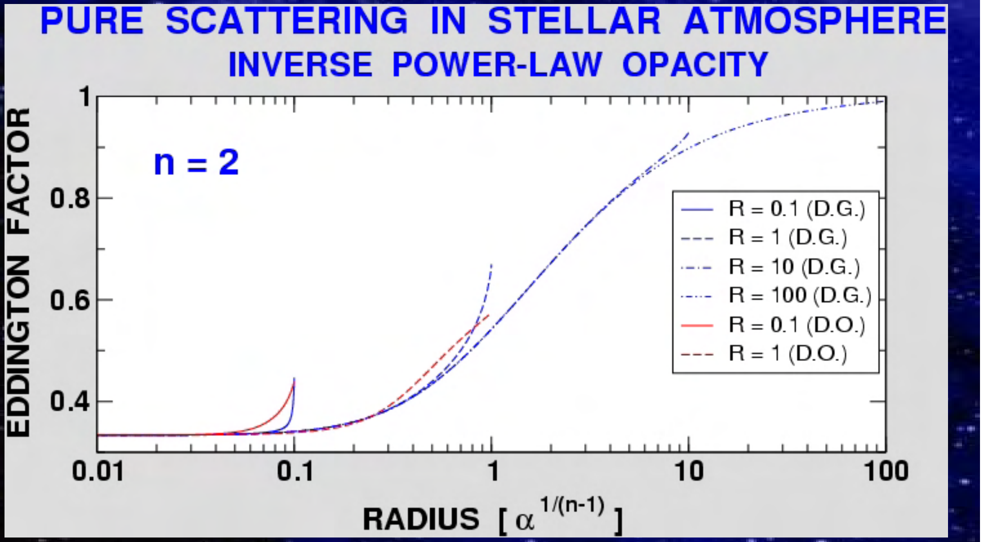


Alternative Transport Techniques

- ⇨Discrete Ordinates (Currently Used)
- ⇨Discontinuous Galerkin (Under Development)

Results from model "Milne" problem:





10X Faster, 10X Less Memory

de Almeida (2003)

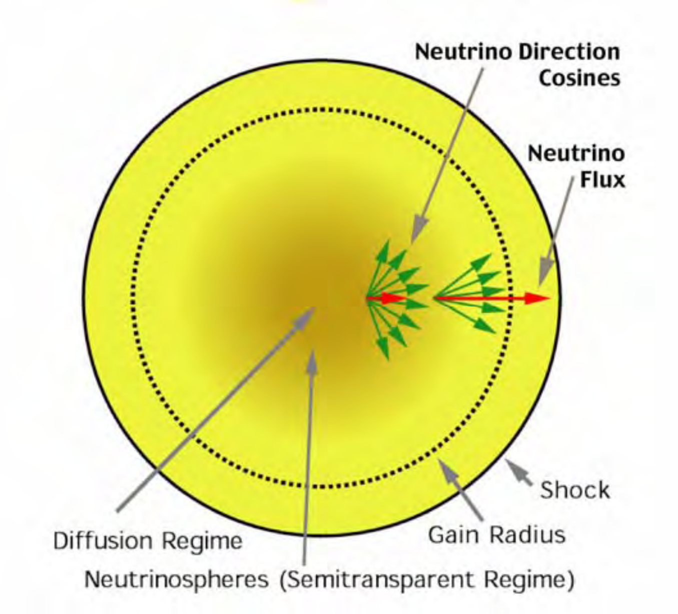
Transport Developments (TSTT)

Adaptive Quadratures (Direction Cosines) for Multidimensional Radiation Transport

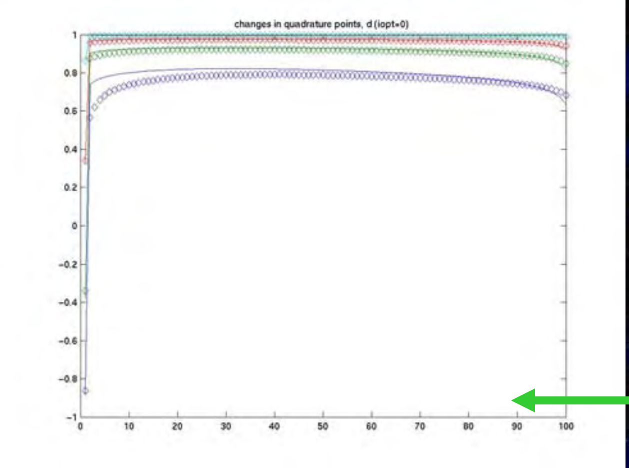
⇨Greatest challenge to completing 3D Boltzmann simulations is memory.

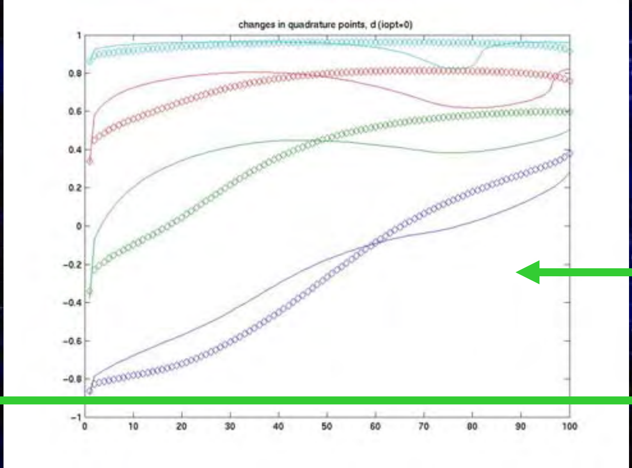
⇨Minimize number of quadratures to minimize memory needs while maintaining physical resolution. (Also important for 1D/2D MGBT.)

⇨Distribute according to “generalized pathlength.”



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

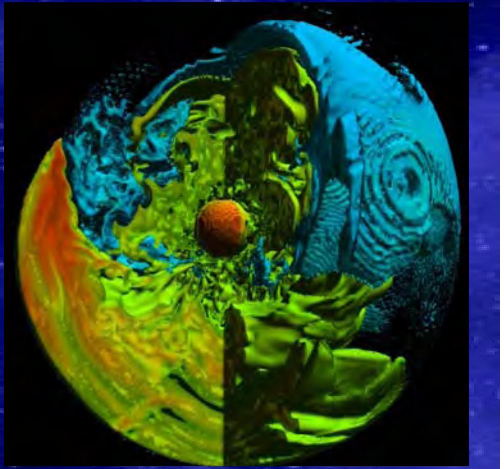




Extended Core

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

$$f(x,y,z,\mu_1,\mu_2,E)$$

$$E_\nu(x,y,z,E)$$

$$F_\nu(x,y,z,E)$$

$$\frac{F_\nu(x,y,z,E)}{E_\nu(x,y,z,E)}$$

Composition

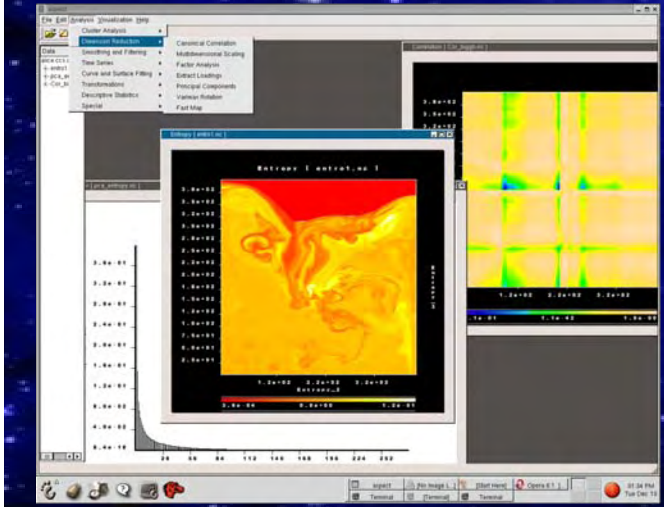
Query the composition of a fluid element.

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

- ⇨**Dataset Size!**
- ⇨**Custom Representations**

Driving developments in...

Samatova et al. (2002)



Data Reduction

Order of magnitude reduction using PCA techniques.

Data Analysis

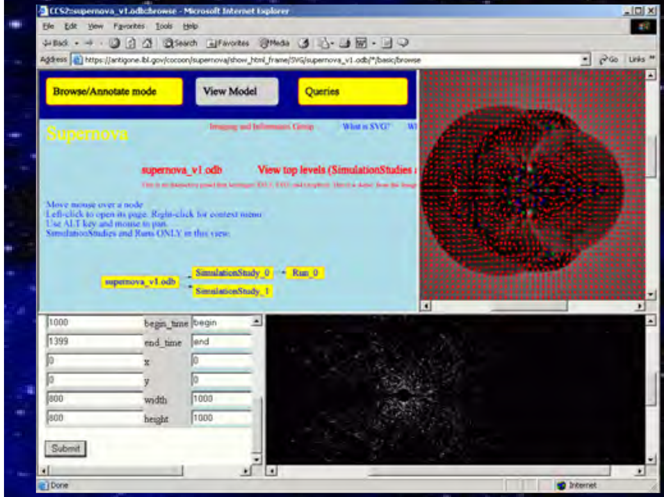
- *Raw Data*
- *Dimensional Compression*
- *PCA, ...*
- *Feature Extraction*
  - *Vortices, …*
  - *Feature-based visualization.*

Integration of Data Analysis and Visualization (ASPECT)

Agent Technology

Raised many issues.

Parvin et al. (2002)



Move mouse over a node
Left-click to open its page. Right-click for context menu
Use ALT key and mouse to pan.
SimulationStudies and Runs ONLY in this view.

1000 begin_time begin
1399 end_time end
0 x 0
0 y 0
800 width 1000
800 height 1000

Potok et al. (2002)

Extensive efforts by SDM and LBL ...

…and visualization (local, remote, collaborative)...

“Off-the-Shelf” Technologies

- ⇨EnSight
- ⇨TSB
- ⇨ParaView

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

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

Custom Visualization (VTK)

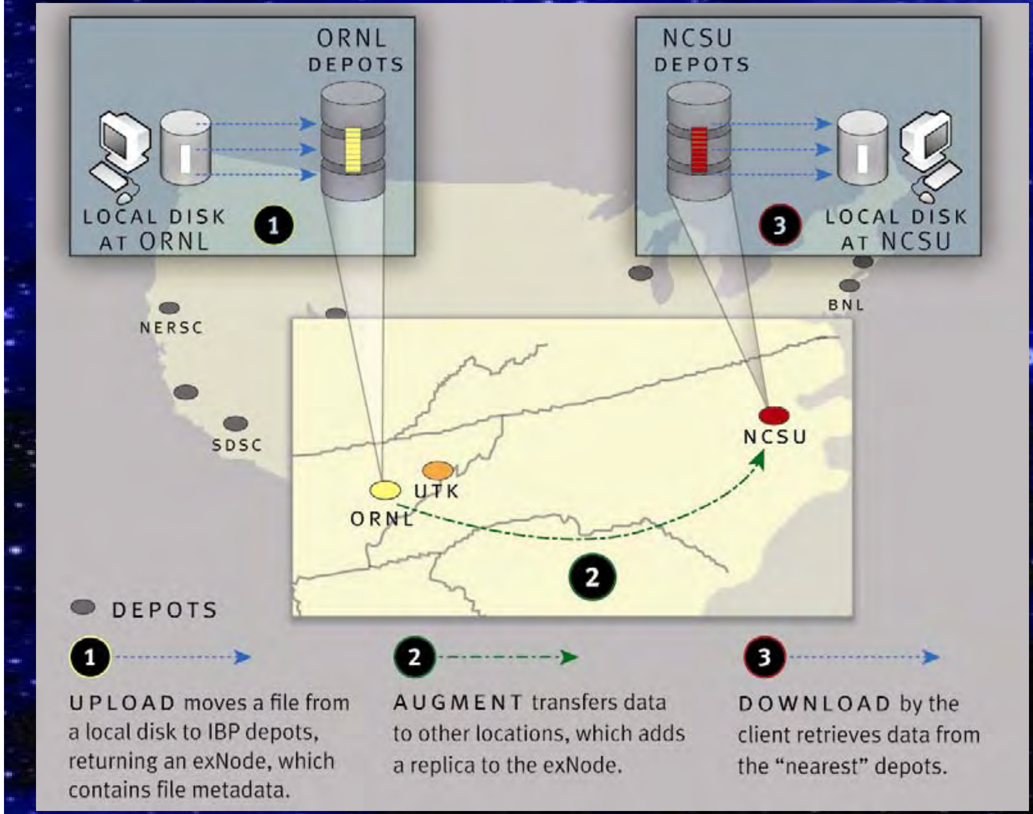
- ⇨Custom Representations
- ⇨Custom Functionality

Integrating visualization with

- ⇨data analysis (SDM collaboration),
- ⇨networking (collaboration with UTK/ORNL groups).

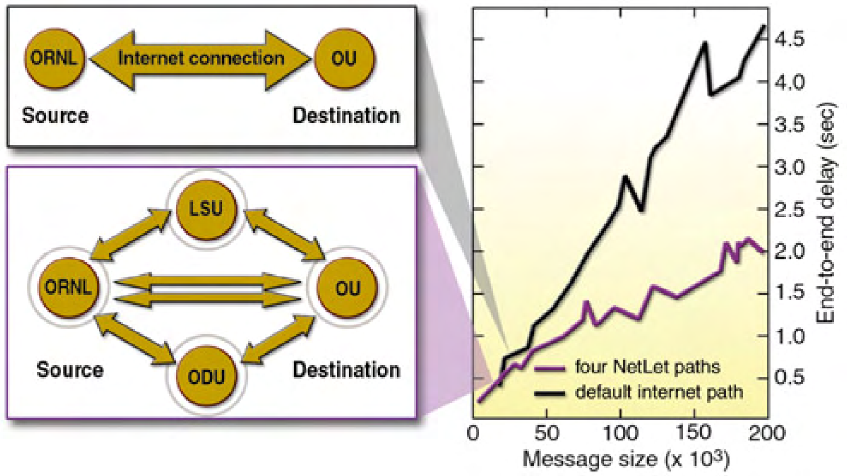
… and networking …

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.



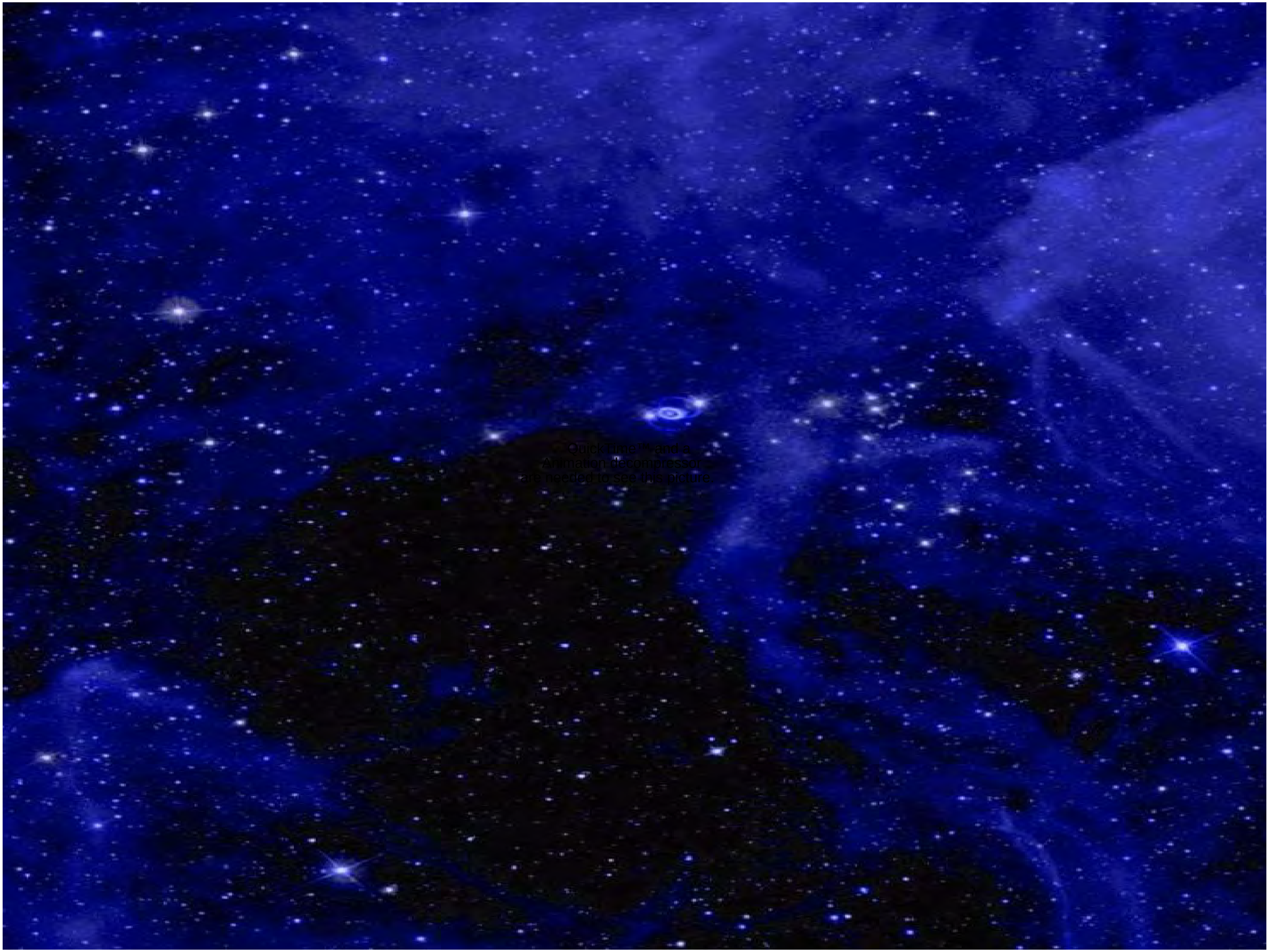
Move data between depots with full available bandwidth.

HRM

LoRS

Layer?

Use LoRS as file service for HRM?



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

Code Performance (PERC)

- 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

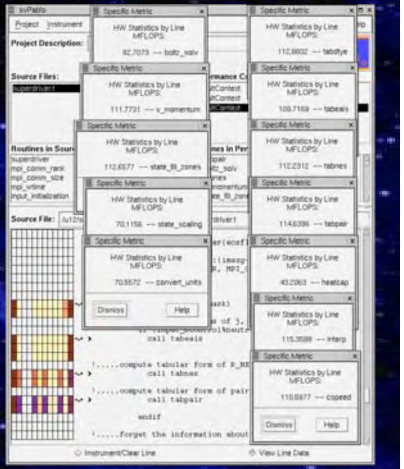
V2D: 2D MGFLD Transport Code

V3D: 3D MGFLD Transport Code (Under Development)

2D/3D Boltzmann Code (Under Development)

Instrument Codes with Performance Tools: SvPablo, Tau

Instrumentation helped improve tools!



Verification and Validation

TSI Code Suite

⇨ ***Hydrodynamics:***

VH-1 (PPM)
ZEPHYR (Finite Difference)

} Verification (Two Approaches, Same Equations)

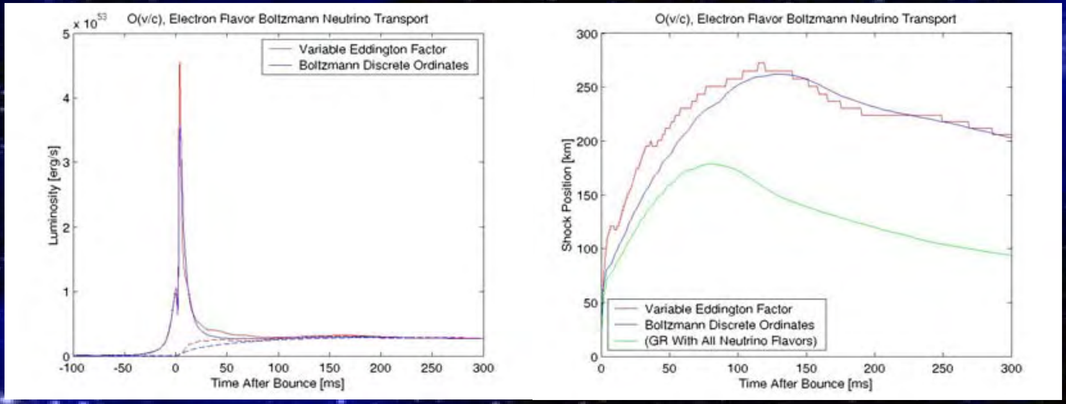
⇨ ***Neutrino Transport:***

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 MGVET Code (Under Development)
2D/3D Boltzmann Code (Under Development)

} Validation (3 Approaches)

Verification

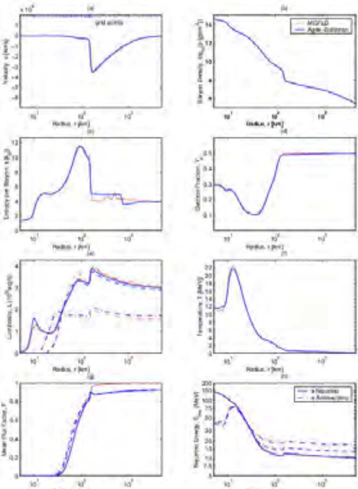


Comparing 2 discretizations of 1D MGBT.
(Liebendoerfer, Rampp, Janka, and Mezzacappa (2003))

⇨ Multifrequency crooked pipe.

⇨ …

Validation



Comparing 1D MGFLD and 1D MGBT.
Liebendoerfer et al. (2002)

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.*

Selected as a testbed application for the ORNL Cray X1 evaluation.

Percentage of Peak
(Single: Single Processor)

	Eagle	Cheetah	Seaborg	X1
AB NES	24% (Single)	12% (Single)		46% (Single)
AB	9% (Single)	5% (Single)	9% (Single)	
V2D			18% (1024)	
GENASIS	30% (Single)	15% (Single)		

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.*

Science Outlook

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.*

Programmatic Comments

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.**