Verification and Validation in Astrophysics

Tomek Plewa

Sandia CSRI Workshop

Tamaya Resort, NM

Outline

Introduction to Astrophysics

- astronomy and astrophysics
- computational astrophysics
- current topics

Laboratory Astrophysics

- HED Physics
- HED Laboratory Astrophysics

Astro V&V Examples

- radiation processes (photoionization, x-ray binaries)
- cosmology (hydrodynamics with self-gravity)
- protoplanetary disks (compressible hydrodynamics with gravity)
- shock-cloud interactions (shock and vorticity dynamics)
- accretion and jet formation (MRI)
- core-collapse (accretion shock, convection, neutrino transport)
- supernova post-explosion hydrodynamics (RMI/RTI)

Discussion

Summary: Lessons Learned

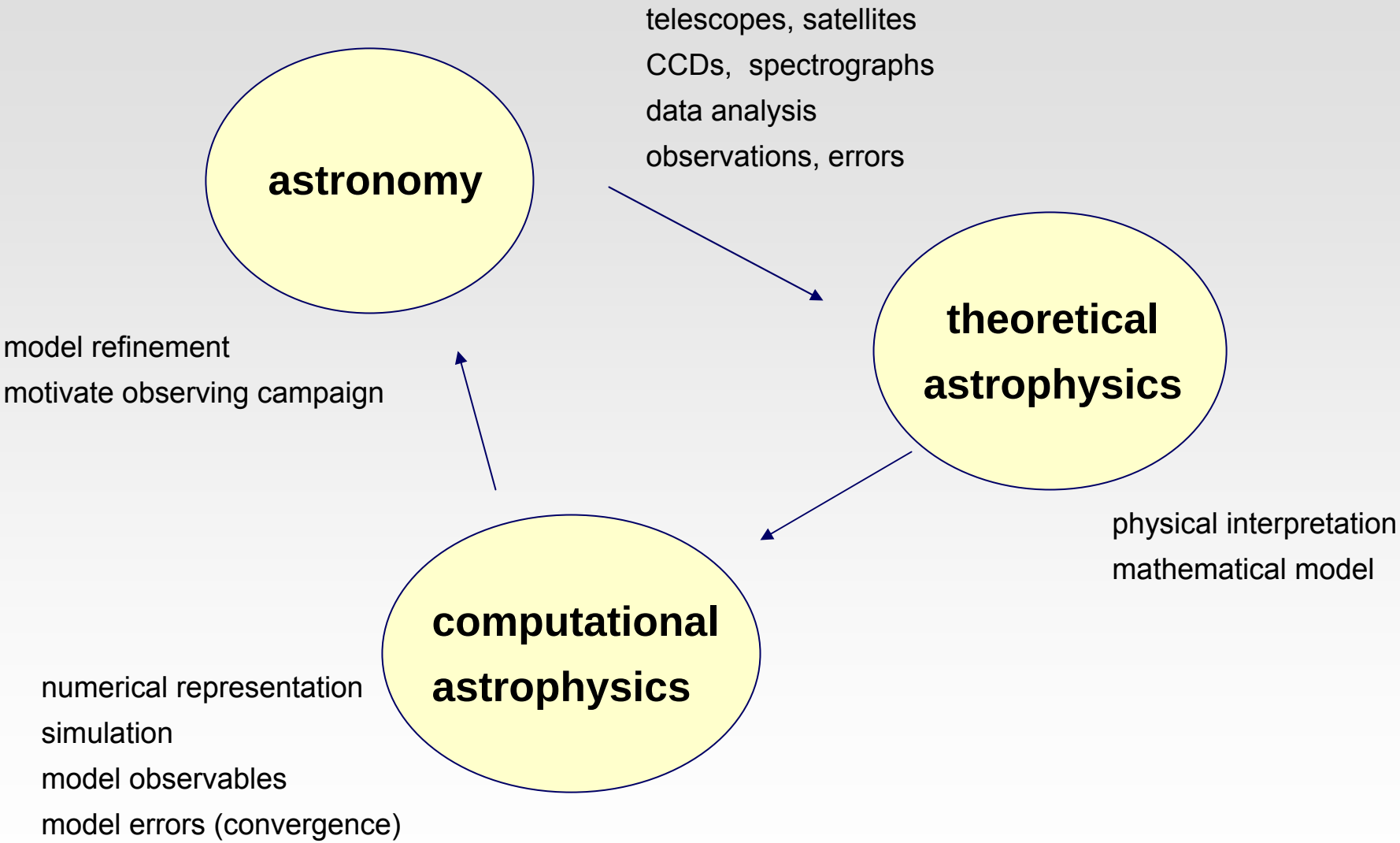
(2004)

- V&V is a **chain of procedures** that has to be strictly followed (Astro)
- Importance of finding **good validation experiment**
- Experiments not considered as **good validation experiments** today may become useful in the future
- The most scientifically attractive experiments are not necessarily **good validation experiments**
- Close interaction with experimentalists, understanding of experimental parameters
- Making next iteration: modifying experiments based on the simulation results, feedback loop

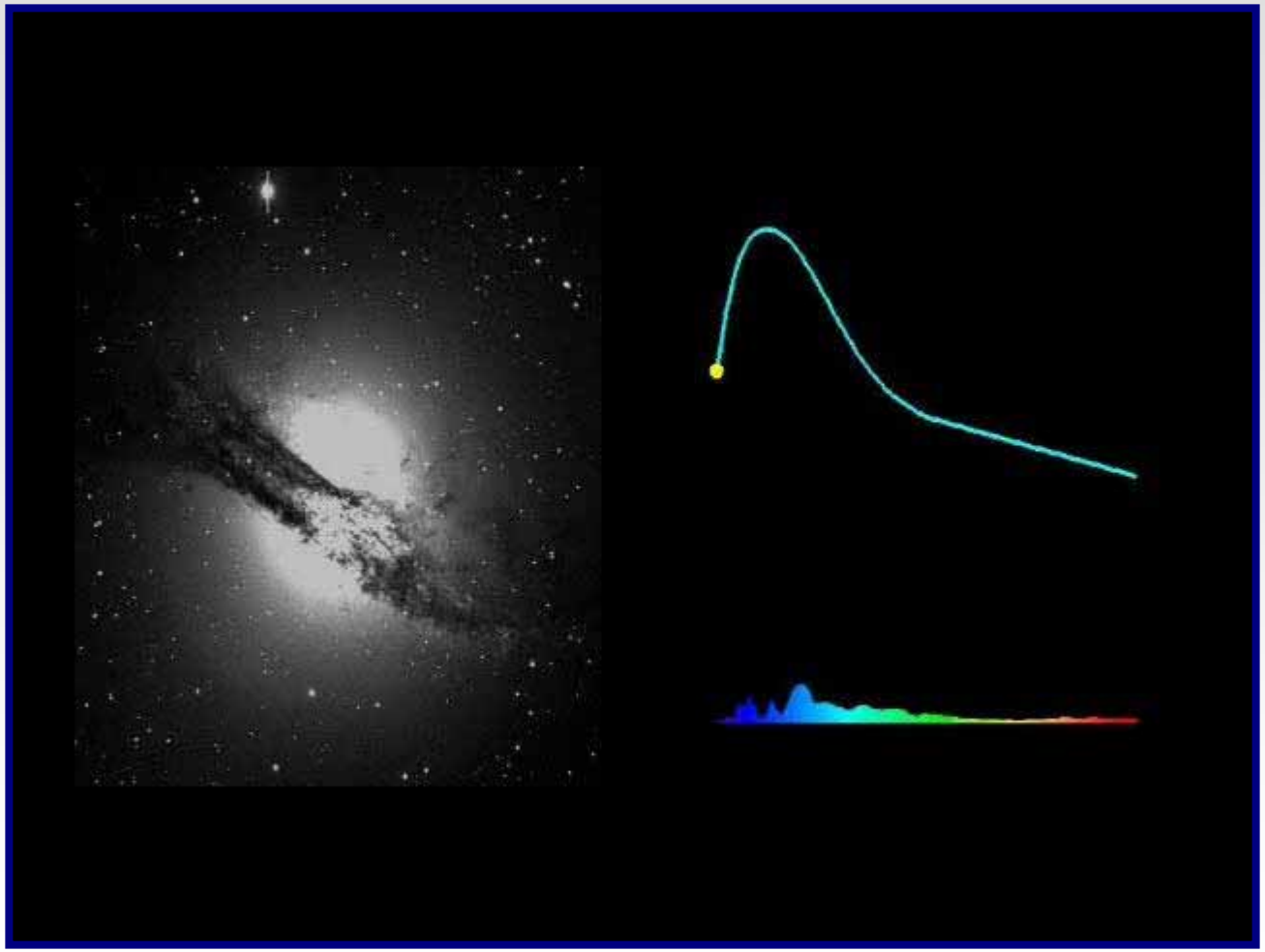
V&V Tools

- SQA: automated tools, coding standards, design procedures (Code)
- Lack of established general framework for verification
- Lack of tools aiding data analysis in validation

Introduction to Astrophysics



Astronomy



P. Nugent (LBNL)

Theoretical Astrophysics

- Observationally driven

- Pure, magneto-, radiation-, SR, and GR hydrodynamics
- Evolutionary processes of large stellar assemblies
- Plasma physics
- Radiative processes
- N-body gravitational systems
- Chemistry of interstellar matter, molecular clouds
- Nuclear physics
- Data (image, spectral) analysis

- Linearization
- Higher-order perturbative analysis
- Order of magnitude estimates
- Statistics

Computational Astrophysics

- A coupled set of PDEs and ODEs.
- **PDEs** across the whole spectrum from elliptic (self-gravity) and parabolic problems (elemental diffusion) to hyperbolic systems (hydrodynamics).
- **ODEs frequently stiff** (nuclear reaction networks). The whole system might be stiff even if the individual components are not.
- One-dimensional problems of limited importance. Most interest in large-scale **multidimensional applications**.
- Temporal and spatial scales may vary vastly. Need methods **adaptive in space and time**. And **subgrid scale** models.
- Limited value of one-time hero-like **demonstration** runs, but important for sponsors.
- Requires **”unlimited” computing power**.

Computational Astrophysics Challenges

- In a single problem ***spatial and temporal scales*** may vary several (> 10) orders of magnitude.

  Ex.: relative flame thickness in thermonuclear supernova flame

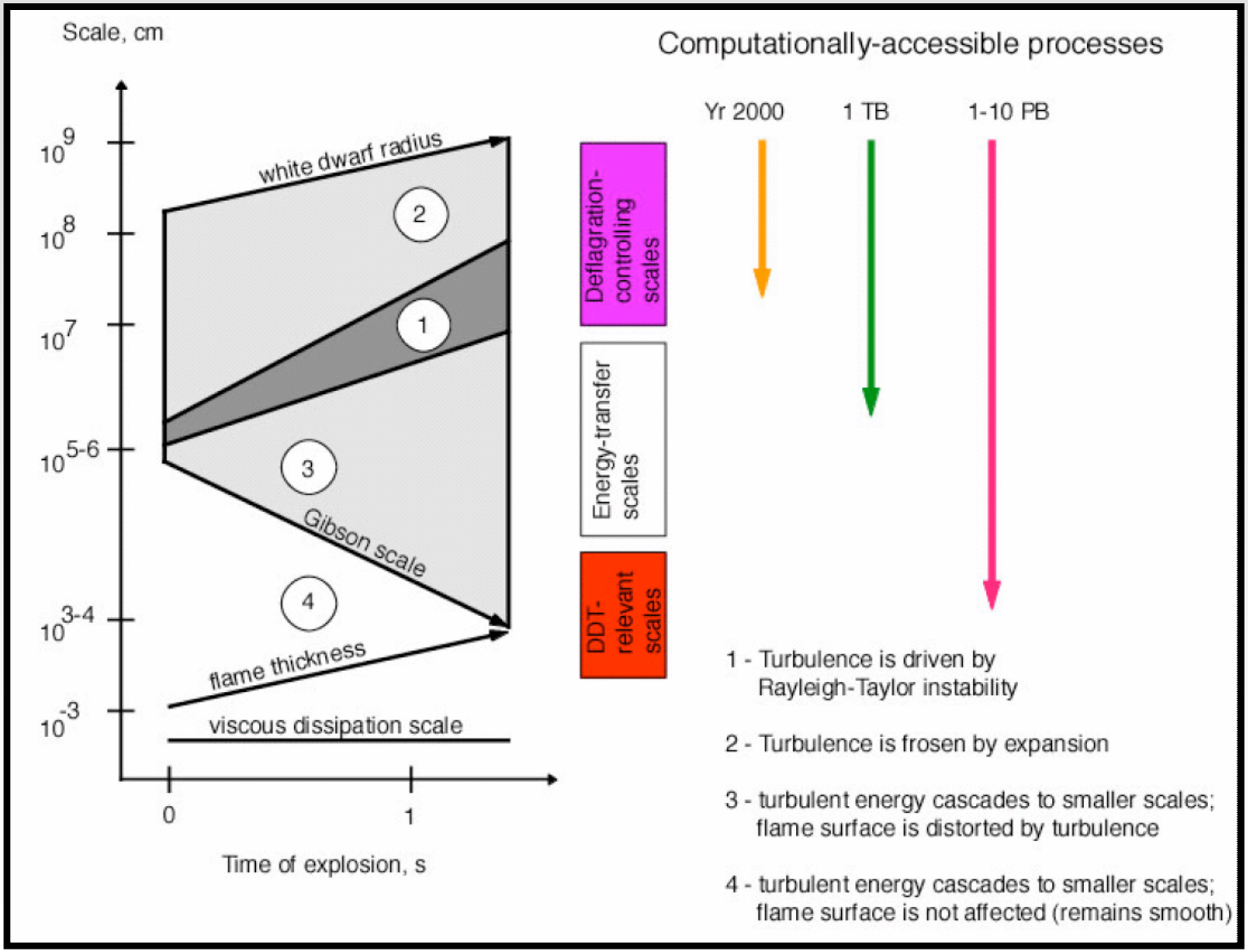
  Ex.: nuclear/hydro timescales in the same problem

- True physical picture is not just only ***indirectly accessible*** but also inherently complex with a rich set of physical processes involved.

- These process are usually ***strongly coupled***. Do we account for that coupling correctly?

- Direct modeling of the whole problem is not always possible (optically thin cooling, deflagrations, star formation). This is similar to ***subgrid scale models*** (RANS, LES).

Example: Thermonuclear Supernova



Khokhlov (2003)

Production Cycle Elements

- Actual science application problem (**right balance** Astro/CS).
- **Algorithmic development** (yields speedups likely exceeding hardware performance increase).
- Computer **implementation development** (single PE/cache efficiency, distributed memory communication, load balancing).
- **Code maintenance** and development system (cvs/svn, solution verification test suite).
- **Data analysis**-oriented (analytics) visualization (server-client model) and data storage system. Absolutely essential to complete production cycle!!

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Discussion

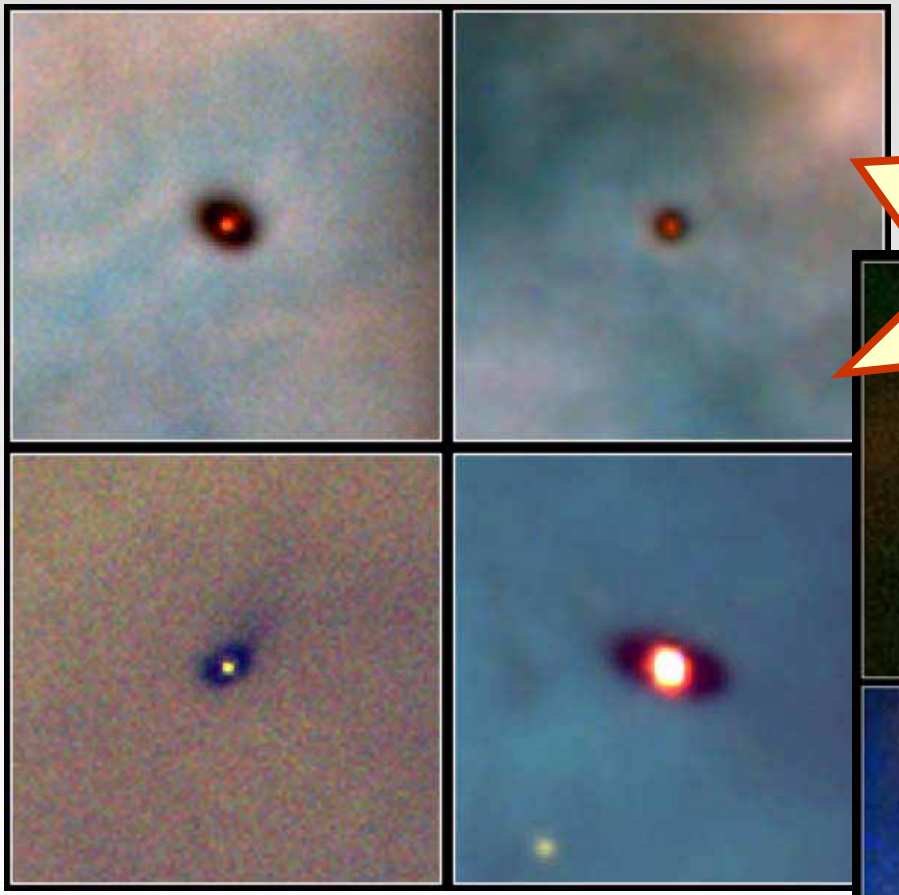
Protoplanets

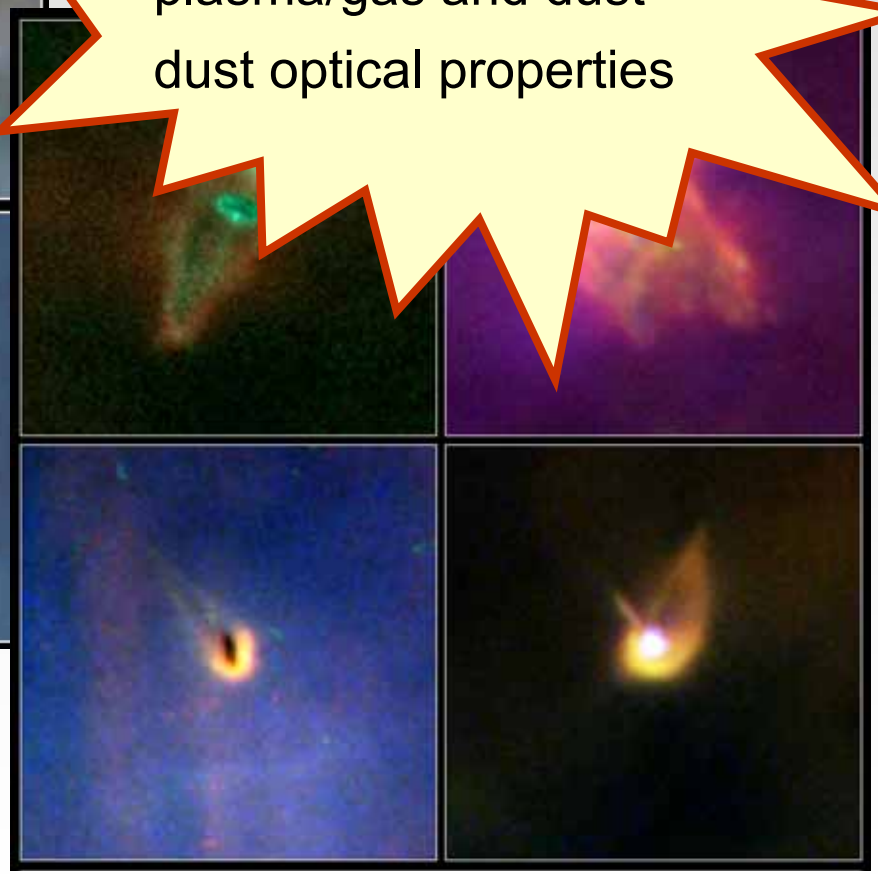
- **We are not alone!** ☺
  - 249 extrasolar planets as of August 8, 2007
  - First spectra reported
- **However…**
  - Most are Jupiter-like on Mercury-like orbits
  - Unlike our own Solar system

The Extrasolar Planets Encyclopaedia:

www.exoplanet.eu

Protoplanets with HST





accretion/MRI/jets/emission

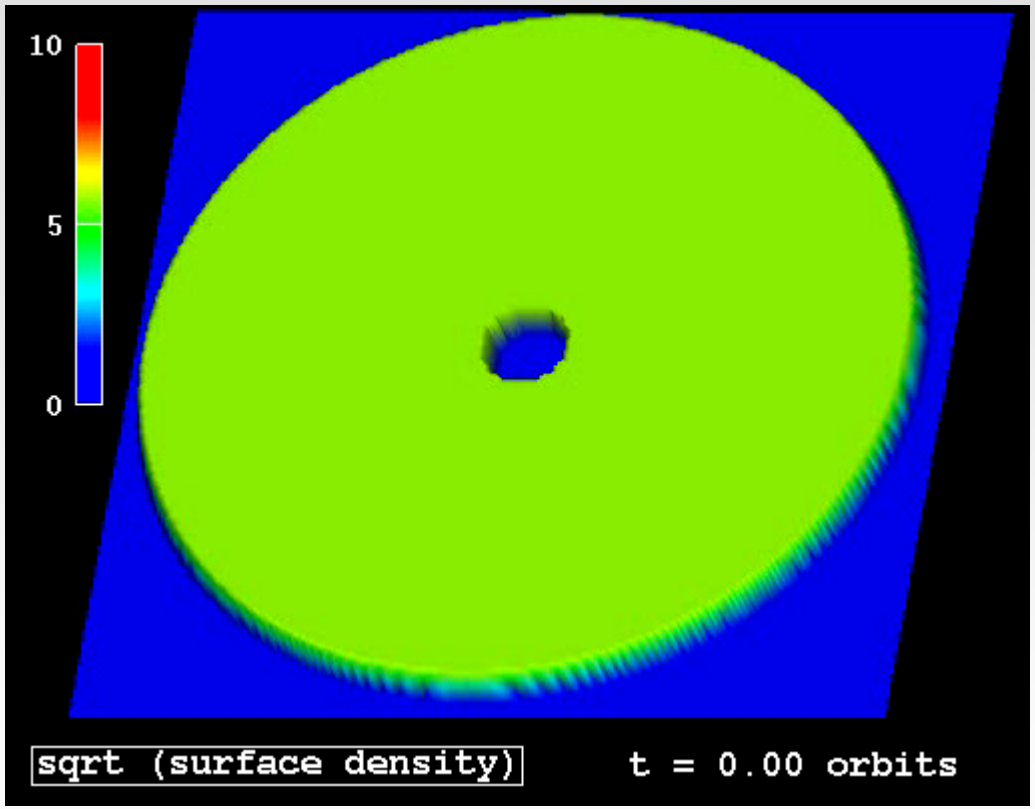
plasma/gas and dust

dust optical properties

Planet formation influenced by formation of the central star(s).

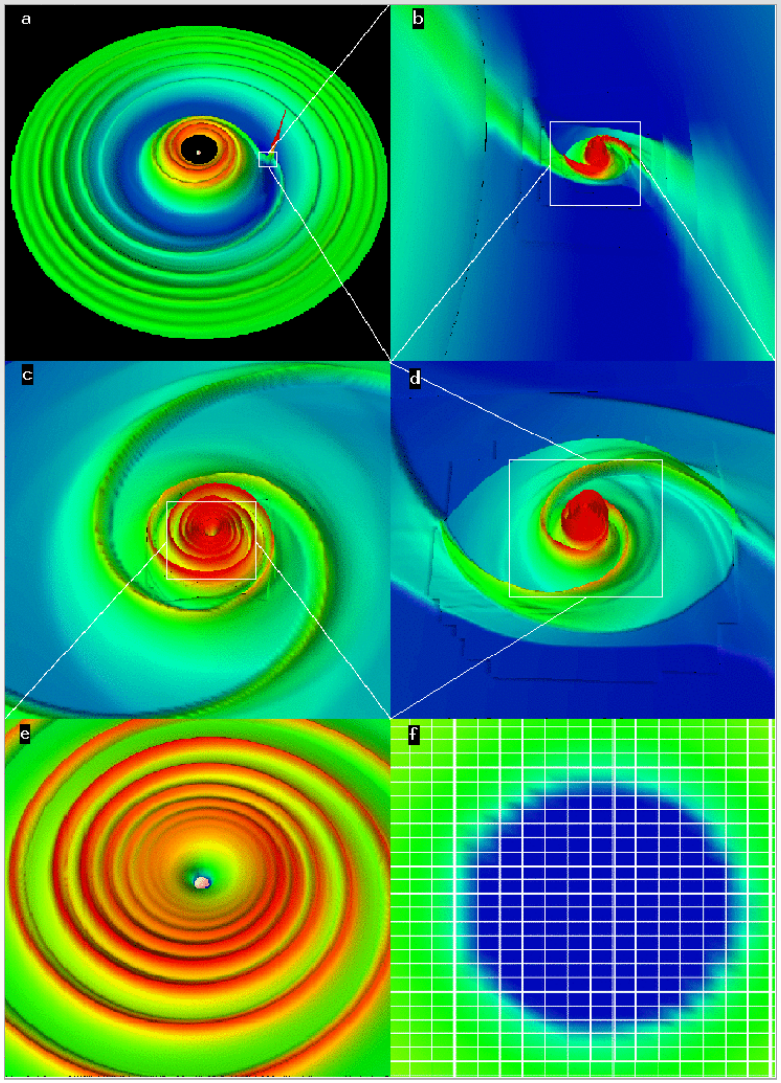
NASA/HST

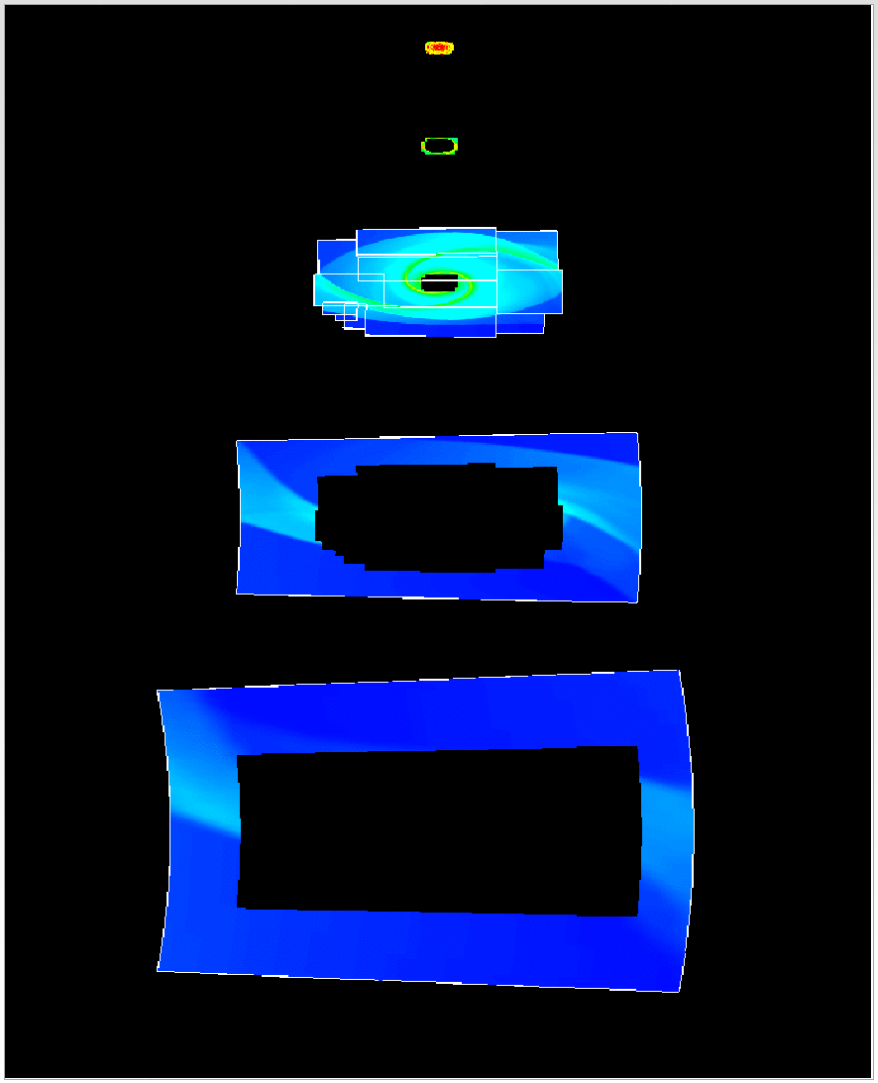
Disk-planet Interaction



Laughlin et al. (2001)

Protoplanetary Disks with AMR

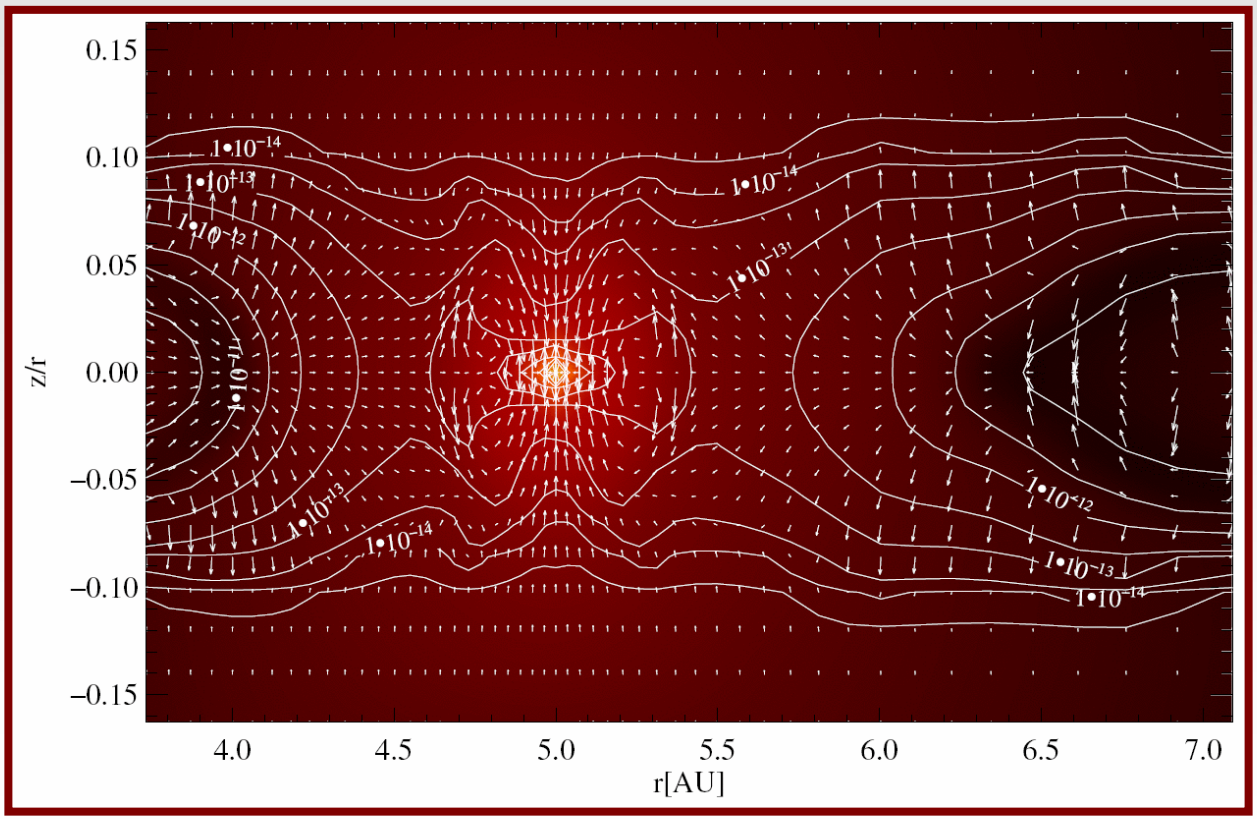




Ciecielag et al. (2002)

Protoplanetary Disk Heating

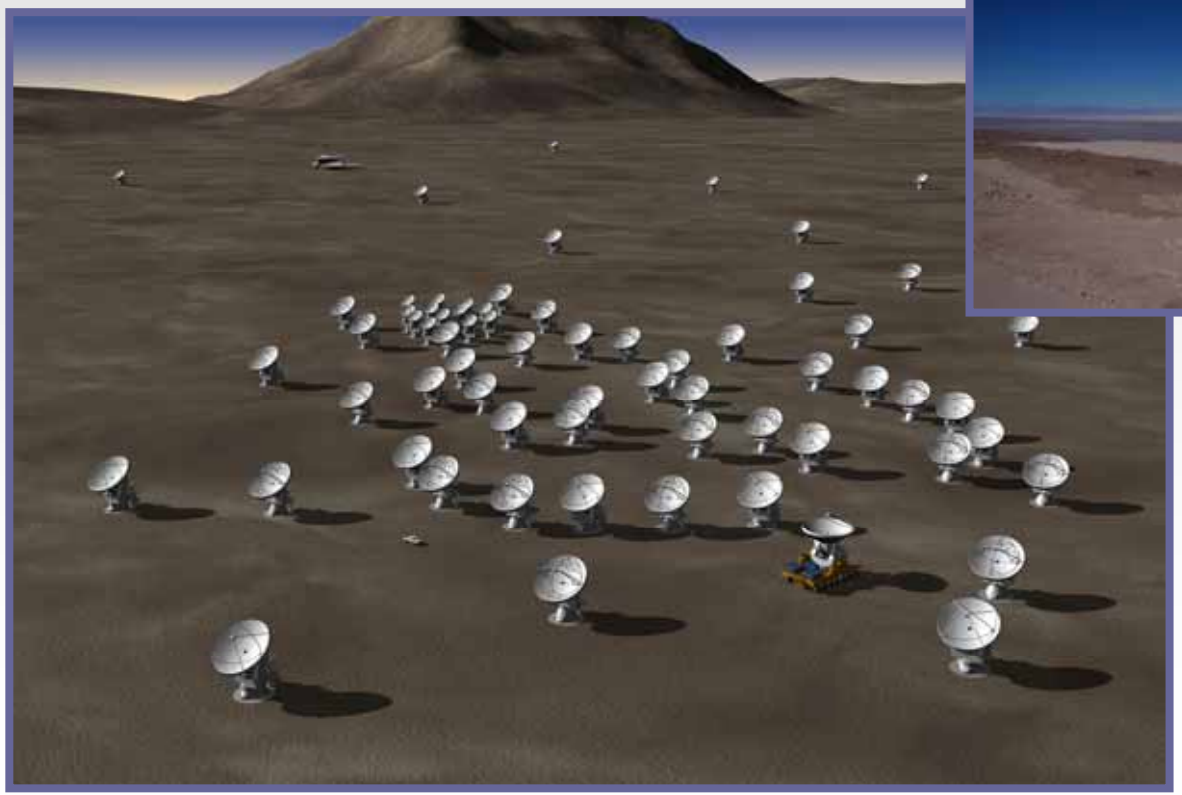
- **Thermal effects**
  - Tidal heating by the planet
  - Three-dimensional off-plane dynamics



Klahr & Kley (2006)

Protoplanets with ALMA

- Atacama Large Millimeter Array
  - One the largest ground-based astronomical projects of this decade
  - Array of 12 meter antennas
  - Baseline of several kilometres



NRAO/ESA/NAOJ

First observations in 2010!!

Protoplanets-related Programs

- **Large EU collaborative projects**
- **NASA**
  - JPL
  - satellite missions
- **Optics and chemistry labs**
  - dust formation
  - dust physical properties
- **MHD labs**
  - MRI experiments in the US (PPPL, LANL) and EU (PROMISE in Germany)
- **Driving observational programs**
  - Atacama Large Milimeter Array (ALMA)
  - Space Interferometry Mission (SIM)
  - Terrestrial Planet Finder (TPF)
  - Very Large Telescope Interferometry (VLTI)

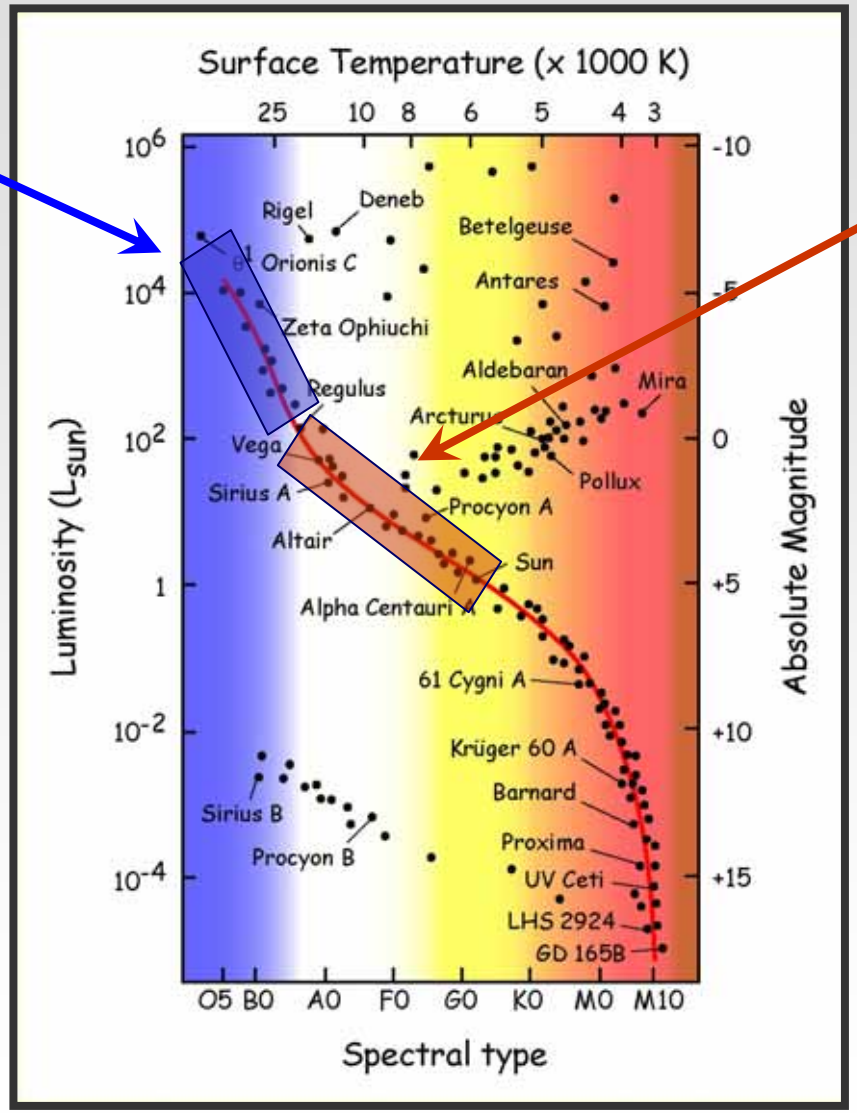
Stellar Evolution Toward Supernovae

- Most related work focused on **nucleosynthesis** and **hydrodynamics** of either stellar interiors or atmospheres
- Long-term evolution can be captured only in 1D; multi-dimensional models are essentially **snapshots in time**
- Model observables require detailed modeling of **stellar atmospheres** (snapshot in time of long-term evolution)

Our Stellar Neighbours

Type II

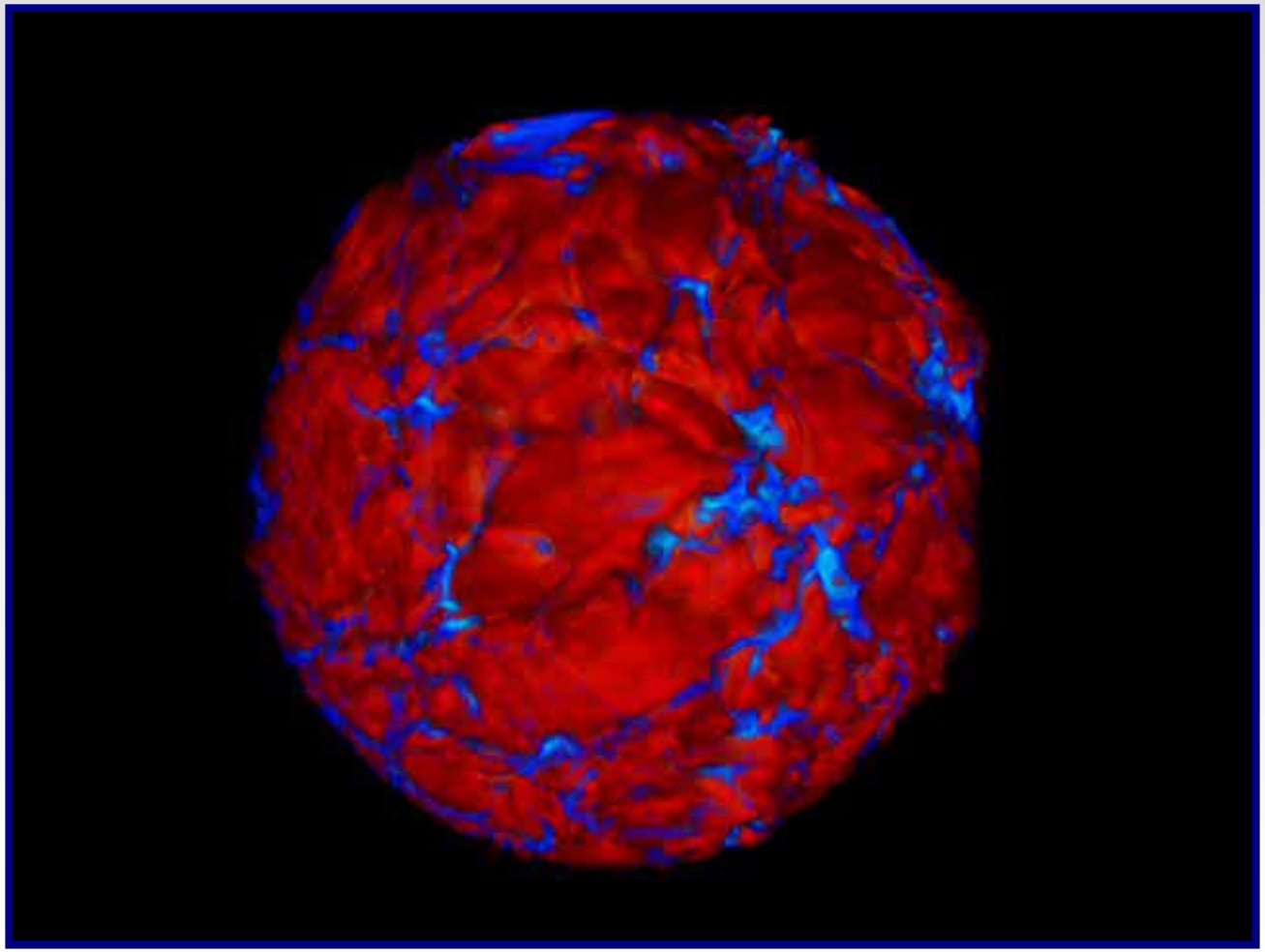
Massive
Single
H-rich



Type Ia

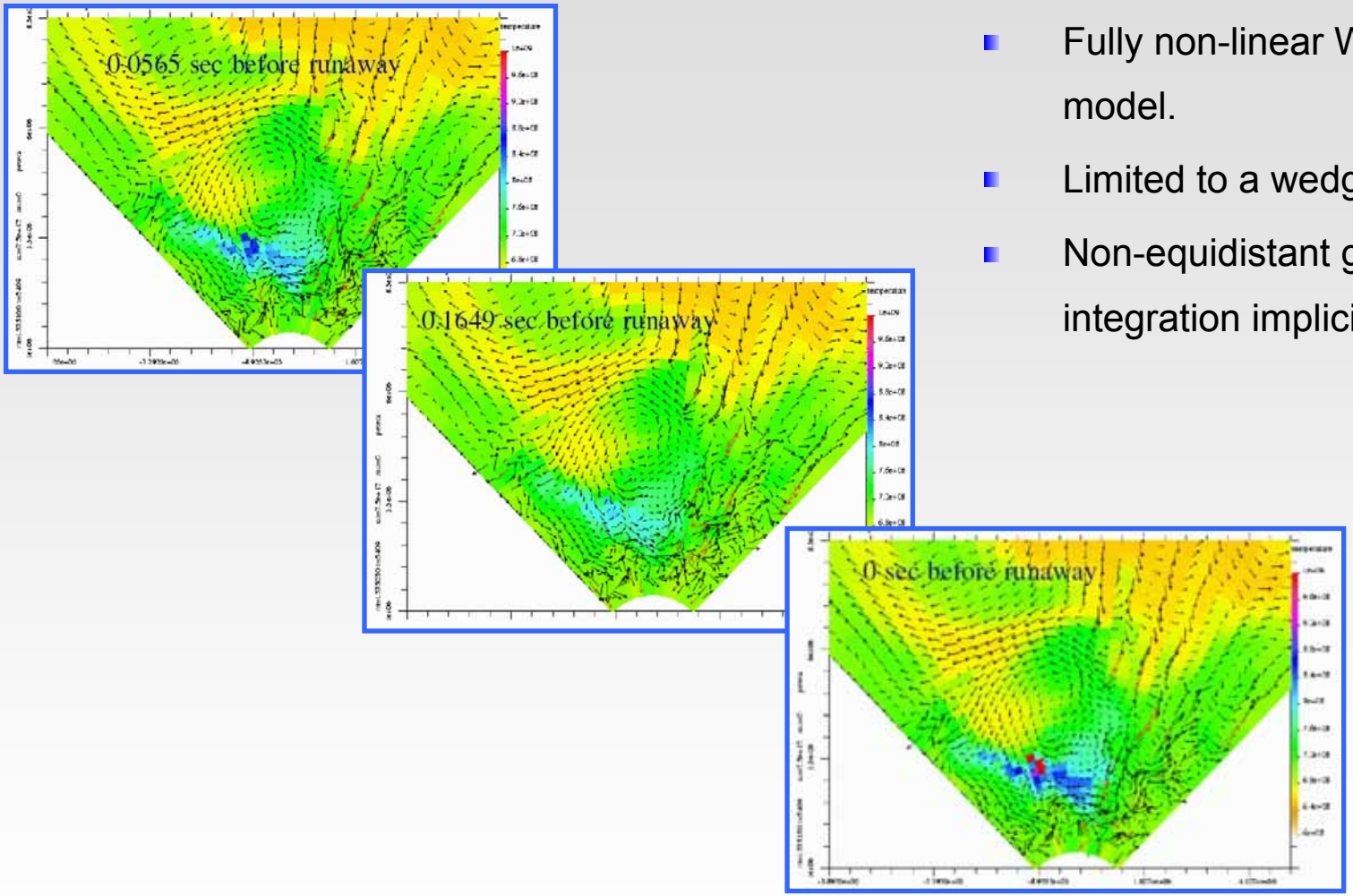
Medium mass
Binary
H/He-free

Giant Convective Star



Woodward et al. (2000)

Thermonuclear SN Ignition Phase



- Fully non-linear WD core model.
- Limited to a wedge in 2D.
- Non-equidistant grid, integration implicit in time.

Höflich & Stein (2002)

Importance of Nuclear Physics

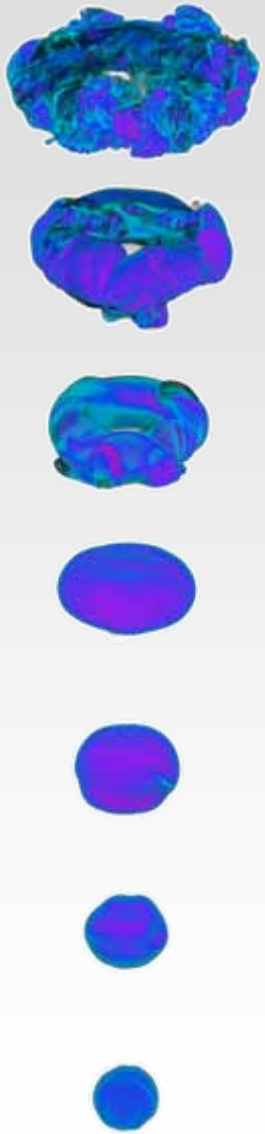
INFLUENCE OF ENHANCEMENT FACTOR f
ONSET OF RUNAWAY

Factor f	C (percent)	r(ignition) (km)
+ 200	26±1	90
+ 50	32.5	86
+ 20	35.5	71
+ 4	36.2	32
+ 1	37.0	27

Höflich & Stein (2002)

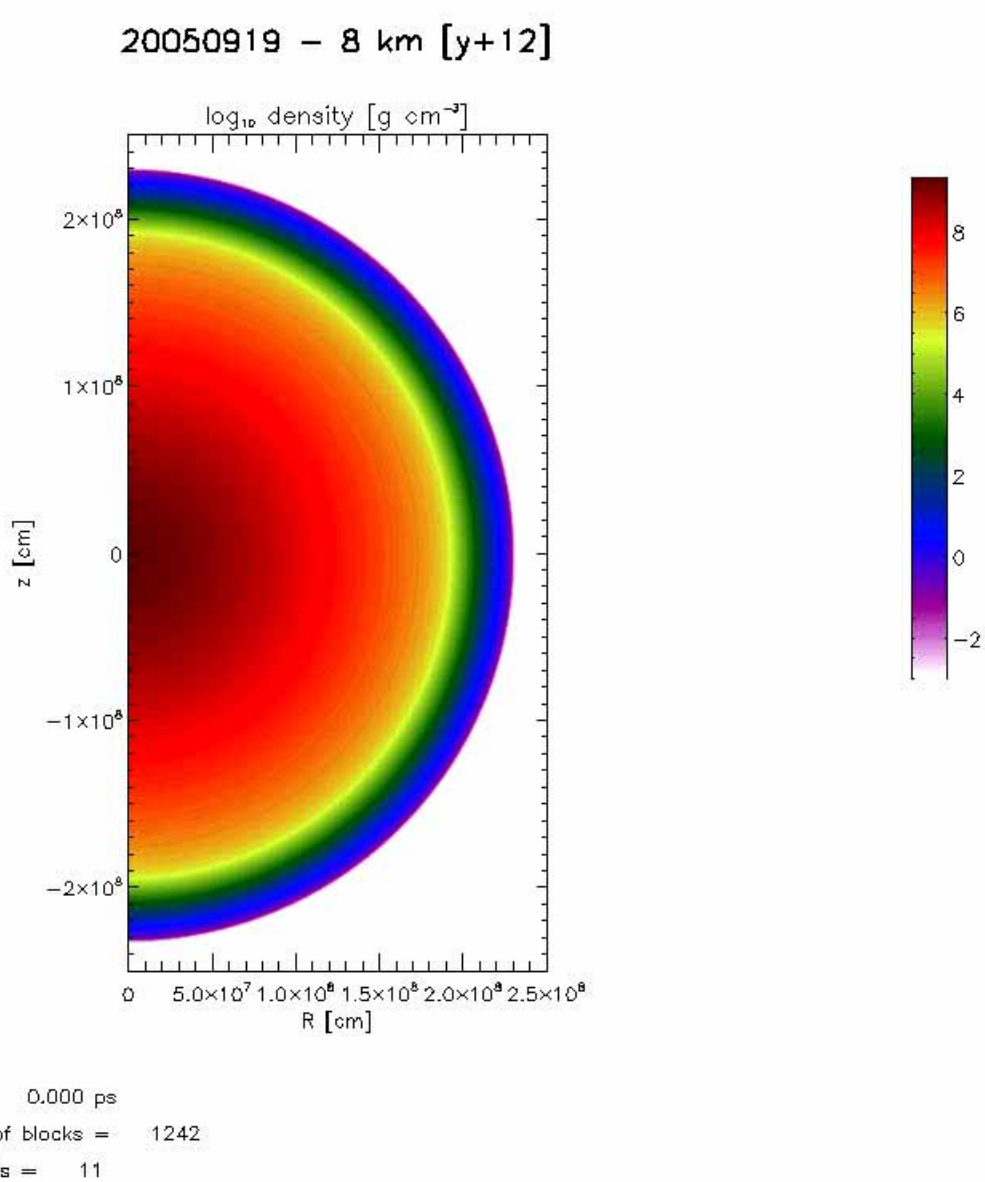
Lessons Learned

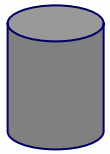
- Ignition at a single point away from the geometric center
- Ignition geometry controlled by reaction rates
- Rotation likely to change flow pattern inducing more small scales
- Highly time-dependent process



Zingale et al. (2006)

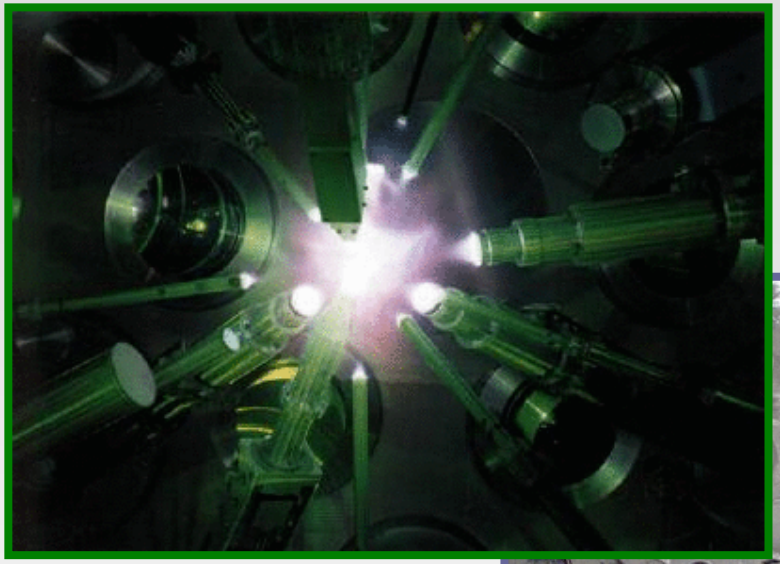
Single-Point Off-Center Ignition



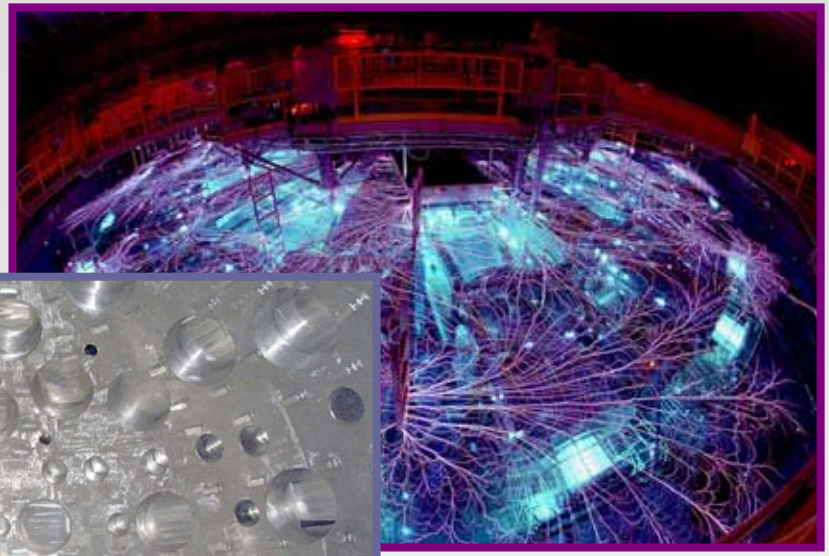


Plewa (2006)

Flavor of Inertial Confinement Fusion

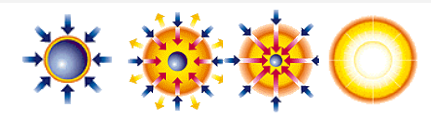


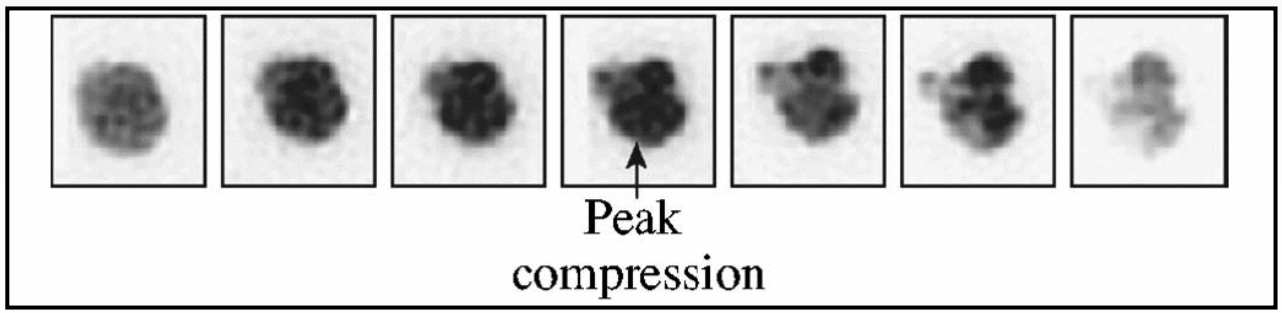
Omega/Rochester



Z-machine/SNL

NIF/LLNL

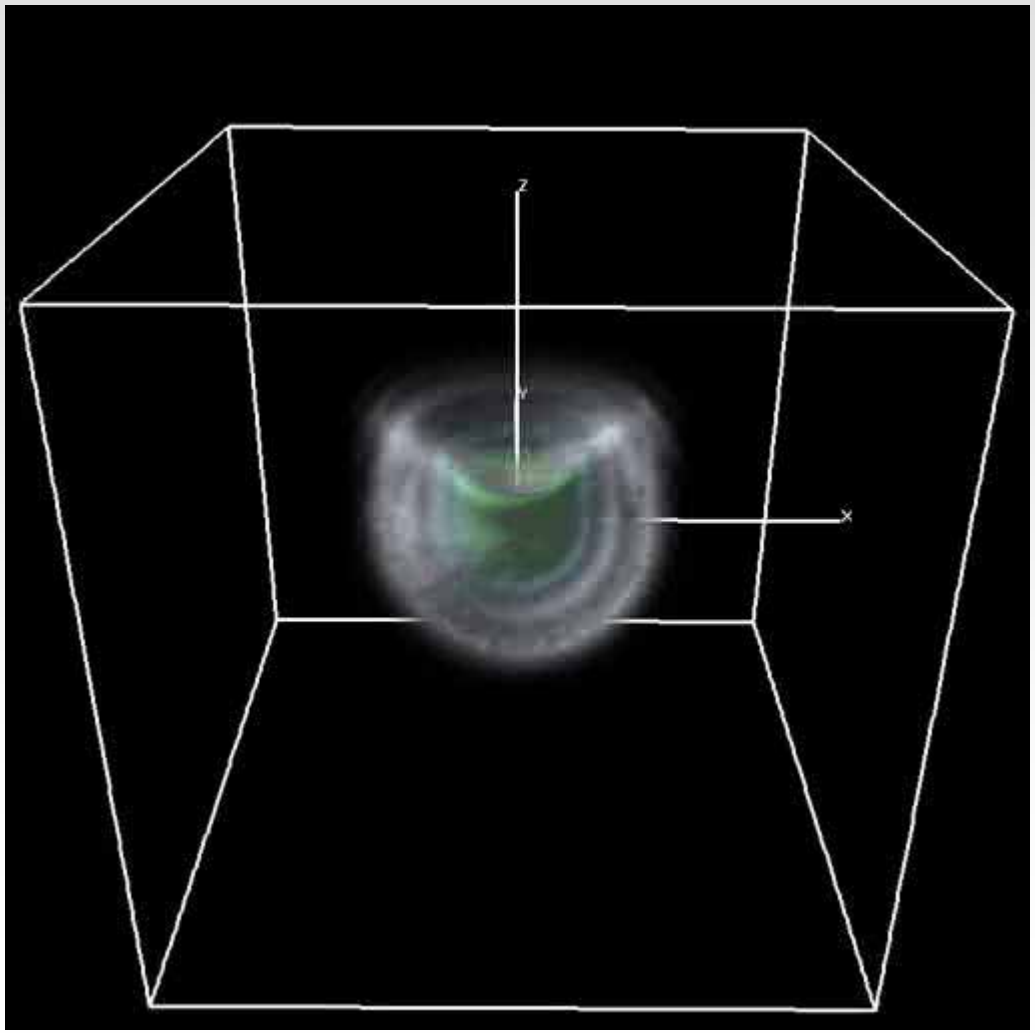




Smalyuk et al. (2007)

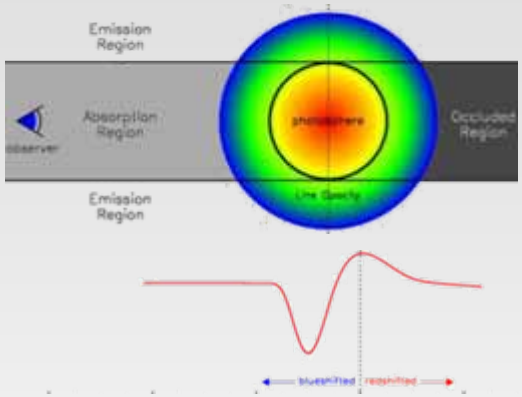
Model Validation – Radiative Transfer

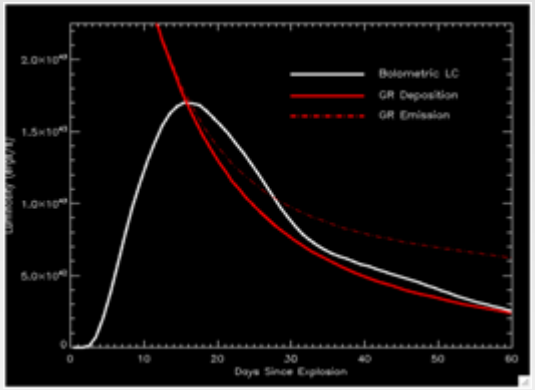
Kasen, Thomas, & Nugent (2006): Multi-dimensional time-dependent Monte Carlo radiative transfer

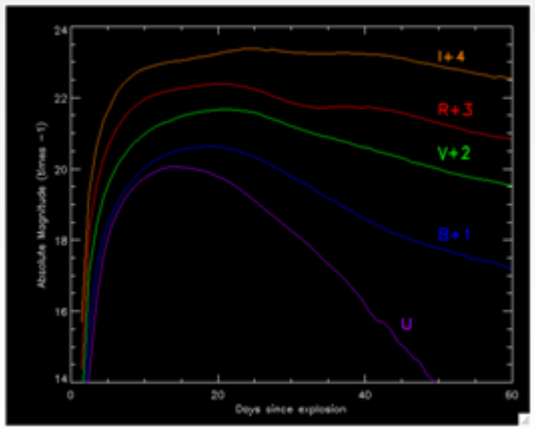


Supernova Model Observables

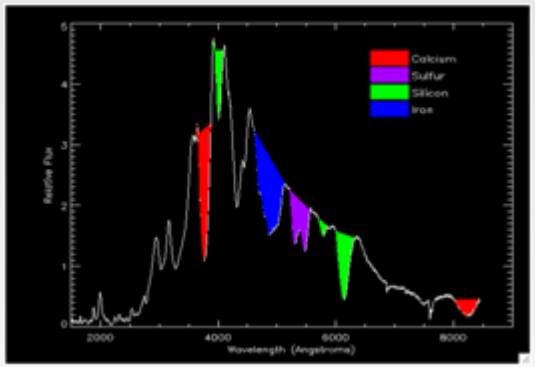
Kasen, Thomas, & Nugent (2006): Multi-dimensional time-dependent Monte Carlo radiative transfer

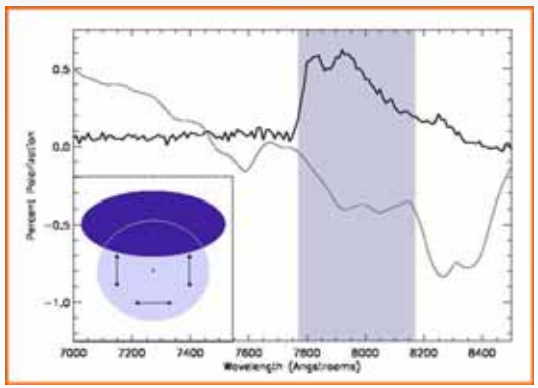




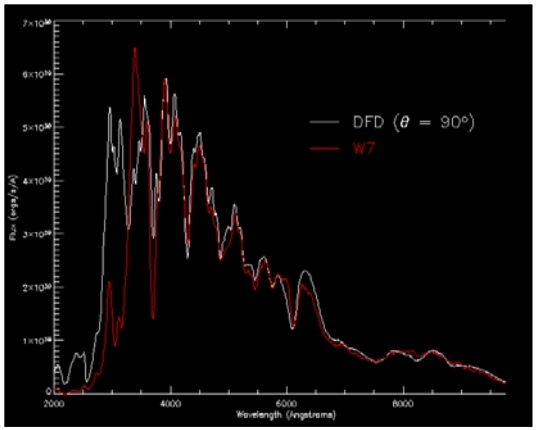


PCA spectrum analysis

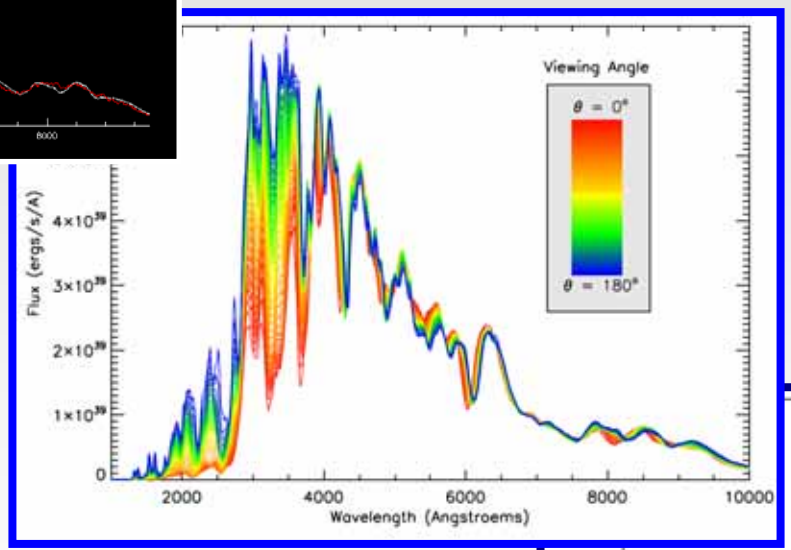




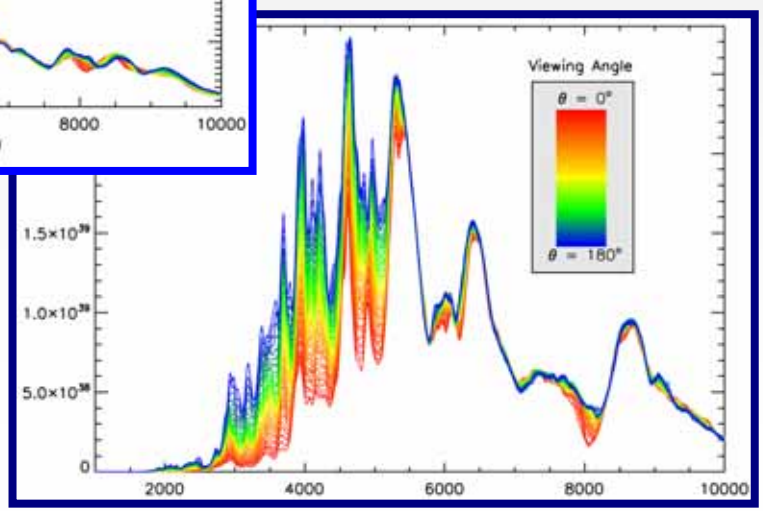
SN Model Validation: Spectroscopy



Y12 @ B_{max}



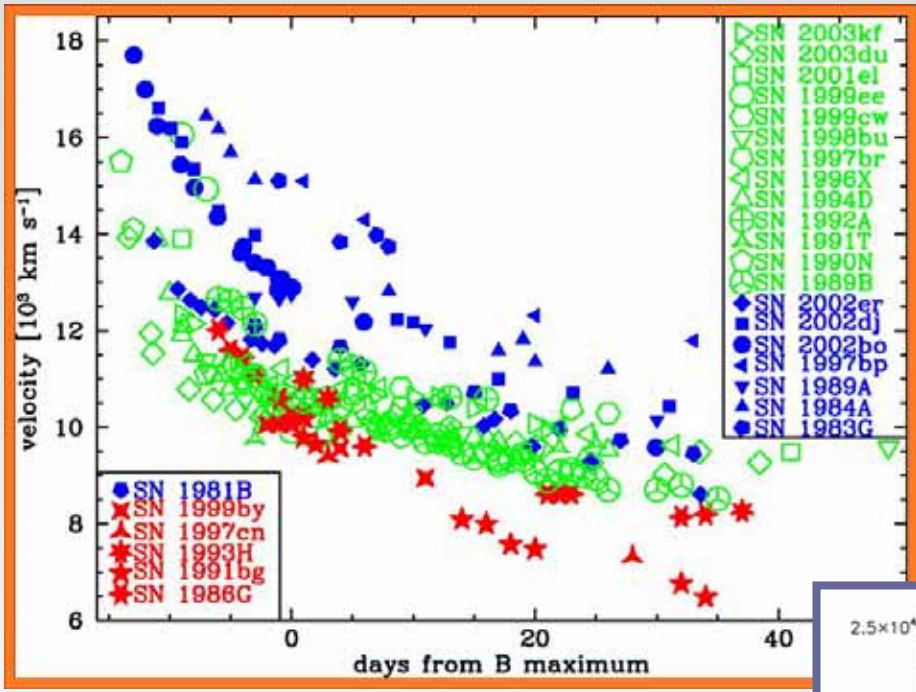
Y12 @ B_{max} + 14



Kasen & Plewa (2007)

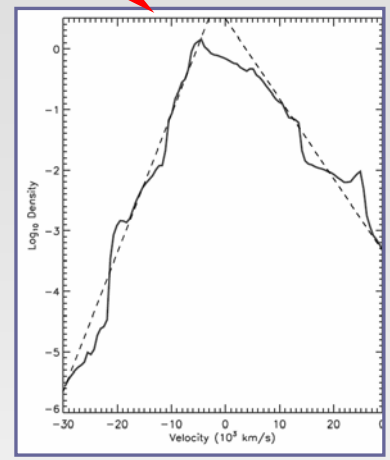
Aspherical IGE core
controlled by the deflagration phase in the DFD model

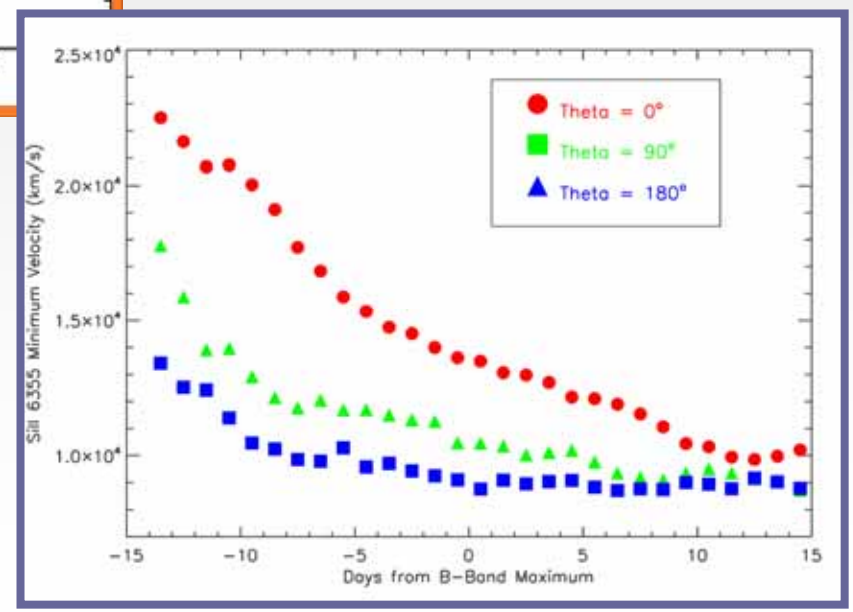
SN Model Validation: Velocity Evolution



Benetti et al. (2005)

7,000 km/s 13,000 km/s

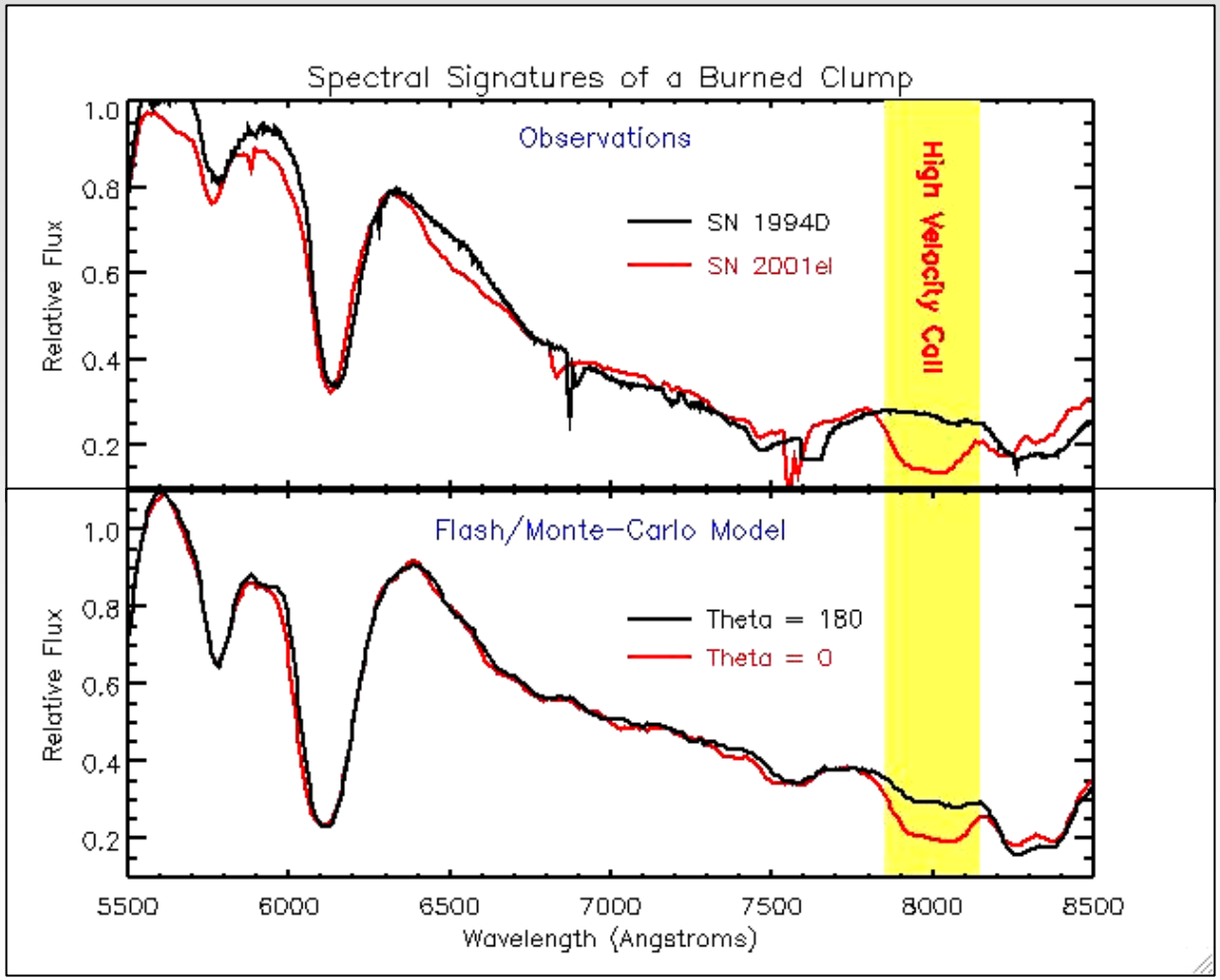




Kasen & Plewa (2007)

Orientation effects
controlled by the deflagration phase in the DFD model

SN Model Validation: Spectral Features



Kasen & Plewa (2005)

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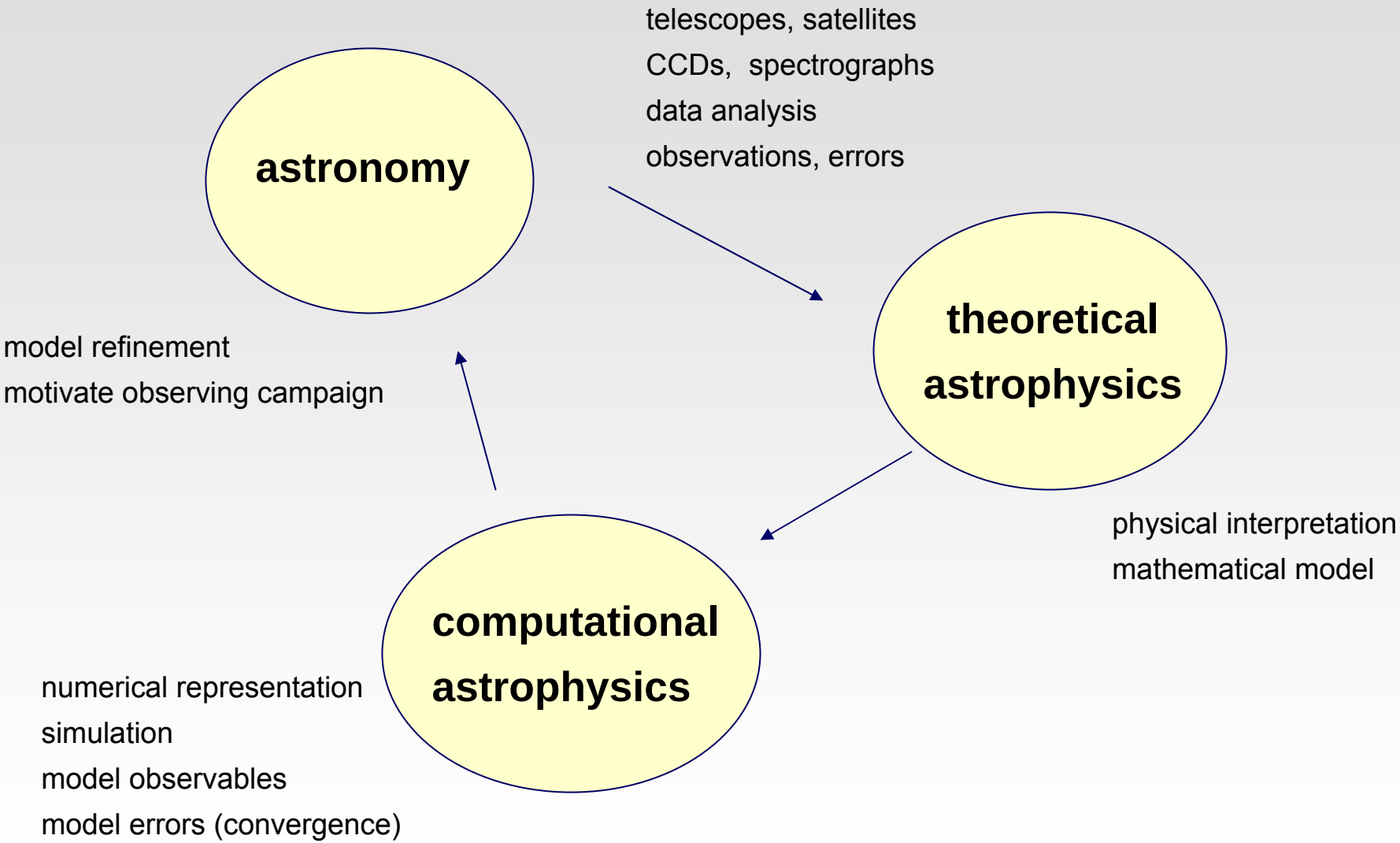
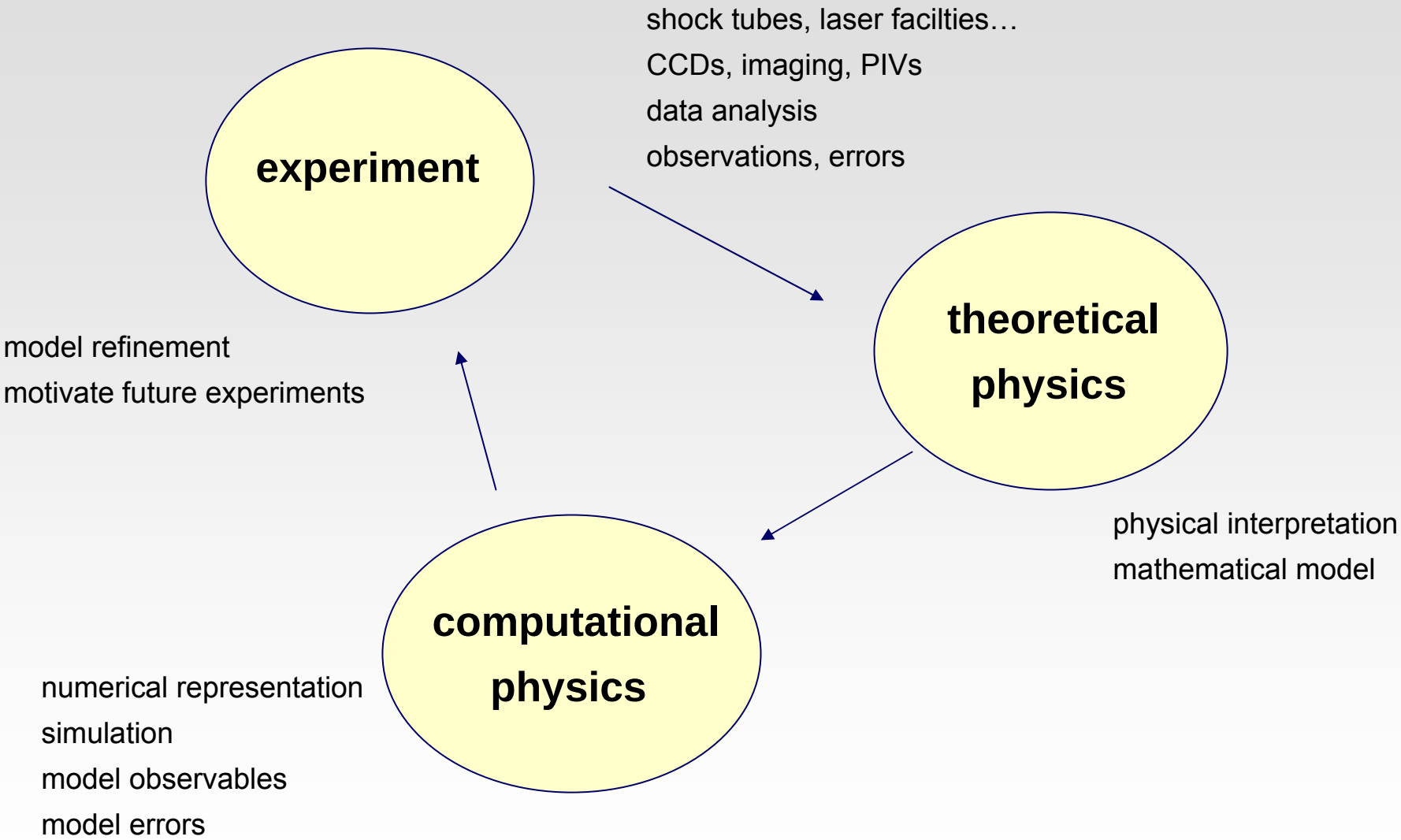
Astrophysics

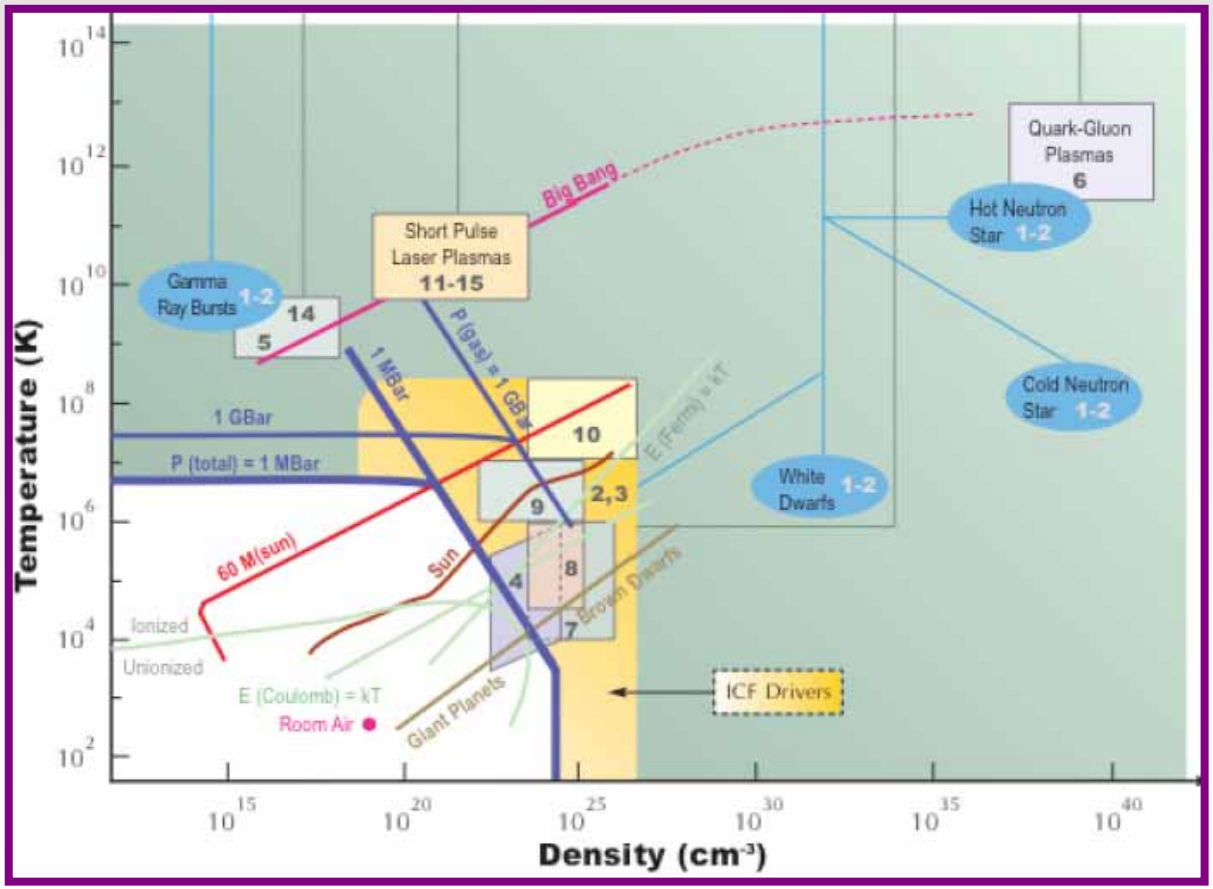


Laboratory Physics



Laboratory Astrophysics

- Astrophysical conditions typically require **very high energy densities**: accessible on lasers (Omega, NIF, Z machine)



Davidson et al. (2004)

High-Energy Density Physics References

Connecting Quarks with the Cosmos (NRC 2002)

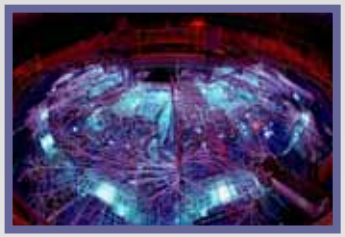
High Energy Density Physics: The X-Games of Contemporary Science (NRC 2003)

The Physics of the Universe (NSTC 2004)

Frontiers for Discovery in High Energy Density Physics (OSTP 2004)

Report of the Dark Energy Task Force (DOE/NASA/NSF 2006)

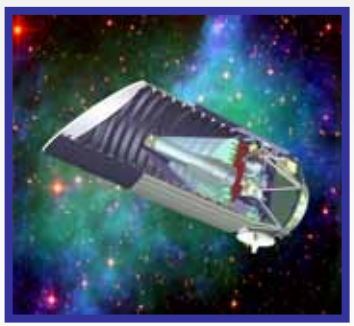
HEDP Experiments

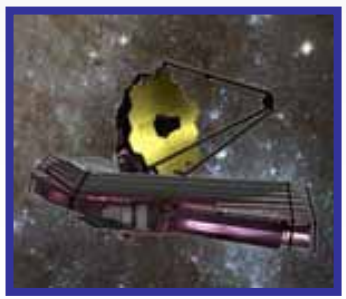


- Heavy ion and particle accelerators (RHIC, RIA…)
- MRI experiments (stellar formation and collapse, jets)
- High energy density physics experiments (U.S., France, UK, Japan, NIF 2011?)
- NIF nuclear physics initiative (LLNL workshop)

Dark-energy related astronomical missions:

- SDSS, SNLS, SN Factory, ESSENCE, HST…
- LSST, Pan-STARRS, South Pole Telescope, GSMT…
- JDEM (2014?), Constellation-X
- JWST (2013?)





High-Energy Density Laboratory Astrophysics

Ablation	nebulae, molecular clouds
Equation of state	planetary interiors
Jets	protostars, active galaxies
Magnetic dynamo	stellar physics, accretion disks
Magnetic reconnection	solar physics, ISM
Nuclear cross sections	stellar evolution, nova/SN/xrb/GRB/etc
Opacities	radiatively driven winds
Particle acceleration	solar physics, SN remnants
Plasma emission	interstellar medium, X-ray binaries
Radiative shocks	SN explosions/remnants, jets, ISM
RMI/RTI interface dynamics	supernovae, stellar interiors
Ultrastrong fields	pulsars, magnetars, GRBs…

HEDLA bi-annual conferences

HEDLA08, March 2008, Caltech (www.hedla.org)

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Discussion

Computational Astrophysics Community

Funding level per group	small
Group size	small
Group expertise	limited
Number of groups	large
Project term	short
Intellectual property protection levels	high
Cross-verification abilities	low
Reusability factor	high
Discovery/funding prospects correlation	high

Example: Photoionization

A photon dominated region code comparison study

Röllig, Abel, Bell, et al., 2006, A&A, 467, 187

We present a comparison between independent computer codes, modeling the physics and chemistry of interstellar photon dominated regions (PDRs). Our goal was to understand the mutual differences in the PDR codes and their effects on the physical and chemical structure of the model clouds, and to converge the output of different codes to a common solution. […]

We established a comprehensive set of reference models for ongoing and future PDR model bench-marking and were able to increase the agreement in model predictions for all benchmark models significantly. Nevertheless, the remaining spread in the computed observables such as the atomic fine-structure line intensities serves as a warning that there is still a considerable uncertainty when interpreting astronomical data with our models.

Example: Cosmology

The Santa Barbara cluster comparison project: a comparison of cosmological hydrodynamics solutions

Frenk, White, Bode, et al., 1999, ApJ, 525, 554

We have simulated the formation of an X-ray cluster in a cold dark matter universe using 12 different codes. The codes span the range of numerical techniques and implementations currently in use, including smoothed particle hydrodynamics (SPH) and grid methods with fixed, deformable, or multilevel meshes. The goal of this comparison is to assess the reliability of cosmological gasdynamical simulations of clusters in the simplest astrophysically relevant case, that in which the gas is assumed to be nonradiative. We compare images of the cluster at different epochs, global properties such as mass, temperature and X-ray luminosity, and radial profiles of various dynamical and thermodynamical quantities. On the whole, the agreement among the various simulations is gratifying, although a number of discrepancies exist. Agreement is best for properties of the dark matter and worst for the total X-ray luminosity. Even in this case, simulations that adequately resolve the core radius of the gas distribution predict total X-ray luminosities that agree to within a factor of 2. Other quantities are reproduced to much higher accuracy. For example, the temperature and gas mass fraction within the virial radius agree to within about 10%, and the ratio of specific dark matter kinetic to gas thermal energies agree to within about 5%. Various factors, including differences in the internal timing of the simulations, contribute to the spread in calculated cluster properties. Based on the overall consistency of results, we discuss a number of general properties of the cluster we have modeled.

Example: Protoplanetary Disks

A comparative study of disc-planet interaction

de Val-Borro, Edgar, Artymowicz, et al., 2006, MNRAS, 370, 529

We perform numerical simulations of a disc-planet system using various grid-based and smoothed particle hydrodynamics (SPH) codes. The tests are run for a simple setup where Jupiter and Neptune mass planets on a circular orbit open a gap in a protoplanetary disc during a few hundred orbital periods. We compare the surface density contours, potential vorticity and smoothed radial profiles at several times. The disc mass and gravitational torque time evolution are analysed with high temporal resolution. There is overall consistency between the codes. The density profiles agree within about 5 per cent for the Eulerian simulations. The SPH results predict the correct shape of the gap although have less resolution in the low-density regions and weaker planetary wakes. The disc masses after 200 orbital periods agree within 10 per cent. The spread is larger in the tidal torques acting on the planet which agree within a factor of 2 at the end of the simulation. In the Neptune case, the dispersion in the torques is greater than for Jupiter, possibly owing to the contribution from the not completely cleared region close to the planet.

Example: Shock-cloud Interaction

Experiment on the mass stripping of an interstellar cloud following shock passage

Hansen, Robey, Klein, & Miles, 2007, ApJ, 662, 379

The interaction of supernova shocks and interstellar clouds is an important astrophysical phenomenon which can lead to mass stripping (transfer of material from cloud to surrounding flow, ``mass loading'' the flow) and possibly increase the compression in the cloud to high enough densities to trigger star formation. Our experiments attempt to simulate and quantify the mass stripping as it occurs when a shock passes through interstellar clouds. We drive a strong shock (and blast wave) using 5 kJ of the 30 kJ Omega laser into a cylinder filled with low-density foam with an embedded 120 μm Al sphere simulating an interstellar cloud. The density ratio between Al and foam is ~9. Time-resolved X-ray radiographs show the cloud getting compressed by the shock (t~5 ns), undergoing a classical Kelvin-Helmholtz roll-up (12 ns) followed by a Widnall instability (30 ns), an inherently three-dimensional effect that breaks the two-dimensional symmetry of the experiment. Material is continuously being stripped from the cloud at a rate which is shown to be considerably larger than what is predicted by laminar models for mass stripping; the cloud is fully stripped by 80-100 ns, 10 times faster than the laminar model. We present a new model for turbulent mass stripping that agrees with the observed rate and that should scale to astrophysical conditions, which occur at even higher Reynolds numbers than the current experiment.

Example: Core-collapse SN radhydro

Supernova simulations with Boltzmann neutrino transport: A comparison of methods

Liebendörfer, Rampp, Janka, & Mezzacappa, 2005, ApJ, 620, 379

Accurate neutrino transport has been built into spherically symmetric simulations of stellar core collapse and postbounce evolution. The results of such simulations agree that spherically symmetric models with standard microphysical input fail to explode by the delayed, neutrino-driven mechanism. Independent groups implemented fundamentally different numerical methods to tackle the Boltzmann neutrino transport equation. Here we present a direct and detailed comparison of such neutrino radiation-hydrodynamics simulations for two codes, AGILE-BOLTZTRAN of the Oak Ridge-Basel group and VERTEX of the Garching group. The former solves the Boltzmann equation directly by an implicit, general relativistic discrete-angle method on the adaptive grid of a conservative implicit hydrodynamics code with second-order TVD advection. In contrast, the latter couples a variable Eddington factor technique with an explicit, moving-grid, conservative high-order Riemann solver with important relativistic effects treated by an effective gravitational potential. The presented study is meant to test our neutrino radiation-hydrodynamics implementations and to provide a data basis for comparisons and verifications of supernova codes to be developed in the future. Results are discussed for simulations of the core collapse and postbounce evolution of a 13 M_{solar} star with Newtonian gravity and a 15 M_{solar} star with relativistic gravity.

Typical UQ Example #1

Sensitivity of p-process nucleosynthesis to nuclear reaction rates in a 25 M supernova model

Rapp, Görres, Wiescher, et al., 2006, ApJ, 653, 474

The astrophysical *p*-process, which is responsible for the origin of the proton-rich stable nuclei heavier than iron, was investigated using a full nuclear reaction network for a Type II supernova explosion when the shock front passes through the O/Ne layer. Calculations were performed with a multilayer model adopting the seed of a preexplosion evolution of a 25 *M* star. The reaction flux was calculated to determine the main reaction path and branching points responsible for synthesizing the proton-rich nuclei. In order to investigate the impact of nuclear reaction rates on the predicted *p*-process abundances, extensive simulations with different sets of collectively and individually modified neutron-, proton-, and -capture and photodisintegration rates have been performed. These results are not only relevant to explore the nuclear-physics-related uncertainties in *p*-process calculations but are also important for identifying the strategy and planning of future experiments.

Typical UQ Example #2

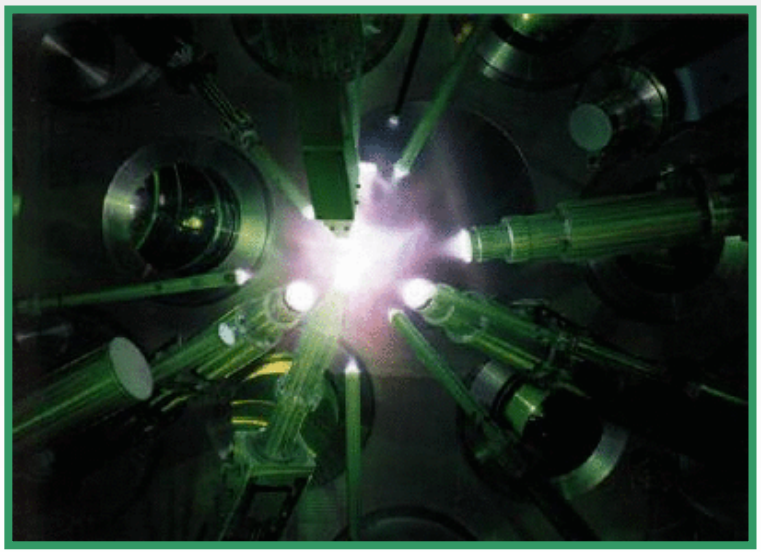
On Variations in the Peak Luminosity of Type Ia Supernovae

Timmes, Brown, & Truran 2003, ApJ, 590, L83

We explore the idea that the observed variations in the peak luminosities of Type Ia supernovae (SNe Ia) originate in part from a scatter in metallicity of the main-sequence stars that become white dwarfs. Previous numerical studies have not self-consistently explored metallicities greater than solar. One-dimensional Chandrasekhar mass models of SNe Ia produce most of their ^{56}Ni in a burn to nuclear statistical equilibrium between the mass shells 0.2 and 0.8 M , for which the electron-to-nucleon ratio Y_e is constant during the burn. We show analytically that under these conditions, charge and mass conservation constrain the mass of ^{56}Ni produced to depend *linearly* on the original metallicity of the white dwarf progenitor. Detailed postprocessing of W7-like models confirms this linear dependence. The effect that we have identified is most evident at metallicities larger than solar and is in agreement with previous self-consistent calculations over the metallicity range common to both calculations. The observed scatter in the metallicity (3 Z) of the solar neighborhood is enough to induce a 25% variation in the mass of ^{56}Ni ejected by SNe Ia. This is sufficient to vary the peak V-band brightness by $|M_V|$ 0.2. This scatter in metallicity is present out to the limiting redshifts of current observations (z 1). Sedimentation of ^{22}Ne can possibly amplify the variation in ^{56}Ni mass to 50%. Further numerical studies can determine if other metallicity-induced effects, such as a change in the mass of the ^{56}Ni-producing region, offset or enhance the variation that we identify.

Example: Supernova in the Lab

- **Rayleigh-Taylor instability** dominates evolution of the shocked supernova envelope material shortly after shock passage
- Primary suspect for the **observed mixing of radioactive material** from the core into the expanding surface layers
- **Scaling laws** (Ryutov's Ma scaling) allow us to identify similar regime in laboratory environment



LLE Rochester

NIF/LLNL

Example: Supernova RT I. Experiment

Assessing Mix Layer Amplitude in 3D Decelerating Interface Experiments

Kuranz, Drake, Dojanowski, et al., 2007, Ap&SS, 307, 115

We present data from recent high-energy-density laboratory experiments designed to explore the Rayleigh Taylor instability under conditions relevant to supernovae. The Omega laser is used to create a blast wave structure that is similar to that of the explosion phase of a core-collapse supernova. An unstable interface is shocked and then decelerated by the planar blast wave, producing Rayleigh Taylor growth. Recent experiments were performed using dual, side-on, x-ray radiography to observe a 3D “egg crate” mode and an imposed, longer-wavelength, sinusoidal mode as a seed perturbation. This paper explores the method of data analysis and accurately estimating the position of important features in the data.

Example: Supernova RT II. Modeling

Flash Code Simulations of Rayleigh-Taylor and Richtmyer-Meshkov Instabilities in Laser-Driven Experiments

Hearn, Plewa, Drake, Kuranz, 2007, Ap&SS, 307, 227

We present two- and three-dimensional simulations involving Richtmyer Meshkov and Rayleigh-Taylor instabilities run with the adaptive mesh refinement code, flash. Variations in the rate of mixing layer growth due to dimensionality, perturbation modes, and simulation resolution are explored. These simulations are designed for detailed comparisons with experiments run on the Omega laser to gain understanding of the mixing processes and to prepare for validation of the Flash code.

Supernovae and Gamma-ray Bursts

- Some of the brightest objects in the Universe, transient
  - Important for cosmology
  - Important for chemical evolution of the Universe
  - But also basic physics
    - Nuclear physics
    - Combustion physics
    - Neutrino physics
    - GR
    - Dark matter

Supernovae and GRBs

Detection

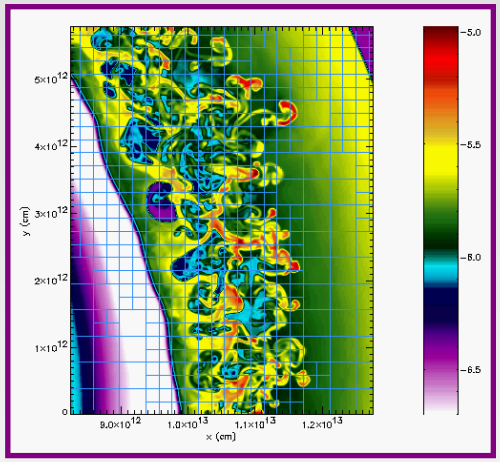
- Telescopes (optical, IR, submm, radio)
- Satellites (optical, IR, xray, gamma ray)
- Sources of gravity waves (LIGO, space interferometry)

Riess et al. (2006)

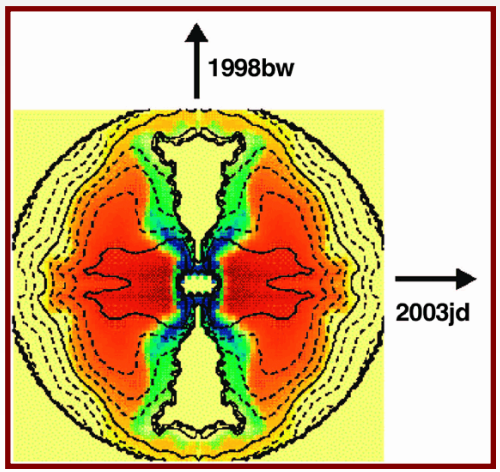
Supernovae and GRBs Numerics

Extremely rich platform for developing simulation technologies.

- **Adaptive discretization**
  - High-order schemes for compressible hydro
- **Radiation transport**
  - Multigrid, linear systems, Boltzmann
- **Thermonunclear physics**
  - Implicit ODE integrators, front tracking
- **Complex EoS**
  - Usually tabulated, fast lookup/consistent interpolation
- **MHD effects**
  - Fast rotation
  - Shear flows
  - Jet formation
- **Relativistic**
  - SR for GRB outflows
  - GR for NS/BH formation



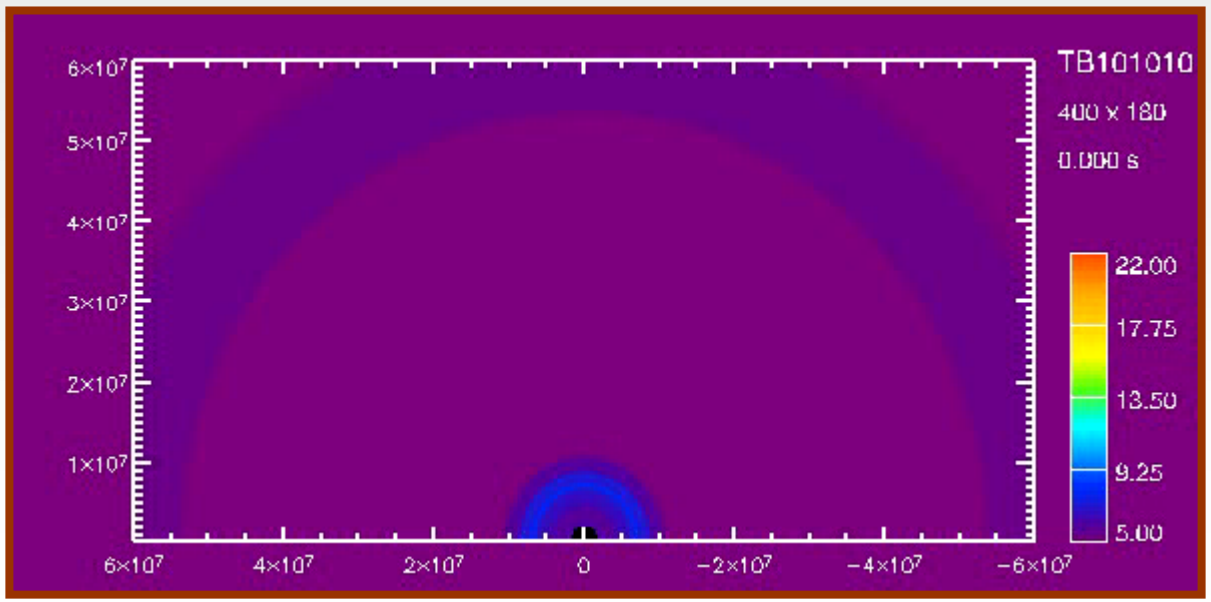
Zingale (2004)



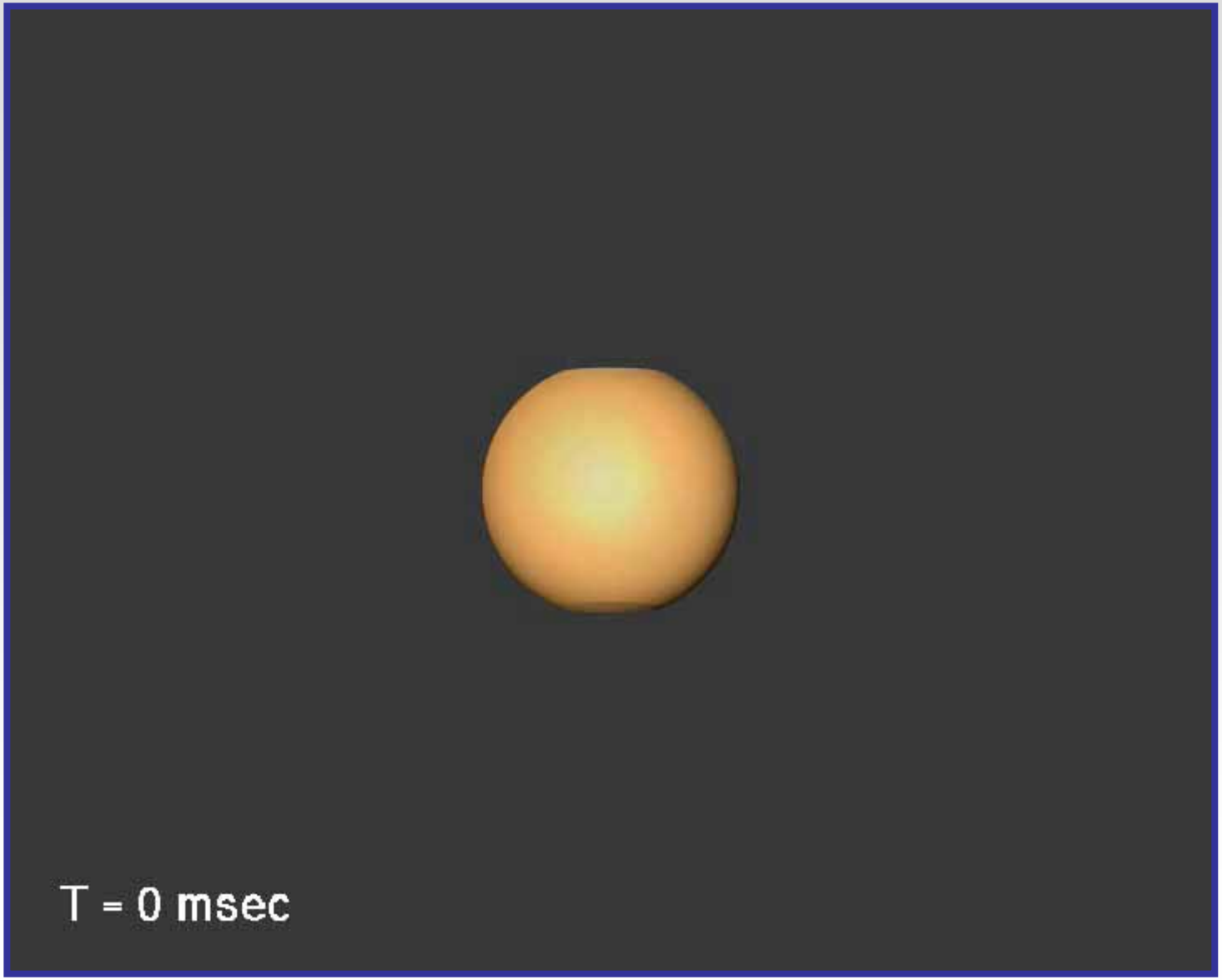
Mazzali et al. (2005)

Core-collapse Supernovae (Type II)

- Massive stars
- Gravity bombs
- Gravitational energy extracted by neutrinos
- Accretion shock originally too weak
- Revived by neutrino heating of the post-shock matter

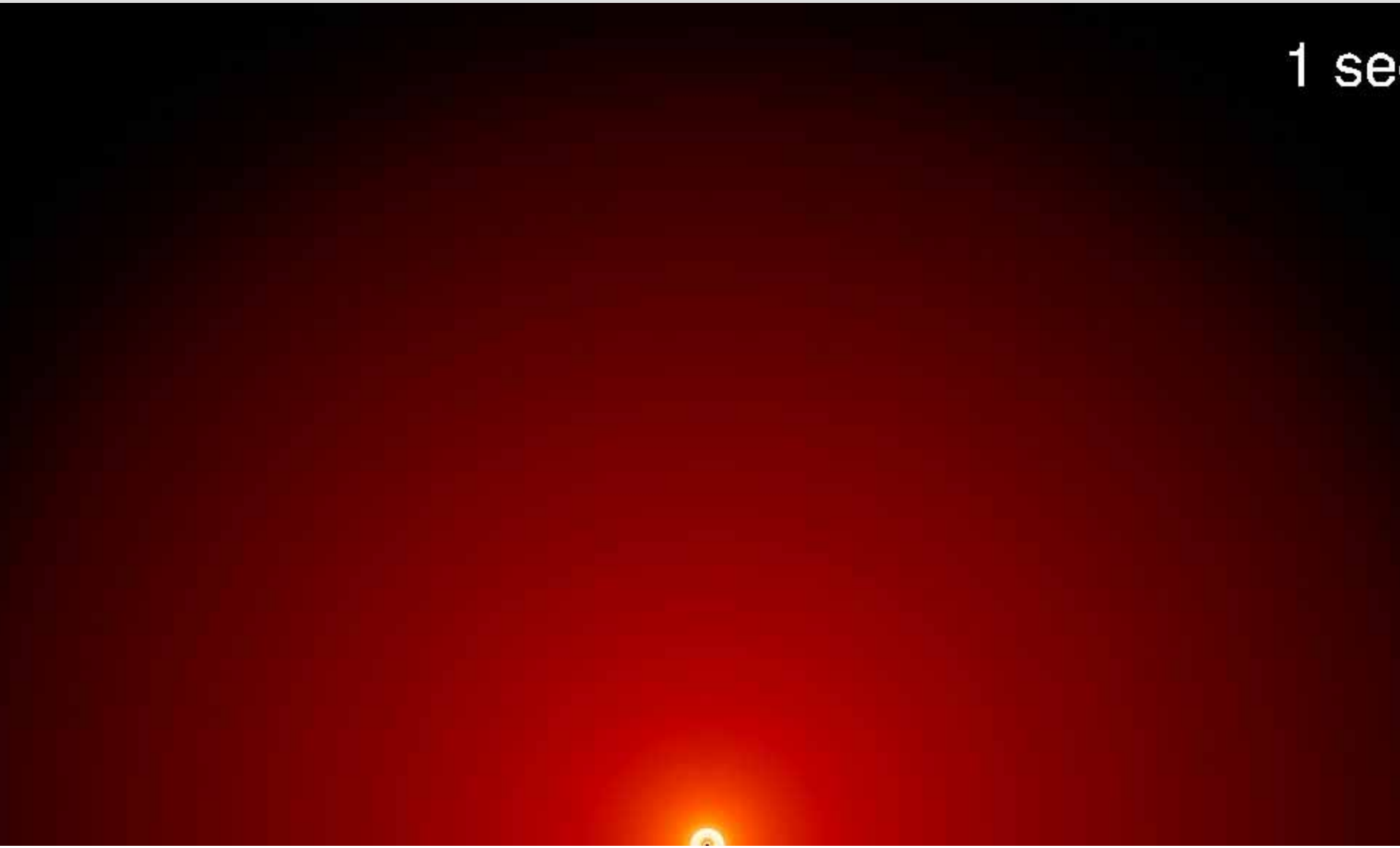


Core-collapse Supernovae (Type II)

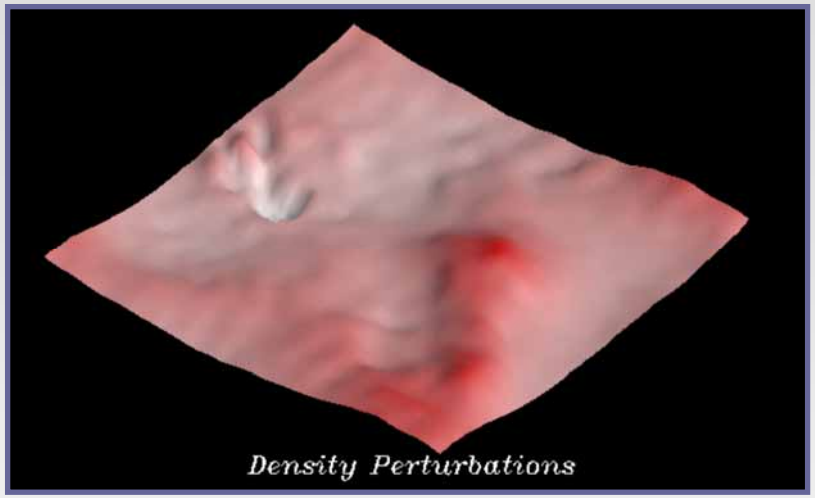


Scheck et al. (2006)

CC SN: Shocking the Envelope

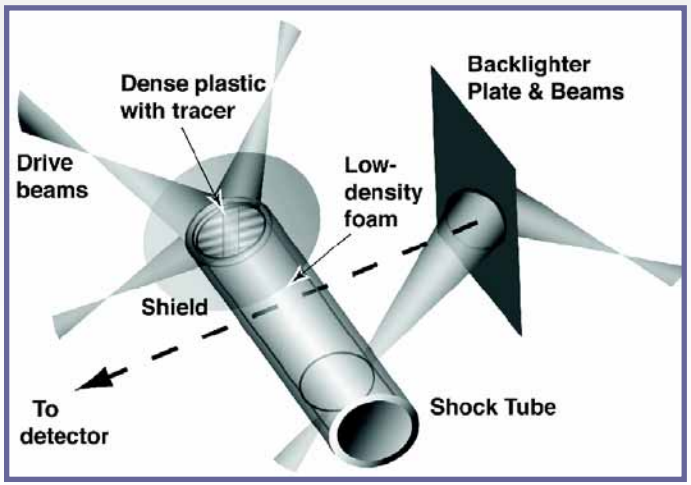


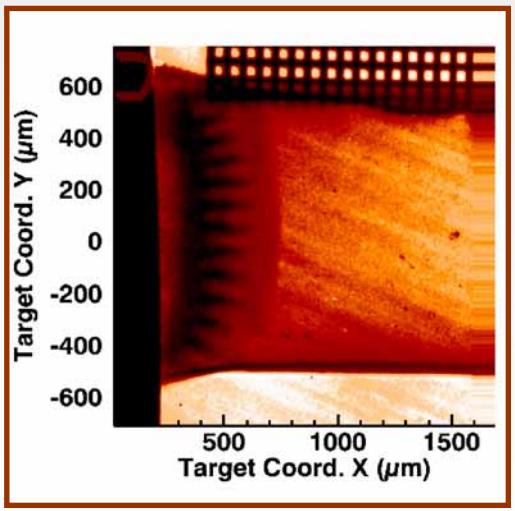
SNRT Project Components



Meakin et al. (2006)

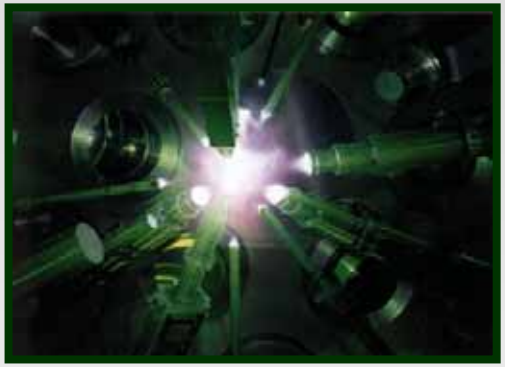
Hearn et al. (2007)





Kuranz et al. (2007)

SNRT Project Outlook



Current Omega shots

- "Realistic" target perturbation definition
- Multidimensional laser pulse shock drive
- Model target improvement

Planning for NIF

- Ignition demonstration still a priority, but…
- Possible demonstration experiments to run early (before 2011)
- Benefits
  - Larger energy
  - Larger volumes
  - Longer timescales
  - Better diagnostic
  - More mass - can use realistic spherical targets!! ☺

Summary

- Notion of V&V in computational astrophysics is present
- Verification uses analytic solutions; (self-)convergence studies done almost exclusively in spatial domain
- Code-to-code comparisons since late1980s; several projects later; growing in popularity
- Validation largely limited to “application to experiment”
- Low relevance is one major factor
- Historically more emphasis on observational rather than laboratory experiments
- UQ is mostly absent due to high “added” cost (a discovery is good enough)

Lessons to Remember

- V&V is a **chain of procedures**
- Need **good validation experiments**
- The most scientifically attractive experiments are not necessarily **good validation experiments**
- Robust, physically-motivated metric
- **Document** anyway: experiments not considered as good validation experiments today may become useful in the future
- **Close interaction with experimentalists**, understanding of experimental parameters
- Making next iteration: modifying experiments based on the simulation results, **closed feedback loop**

Questions and discussion