RADMC-3D

A publicly available radiative transfer program

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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

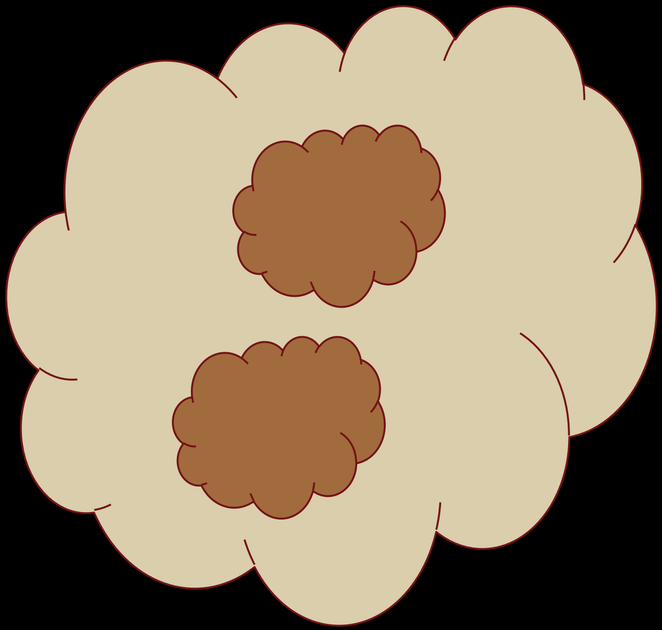
- Continuum radiative transfer (dust)
- Gas line transfer (for now only LTE, LVG, OpThin)
- Polarization
  - Scattering (off randomly oriented dust particles)
  - Thermal polarization (though simplified)
- Various sources of energy:
  - Stars
  - Continuous distributions of stars (for galaxies)
  - Viscous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

RADMC-3D Features

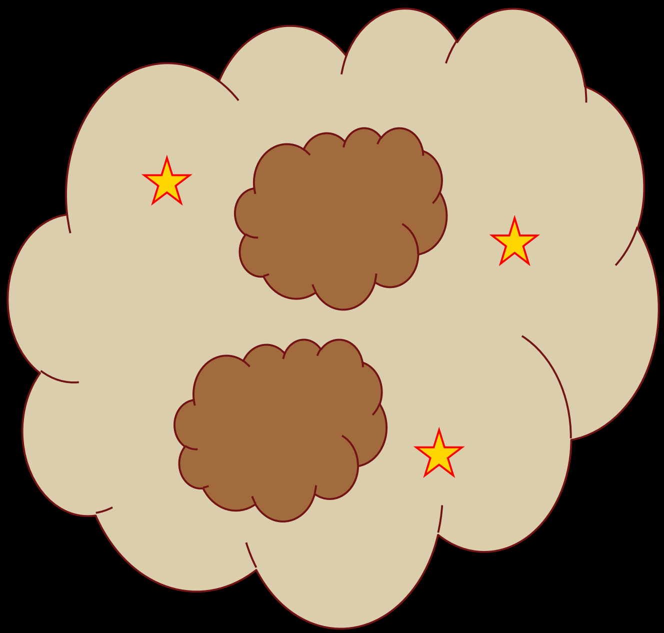
- 1-D, 2-D and 3-D models
- Cartesian or spherical coordinates
- Various gridding possibilities:
  - Regular
  - Oct-tree Mesh Refinement or
  - Patch-based Mesh Refinement
- Interface with:
  - FLASH
  - RAMSES (thanks, Benoit Commercon)
  - PLUTO (thanks, Mario Flock)

How RADMC-3D works

A model begins with a density distribution...



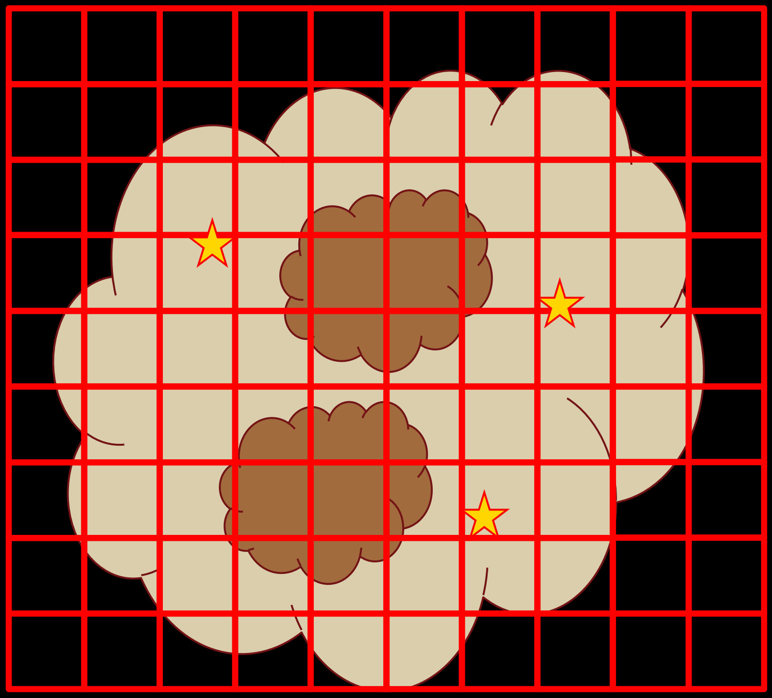
Add stars...



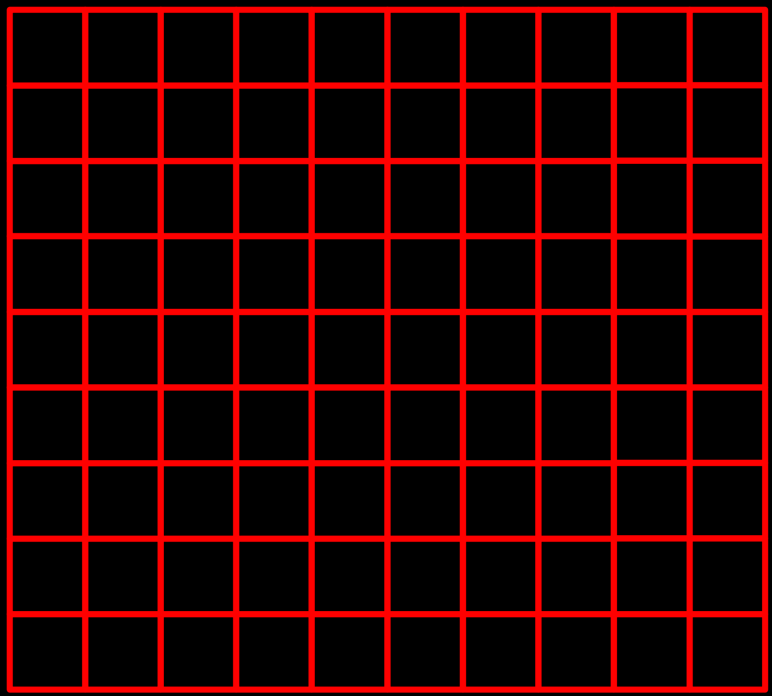
Stellar data in stars.inp

```
2                          ← format number (just keep it at 2)
1 150                      ← nr of stars and nr of wavelength sampling points

  R_star [cm]     M_star [g]      x-position [cm]  y-position [cm]  z-position [cm]
 6.960000e+10  1.988920e+33  0.000000e+00  0.000000e+00  0.000000e+00

 1.000000e-01
 1.236673e-01
 1.529360e-01
 1.891319e-01
 2.338943e-01
 2.892508e-01
 3.577086e-01
 4.423686e-01             ← Wavelength sampling points
 5.470654e-01
 6.765410e-01
 8.366600e-01
 1.034675e+00
 1.279555e+00
 1.582391e+00
 1.956900e+00
 2.420045e+00
 2.992805e+00
 3.701121e+00
 4.577077e+00             Below: Spectrum of star in erg/cm^2/s/Hz as seen at 1 pc
 5.660348e+00                    OR simply T_star (then producing a Blackbody spectrum)
 7.000000e+00
```

Map the density on a grid...



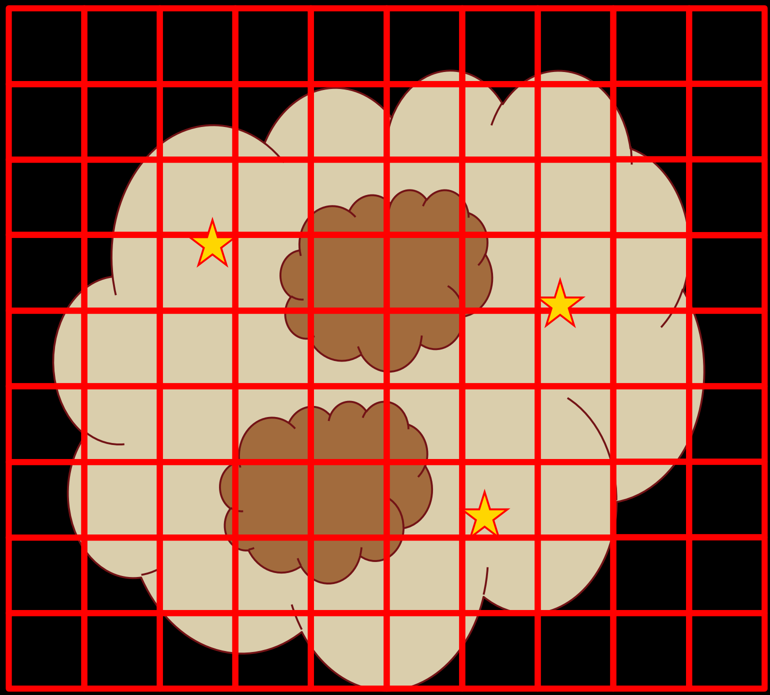
The grid is defined in amr_grid.inp



The grid is defined in amr_grid.inp

1	← format number (just keep it at 1)
0	← Adaptive Mesh Refinement style (here: 0 = regular grid)
0	← Coordinate system (0 = cartesian, 100 = spherical)
0	← (forget about this ;-))
1 1 1	← Which directions are active (all three = 3D)
32 32 32	← Nr of cells in each direction
-1.495980e+14	
-1.402481e+14	
-1.308982e+14	
-1.215484e+14	
-1.121985e+14	
-1.028486e+14	
-9.349875e+13	
-8.414888e+13	
-7.479900e+13	← x-coordinates
-6.544912e+13	
-5.609925e+13	
-4.674938e+13	
-3.739950e+13	
-2.804962e+13	
-1.869975e+13	
-9.349875e+12	
0.000000e+00	(further down: y coordinates and z coordinates)
9.349875e+12	
1.869975e+13	
2.804962e+13	

Map the dust density on this grid...



Dust density is defined in dust_density.inp

```
1
32768
1
 3.585493e-19
 4.532487e-19
 5.640772e-19
 6.911218e-19
 8.336520e-19
 9.899863e-19
 1.157411e-18
 1.332172e-18
 1.509549e-18
 1.684023e-18
 1.849538e-18
 1.999827e-18
 2.128805e-18
 2.230969e-18
 2.301787e-18
 2.338035e-18
 2.338035e-18
 2.301787e-18
 2.230969e-18
 2.128805e-18
 1.999827e-18
 1.849538e-18
 1.684023e-18
```

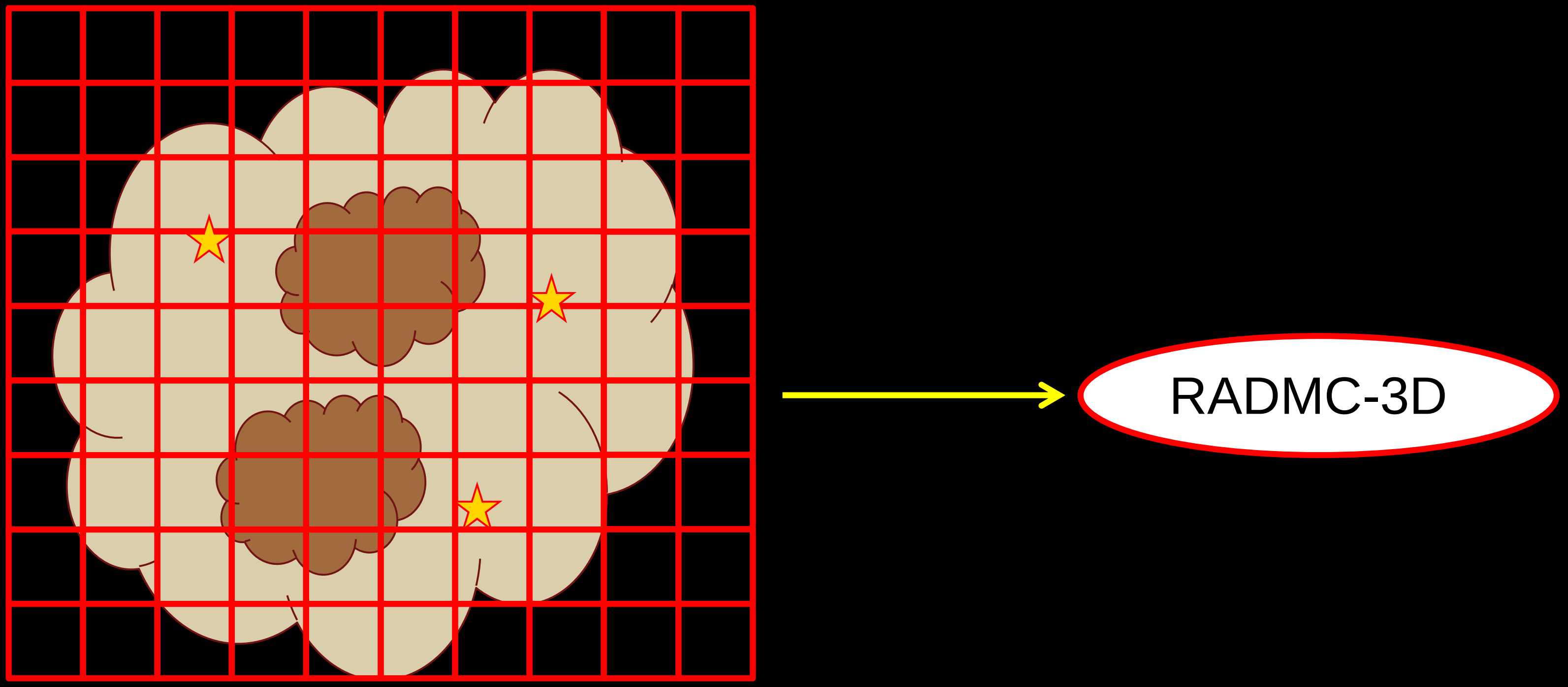
← format number (just keep it at 1)

← nr of cells

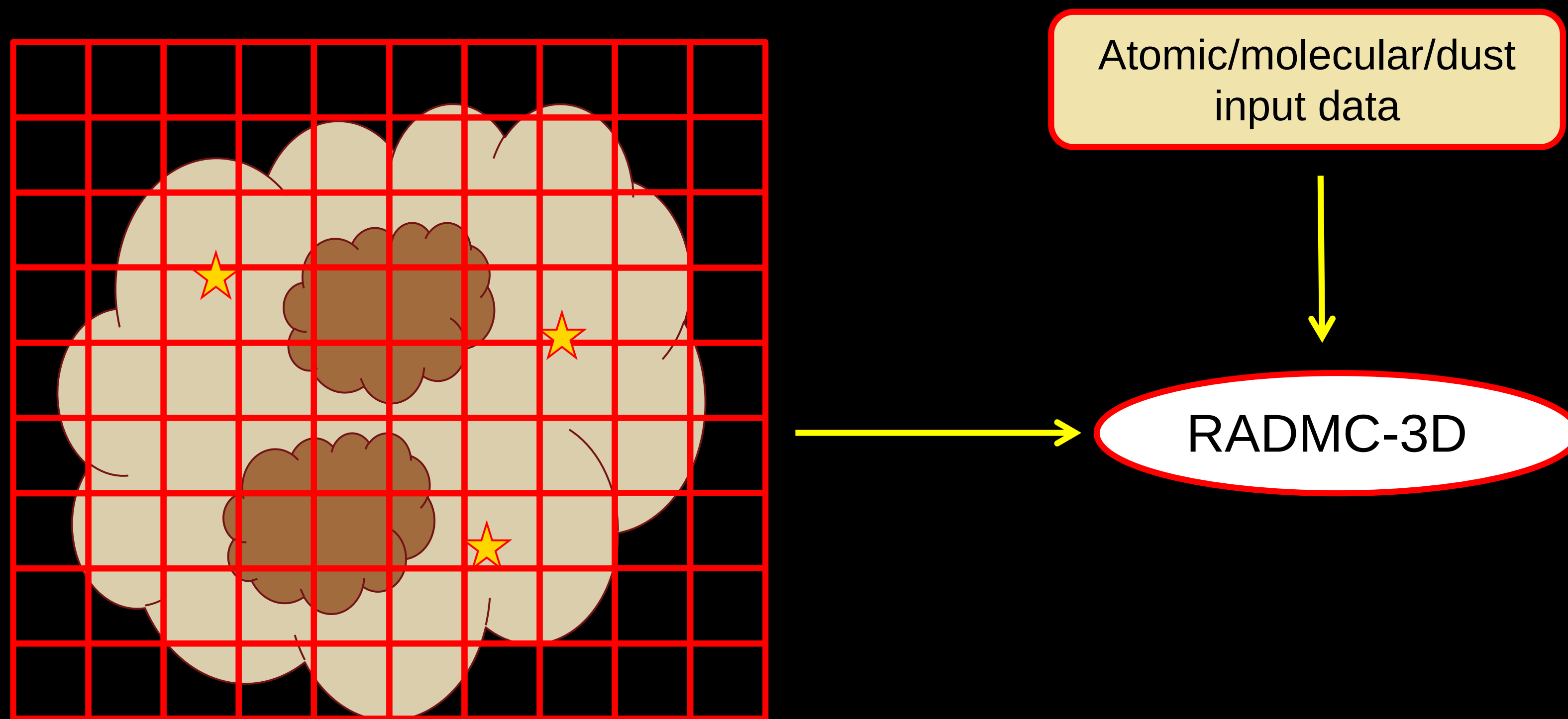
← nr of dust species (or grain size samples)

← dust density in g/cm^3 in each cell (x-direction is inner loop)

Pass these numbers to RADMC-3D...

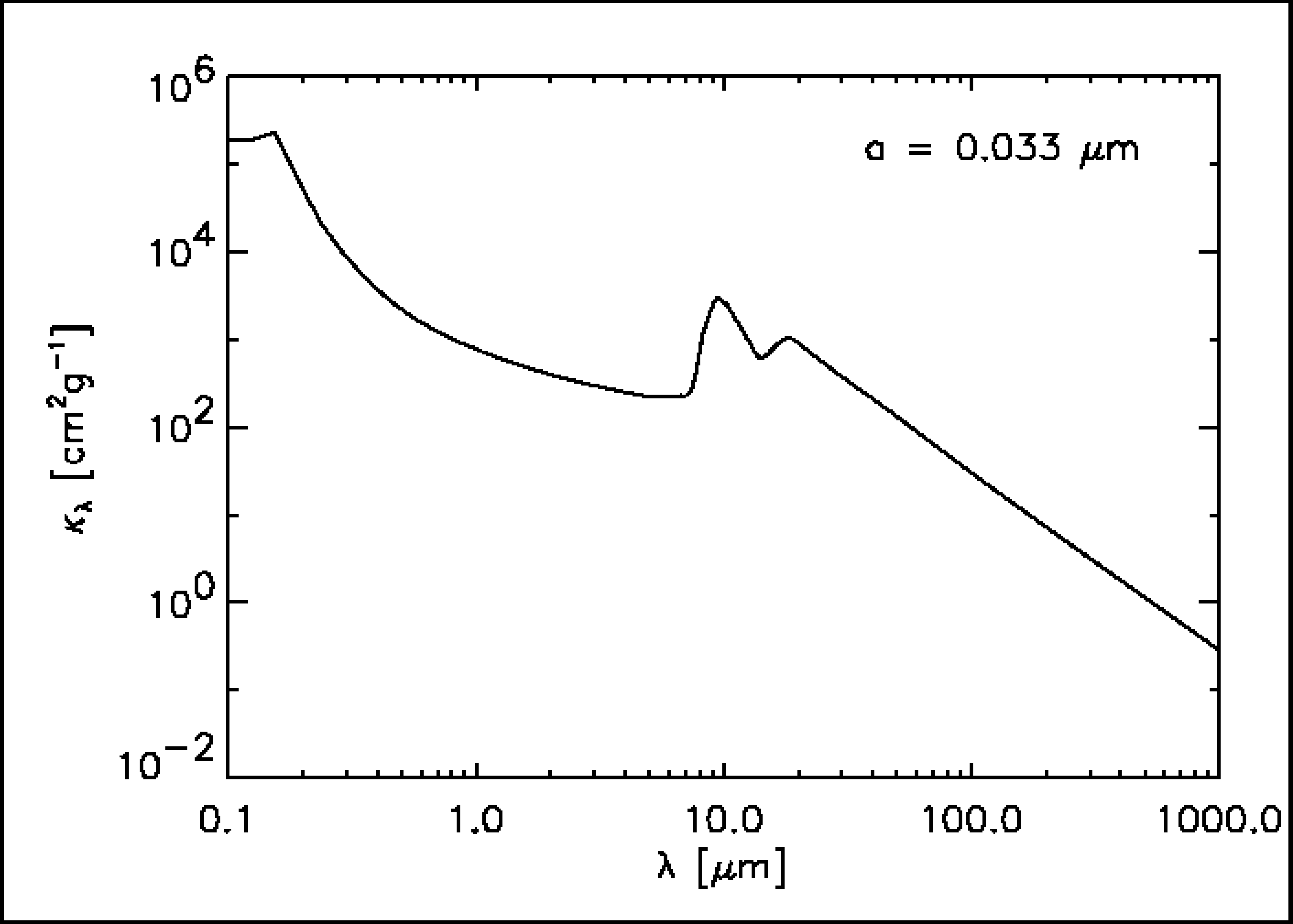


Also give RADMC-3D physical data...



Input: Dust opacity

Opacity of amorphous silicate



Input: Dust opacity

Opacity of amorphous silicate: File = dustkappa_silicate.inp

```
           2          ← format number (just keep it at 2)
         400          ← nr of wavelength sampling points
 Wavel [micron]    kappa_abs [cm^2/g]  kappa_scat [cm^2/g]
 0.102927E+00  0.108810E+05  0.277522E+05
 0.105940E+00  0.114659E+05  0.286342E+05
 0.109041E+00  0.120737E+05  0.295038E+05
 0.112233E+00  0.127084E+05  0.303582E+05
 0.115519E+00  0.133746E+05  0.311906E+05
 0.118901E+00  0.140758E+05  0.319903E+05
 0.122381E+00  0.148124E+05  0.327439E+05
 0.125964E+00  0.155804E+05  0.334388E+05
 0.129652E+00  0.163725E+05  0.340652E+05
 0.133447E+00  0.171797E+05  0.346178E+05
 0.137354E+00  0.179938E+05  0.350955E+05
 0.141375E+00  0.188093E+05  0.354996E+05
 0.145514E+00  0.196246E+05  0.358319E+05
 0.149774E+00  0.204421E+05  0.360928E+05
 0.154158E+00  0.212660E+05  0.362802E+05
 0.158671E+00  0.221011E+05  0.363901E+05
 0.163316E+00  0.229507E+05  0.364170E+05
 0.168097E+00  0.238149E+05  0.363553E+05
 0.173018E+00  0.246899E+05  0.362002E+05
 0.178083E+00  0.255677E+05  0.359493E+05
dustkappa_silicate.inp
```

Input: Line data

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

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

Input: Line data

- Example: LAMDA file: molecule_co.inp

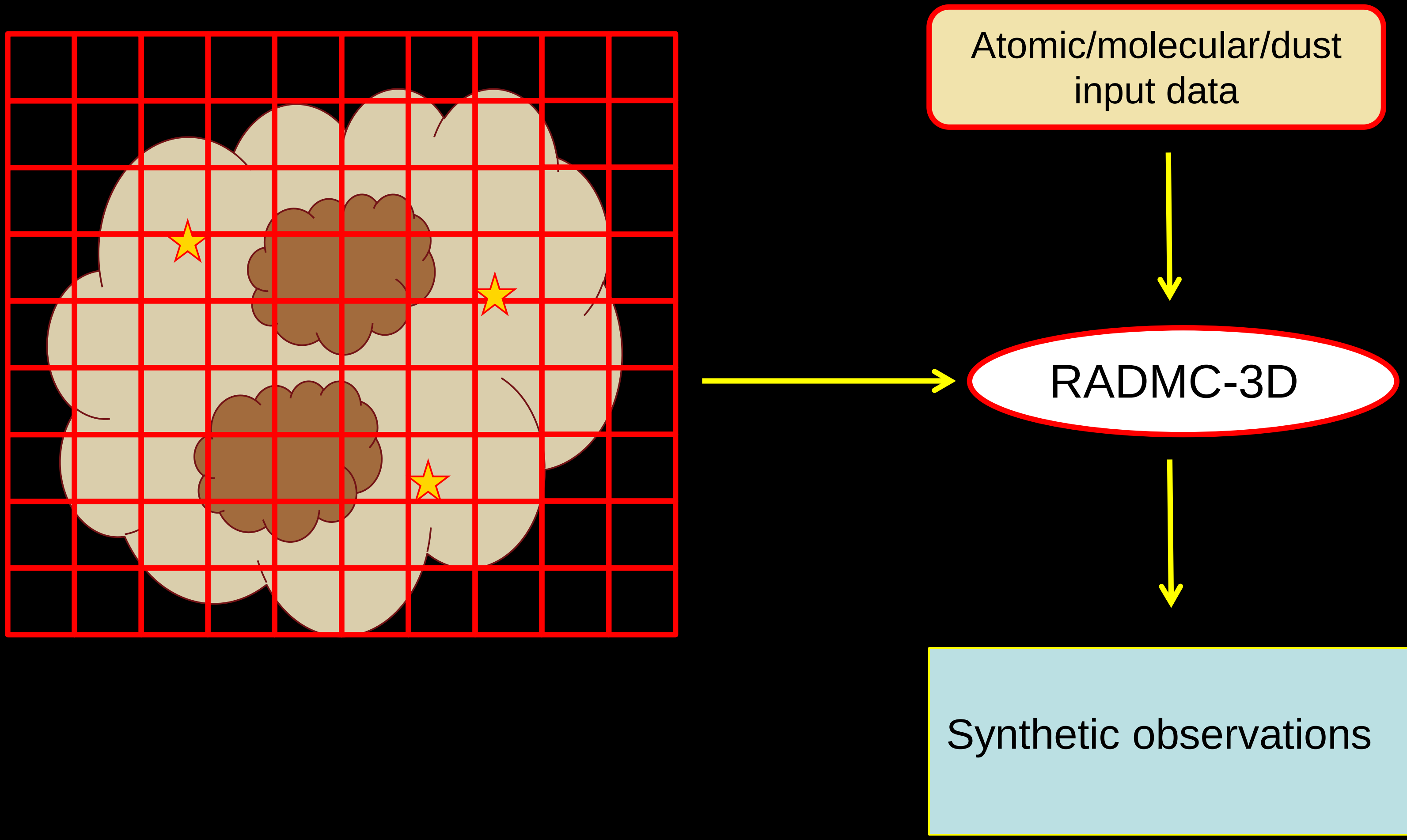
```
!MOLECULE
CO
!MOLECULAR WEIGHT
28.0
!NUMBER OF ENERGY LEVELS
41
!LEVEL + ENERGIES(cm^-1) + WEIGHT + J
    1     0.000000000    1.0      0
    2     3.845033413    3.0      1
    3    11.534919938    5.0      2
    4    23.069512649    7.0      3
    5    38.448164669    9.0      4
    6    57.670329083   11.0      5
    7    80.735459105   13.0      6
    8   107.642407981   15.0      7
    9   138.390328288   17.0      8
   10   172.978074417   19.0      9
   11   211.404098498   21.0     10
   12   253.667154063   23.0     11
   13   299.765594677   25.0     12
   14   349.697573572   27.0     13
```

Input: Line data

- Example: LAMDA file: molecule_co.inp

```
   39  2835.762724236   77.0    38
   40  2984.270676211   79.0    39
   41  3136.509541175   81.0    40
!NUMBER OF RADIATIVE TRANSITIONS
40
!TRANS + UP + LOW + EINSTEINA(s^-1) + FREQ(GHz) + E_u(K)
    1     2     1   7.203e-08     115.2712018       5.53
    2     3     2   6.910e-07     230.5380000      16.60
    3     4     3   2.497e-06     345.7959899      33.19
    4     5     4   6.126e-06     461.0407682      55.32
    5     6     5   1.221e-05     576.2679305      82.97
    6     7     6   2.137e-05     691.4730763     116.16
    7     8     7   3.422e-05     806.6518060     154.87
    8     9     8   5.134e-05     921.7997000     199.11
    9    10     9   7.330e-05    1036.9123930     248.88
   10    11    10   1.006e-04    1151.9854520     304.16
   11    12    11   1.339e-04    1267.0144860     364.97
   12    13    12   1.735e-04    1381.9951050     431.29
   13    14    13   2.200e-04    1496.9229090     503.13
   14    15    14   2.739e-04    1611.7935180     580.49
   15    16    15   3.354e-04    1726.6025057     663.35
   16    17    16   4.050e-04    1841.3455060     751.72
```

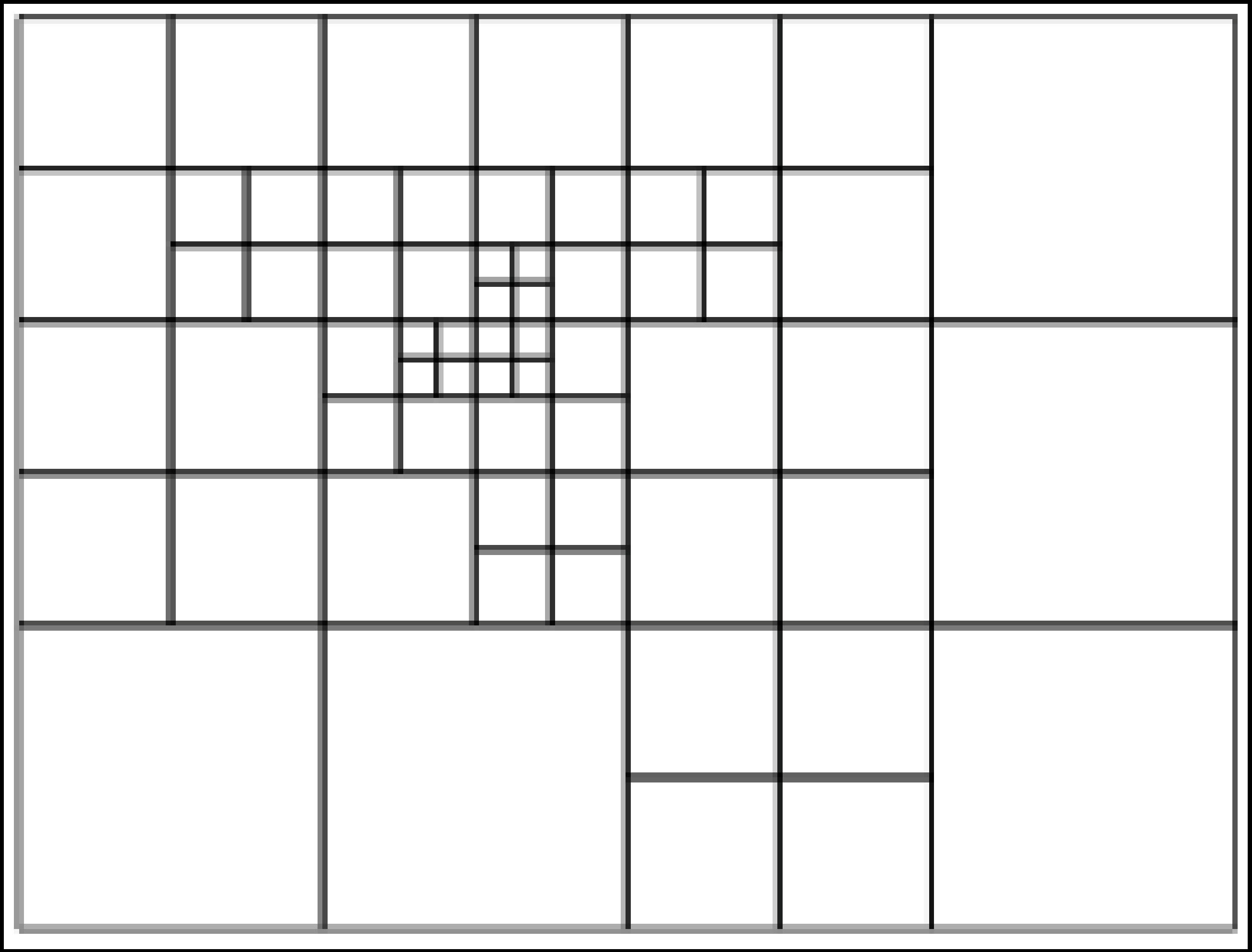
Now it can produce synthetic observations...



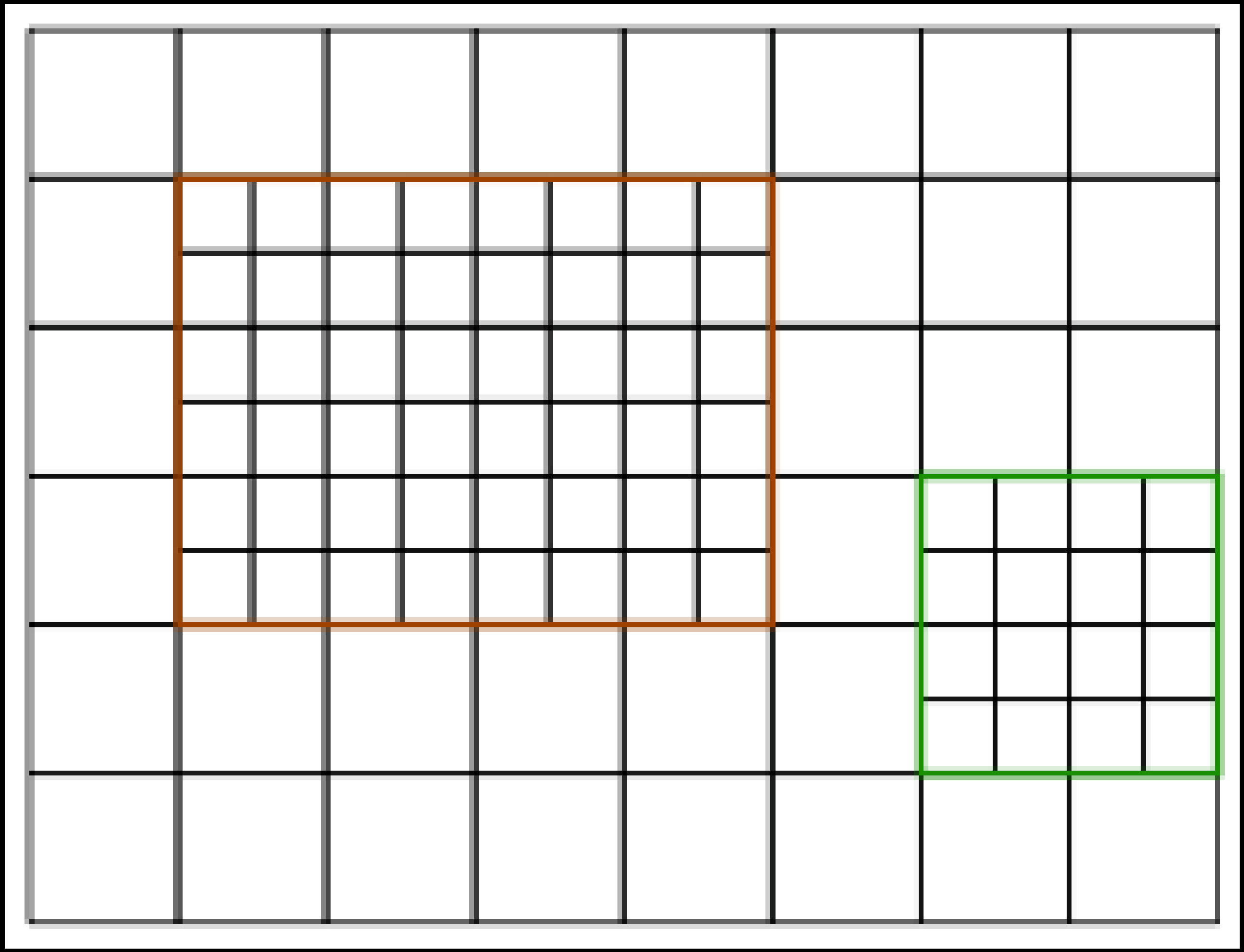
Example observation: image.out

```
          1                              ← format number
        100            100               ← number of pixels in x and y direction in image
          1                              ← number of wavelengths
  1496000000000.0000         1496000000000.0000          ← pixel size in x and y direction [cm]
0.1000000000000E+02                      ← wavelength(s) in micron

0.85840416641744E-12
0.86120137734098E-12
0.85343711679501E-12
0.84119848246107E-12
0.83704389758274E-12
0.83770141176467E-12
0.84088198540427E-12
0.84745088377258E-12
0.86119210411486E-12                    ← image: intensity I_nu for each pixel 9x-dir is inner loop)
0.87557632864847E-12
0.88284765130151E-12
0.87687874565191E-12
0.87051581423311E-12
0.86998928963052E-12
0.87201905465402E-12
0.86828892598439E-12
0.86329118261484E-12
0.86633272040454E-12
0.87816202433684E-12
0.86690106620810E-12
```

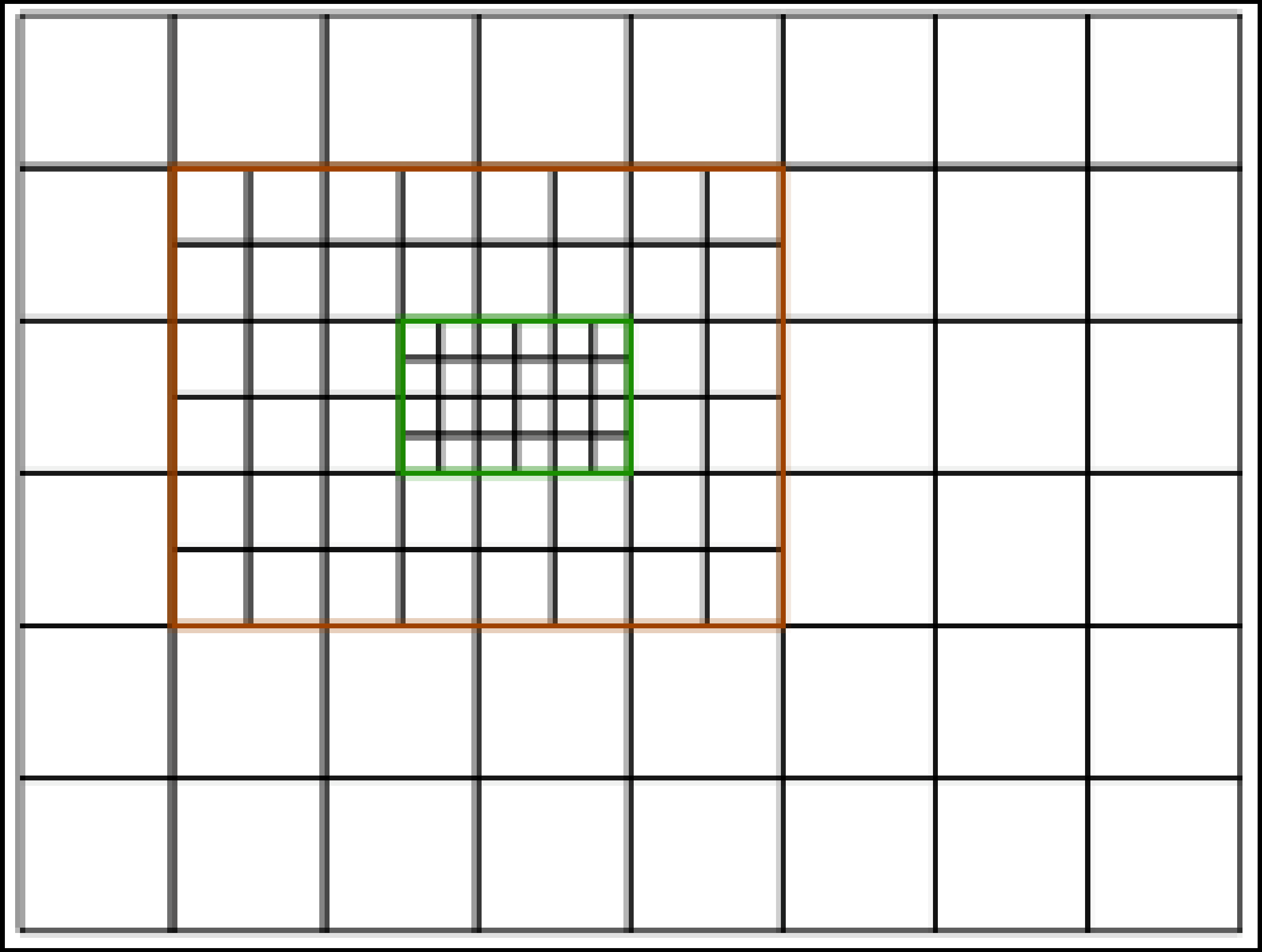
AMR Grid Structure: Oct tree



AMR Grid Structure: Patch-based



AMR: Patch-based, recursive



Coordinates

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

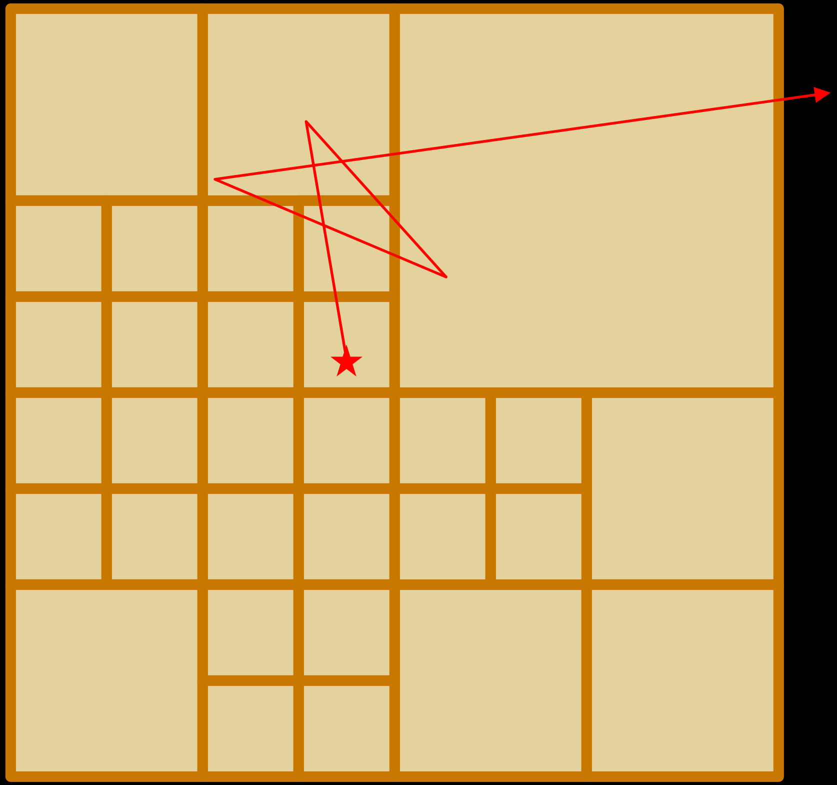
- In all these coordinate systems the AMR is possible.

Interfaces from well-known codes

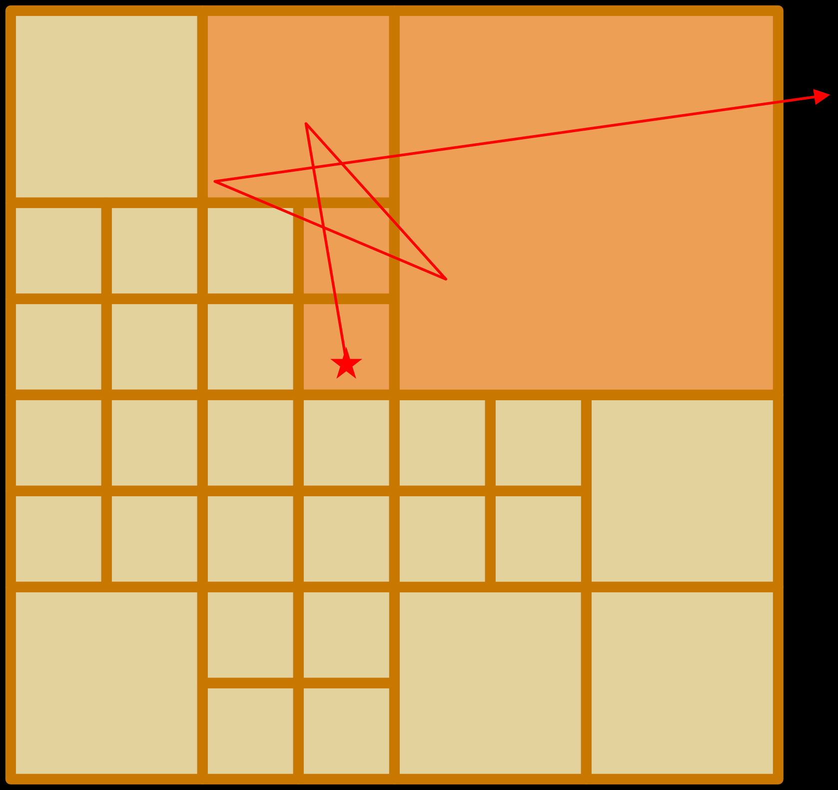
- FLASH
- RAMSES
- PLUTO
- ZEUS

Dust continuum radiative transfer

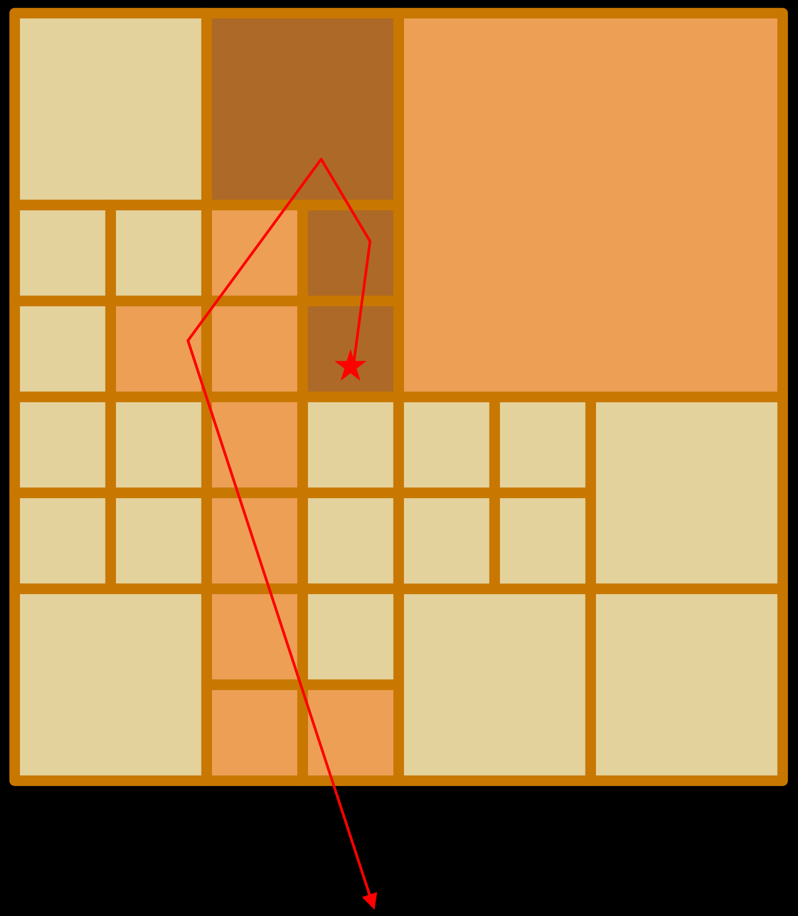
Stage 1: Monte Carlo Dust Temperature



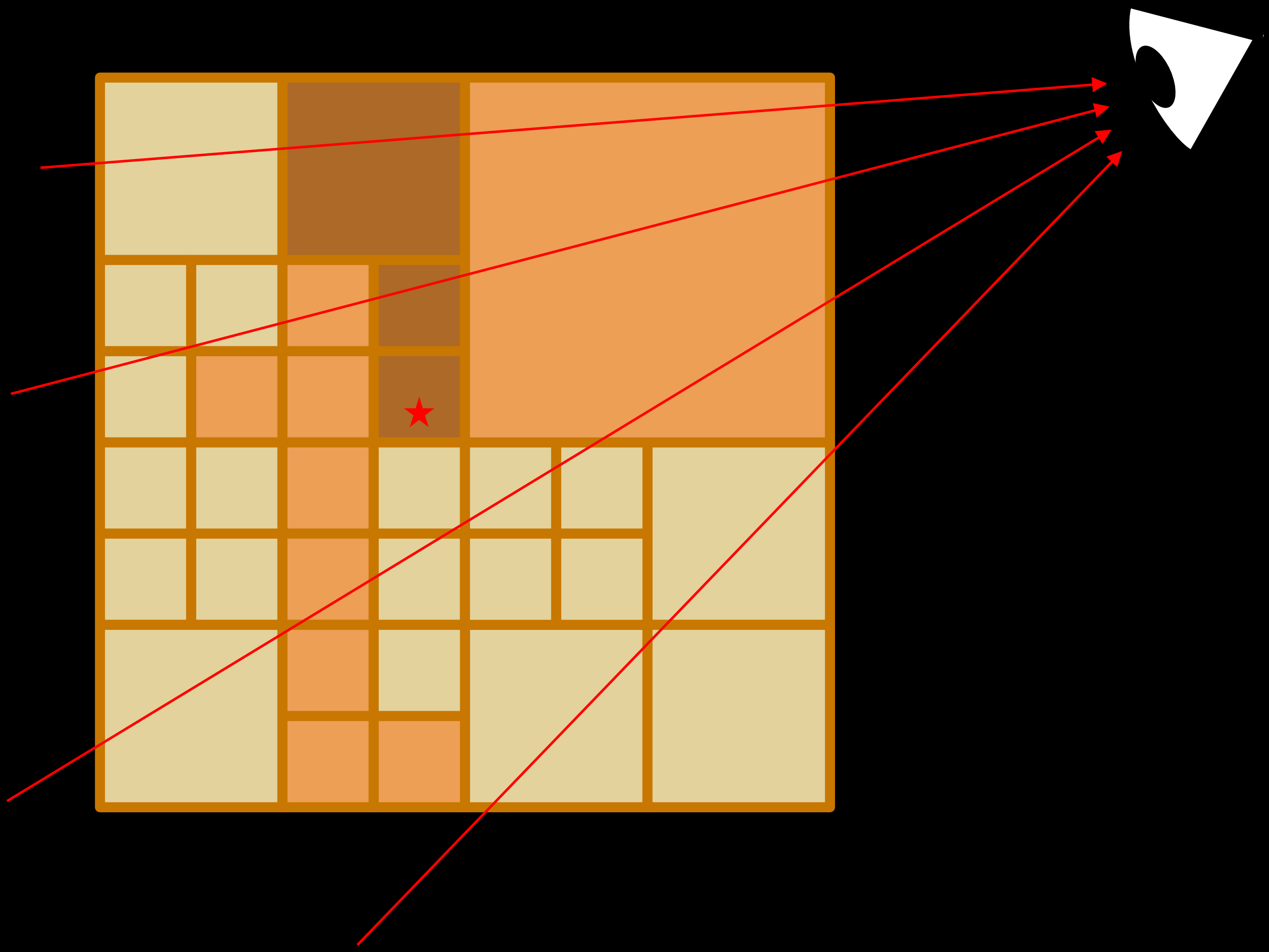
Stage 1: Monte Carlo Dust Temperature



Stage 1: Monte Carlo Dust Temperature

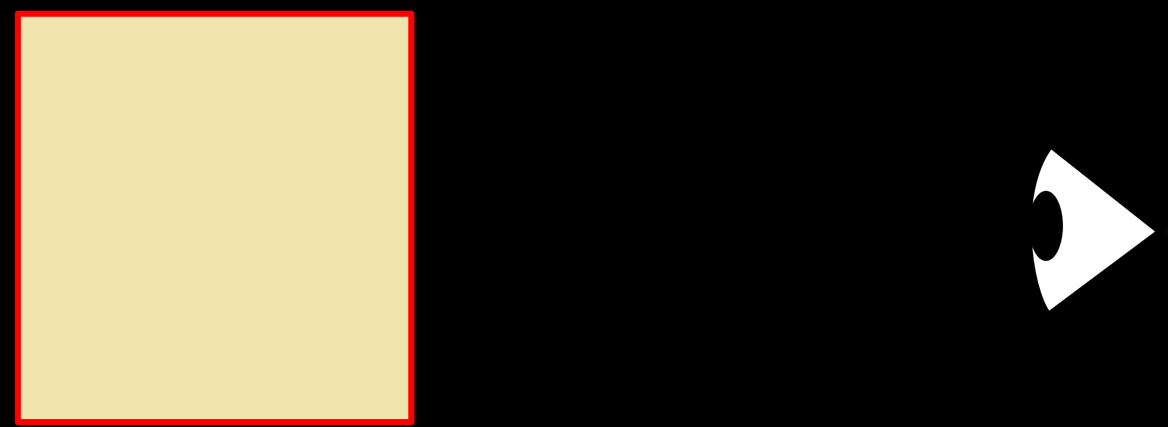


Stage 2: Ray tracing



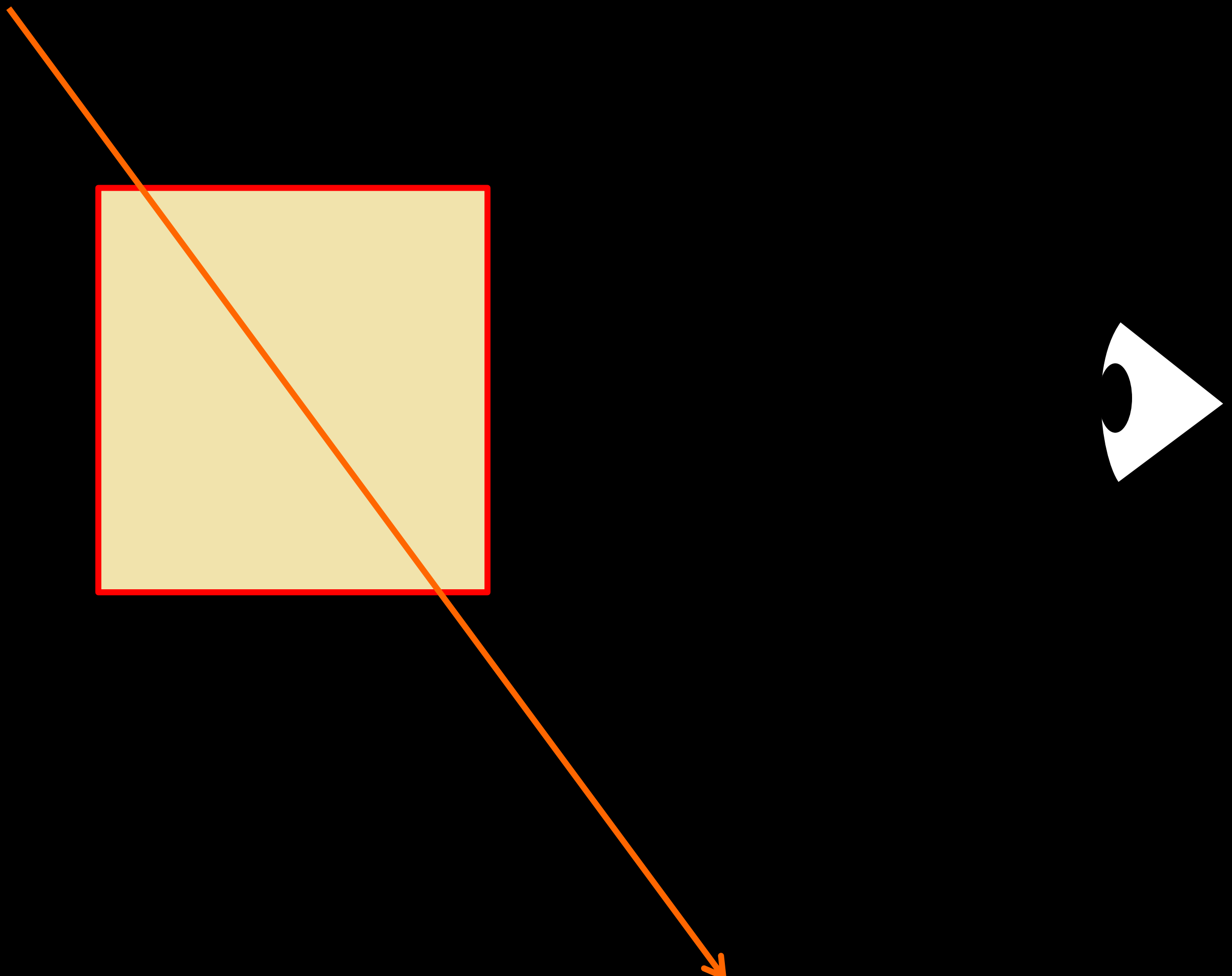
Treatment of scattering off dust grains

Using a scattering source function



Treatment of scattering off dust grains

Using a scattering source function

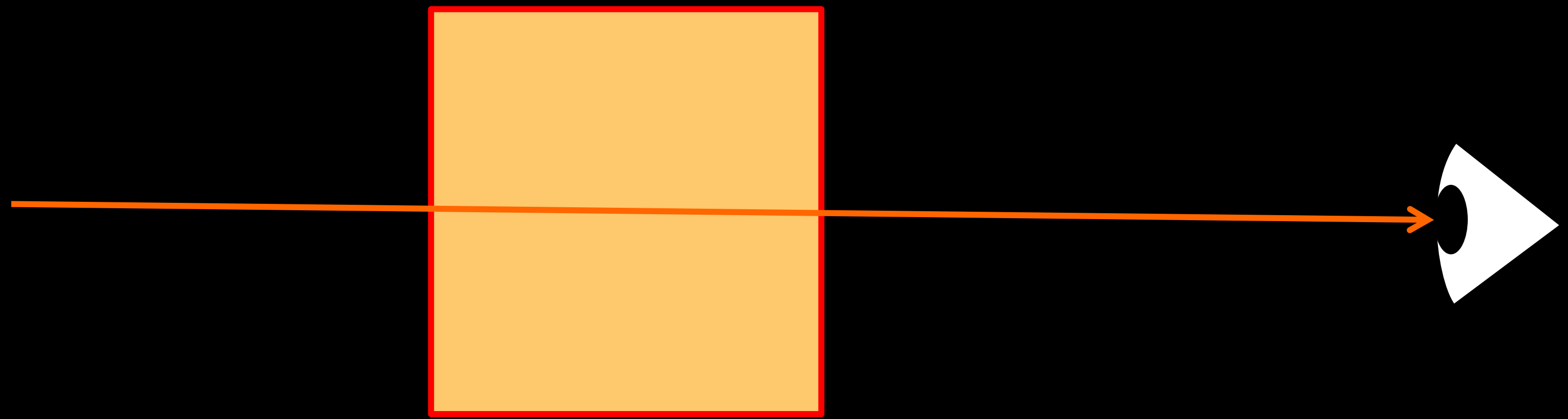


Treatment of scattering off dust grains

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)

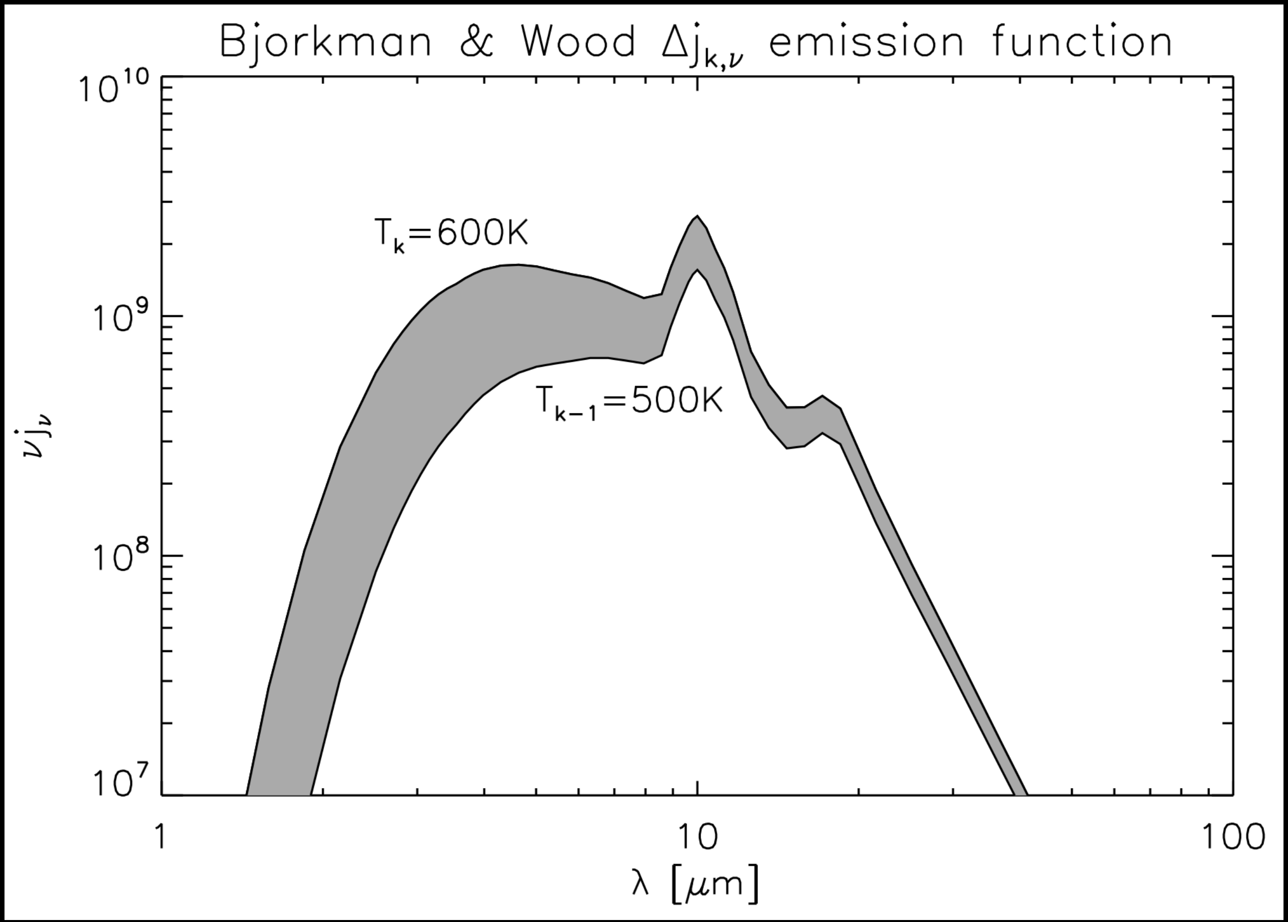
Method = Bjorkman & Wood (2001) algorithm:

- 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

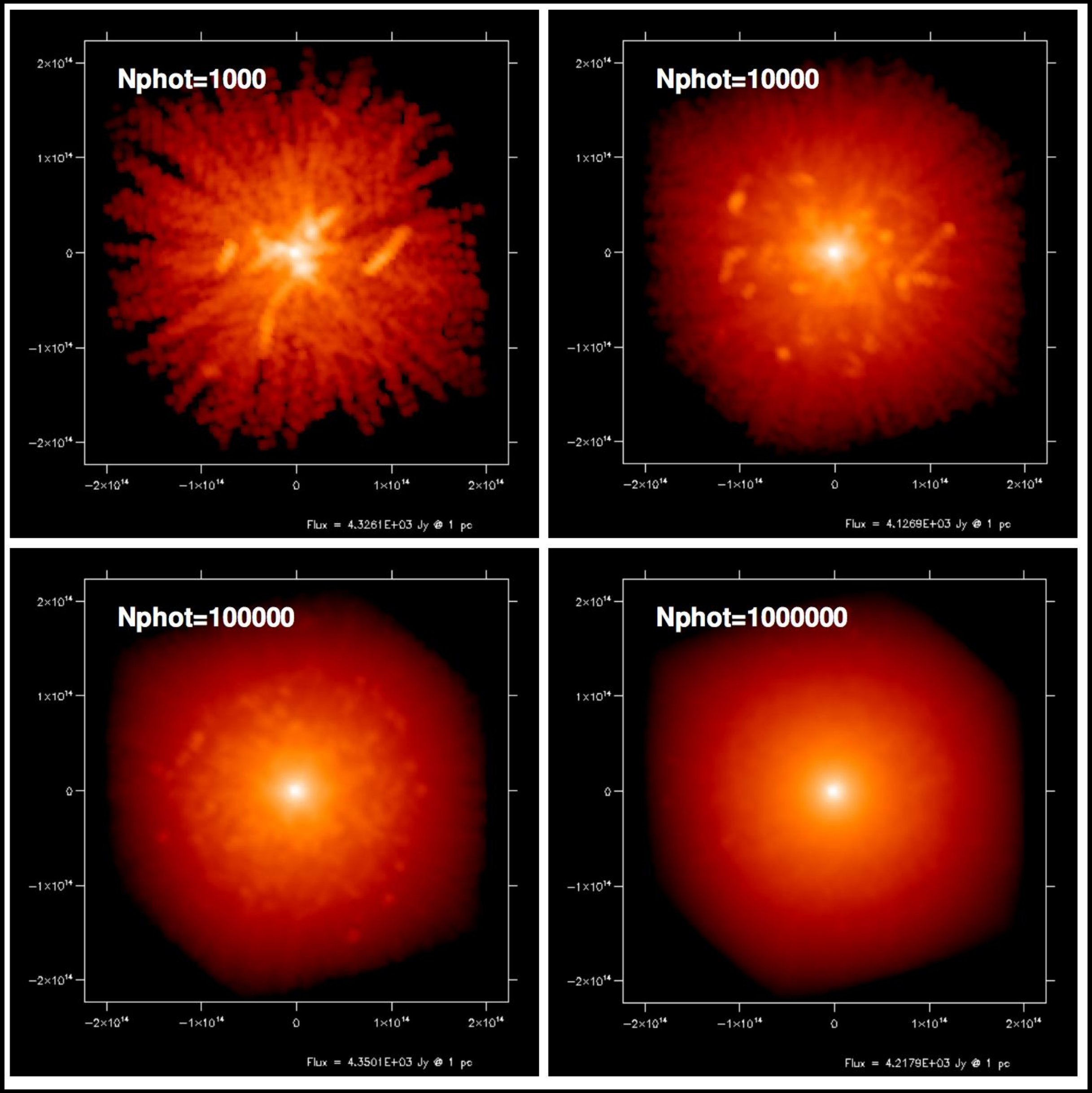
Line radiative transfer

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

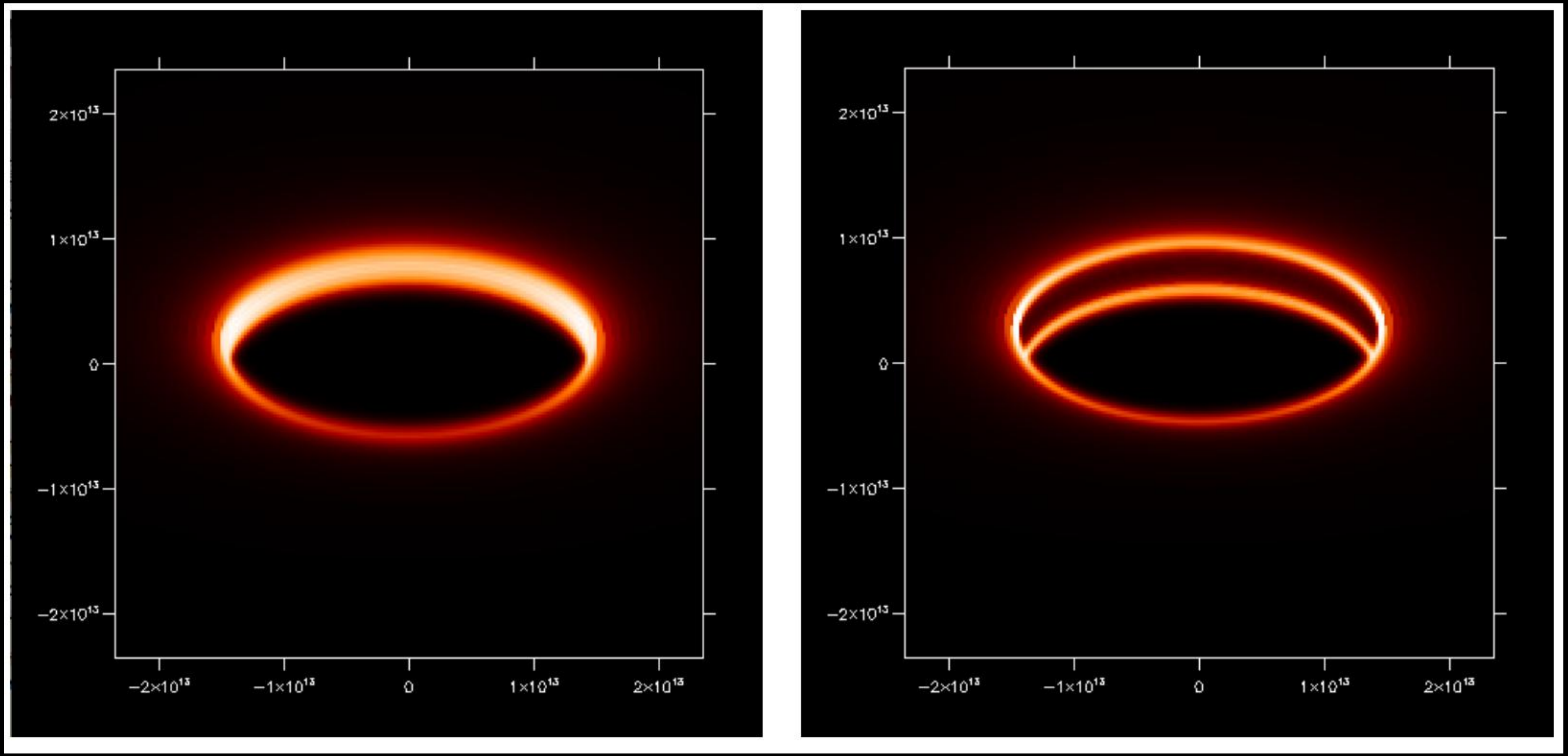
The pitfalls of raytracing...

Too low photon statistics

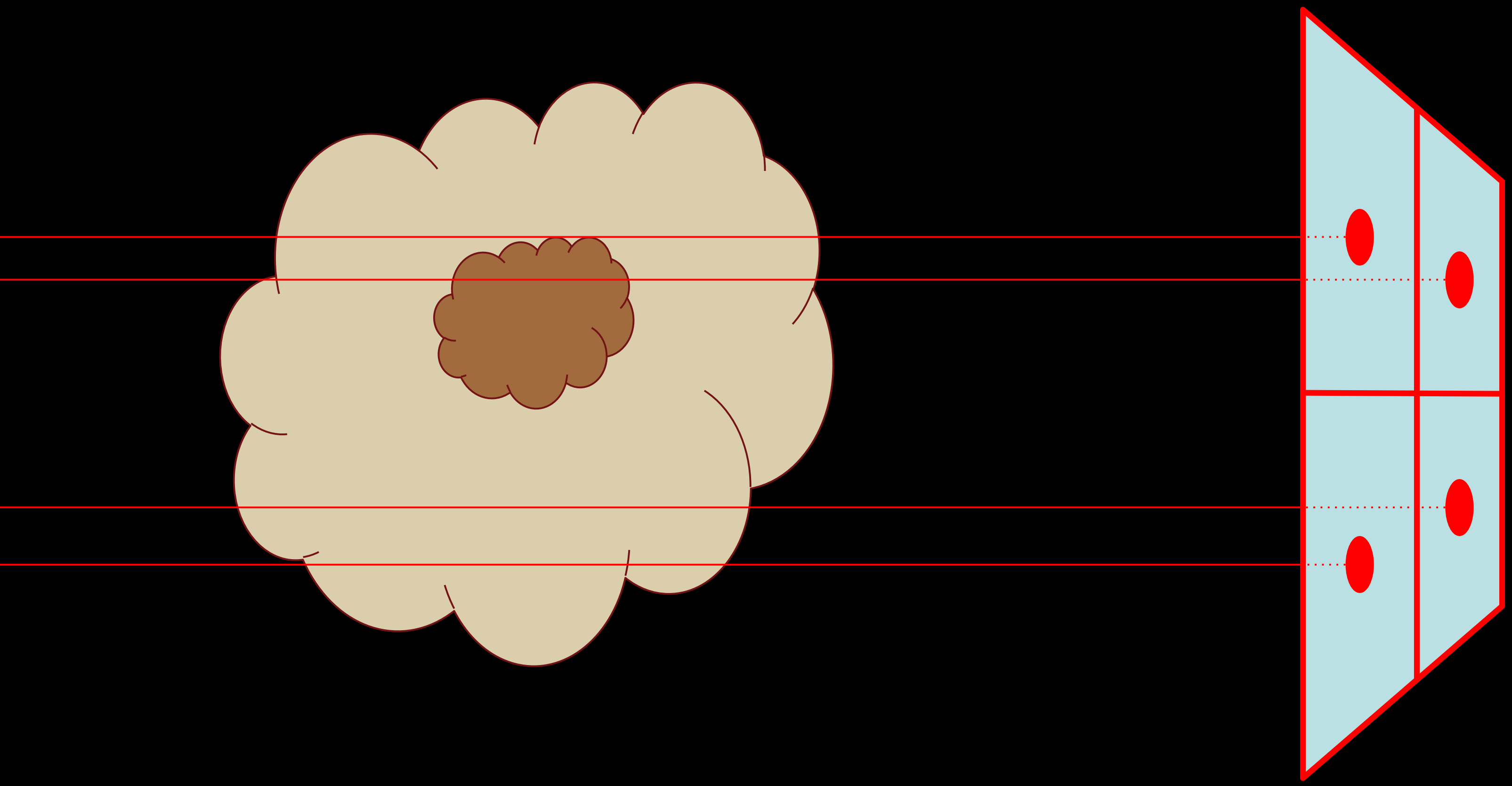


Too low spatial resolution

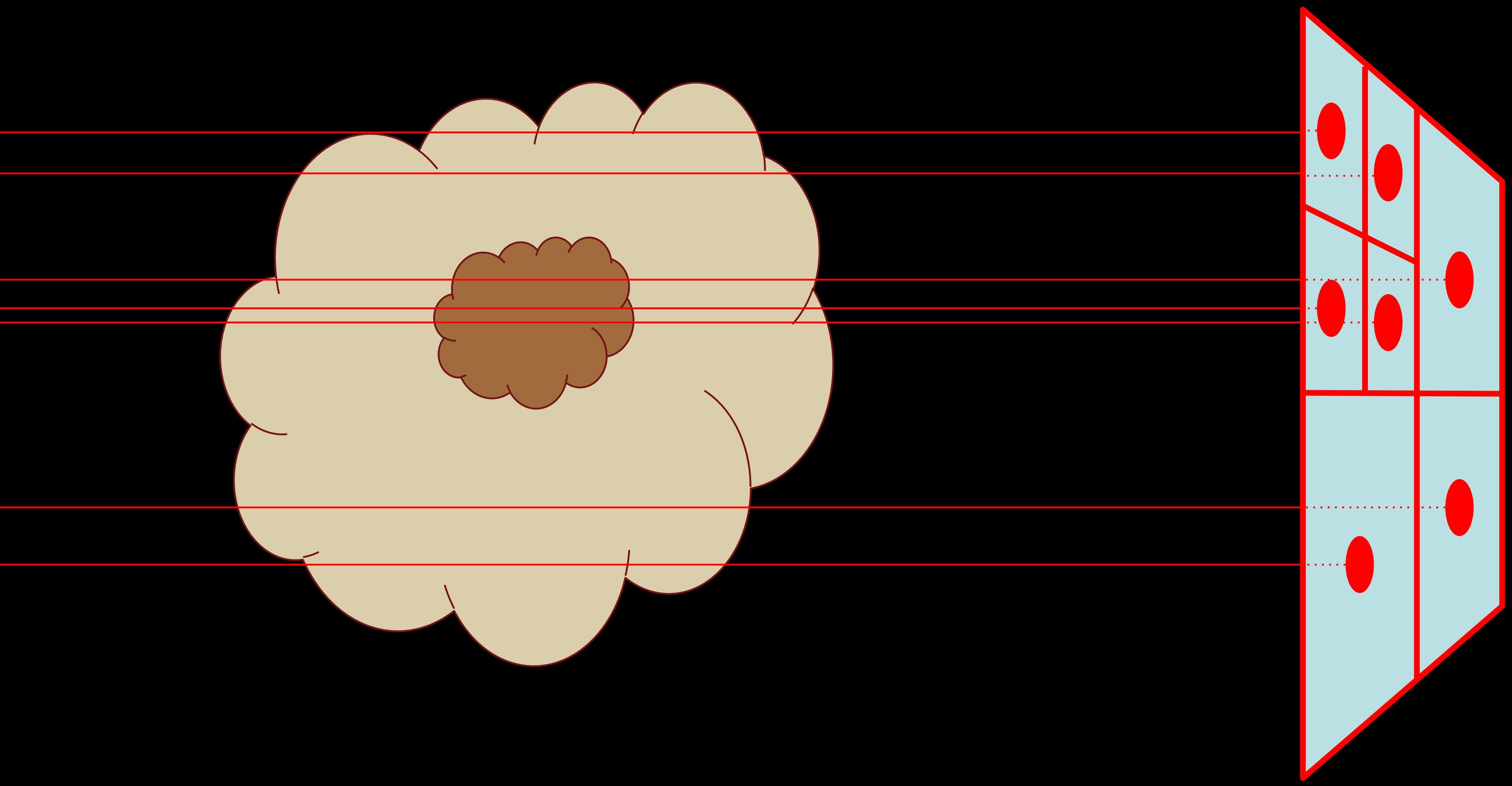
Example: Inner edge of a protoplanetary disk



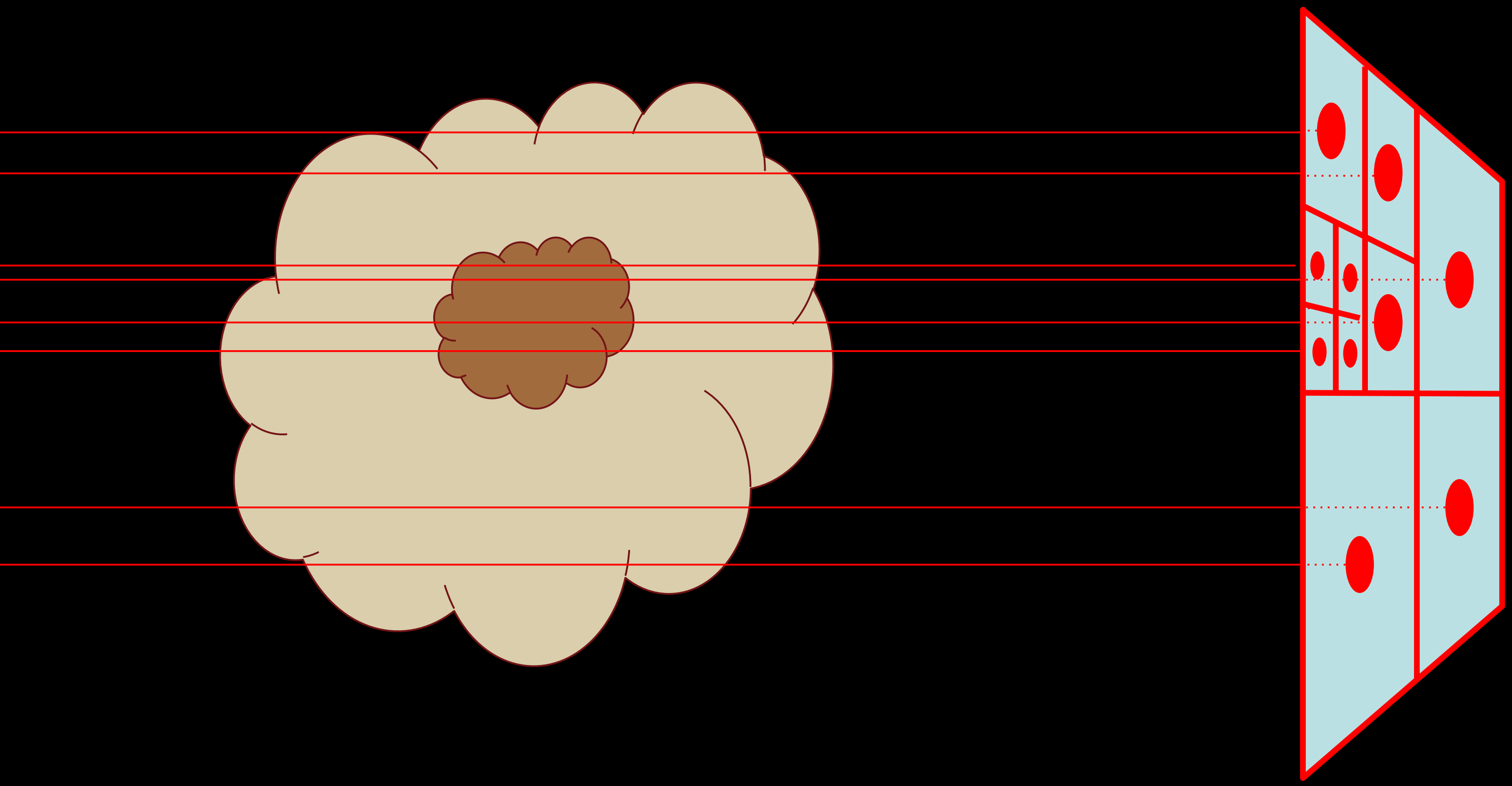
Recursive sub-pixeling of images



Recursive sub-pixeling of images



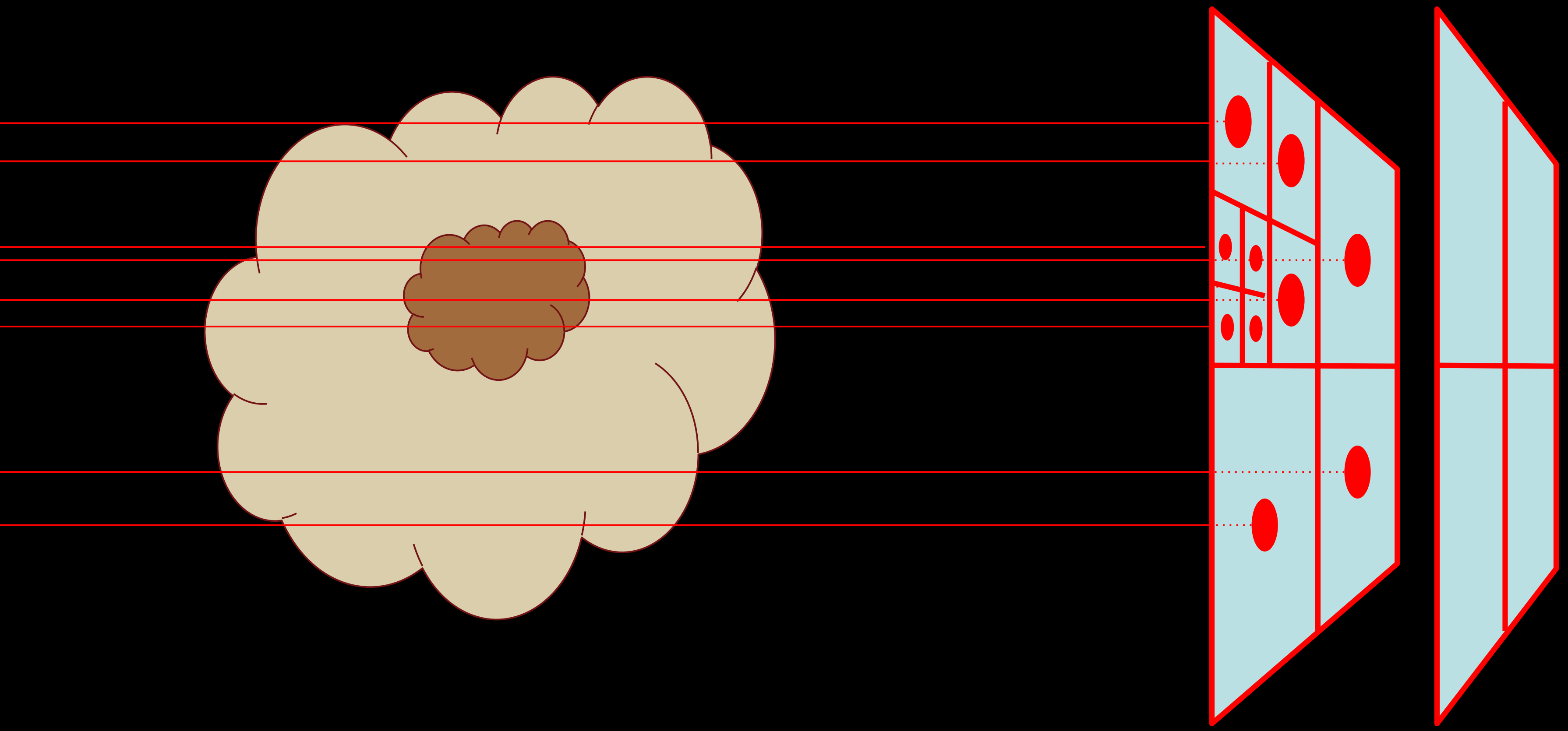
Recursive sub-pixeling of images



Necessary for obtaining the correct flux

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

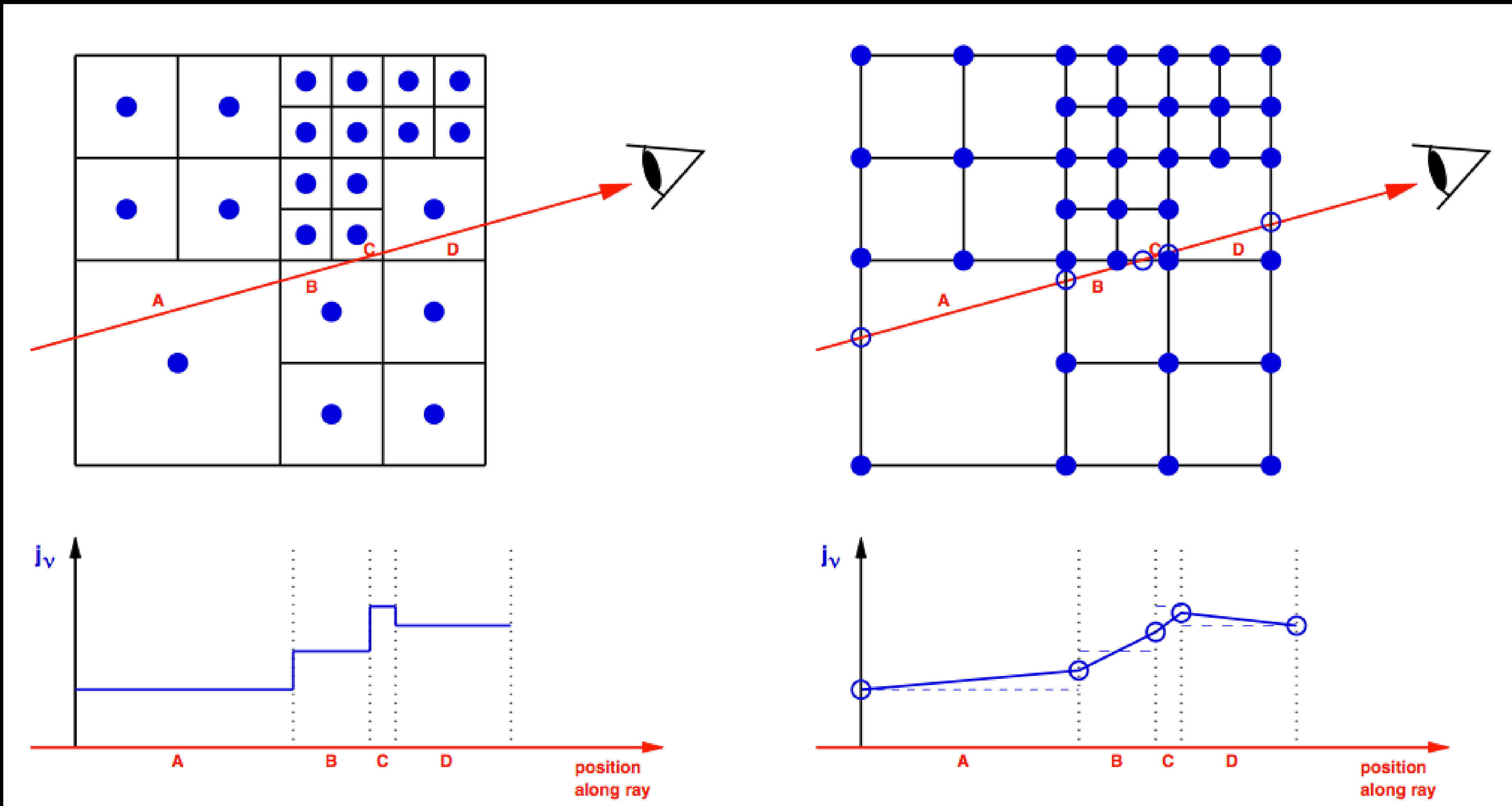
Recursive sub-pixeling of images



Necessary for obtaining the correct flux

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

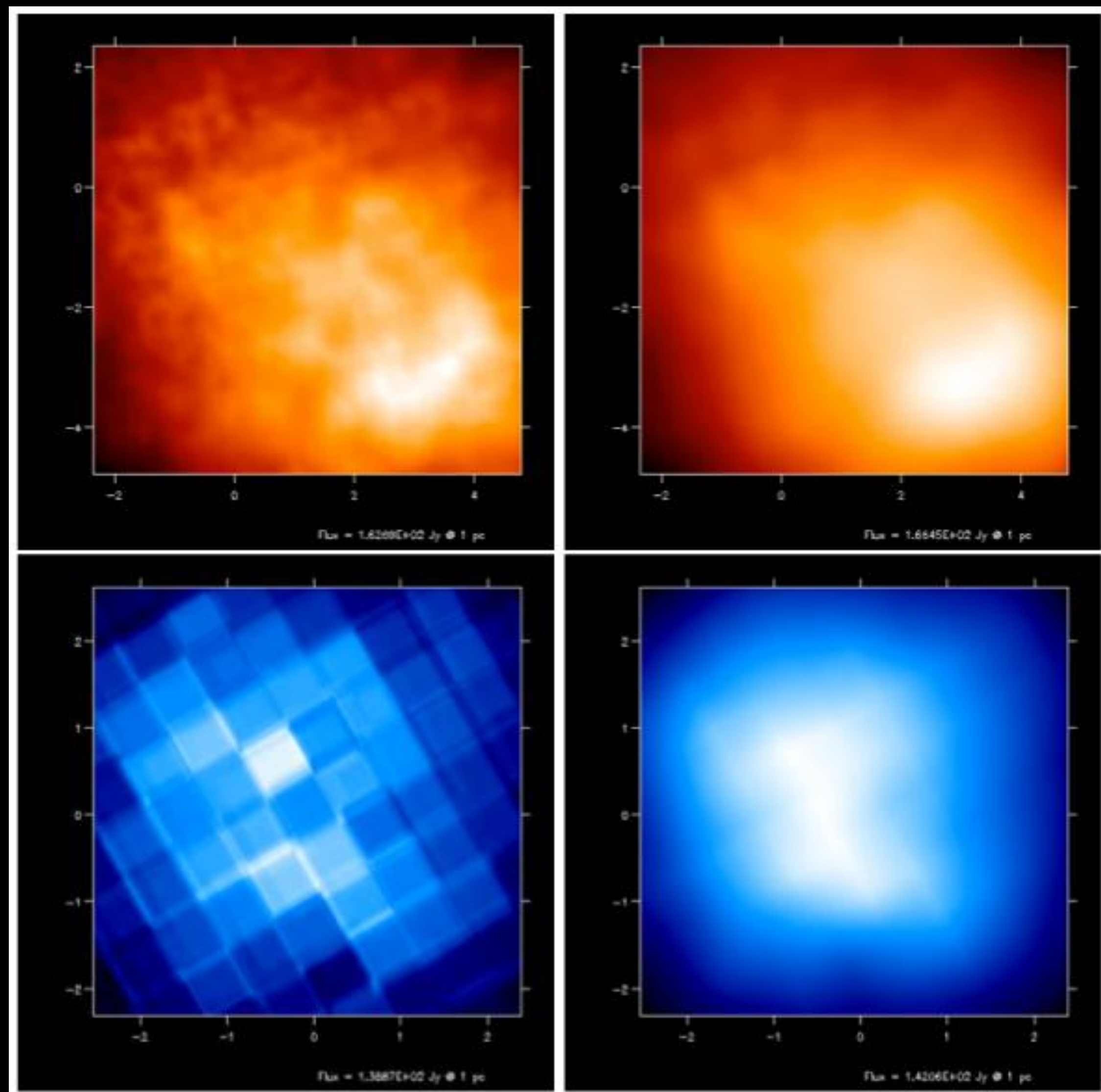
Second order ray-tracing



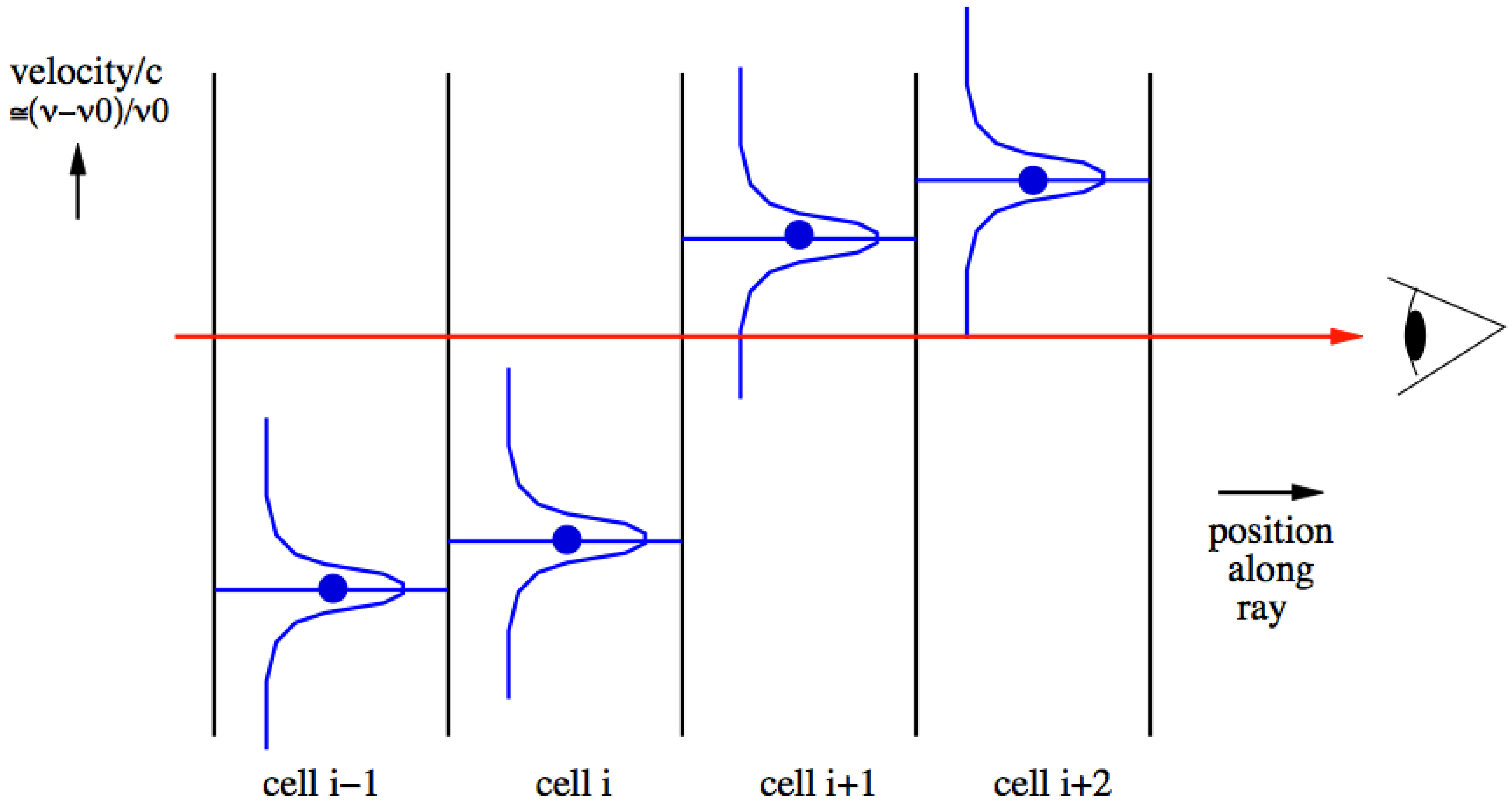
Useful for obtaining smoother images

Second order ray-tracing

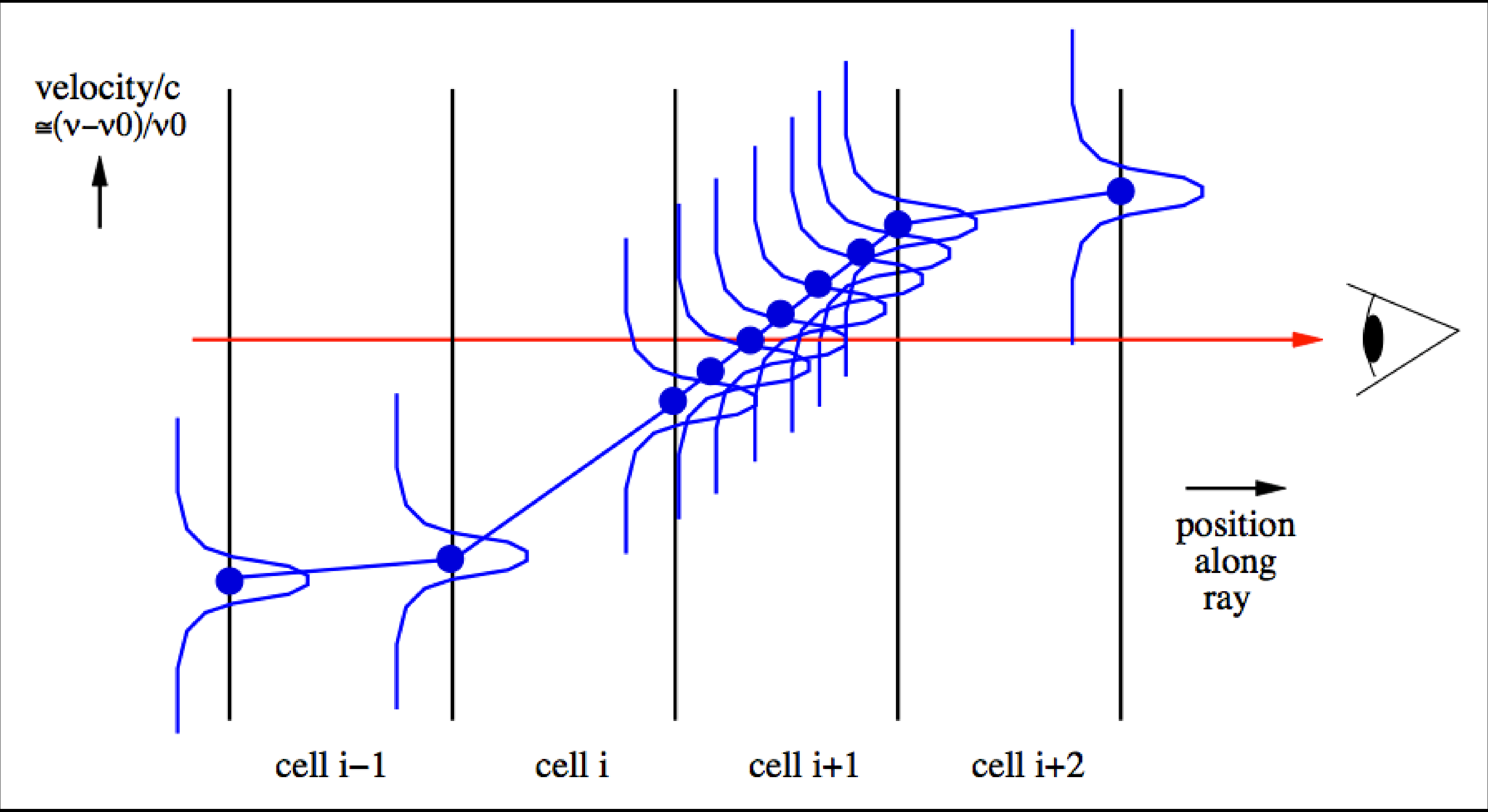
First order integration: Second order integration:



Line transfer: Doppler Catching...



Line transfer: Doppler Catching...



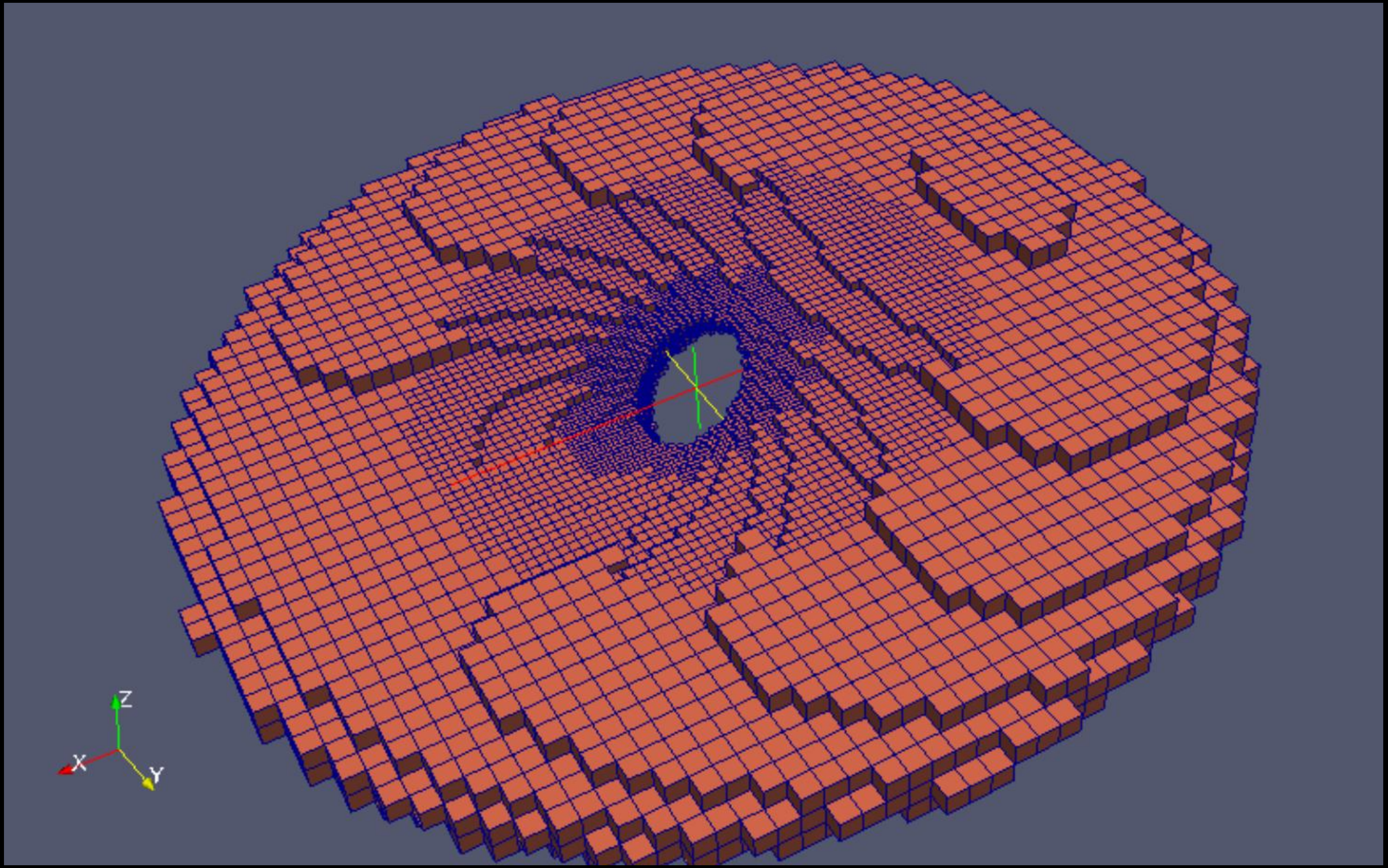
Necessary when there are strong velocity gradients

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.

VTK support

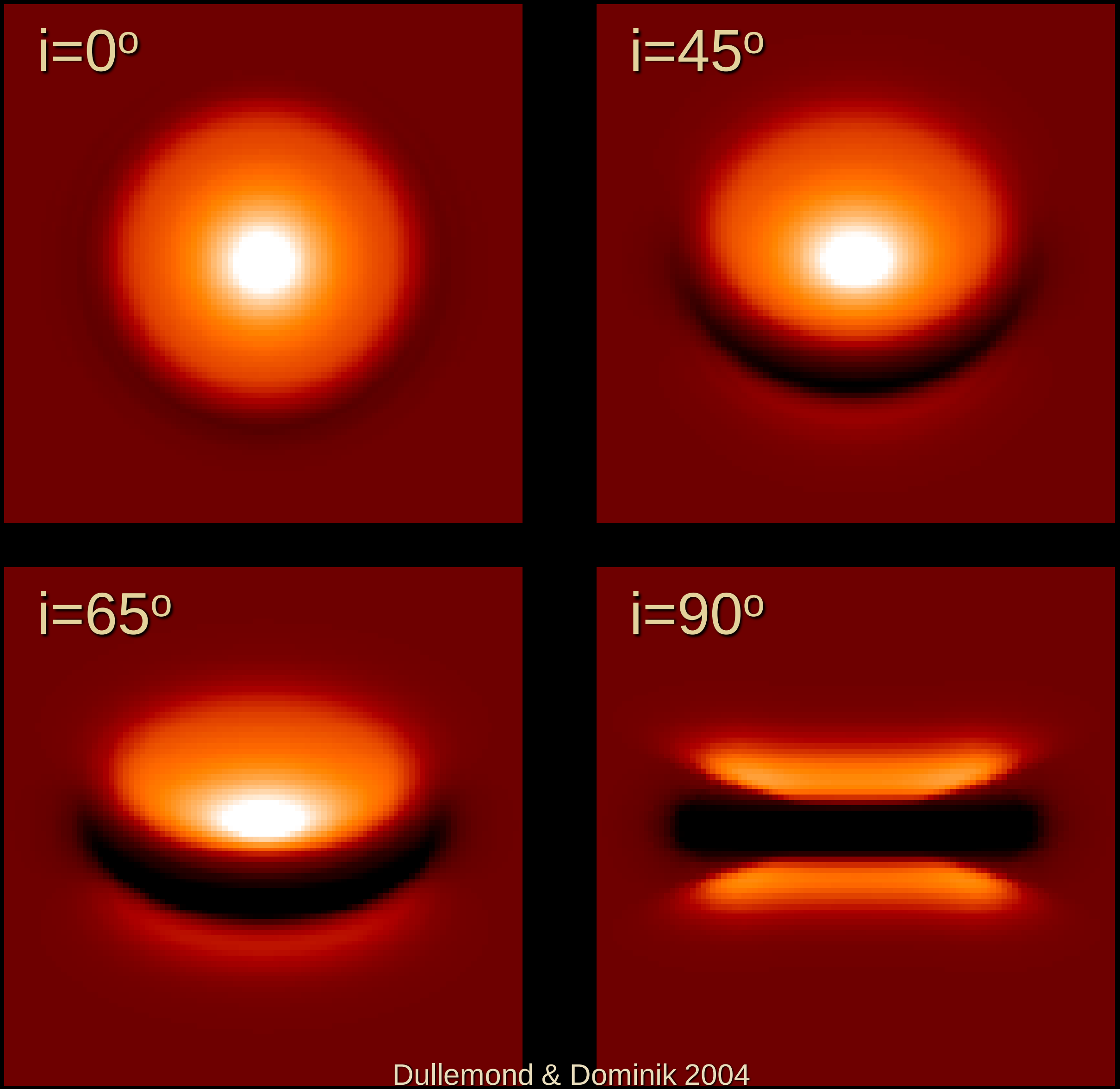


For coupling, e.g., to PARAVIEW

Examples

Example: Protoplanetary Disk

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



Dullemond & Dominik 2004

Example: Protoplanetary Disk

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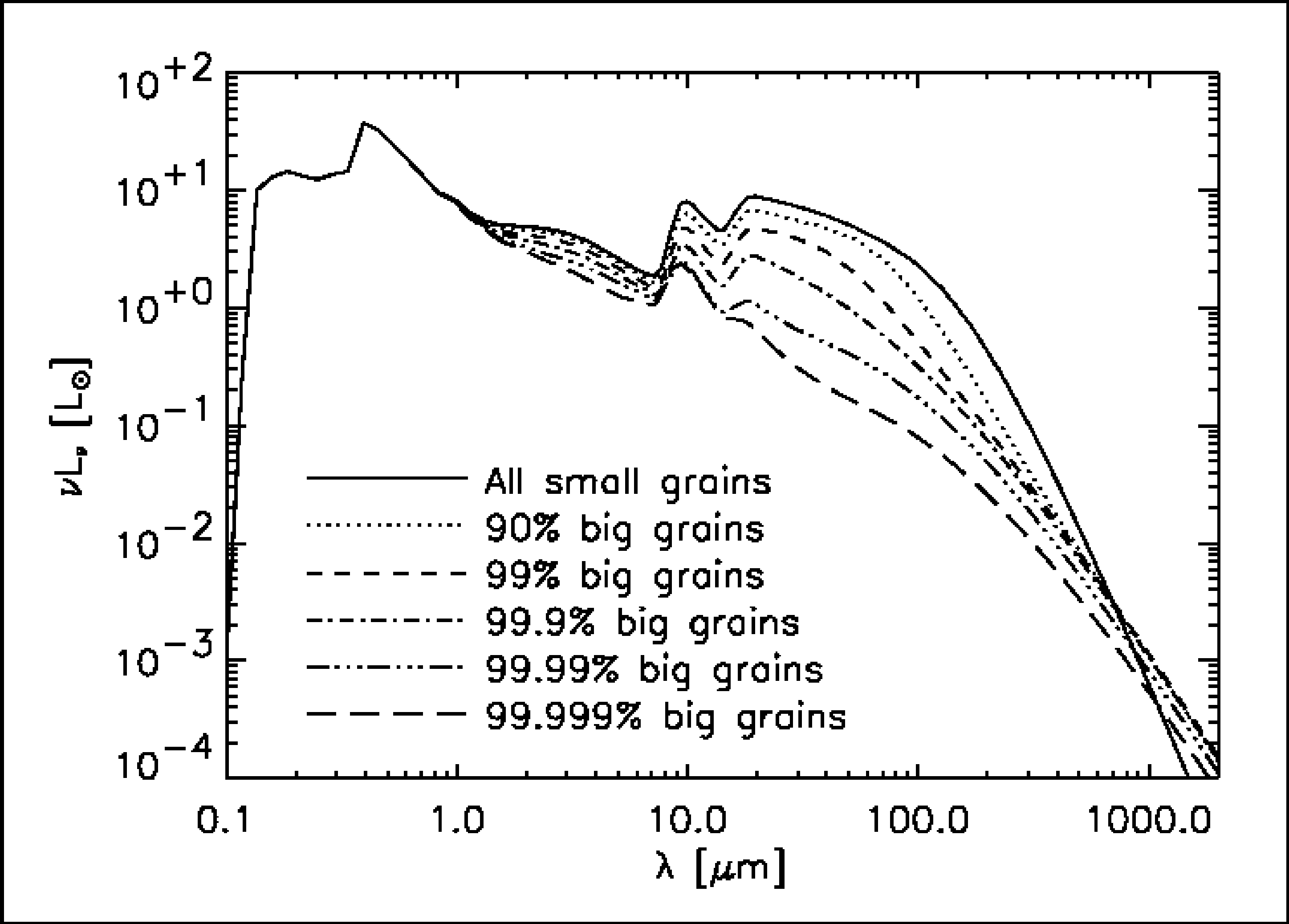

Dullemond & Dominik 2004

Example: Protoplanetary Disk

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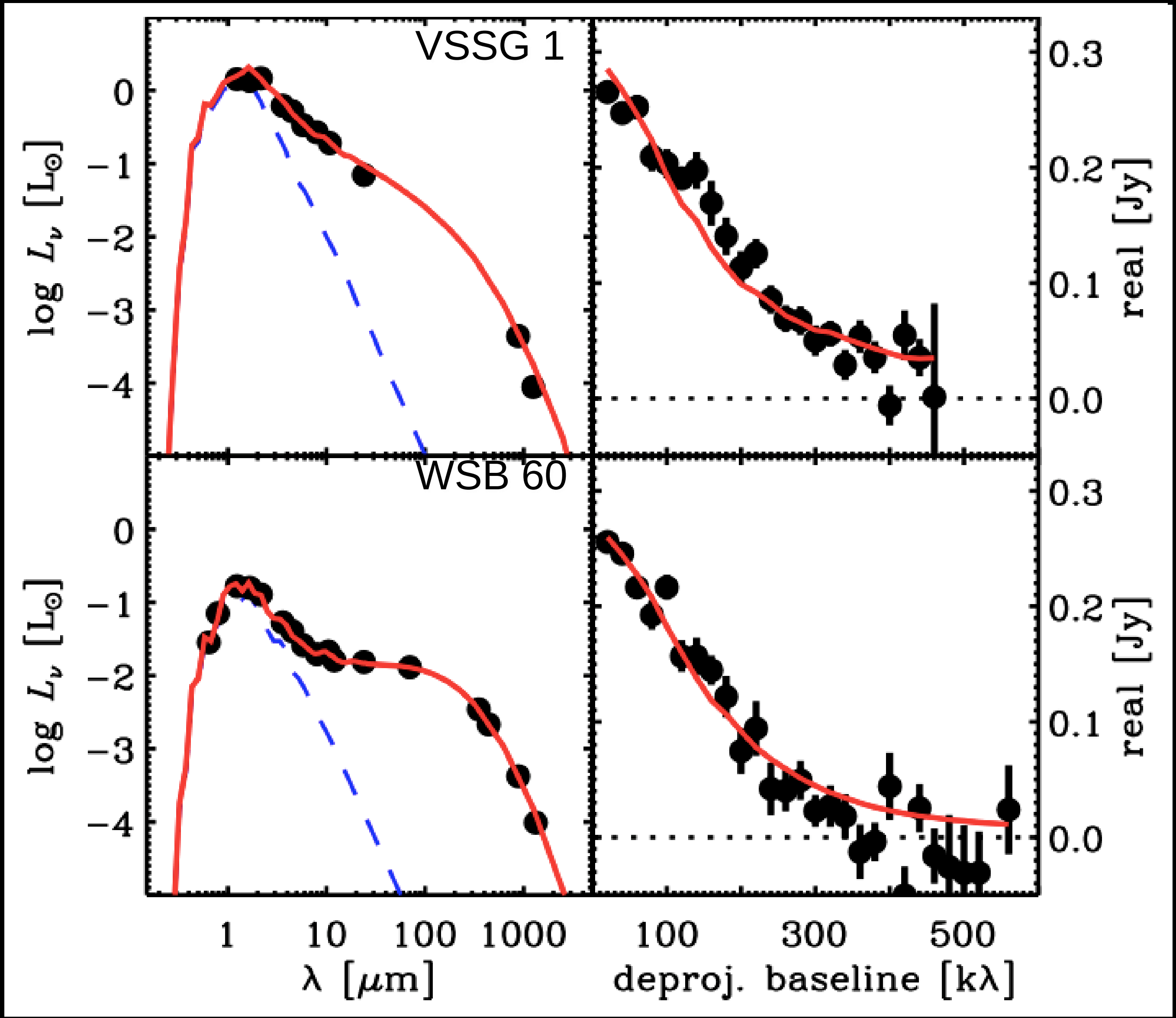
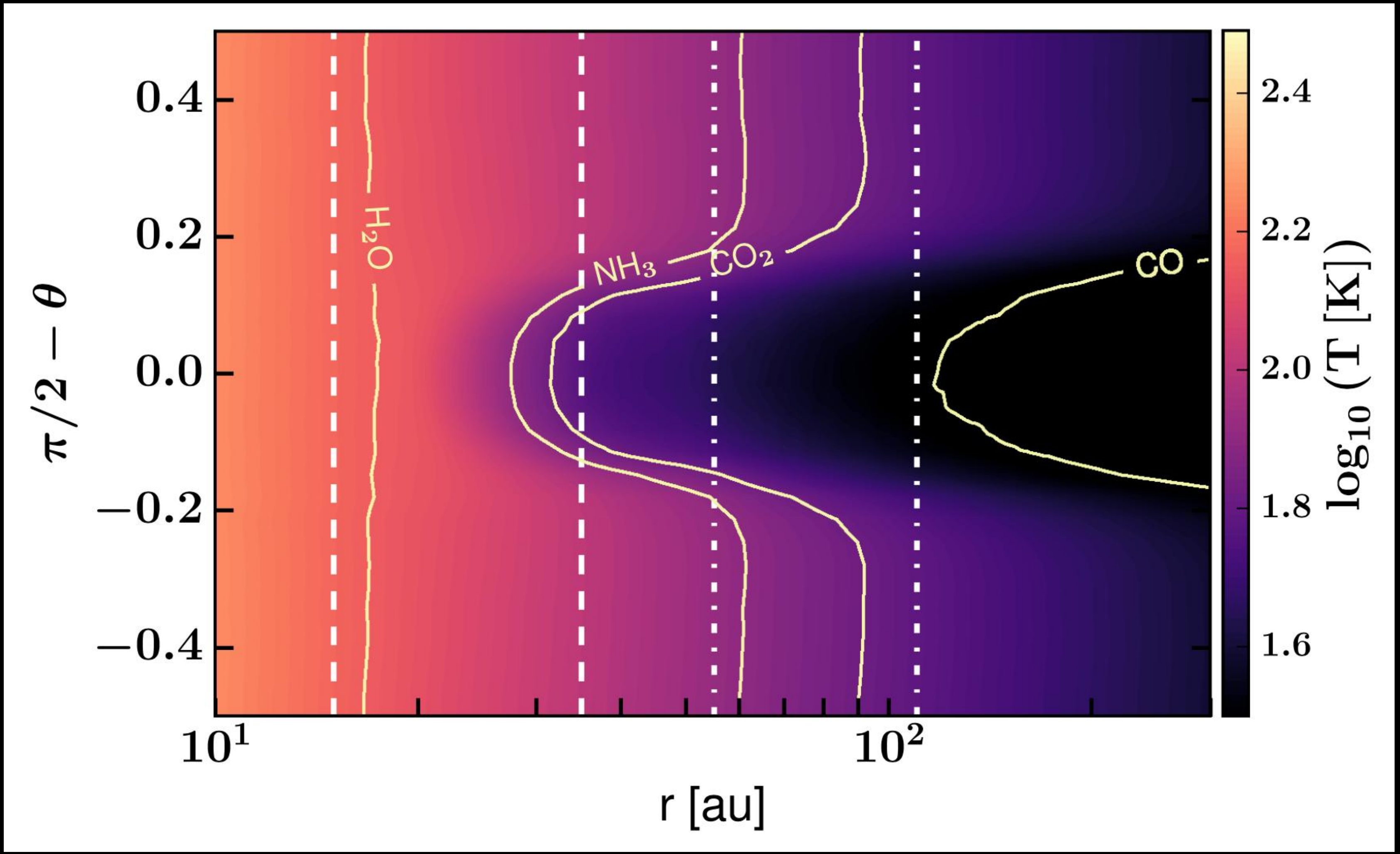


SED + millimeter resolved maps (=visibility values)

Andrews et al. 2009

Example: Protoplanetary Disk

Temperature structure and effect on volatiles

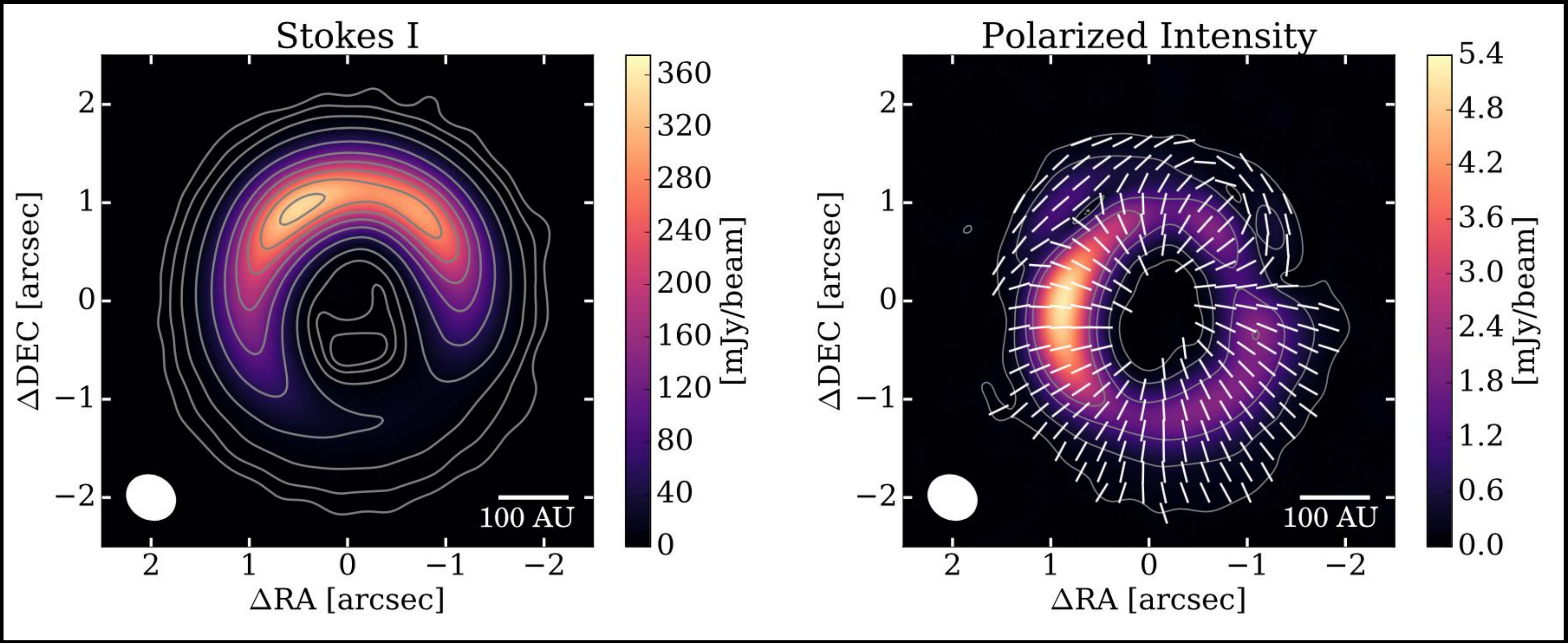


Pohl et al. (2017)

Example: Protoplanetary Disk

Polarized mm-emission by scattering

ALMA Observations

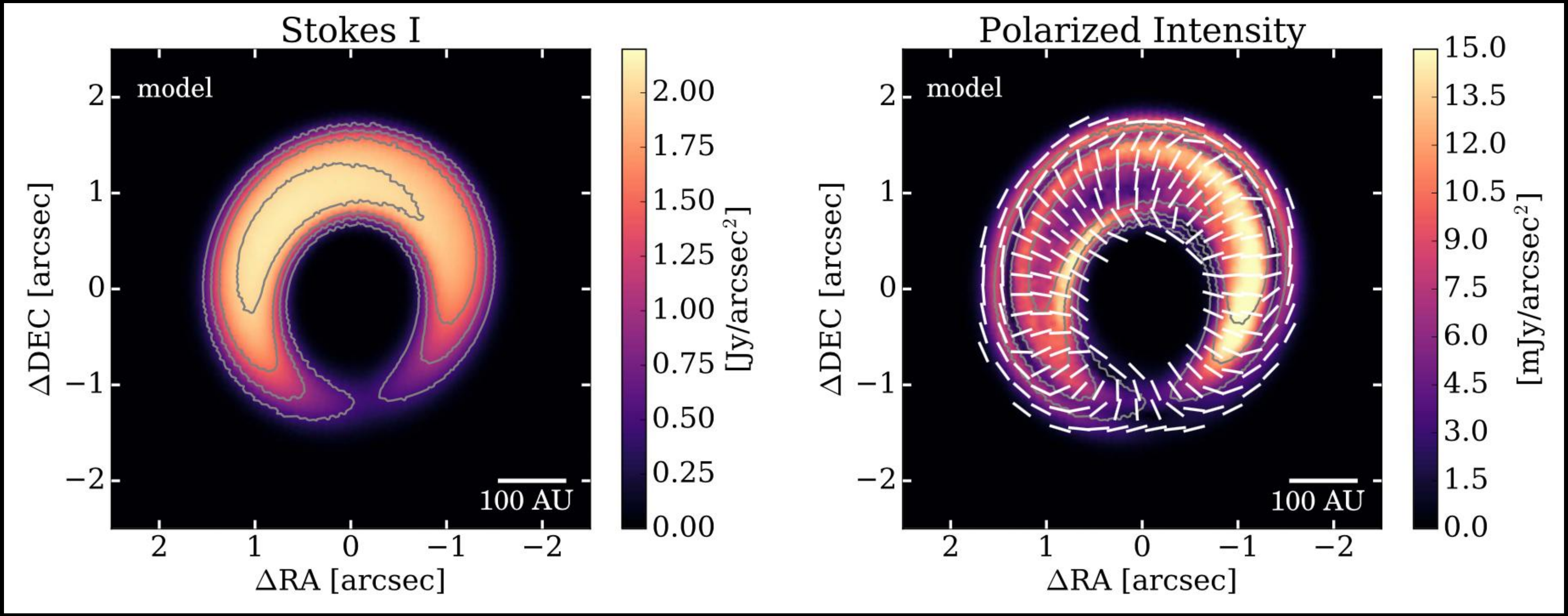


Kataoka et al. (2016)

Example: Protoplanetary Disk

Polarized mm-emission by scattering

RADMC-3D Model Predictions



Kataoka et al. (2016)

Example: Protoplanetary Disk

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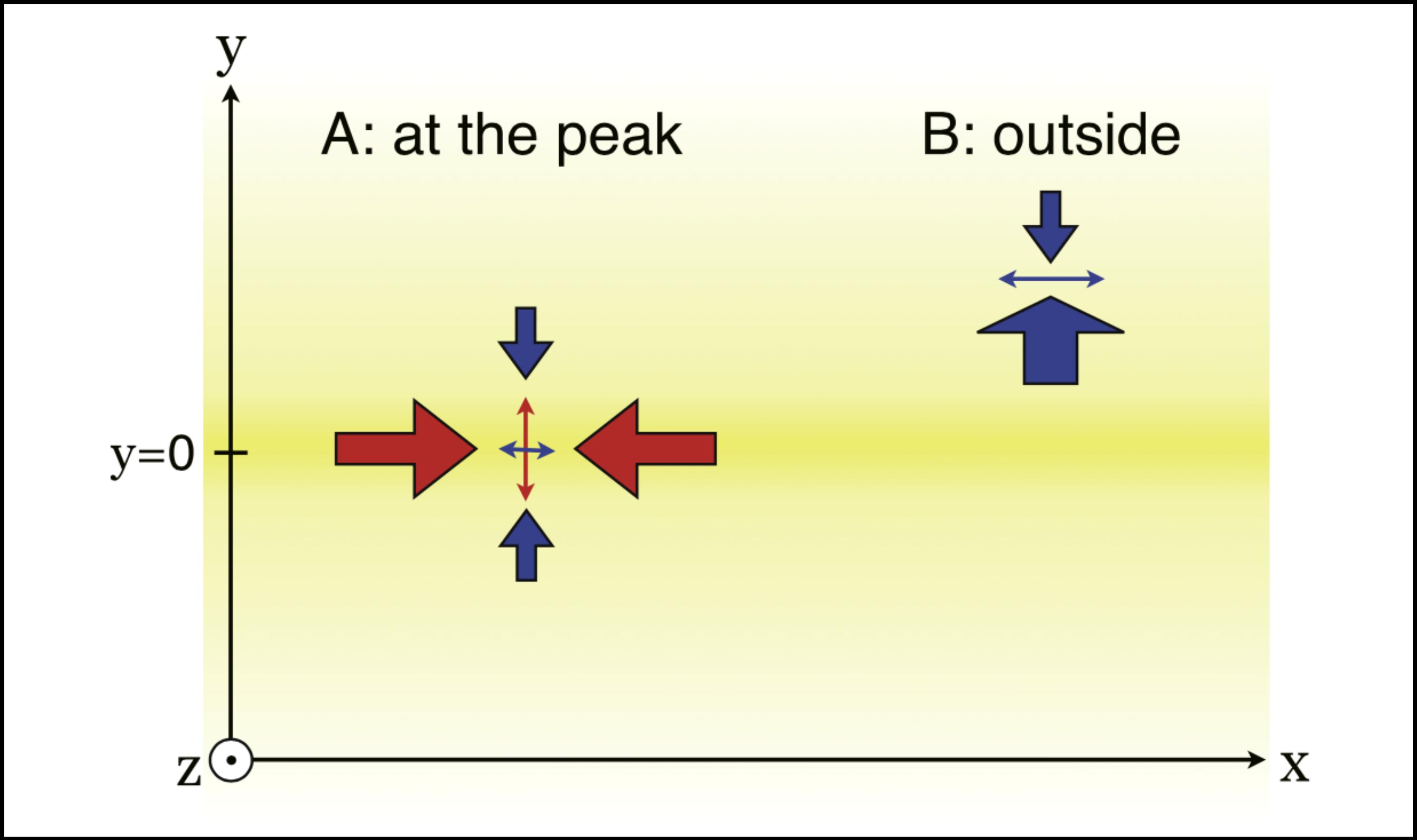
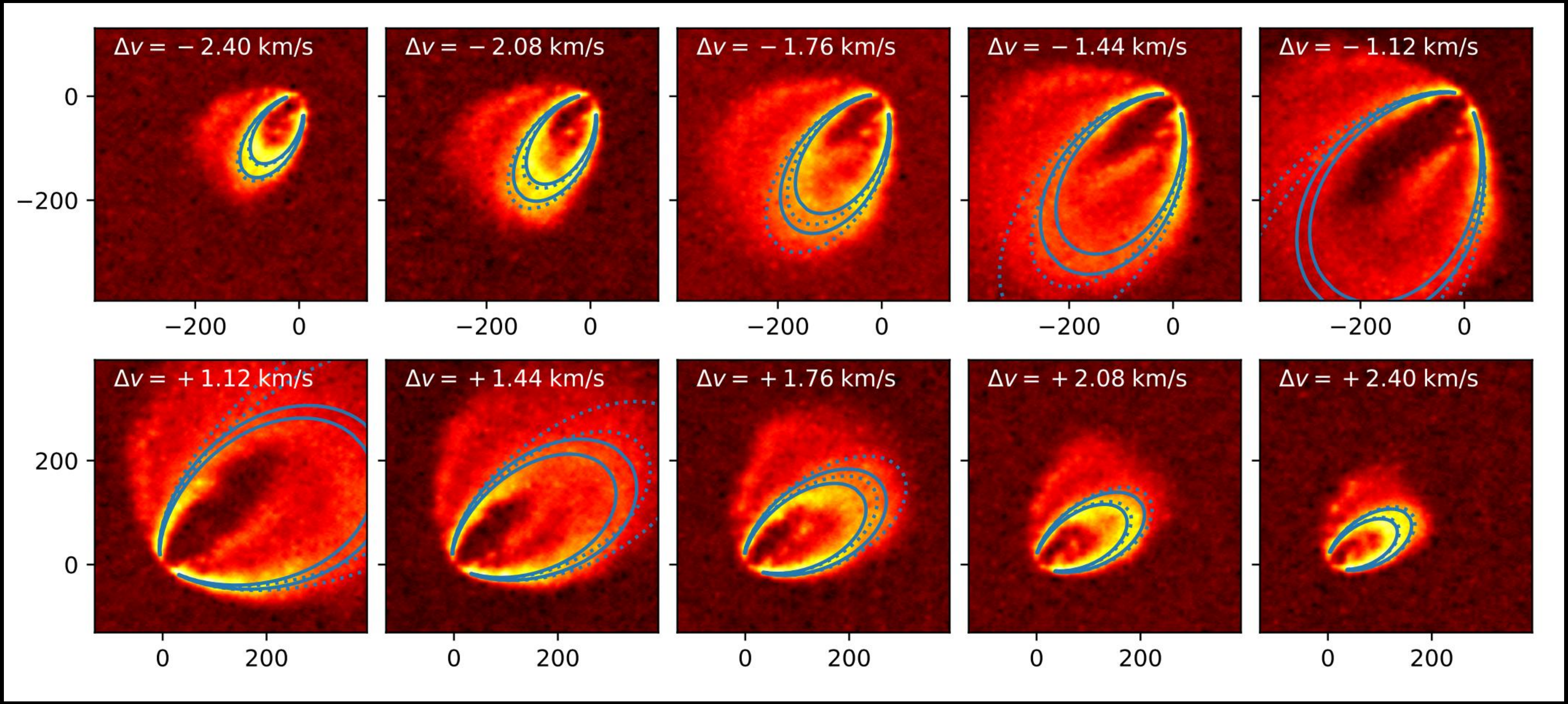


Kataoka et al. (2016)

Example: Protoplanetary Disk

Channel maps

ALMA Observations (Isella et al. 2018)

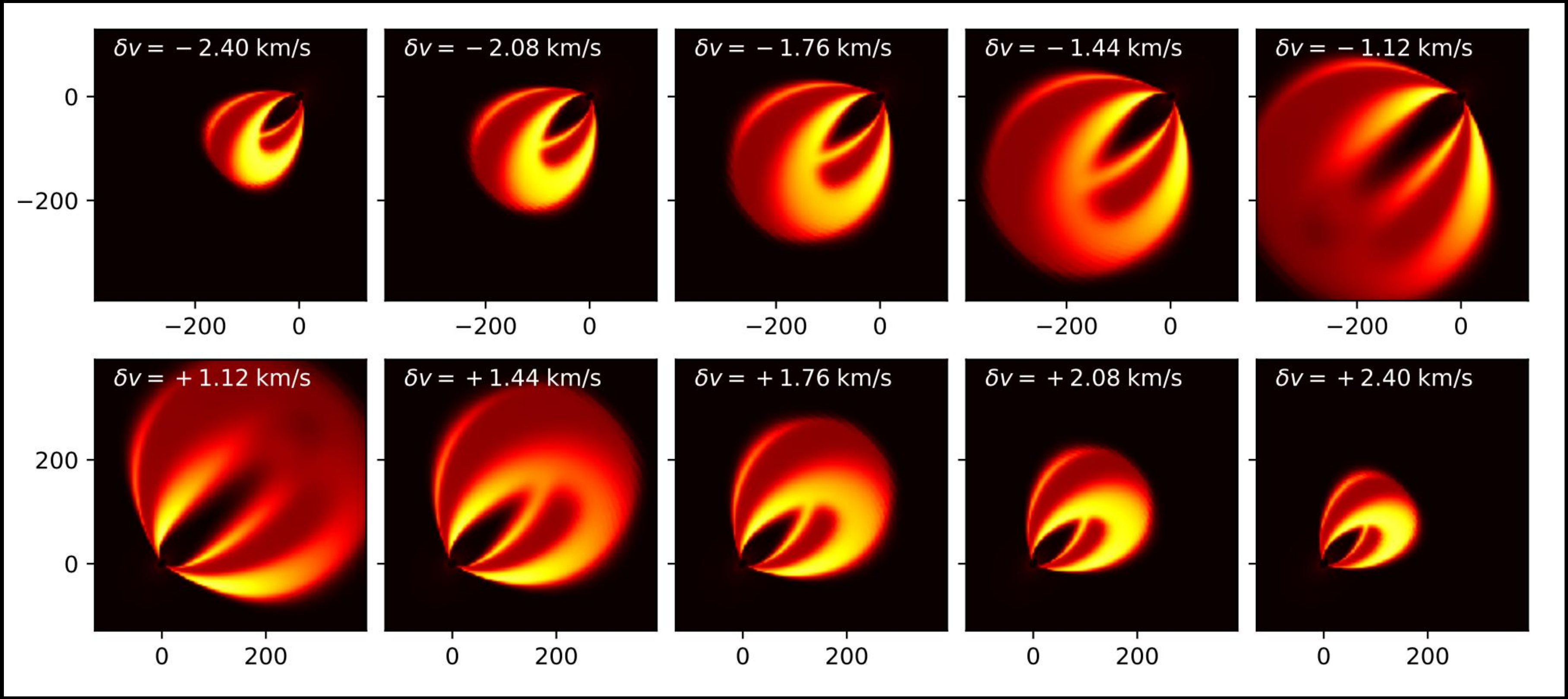


Dullemond et al. (submitted)

Example: Protoplanetary Disk

Channel maps

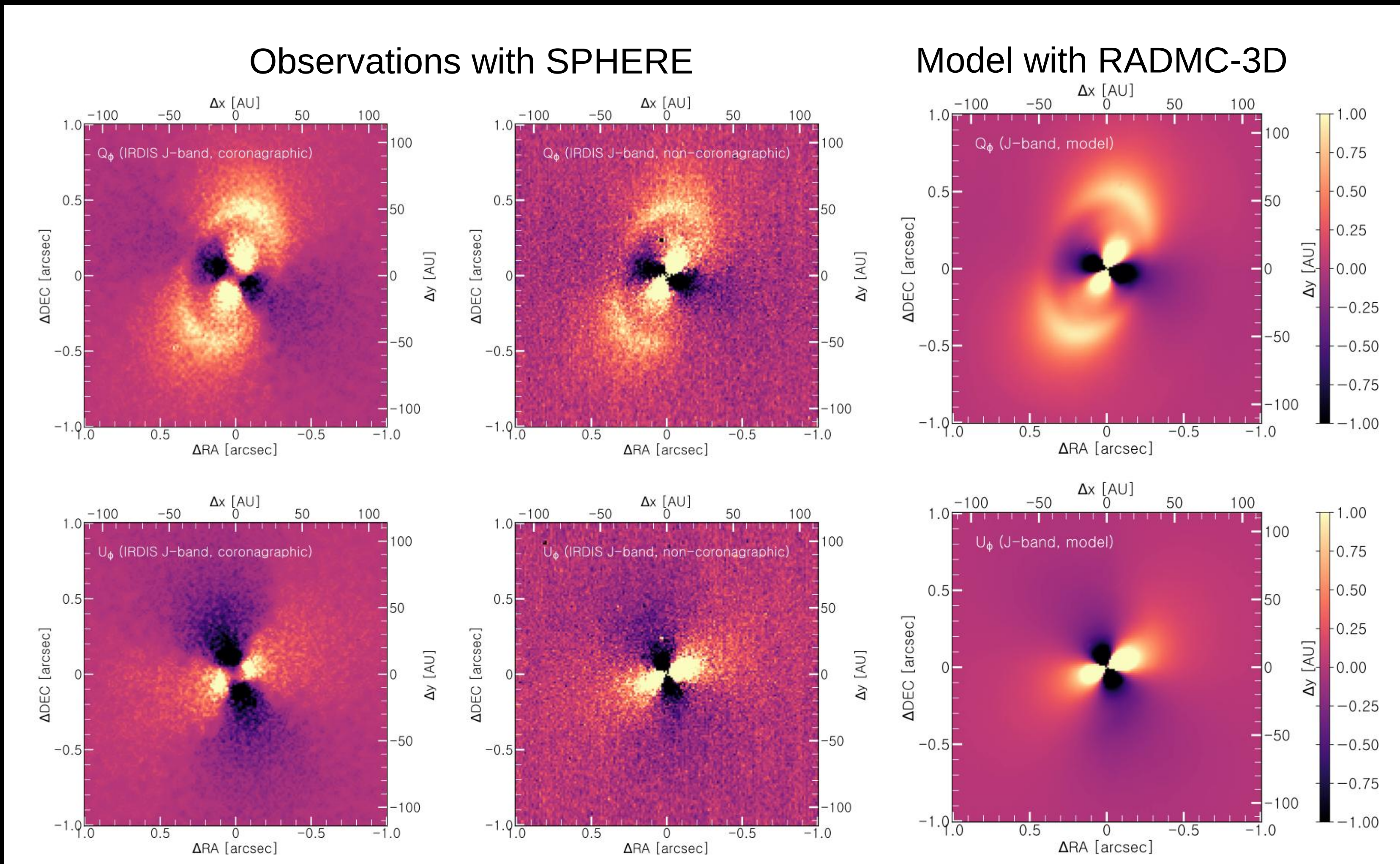
RADMC-3D Model



Dullemond et al. (submitted)

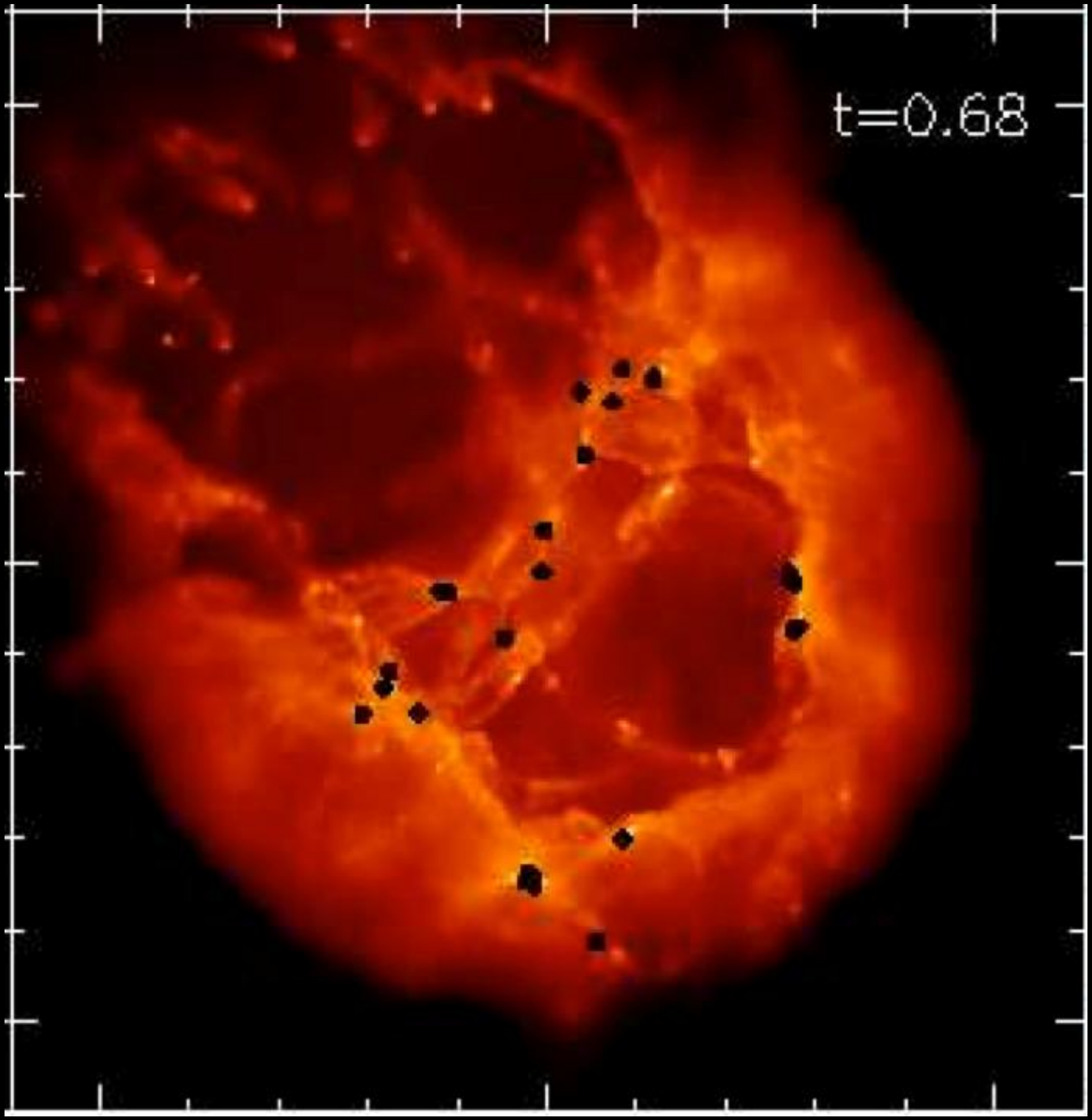
Example: Protoplanetary Disk

Polarized scattered light of PDS 70
(the disk with the 2 planets)



Keppler et al. 2018

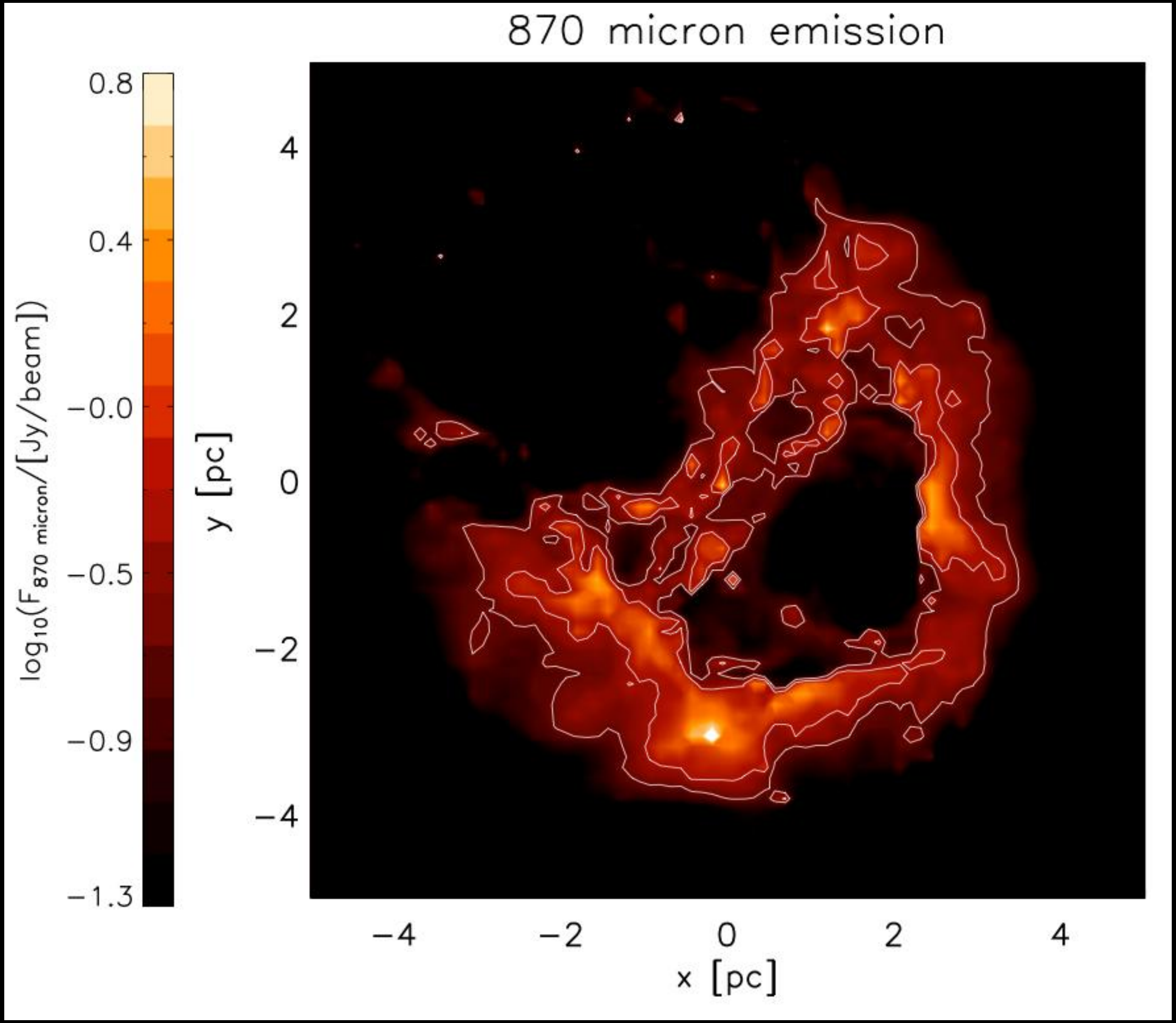
Example: Models of HII regions



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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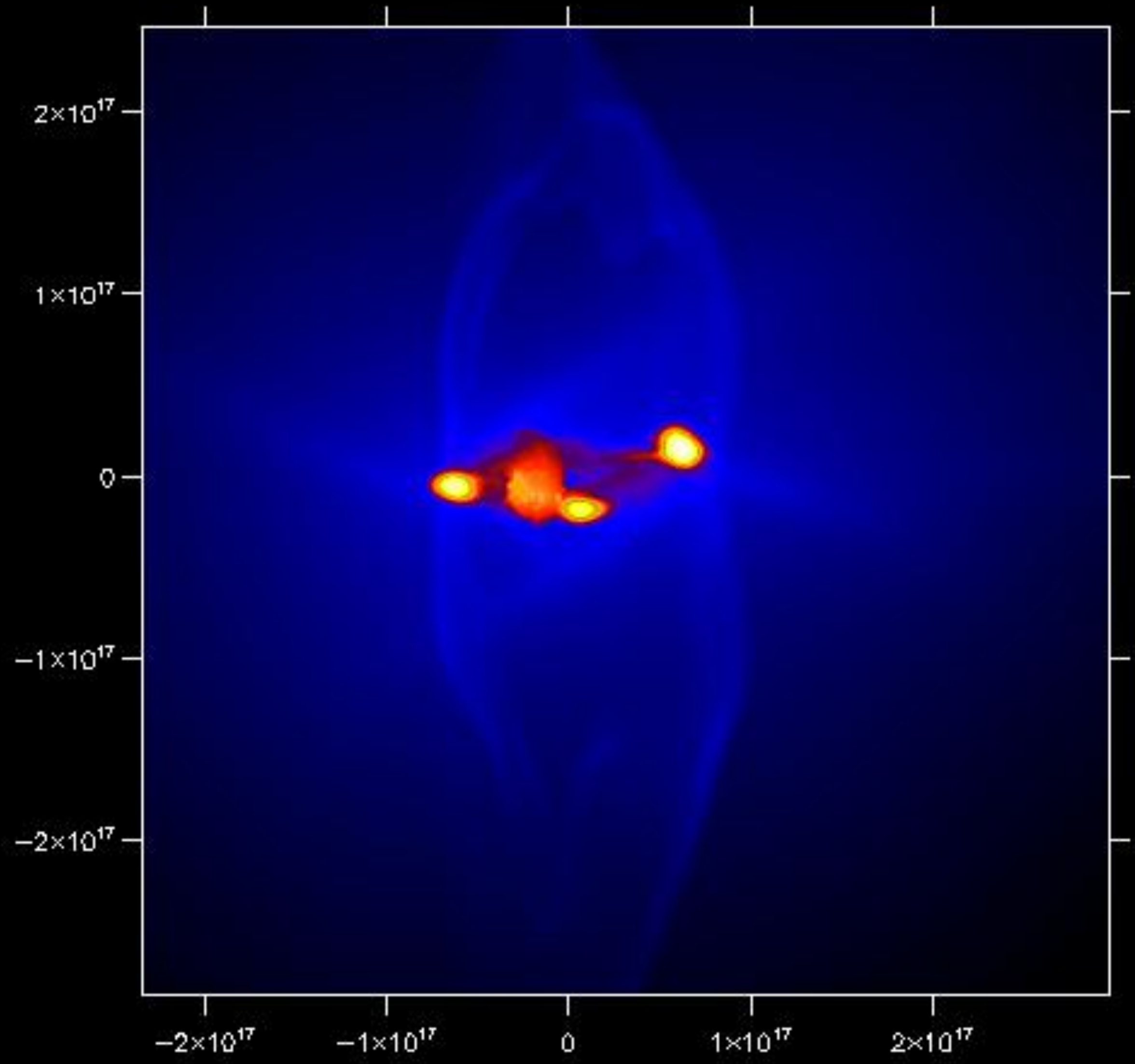
Viewing perspective of compact HII regions

Peters et al. 2010



Viewing perspective of compact HII regions

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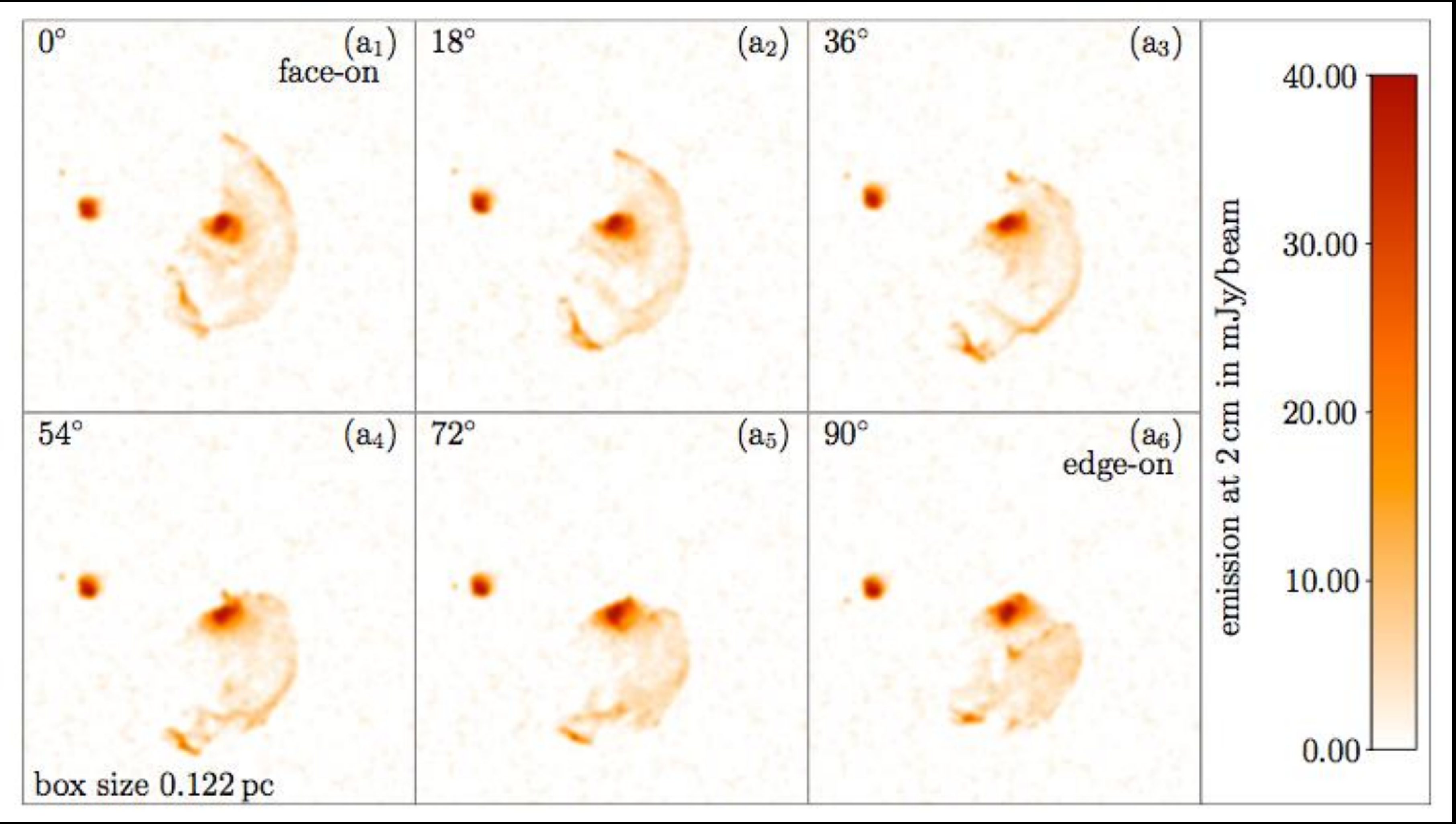
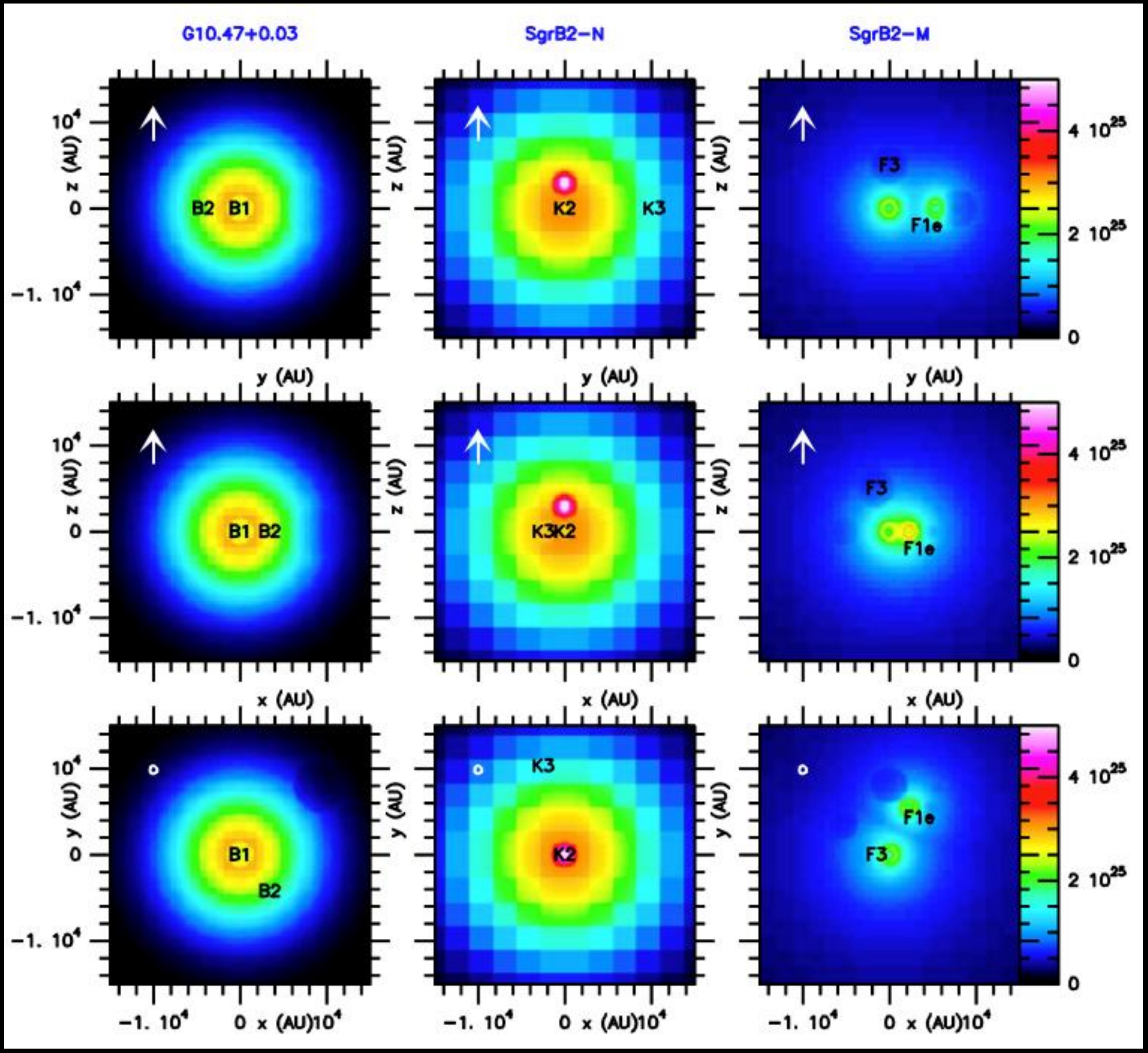


Example: Line transfer in SF regions

Model of HCN emission around young massive stars.



Rolffs, Schilke et al. 2011

Example: Line transfer in SF regions

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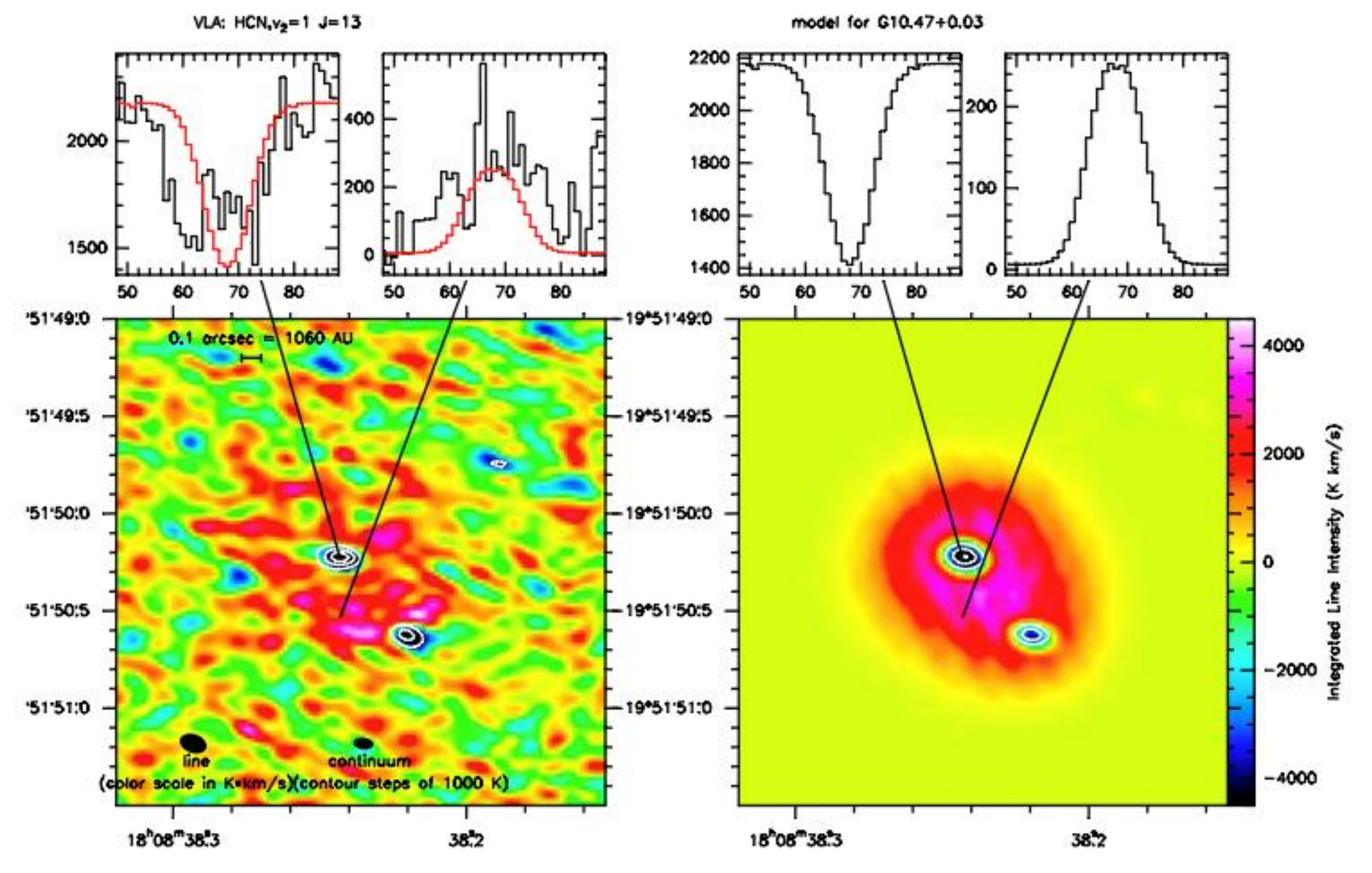
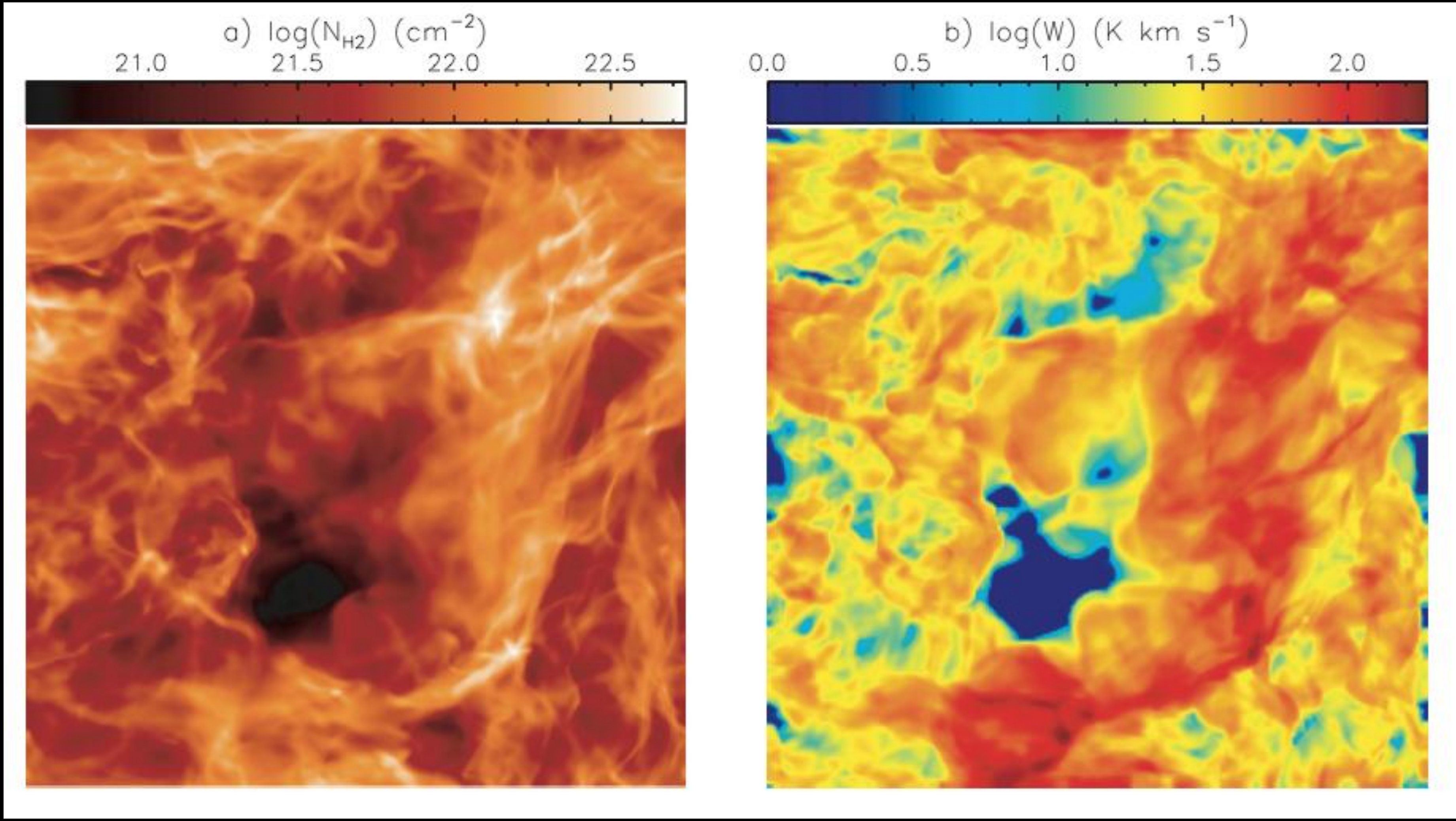


Rolffs, Schilke et al. 2011

The CO X-factor in the turbulent ISM

Shetty et al. 2011a/b



The CO X-factor in the turbulent ISM

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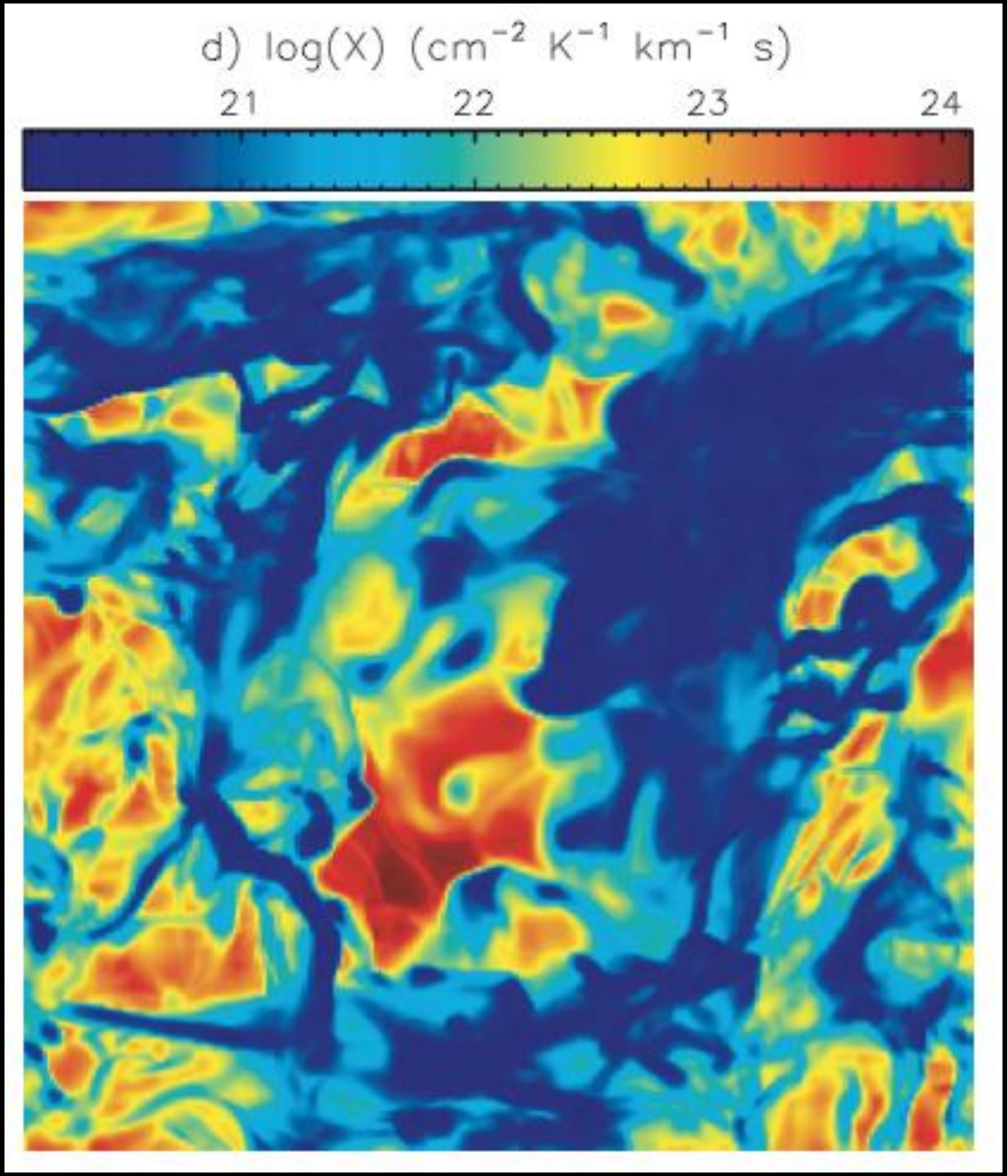
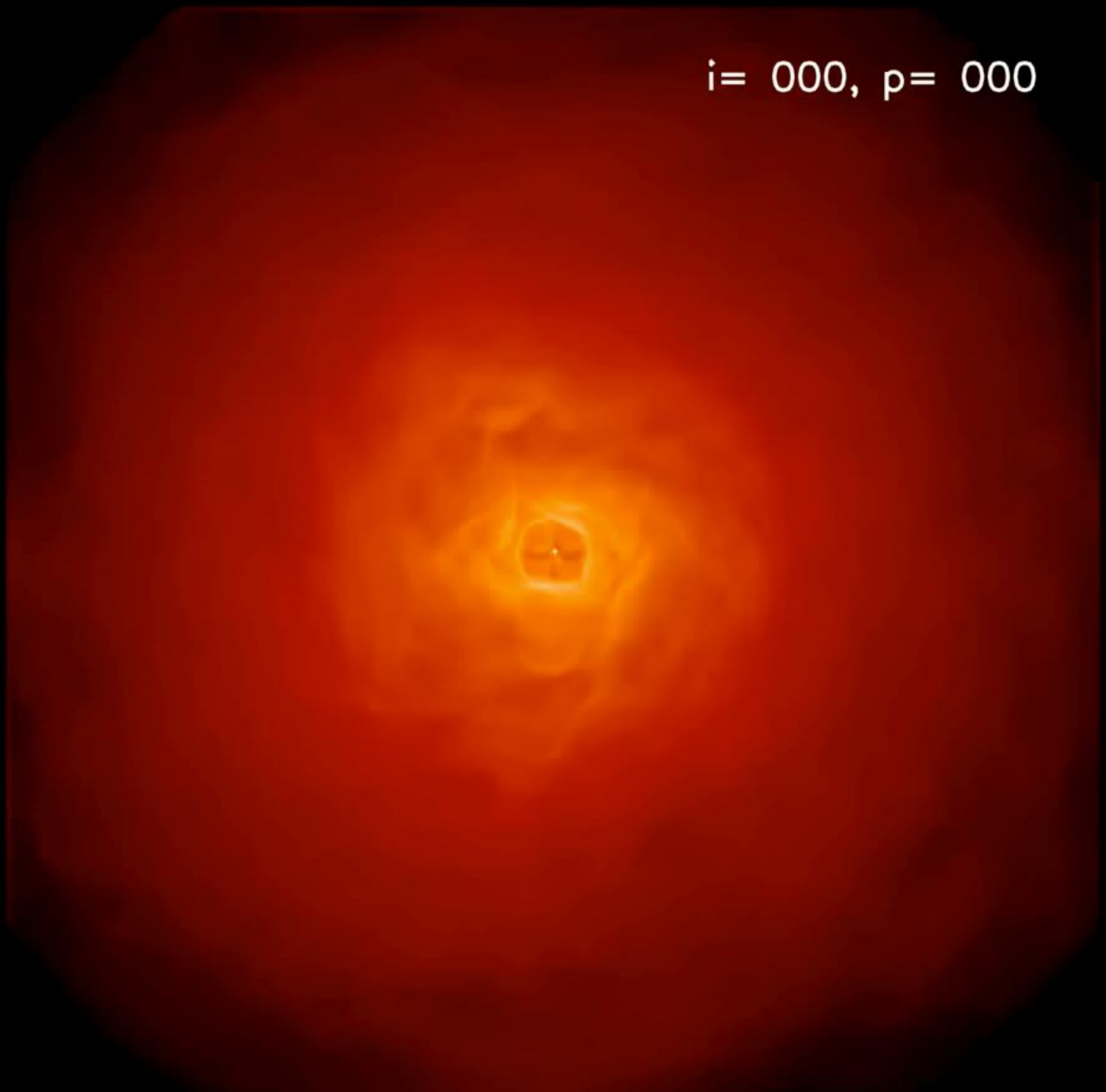


Example of AGN model



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