Present and Future Computing Requirements

Radiative Transfer of Astrophysical Explosions

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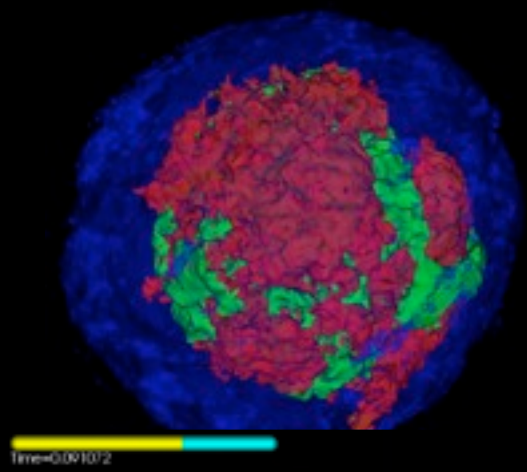
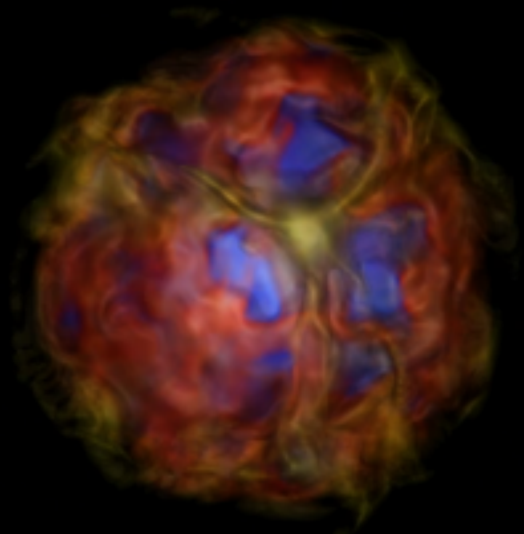
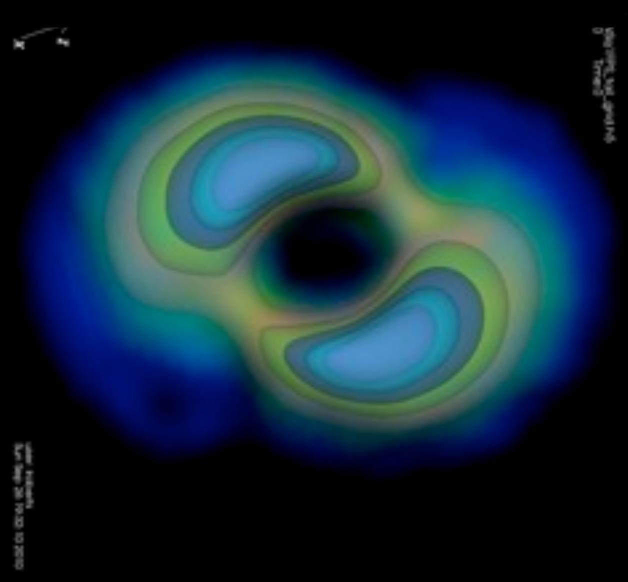
topics and open questions







- thermonuclear supernova:

  What are the progenitors: 1 or 2 white dwarfs?
  How does the nuclear runaway ignite and develop?
  How regular are these "standard candles" for cosmology?

- core collapse supernovae:

  Does the neutrino driven explosion mechanism work?
  How does neutrino physics (e.g., flavor oscillations) affect the observable burst and nucleosynthesis of heavy elements?

- neutron star mergers:

  What amount of heavy elements (r-process) is produced?
  What are the electromagnetic counterparts to these gravitational wave sources?

connect to observatories (PTF, nuStar, LSST),
neutrino detectors, FRIB, GR-wave detectors

Project Overview

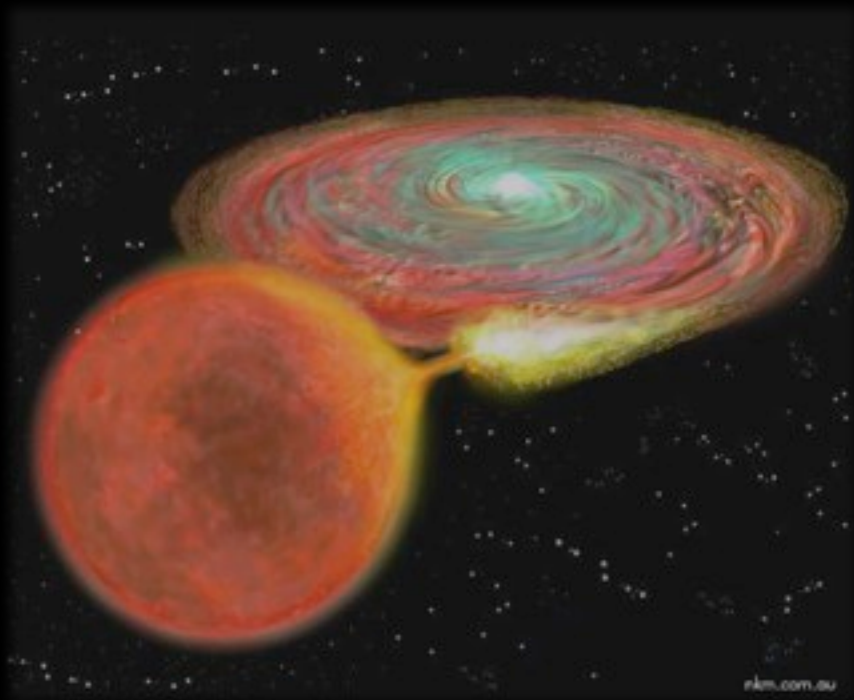
Our goal is to address fundamental questions concerning the nature of supernovae, neutrinos and the nucleosynthesis of the heavy elements using 3-dimensional multi-physics simulations of astrophysical explosions.

We emphasize the prediction of observables (photon/neutrino light curves and spectra) that can be directly compared to observations, in order to validate or falsify competing theoretical scenarios.

Two example goals for next ~3 years

Carry out the 3-D radiation-hydrodynamical simulation of core collapse supernovae with neutrino transport treated in multi-group flux limited diffusion (CASTRO code)

Calculate higher resolution, higher fidelity light curves and spectra (neutrinos and photons) for several 3-D models of all types of supernovae (SEDONA code)



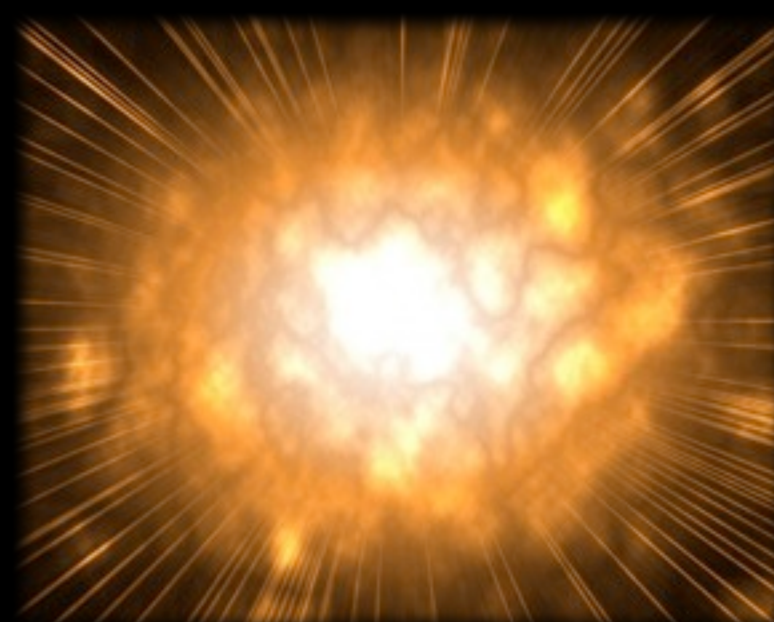
<u>presupernova evolution</u>

<u>stellar evolution & ignition</u>
3-D convection
low mach number
hydrodynamics

e.g., *MAESTRO*

<u>explosion</u>
t ~ seconds/minutes
hydrodynamics (AMR)
gravity
nuclear burning
neutrino transport

e.g. *CASTRO*



<u>light curves/spectra</u>
t ~ months
radioactive decay
gamma-ray/optical photon
transport
(non-equilibrium) atomic
physics

e.g., SEDONA

current HPC methods

Codes

Sedona (implicit monte carlo transport + atomic microphysics)
CASTRO (hydrodynamics + flux limited diffusion)
Maestro (low mach number hydrodynamics)
Phoenix (S_n NLTE radiative transfer)
Nyx (Castro + particle in cell dark matter)

Algorithms used

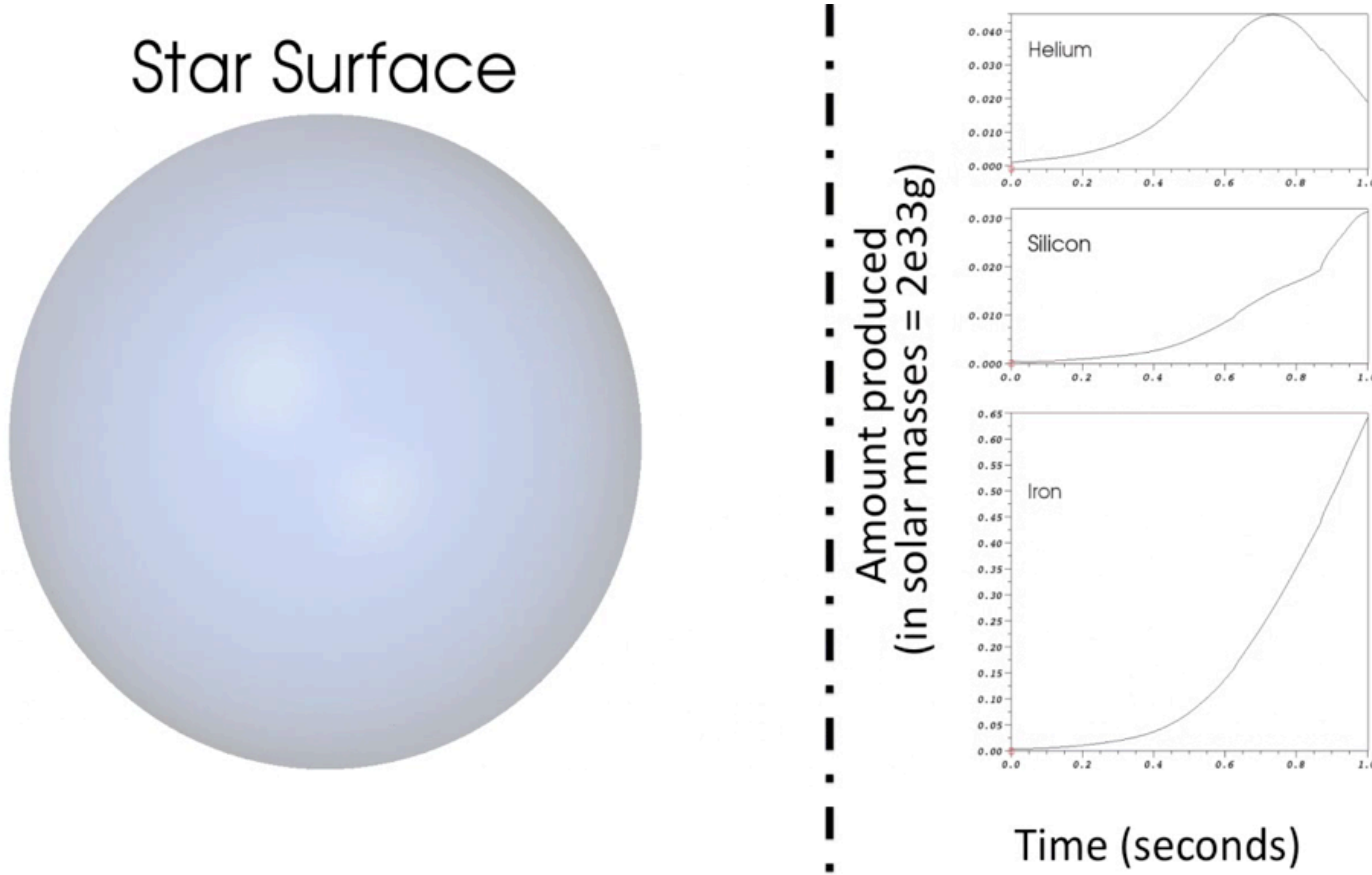
Monte Carlo, multi-grid solvers, sparse matrix solvers
compressible finite volume Godunov hydrodynamics
parallelization: hybrid MPI/OpenMPI

Architectures currently used:

Cray XT4-5, XE6: Franklin, Hopper (NERSC) Jaguar (NCCS)
Linux Clusters @ UCB, LBNL

Quantities affecting problem size:

spatial and wavelength resolution
# of monte carlo particles (signal to noise)
# of atomic lines/levels used for opacity/emissivity calculation

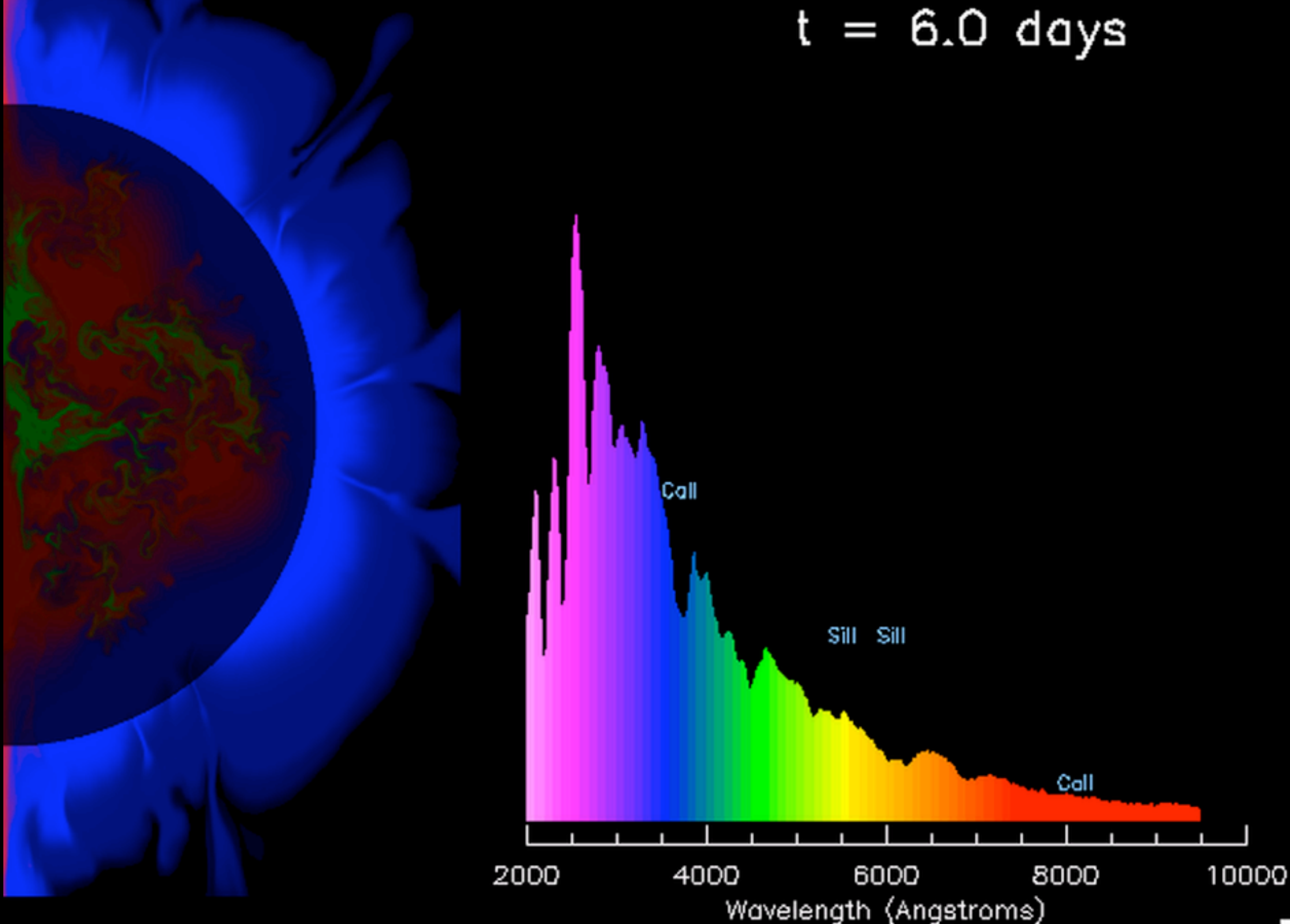


deflagration model of a type Ia supernova with CASTRO

credit: Hank Childs, Haitao Ma, Stan Woosley

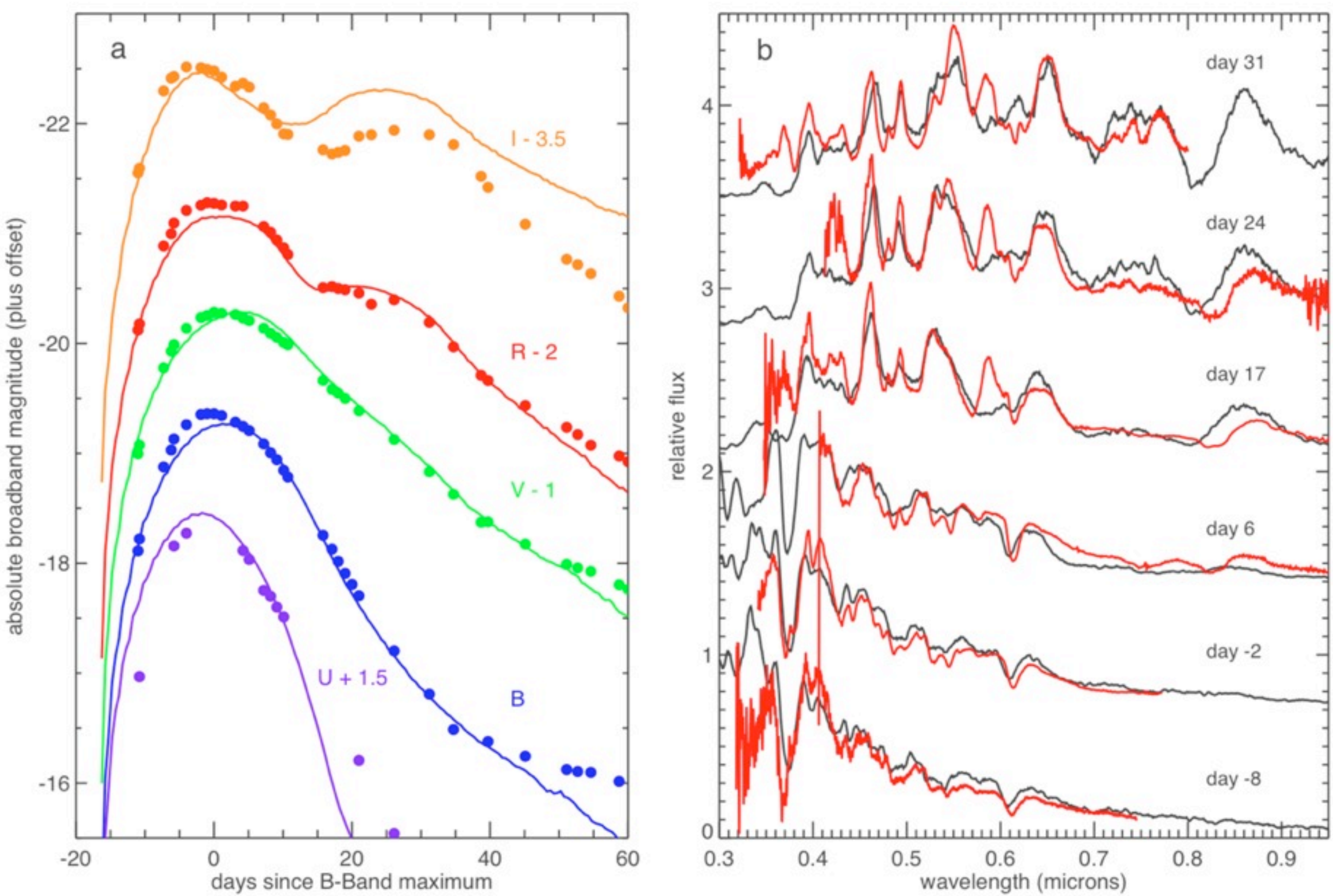
SEDONA light curve/spectrum calculation

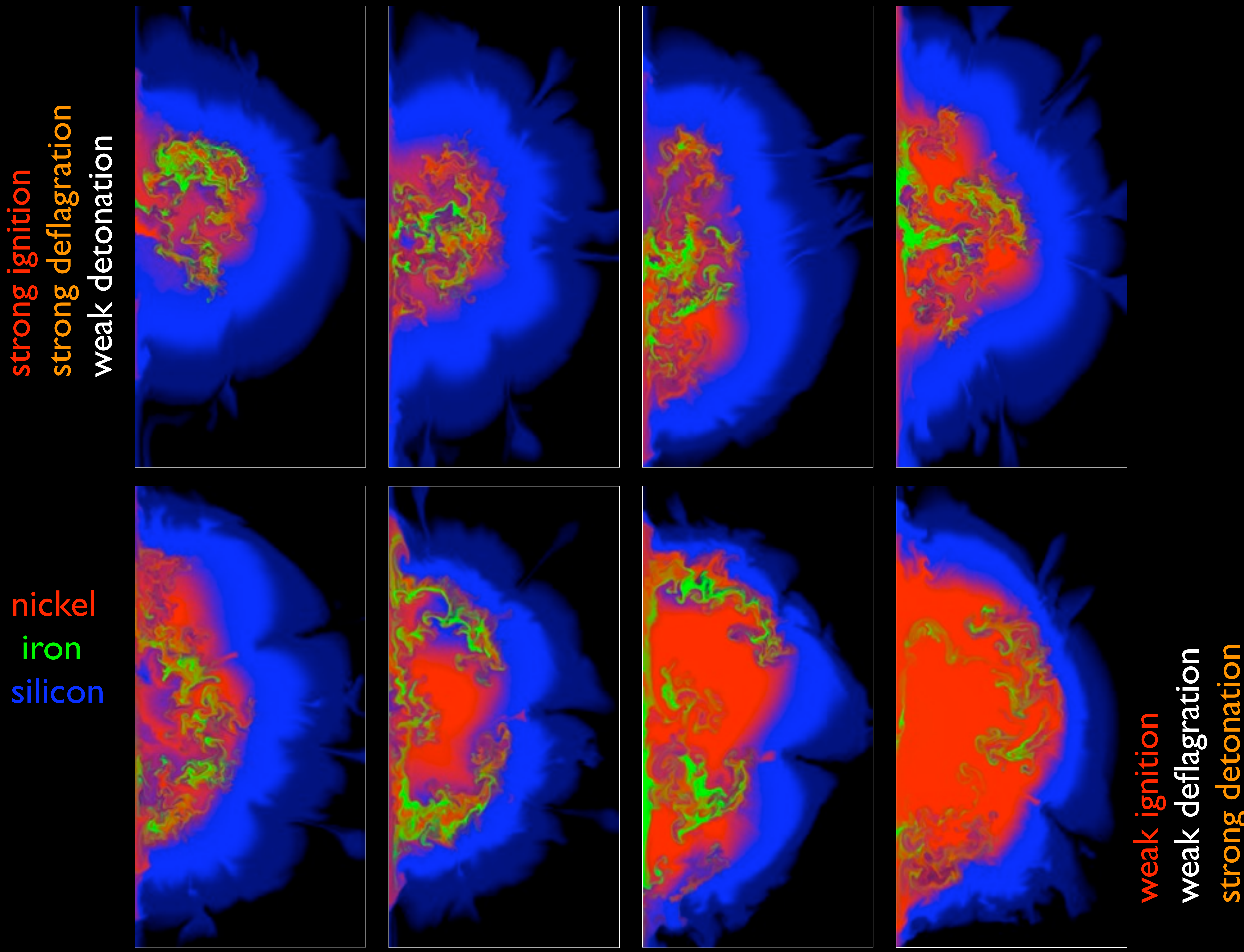
SEDONA light curve/spectrum calculation



validation against astronomical observation

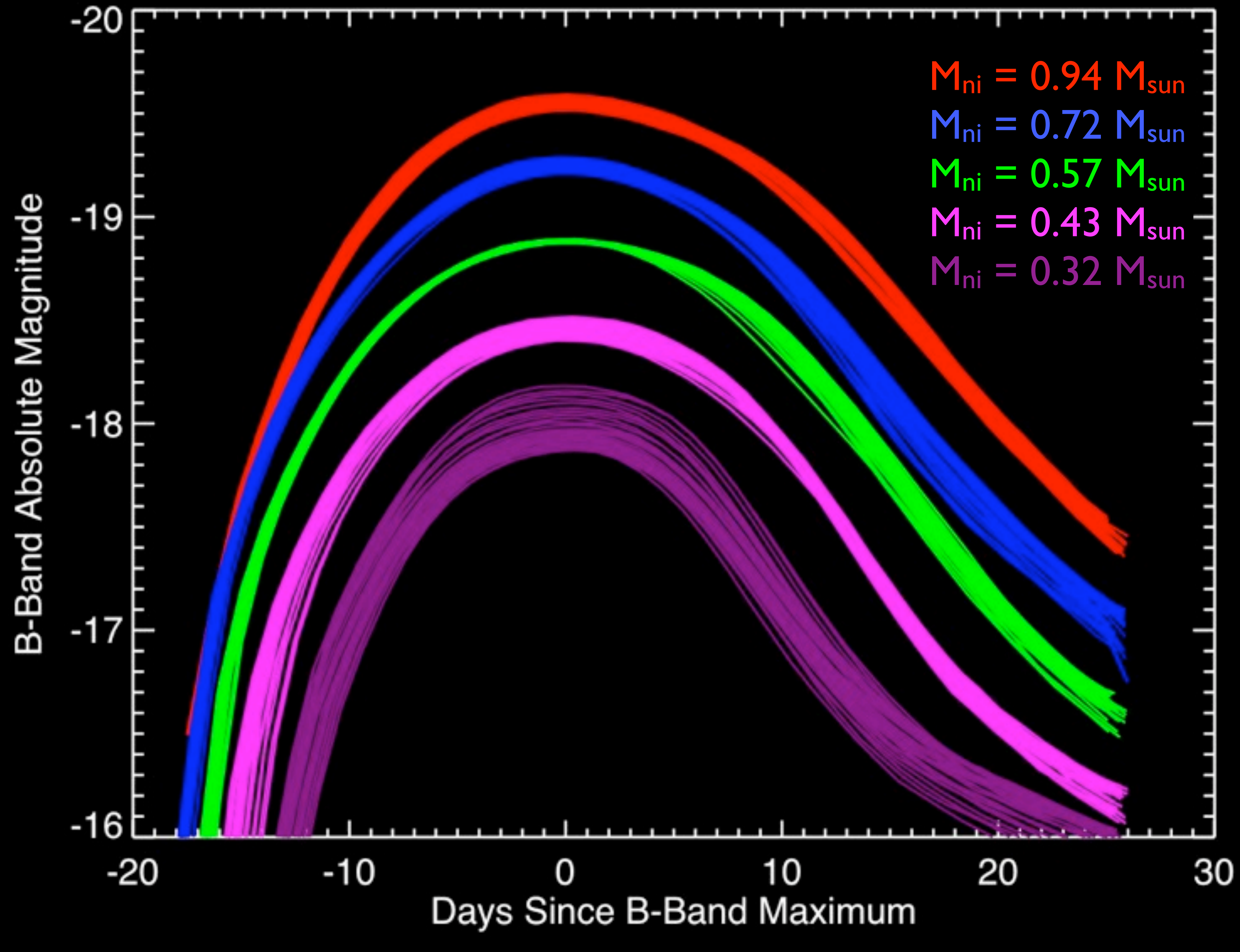
e.g., kasen et al (2009)




strong ignition
strong deflagration
weak detonation
nickel
iron
silicon
weak ignition
weak deflagration
strong detonation

models variations in brightness/duration

dependence on initial conditions, viewing angle



Transport Problem

radiation transfer equation

$$\frac{dI}{ds} = -\kappa I + \eta$$

$I(x, y, z, \lambda, \theta, \phi)$ radiation specific intensity

$\eta(x, y, z, \lambda)$ gas emissivity

$\kappa(x, y, z, \lambda)$ gas opacity

formally a 6 dimensional problem $\longrightarrow$

generally more computationally and memory intensive than hydrodynamics

opacity and emissivity depend on complex microphysics (equation of state) which itself depends on the transport of the radiation field (strong non-linear coupling - implicit methods)

transport methods

multi-group flux limited diffusion (MGFLD)

ignore θ,φ, keep λ dependence, multi-grid methods to solve mixed-frame diffusion equation (hypre library, LLNL)

CASTRO code (coupled to 3-D AMR hydrodynamics)

implicit monte carlo transport

mixed-frame stochastic particle propagation; retains the full angle, wavelength, & polarization information

SEDONA code (assumes free expansion)

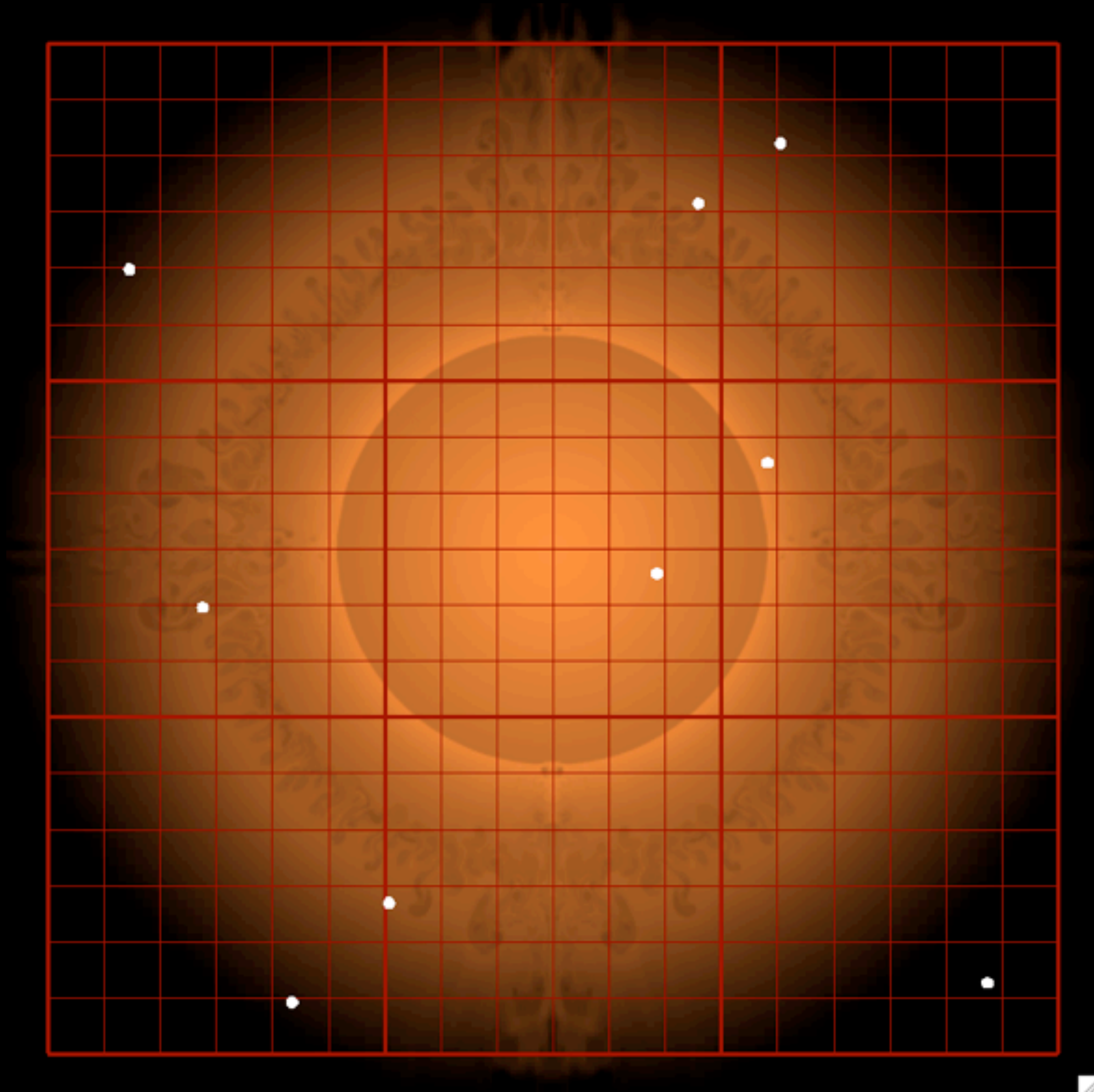
S_n methods

co-moving frame formal solution of transport equation for discretized angles

e.g., PHOENIX code

implicit monte carlo transport

stochastic particle propagation



particle count

very large number of particles needed to overcome statistical noise: S/N ~ $N^{1/2}$

strategy: replicate on multiple cores (nearly perfect scaling)

domain decomposition

node memory determines size of local domain and hence amount of communication at boundaries

load balancing

more work on regions with high particle counts, high scattering probability (opacity)

strategies: population control, adaptive refinement, replicate heavily loaded zones

2-D planar shock problem

non-equilibrium radiative shock (e.g., ensman 1994)

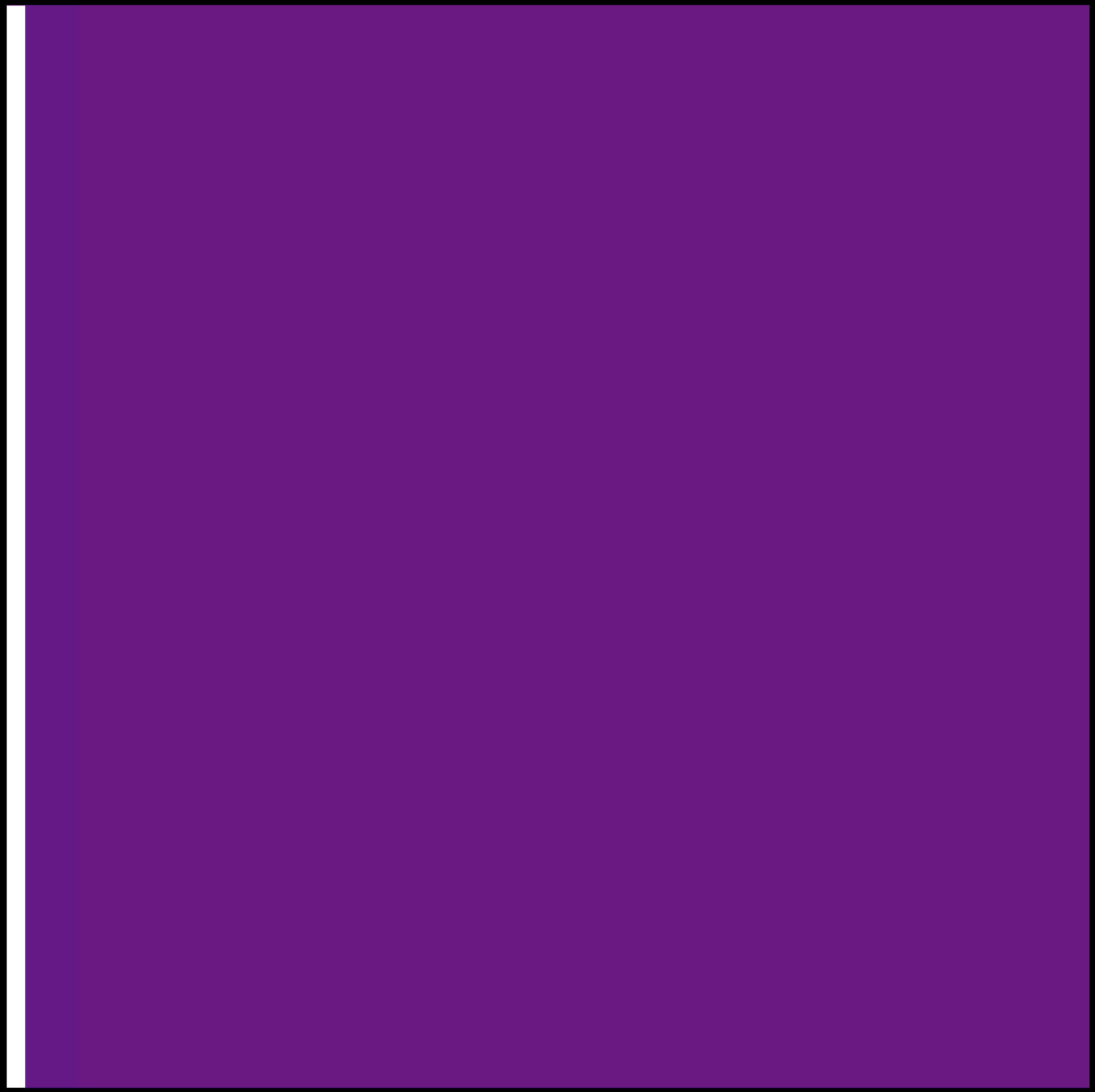
gas temperature

radiation temperature

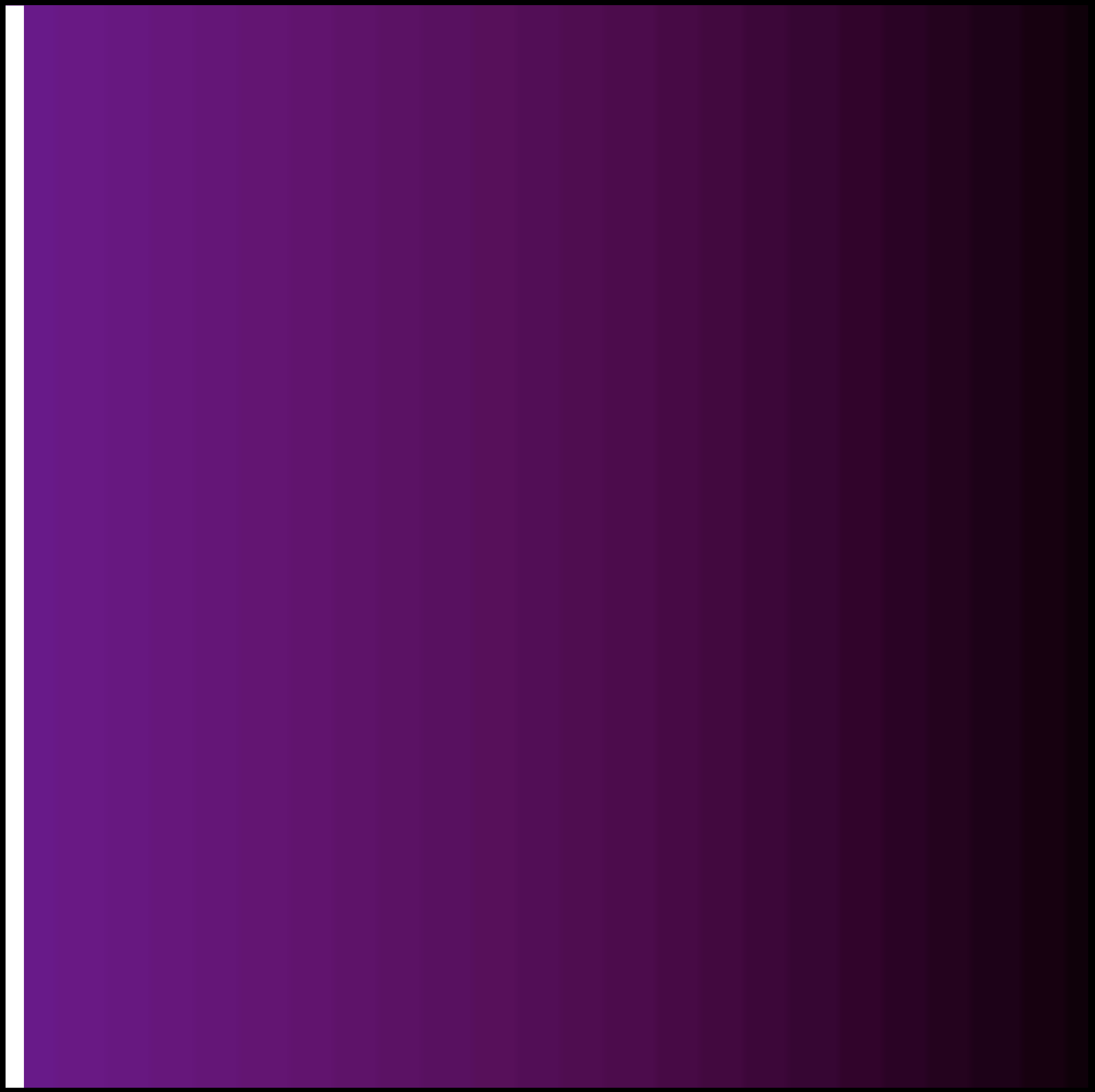
2-D planar shock problem

non-equilibrium radiative shock (e.g., ensman 1994)

gas temperature

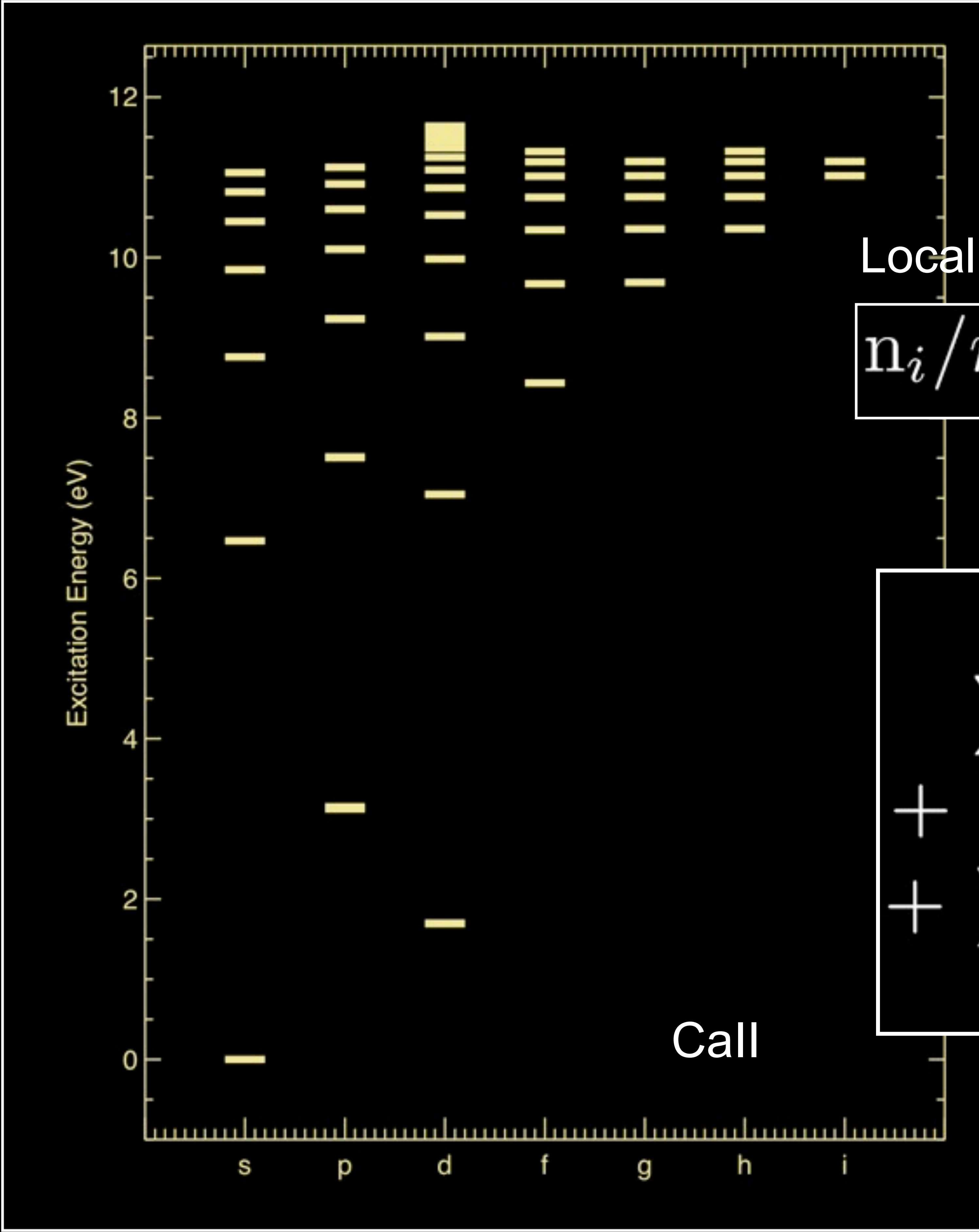


radiation temperature



microphysics

~1GB atomic data



Local Thermodynamic Equilibrium (LTE)

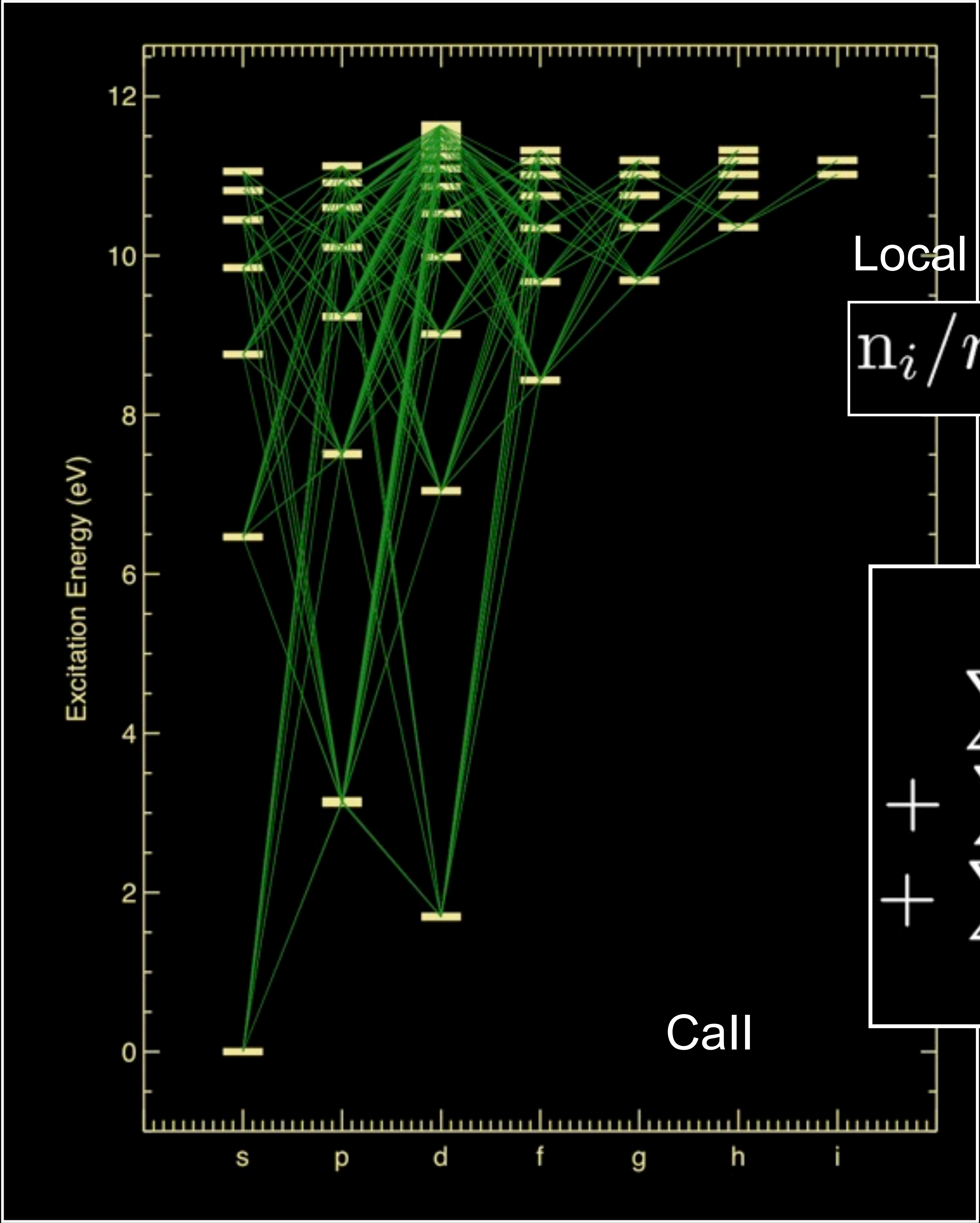
$$\boxed{n_i/n_j = \frac{g_i}{g_j}\exp(-\Delta E/kT)}$$

non-equilibrium (NLTE)

$$\boxed{\begin{aligned} &\partial n_i/\partial t = \\ &\sum_{j\neq i}(n_j R_{ji} - n_i R_{ij}) \\ &+ \sum_{j\neq i}(n_j C_{ji} - n_i C_{ij}) \\ &+ \sum_{j\neq i}(n_j G_{ji} - n_i G_{ij}) \\ &= 0 \end{aligned}}$$

nxn matrix, where n = number of atomic levels (sparsity depends on number of transitions included)

microphysics



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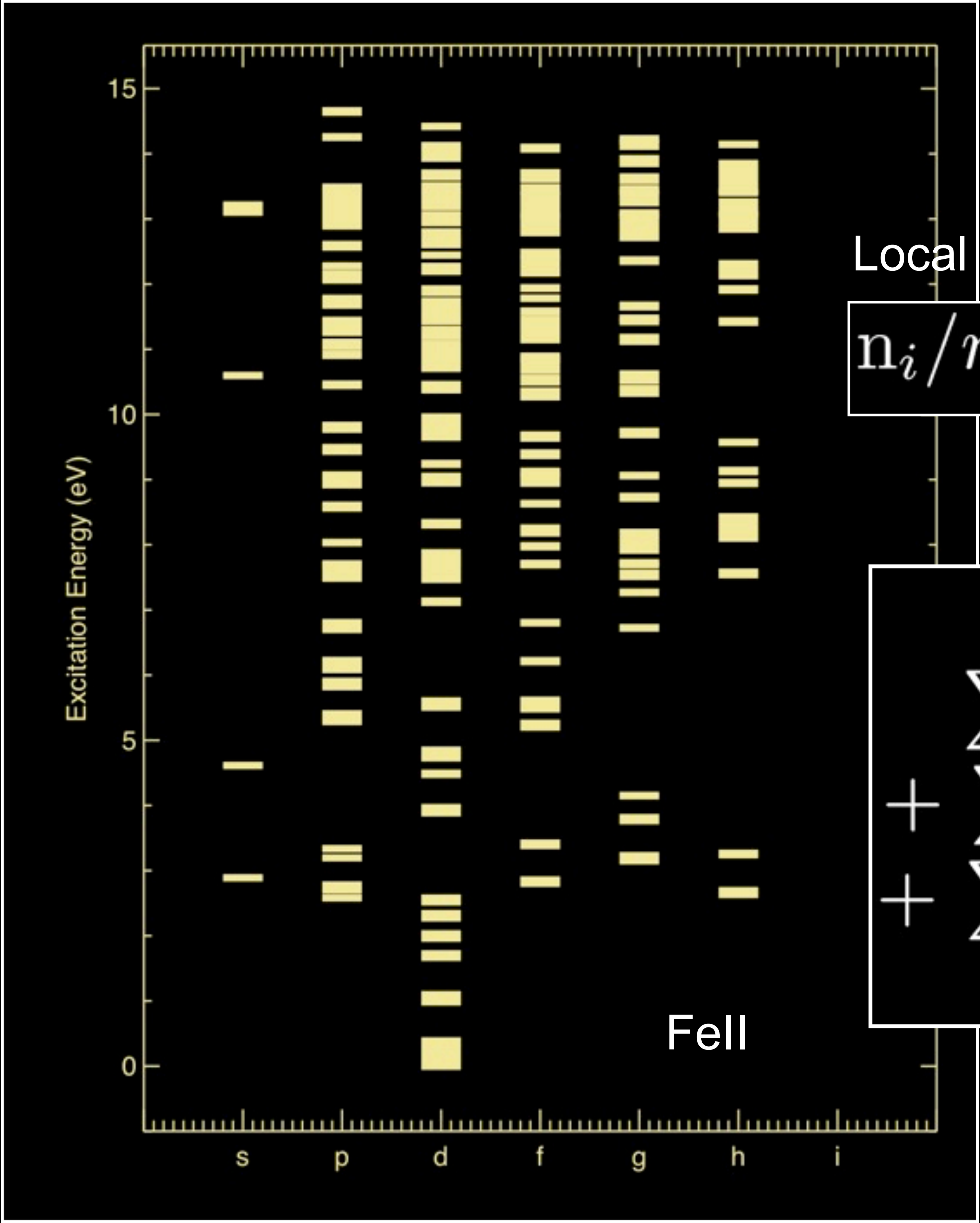

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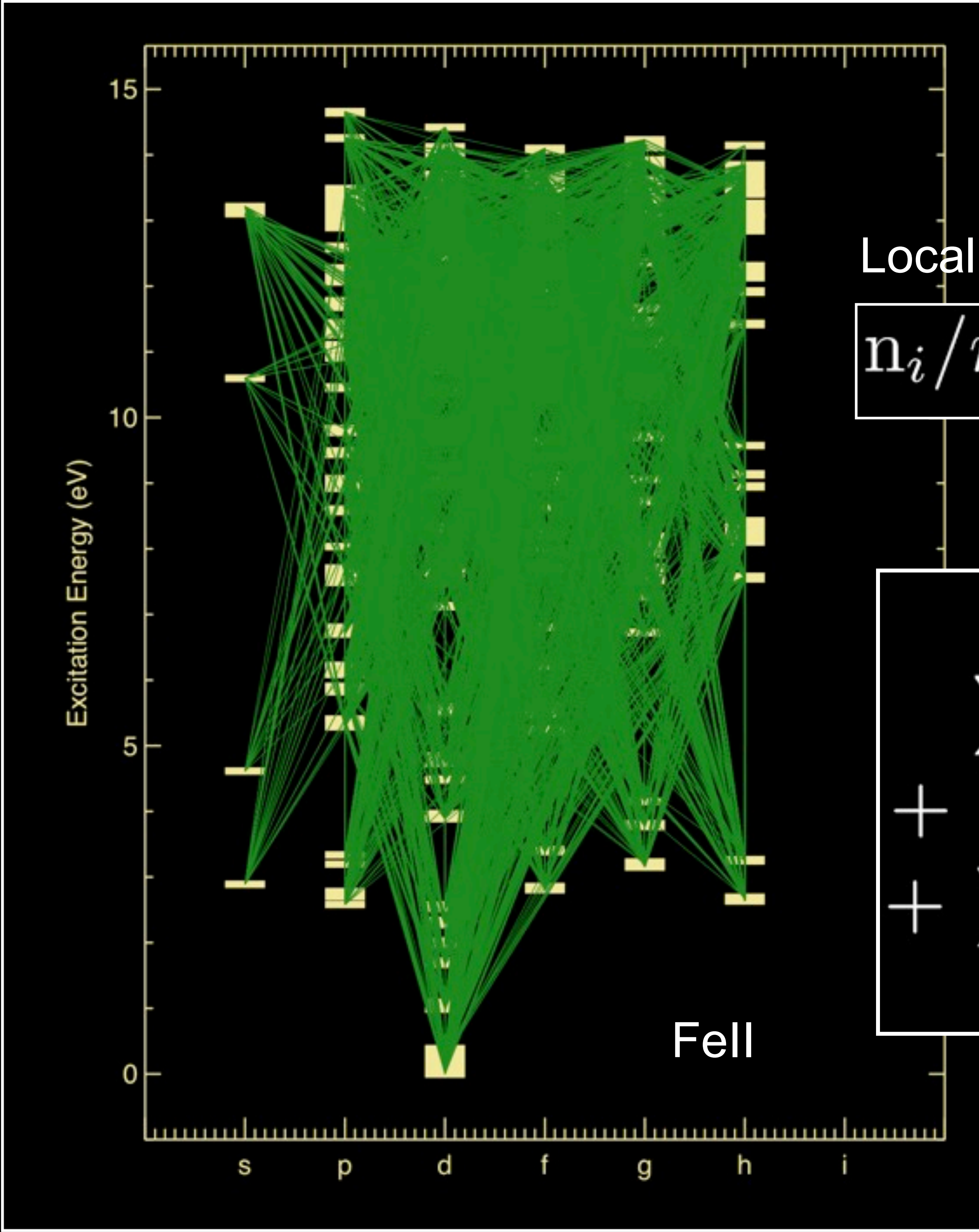

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code profile (sedona)

light curve calculations

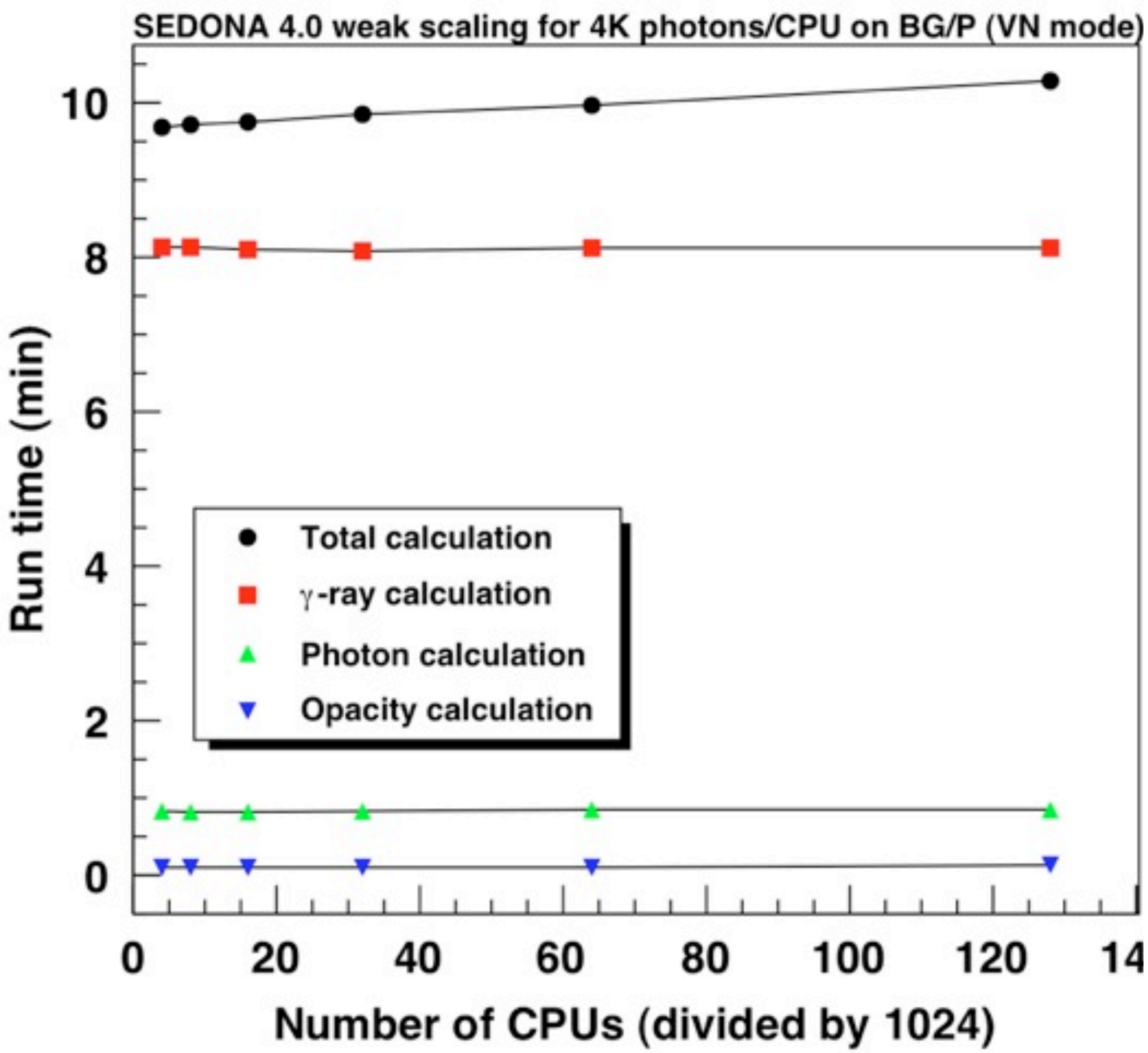
	prior 2D	current 3D	future 3D
resolution	$n_x = 100^2$ $n_l = 5000$	$n_x = 100^3$ $n_l = 1000$	$n_x = 512^3$ $n_l = 10{,}000$
grid size	~1 GB	~10 GB	~10 TB
particles	$\sim 10^8$	$\sim 10^9$	$\sim 10^{10}$ - 10^{11}
total memory	~10 GB	~100 GB	~10 TB
input	~1 GB	~1 GB	~20 GB
output	~1 GB	~100 GB	~100 GB
cores	1,000-10,000	~10,000	100,000+
execution time	10,000 hours	100,000 hours	1-10 M hours

code profile (castro)

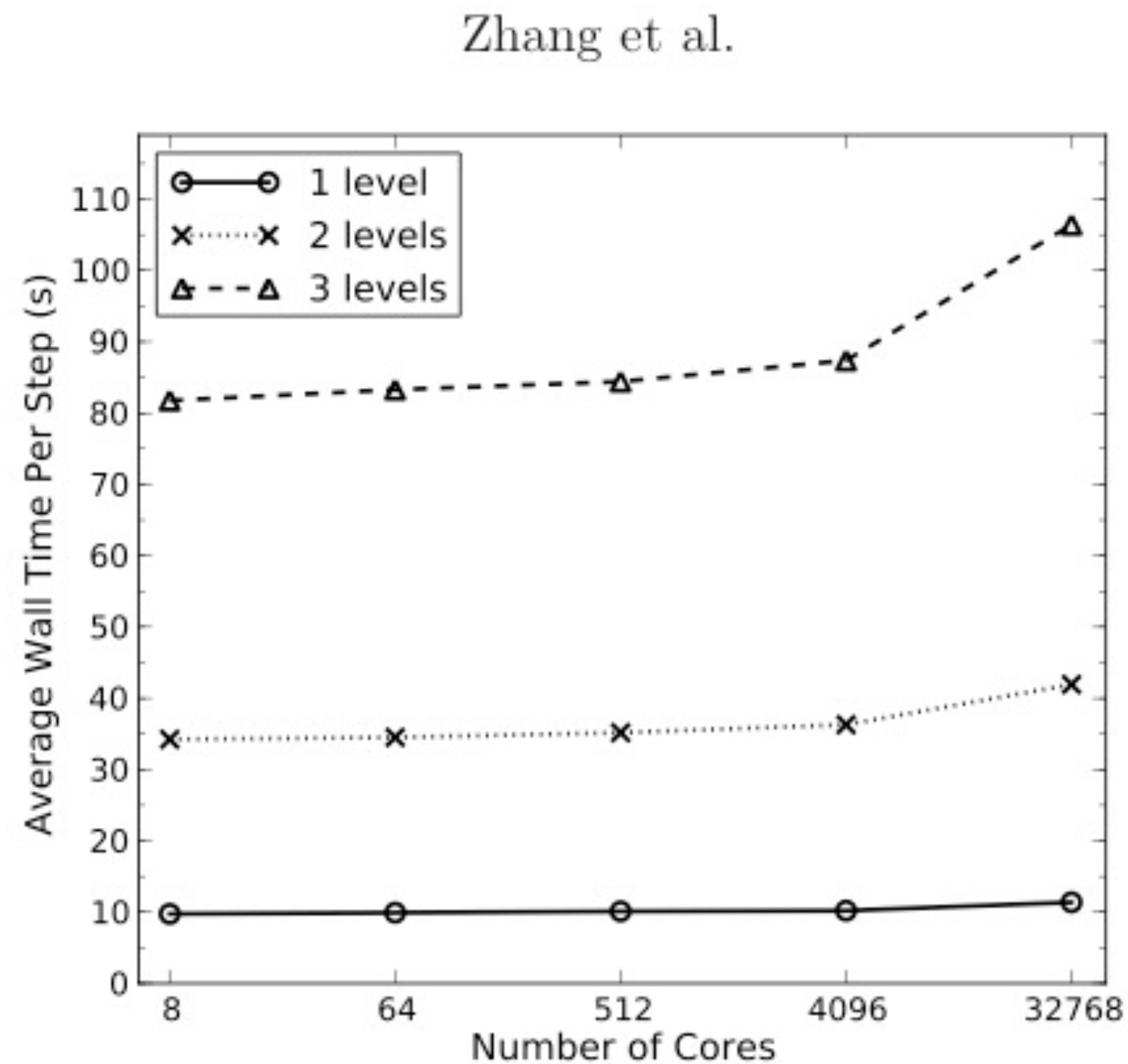
core collapse supernova simulation

	future 3D
resolution	$n_x = 1000^3$, $n_l = 64$ 4 level AMR
total memory	~50 TB
output	2 TB (checkpoint)
cores	100,000+
execution time	30 M hours

computational expense of neutrino radiation transport roughly $n_l \sim 64$ times more than that of hydrodynamics



sedona 2D spectrum
(full replication)



castro radiative blast wave
(grey flux limited diffusion)
zhang et al., 2011

HPC usage and methods for next 3-5 years

Changes to compute/memory load

Increases by a factor of ~10-100

Changes to data read/written

similar input/output files; larger checkpoints (1-10 TB of particles)

Upcoming changes to code/methods/approaches

Increase effective resolution by implementing adaptive grids in SEDONA within the BoxLib AMR framework.

Improved load balancing

Strategy for many-core, accelerator systems

Run individual particle propagation on multi-cores/accelerators within the local domain (as in current hybrid MPI/openMP approach) assuming sufficient memory to avoid excessive communication hit.

summary

What new science results might be afforded by improvements in NERSC computing hardware, software and services?

Well-resolved 3-D simulations of core collapse supernova explosions, light curves and spectra (including non-equilibrium effects for select species) illuminating the fundamental questions in the astrophysics and nuclear physics of these events.

Recommendations on NERSC architecture, system configuration and the associated service requirements needed for your science

Maintain reasonably large memory resources per node.
Visualization/analytics capabilities, comparative analysis of large data sets

What significant scientific progress could you achieve over the next 3 years with access to 50X NERSC resources?

Higher resolution calculations will evaluate degree of convergence.

Outcome of supernova simulations are sensitive to progenitor star properties, ignition conditions, hydrodynamical instabilities, uncertainties in input physics
$\longrightarrow$ need parameter studies!