Time-dependent RT, hydrodynamics, post-processing hydrodynamics, synthetic observables

Tim Harries

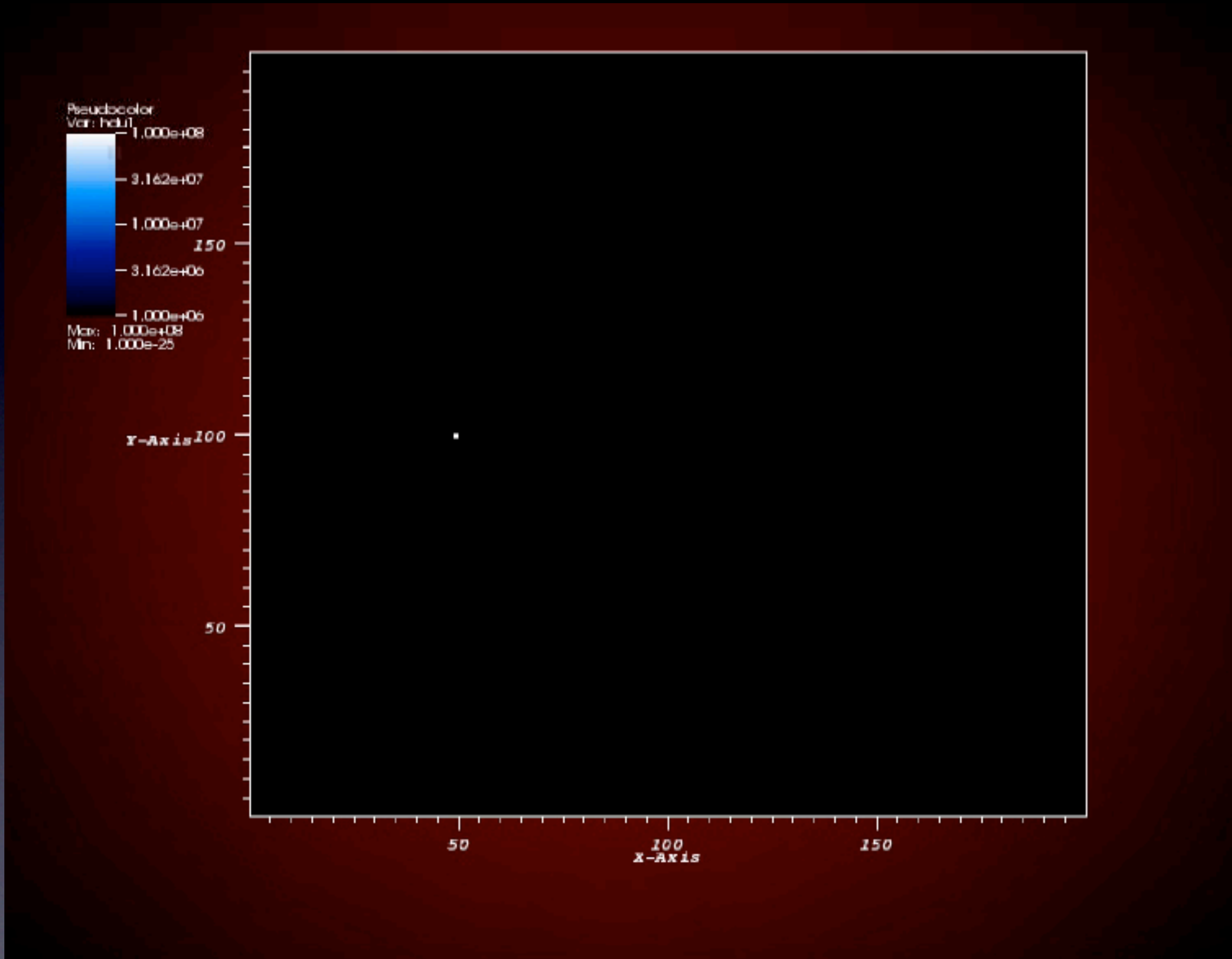
UNIVERSITY OF EXETER

St. **A**ndrews **M**onte **C**arlo **S**ummer **S**chool 2013

Time-dependent RT

Harries, 2012, MNRAS, 416, 1500

- Many interesting phenomena occur out of equilibrium
- Traditionally time-dependent calculations employ flux-limited diffusion
  - Grey
  - Flux-limiter is essentially arbitrary
  - Radiation field can diffuse around obstacles


Pseudocolor
Var: helu1
1.000e+08
3.162e+07
1.000e+07
3.162e+06
1.000e+06
Max: 1.000e+08
Min: 1.000e-25
150
Y-Axis
100
50
50
100
X-Axis
150

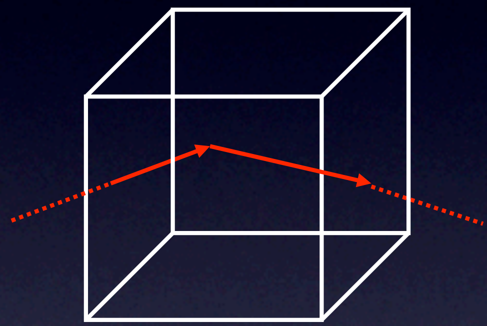
New MC algorithm

- Photon packets are used to determine the radiation energy density
- Matter interaction terms integrated explicitly
- Method effective in both the optically thick, and crucially, the optically thin (free streaming) limit

$$\dot{E} = 4\pi \int_0^\infty k_\nu B_\nu d\nu \qquad \dot{A} = 4\pi \int_0^\infty k_\nu J_\nu d\nu$$

$$u_{r,\nu} = 4\pi J_\nu d\nu / c$$

$$u_{r,\nu} = \frac{1}{\Delta t} \frac{1}{V} \frac{1}{c} \sum \epsilon_\nu \ell$$



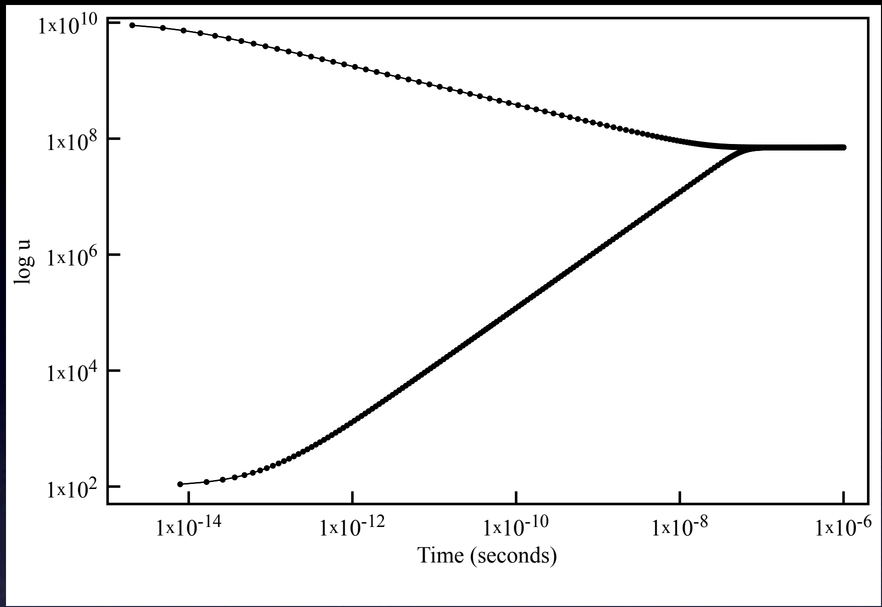
$$\dot{A} = \frac{1}{V} \frac{1}{\Delta t} \sum k \epsilon \ell$$

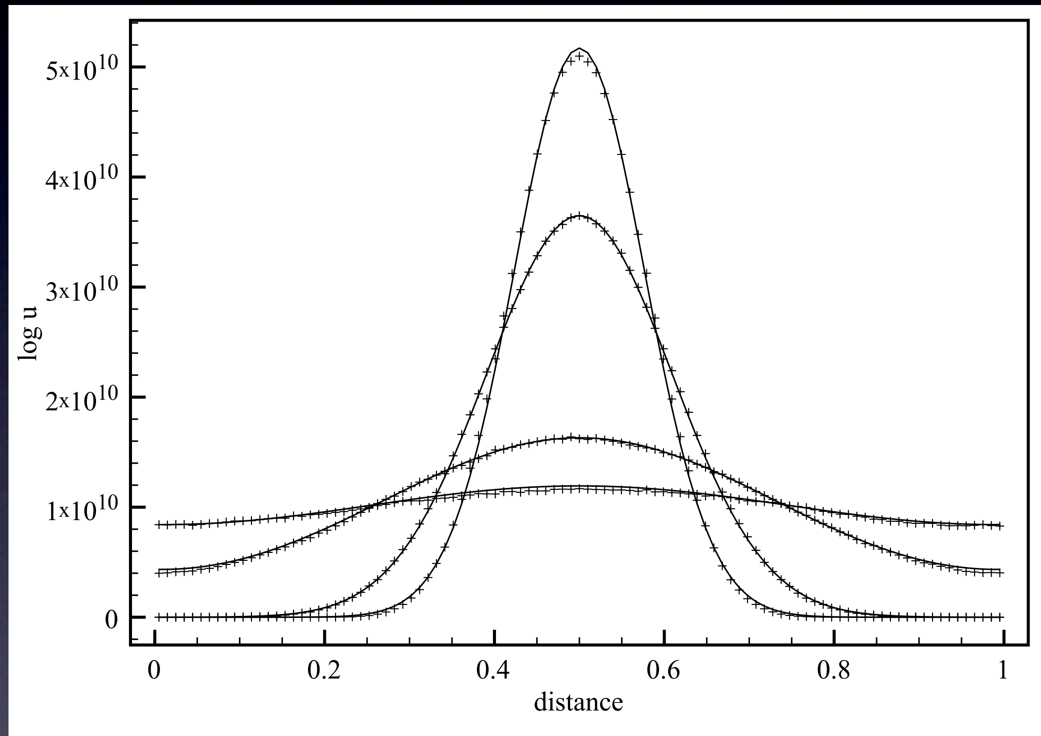
$$\dot{u}_r = \dot{E} - \dot{A} \qquad \dot{u}_g = \dot{A} - \dot{E}$$

$$u_g^{n+1} = u_g^n + (\dot{A} - \dot{E}) \Delta t$$

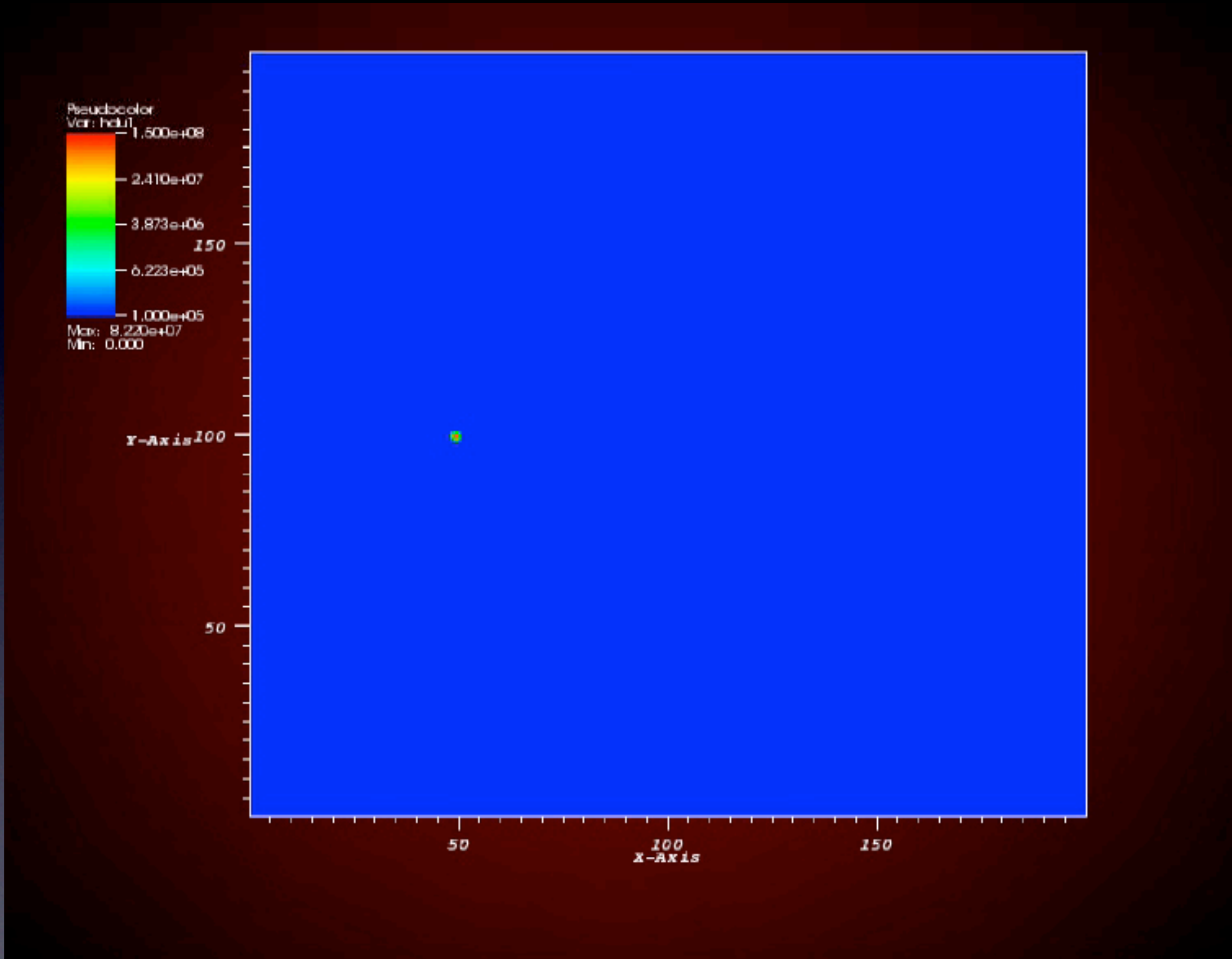
$$\frac{du_g}{dt} = c\kappa u_r - 4\pi\kappa B(u_g)$$

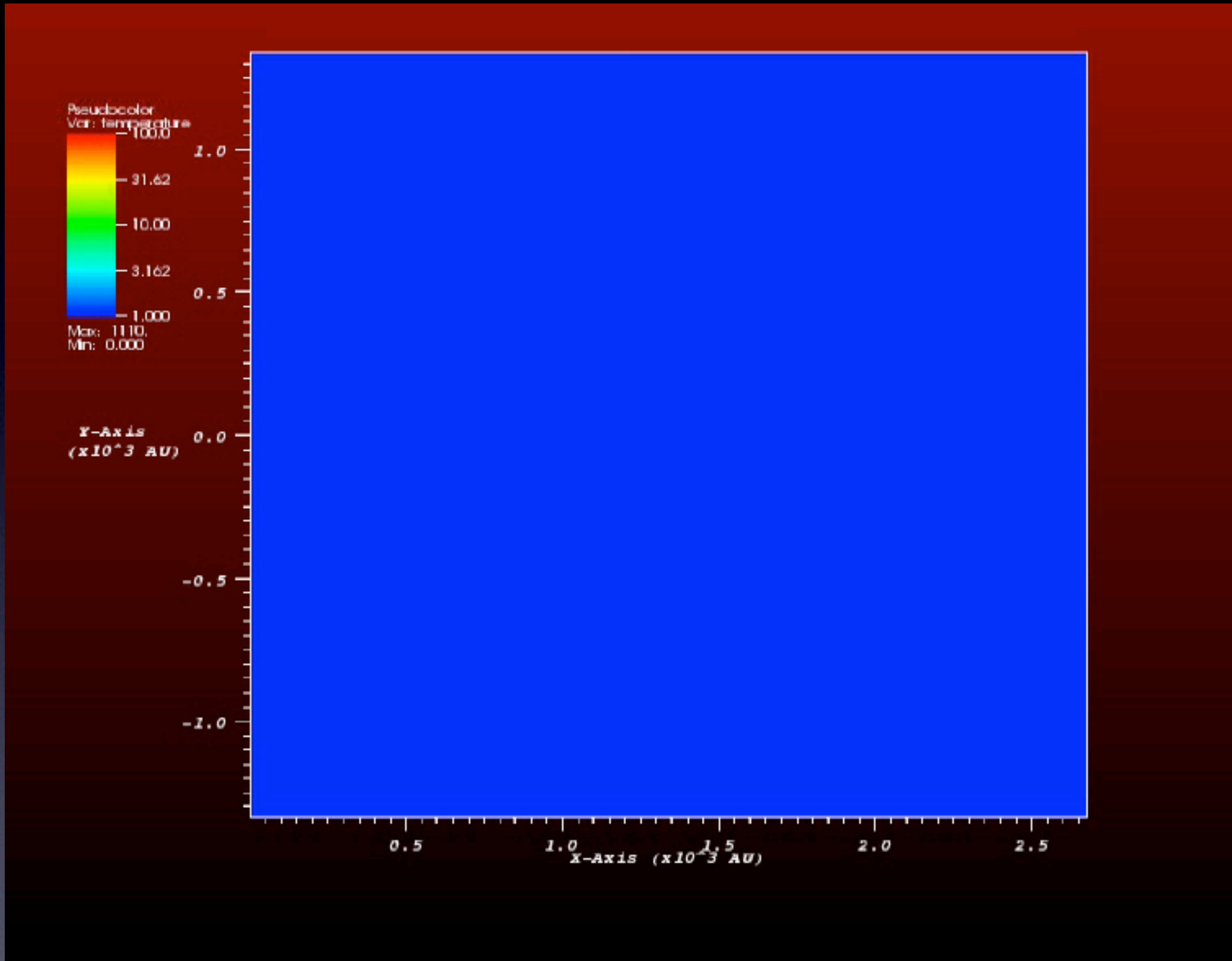
$$\frac{du_r}{dt} = -D\frac{d^2u_r}{dx^2} \qquad D = \frac{c}{\kappa}$$

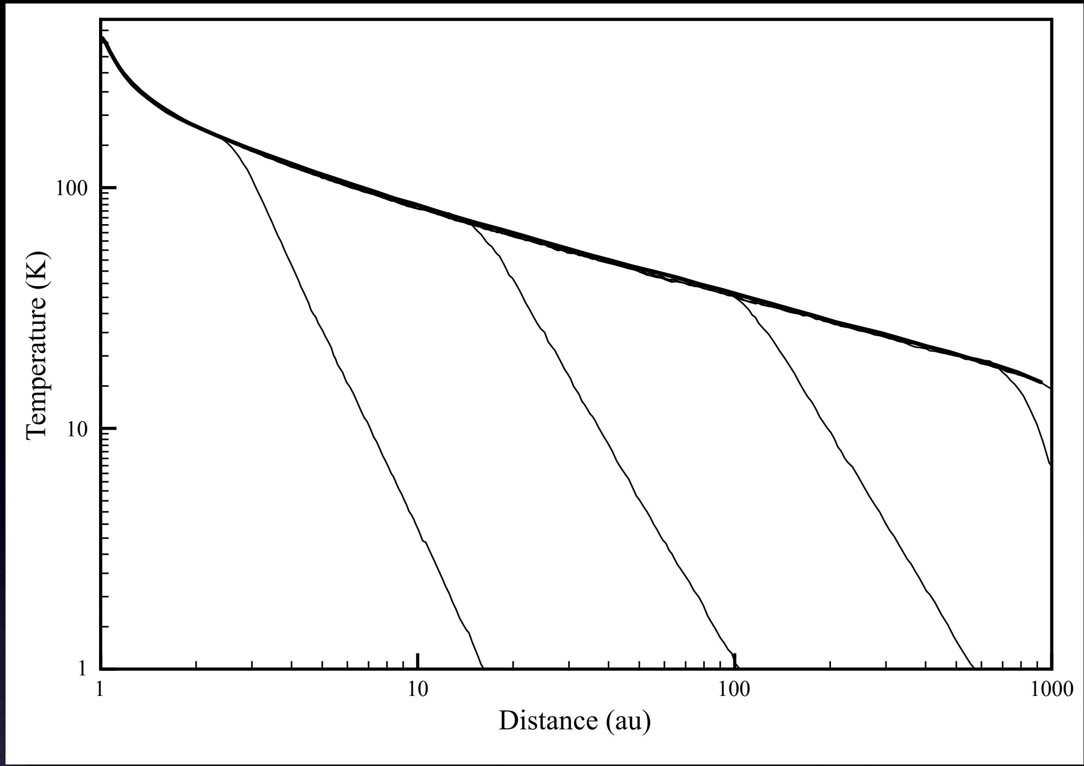




$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$$


Pseudocolor
Var: halu1
1.500e+08
2.410e+07
3.873e+06
6.223e+05
1.000e+05
Max: 8.220e+07
Min: 0.000
150
Y-Axis 100
50
50
100
X-Axis
150


Pseudocolor
Var: temperature
100.0
31.62
10.00
3.162
1.000
Max: 1110.
Min: 0.000
Y-Axis
(x10^3 AU)
1.0
0.5
0.0
-0.5
-1.0
0.5
1.0
1.5
2.0
2.5
X-Axis (x10^3 AU)



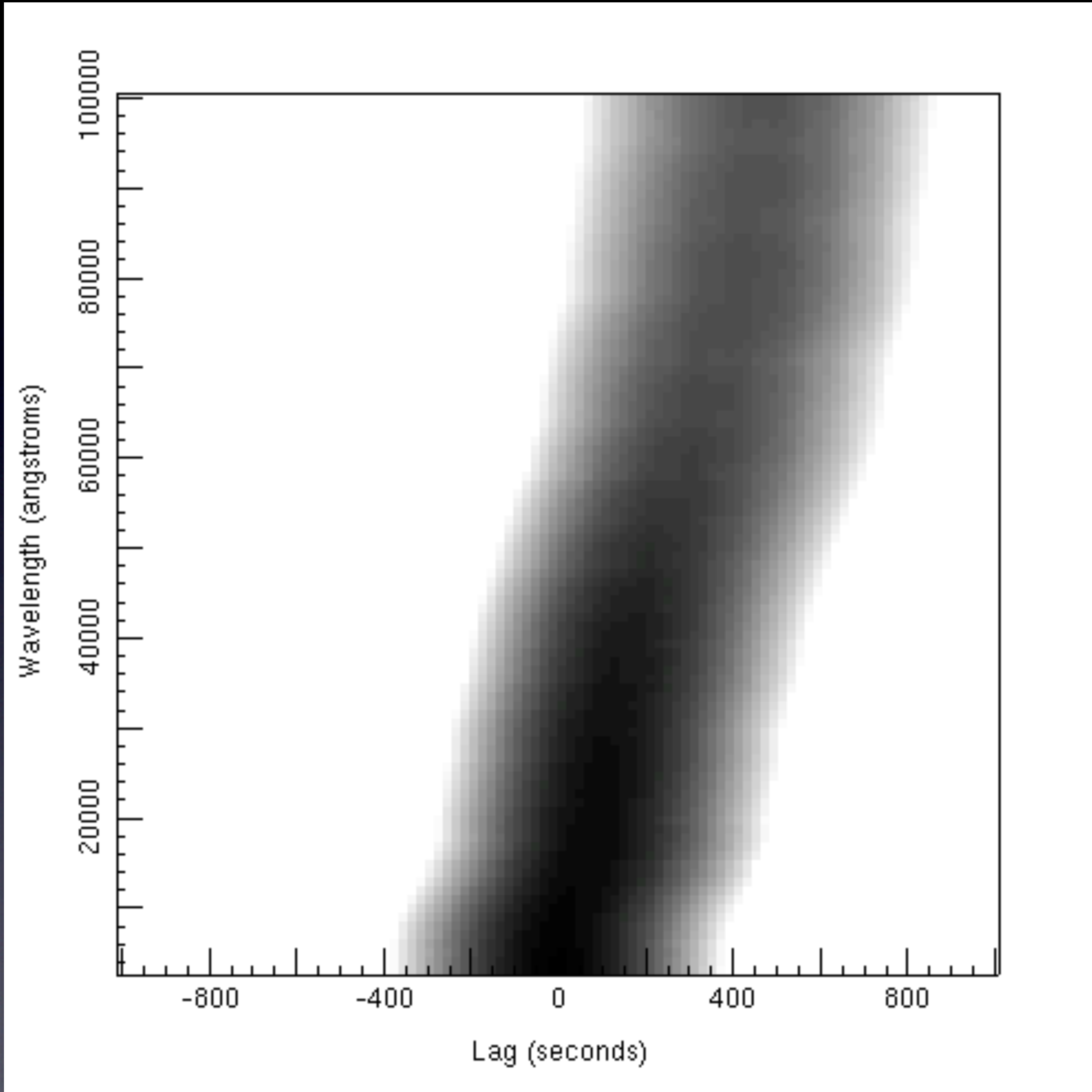
The disc midplane temperature for the Pascucci benchmark disc. The heavy line shows the benchmark temperature distribution, while the other lines show (from the left) snapshots at $t = 3.1 \times 10^4$ s, $t = 1.02 \times 10^6$ s, $t = 3.3 \times 10^7$ s, and $t = 1.05 \times 10^9$ s.

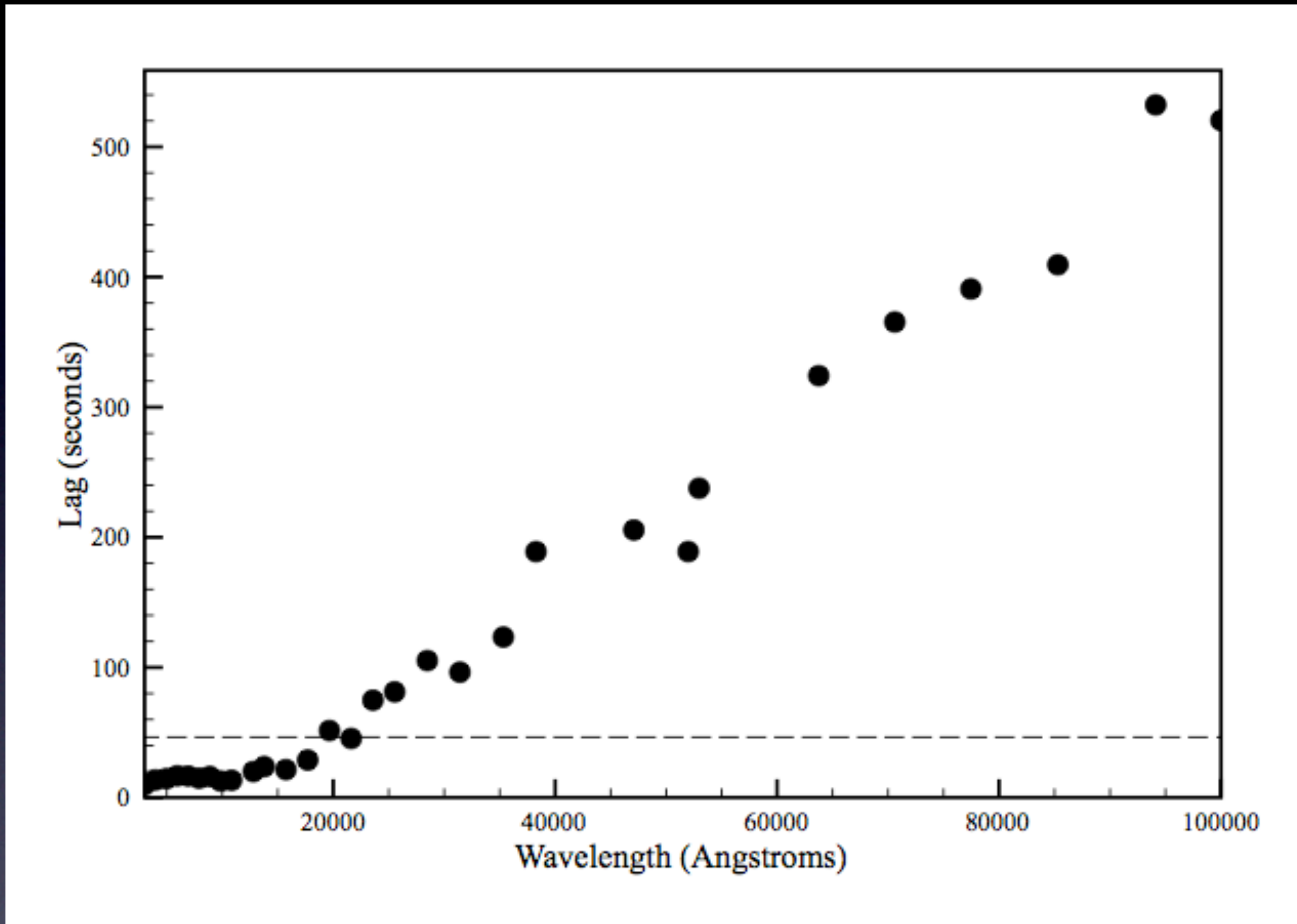
An application

- Standard flared disc (alpha=2.125, beta=1.125, r_{inner}=5 R_*, r_{outer}=300AU, m_{disc}=0.01M_*)
- Illuminated by a typical CTTS (T_{eff} = 4000K, R=2 solar radii)
- Accretion rate sinusoidally varies over a period of 24h (1-5 × 10^{-8} solar masses per year).

An application

- Additional blue continuum will heat the disc, which will emit more near/mid-IR radiation
- There will be a time-delay between the blue continuum and the disc's response
    - Photon flight time
    - Thermal lag


100000
80000
60000
40000
20000
Wavelength (angstroms)
-800
-400
0
400
800
Lag (seconds)


Lag (seconds)
500
400
300
200
100
0
20000
40000
60000
80000
100000
Wavelength (Angstroms)

A new RHD method

RHD summary

$$\frac{d\rho}{dt} + \rho\nabla\cdot\mathbf{v} = 0$$ Continuity equation

$$\rho\frac{d\mathbf{v}}{dt} = -\nabla P - \nabla\phi + \mathbf{F}_{\rm rad}$$ Momentum equation

$$P = \mathrm{func}(\rho, T)$$ Equation of state

$$\mathbf{F}_{\rm rad} = \frac{1}{c}\int_0^{4\pi}\int_0^{\infty}\kappa_\nu I_\nu d\nu d\Omega$$ Radiation pressure

Flux-limited diffusion

$$f = -D\nabla E \qquad\qquad D = \frac{c}{3\kappa}$$

Note that this is (usually) a grey approximation (opacity frequency dependence is bundled up in the Rosseland mean), and the photons are assumed to diffuse (valid in optically thick regions only).

Radiation Pressure (I)

momentum per photon packet $\mathbf{p}_{\text{packet}} = \frac{\epsilon}{c}\hat{\mathbf{u}}$

The difference in momentum between packets entering and leaving a cell gives net momentum change of a cell

$$\Delta \mathbf{p}_{\text{cell}} = \sum_{m} \mathbf{p}_{\text{packet,in}} - \sum_{n} \mathbf{p}_{\text{packet,out}}$$

m = photon packets entering cell

n = photon packets leaving cell

$$\mathbf{F}_{\text{cell,radiation}} = \frac{\Delta \mathrm{p}_{\text{cell}}}{\Delta t}$$

Radiation Pressure (II)

Alternatively we can use an estimator of the flux to obtain the radiative force on a cell

$$\mathbf{F}_{\mathrm{rad}} = \frac{1}{V}\frac{1}{\Delta T}\frac{\epsilon}{c}\sum \ell k_\nu \hat{\mathbf{u}}$$

This estimator is better in the optically thin limit.

This force is used to update the momentum in the hydrodynamics step

Interleaving radiation and hydrodynamics steps gives an RHD code.

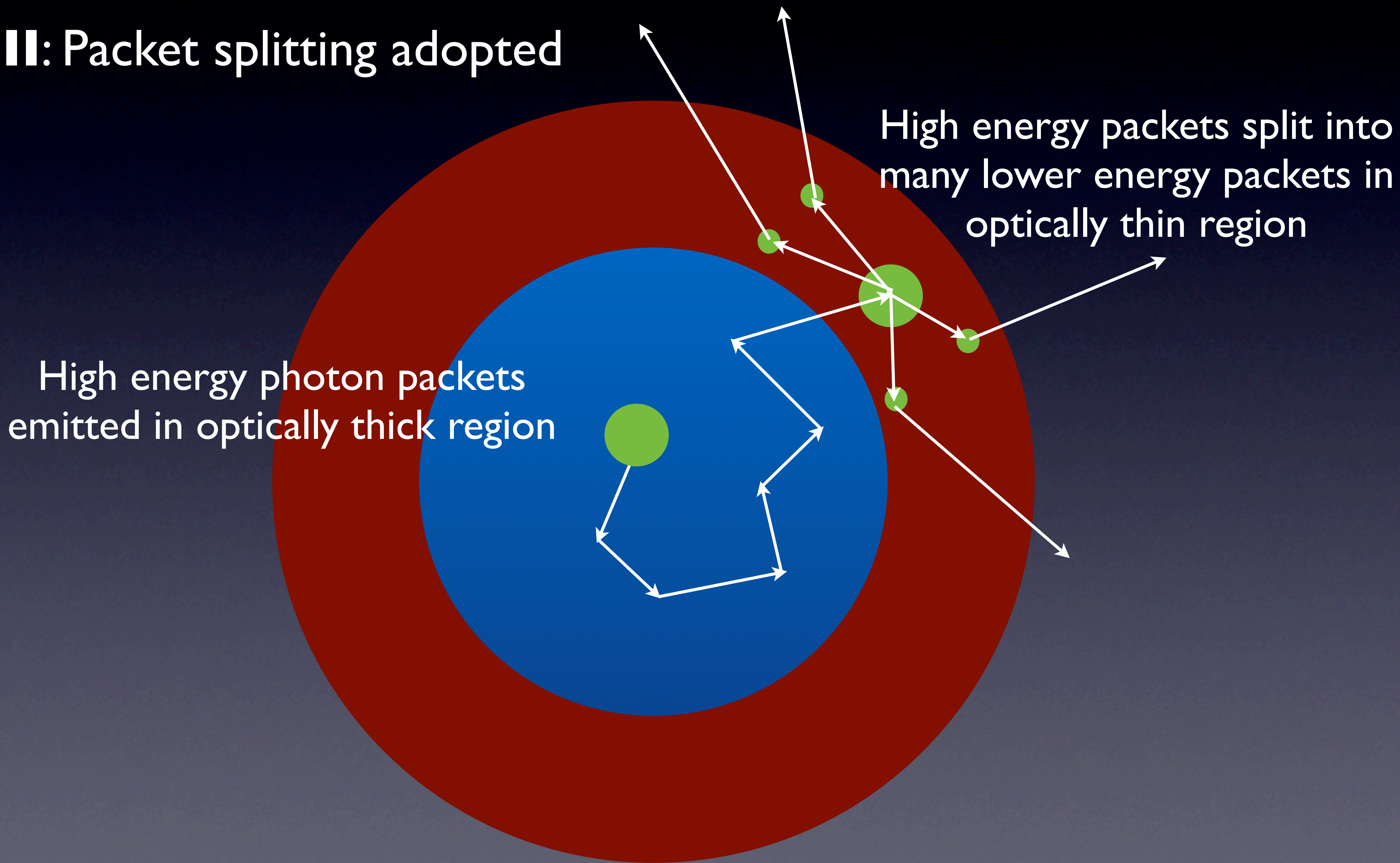
There are drawbacks....

Many millions of photon packets must be tracked in order to correctly estimate the mean intensity

Each photon packet must undergo a random walk encompassing (perhaps) many thousands of absorptions and re-emissions.

I: Photon packets propagated using modified random walk in optically thick regions (Min et al., 2009, *A&A*, **497**, 155)

II: Packet splitting adopted

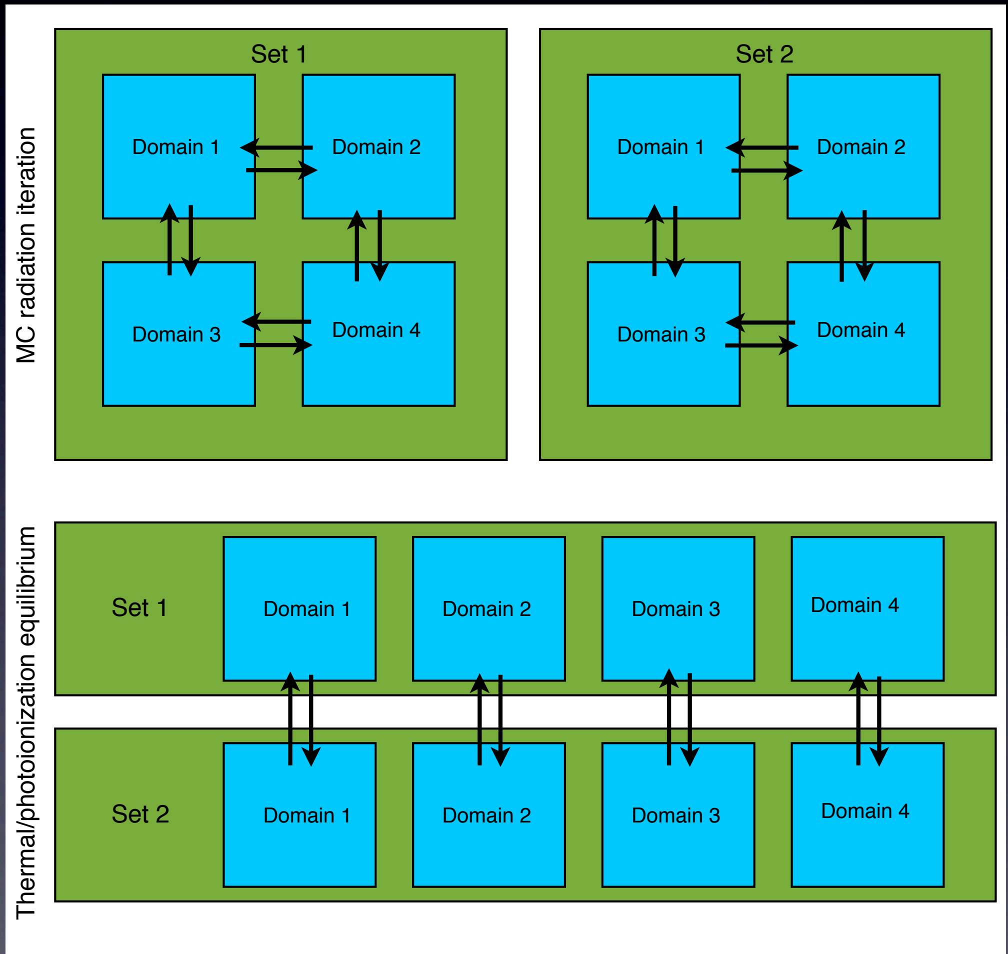


Each MC packet is an independent event

Scales very well under parallelization

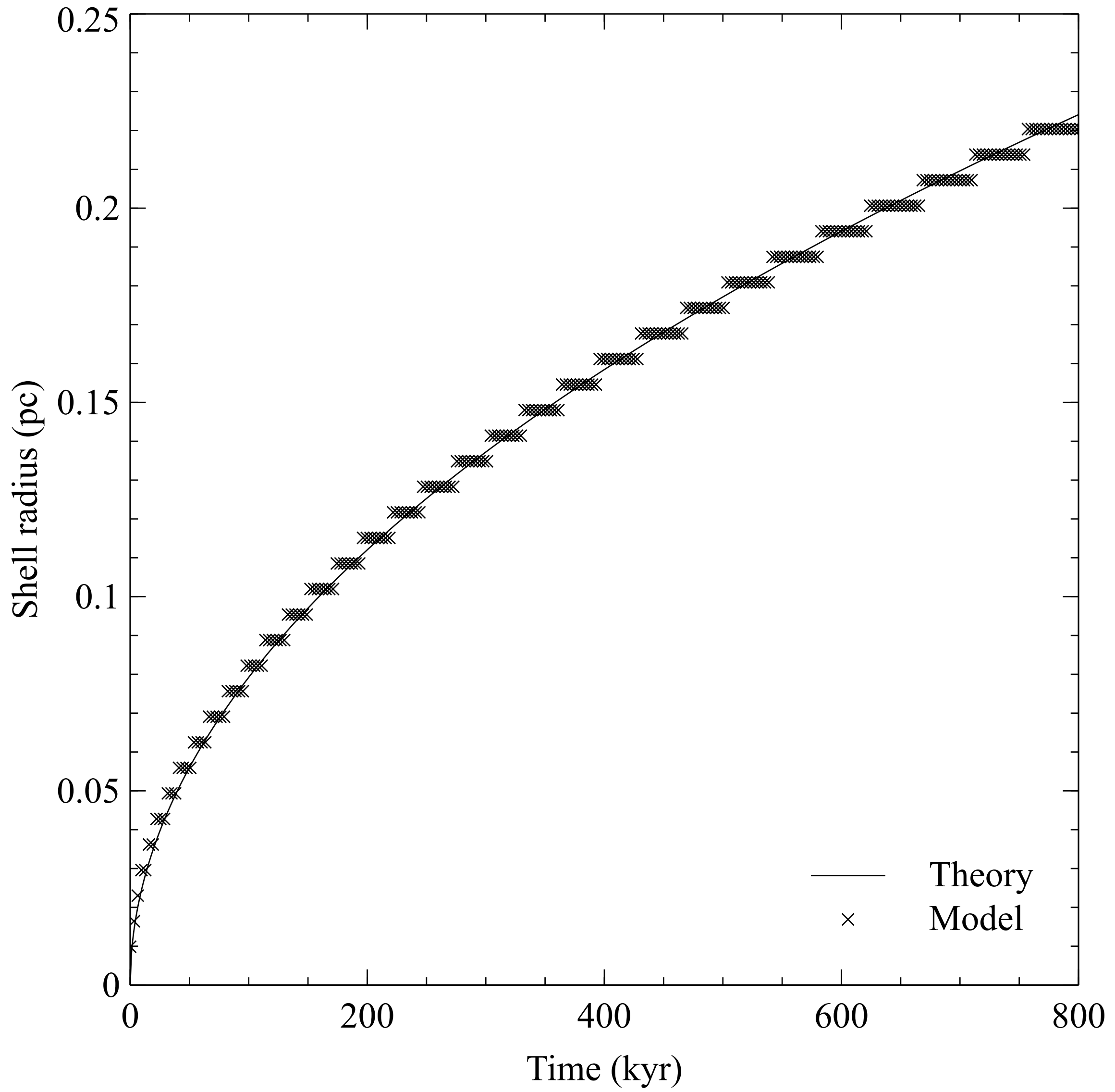
But communication of photon packets between domains of domain decomposed hydrodynamics is a bottleneck...

Solve this by having many instances of the entire computational domain



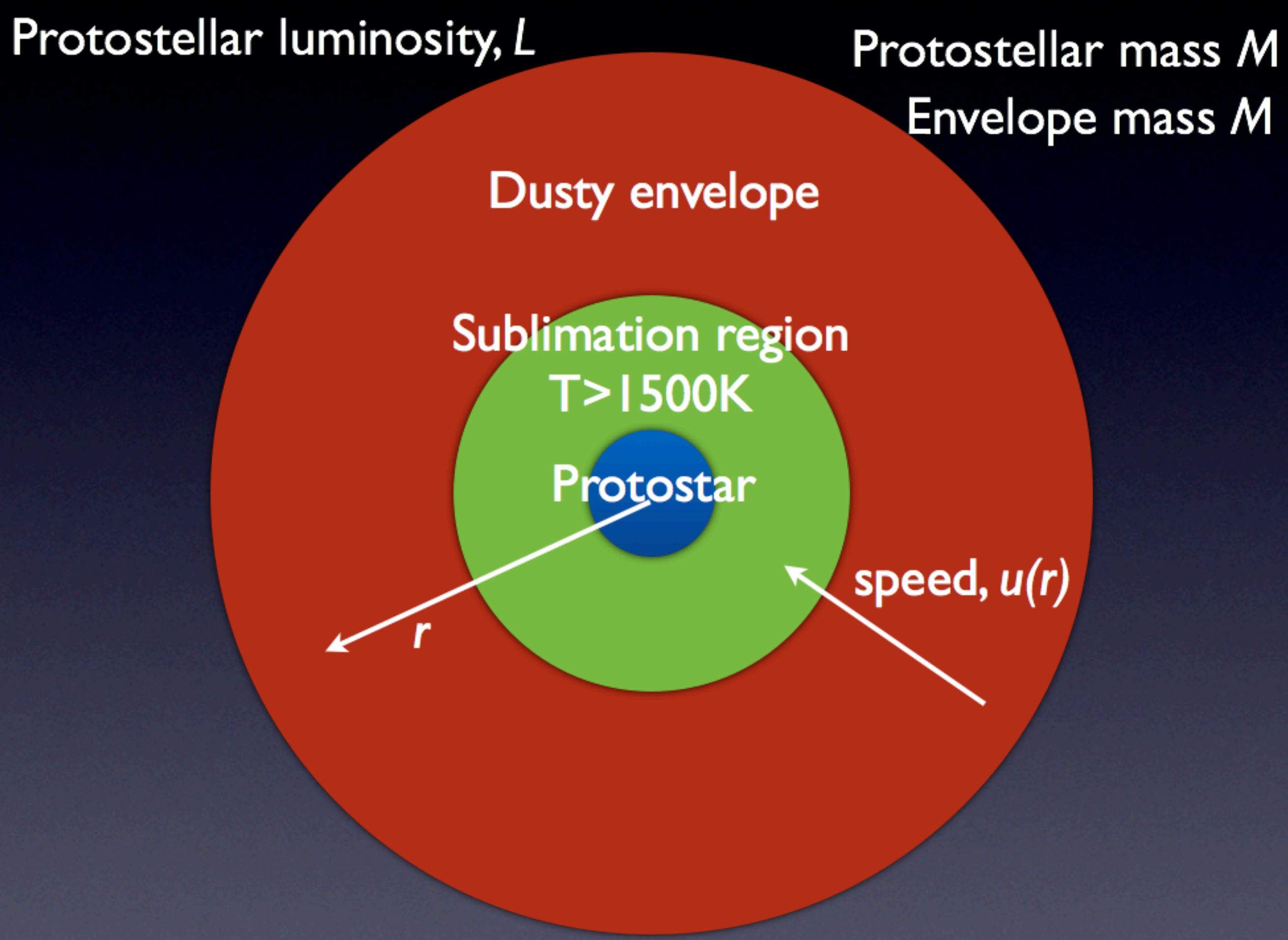
Each of the *i* sets does *N*/*i* photon packets

At the end of each photon packet loop the temperatures, ionization states etc are reduced over the *i* sets

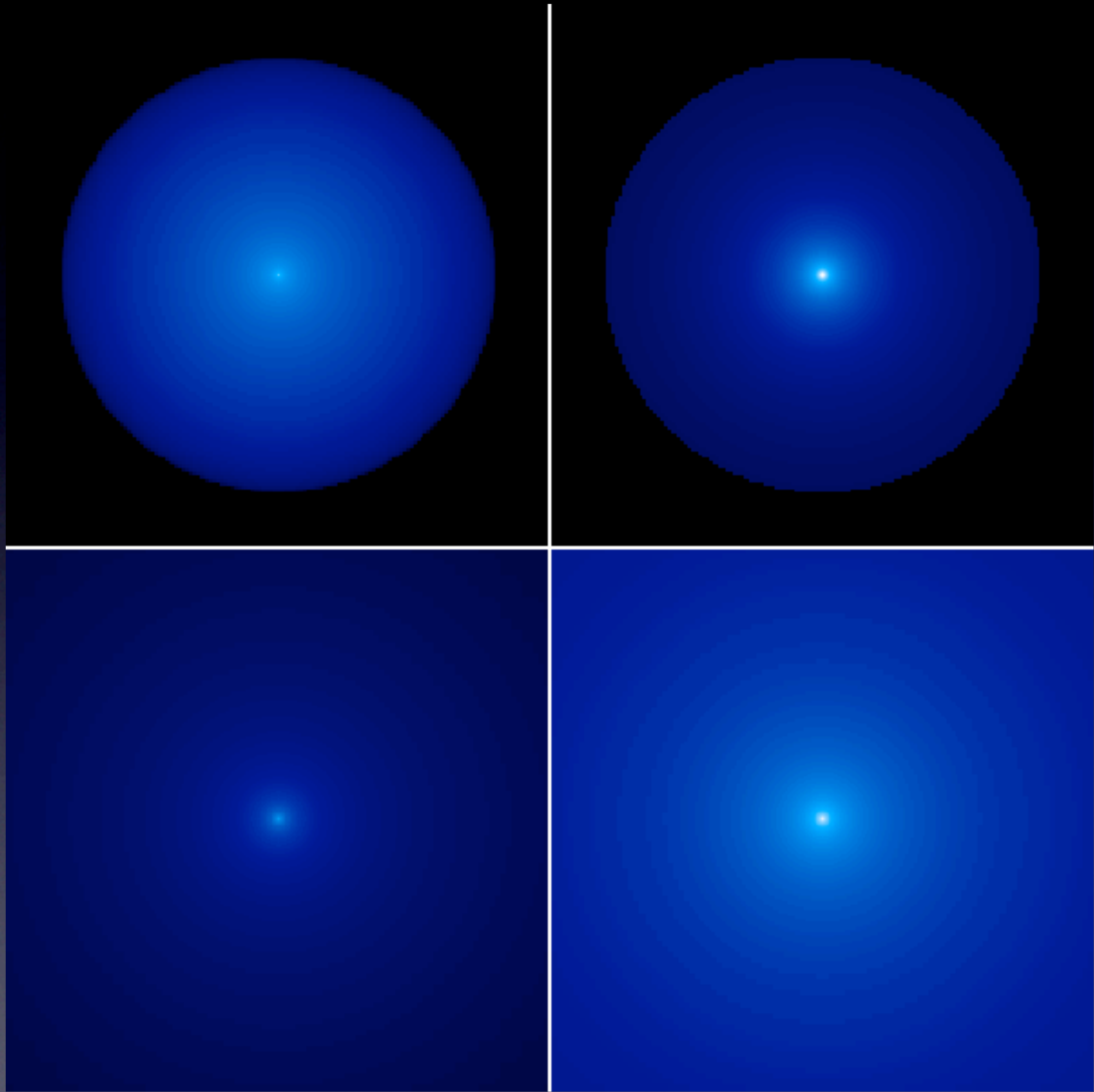


0.25
0.2
0.15
0.1
0.05
0
Shell radius (pc)
0
200
400
600
800
Time (kyr)
Theory
Model

Massive star formation

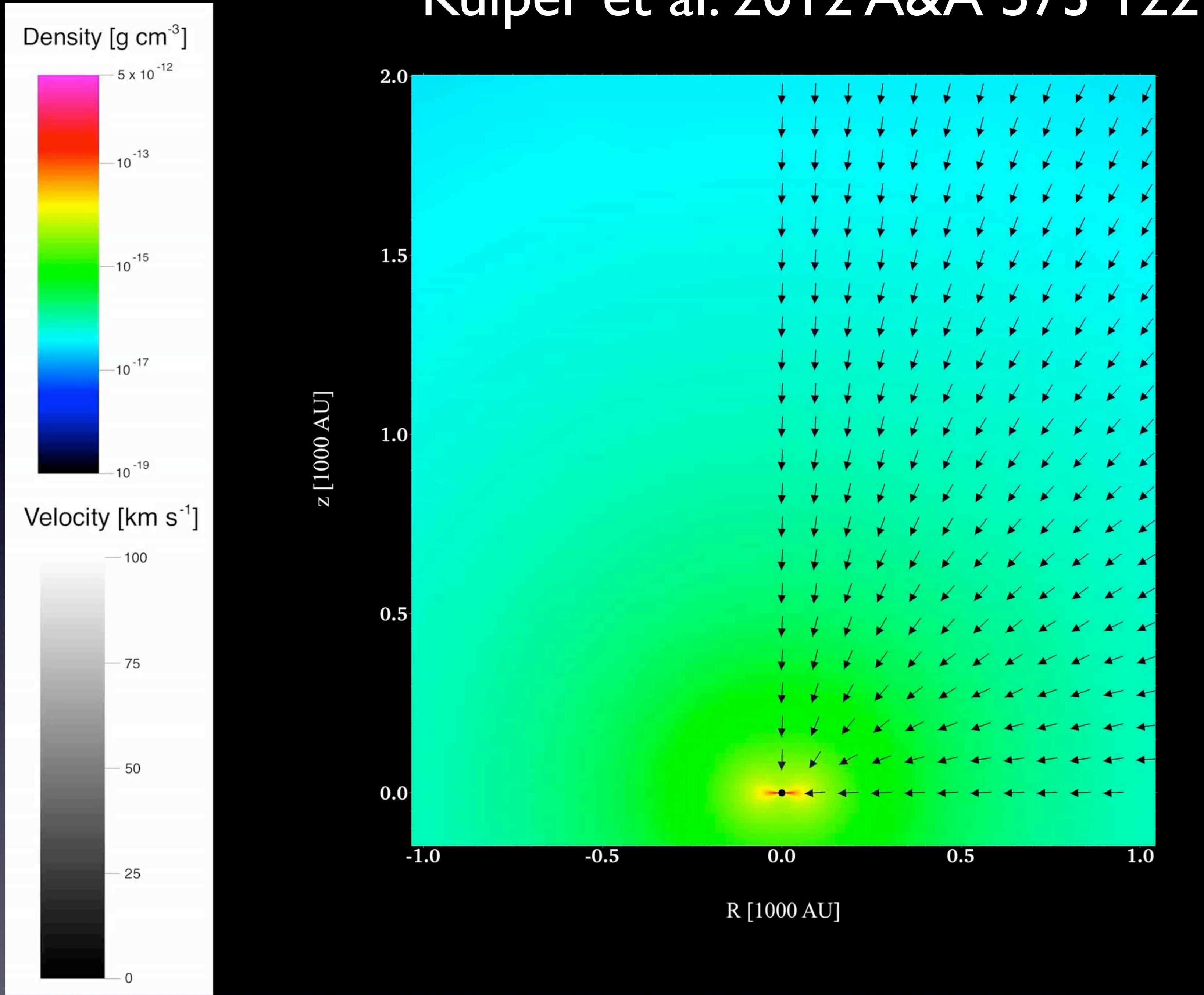


Larson & Starrfield, 1971, *A&A*, **13**, 190

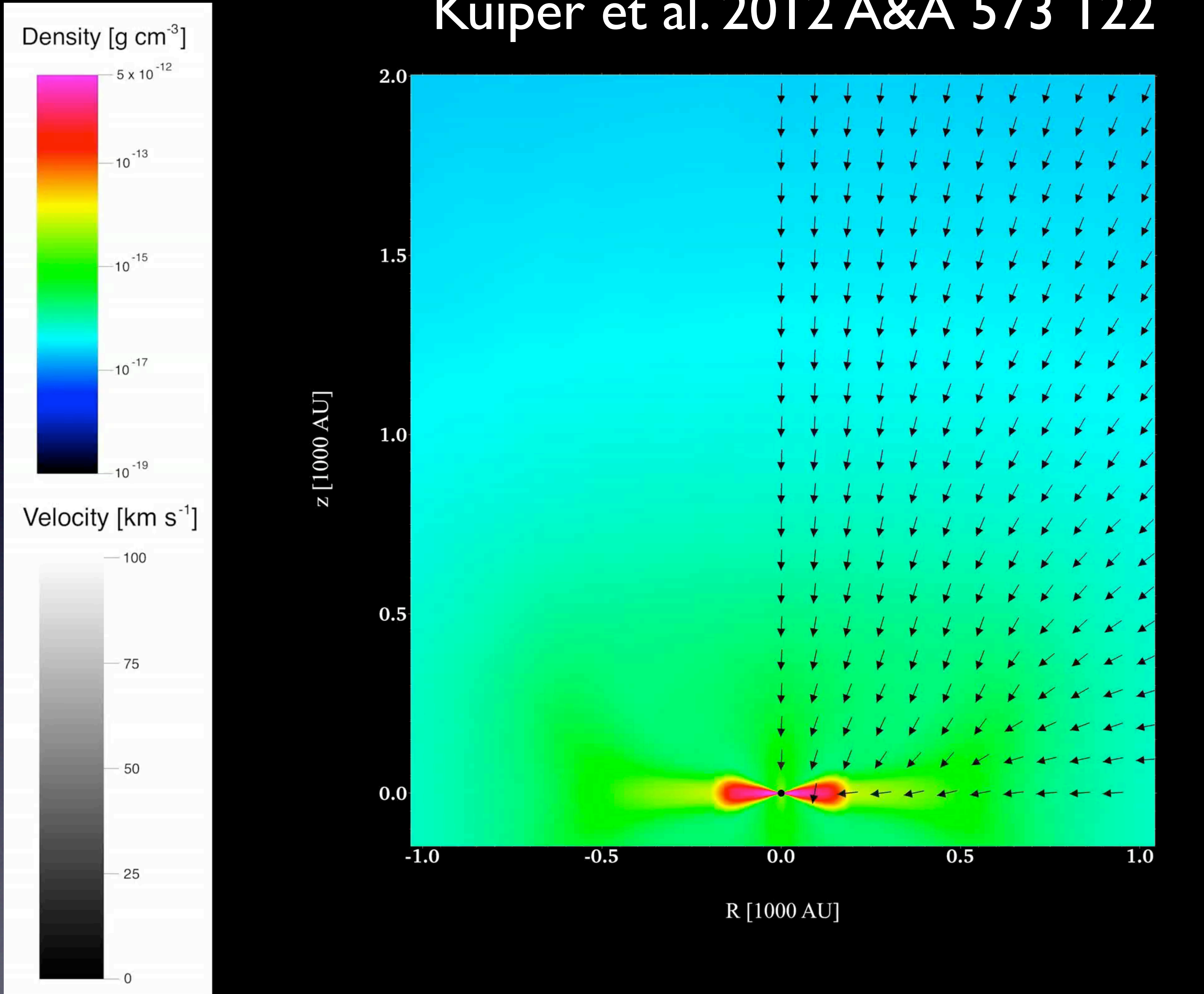


Krumholz et al. 2009 Science 323 754

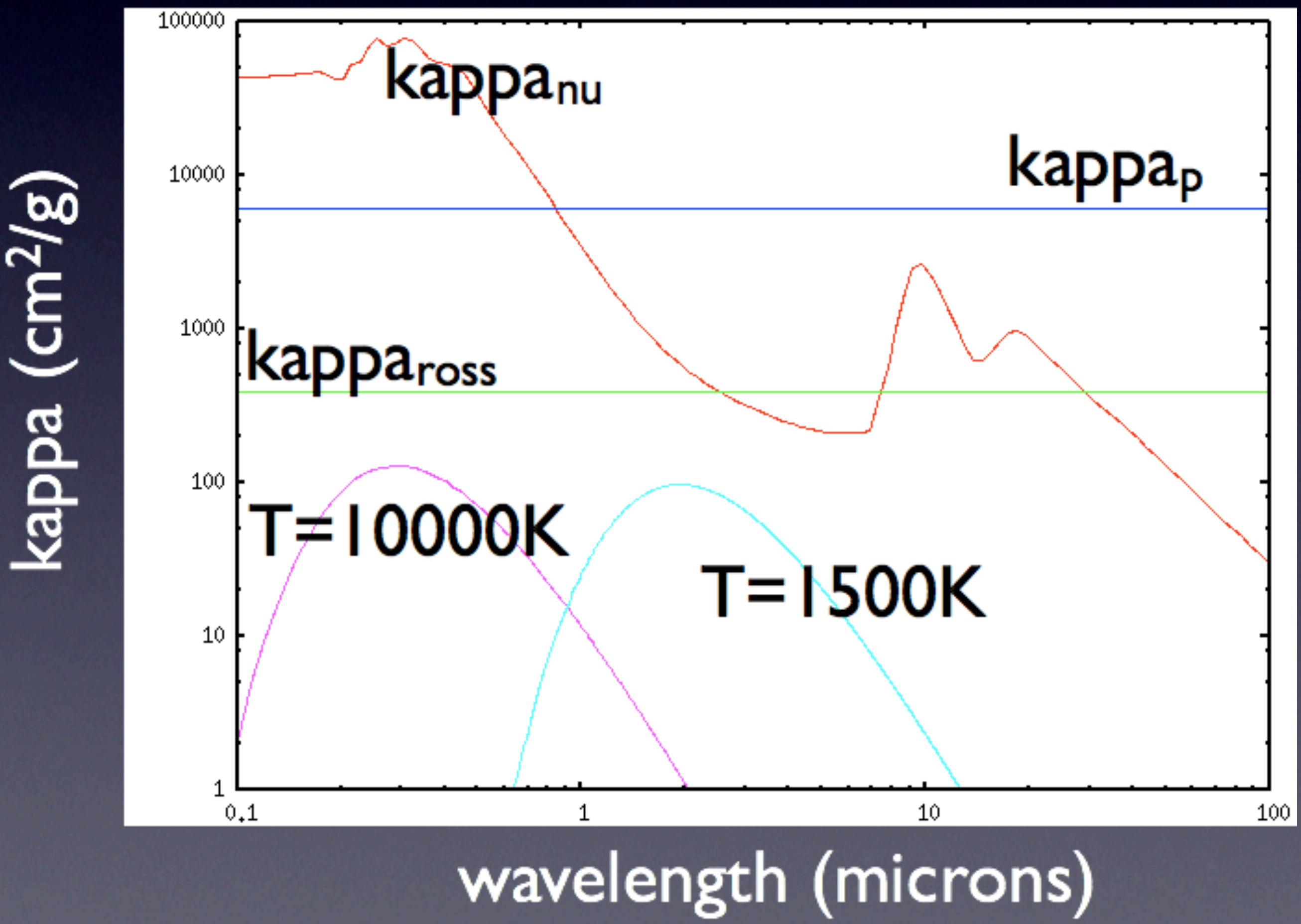
Kuiper et al. 2012 A&A 573 122

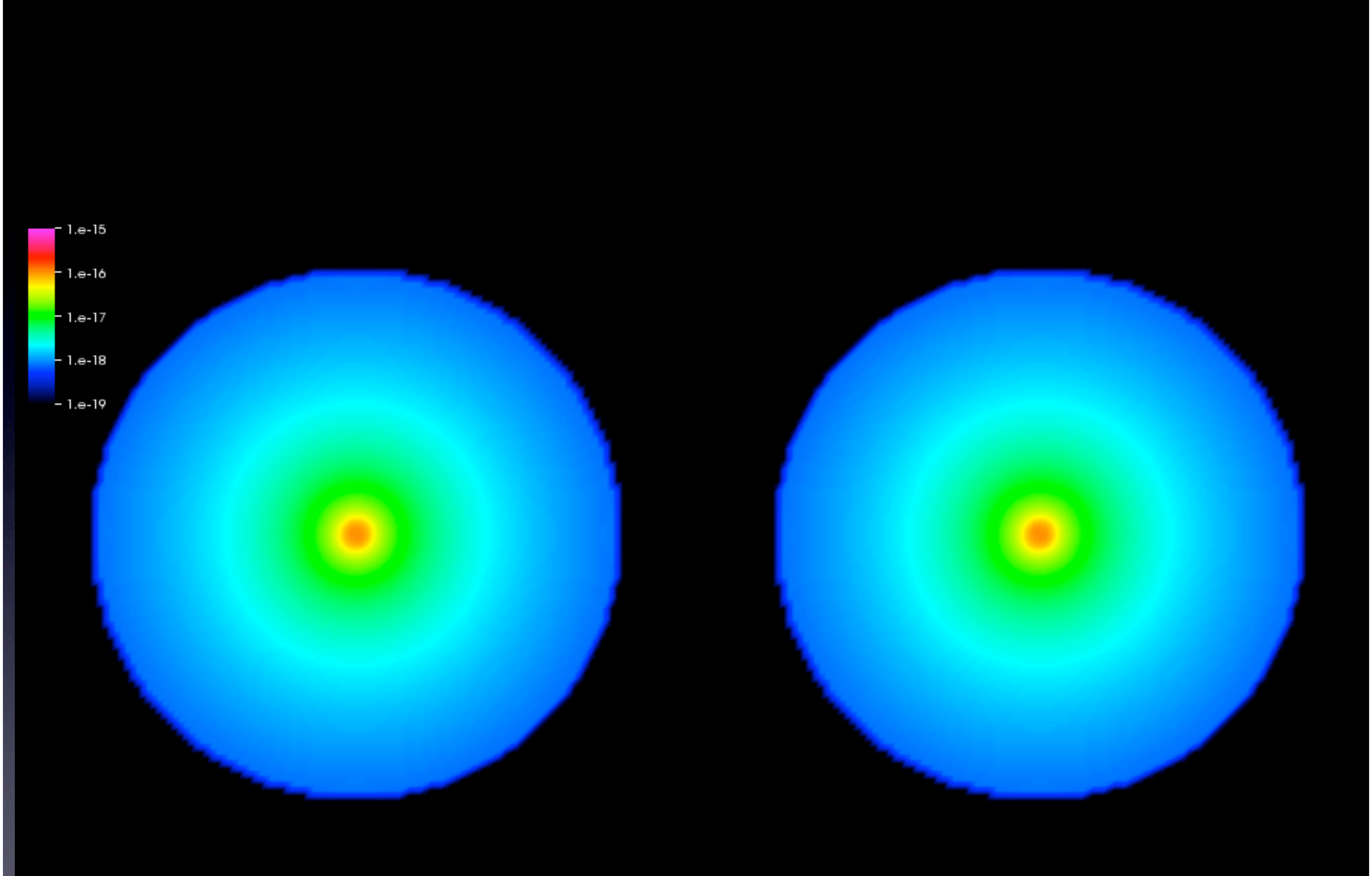


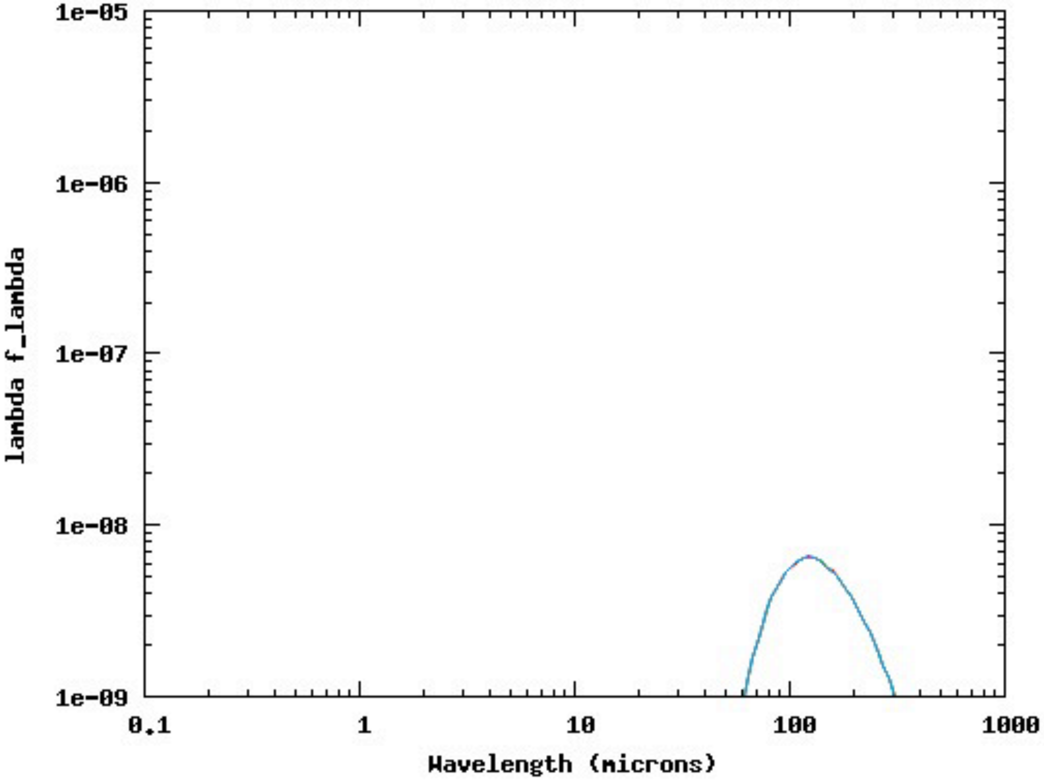
Kuiper et al. 2012 A&A 573 122

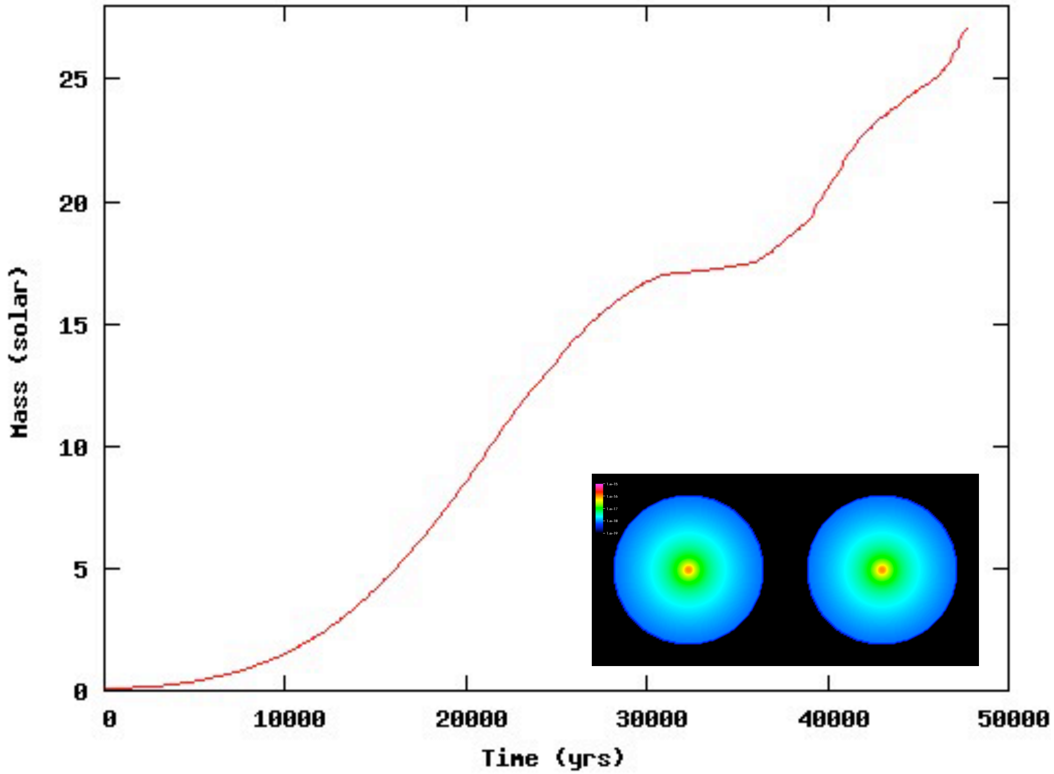


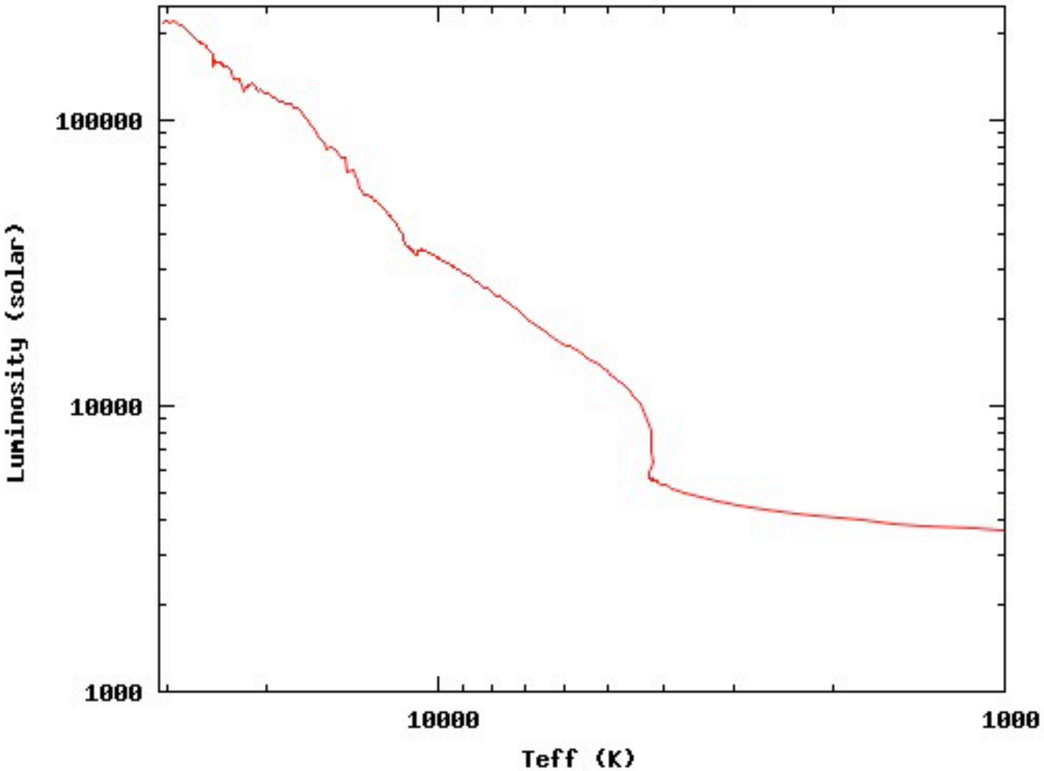
$$\mathbf{a}_{\rm rad,FLD} = \kappa_{\rm Ross}(T_{\rm sub})\frac{L_*}{4\pi r_{\rm sub}^2 c} \qquad \mathbf{a}_{\rm rad} = \kappa_{\rm Planck}(T_*)\frac{L_*}{4\pi r_{\rm sub}^2 c}$$

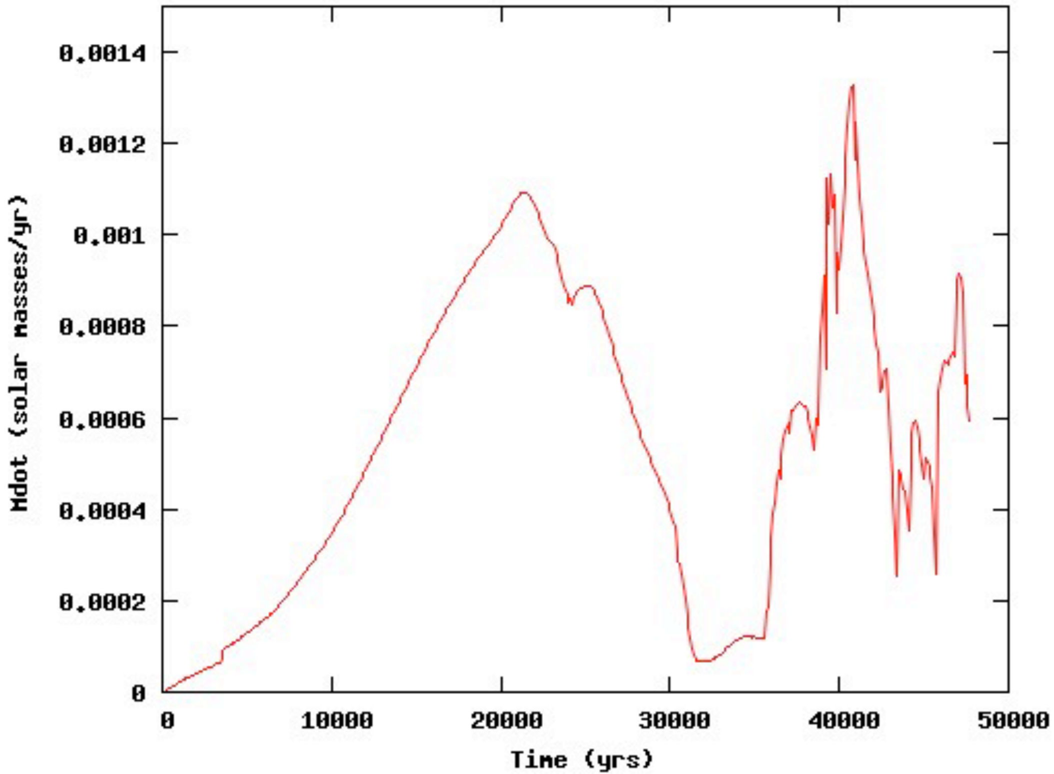



1.e-15
1.e-16
1.e-17
1.e-18
1.e-19


1e-05
1e-06
1e-07
1e-08
1e-09
lambda f_lambda
0.1
1
10
100
1000
Wavelength (microns)


25
20
15
10
5
0
Mass (solar)
0
10000
20000
30000
40000
50000
Time (yrs)


100000
10000
1000
Luminosity (solar)
10000
1000
Teff (K)


0.0014
0.0012
0.001
0.0008
0.0006
0.0004
0.0002
0
Mdot (solar masses/yr)
0
10000
20000
30000
40000
50000
Time (yrs)

The TORUS code

http://www.astro.ex.ac.uk/people/th2/torus_html/homepage.html

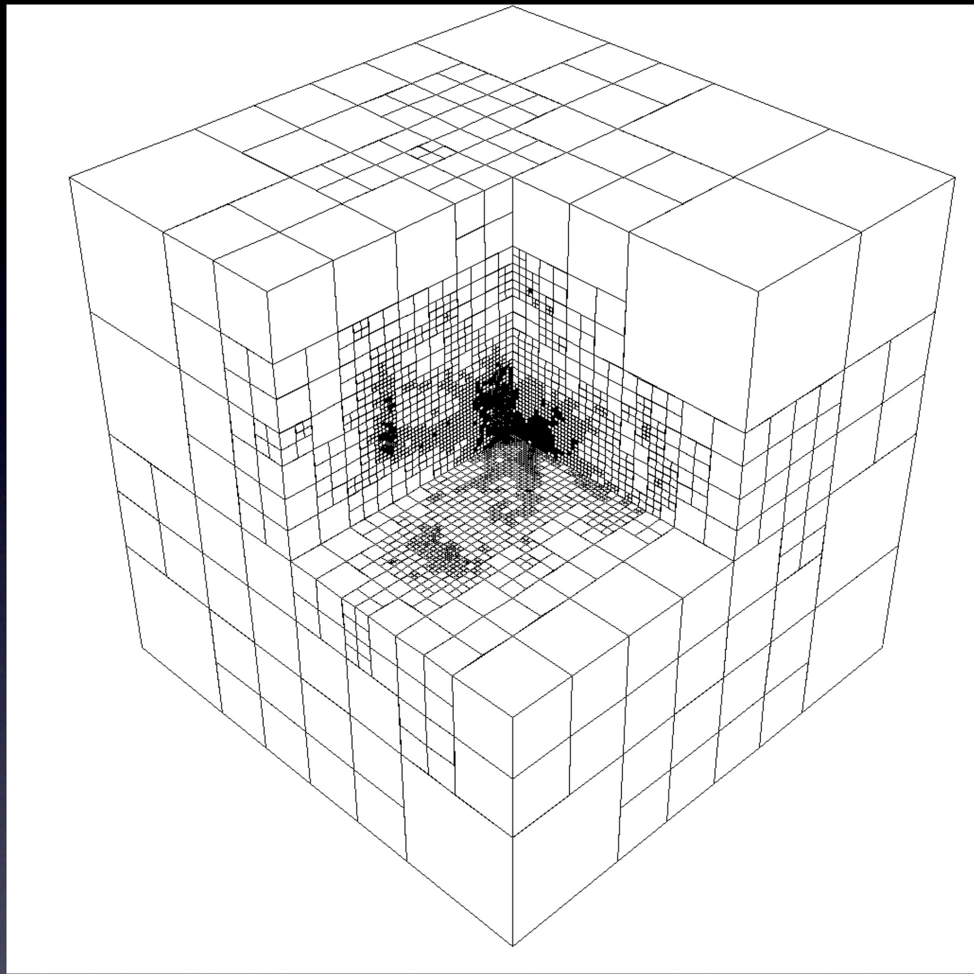
- Flexible tool for computing images and spectra for a wide variety of objects with circumstellar material, e.g.
  - O-star and WR star winds (atomic lines and continuum)
  - Symbiotic binary stars (Raman scattered lines)
  - Classical T Tauri stars (atomic lines and dust continuum)
  - Herbig Ae/Be stars (dust continuum)
  - Stellar clusters (dust continuum)
  - Molecular Clouds (molecular lines and dust continuum)
  - Spiral galaxies (21cm line)

Technical aspects

- Written in modular Fortran 90 (code base is ~150,000 lines)
- Stored in SVN
- Parallelized under MPI and openMP
- Minimal external libraries required (MPI plus cfitsio if you wish to create FITS output)
- Test suite run nightly
- Compiles on a wide variety of architectures

Numerical aspects

- Variables (density, temperature, velocity etc) held on an adaptive mesh
  - Either 3D cartesian (octal tree)
  - or 2D cylindrical (quad tree)
  - or 3D cylindrical polar (mixture of octal/quad)



Science aspects

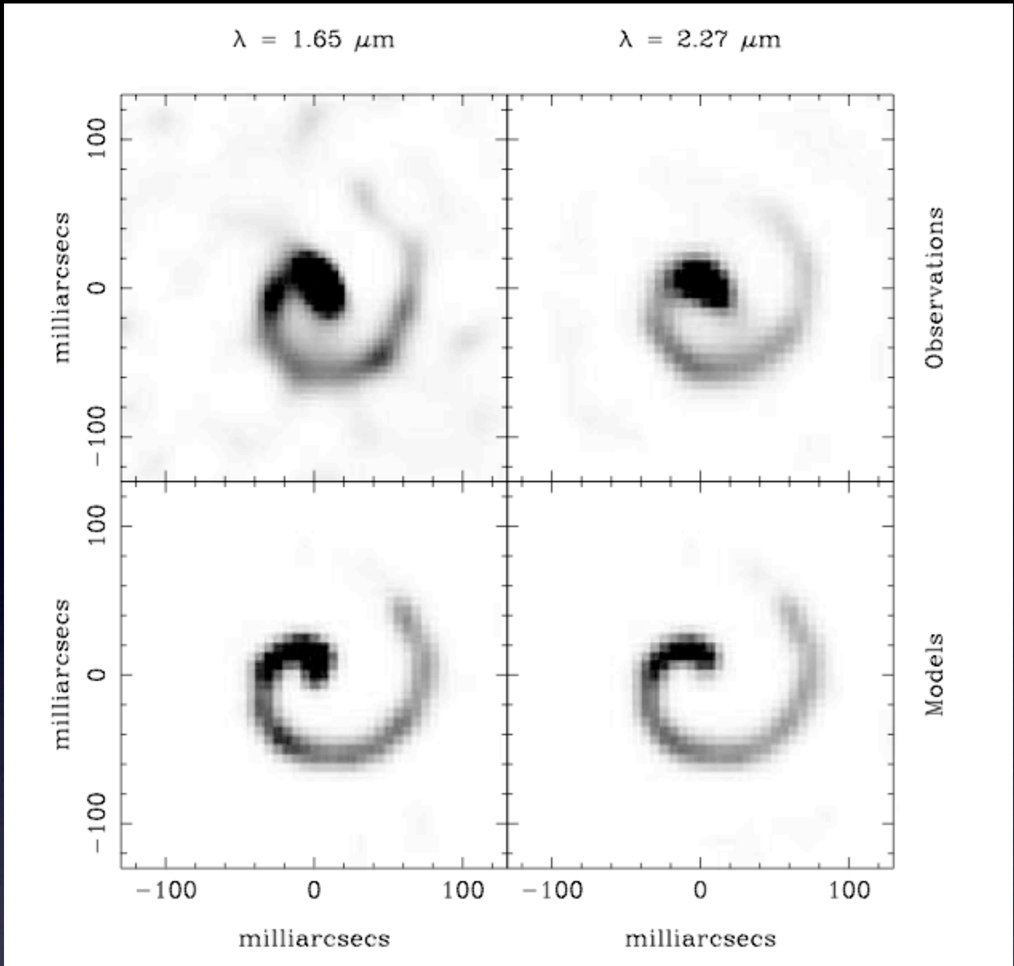
- Atomic spectral lines
  - Solves statistical equilibrium using either the Sobolev approximation or in the co-moving frame
  - Does **not** currently perform radiative equilibrium for the atomic case (i.e. need a temperature structure)
  - Line transfer followed in all four Stokes intensities (spectropolarimetry)

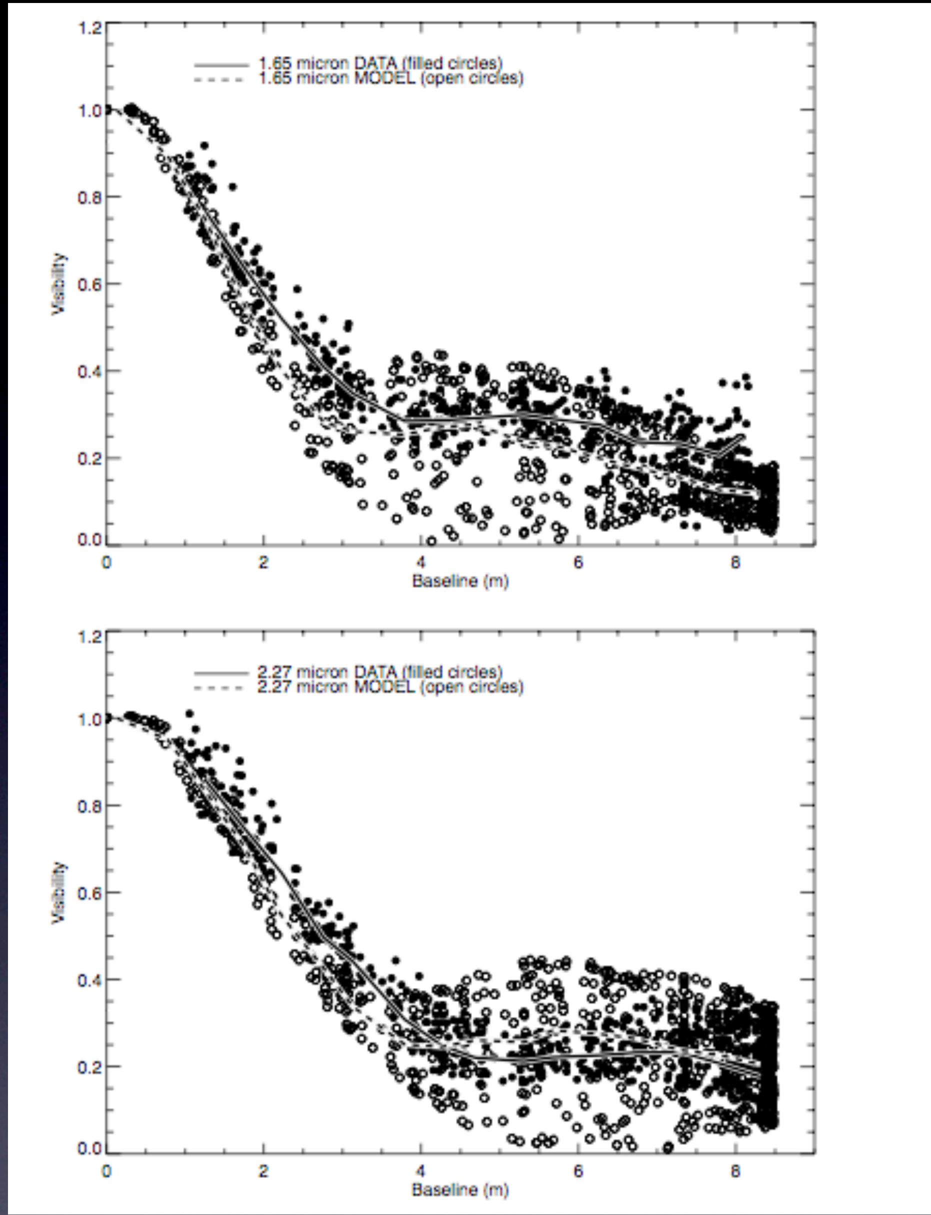
Science aspects

- Photoionization (truly work in progress)
  - Monte-Carlo estimators for the photoionization rate
  - Full radiative equilibrium inc. dust
  - Similar method to (but not as detailed in atomic physics as) Barbara Ercolano's *Mocassin* code and Kenny's photoionization code

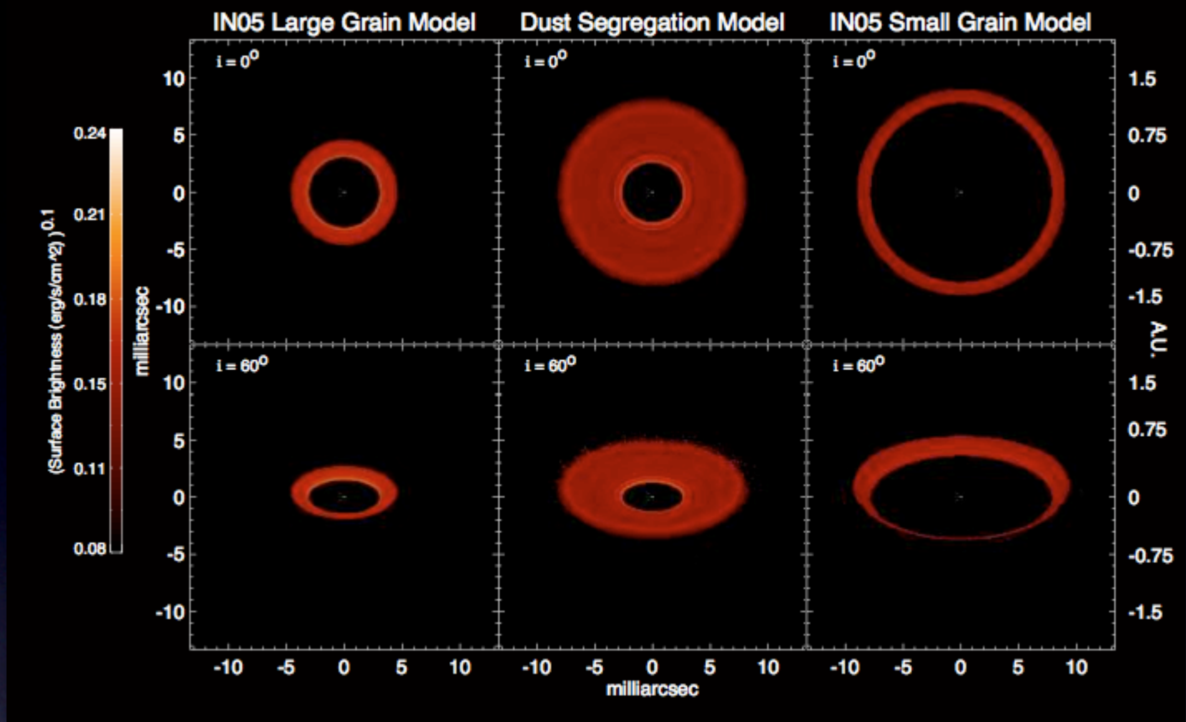
Science aspects

- Dust continuum transfer
  - Radiative equilibrium solving using Lucy's (1999, *A&A*, **344**, 282) Monte-Carlo algorithm
  - Multiple dust species, dust sublimation, vertical hydrostatic equilibrium in discs
  - Stokes intensities followed (polarization images, spectra)





Harries, Monnier, Symington & Kurosawa (2004)



Tannirkulam et al. , 2008, *ApJ*, **689**, 513

Tannirkulam et al. , 2008, *ApJ*, **677**, 51

Tannirkulam et al. , 2007, *ApJ*, **661**, 374

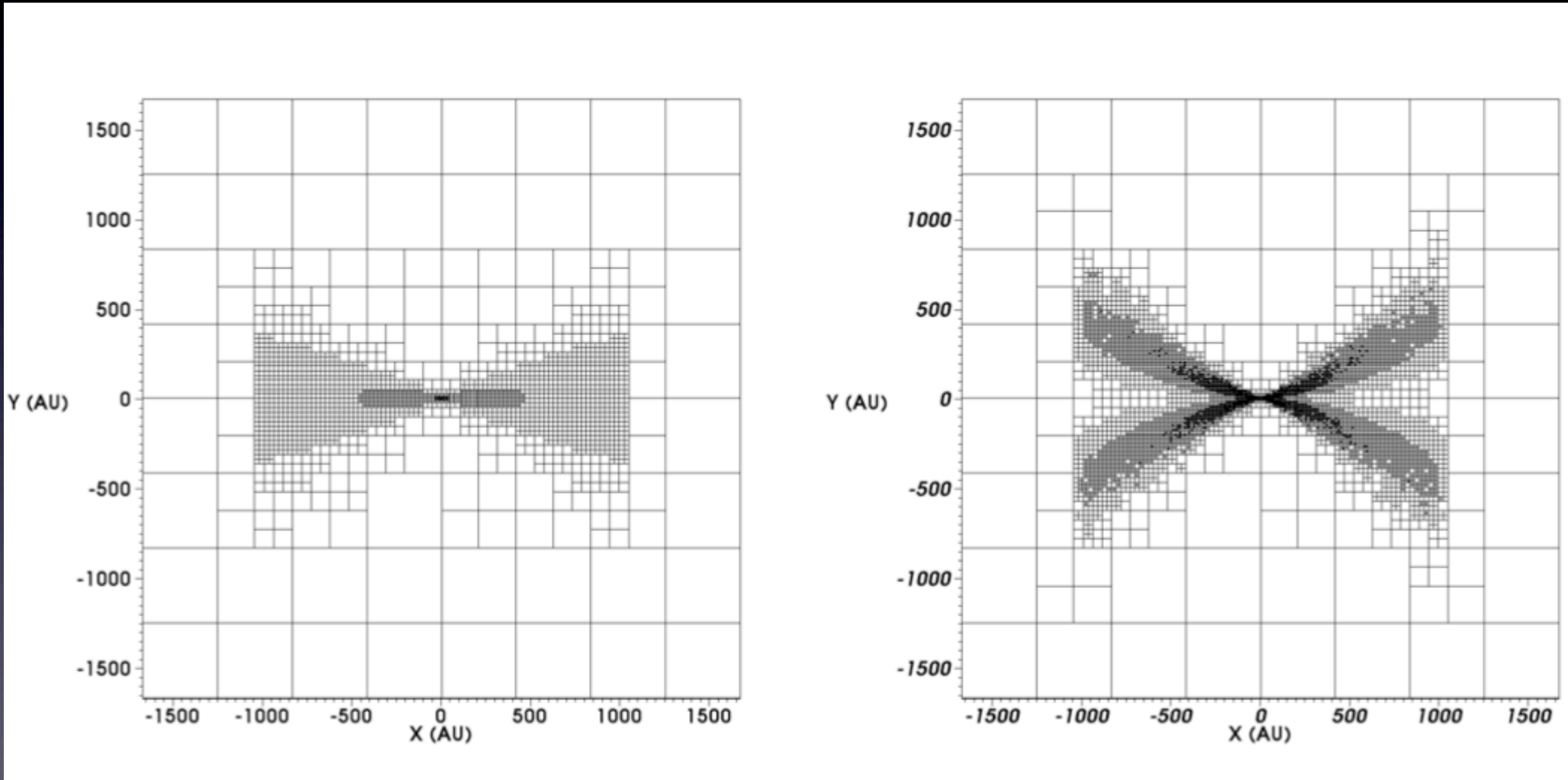
Post-processing hydro simulations

- Gridding SPH simulations
- Resolution issues

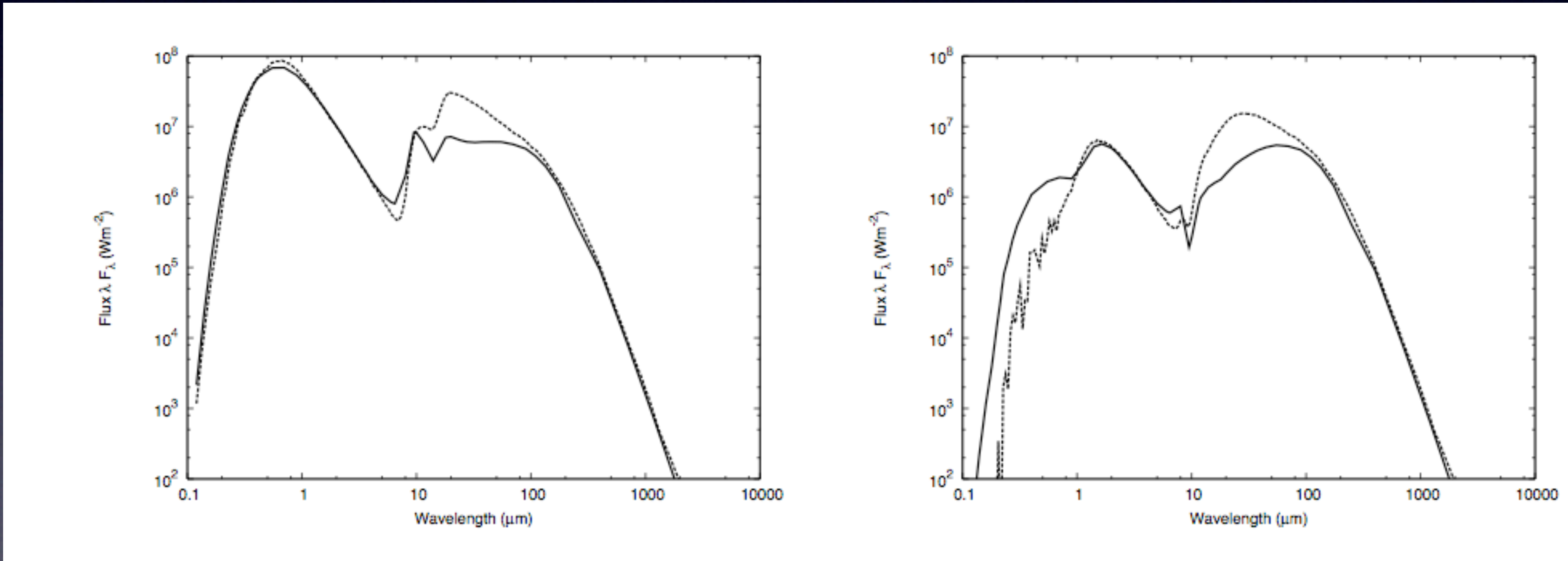
- NB the spatial resolution required for hydrodynamics is often significantly lower than that required for radiation transport!

Acreman et al. 2010, MNRAS, 403, 1143

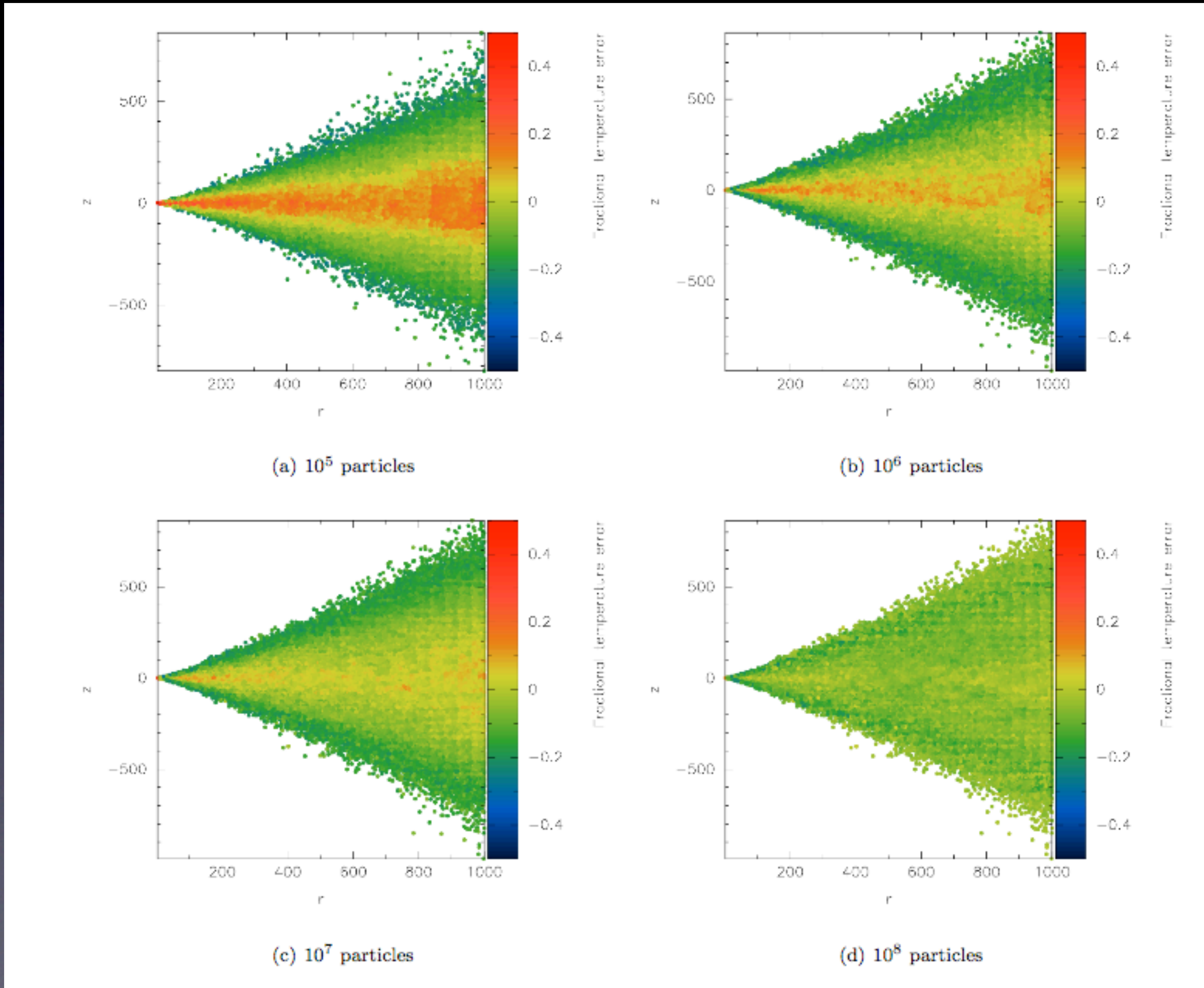
Splitting on mass or splitting on density gradient?



Benchmark SEDs at two inclinations for 100,000 particle SPH simulation



Fractional temperature errors compared to benchmark

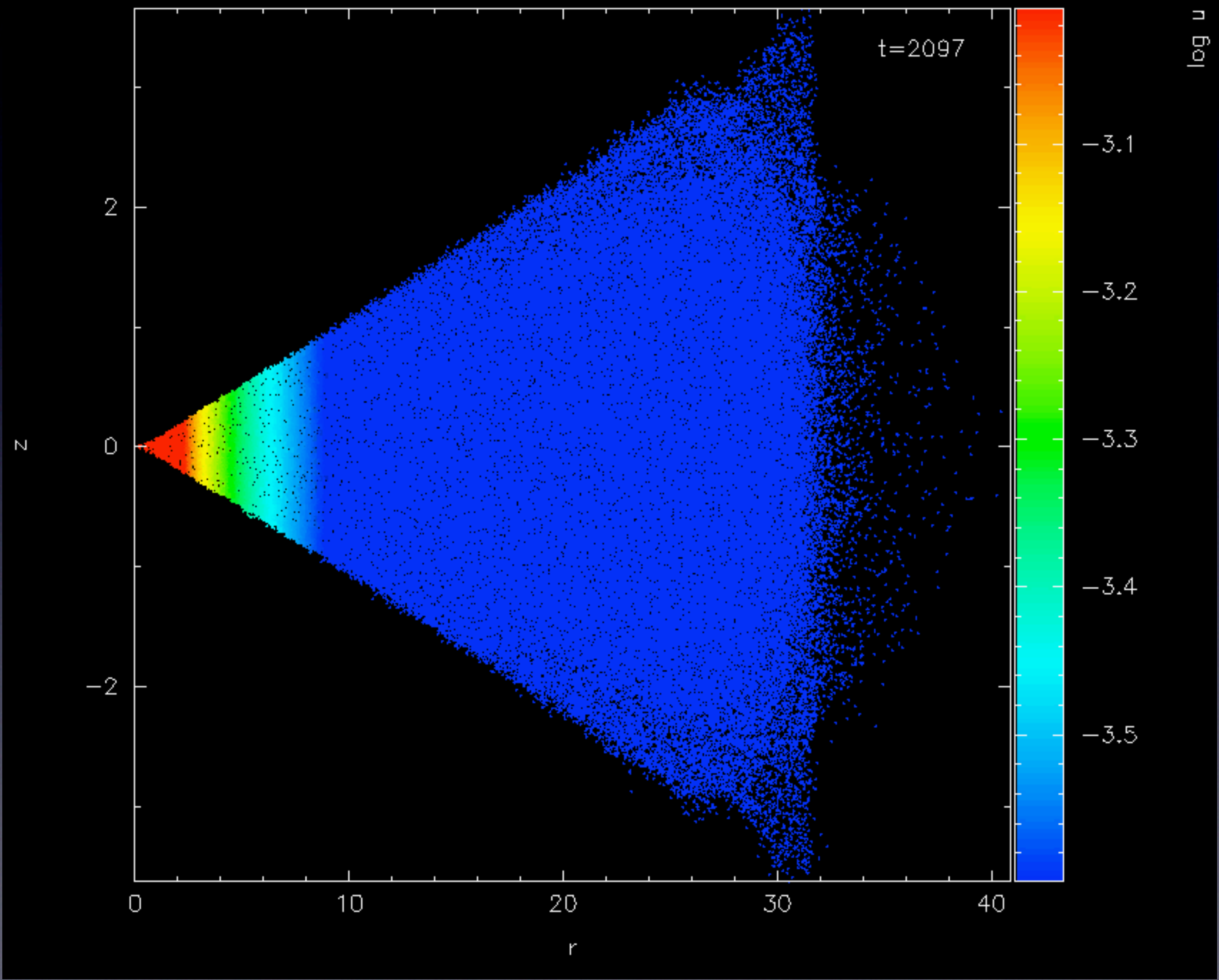


(a) 10^5 particles

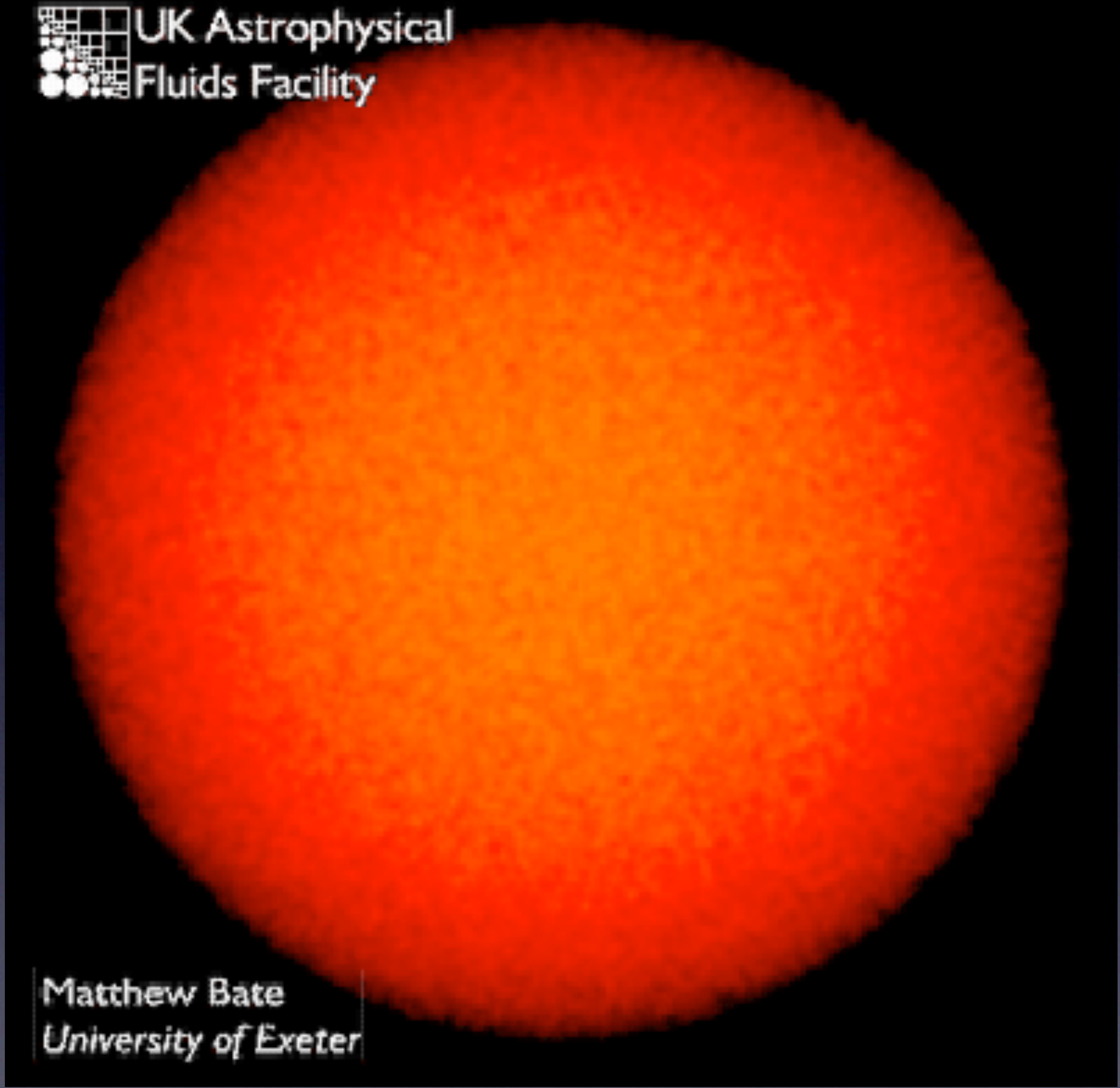
(b) 10^6 particles

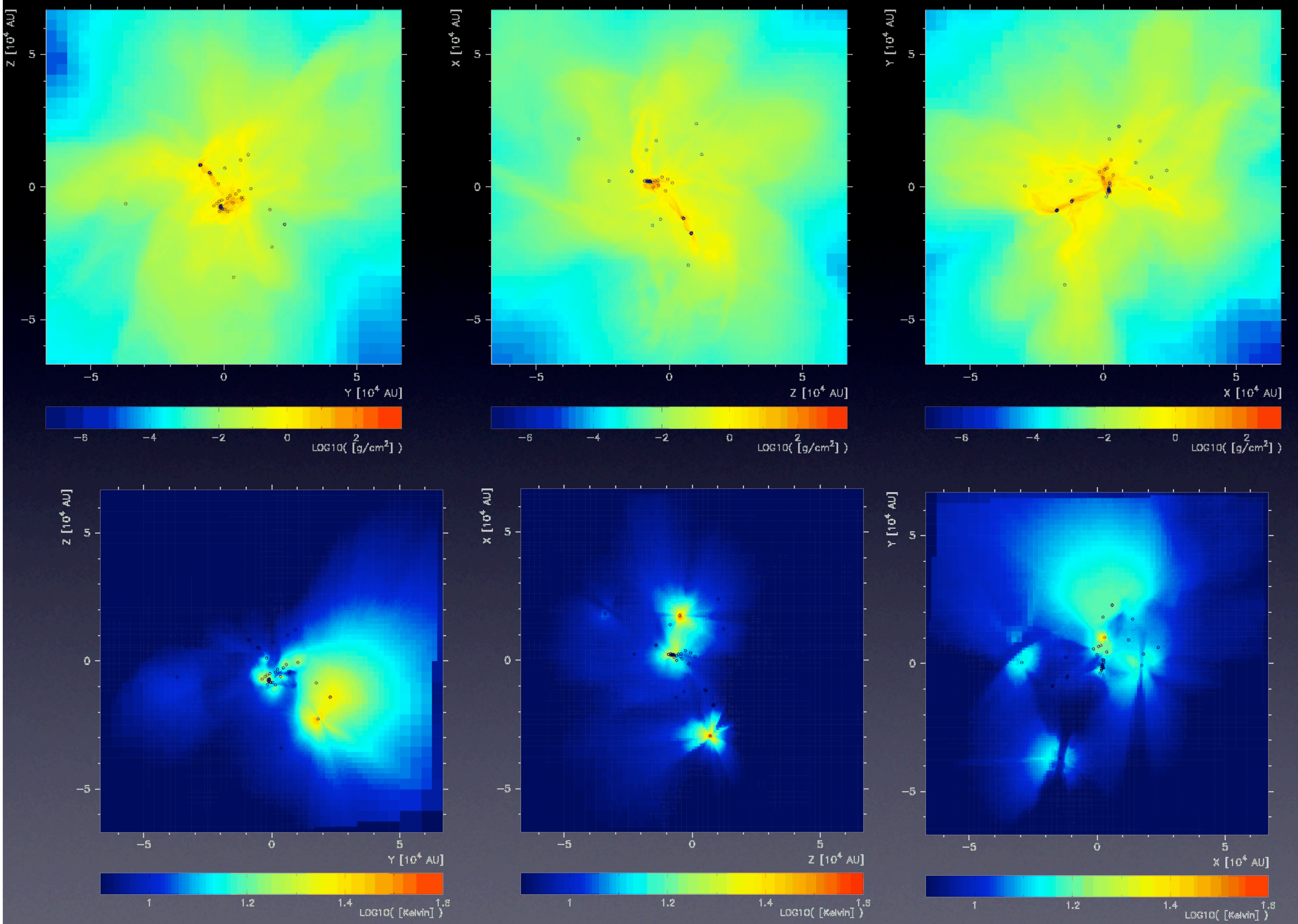
(c) 10^7 particles

(d) 10^8 particles

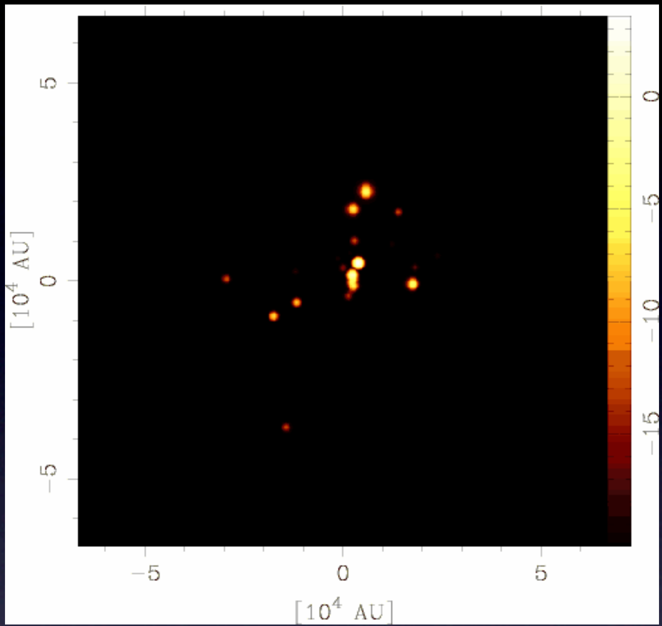


t=2097
z
r
log u
0
10
20
30
40
2
0
−2
−3.1
−3.2
−3.3
−3.4
−3.5

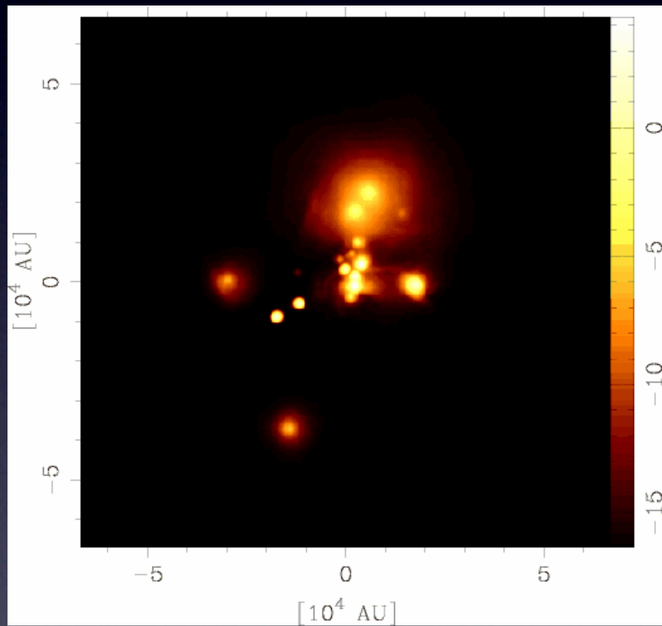

UK Astrophysical
Fluids Facility
Matthew Bate
University of Exeter


Z [10^4 AU]
Y [10^4 AU]
LOG10([g/cm^2])
X [10^4 AU]
Z [10^4 AU]
LOG10([g/cm^2])
Y [10^4 AU]
X [10^4 AU]
LOG10([g/cm^2])
Z [10^4 AU]
Y [10^4 AU]
LOG10([Kelvin])
X [10^4 AU]
Z [10^4 AU]
LOG10([Kelvin])
Y [10^4 AU]
X [10^4 AU]
LOG10([Kelvin])

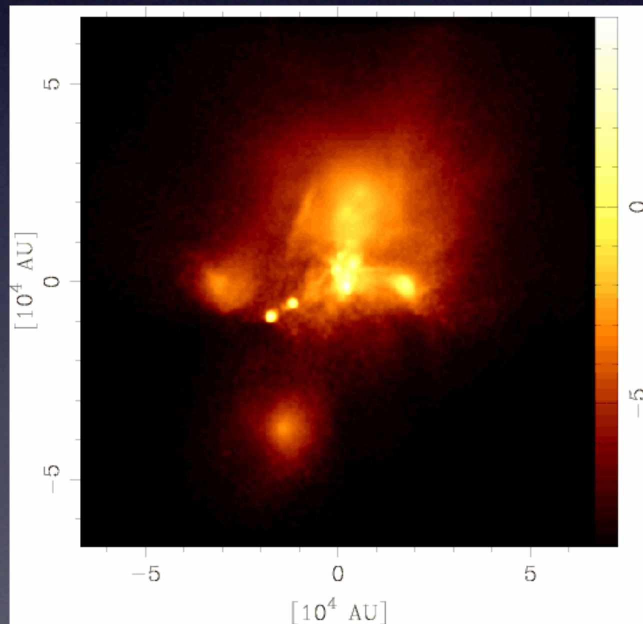
24 micron

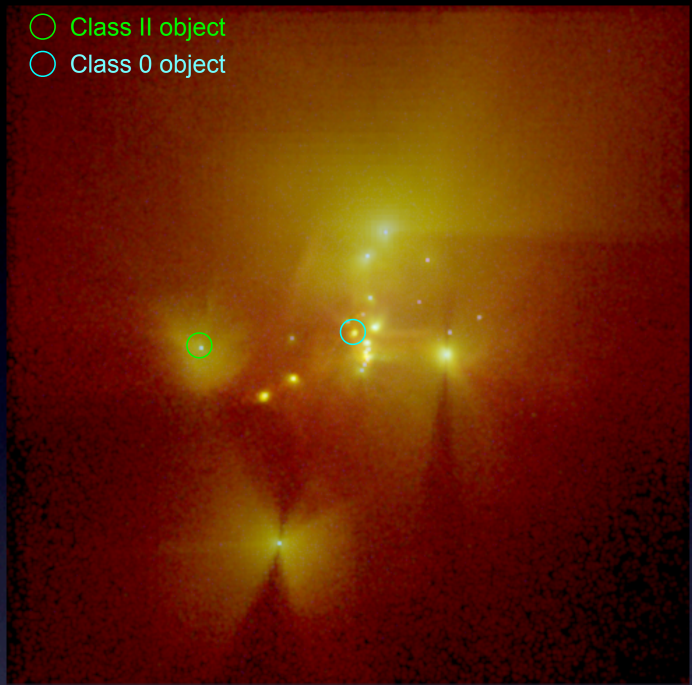


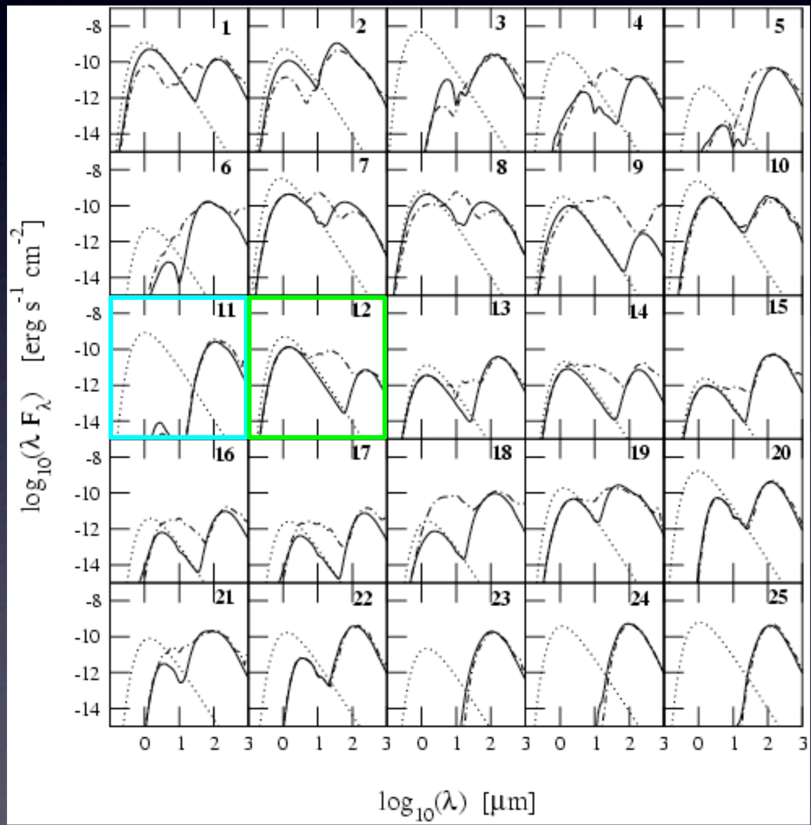
70 micron



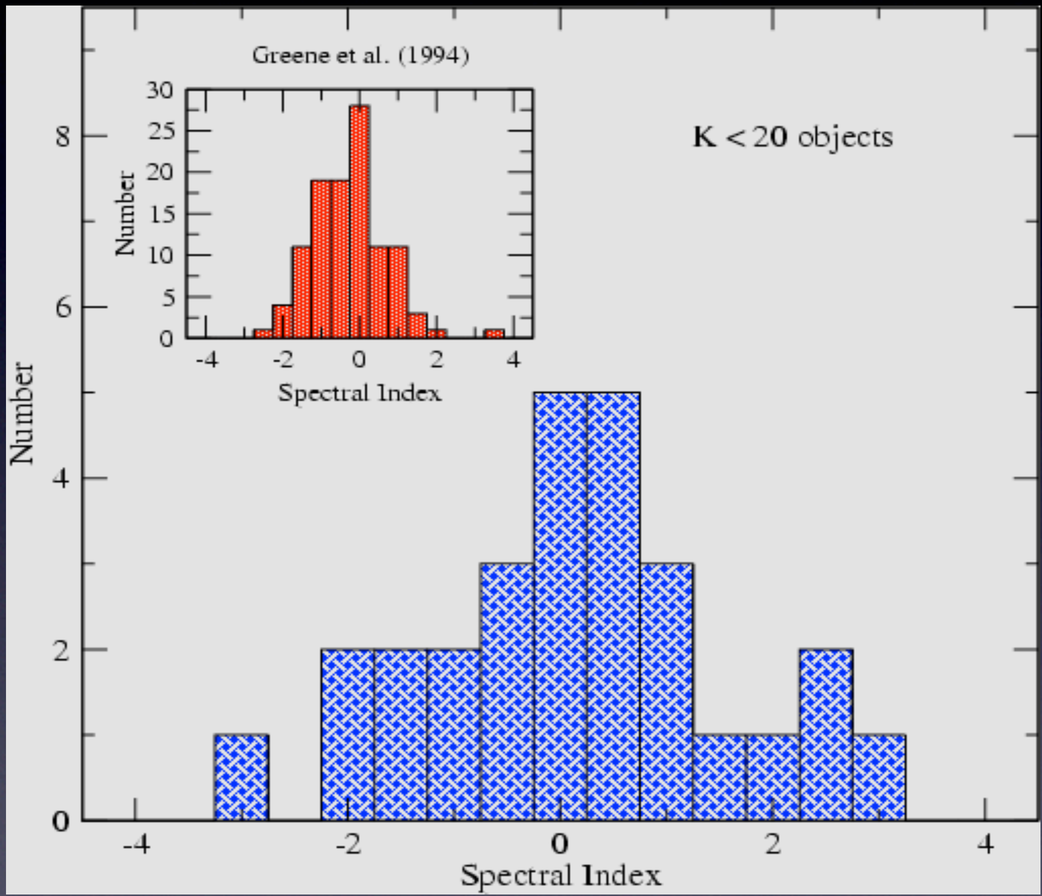
160 micron




Class II object
Class 0 object


$\log_{10}(\lambda F_\lambda)$ [erg s^{-1} cm^{-2}]
$\log_{10}(\lambda)$ [μm]

Spectral index distribution
(Slope of SED between 2.2-10 μm)

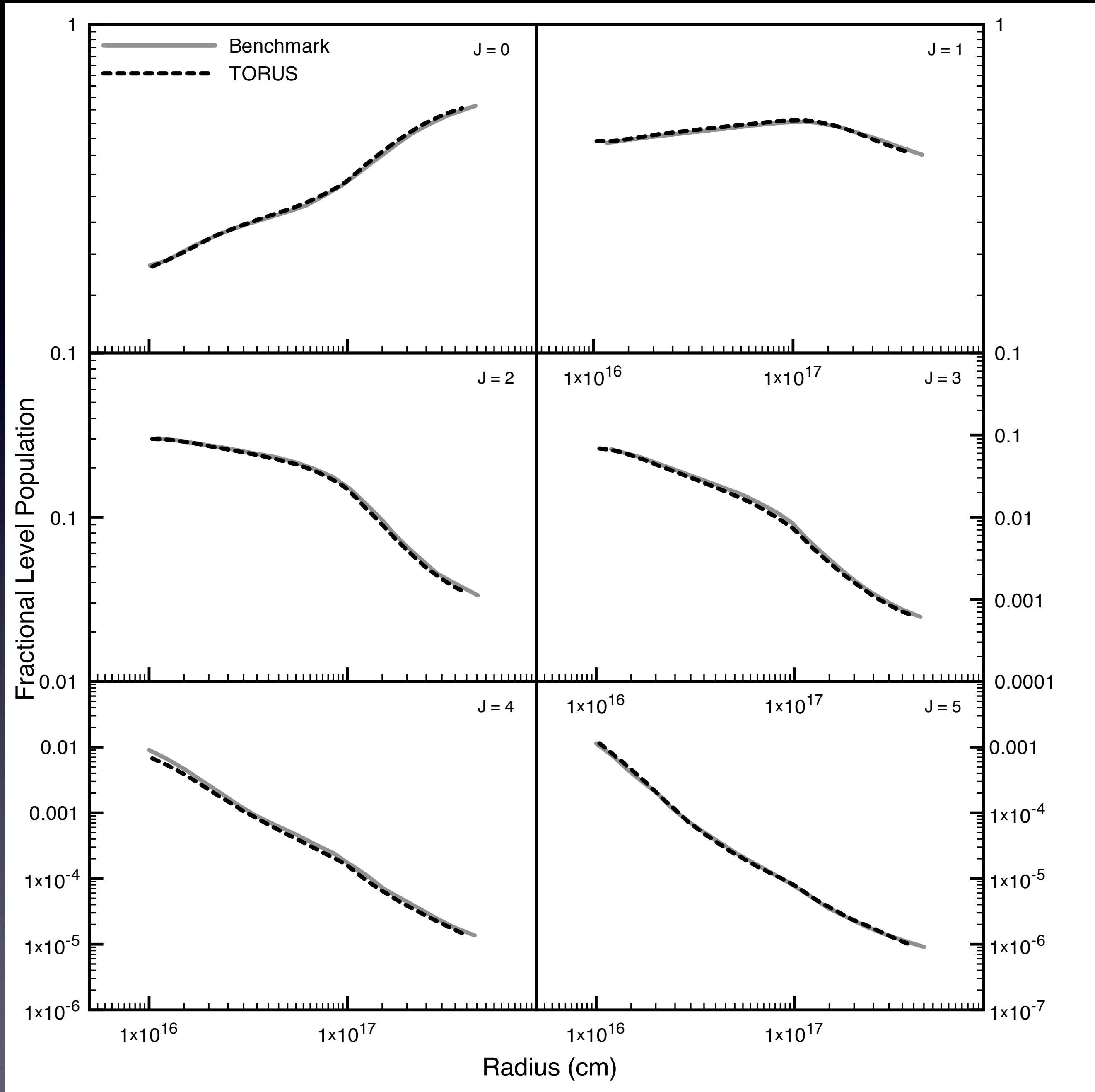


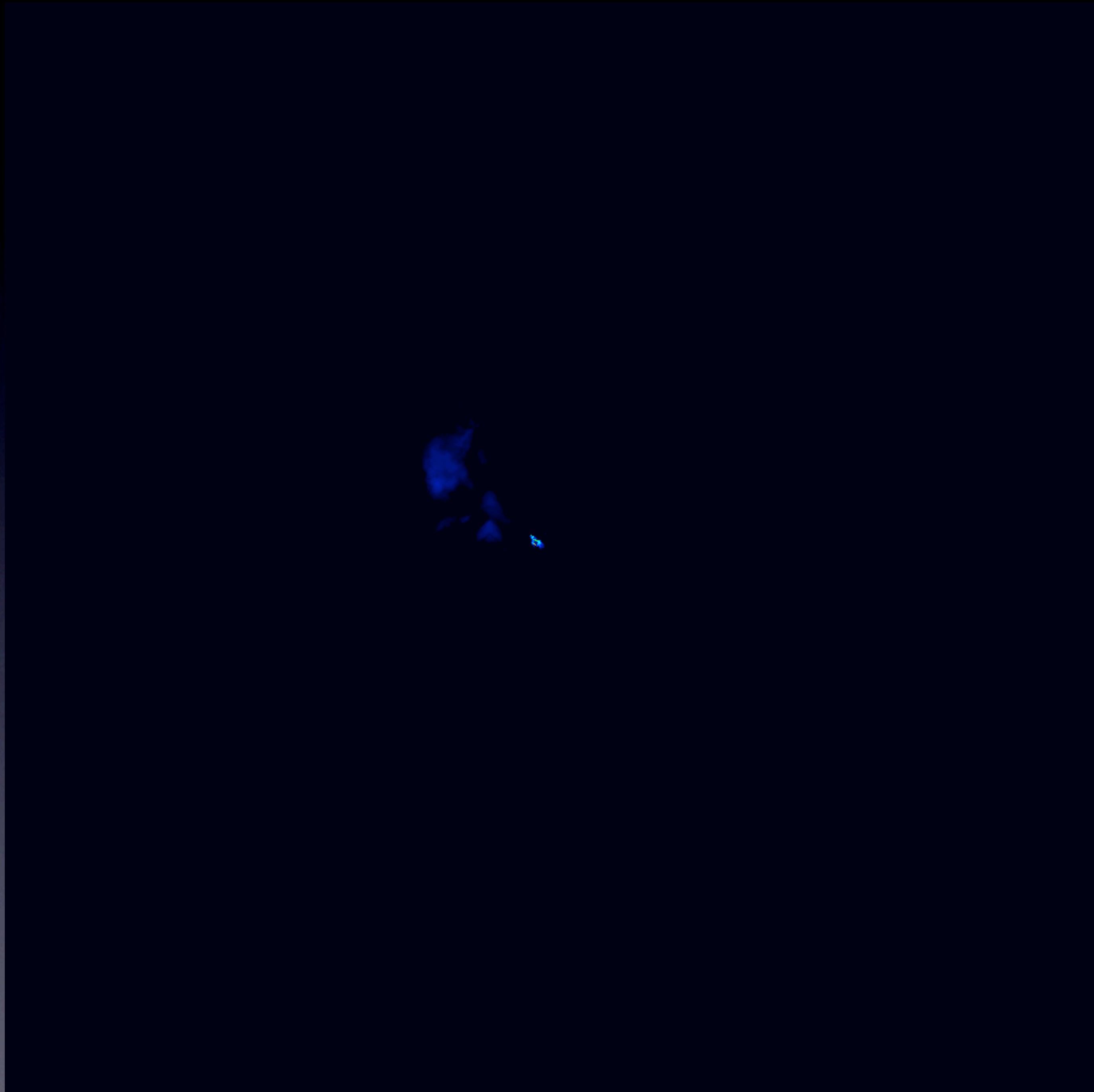
Red histogram shows results for rho Oph by Greene et al. (1994).

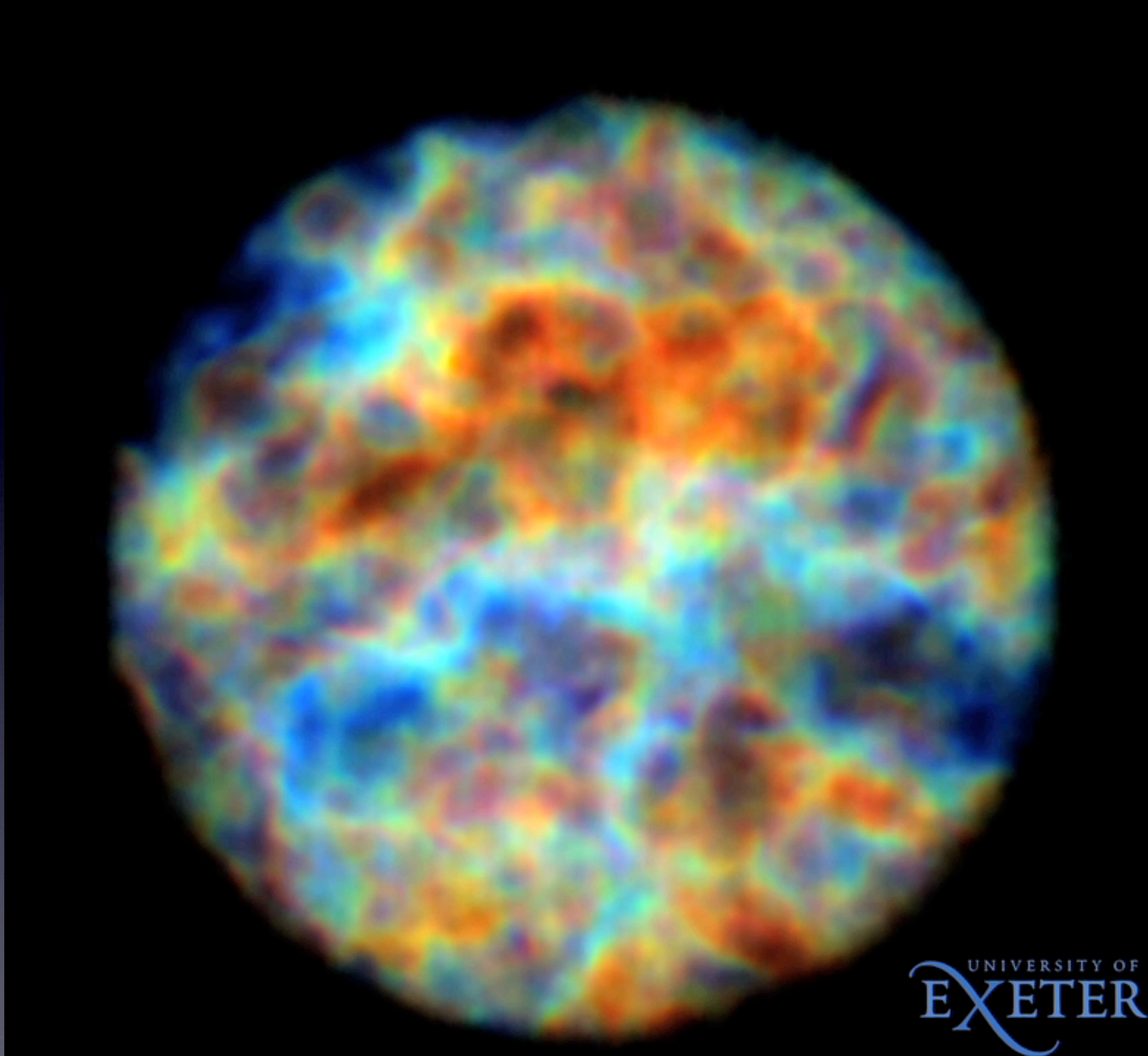
Molecular lines

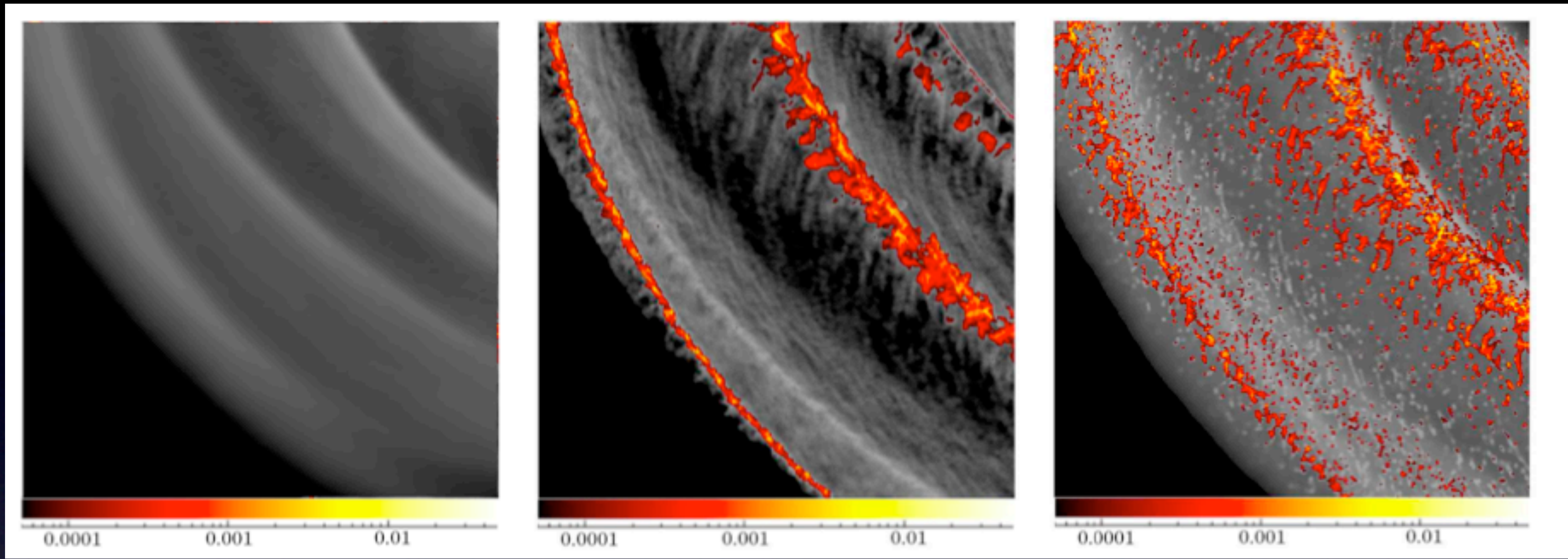
- David Rundle's PhD thesis
- Statistical equilibrium solved using co-moving frame transfer with Monte-Carlo direction sampling (modified version of the MC accelerated lambda iteration method of Hogerheijde & van der Tak 2001)

HCO^+ J=1 to 0 (89.2 GHZ)






UNIVERSITY OF
EXETER



Acreman, Douglas, Dobbs and Brunt, "Synthetic HI observations of a simulated spiral galaxy", MNRAS submitted.

Douglas, Acreman, Dobbs and Brunt, "A Synthetic 21-cm Galactic Plane Survey of an SPH Galaxy Simulation", MNRAS, submitted.

Using TORUS

- The publicly available version is at

  http://www.astro.ex.ac.uk/people/th2/torus_html/homepage.html

- This version contains the code for performing dust radiative equilibrium and calculating images and SEDs
- A version with molecular line transfer, atomic line transfer, and photoionisation is available to collaborative users (those who will work closely with the Exeter Group)

Installing TORUS

- You will need
  - The source code and data files (grain optical constants) from the TORUS pages
  - The cfitsio library (if you want write or read FITS images)

    http://heasarc.gsfc.nasa.gov/fitsio/

  - The VISIT visualisation code (to view the AMR mesh. Binaries are available from

    https://wci.llnl.gov/codes/visit/

Running TORUS

- There is a user manual on the TORUS website
- TORUS models are set up using a parameters file that is text file containing keywords and values

Part of a TORUS parameters file

```
! Torus parameter file for 2D benchmark disc
! See Pascucci et al, 2004, A&A, 417, 793

dustphysics T   ! use dust microphysics

radeq T  ! perform a radiative equilibrium calculation

! AMR grid parameters

readgrid F   ! we aren't reading a grid, we will set one up from scratch
writegrid F  ! we don't need to write out the AMR file - we just need SEDs
amrgridsize 4.e6 ! the linear size of the top-level AMR mesh in units of 10^10 cm
amr2d T  ! this is a 2d (cylindrical) model

! grid smoothing switches

smoothgridtau T  ! smooths the grid for optical depth, in order to resolve disc photosphere
dosmoothgrid T   ! smooth the grid for jumps in cell refinement
smoothfactor 3.0 ! make sure that neighbouring cells are not only one AMR depth apart


! Source parameters

nsource 1  ! there is just one source
radius1 1.  ! it has a radius of 1 solar radius
teff1 5800.  ! the source effective temperature
contflux1 blackbody ! the continuum flux is assumed to be a blackbody
mass1 1.   ! the source has a mass of one solar mass
sourcepos1 0. 0. 0  ! it is located at the grid cntre

! Geometry specific parameters

geometry benchmark  ! this is the Pascucci (2004) benchmark
rinner 1. ! inner disc radius (AU)
router 1000. ! outer disc radius
height 125. ! disc scaleheight at 100 AU (in AU)
rho 8.16136e-18  ! density at inner edge midplane (g/cc)

! Dust grain properties

iso_scatter T      ! Assume isotropic scattering (assumed by benchmark)
graintype1 draine_sil  ! Draine silicates
grainfrac1 0.01    ! grain mass fraction (in terms of gas)
amin1 0.12         ! minimum grain size (microns)
amax1 0.1201       ! maximum grain size (microns)
qdist1 0.01        ! power law index (flat)
```

What to do next

- If you want to install and run a test model using TORUS then please feel free
- Try running the sample parameters file from the web (a dusty disc) and calculate some SEDs and images...

Have fun!