RADMC-3D

A publicly available radiative transfer program

C.P. Dullemond
Institute for Theoretical Astrophysics (ITA/ZAH), University of Heidelberg
With help from: R. Shetty, T. Peters, A. Juhasz, B. Commercon, M. Flock
and many beta-testers

Two „kinds“ of radiative transfer

- In dynamic models:
  - Must be extremely fast (RT=bottle neck)
  - High accuracy not feasible (not really necessary)
  - Using mean opacities, flux lim diffusion, simplex-style
  - Must be as parallellizable as hydro
  - Complex on MPI

- Post-processing, for comparison to observations:
  - Must be very accurate, and frequency dependent
  - Must include complex radiative physics (lines,dust)
  - Must not necessarily be extremely fast
  - Can often be done on shared-memory machines

RADMC-3D Goals

- Compute synthetic observations from models:
  - Images
  - Spectra
  - ...and their combination: PV Diagrams etc

- Processes currently included:
  - Dust thermal emission, extinction, scattering
  - Line emission, extinction: LTE / simple non-LTE

- What it will *not* do:
  - Add noise, simulate instrument response

RADMC-3D philosophy

- Publicly available without strings attached
- Very flexible...
  - Any density distribution (1D,2D,3D) provided as:
    - List of numbers at grid points provided as input file
    - User-defined analytic function
  - Various coordinates: Cartesian / Spherical
  - Various grid-types: Regular / AMR / Patches
  - Various emission processes: Dust, Lines, User-defined
- ...yet relatively easy to use:
  - Well-documented (extensive manual)
  - Many simple example models
  - Out-of-the-box compilation and installation
  - Graphical User Interface for image-production

RADMC-3D Features

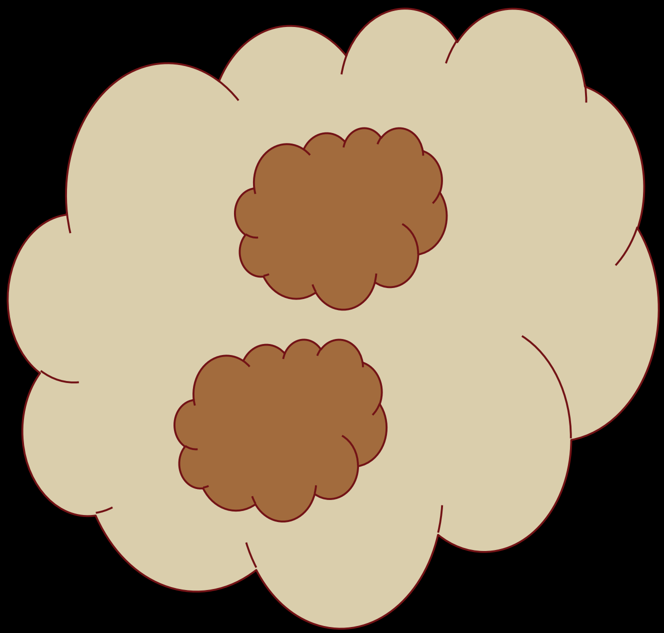
- Continuum radiative transfer (dust)
- Gas line transfer (for now only LTE, LVG, OpThin)
- Polarization
  - Scattering (off randomly oriented dust particles)
  - Thermal polarization (though simplified)
- Various sources of energy:
  - Stars
  - Continuous distributions of stars (for galaxies)
  - Viscous heating
  - External irradiation / interstellar radiation field
- Multi dust components, each with own density distribution and independent temperatures

RADMC-3D Features

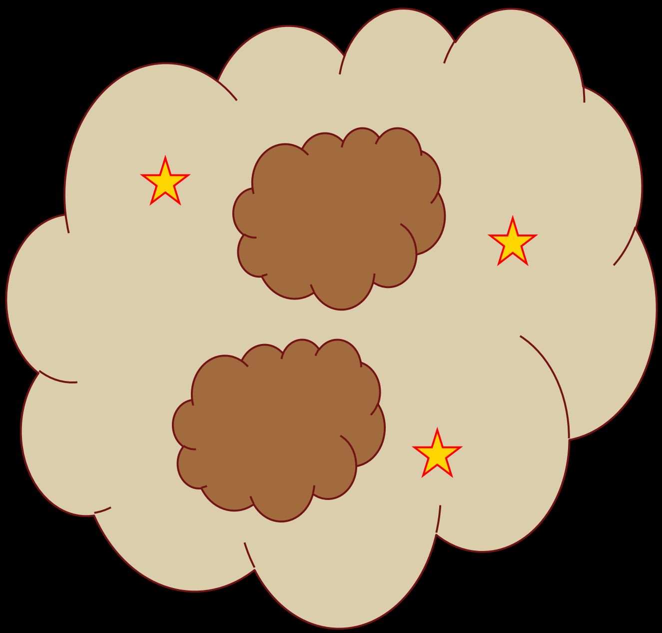
- 1-D, 2-D and 3-D models
- Cartesian or spherical coordinates
- Various gridding possibilities:
  - Regular
  - Oct-tree Mesh Refinement or
  - Patch-based Mesh Refinement
- Interface with:
  - FLASH
  - RAMSES (thanks, Benoit Commercon)
  - PLUTO (thanks, Mario Flock)

How RADMC-3D works

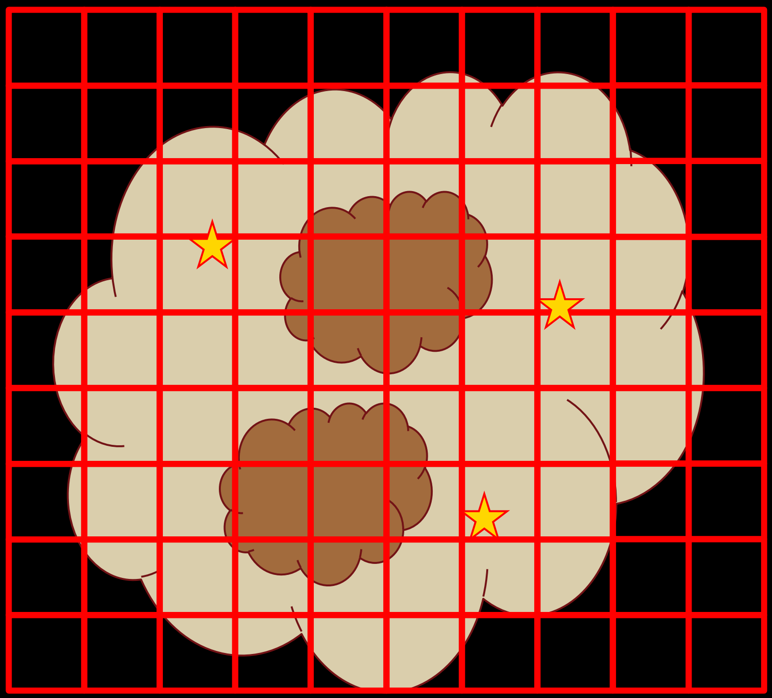
A model begins with a density distribution...



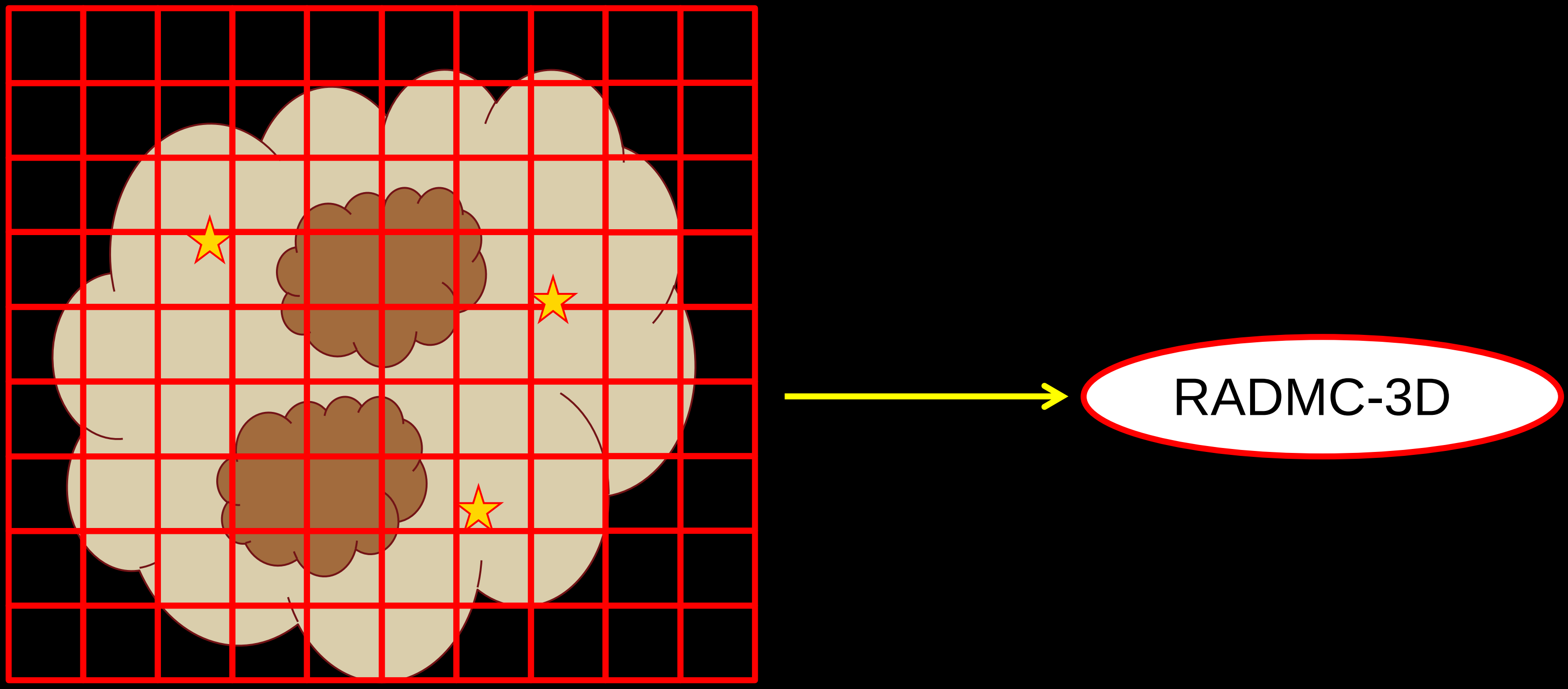
Add stars...



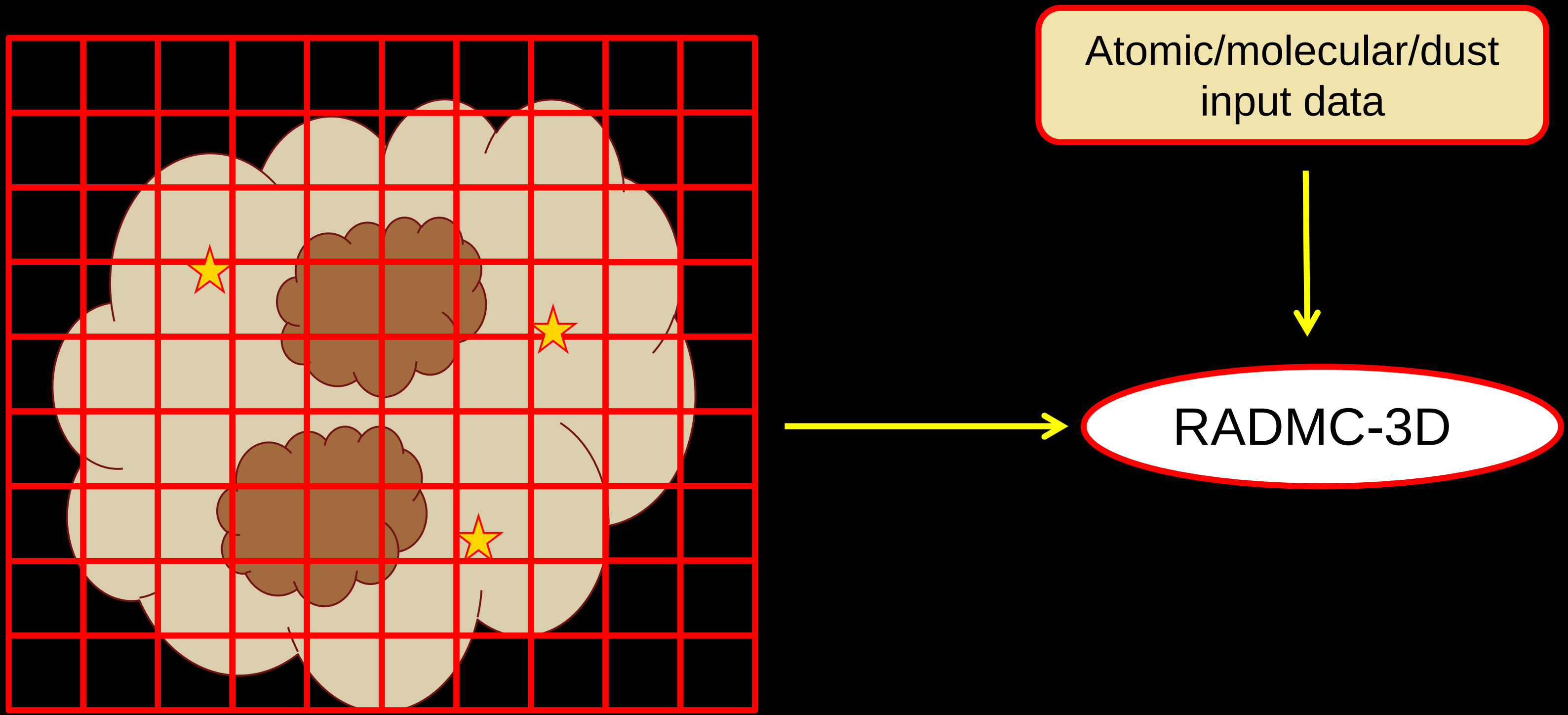
Map the density on a grid...



Pass these numbers to RADMC-3D...

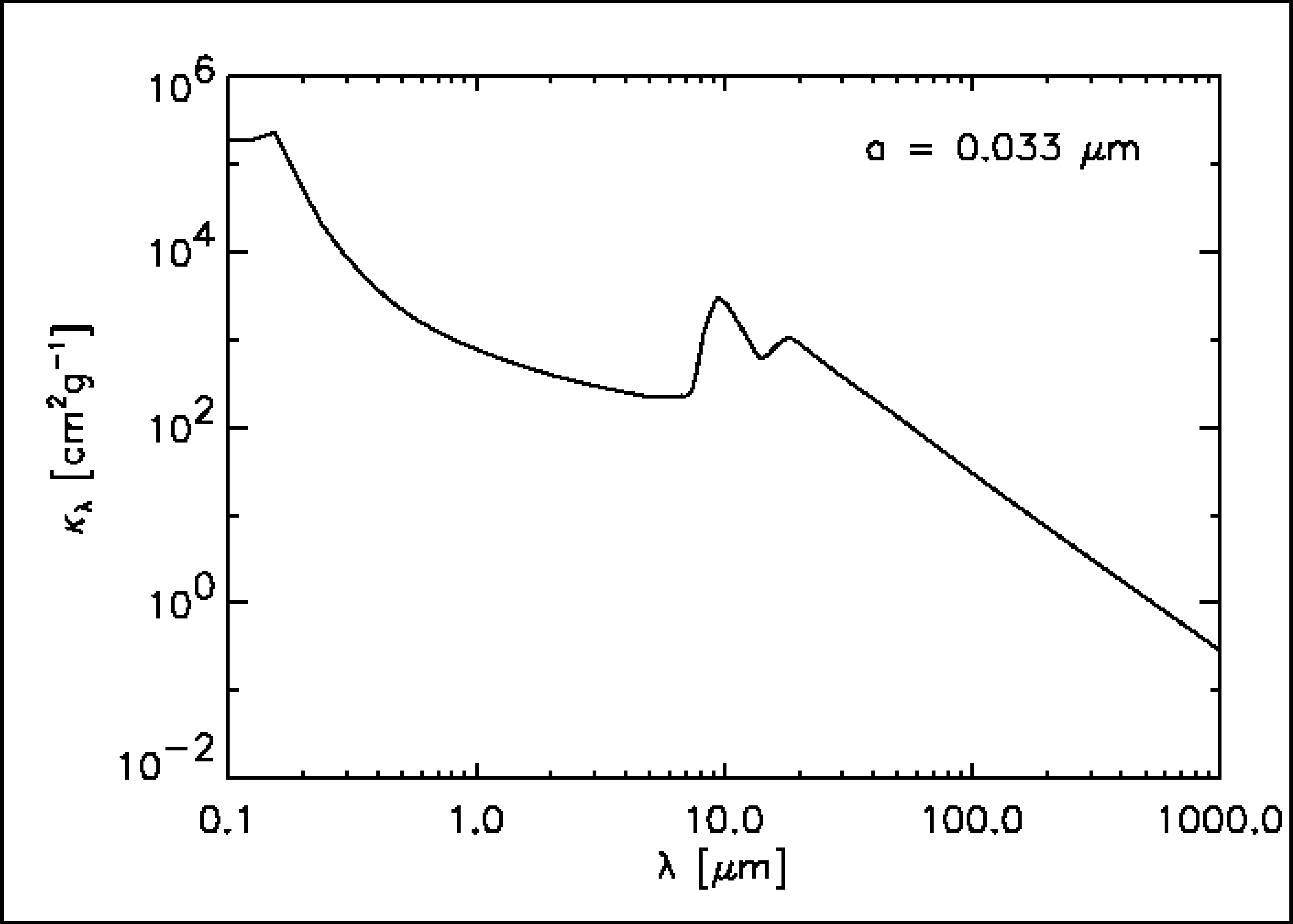


Also give RADMC-3D physical data...



Input: Dust opacity

Opacity of amorphous silicate

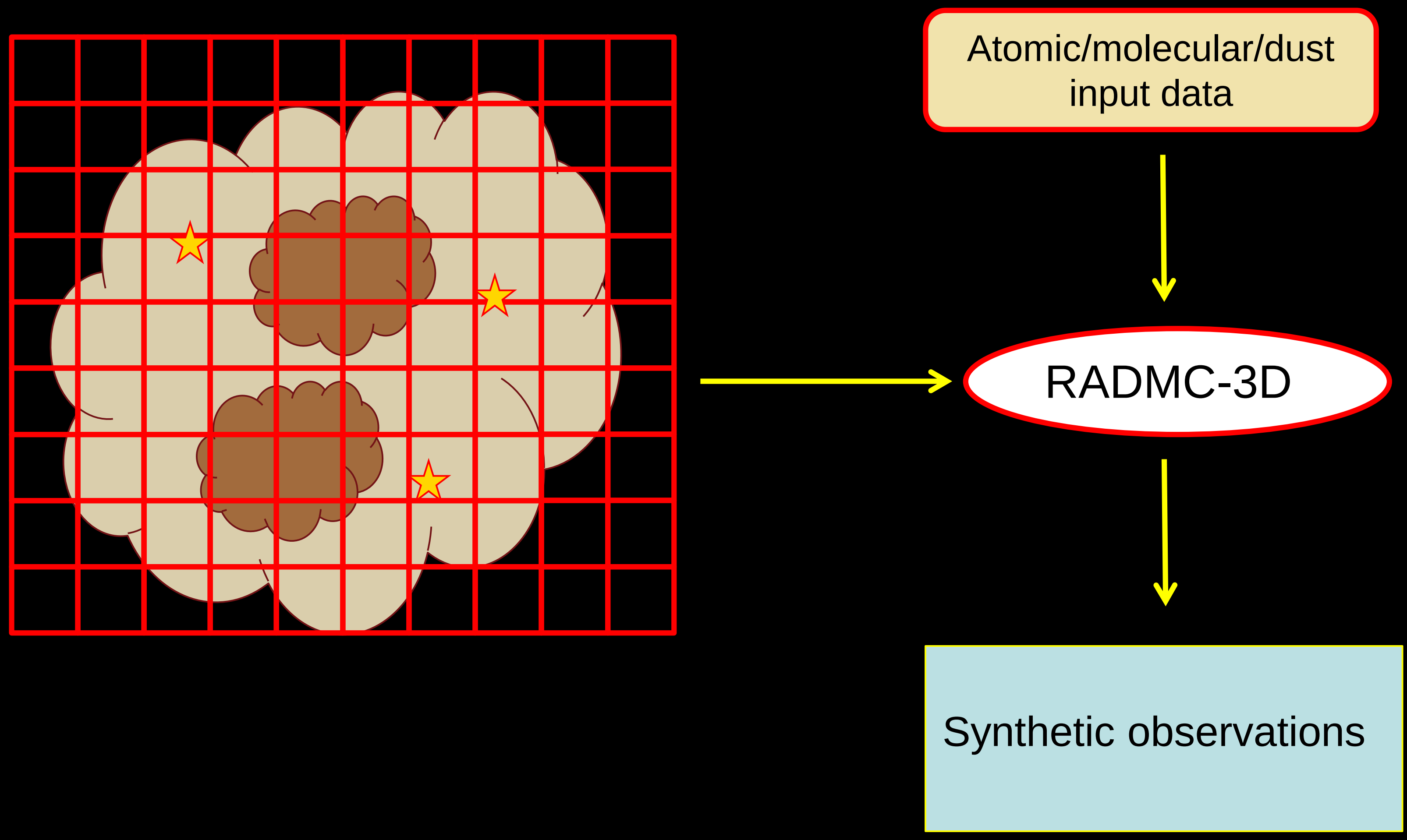


Input: Line data

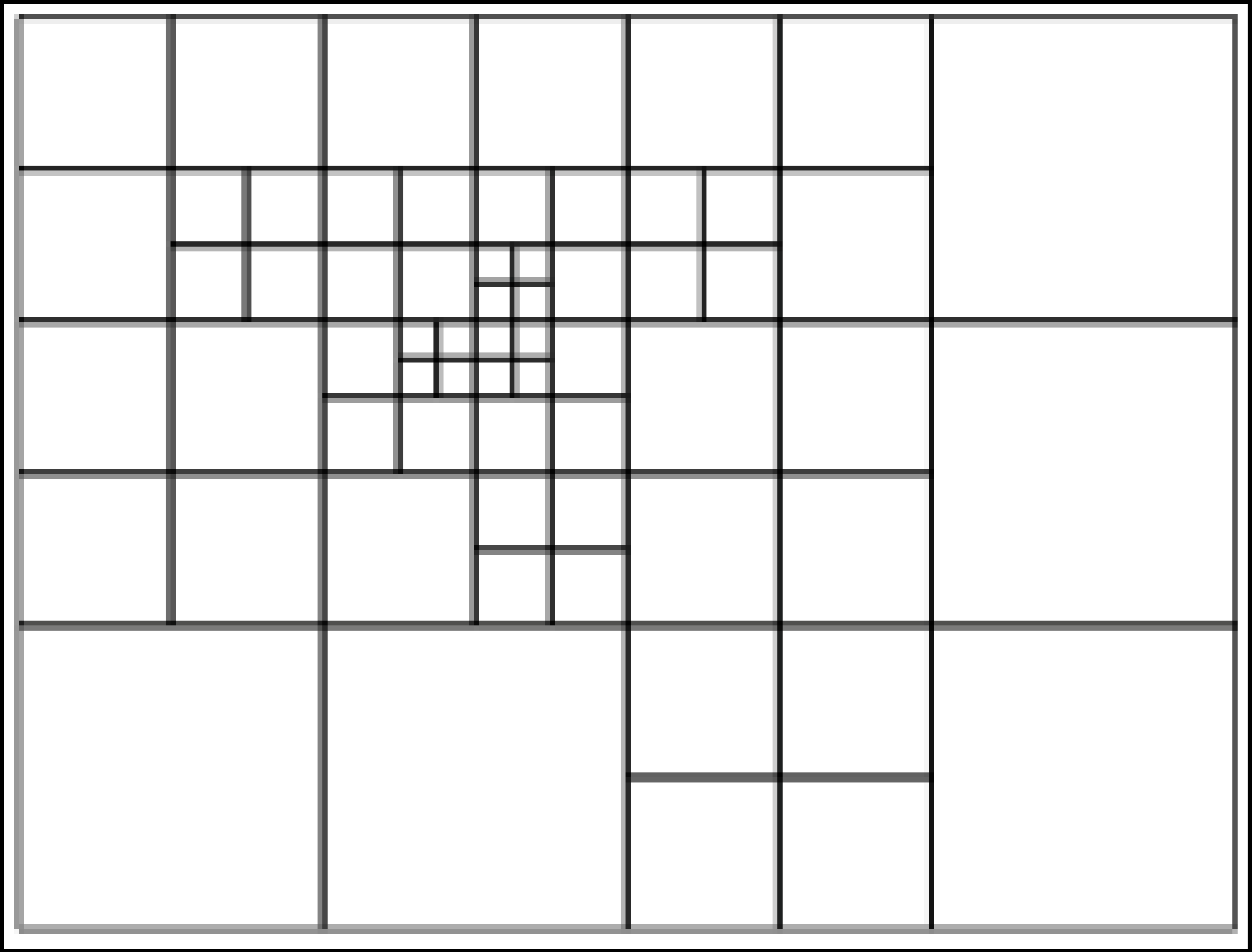
- Levels: Energies, degeneracies
- Transitions: A-coefficients
- Collisional data

- Various databases now readable:
  - Leiden
  - HITRAN (linelist)
  - ...

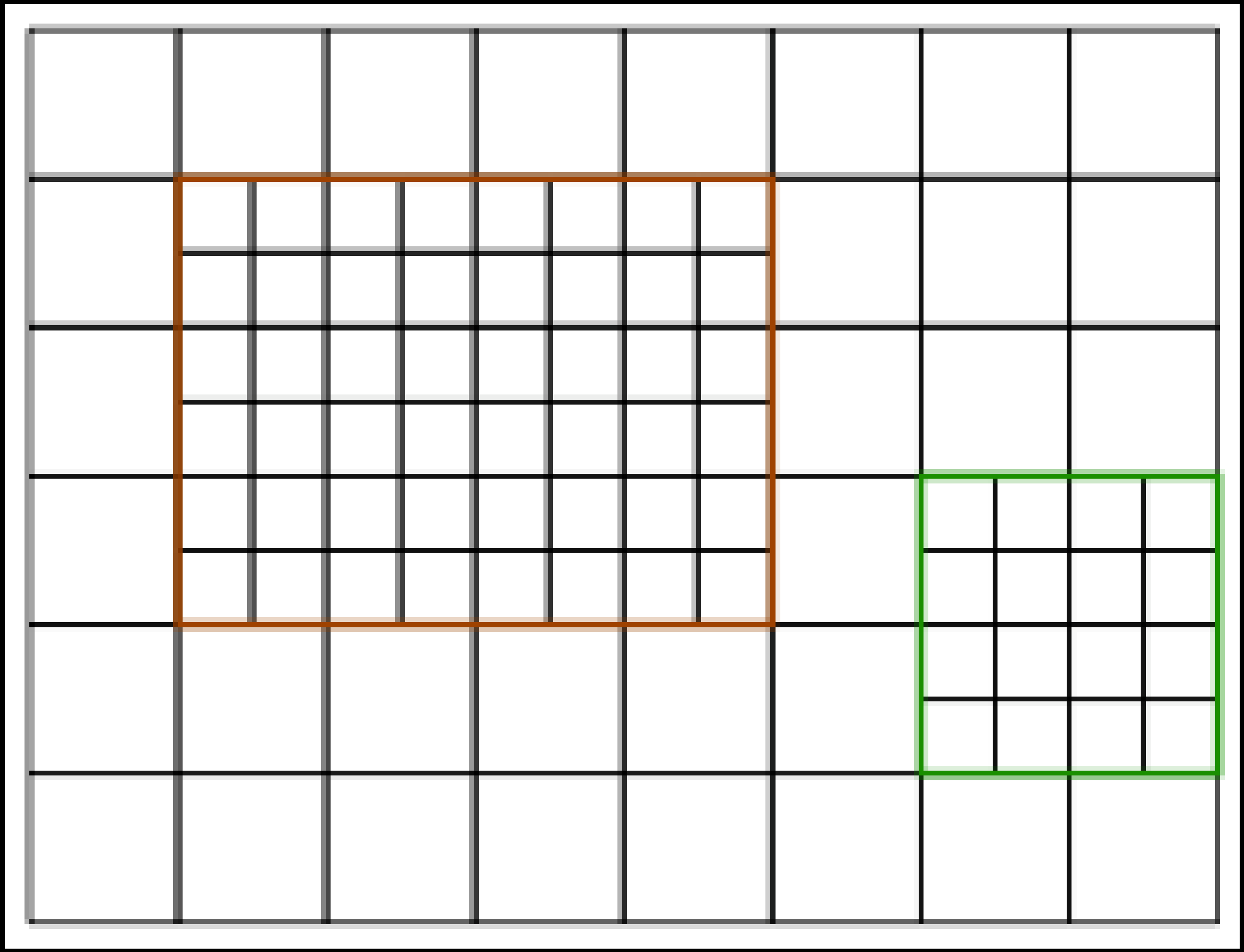
Now it can produce synthetic observations...



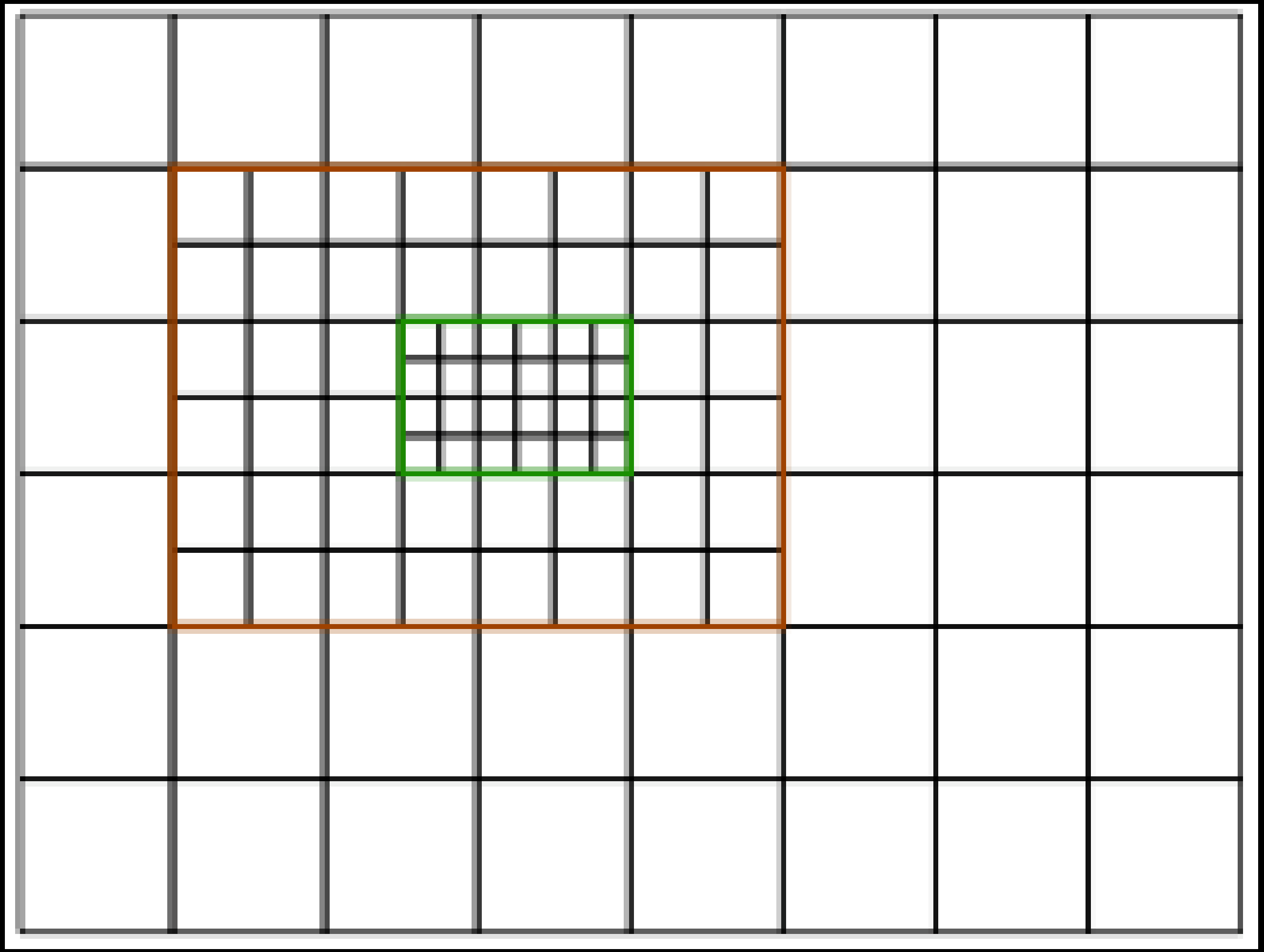
AMR Grid Structure: Oct tree



AMR Grid Structure: Patch-based



AMR: Patch-based, recursive



Coordinates

- Cartesian: 3D
- Spherical: 1D, 2D, 3D

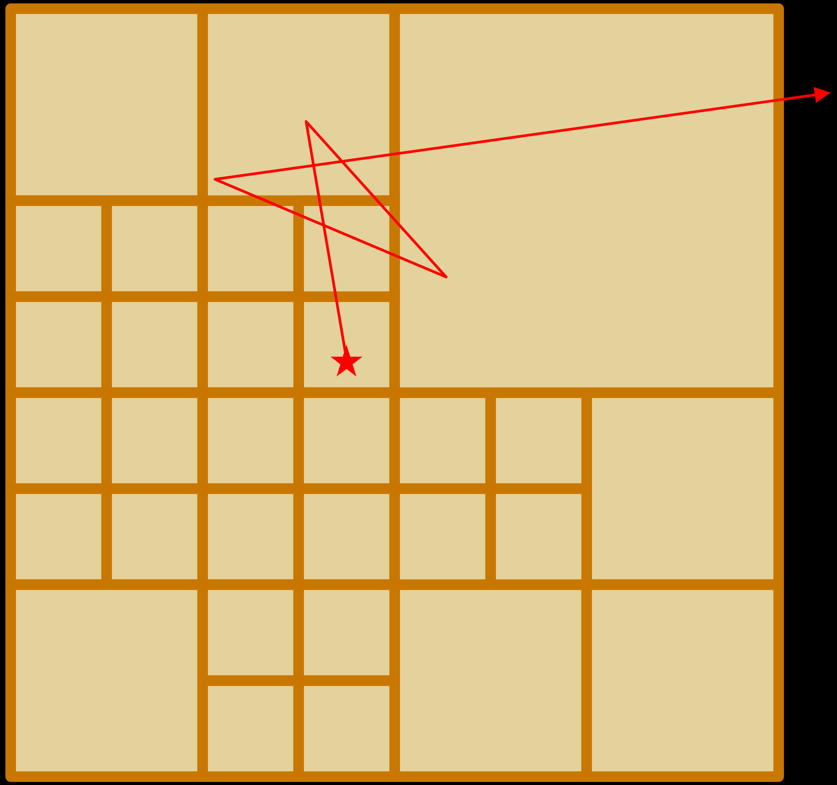
- In all these coordinate systems the AMR is possible.

Interfaces from well-known codes

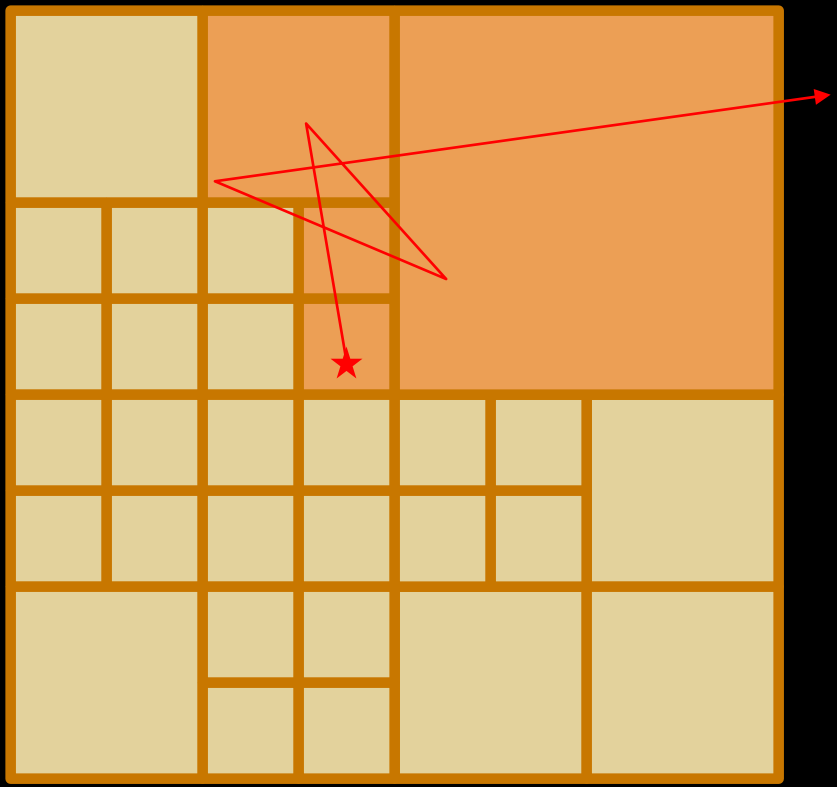
- FLASH
- RAMSES
- PLUTO
- ZEUS

Dust continuum radiative transfer

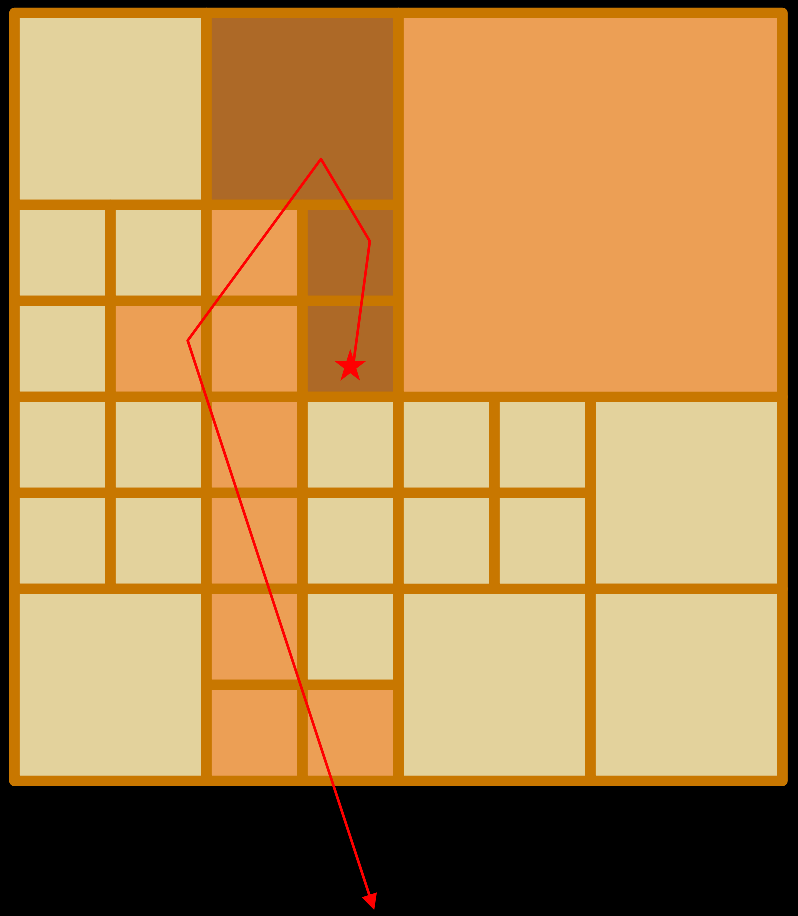
Stage 1: Monte Carlo Dust Temperature



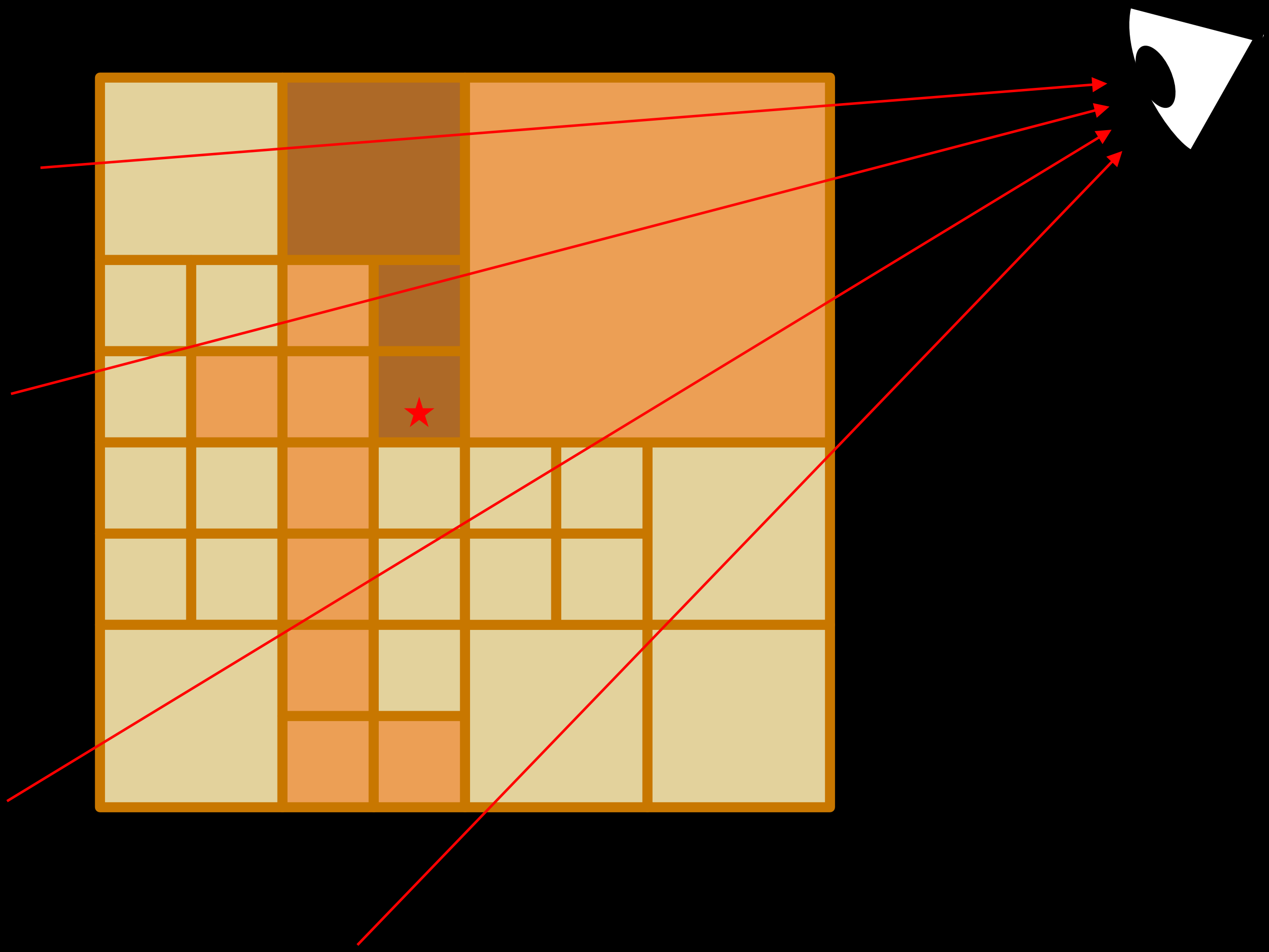
Stage 1: Monte Carlo Dust Temperature



Stage 1: Monte Carlo Dust Temperature

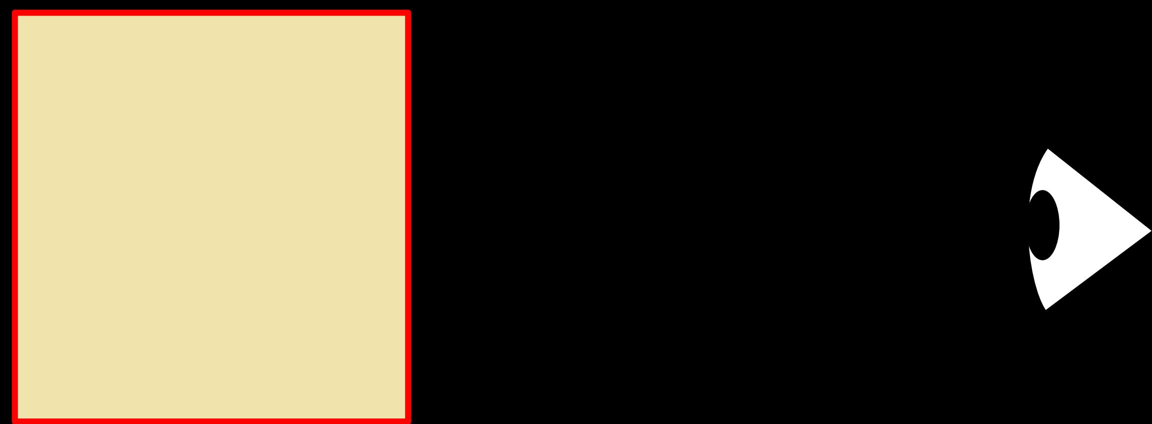


Stage 2: Ray tracing



Treatment of scattering off dust grains

Using a scattering source function



Treatment of scattering off dust grains

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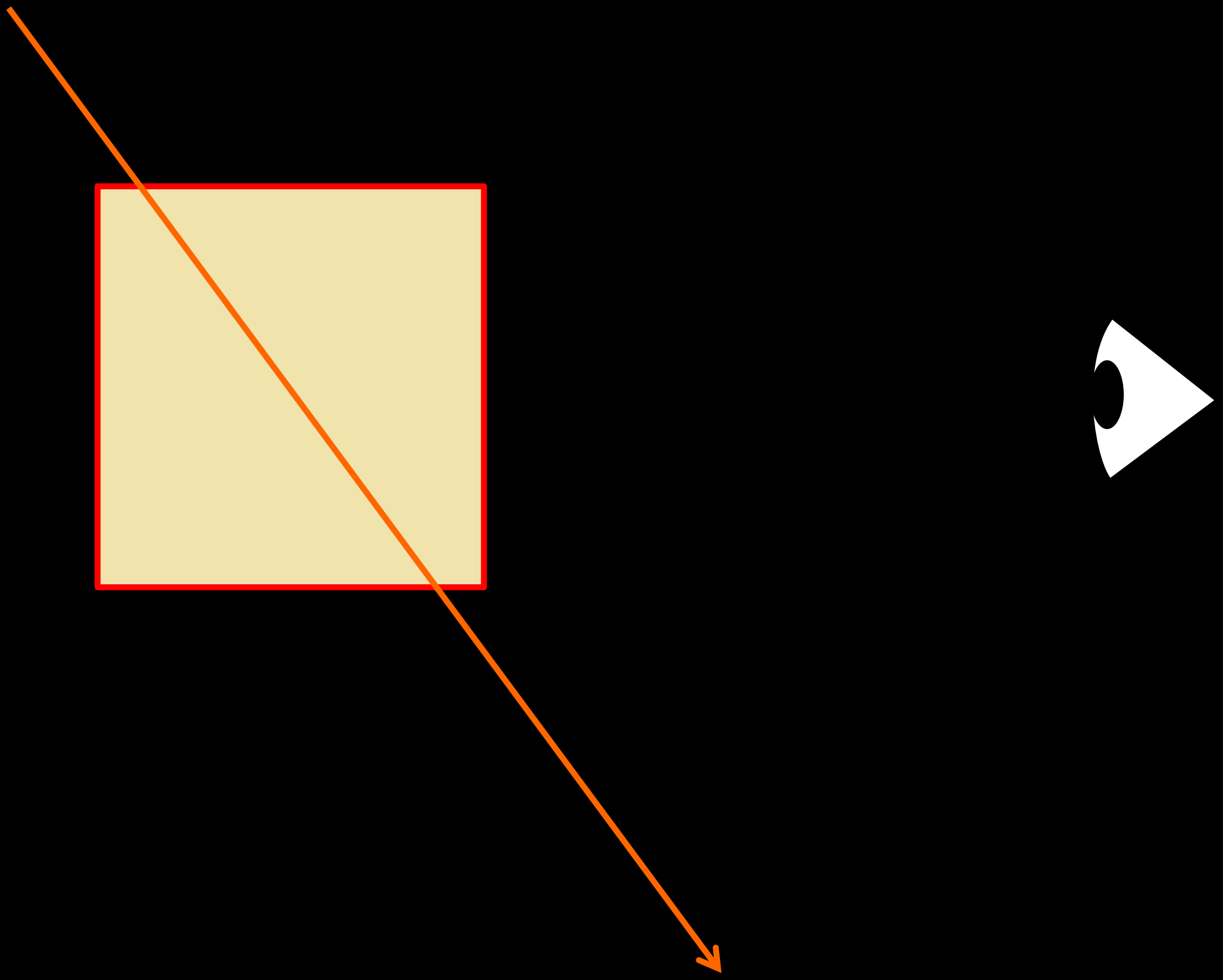
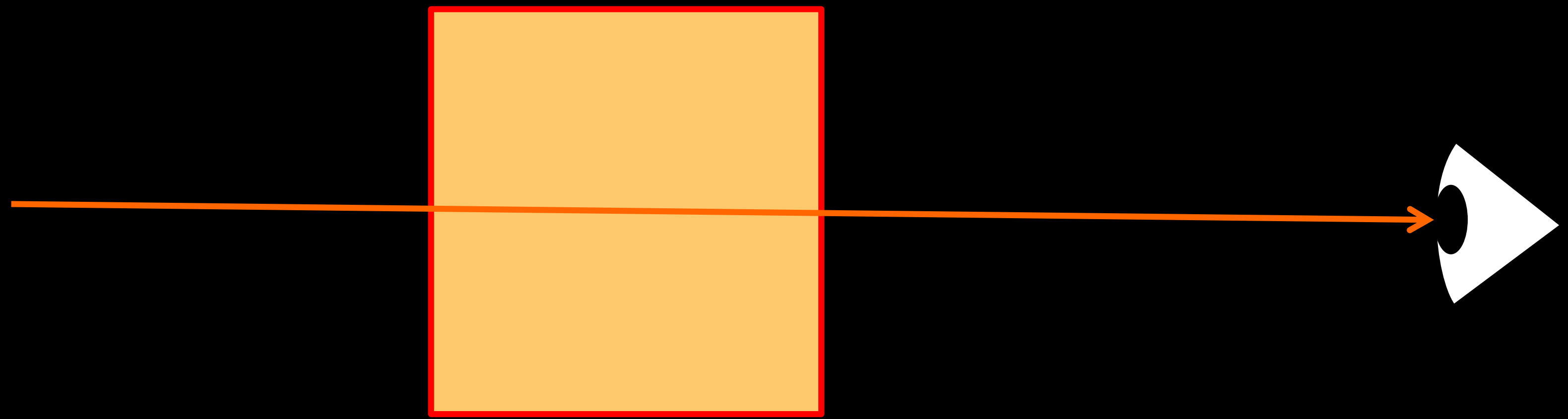


Treatment of scattering off dust grains

Using a scattering source function

Treatment of scattering off dust grains

Using a scattering source function



RADMC-3D Method of Dust RT

- First do an *all-frequency* Monte Carlo calculation for the dust temperature
- Then do ray-tracing for the images/spectra
  - Before each image (i.e. at each wavelength): do a *monochromatic* Monte Carlo calculation for the scattering source function.

About Step 1 (thermal Monte Carlo)

Method = Bjorkman & Wood (2001) algorithm:

- The main idea behind the BW method:
  Treat each absorption-reemission event similar to a scattering event.
- Like scattering Monte Carlo: Build up energy in each cell to compute the source function (in this case to be precise: the dust temperature)
- Difference to scattering event:
  - Scattering changes angle, but keeps frequency
  - Abs/reemis event changes angle *and* frequency

About Step 1 (thermal Monte Carlo)

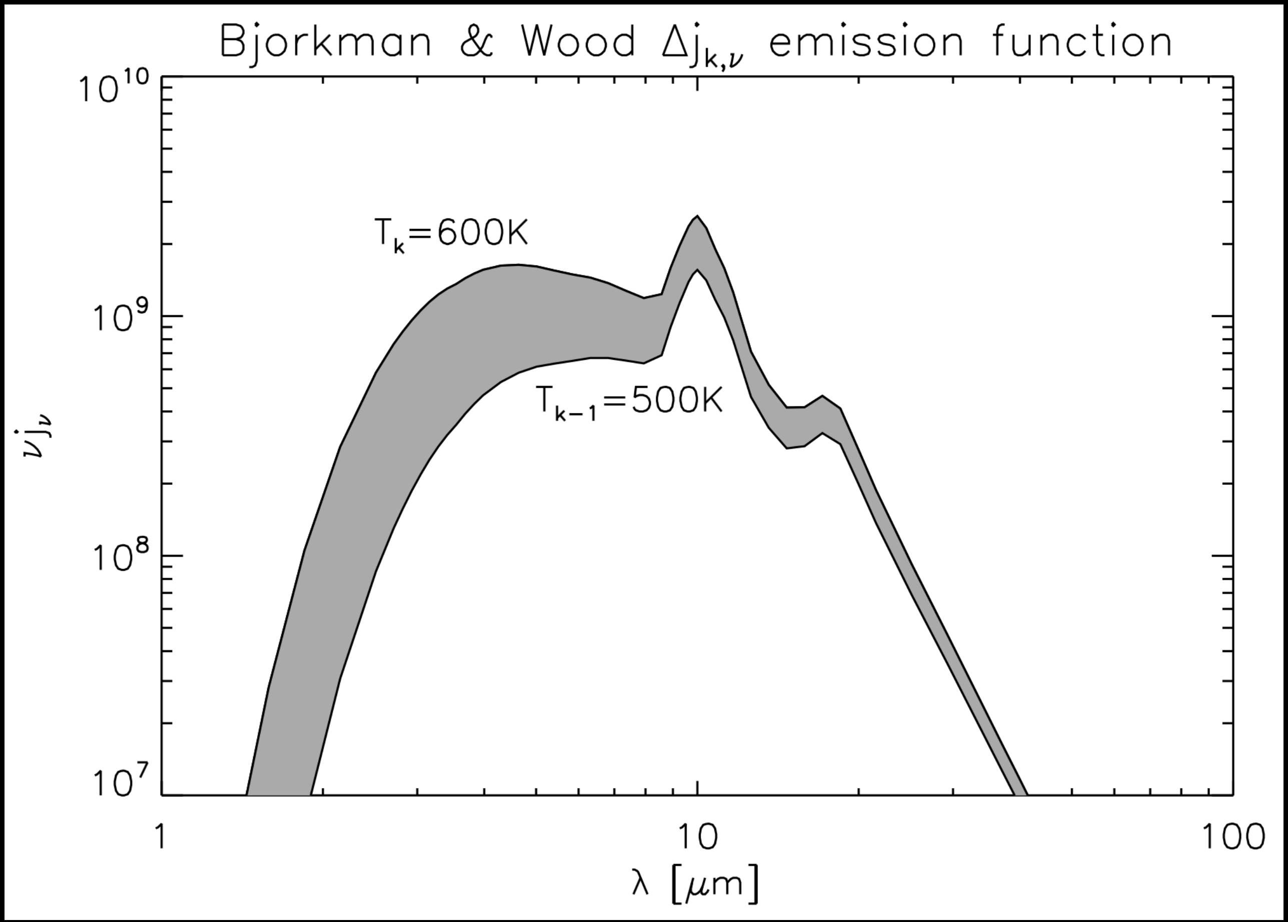
Method = Bjorkman & Wood (2001) algorithm:

- Question: which frequency to take at each absorption-reemission event?
  Answer: Use the Planck function
- Tiny catch: Since T increases with "time" (= photon packages launched), which Planck function should we use?
  Answer: What about the "current" one?
- Tiny catch: Previous events used "wrong" (too low) temperature. How can we aposteriori correct for that?
- Answer: Use difference $B(T_{curr}) - B(T_{prev})$

About Step 1 (thermal Monte Carlo)

Method = Bjorkman & Wood (2001) algorithm:

- Answer: Use difference $(B(T_{curr}) - B(T_{prev}))\ \rho\ \kappa_\nu$



About Step 1 (thermal Monte Carlo)

Method = Bjorkman & Wood (2001) algorithm:

Advantages:

- Excellent luminosity conservation
- No convergence checking needed
- Extremely stable!

Drawbacks:

- Photons might get "stuck" (though never permanently) in ultra-high-τ regions. But: Lambda Iteration would lead to fake convergence. So BW is safer.
- Does not work for temperature-dependent κ_ν

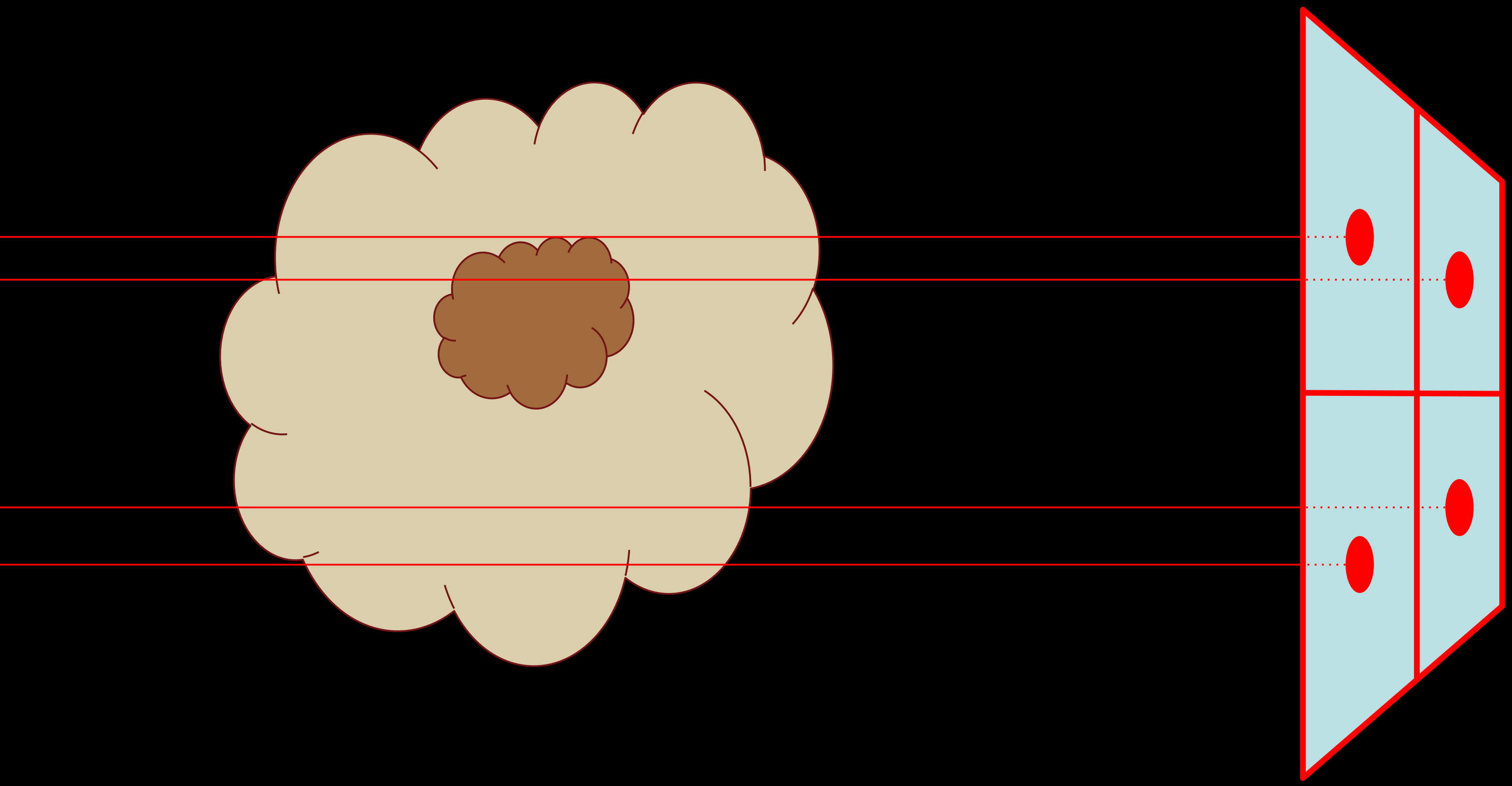
Line radiative transfer

Line transfer with RADMC-3D

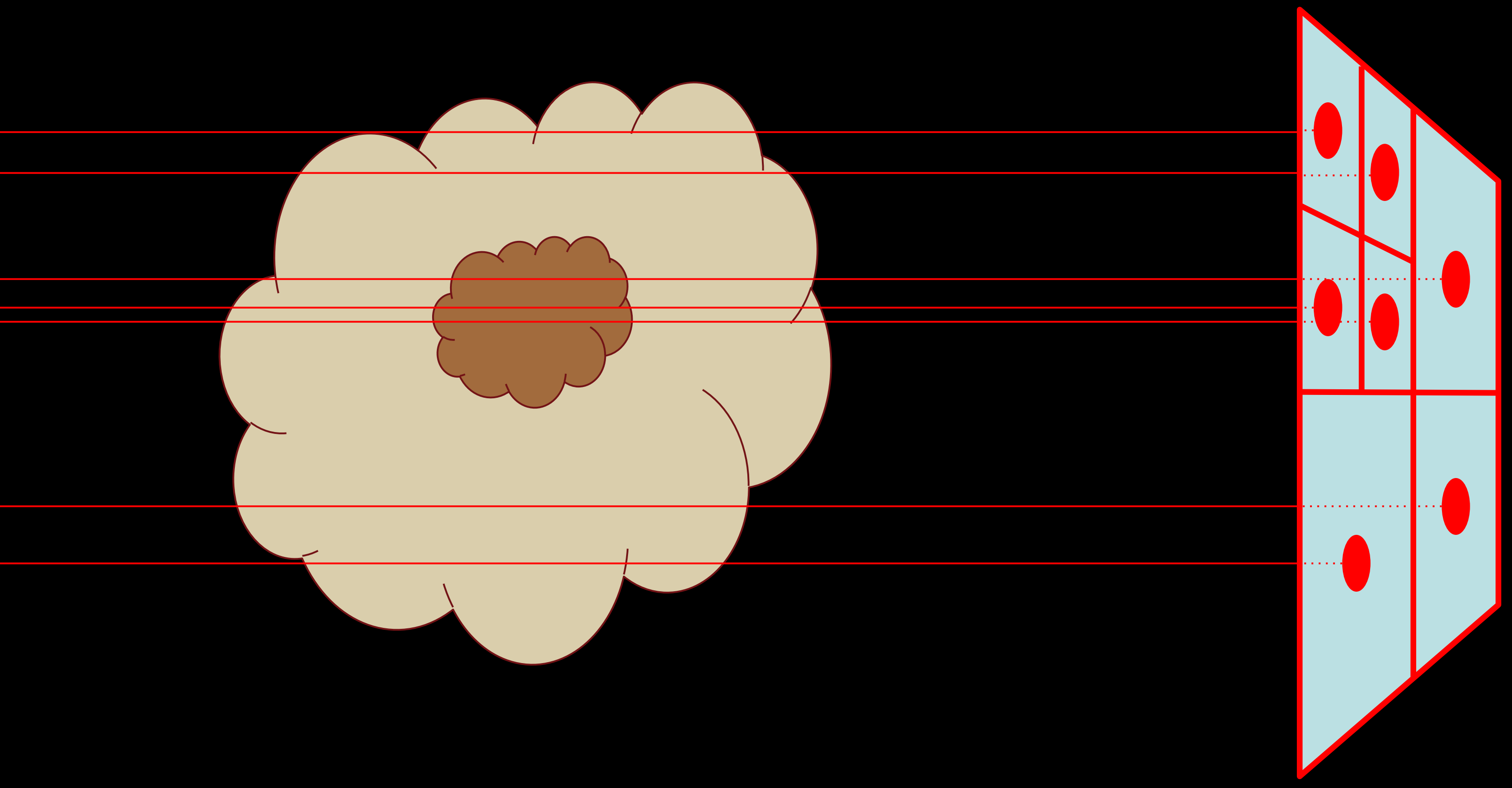
- At the moment the following modes are possible:
  - LTE
  - LVG (Sobolev)
  - Optically thin populations
- Full non-LTE not yet possible
- But:
  - Lines and dust continuum can be combined
  - Velocities included

The pitfalls of raytracing...

Recursive sub-pixeling of images



Recursive sub-pixeling of images



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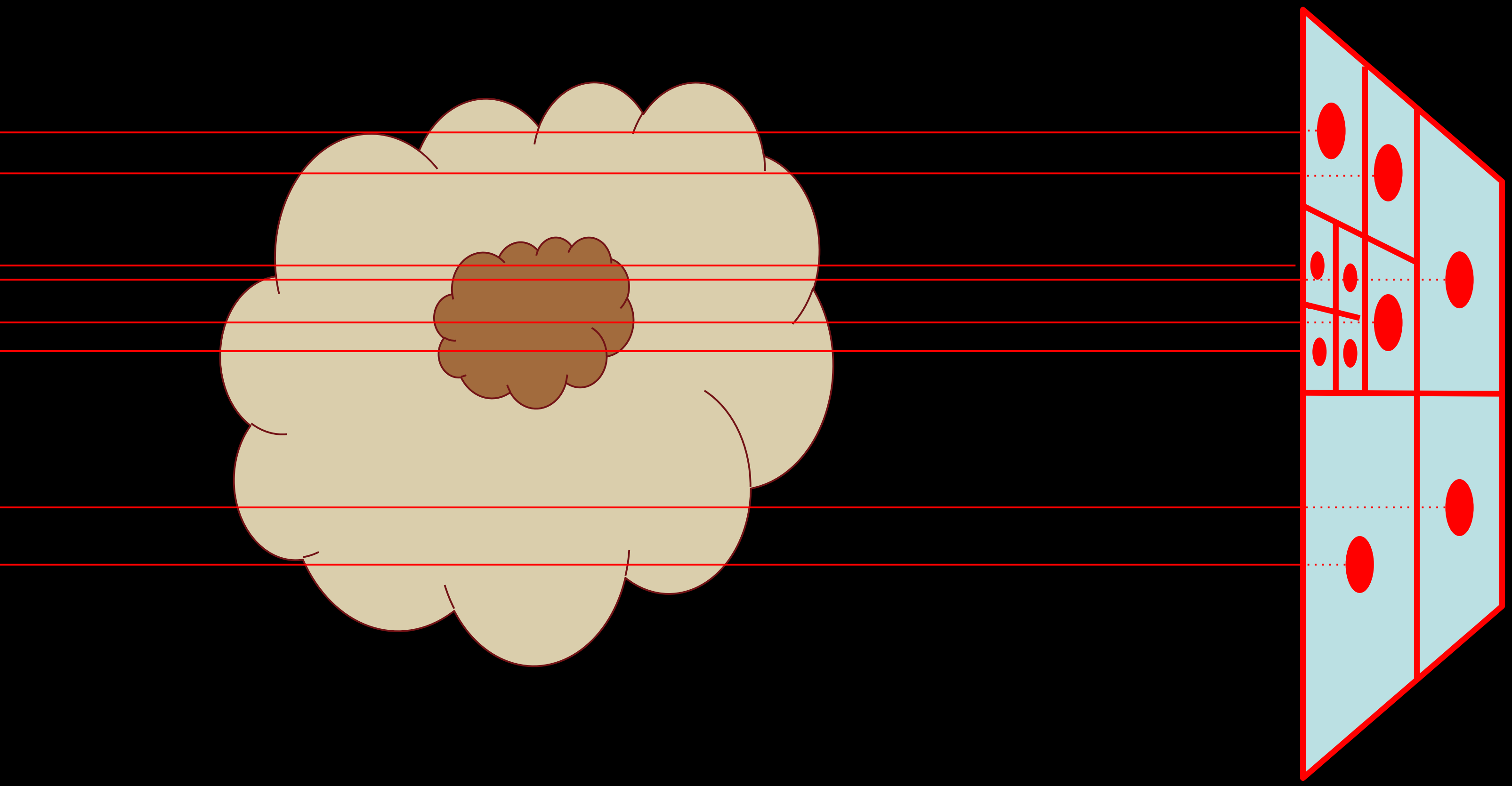
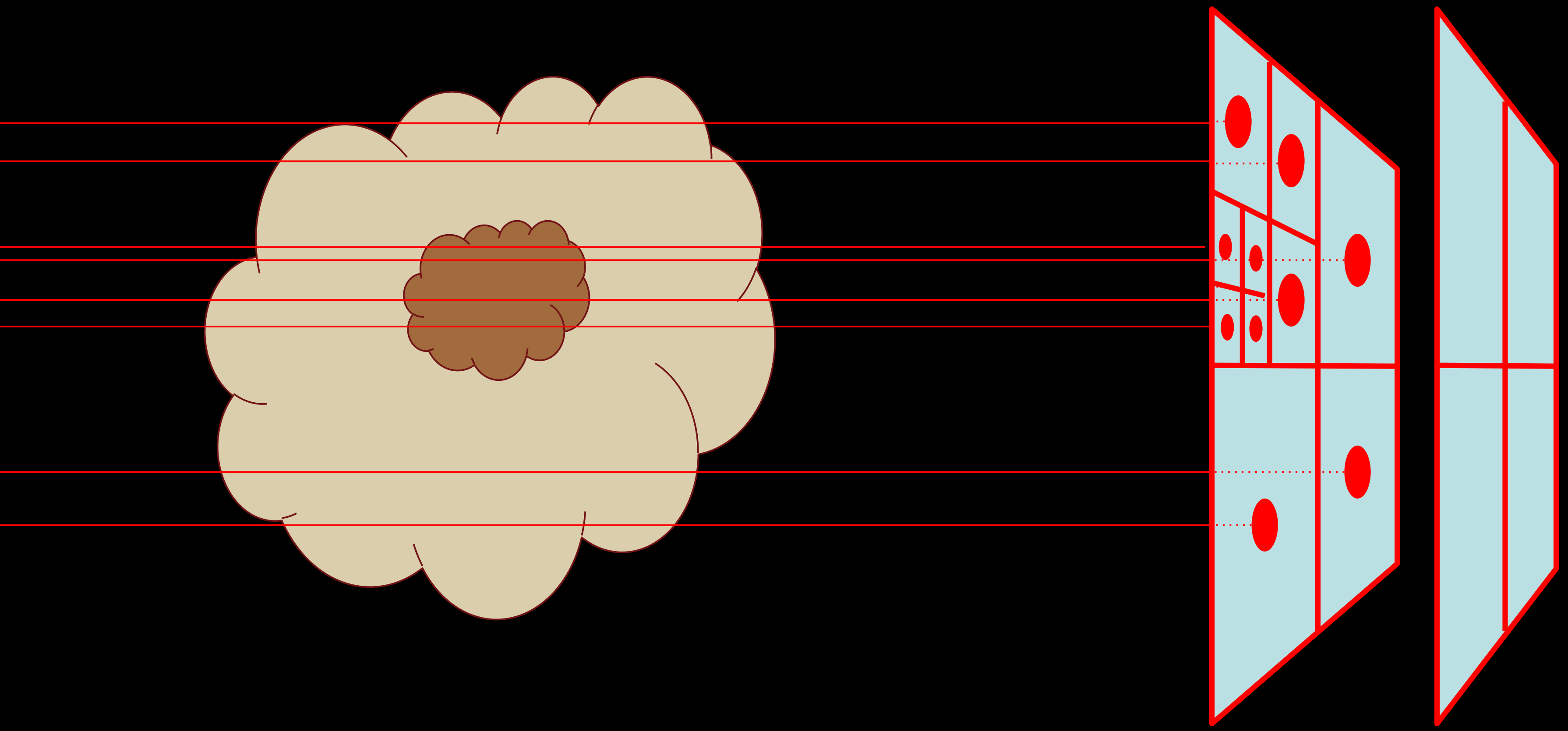


Necessary for obtaining the correct flux

See also the Voronoi method by Christian Brinch as an alternative method

Recursive sub-pixeling of images



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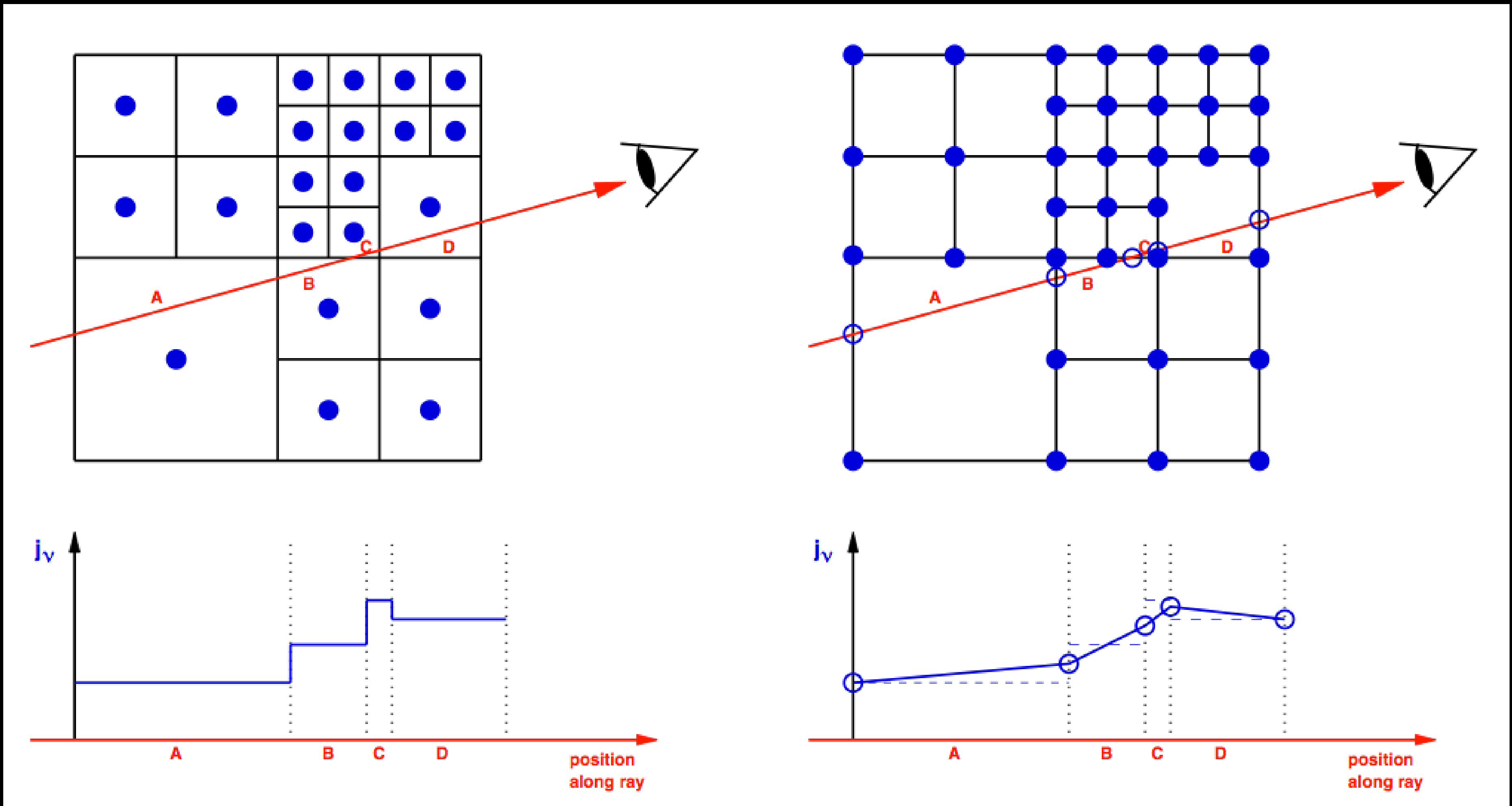
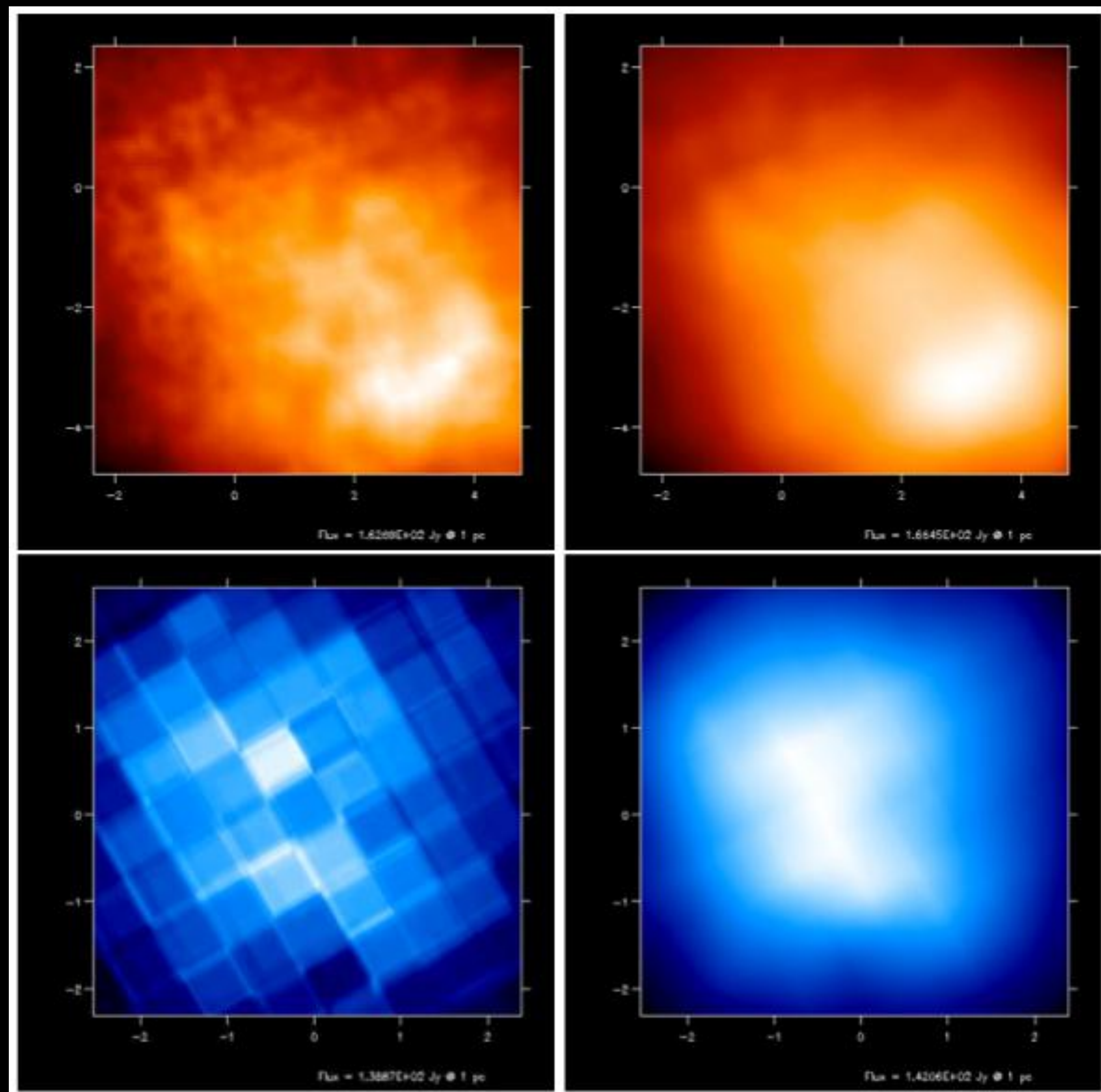
Second order ray-tracing



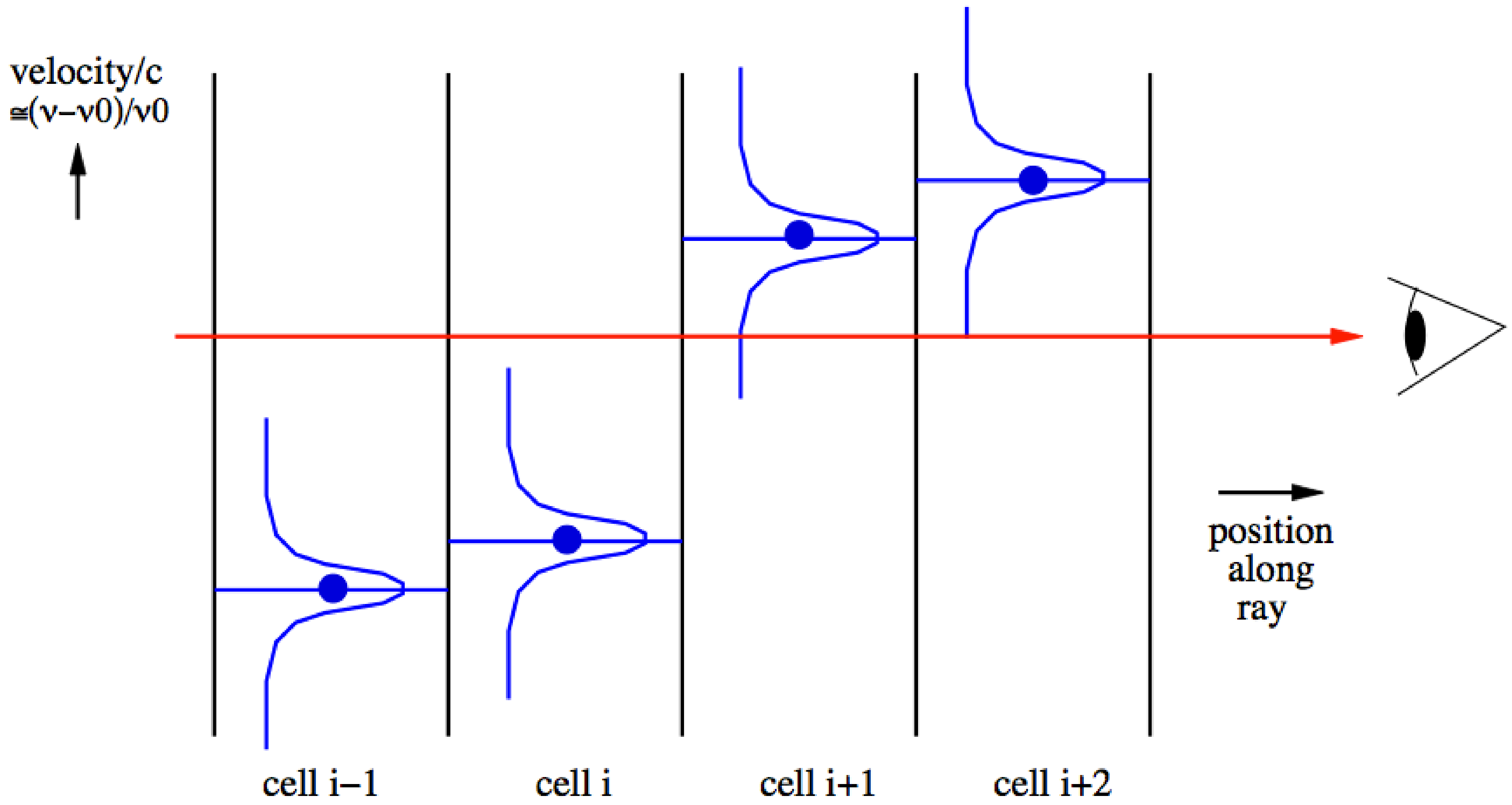
Useful for obtaining smoother images

Second order ray-tracing

First order integration: Second order integration:



Line transfer: Doppler Catching...



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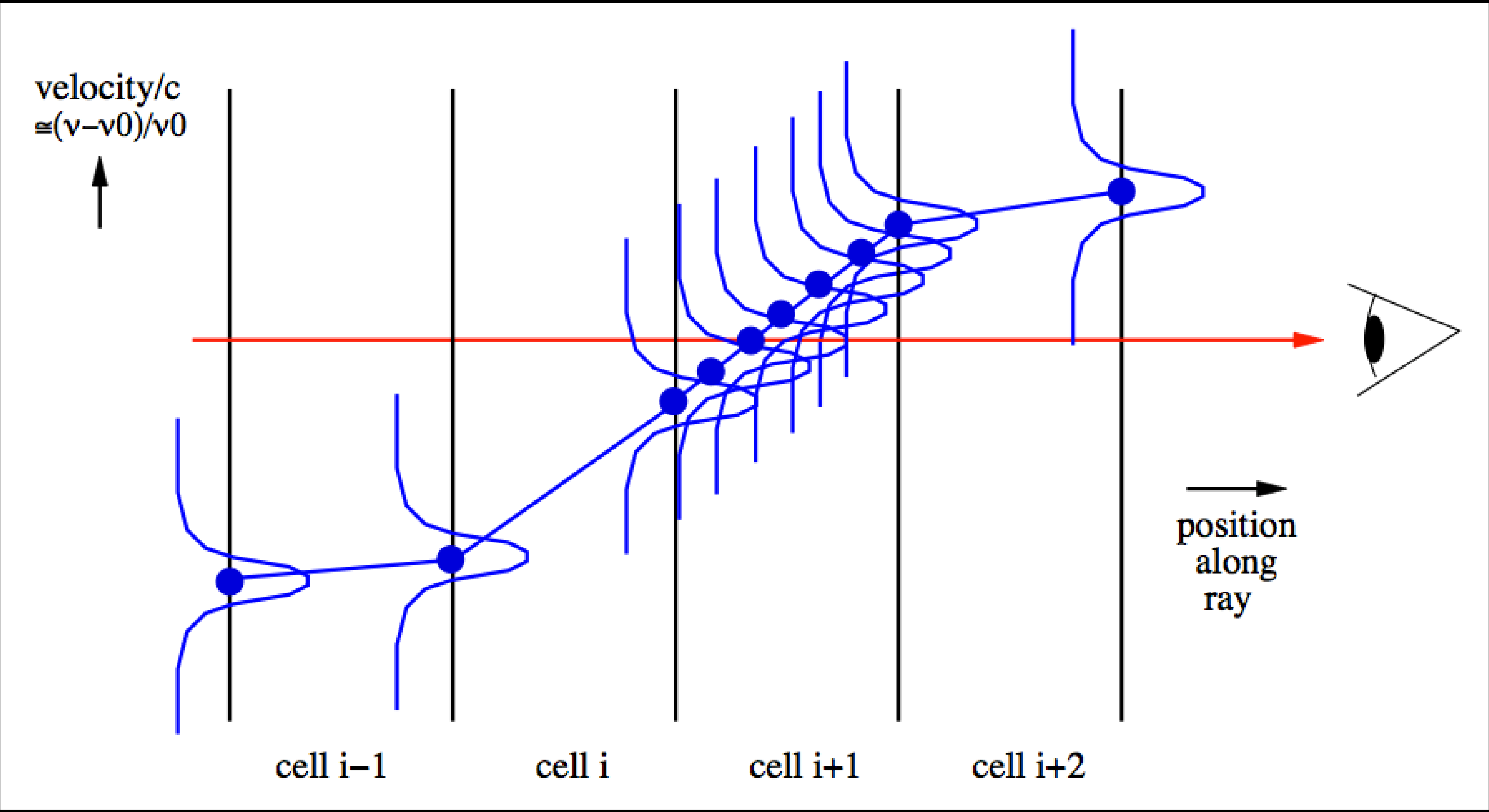


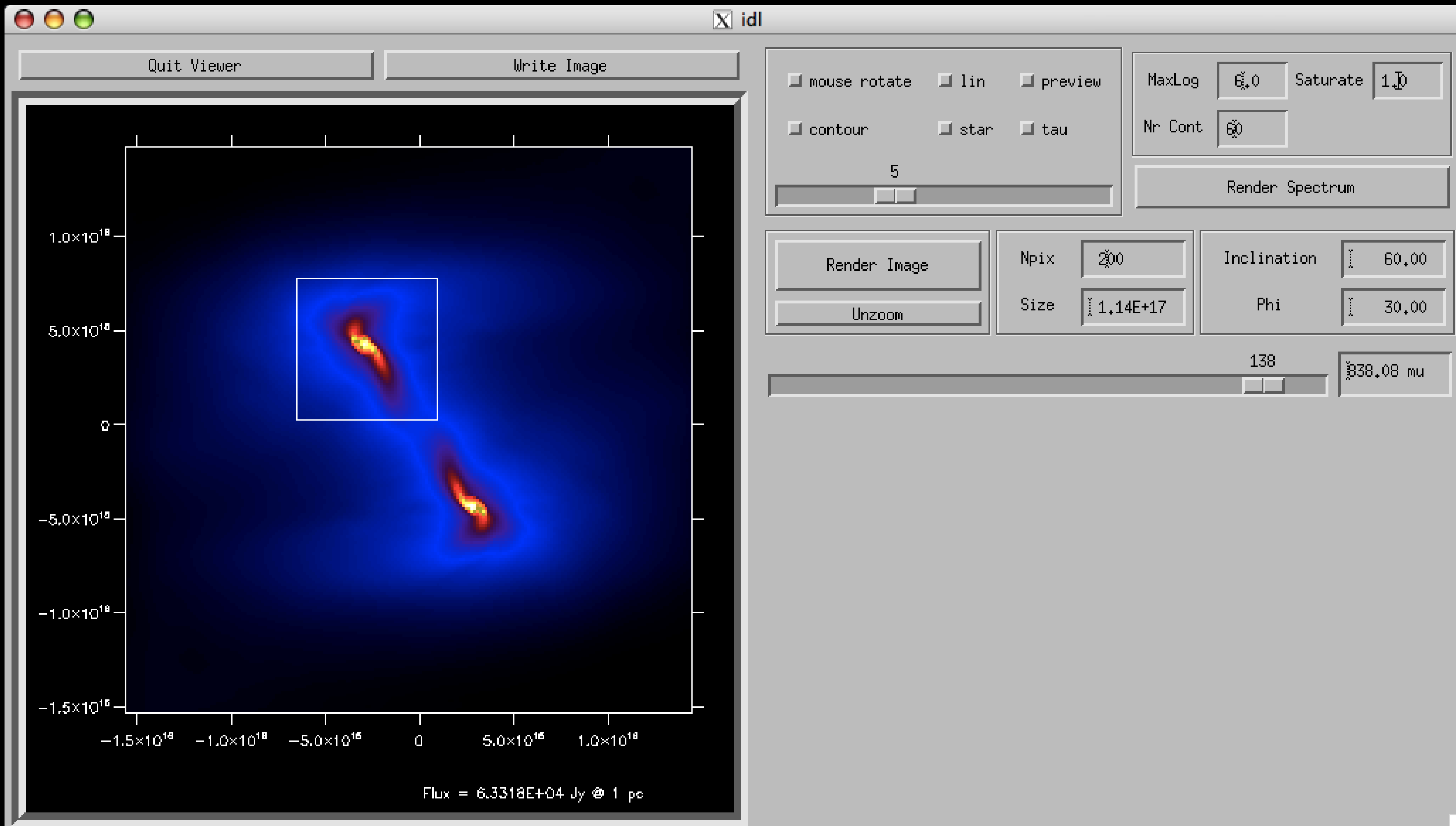
Necessary when there are strong velocity gradients

Some useful features of RADMC-3D

Add your own components

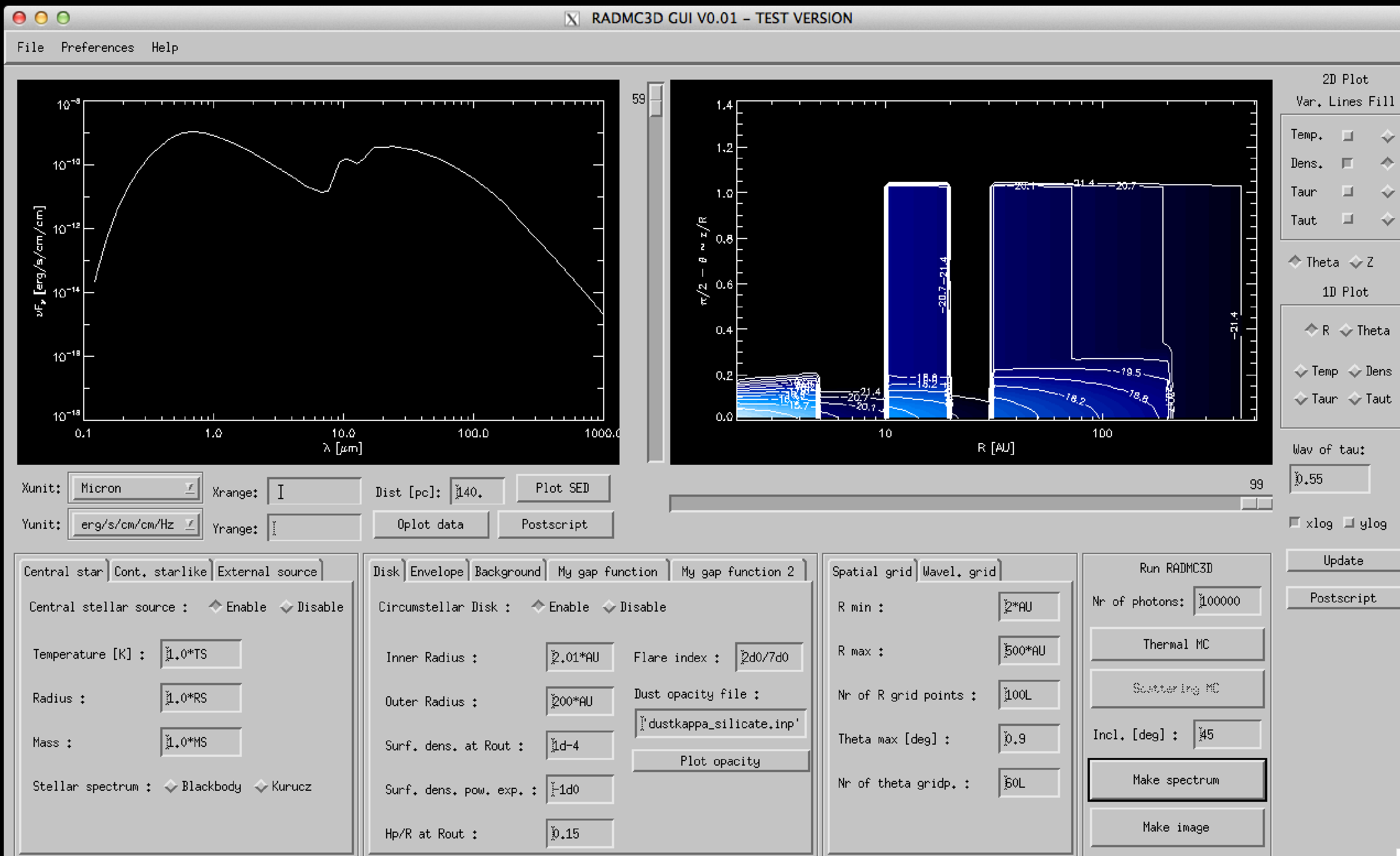
- RADMC-3D has a userdef_module.f90 module
  - Allows you to add physics and special-purpose modes into the code without the need for editing the main code!
  - This module is in your local model directory, all the rest of the code remains in main directory.

Graphical User Interface for Images

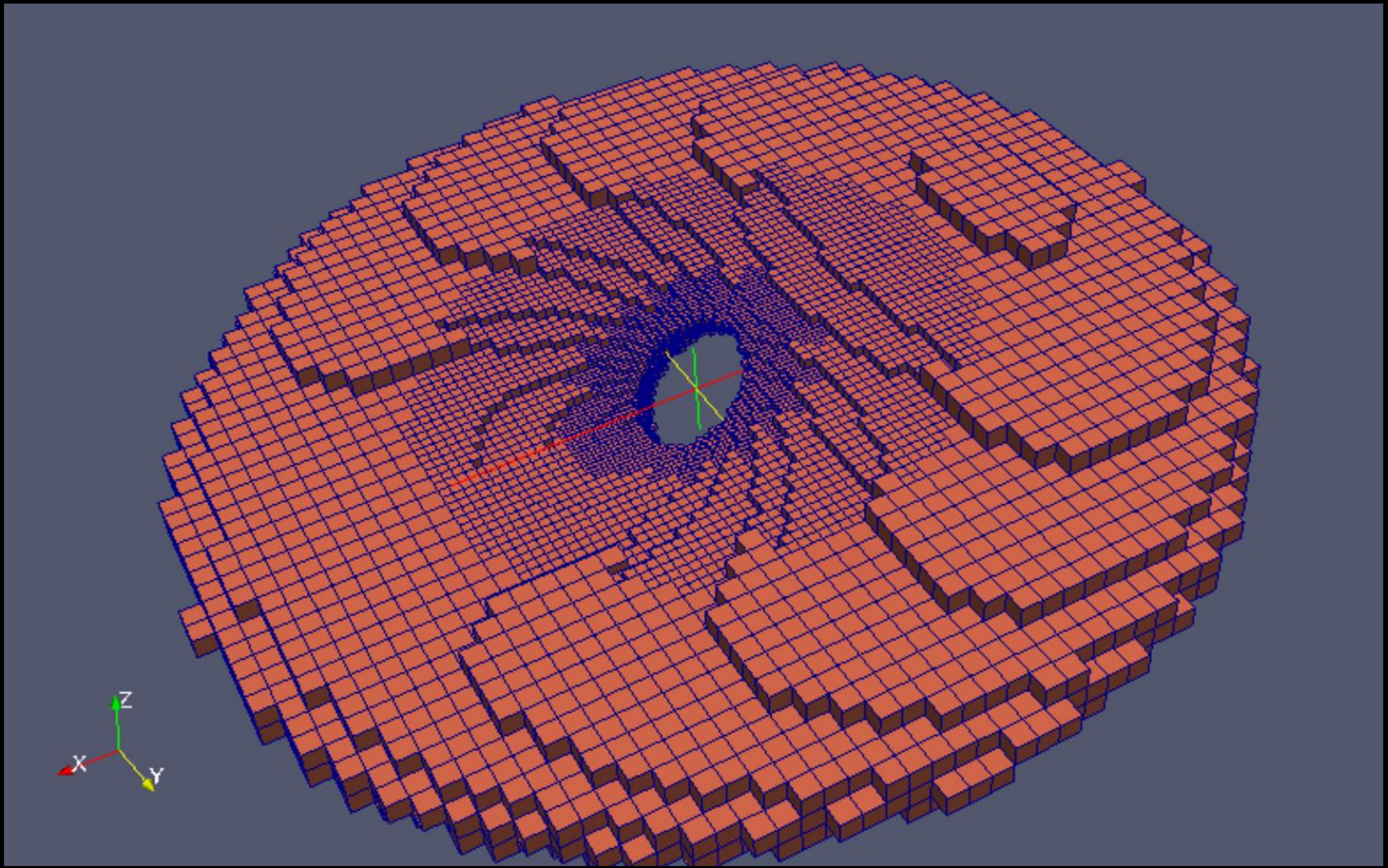


Graphical User Interface for Disk Models

By Attila Juhasz (IoA Cambridge)



VTK support

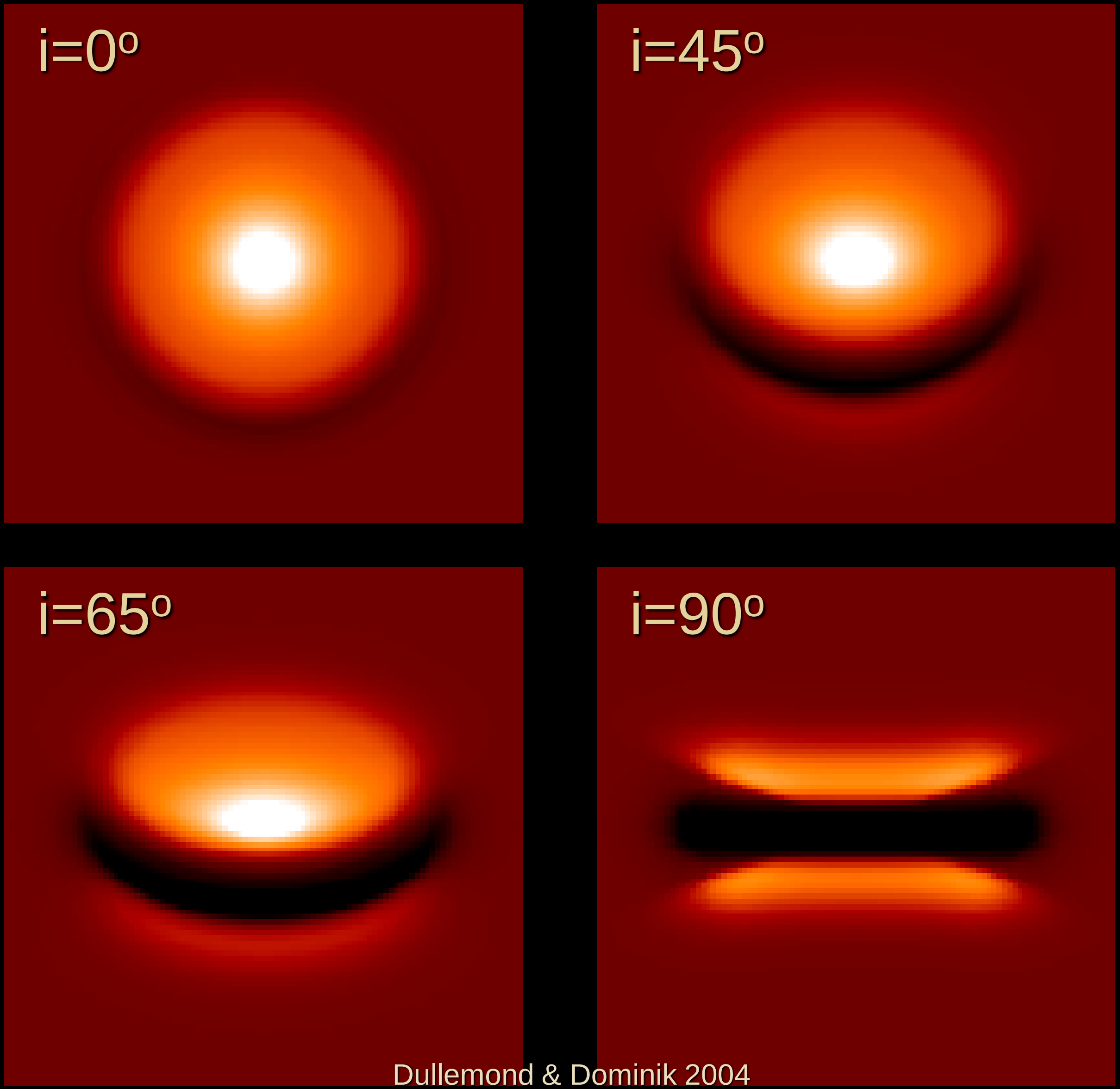


For coupling, e.g., to PARAVIEW

Examples

Example: Protoplanetary Disk

Done with RADMC-2D (predecessor to RADMC-3D)



Dullemond & Dominik 2004

Example: Protoplanetary Disk

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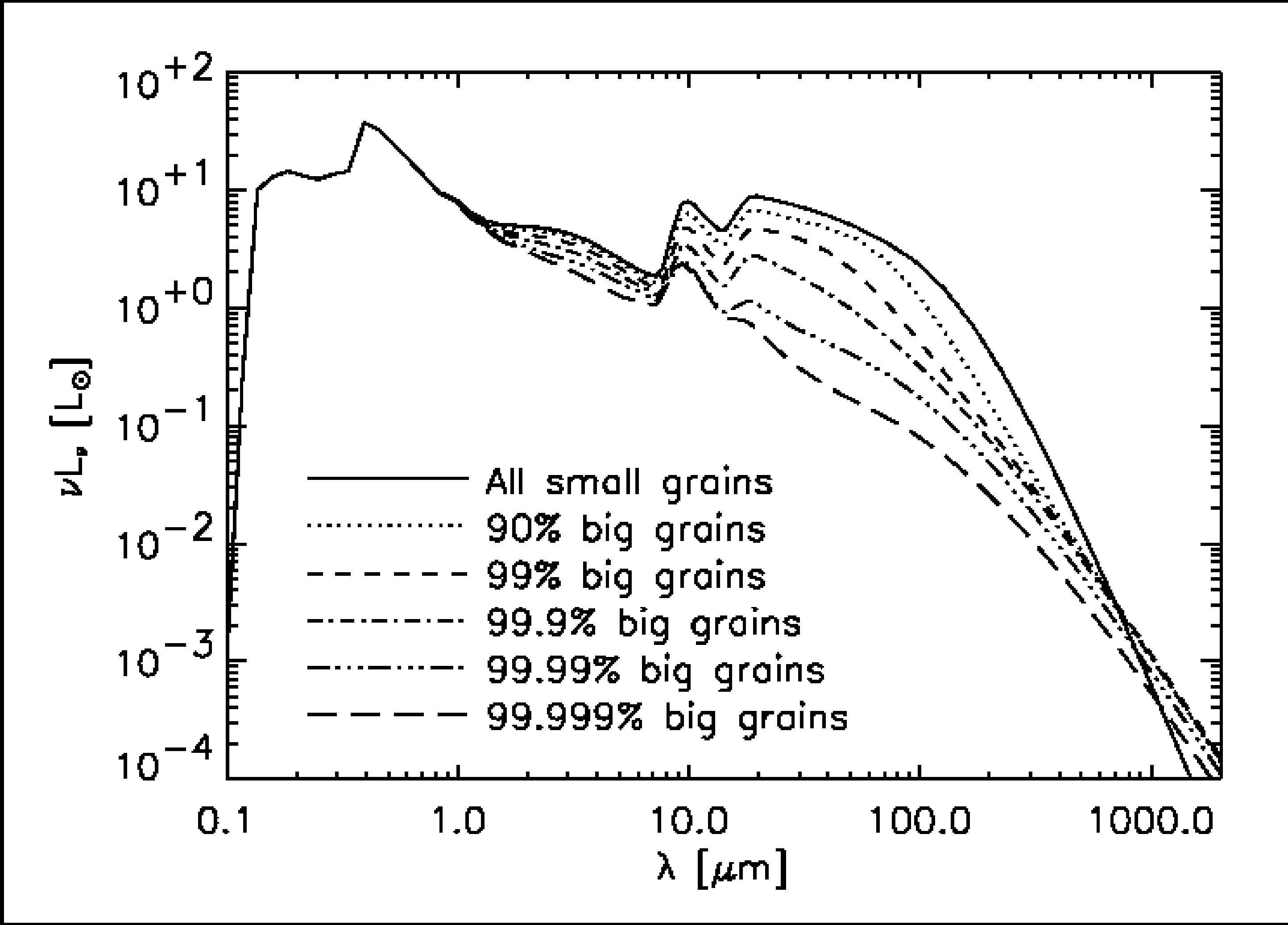

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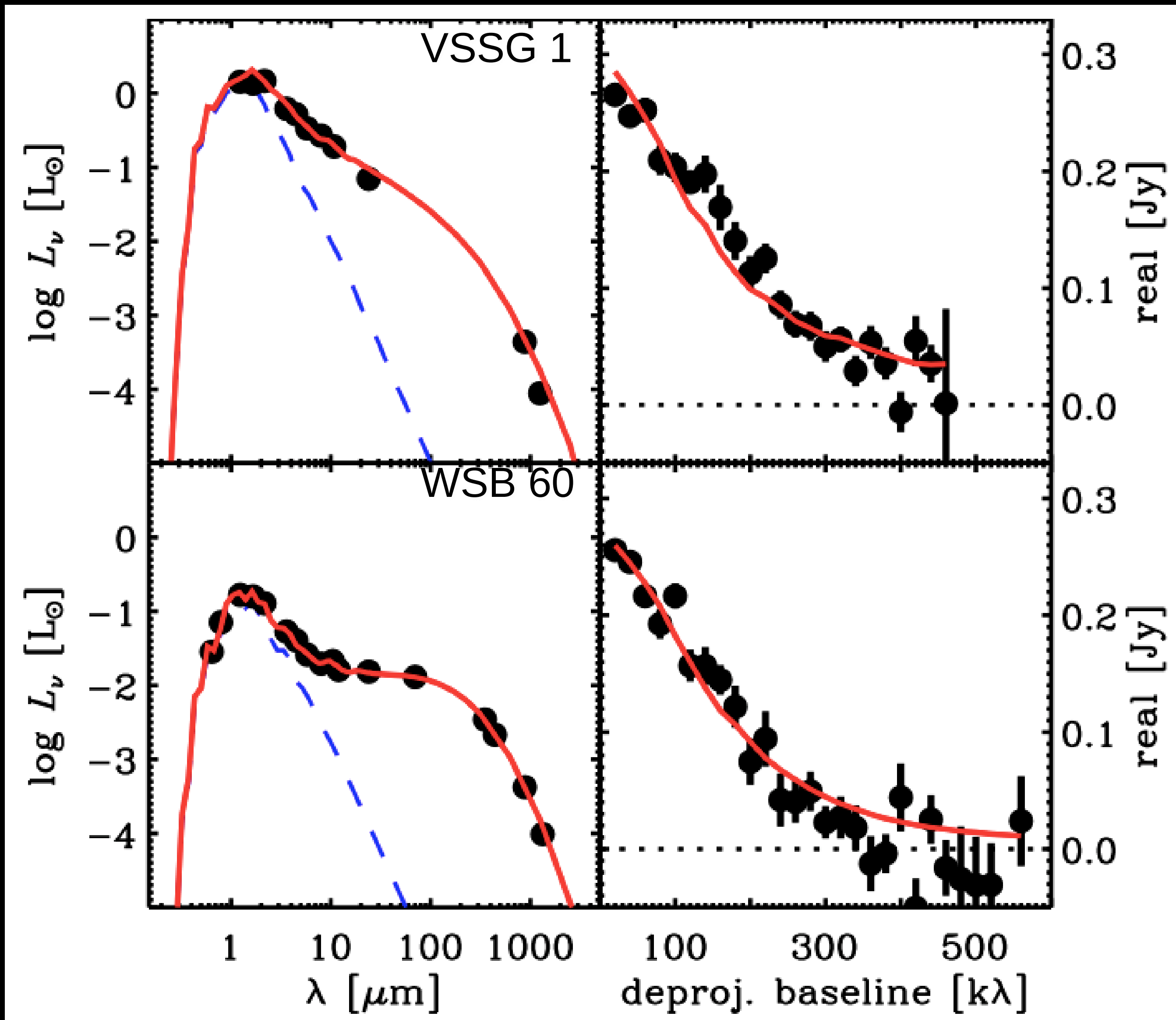
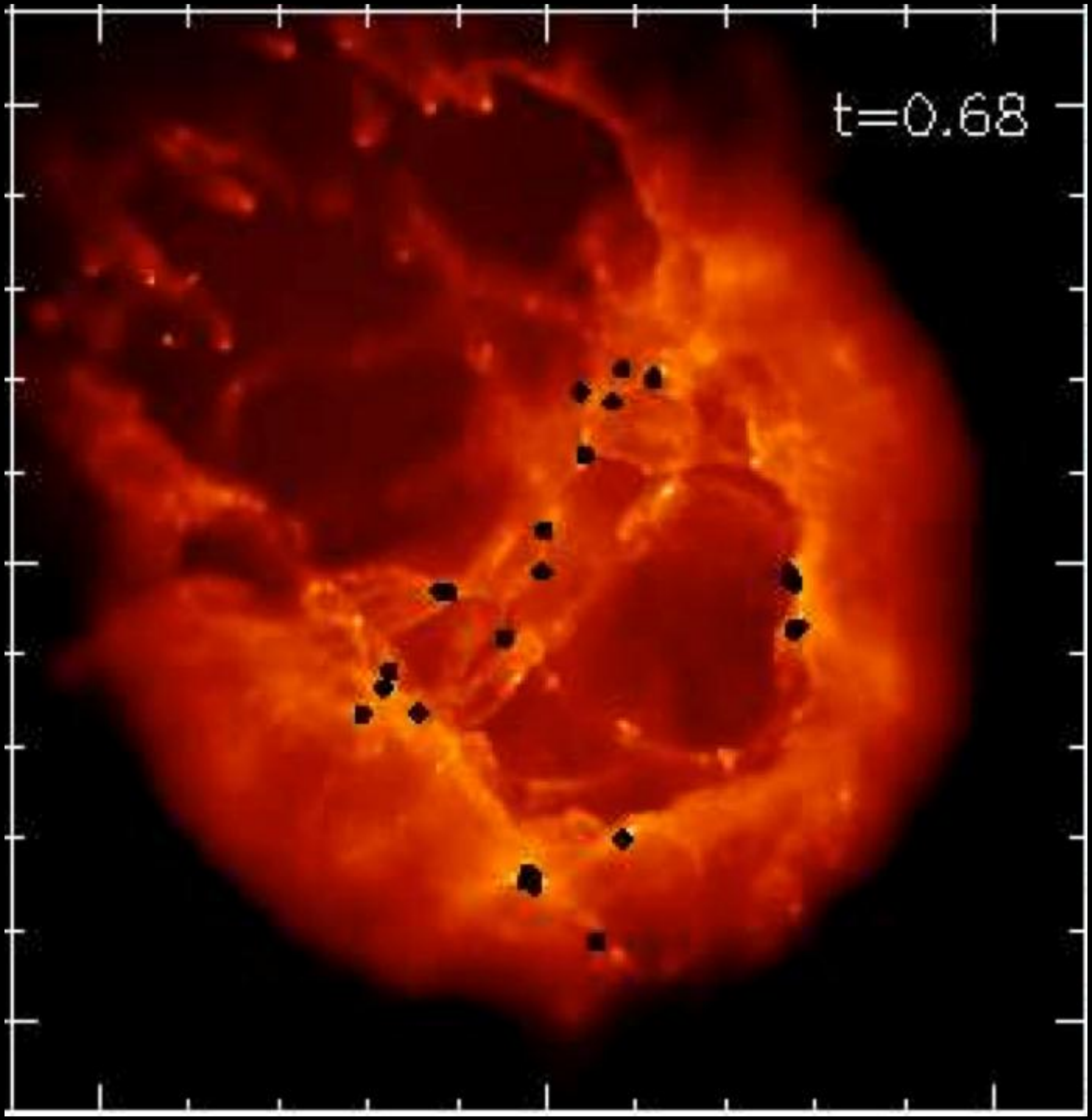


SED + millimeter resolved maps (=visibility values)

Andrews et al. 2009

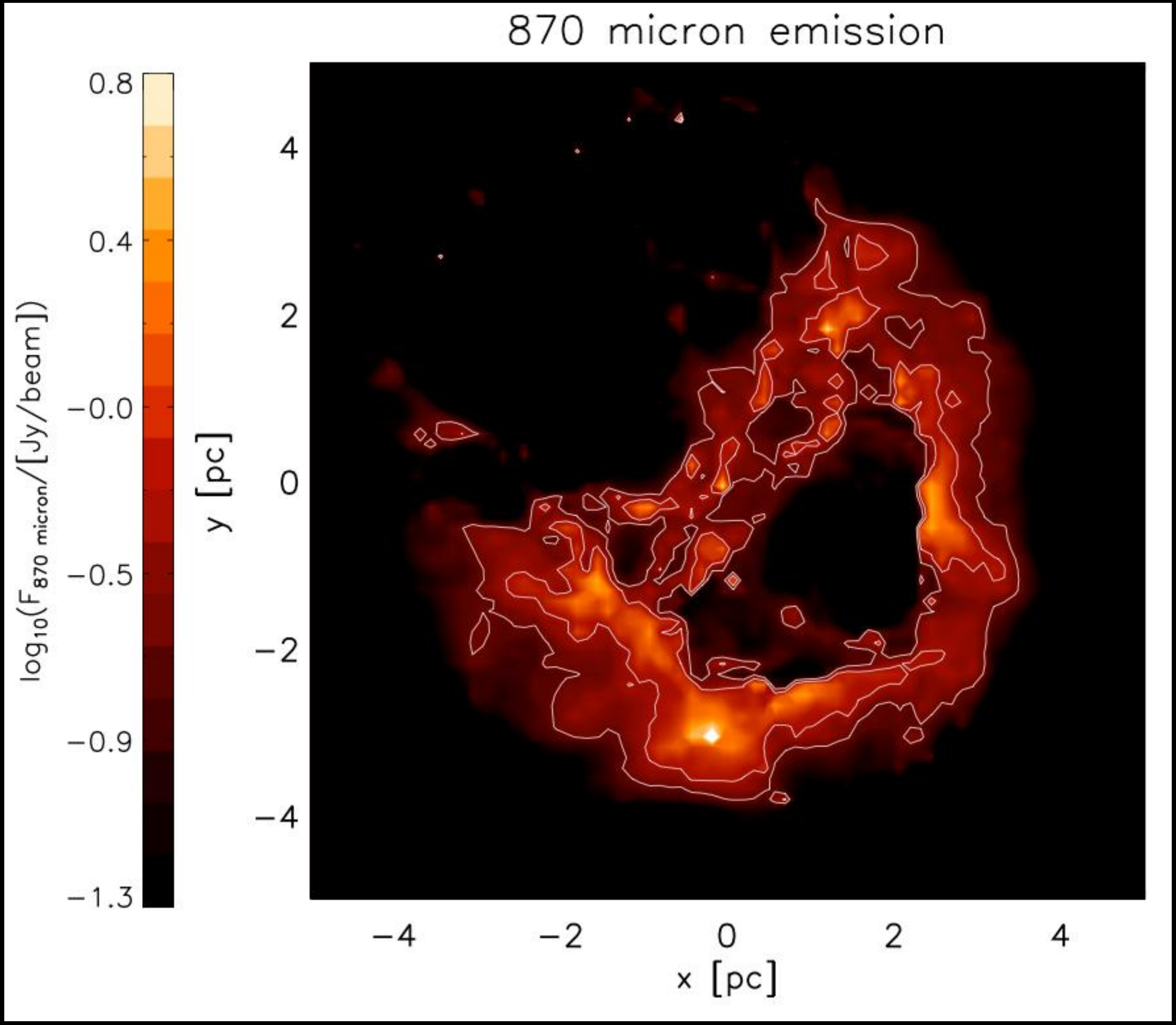
Example: Models of HII regions



SPH Model of a star forming region with an HII bubble ripping the cloud apart.

Credit: Stefanie Walch
Cardiff and MPA-Garching

Example: Models of HII regions



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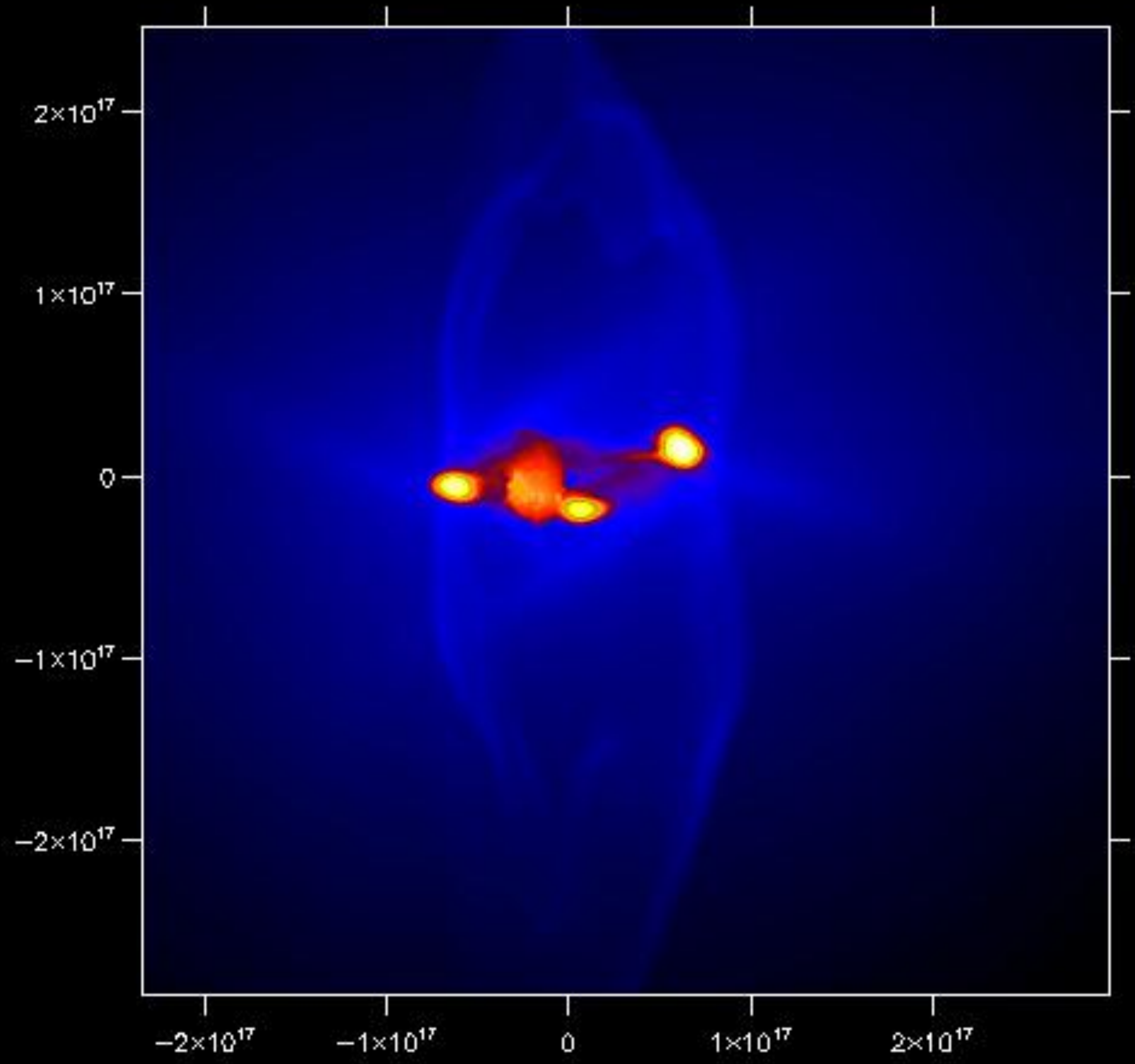
Viewing perspective of compact HII regions

Peters et al. 2010



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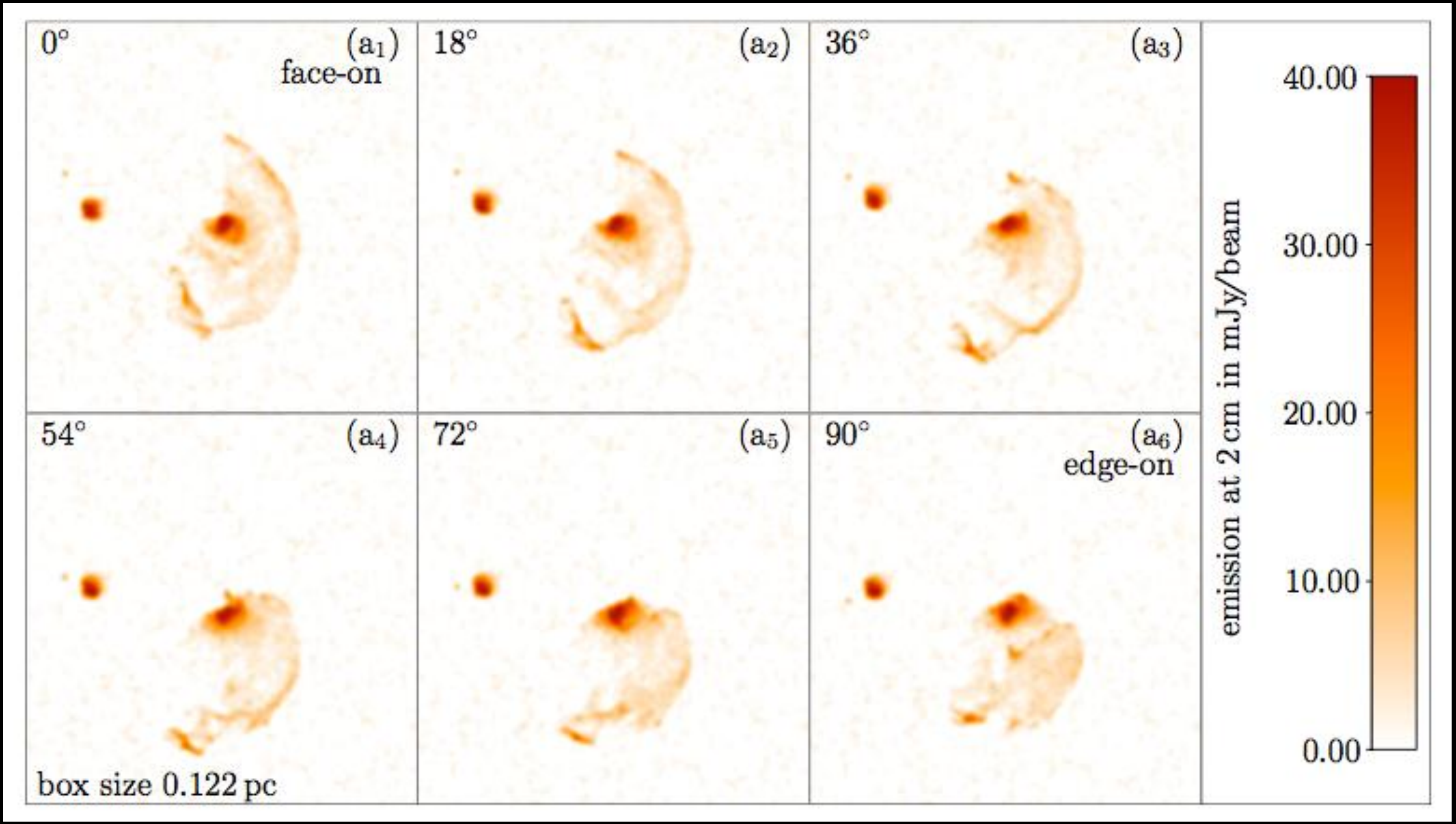
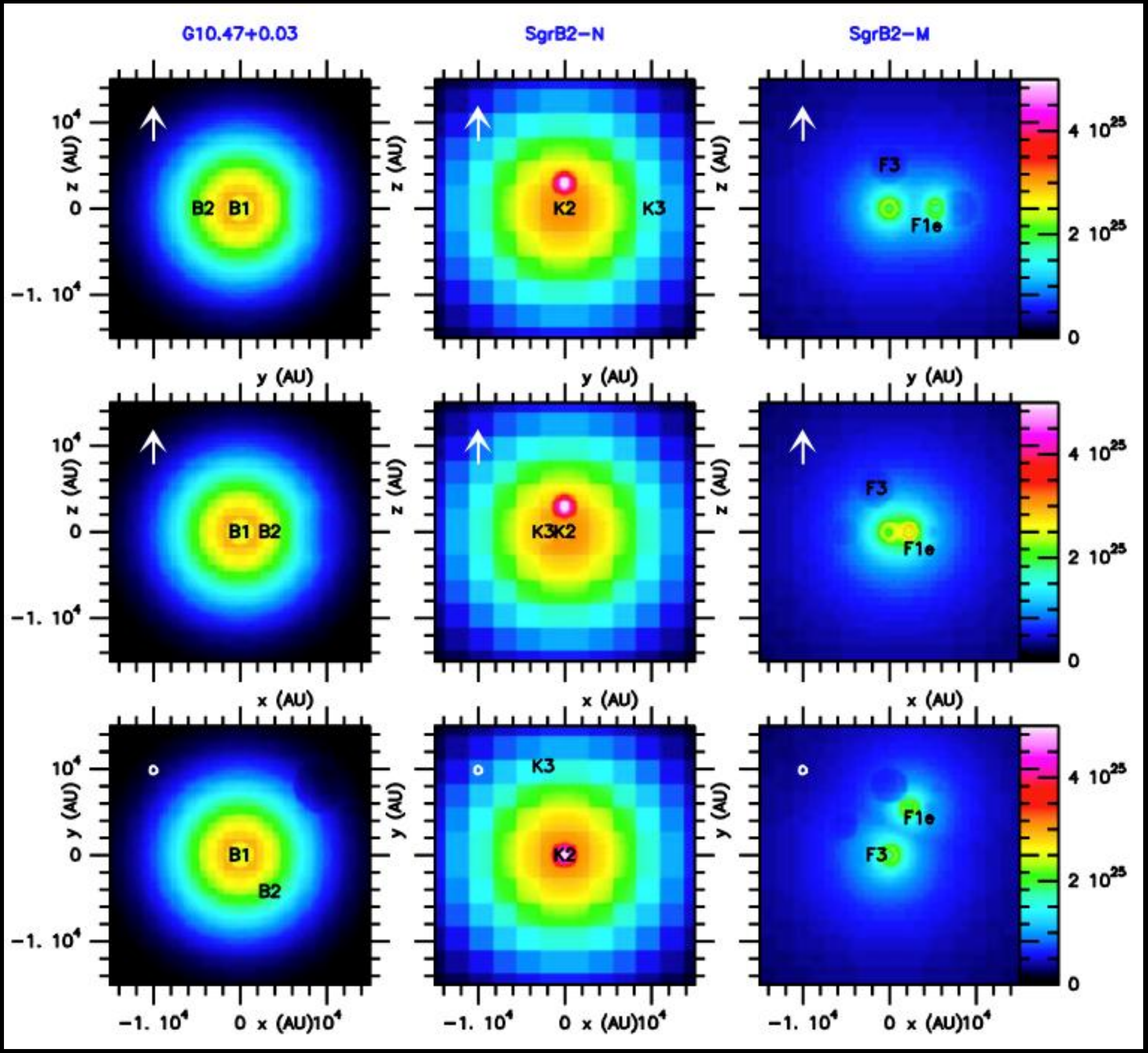


Example: Line transfer in SF regions

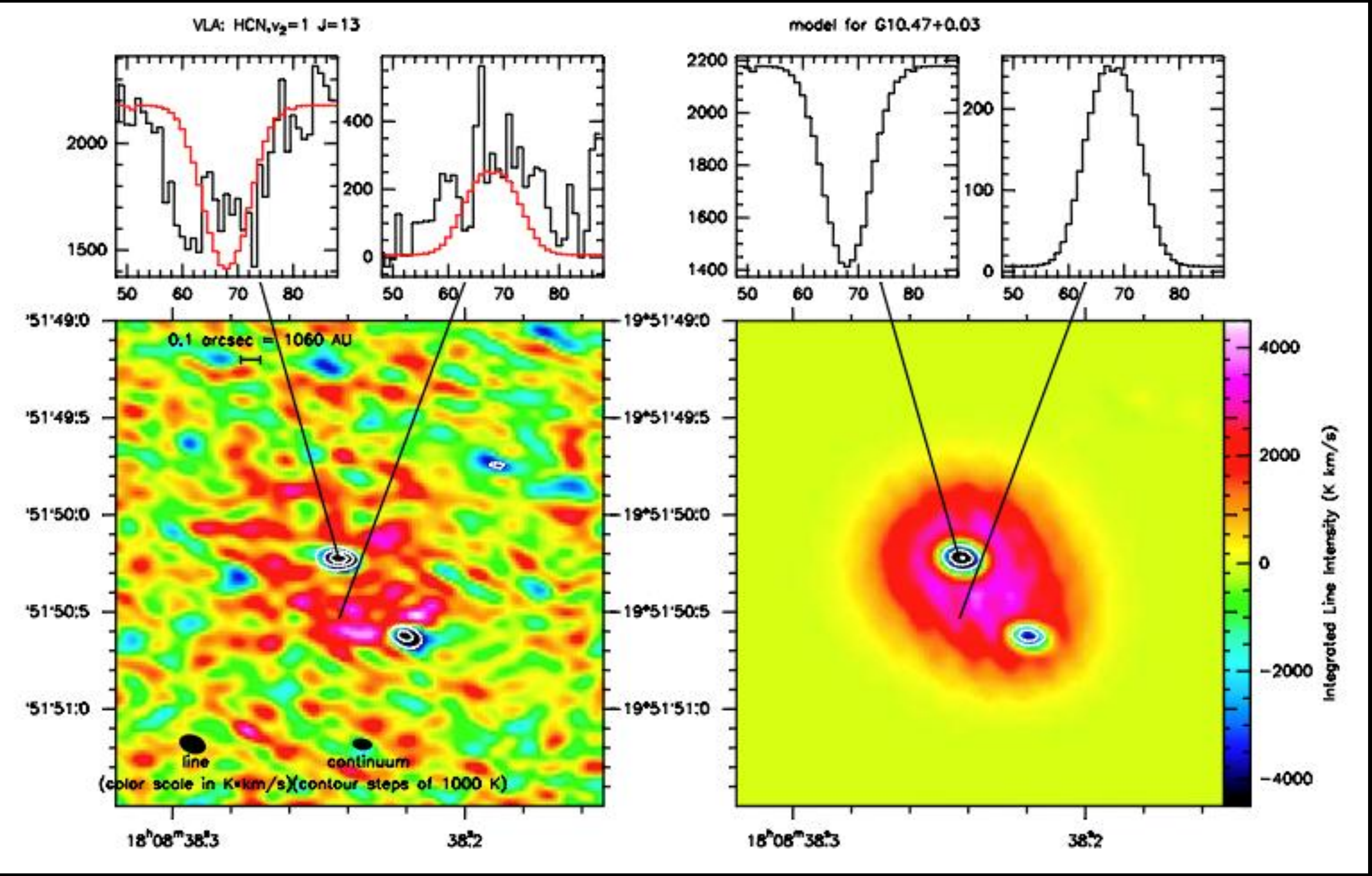
Model of HCN emission around young massive stars.



Rolffs, Schilke et al. 2011

Example: Line transfer in SF regions

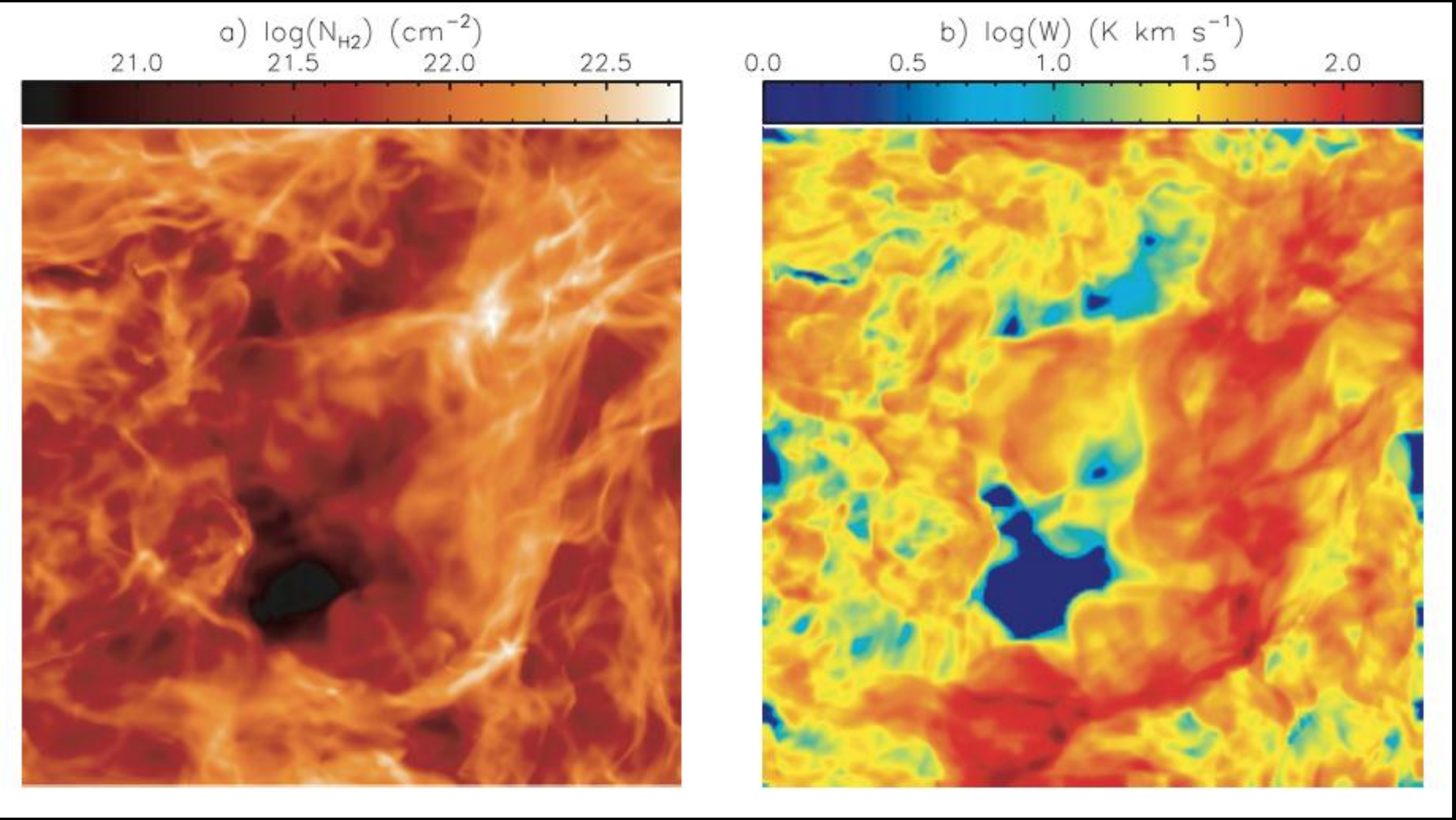
Model of HCN emission around young massive stars.



Rolffs, Schilke et al. 2011

The CO X-factor in the turbulent ISM

Shetty et al. 2011a/b



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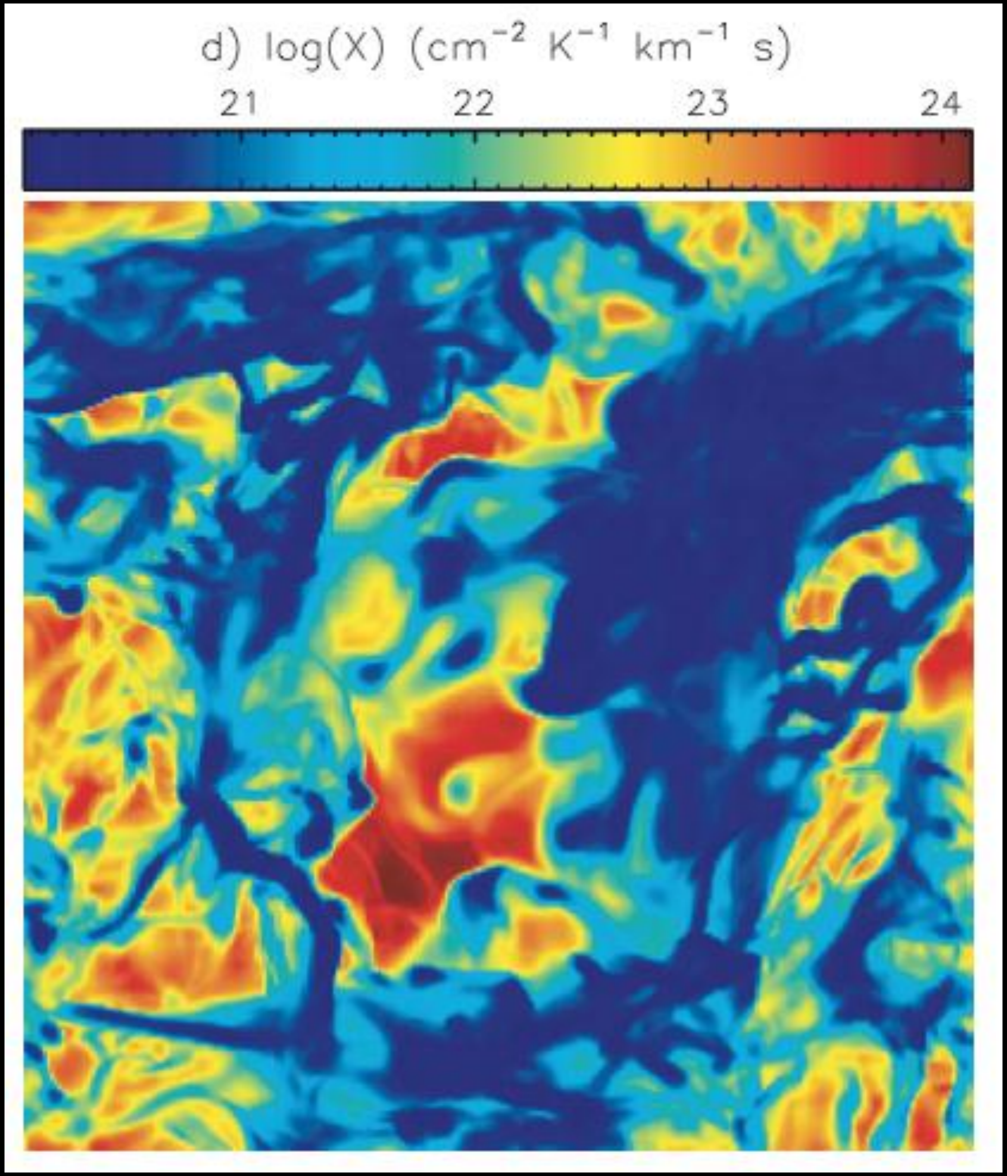
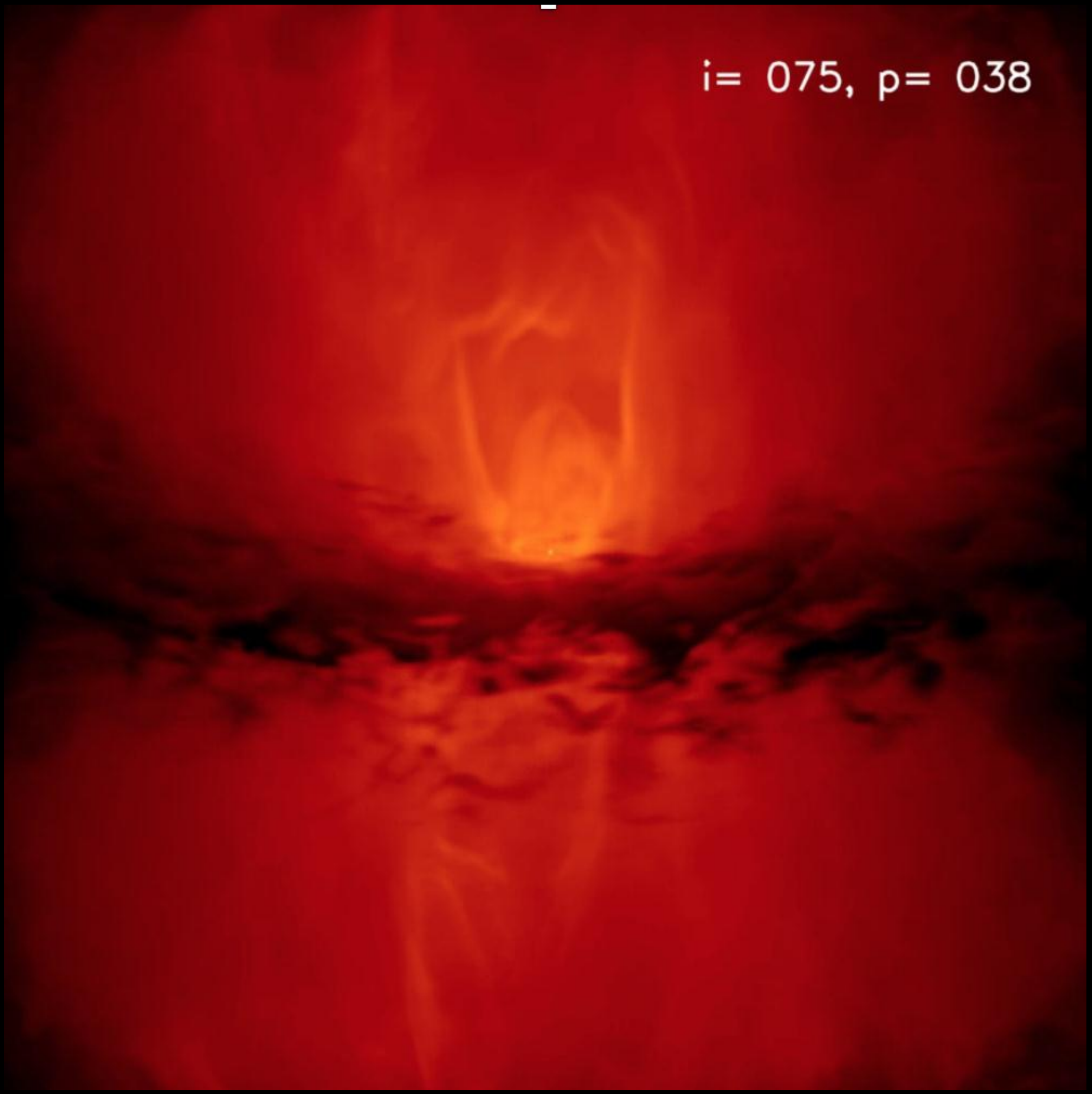


Example of AGN model



K. Wada, M. Schartmann and R. Meijerink (2016) ApJ, 828, L19

Issues of parallelization

- Currently RADMC-3D = OpenMP
- MPI distributed memory is hard. But a simple trick is possible:
  - Each node has FULL grid (possibly memory issue for large models)
  - Partly “embarrassingly parallel”:
    - Let 8 nodes do MC for 5 minutes
    - Then add all cell-energies (gather)
    - Redistribute (broadcast)
    - Recompute the new temperatures
    - Do another 5 minutes etc.

Availability

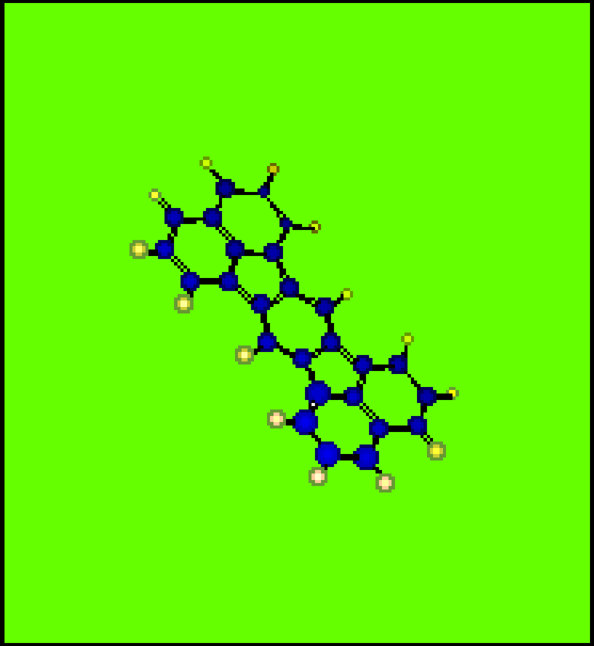
- URL: http://www.ita.uni-heidelberg.de/~dullemond/radtrans/radmc-3d/
- Current version: 0.41
- Publically available
- For your convenience:
  - Extensive manual
  - Several simplistic example setups
  - Several more complex examples
  - Forum (PHPBB)
- GOAL:
  - Easy to use in simple way (complexities hidden)...
  - ...but if you want: Lots of flexibility + possibilities

Very-near future stuff:

Quantum-heating & PAHs

Polycyclic Aromatic Hydrocarbons

Molecules or dust grains?



Polycyclic Aromatic Hydrocarbons

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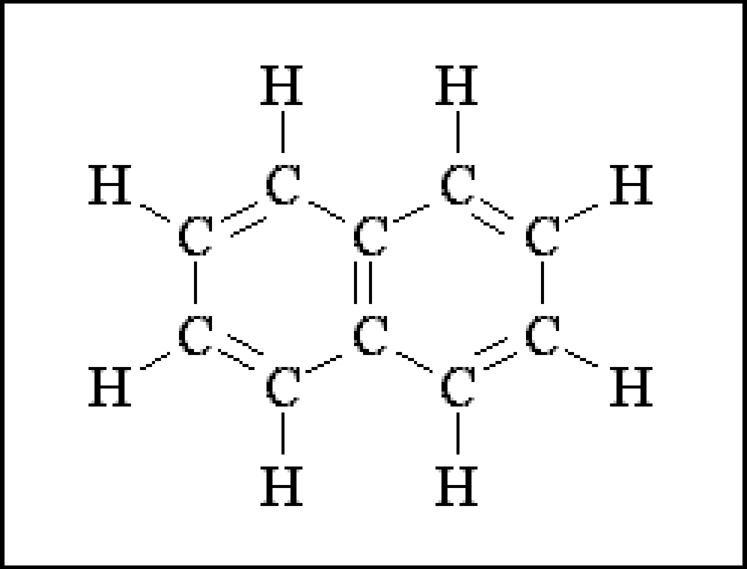
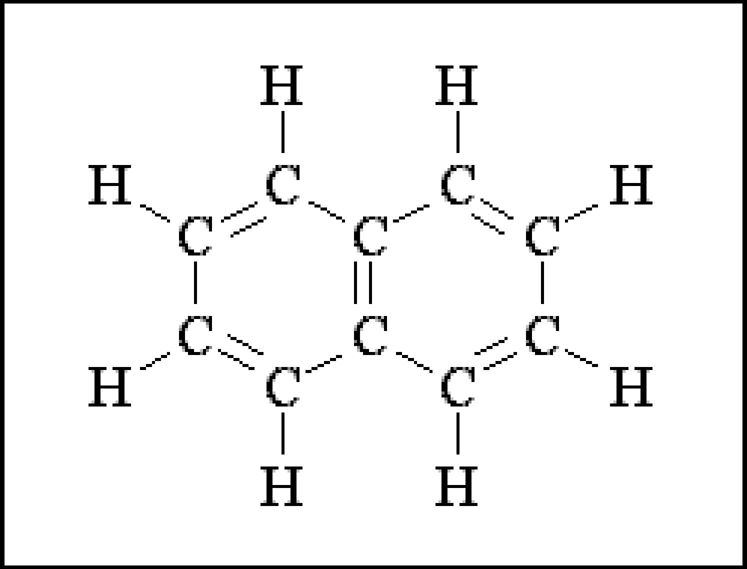


Naphthalene

$C_{10}H_8$

Polycyclic Aromatic Hydrocarbons

Molecules or dust grains?



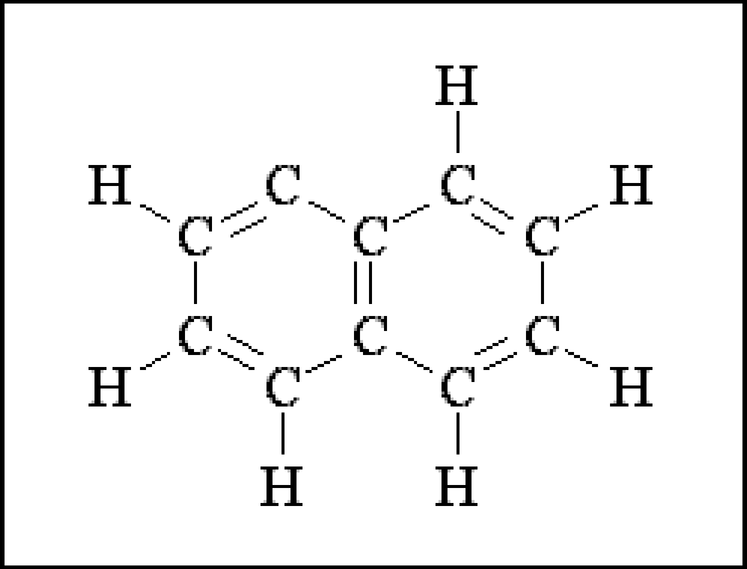
Dehydrogenation

Naphthalene

$C_{10}H_8$

Polycyclic Aromatic Hydrocarbons

Molecules or dust grains?



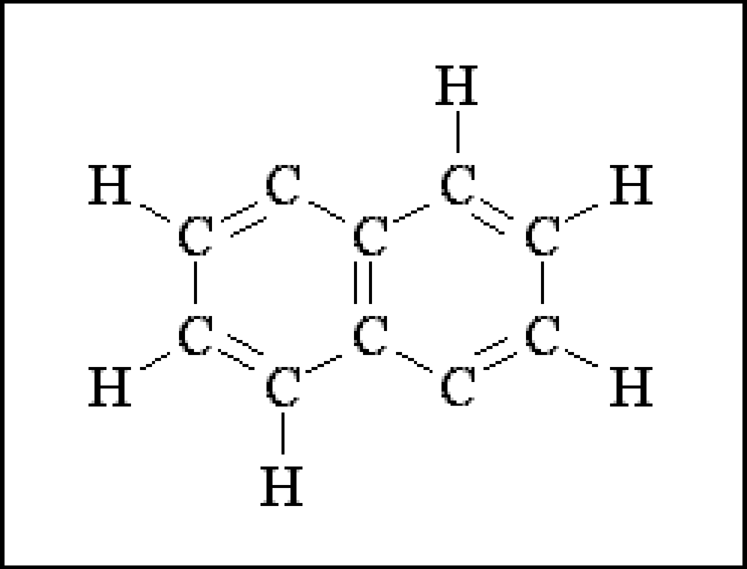
Dehydrogenation

Naphthalene

$C_{10}H_7$

Polycyclic Aromatic Hydrocarbons

Molecules or dust grains?



Dehydrogenation

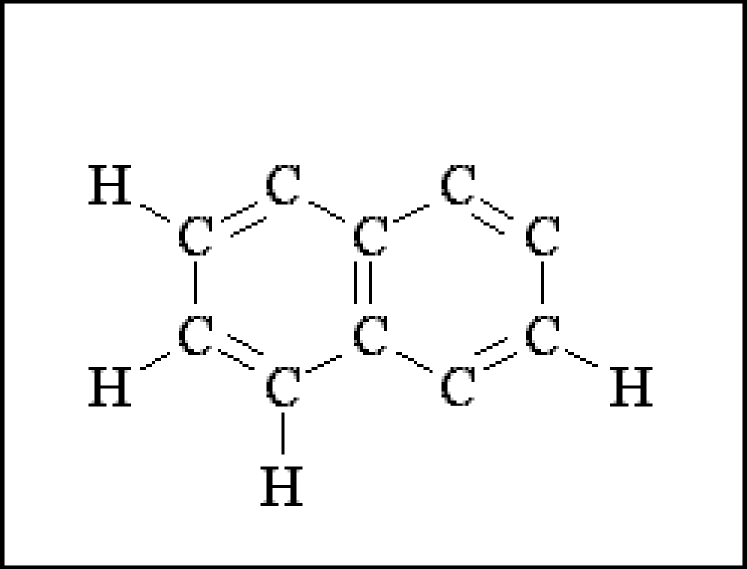
Naphthalene

$C_{10}H_6$

Polycyclic Aromatic Hydrocarbons

Molecules or dust grains?

Dehydrogenation

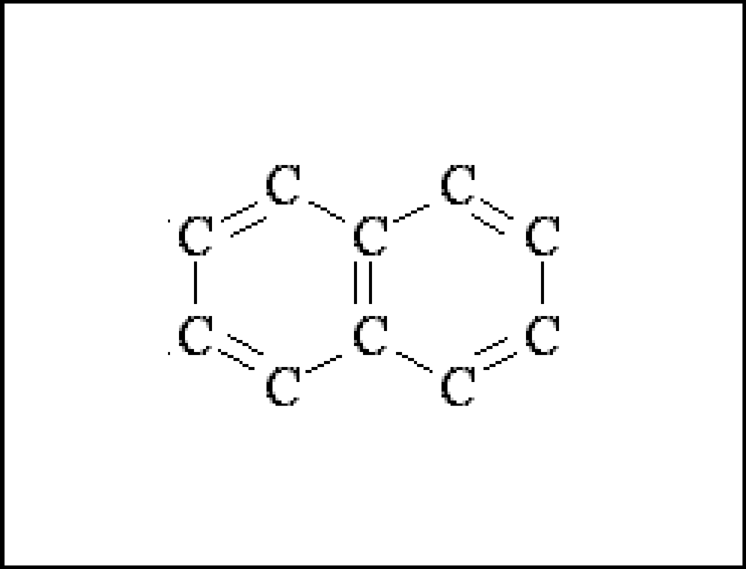


Naphthalene

$C_{10}H_4$

Polycyclic Aromatic Hydrocarbons

Molecules or dust grains?



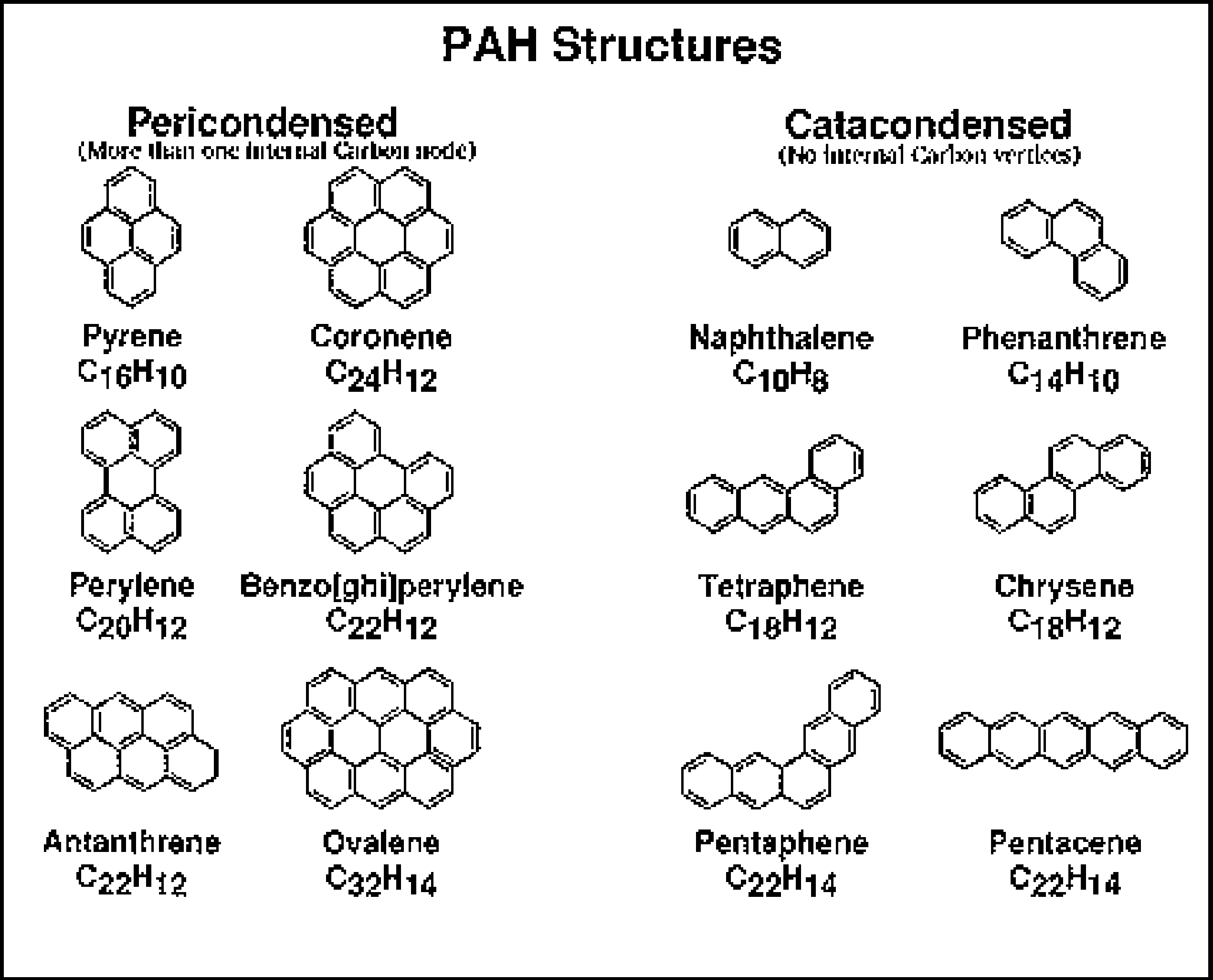
Dehydrogenation

Naphthalene

C_{10}

Polycyclic Aromatic Hydrocarbons

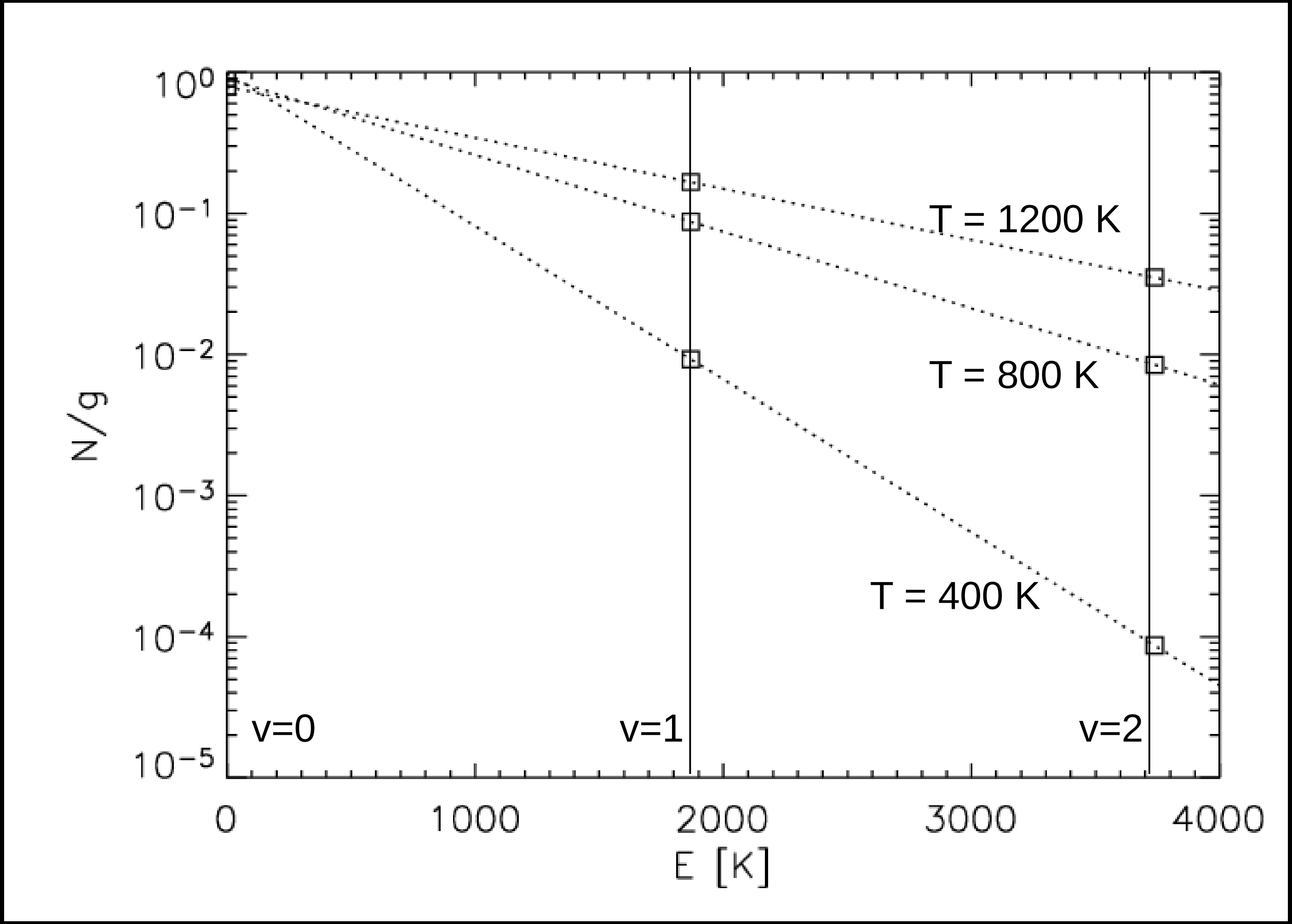
Molecules or dust grains?



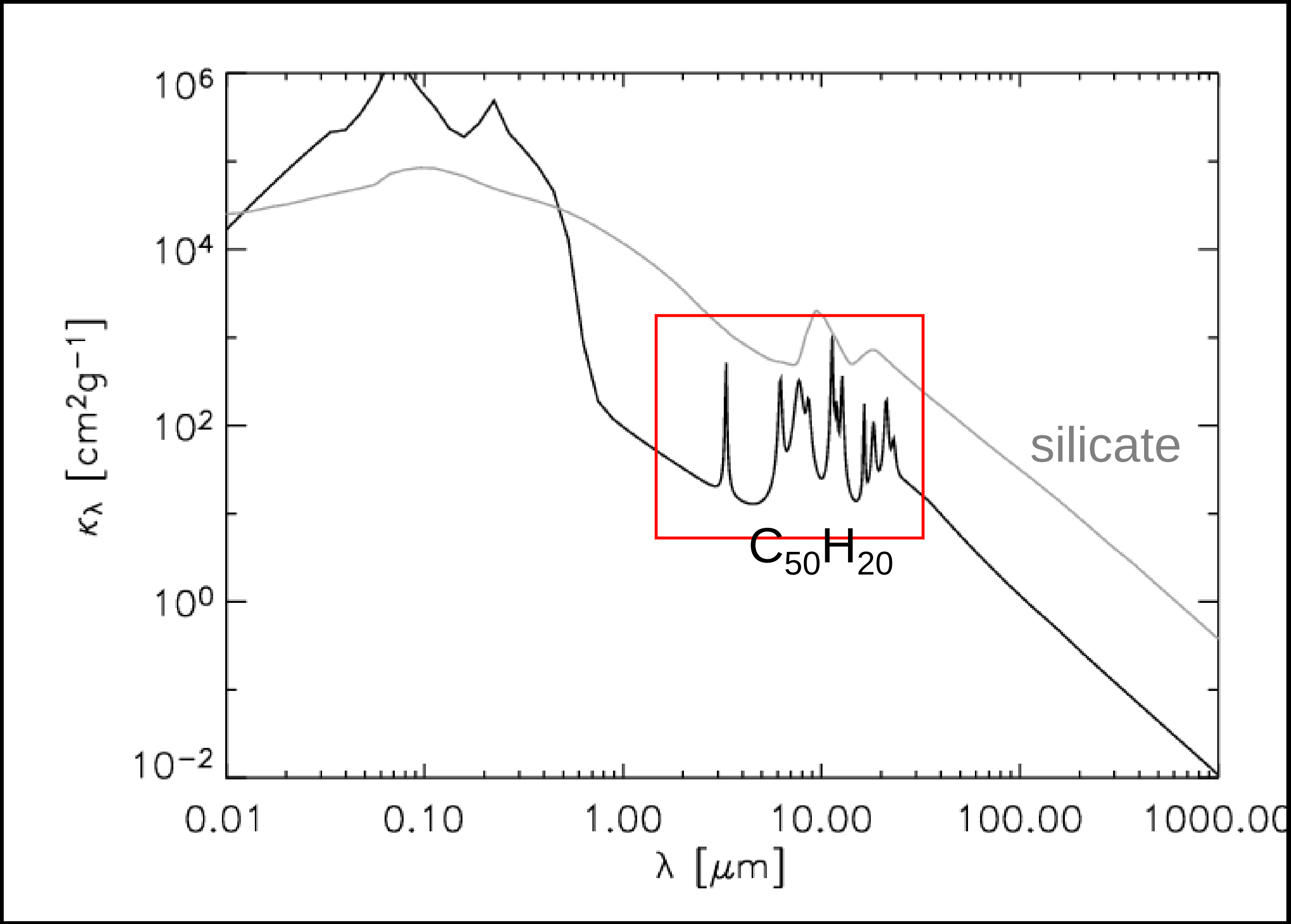
Polycyclic Aromatic Hydrocarbons

Molecules or dust grains?

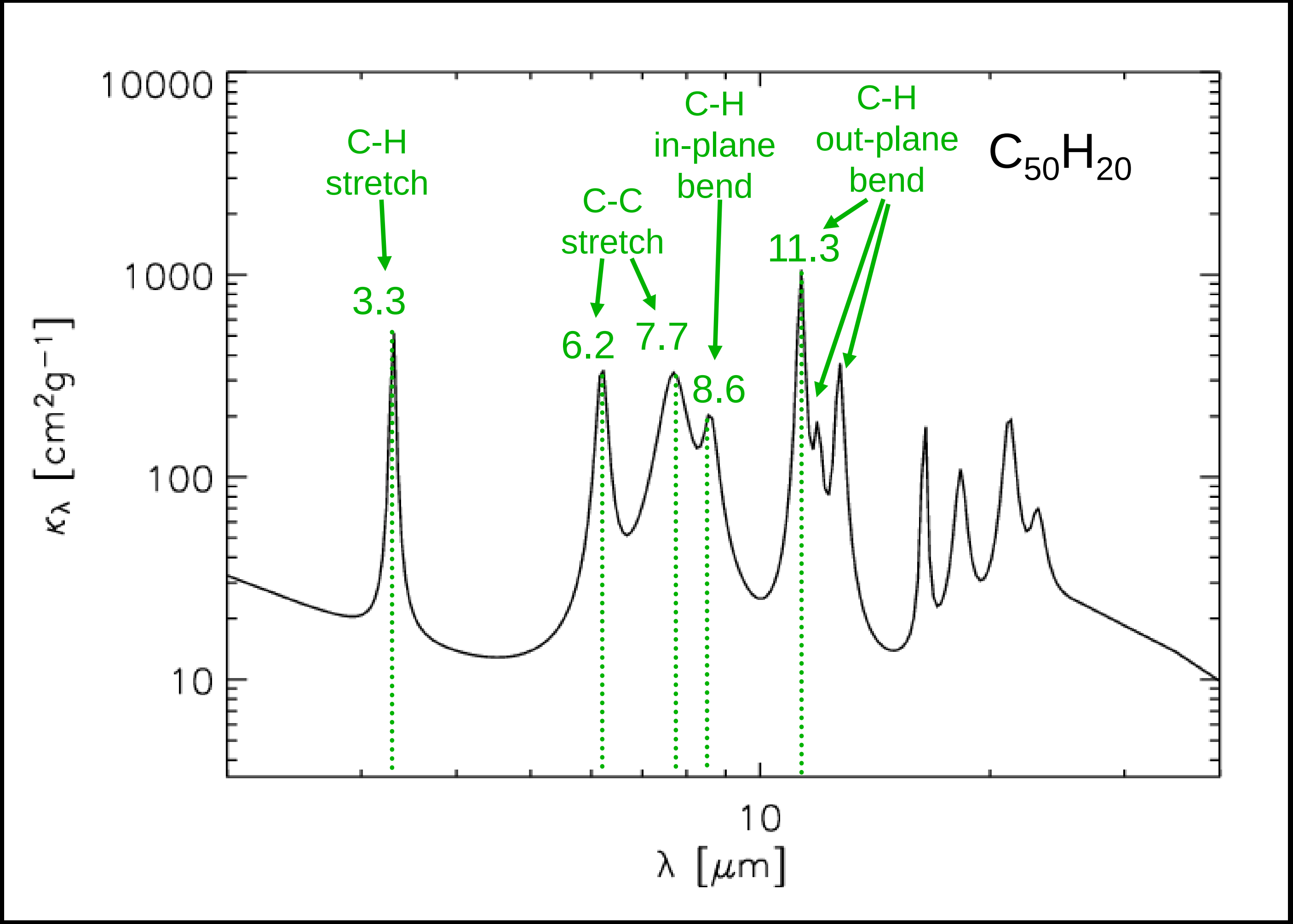
C-C
stretch
vibration



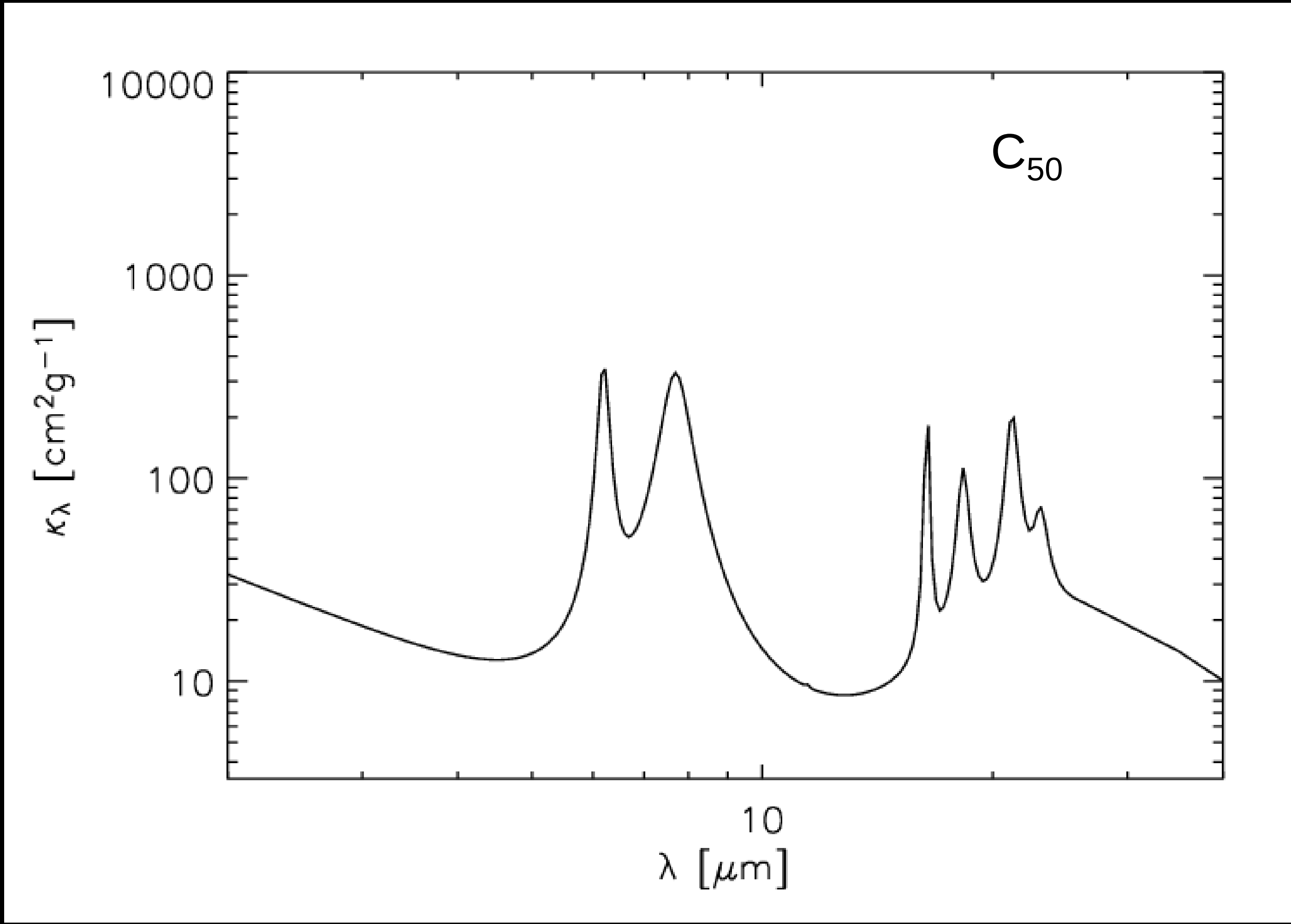
PAH opacity: Li & Draine model



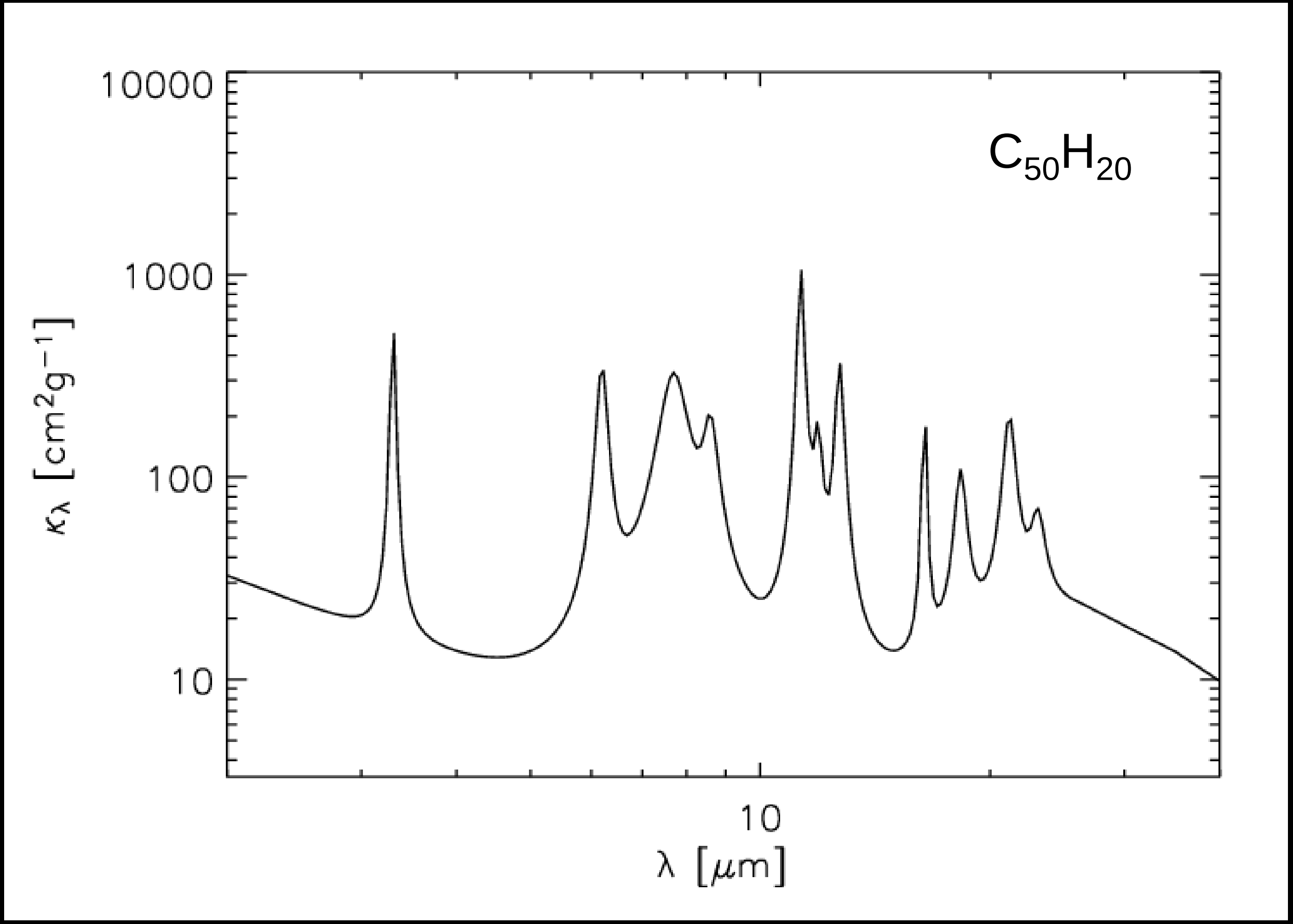
PAH opacity: Li & Draine model



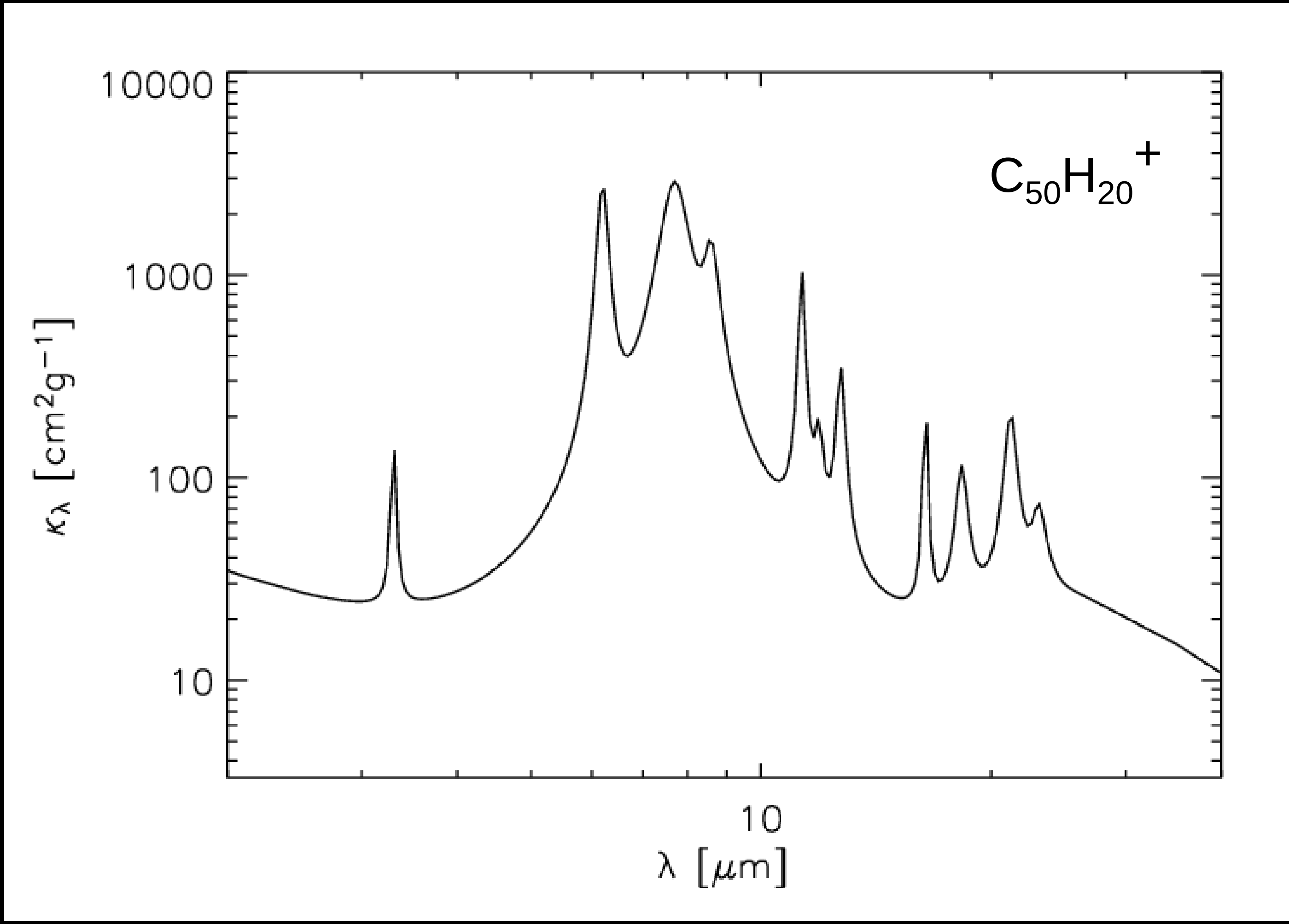
PAH opacity: Li & Draine model



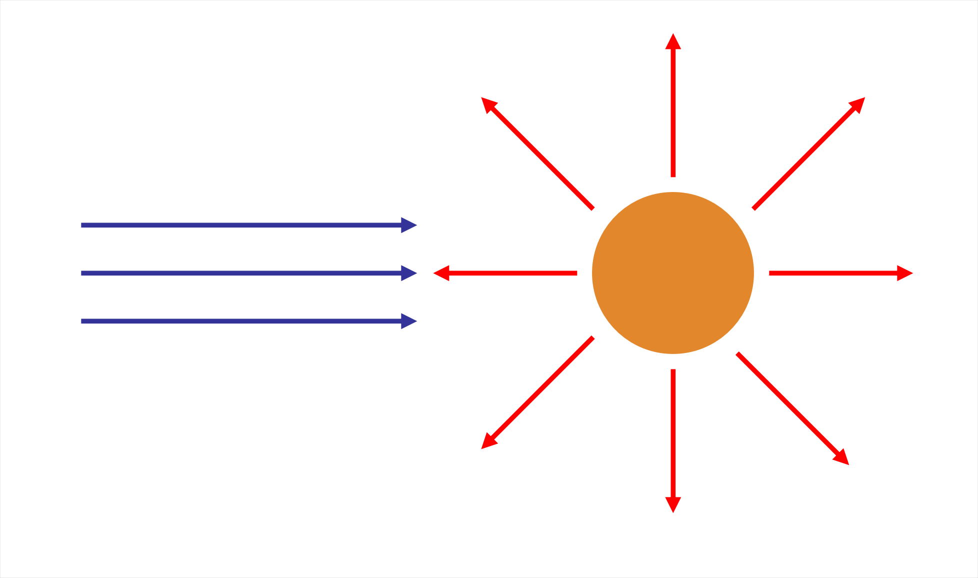
PAH opacity: Li & Draine model



PAH opacity: Li & Draine model



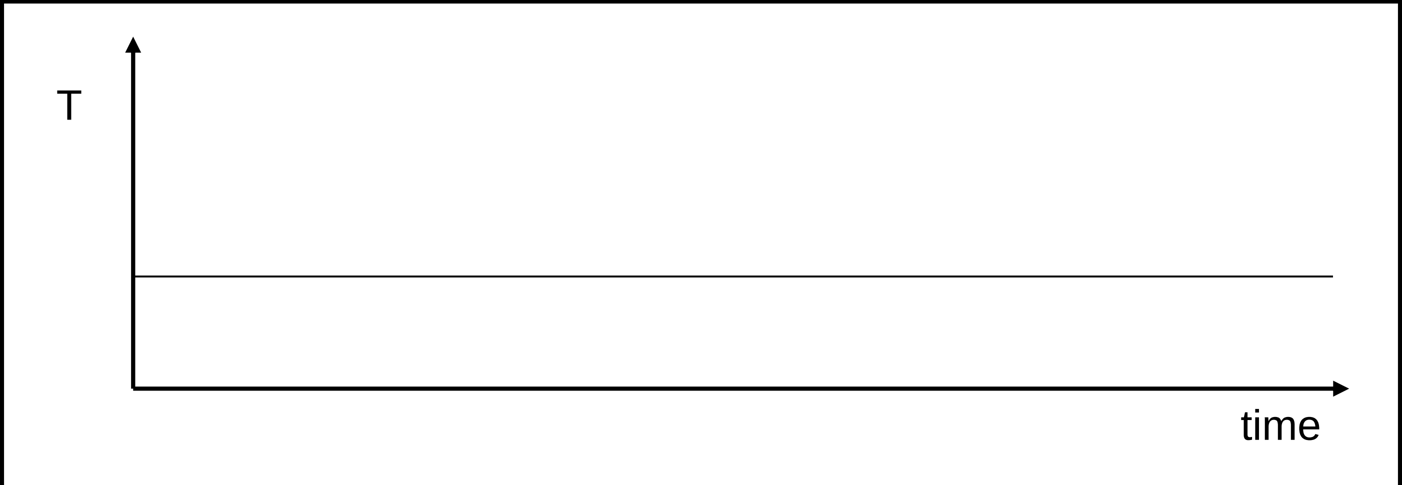
Big grains: thermal equilibrium



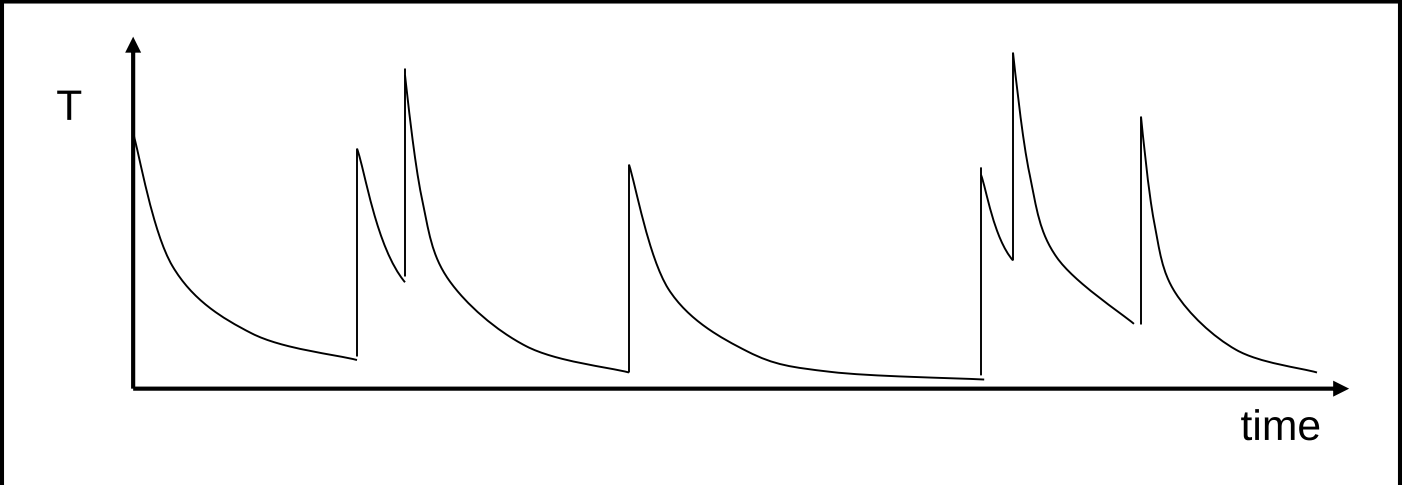
$$\int B_n(T)\,k_n\,dn = \frac{1}{p}\int F_n\,k_n\,dn \quad \longrightarrow \quad T$$

Thermal vs. Quantum

Big grain:
thermal
equilibrium

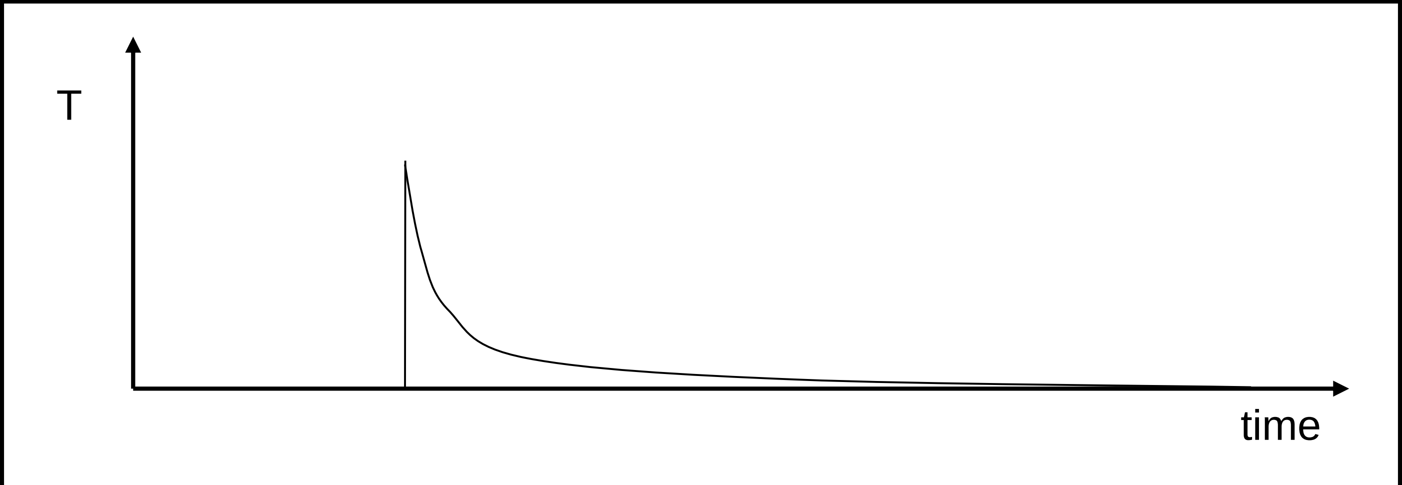


Small grain:
quantum
fluctuations

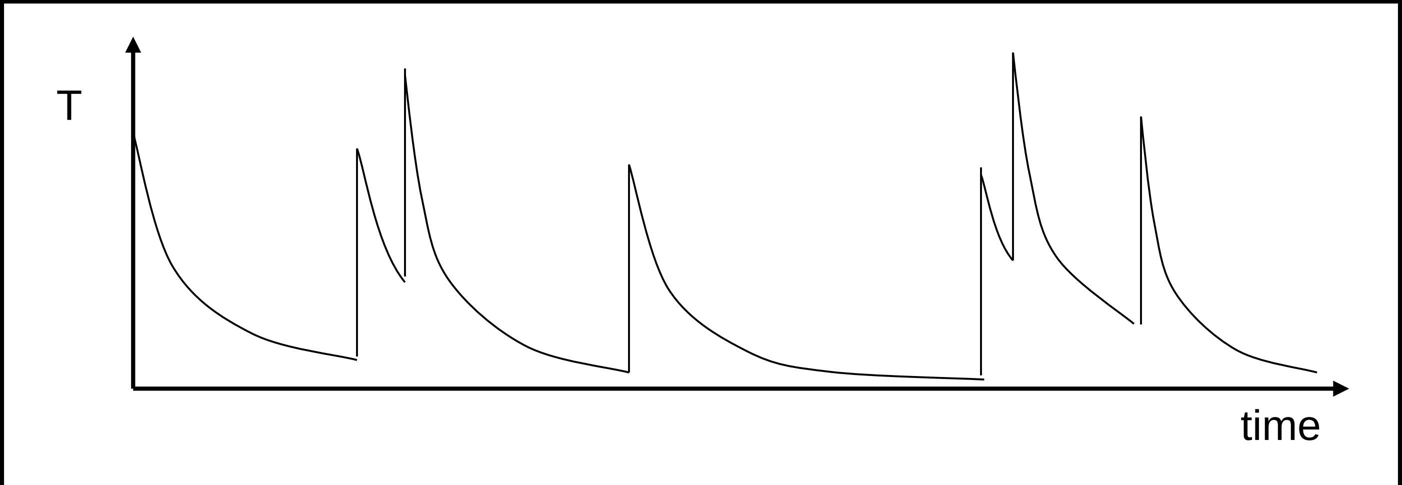


Single- vs. Multi-photon

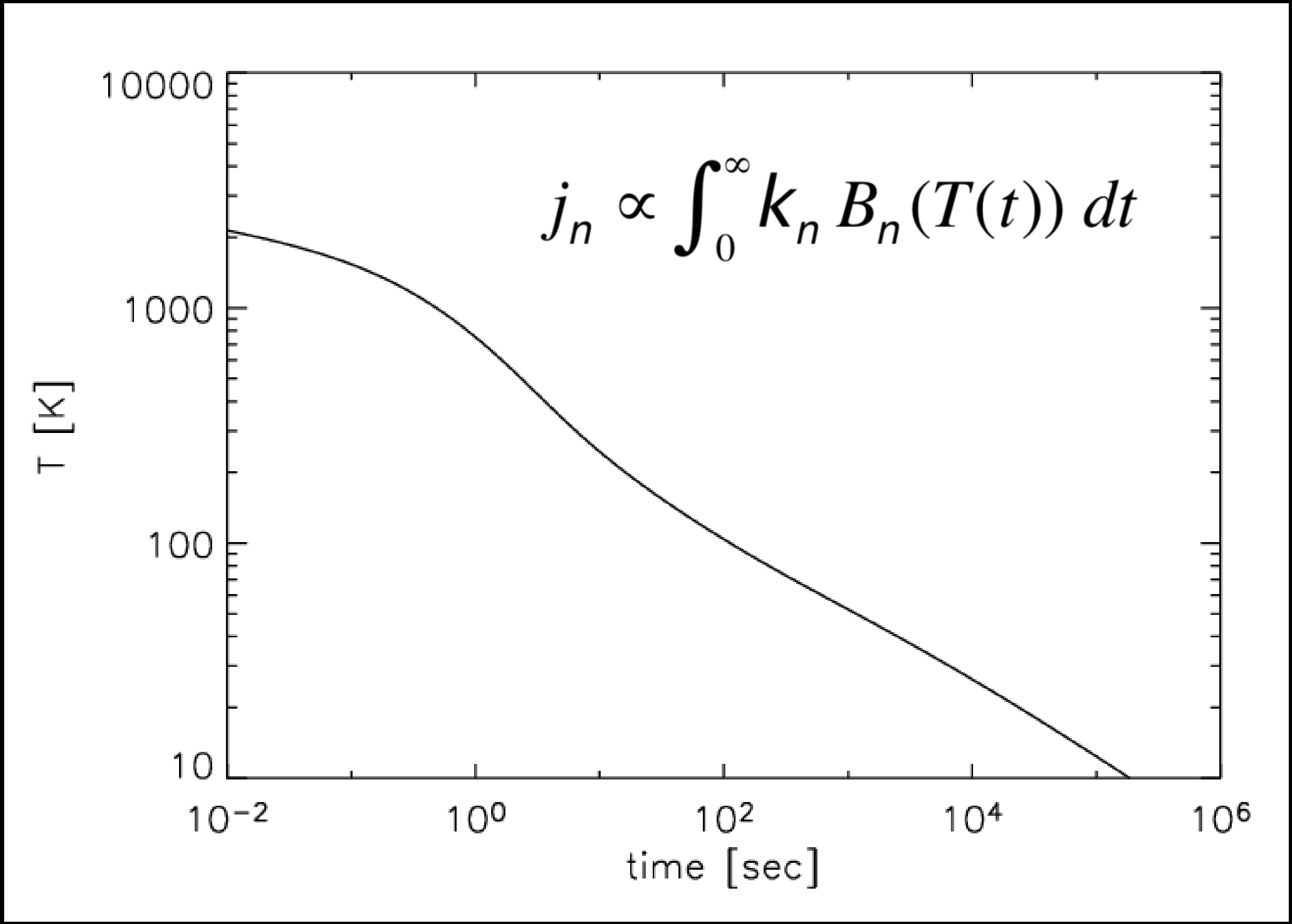
Single-
photon



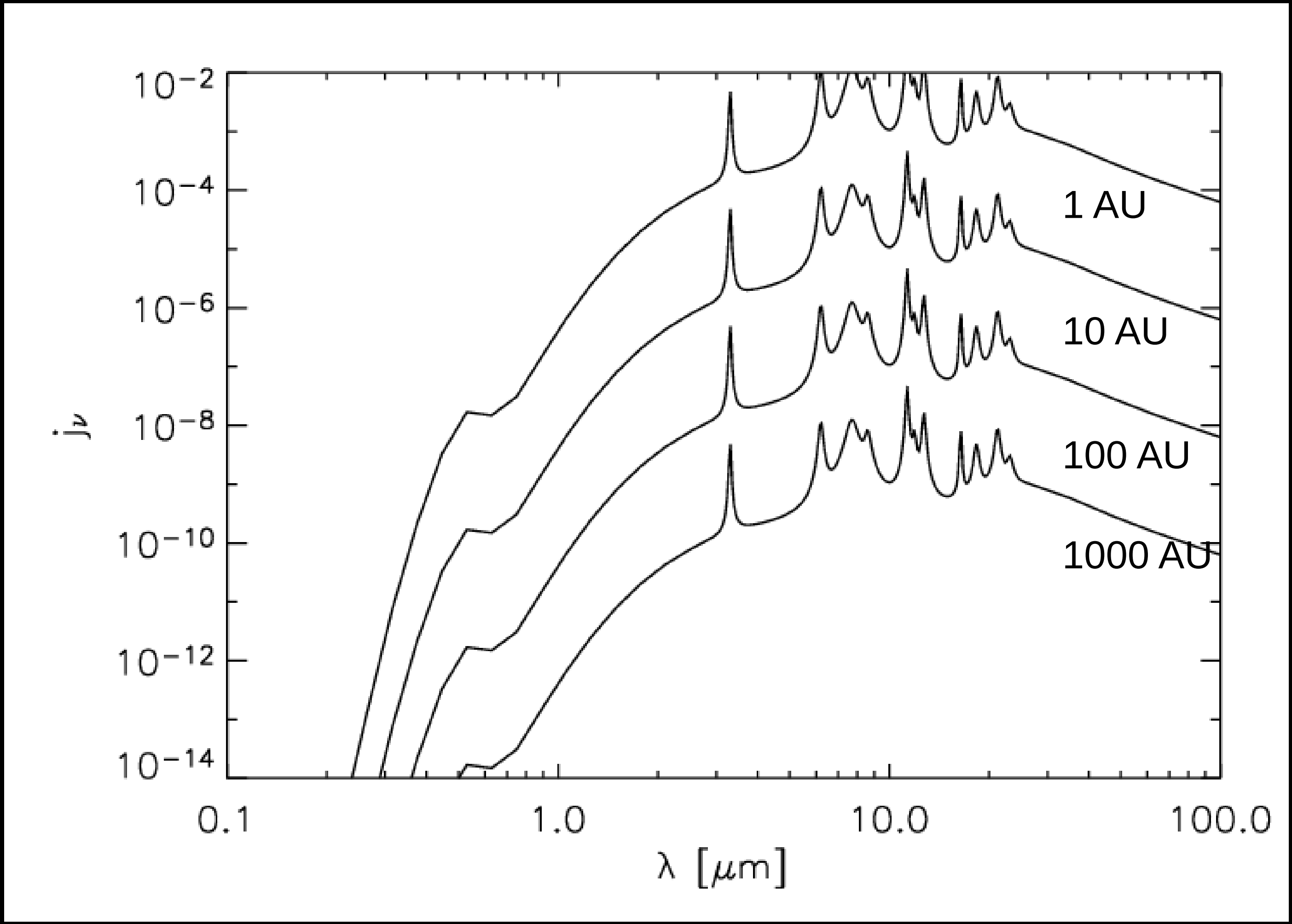
Multi-
photon



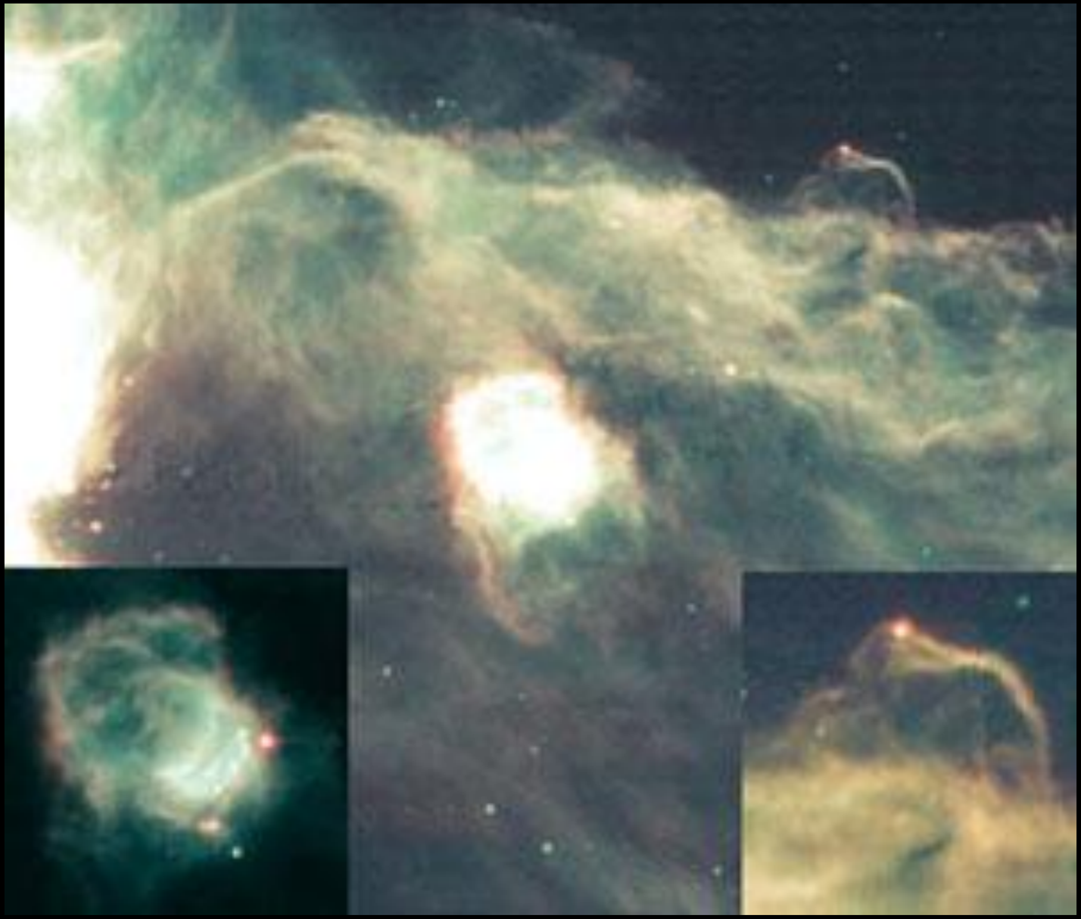
Cooling curve



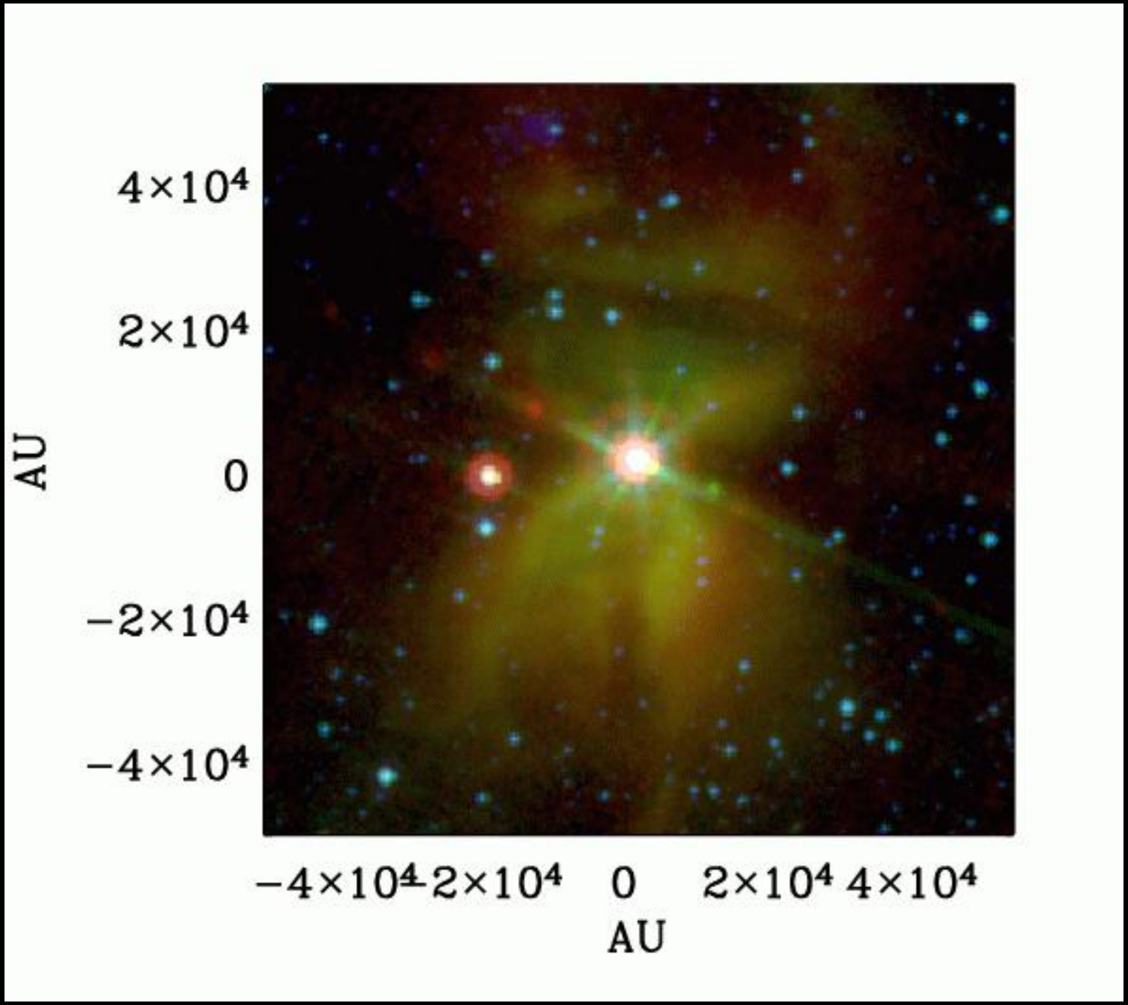
Emissivity after single excitation



PAH emission: usually extended



Near-IR PAH emission far from star:

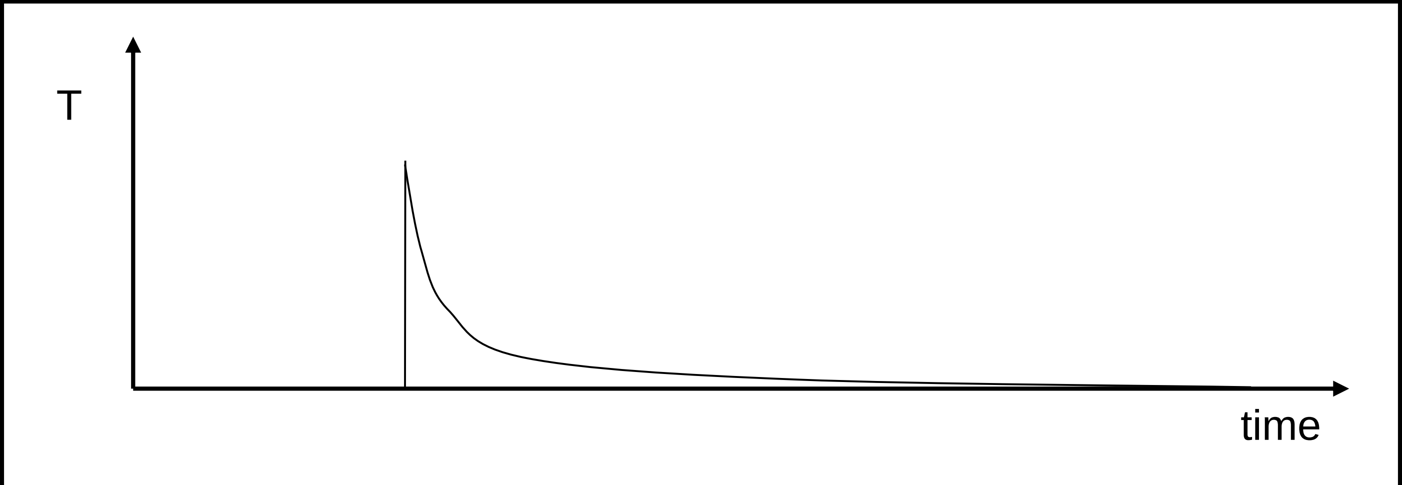


VV Serpens: Spitzer IRAC image

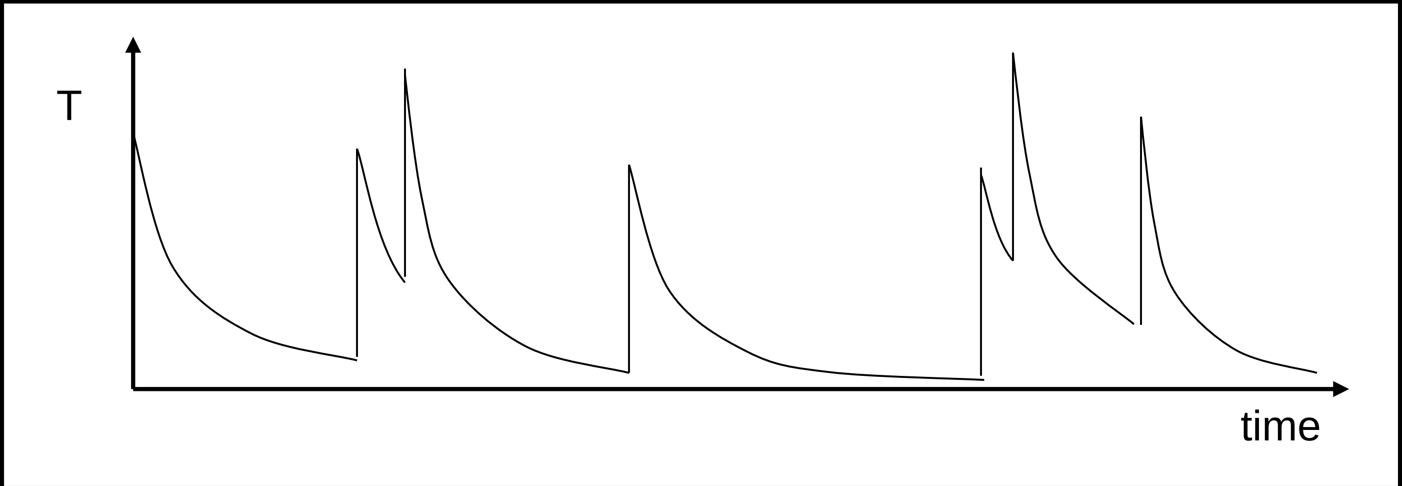
Pontoppidan, Dullemond et al. 2006

Single- vs. Multi-photon

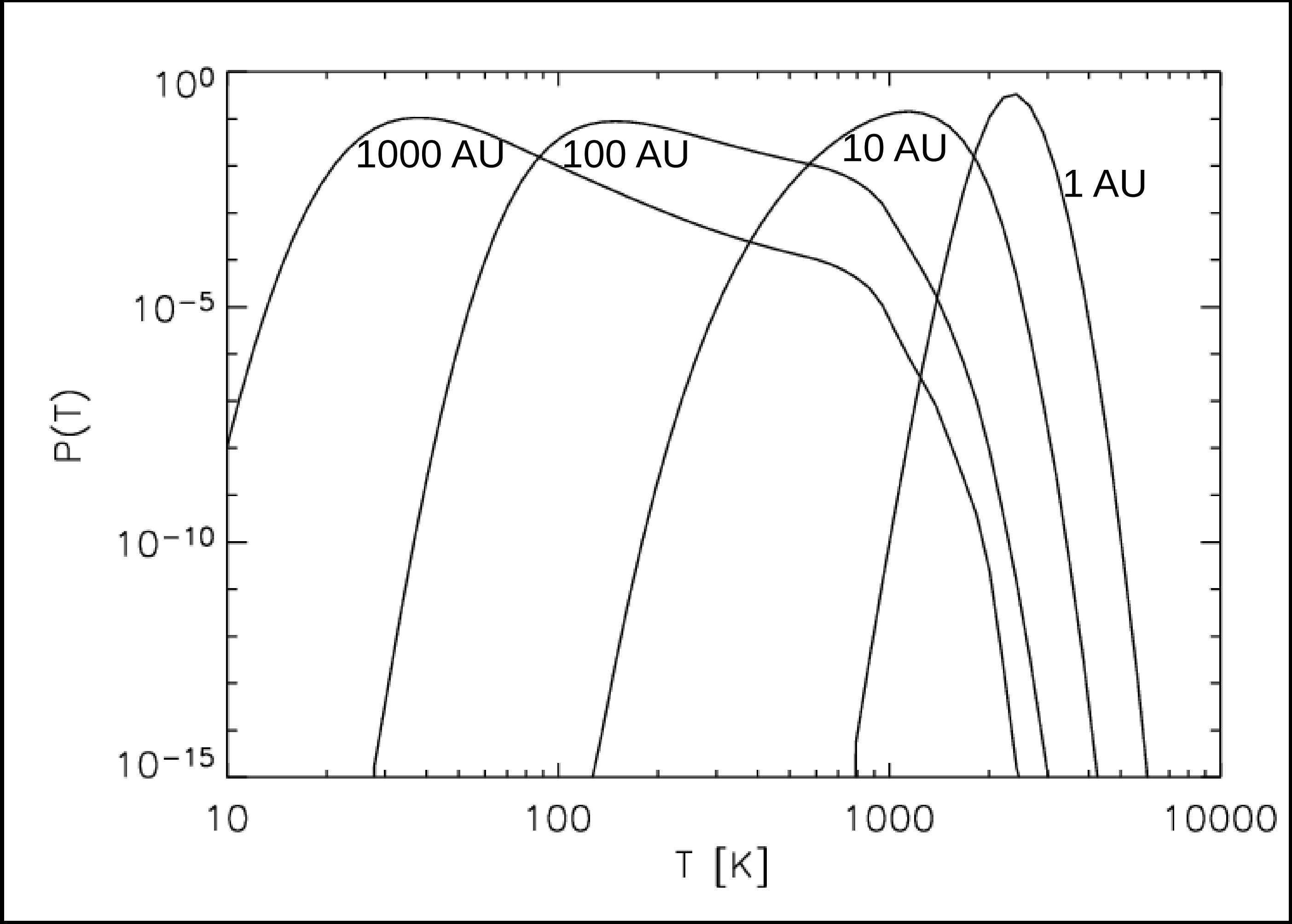
Single-photon



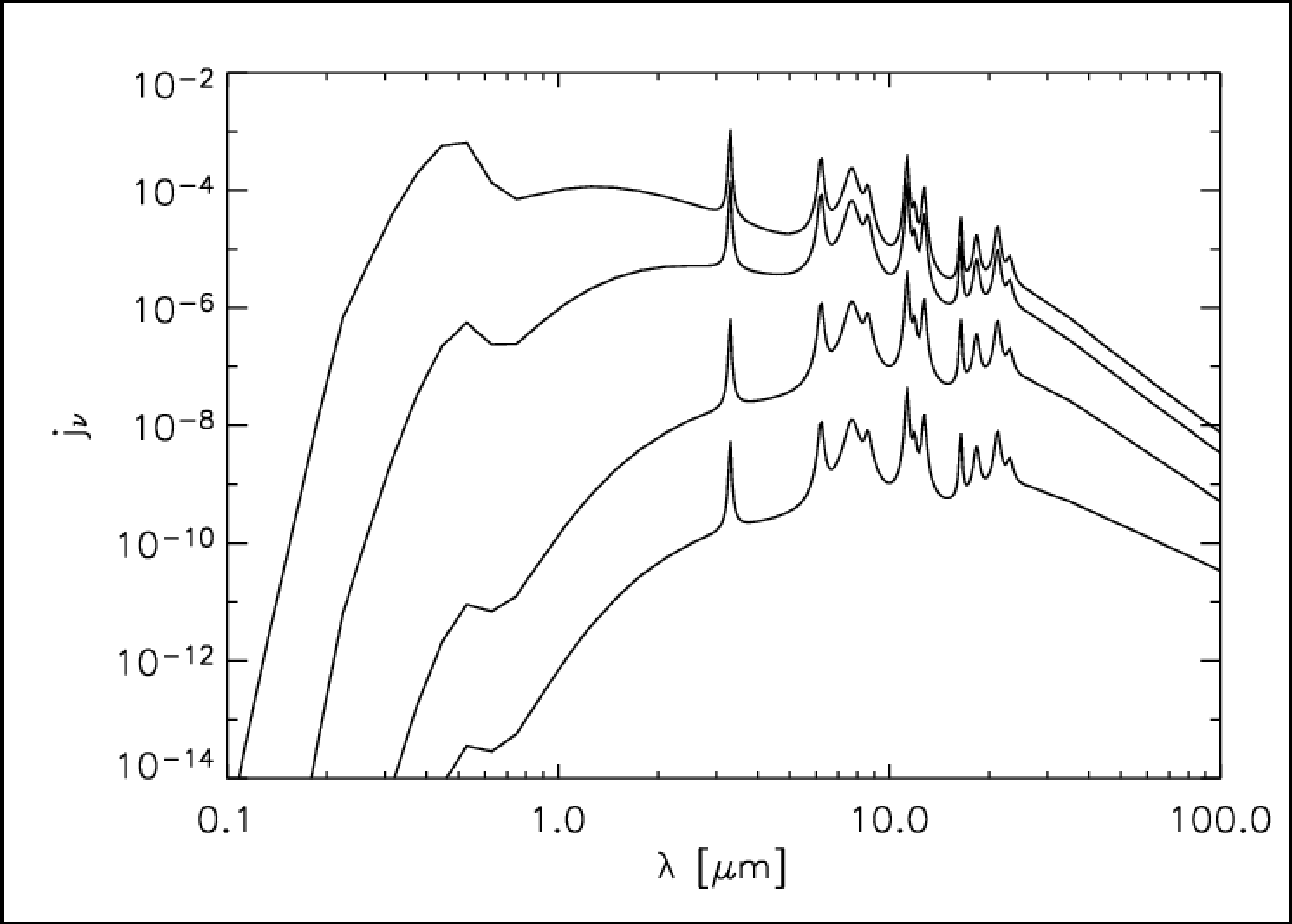
Multi-photon



Temperature distribution function



Emissivity with P(T)



Emissivity after single excitation