PAH in 3D

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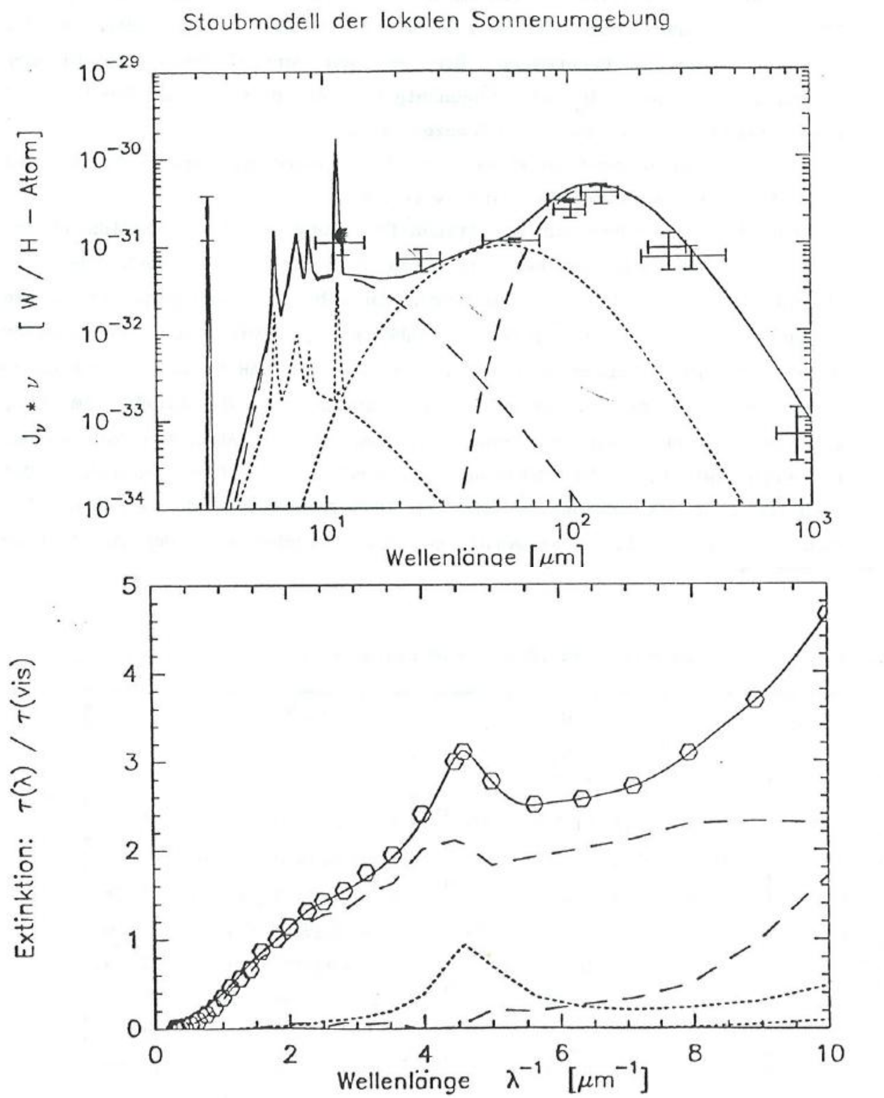
Endrik Krűgel

- Dust model of the ISM
- PAH bands in starburst nuclei
- Monte Carlo radiative transfer
- PAH destruction in T Tauri disks

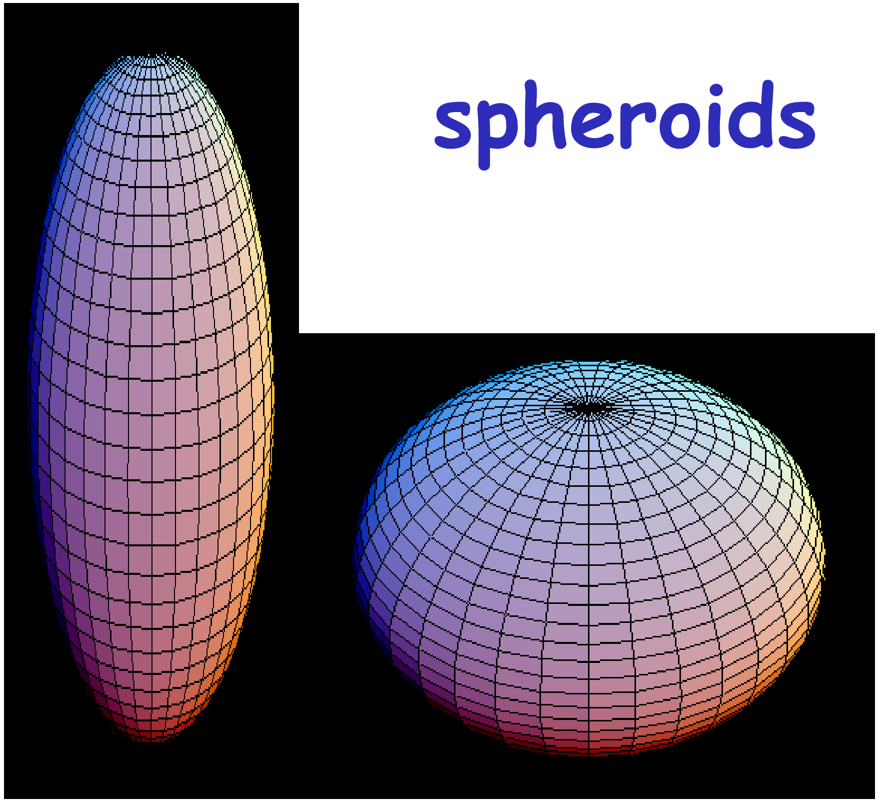
dust'1990



Staubmodell der lokalen Sonnenumgebung
$J_\nu * \nu$ [W / H – Atom]
10^{-29}
10^{-30}
10^{-31}
10^{-32}
10^{-33}
10^{-34}
10^1
10^2
10^3
Wellenlänge [μm]
Extinktion: τ(λ) / τ(vis)
0
1
2
3
4
5
0
2
4
6
8
10
Wellenlänge λ^{-1} [μm^{-1}]

1: polarisation

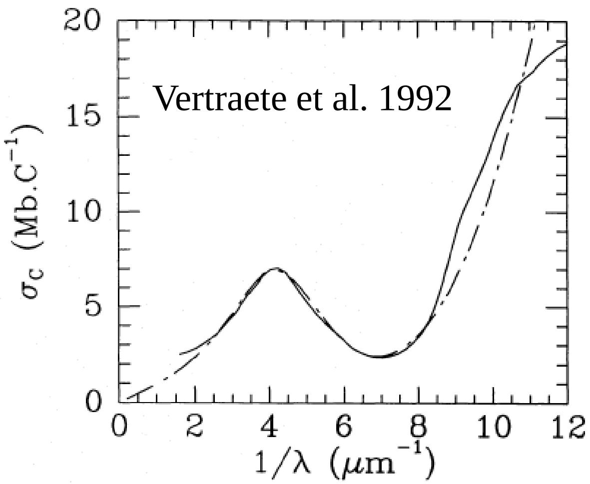
spheroids

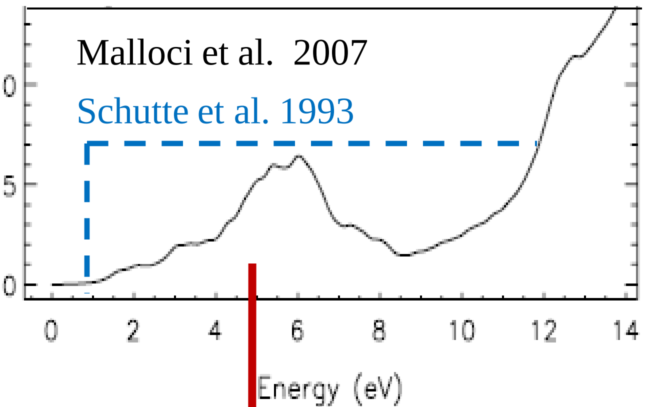


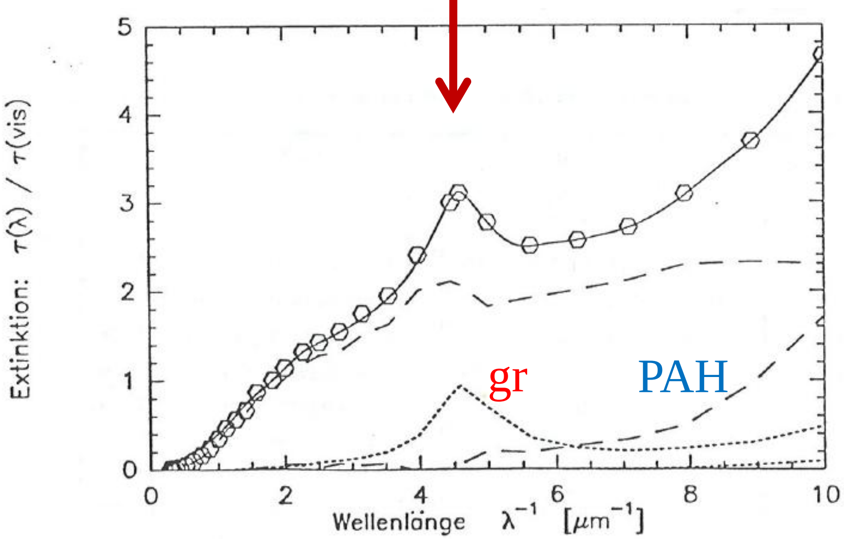
Voshchinnikov (2004)

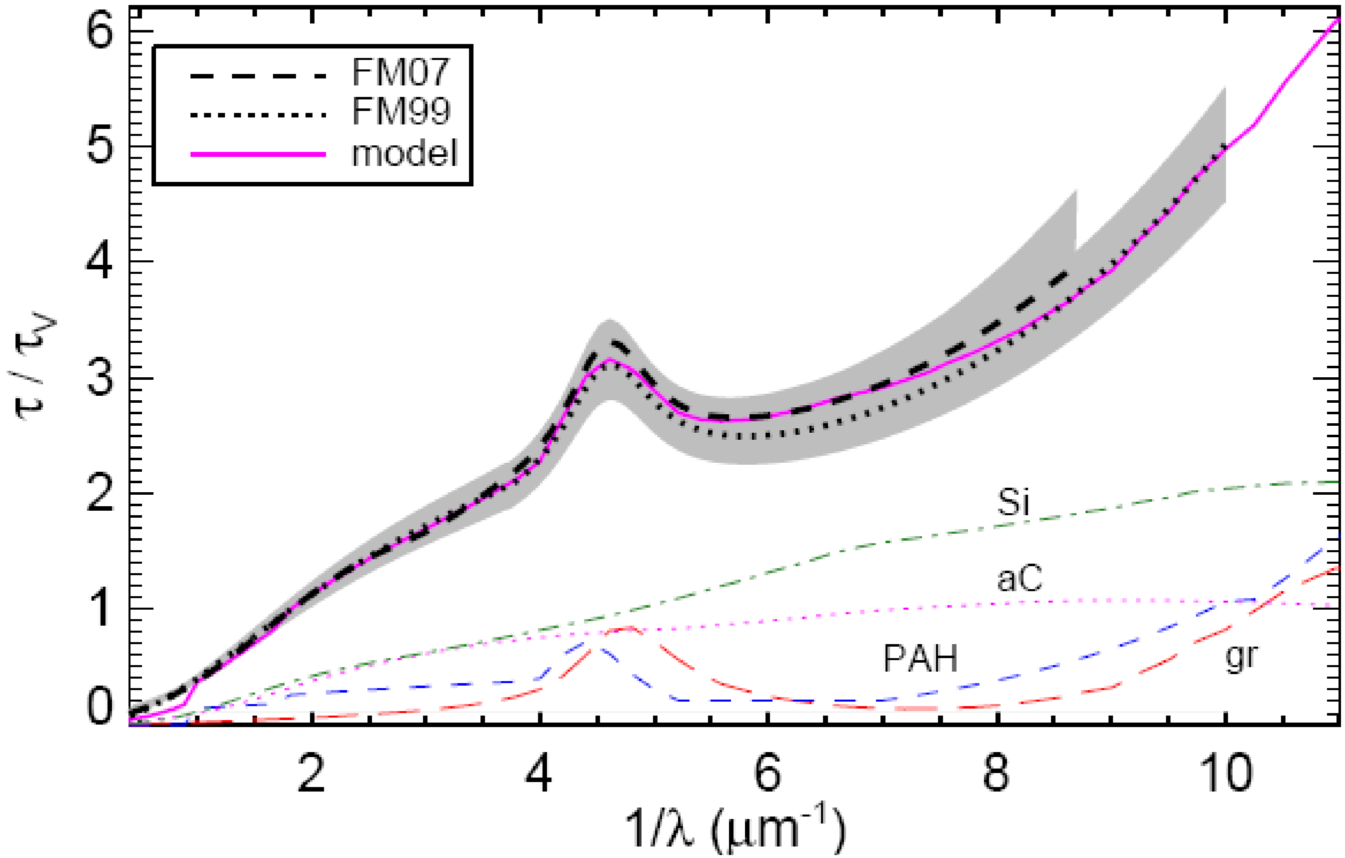
PAH in 3D

2: "2200" bump +
3: PAH absorption









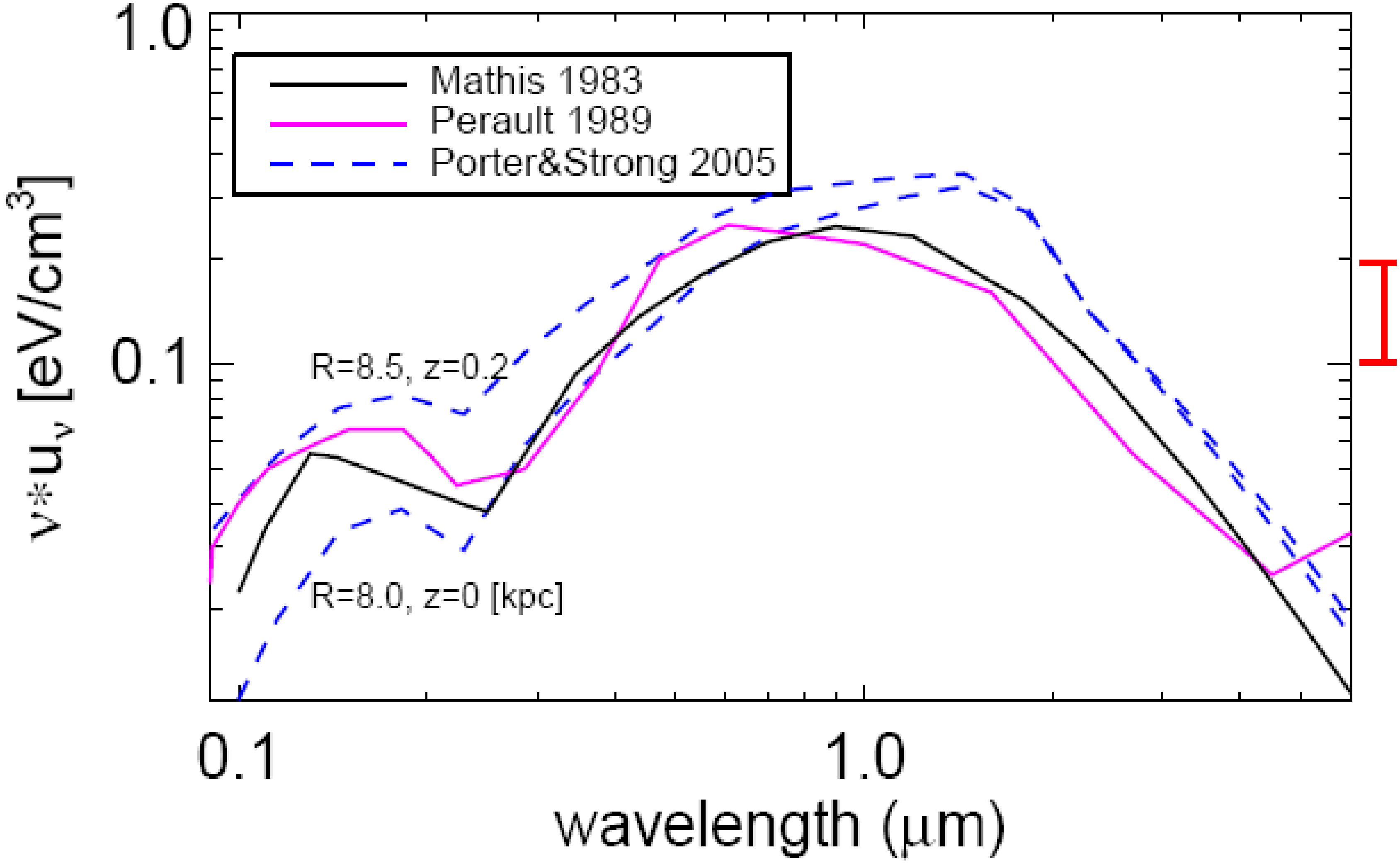
Si + aC : 60Å < a < 0.2-0.3μm, $\sim a^{-3.5}$

Graphite : 5Å < a < 80 Å , $\sim a^{-3.5}$

PAH : 30, 200 C

ISM [g] : 0.66Si + 0.22aC + 0.07gr + 0.05 PAH [g]

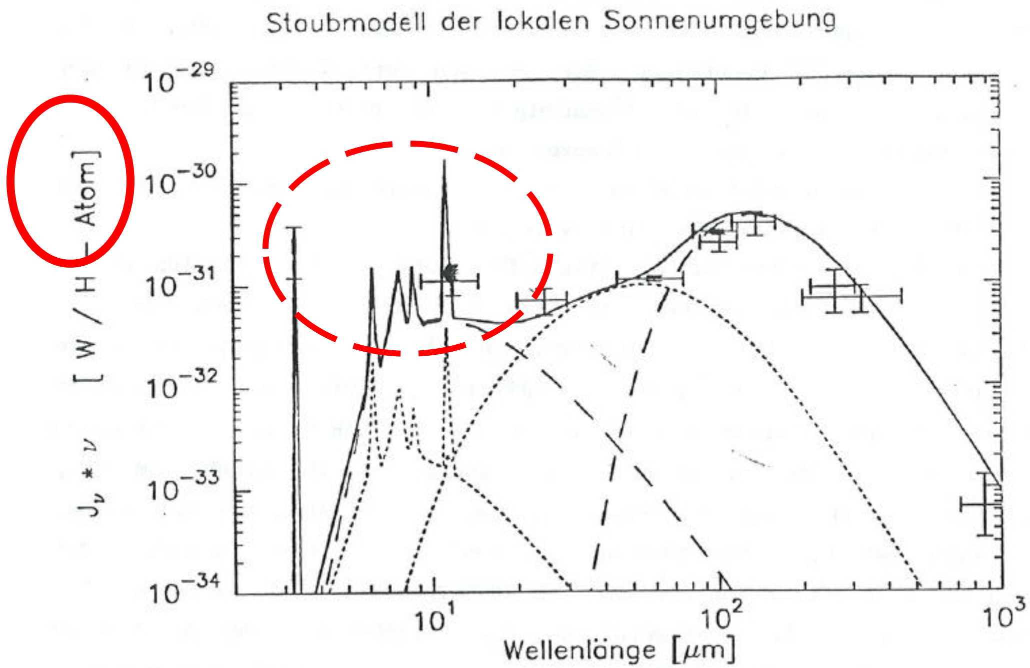
mean ISRF


1.0
0.1
ν*u$_ν$ [eV/cm^3]
Mathis 1983
Perault 1989
Porter&Strong 2005
R=8.5, z=0.2
R=8.0, z=0 [kpc]
0.1
1.0
wavelength (μm)

PAH in 3D

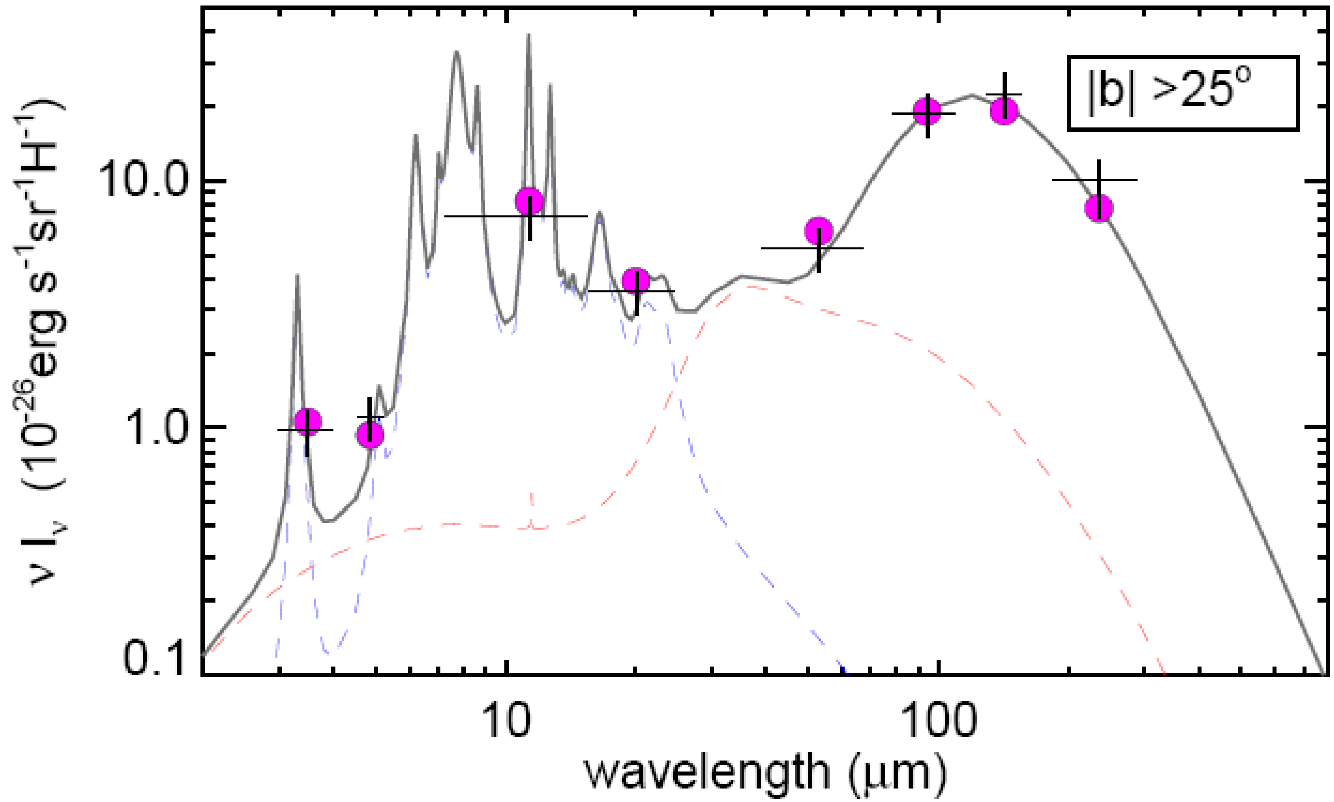
4: abundance +

5: PAH bands



"Carbon crisis"

abundances [ppm]: 31Si + 150aC + 50gr + 30PAH


|b| >25°
10.0
1.0
0.1
10
100
wavelength (μm)
ν I_ν (10^-26 erg s^-1 sr^-1 H^-1)

PAH in 3D

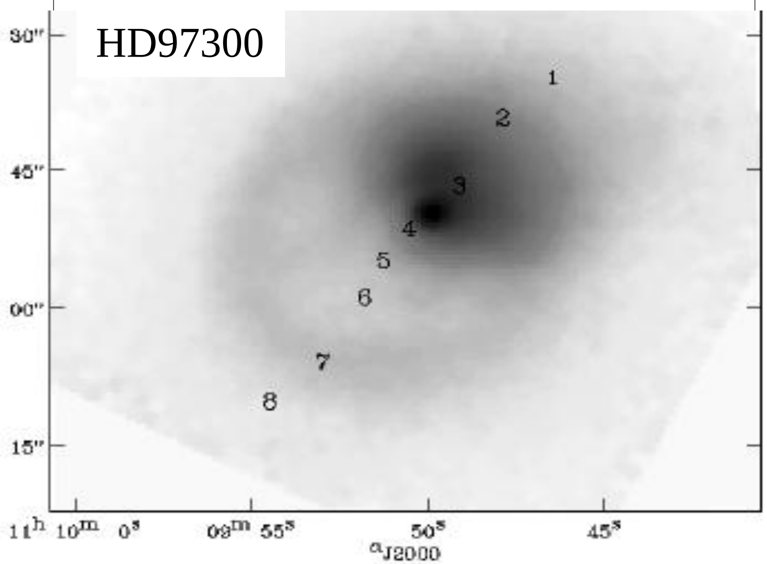
ISO

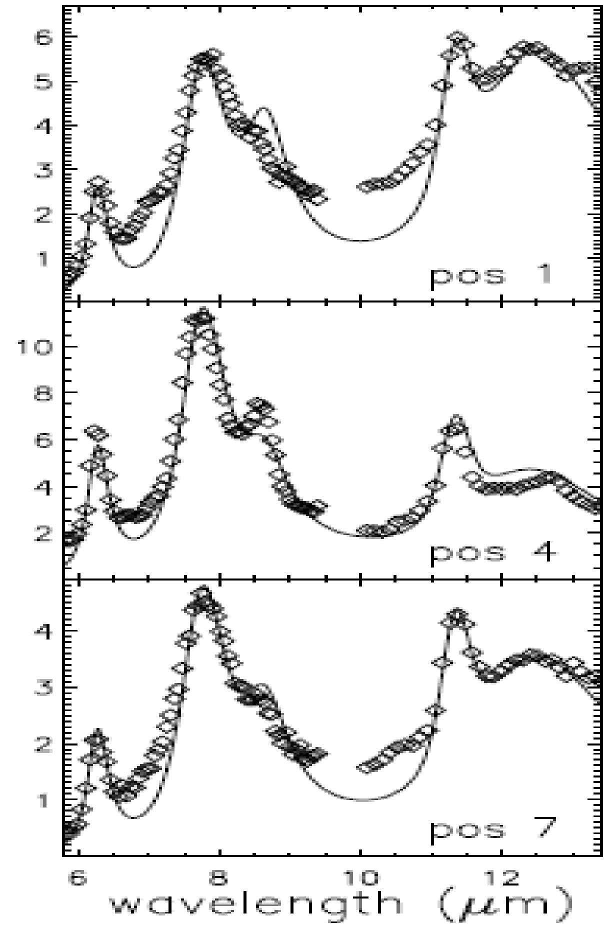
Lorentzian profile

$$\sigma_\nu = \frac{\sigma}{2\pi} \cdot \frac{\gamma}{(\omega - \omega_0)^2 + (\gamma/2)^2}$$

Table 1. PAH Properties

λ (Å)	$\sigma^{\dagger}$ $(10^{-21}\mathrm{cm}^2\mu\mathrm{m})$	$\sigma^{\ddagger}$ $(10^{-21}\mathrm{cm}^2\mu\mathrm{m})$	γ $(10^{12}\mathrm{s}^{-1})$
6.3	1.8	1.8	16
7.8	4.6	12	24
8.6	6.7	6	18
11.3	17	40	5
12.5	17	19	29

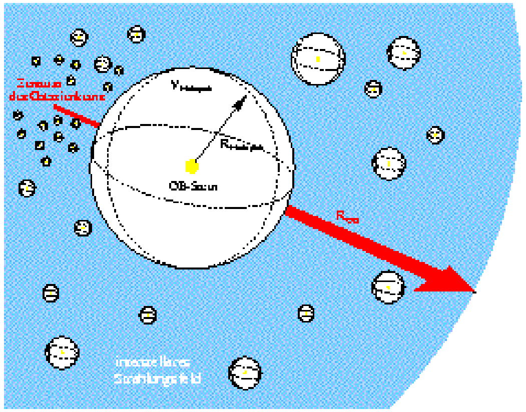


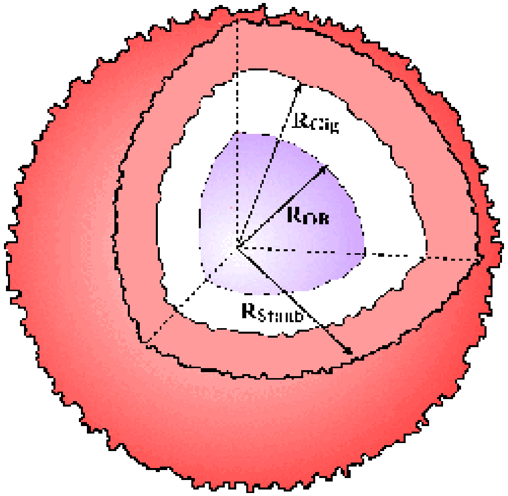


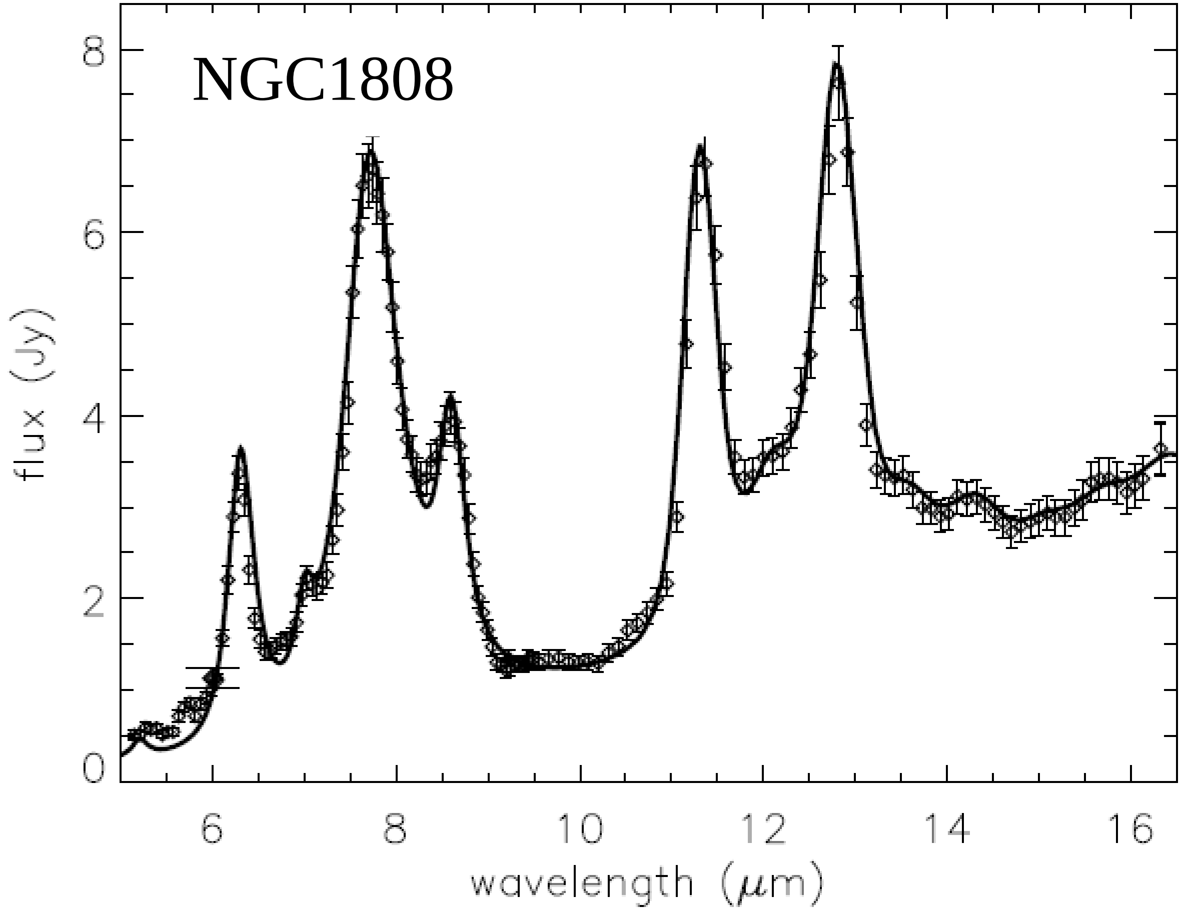
Boulanger et al. (1998)

Siebenmorgen et al. (1998)

Radiative transfer in SB







Siebenmorgen et al. (2001)

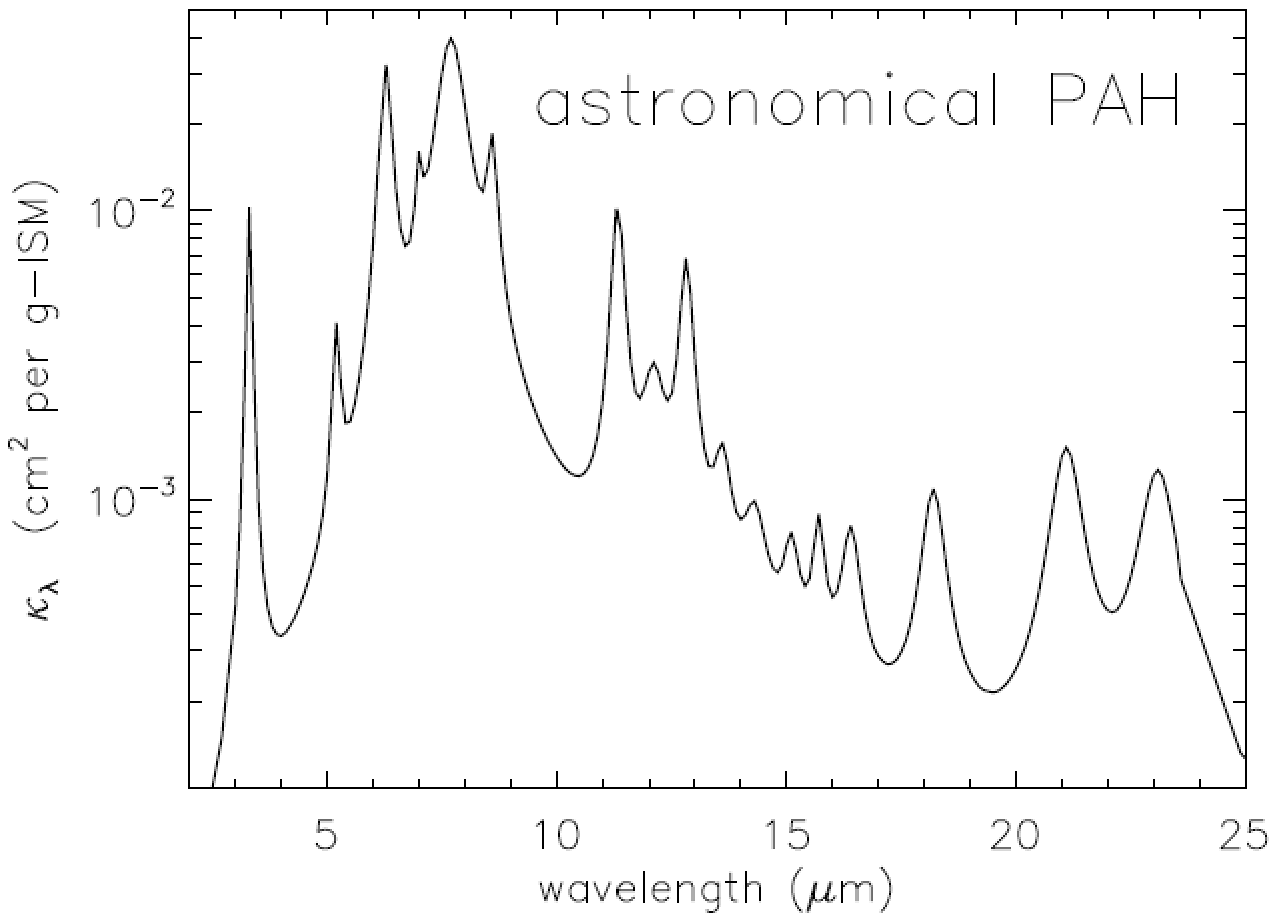
post ISO

17 features

Table 2. Astronomical PAH.

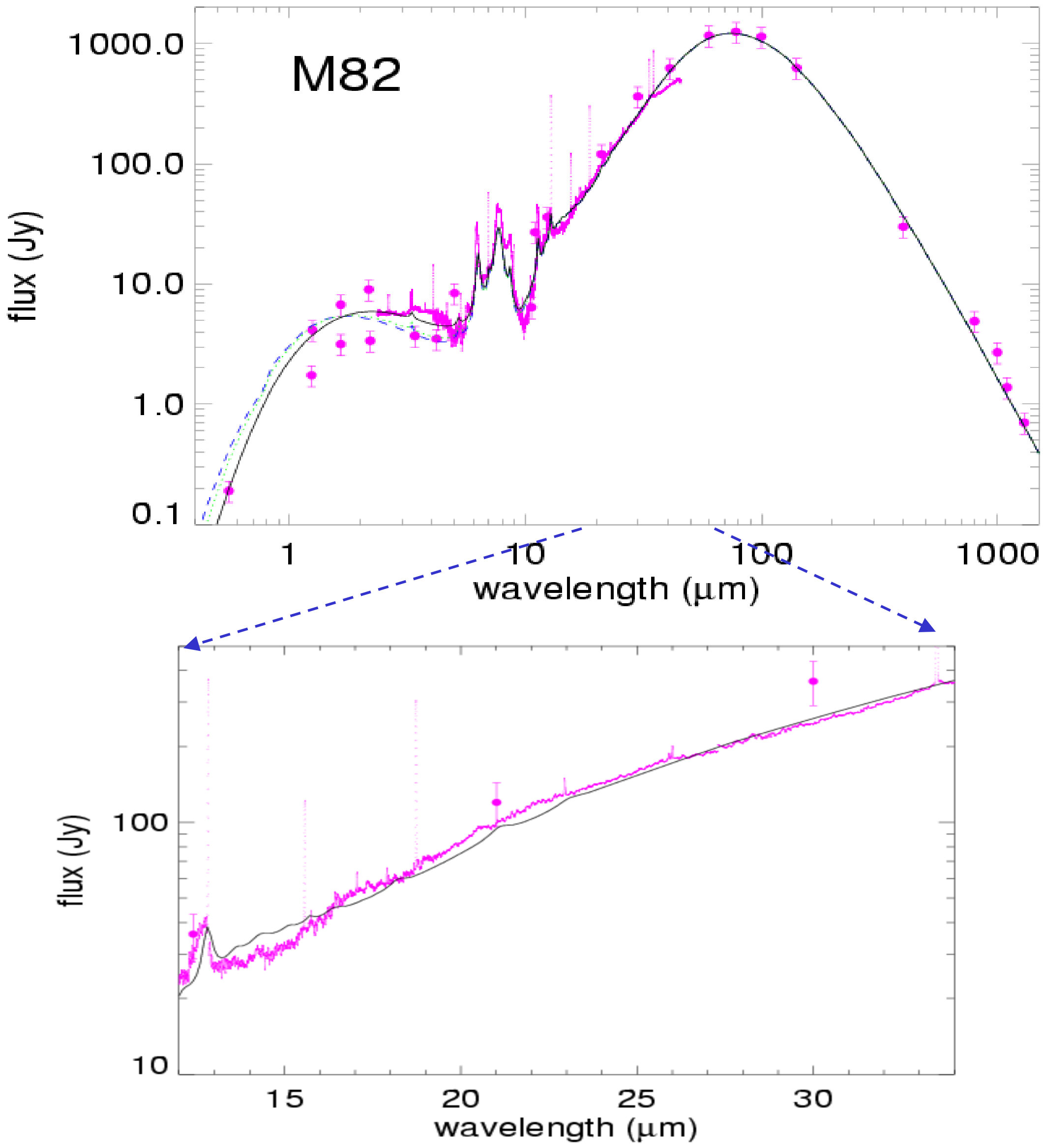
(1) Wavelength λ_0 μm	(2) Damping Constant γ 10^{12} s^{-1}	(3) Integrated Cross Section $\sigma_{\rm int}$ 10^{-22} cm^2 μm	(4) Mode	(5) Remarks
3.3	20	12	C–H stretch	no data
5.2	12	1.1	C–C vibration	tentative
6.2	14	21	C–C vibration	
7.0	5.9	12.5	C–H?	
7.7	22	55	C–C vibration	
8.6	6	35	C–H in-plane bend	
11.3	4	36	C–H solo out-of-plane bend	
11.9	7	12	C–H duo out-of-plane bend	
12.8	3.5	28	C–H trio out-of-plane bend	
13.6	4	3.7	C–H quatro out-of-plane bend	tentative detection
14.3	5	0.9	C–C skeleton vibration	first extragalactic detection
15.1	3	0.3	C–C skeleton vibration	tentative detection
15.7	2	0.3	C–C skeleton vibration	first extragalactic detection
16.4	3	0.5	C–C skeleton vibration	data do not cover full band
18.2	3	1.0	C–C skeleton vibration	no data
21.1	3	2.0	C–C skeleton vibration	no data
23.1	3	2.0	C–C skeleton vibration	no data

post ISO



Siebenmorgen et al. (2001)

post Spitzer



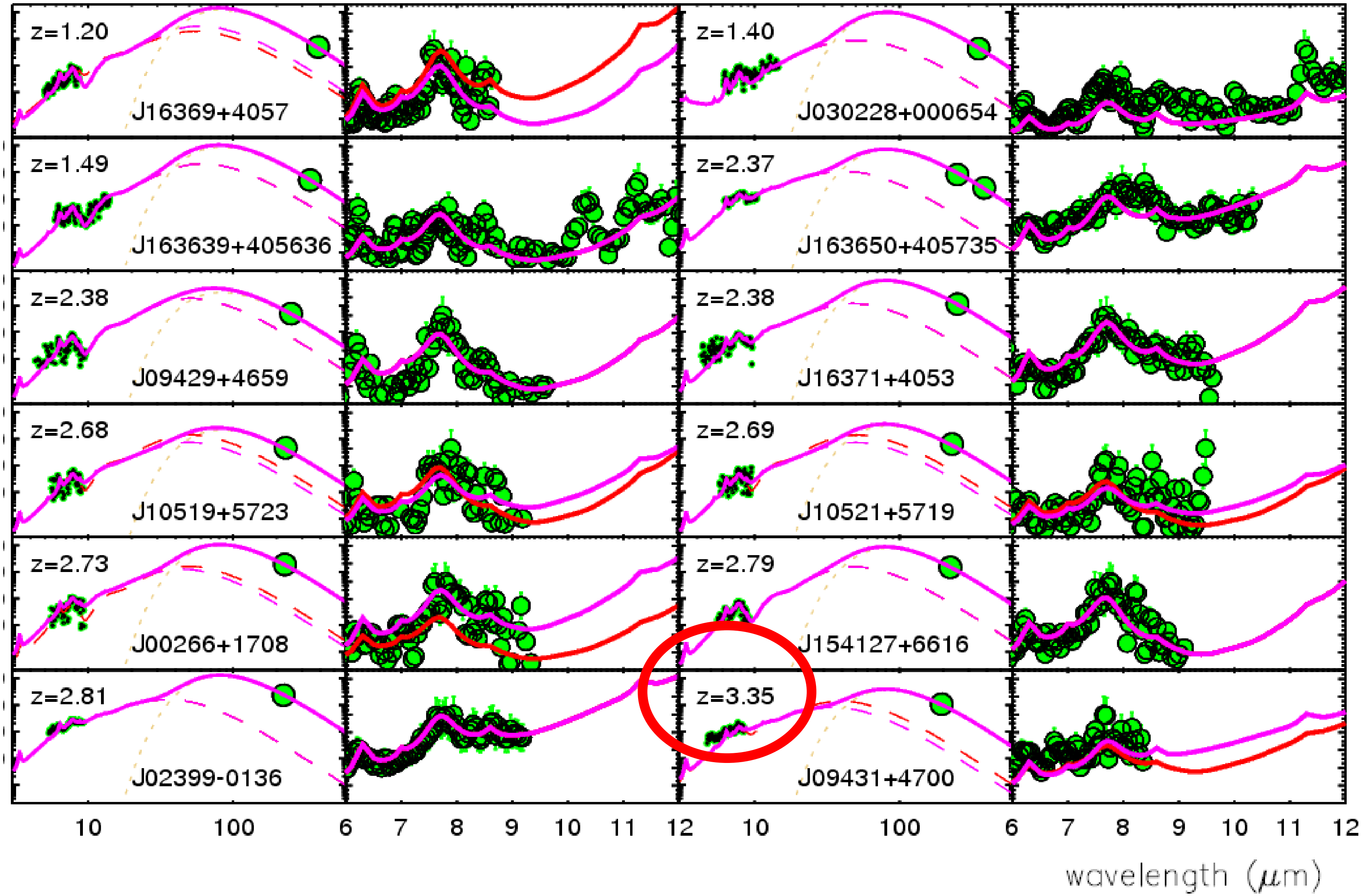
Siebenmorgen et al. (2007)

SED model grid:

- luminosity
- size
- mass

PAH in 3D

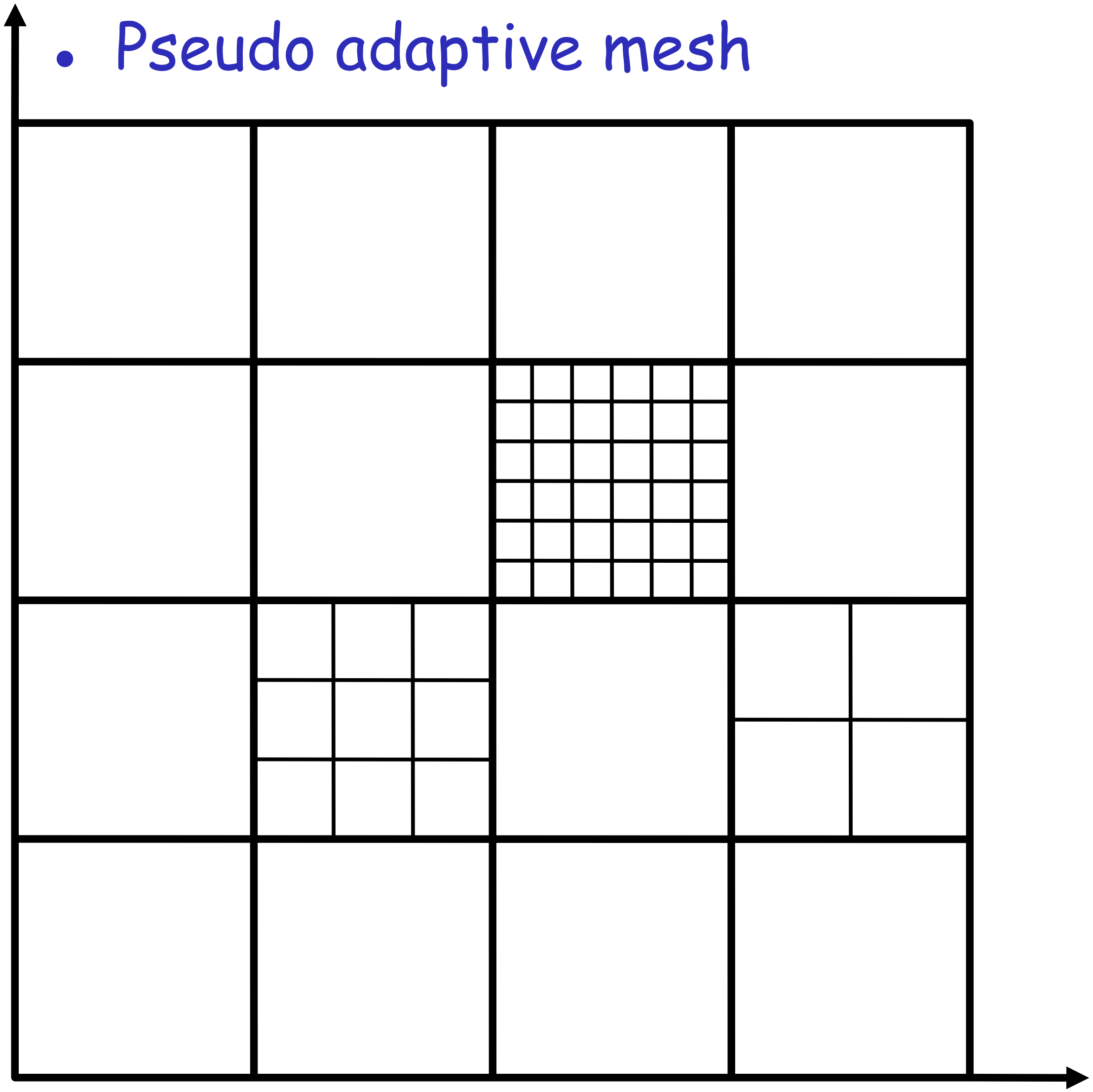
high z



Efstathiou & Siebenmorgen (2009)

Monte Carlo

- Arbitrary dust distribution
- Pseudo adaptive mesh

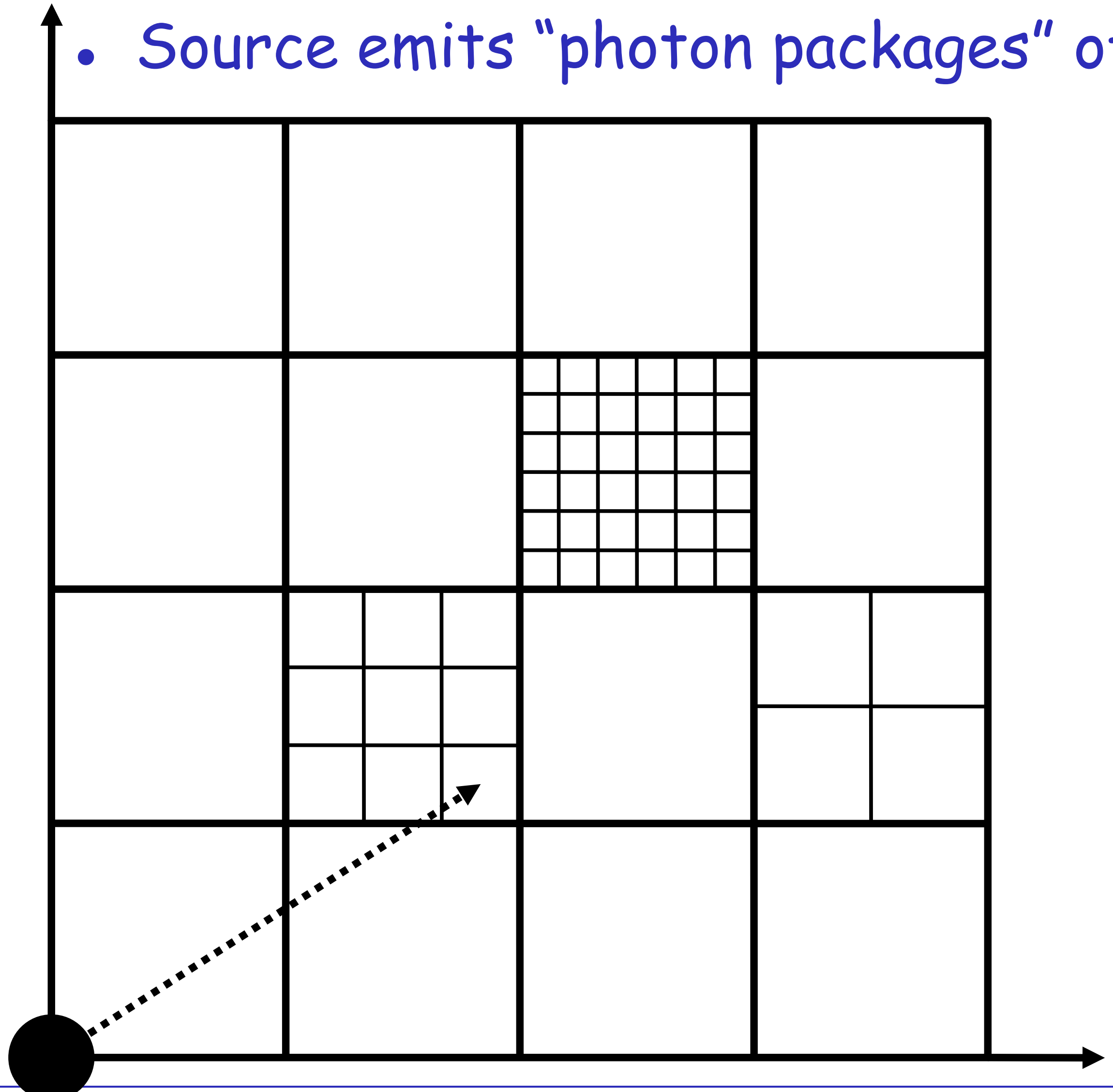


1. geometry

Original code by Krűgel (2006)

Monte Carlo

- Source emits "photon packages" of equal energy

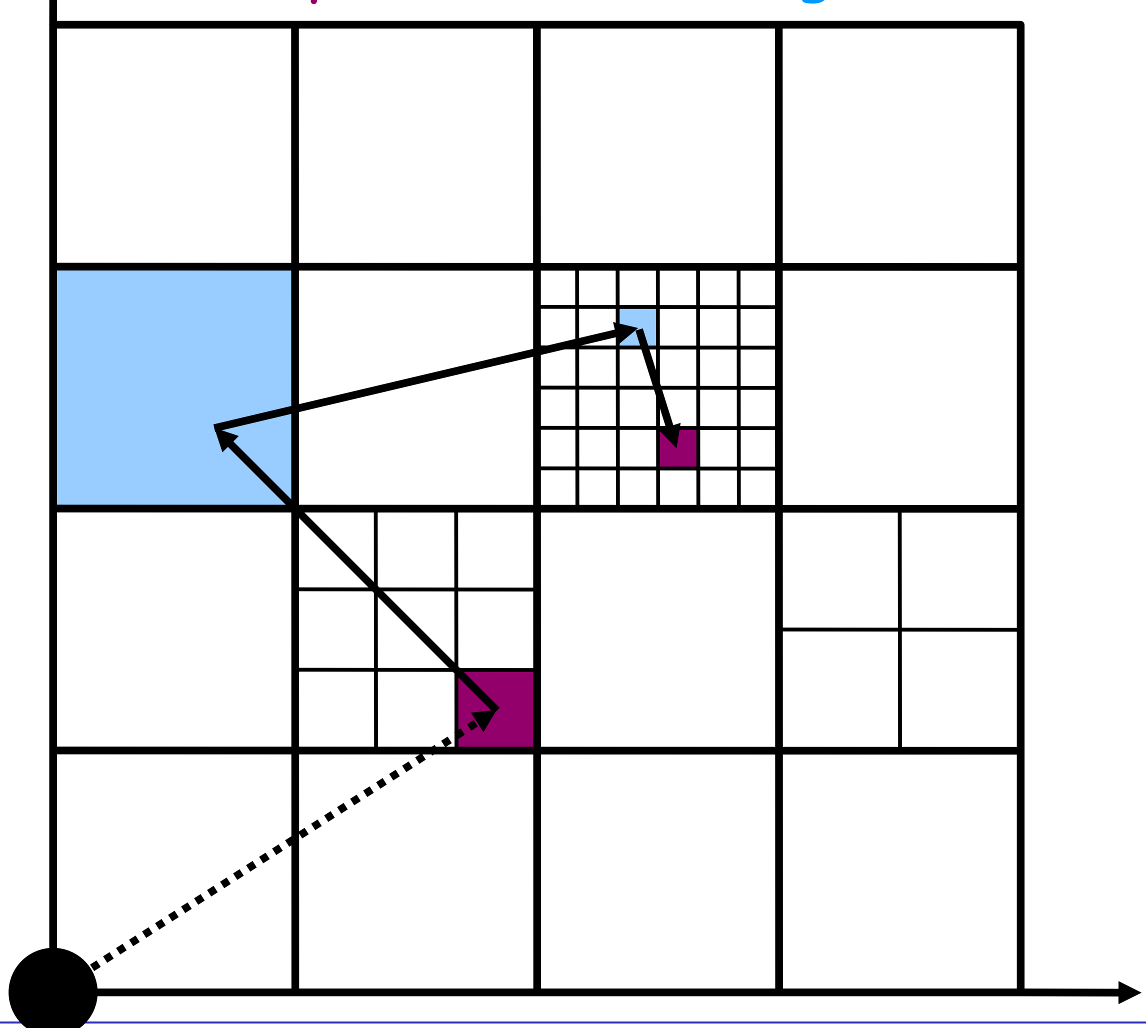


1. geometry
2. source

Monte Carlo

$\tau = -\ln(\zeta)$

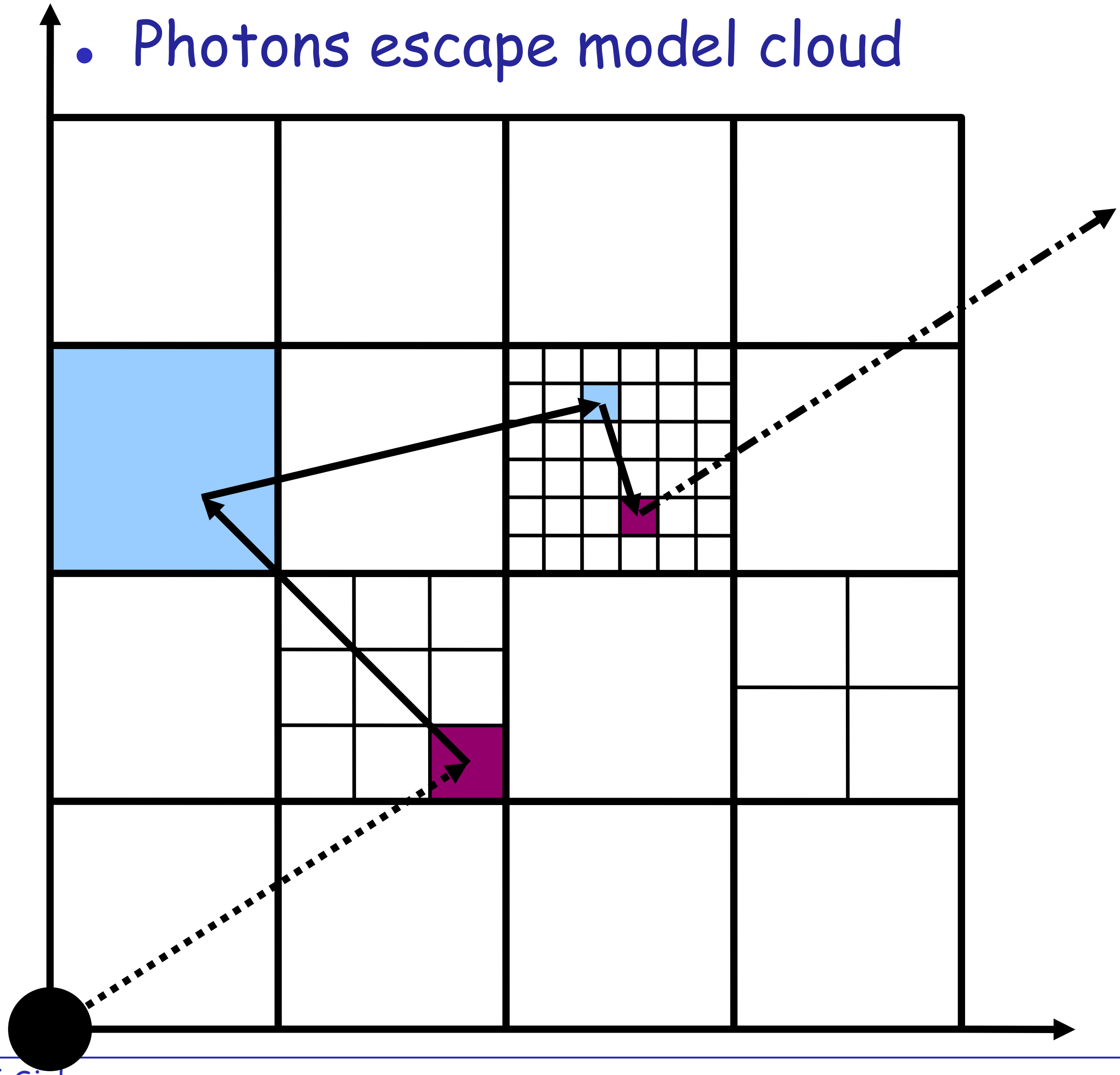
- absorption / scattering / no interaction



1. geometry
2. source
3. inter-action
4. dust temperature

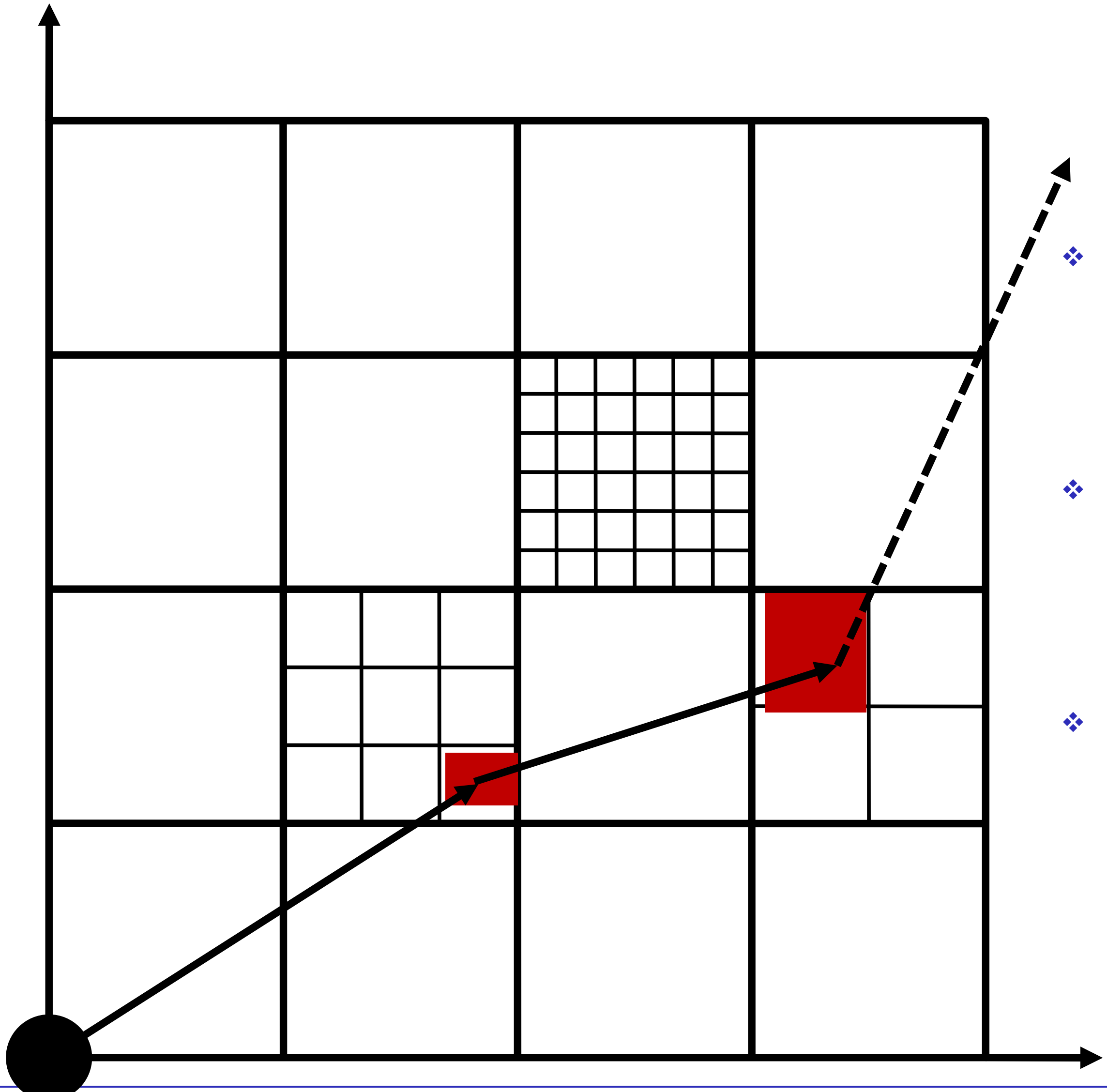
Monte Carlo

- Photons escape model cloud



1. geometry
2. source
3. inter-action
4. temperature
5. detection

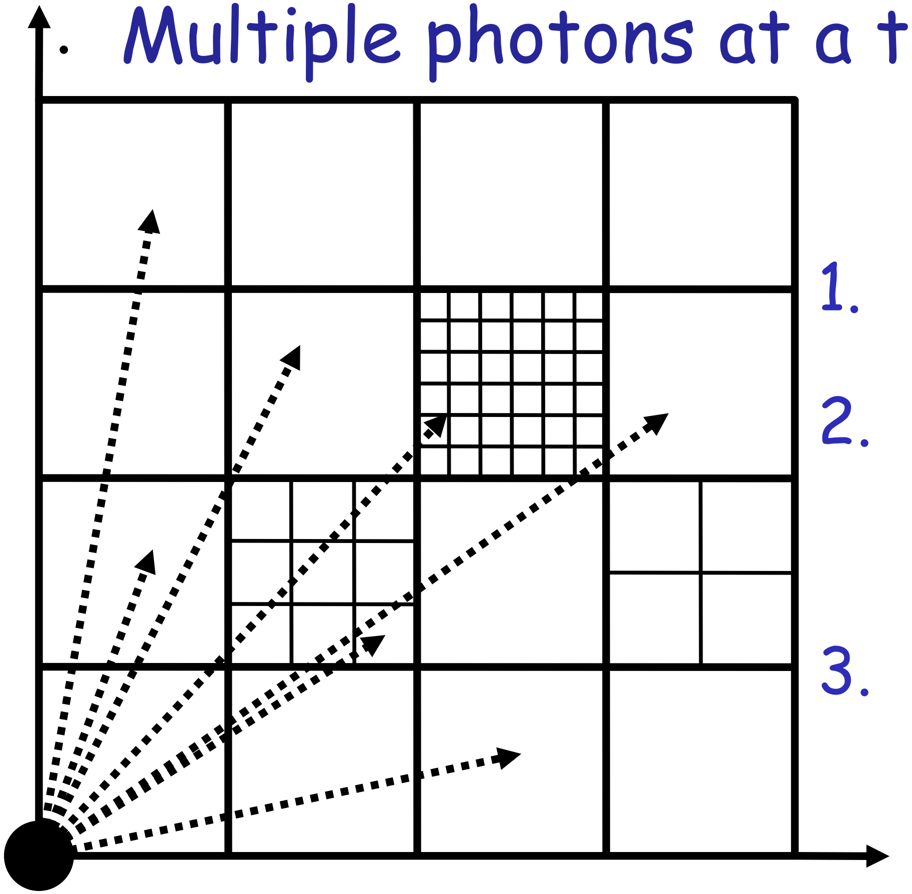
Monte Carlo + PAH



- store PAH absorption events of each cell
- compute PAH emission
- neglect PAH self absorption

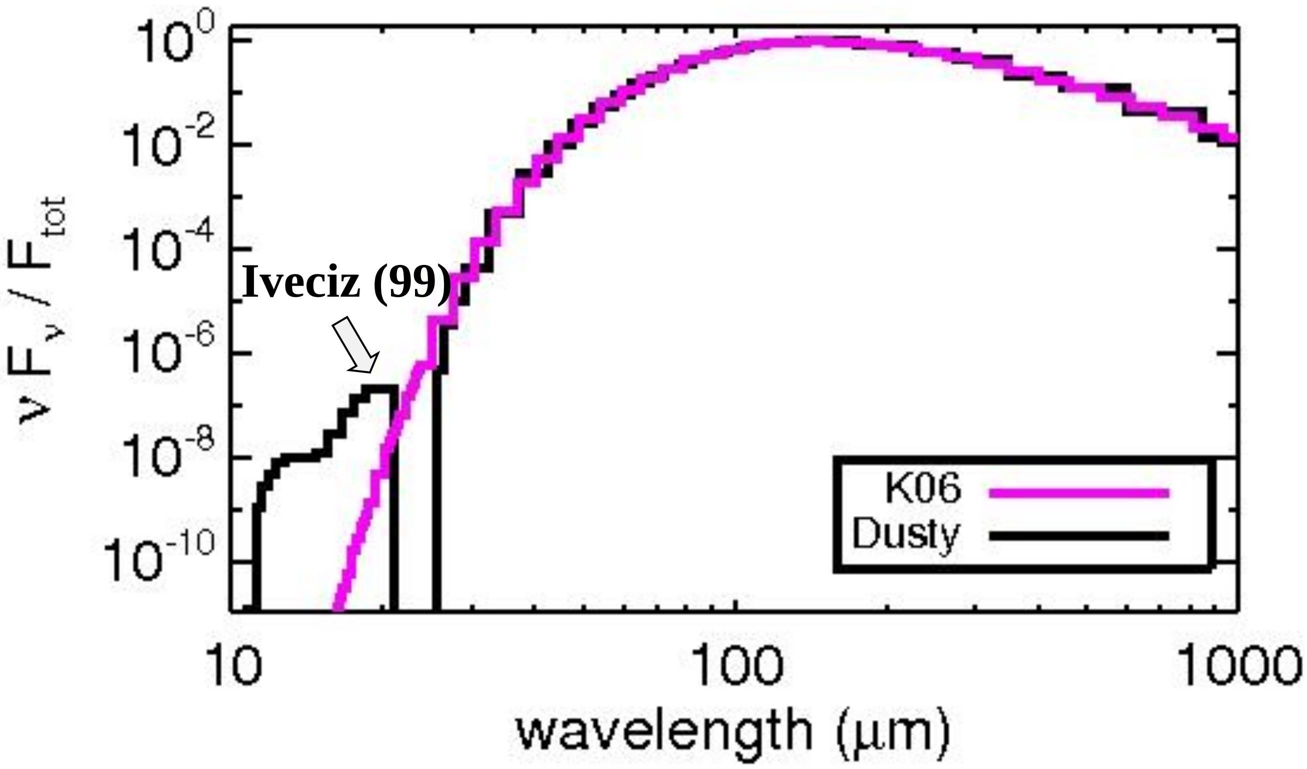
MC parallelization

- Multiple photons at a time:

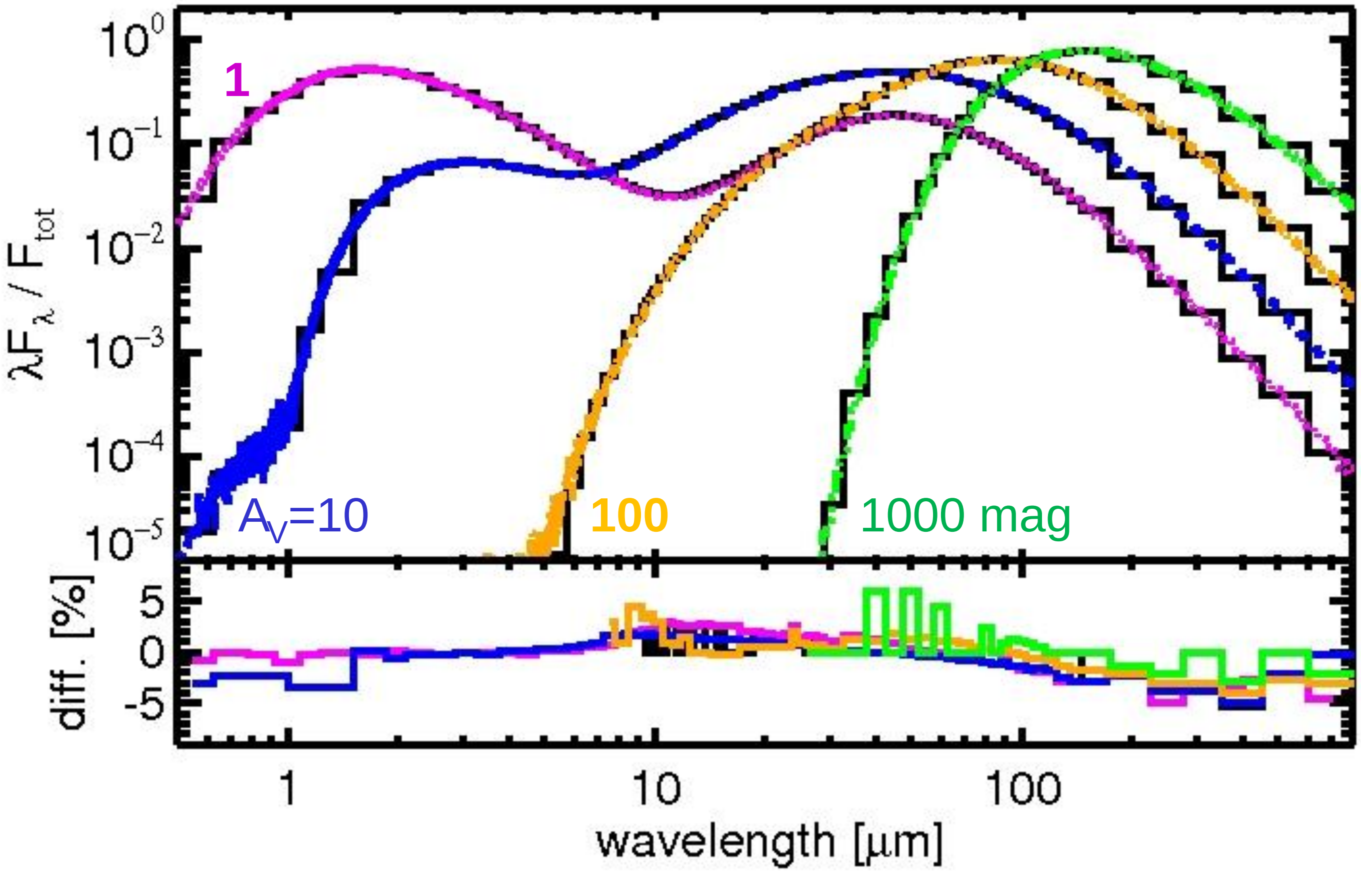


1. Cell locked when hit by photon
2. Parallel random number generator (Mersene Twister)
3. Computer games ⟹ Graphical Processing Units (CUDA)

1D benchmark sphere



1D benchmark sphere



T_* = 2500K

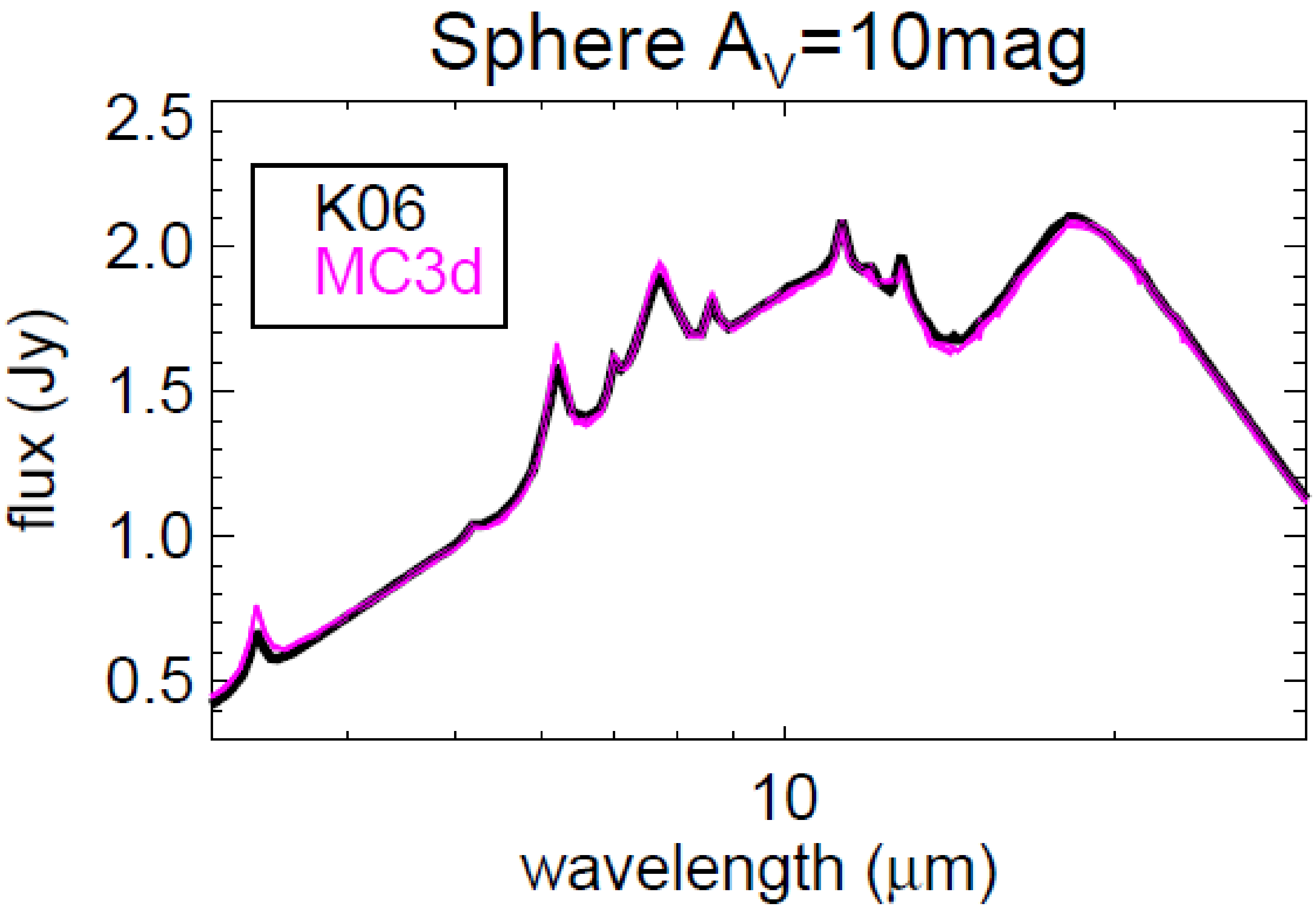
ρ(r) = const.

~5% for $\tau \longrightarrow 0$

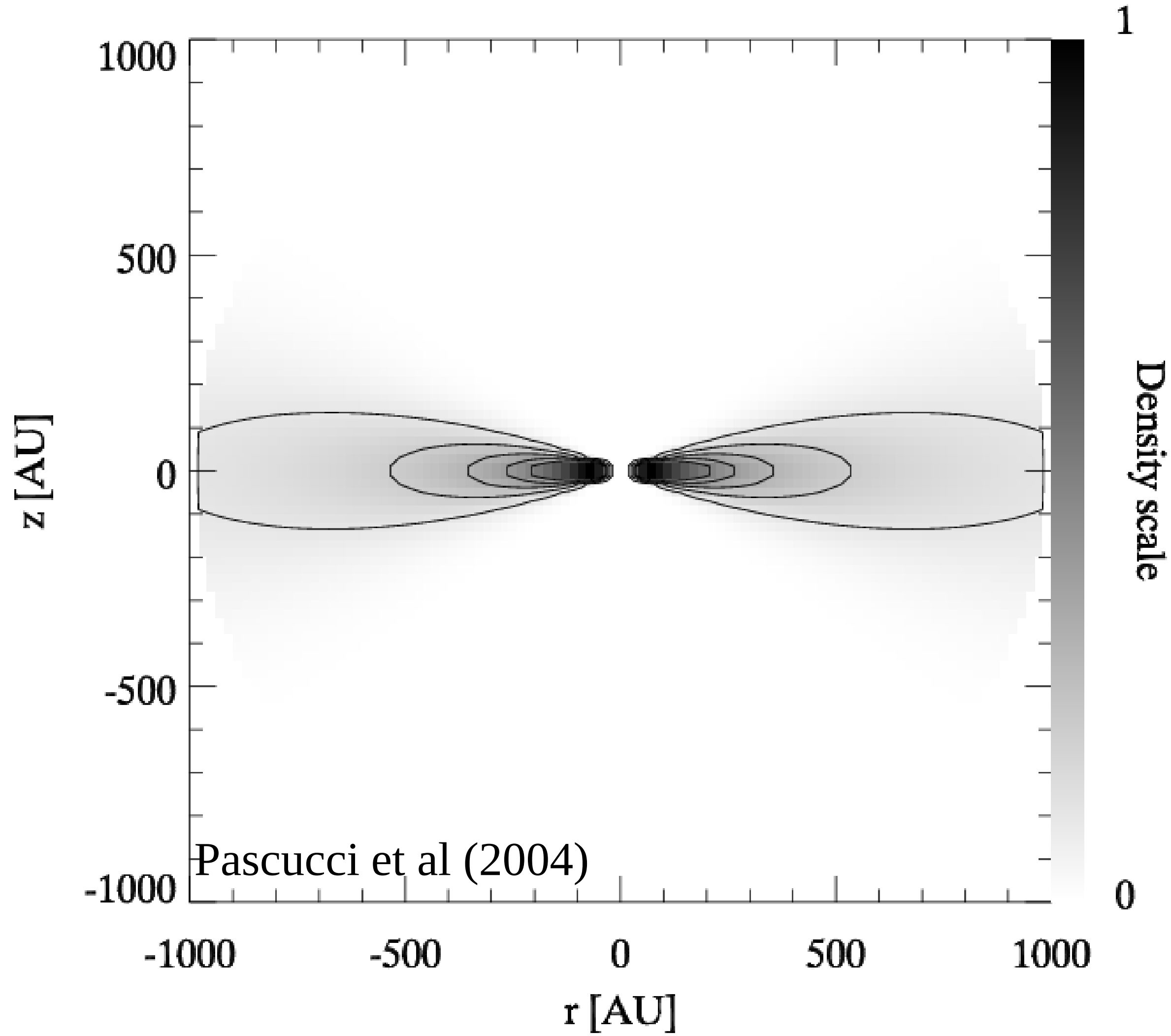
MC methods

Method	**Parallelization**	**Advantage**	**Time** Benchmark sphere τ~1000)
Lucy	YES (but floating)	Optical thin	>1h
Bjorkman & Wood	Partly (not independent)	No iteration	5min
our	YES	GPU	<1min

Monte Carlo + PAH



2D benchmark



Disk:

$T_* = 5800K$

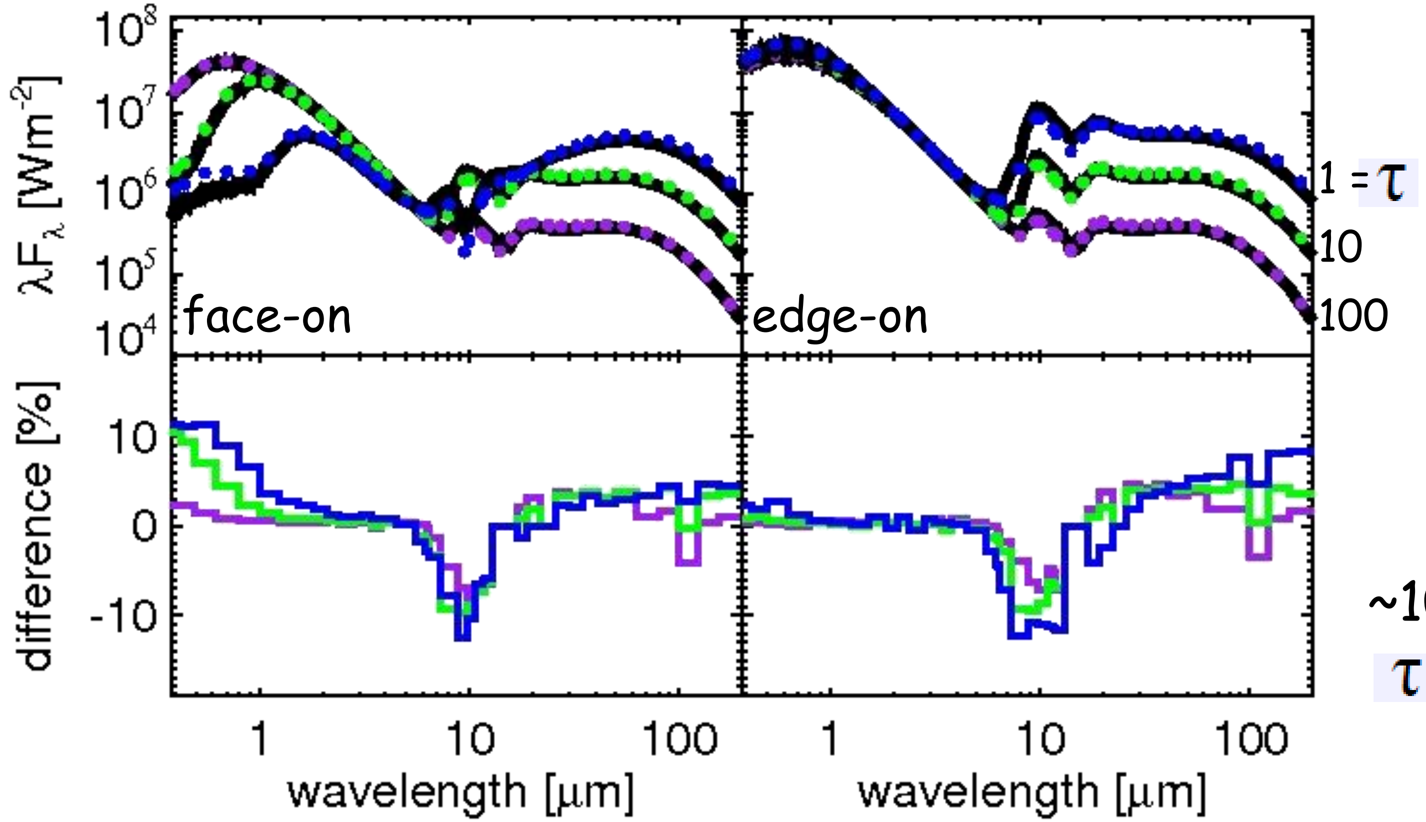
$L_* = L_{sun}$

$\rho(r)$: hydro static equilibrium

(Chiang & Goldreich 1997)

PAH in 3D

2D benchmark disk

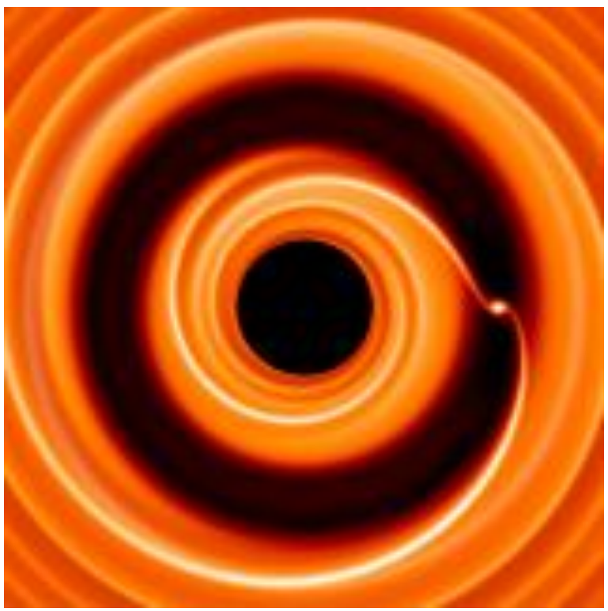


~10% for

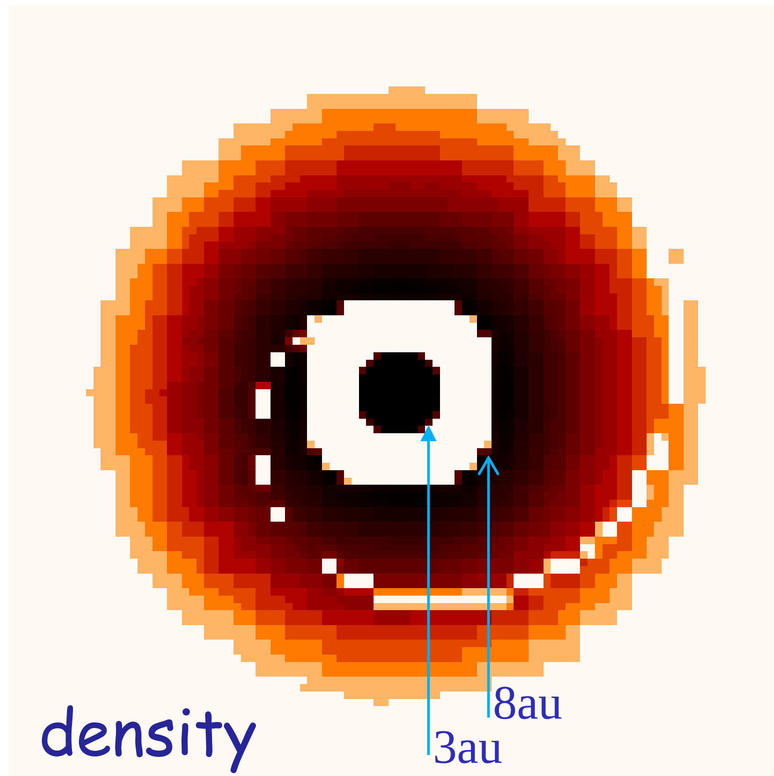
$\tau \rightarrow 0$

3D

proto-planetary disk
+ spiral



MHD (Fargo)



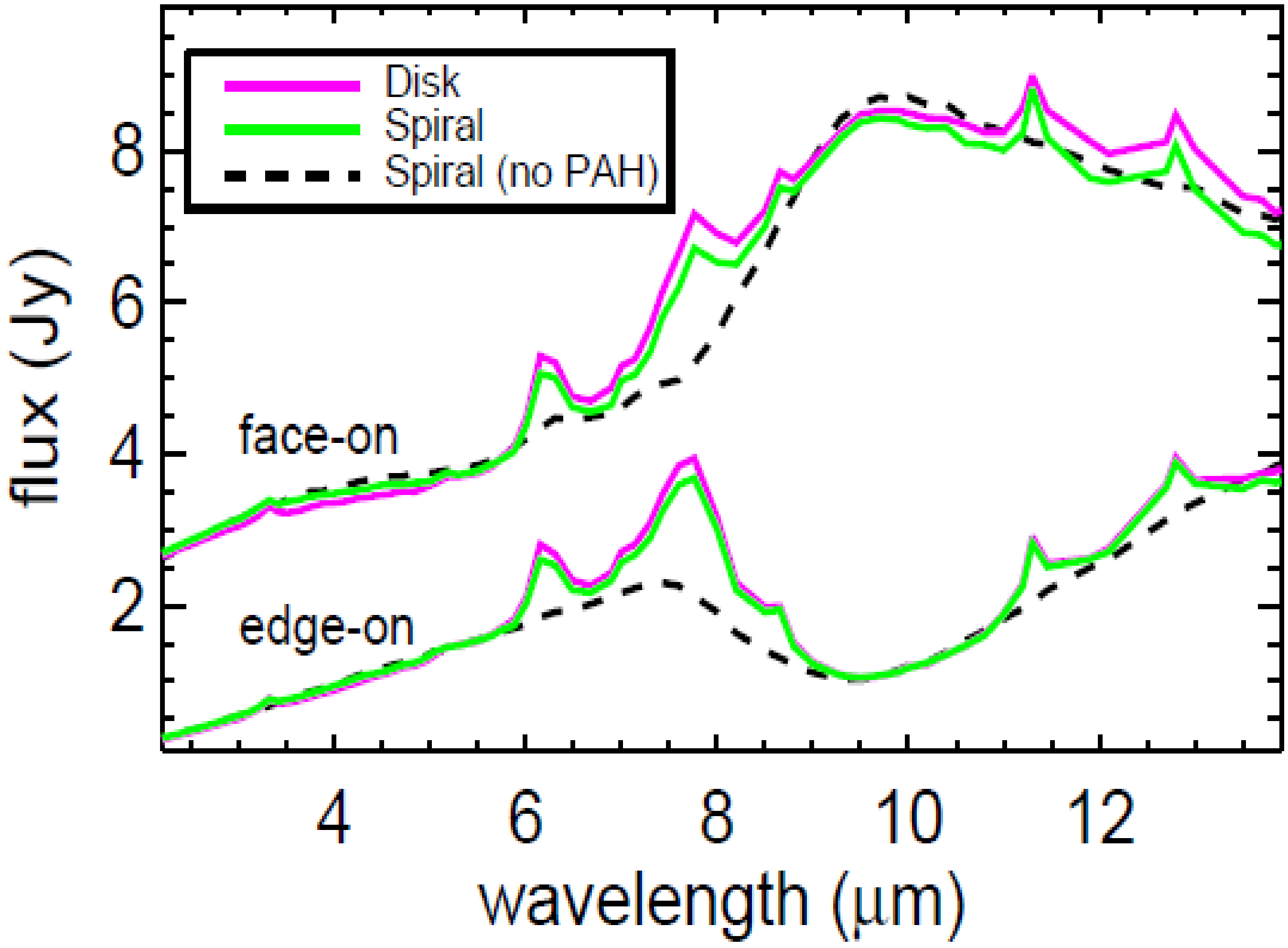
density

$T_* = 5800K$

$L_* = L_{sun}$

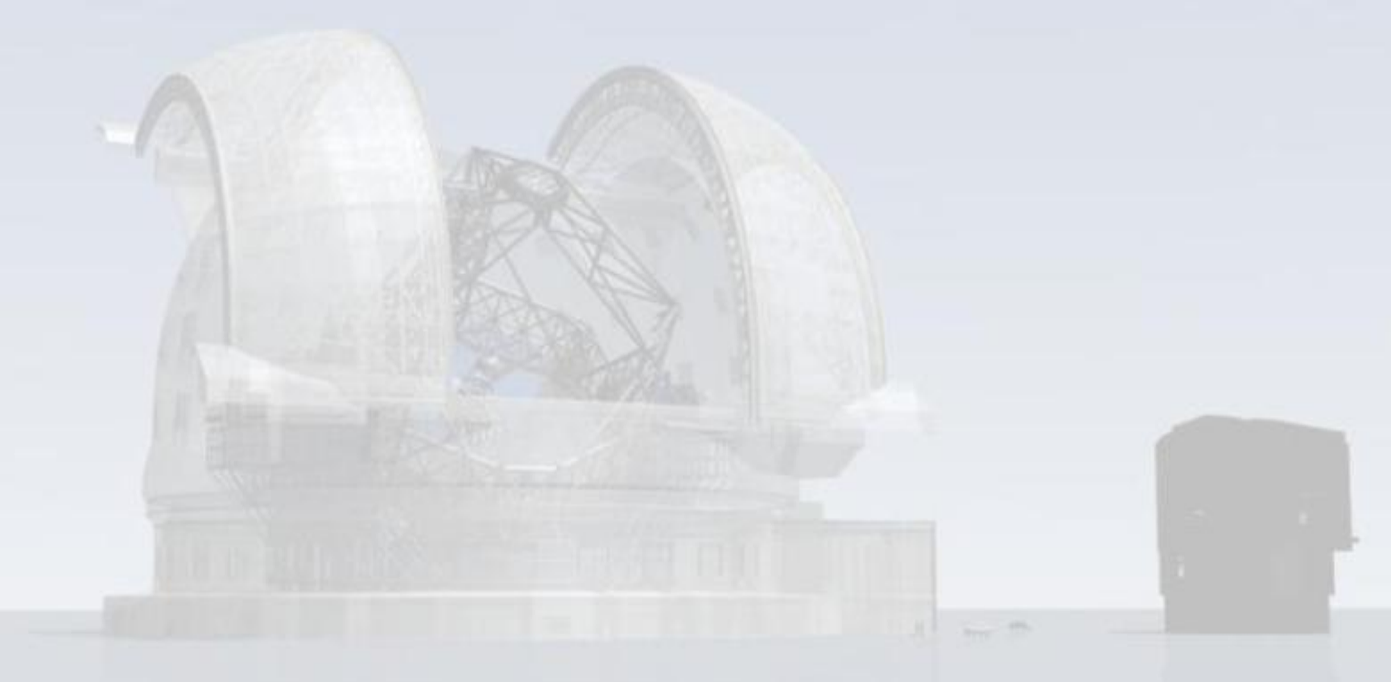
$A_V = 10mag$

3D
proto-planetary disk + spiral



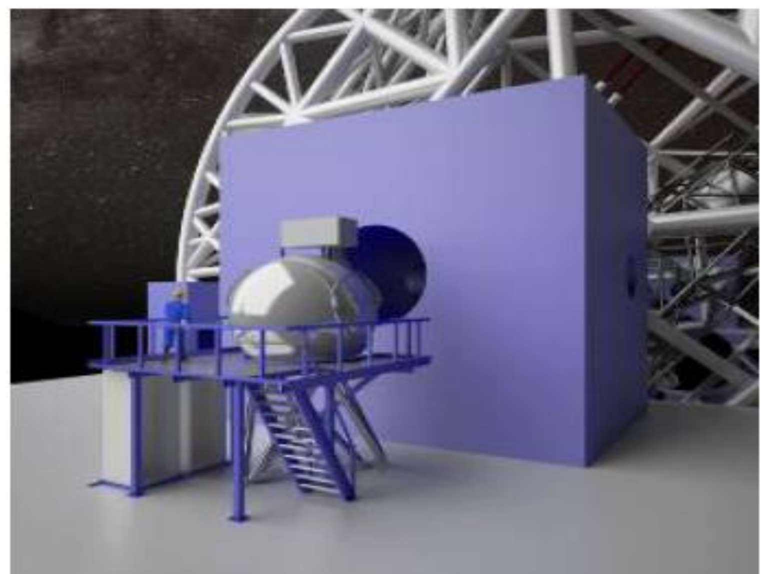
ELT 42m

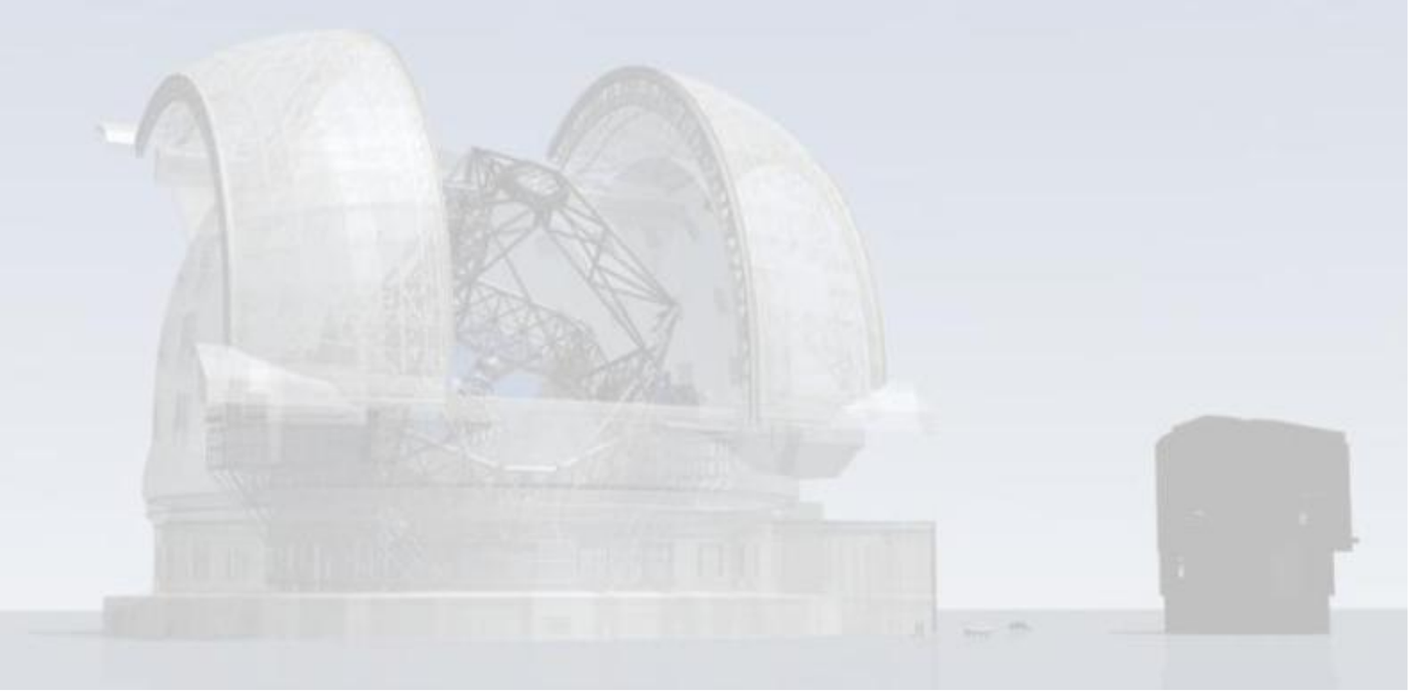
PAH imaging



METIS

Mid-infrared
E-ELT Imager and
Spectrograph





ELT 42m

PAH imaging

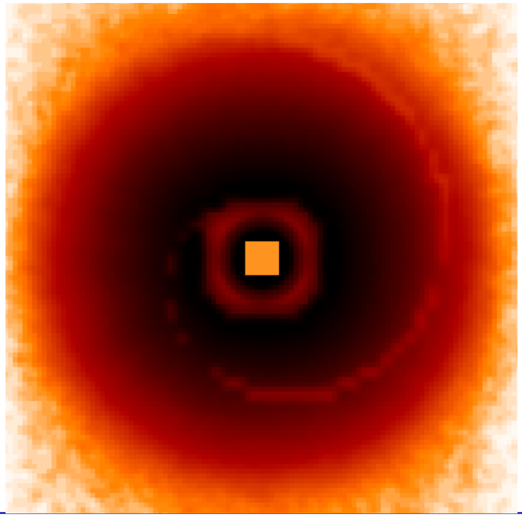
D = 50pc

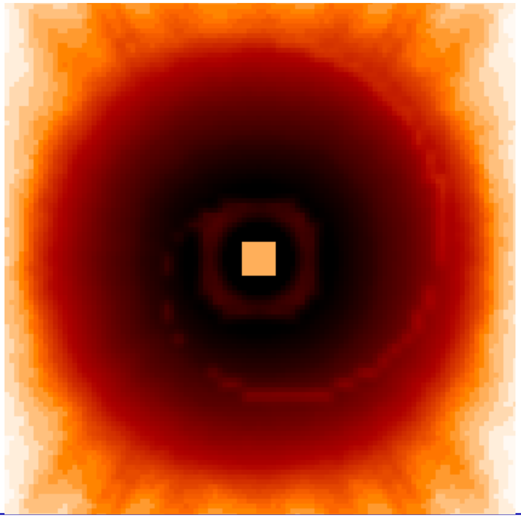
50mas

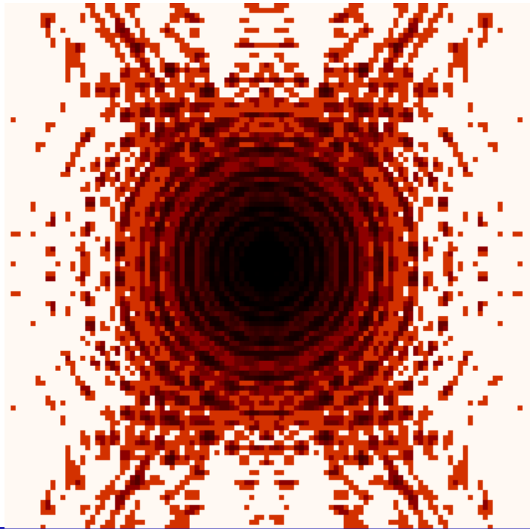
at 11.3μm

dual band + coronograph

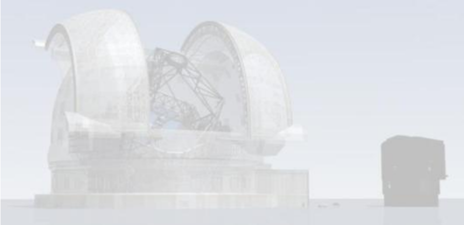
PSF

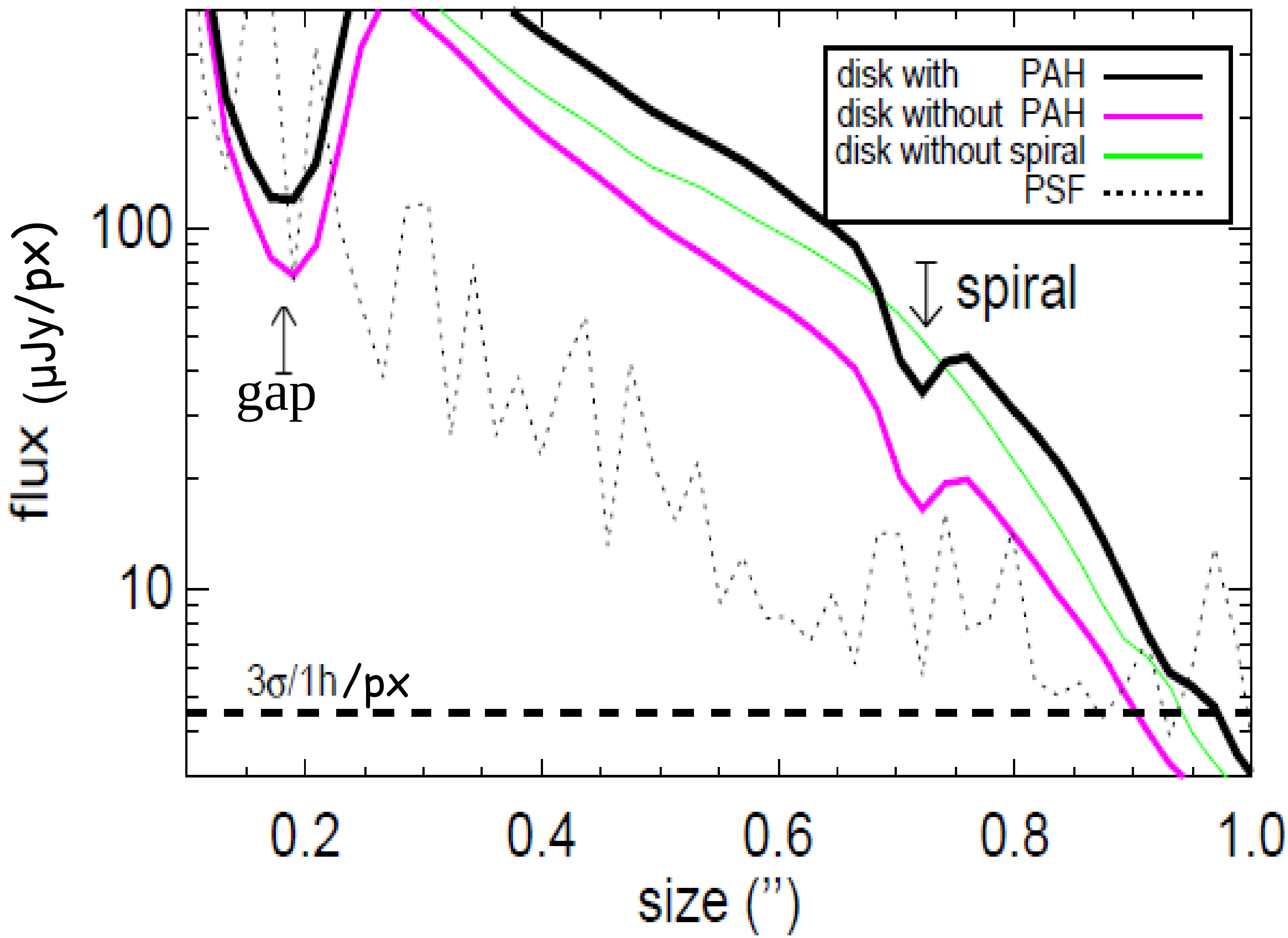






PAH in 3D





PAH imaging

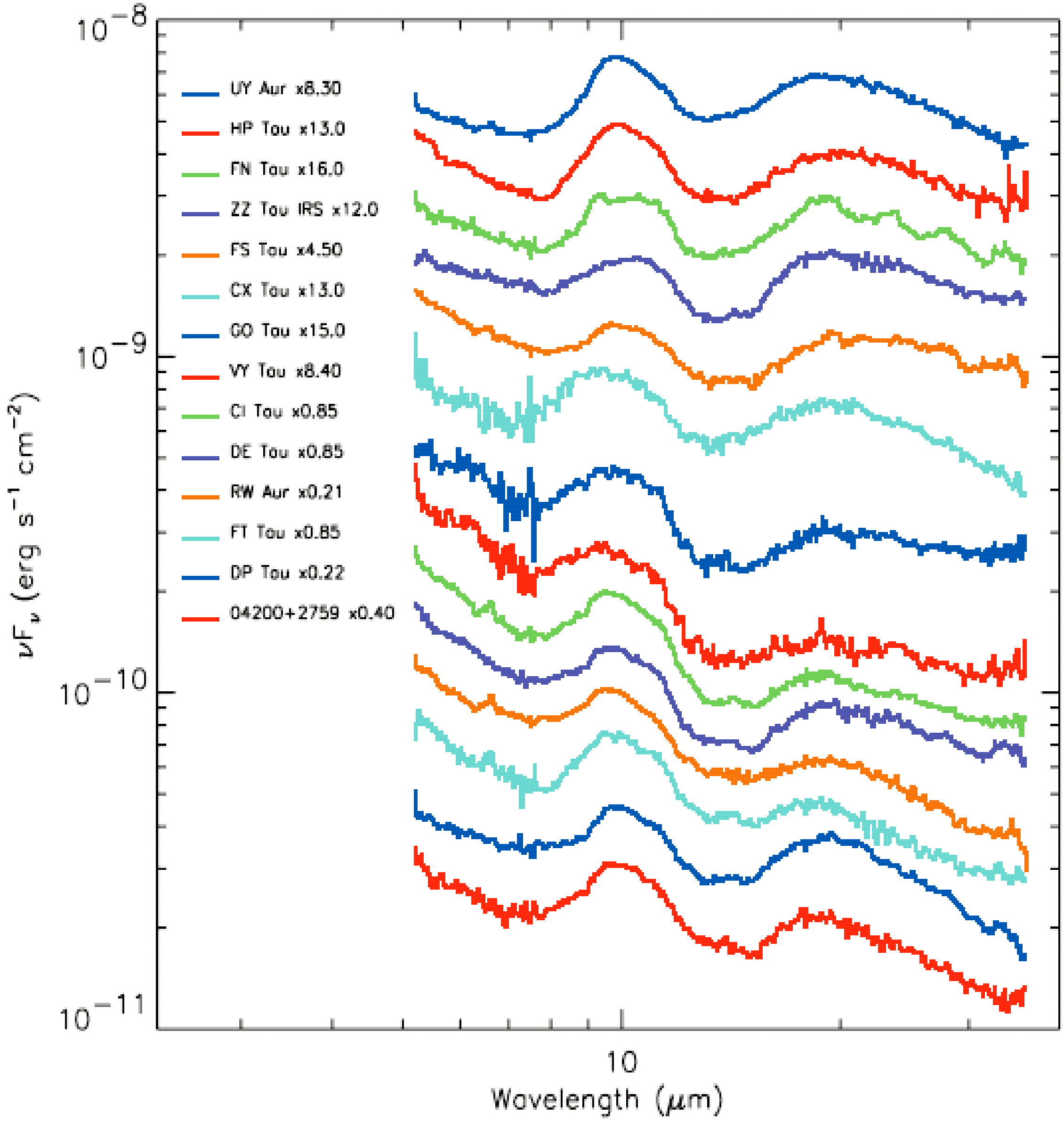
D = 50pc

50mas

at 11.3μm

T Tauri stars

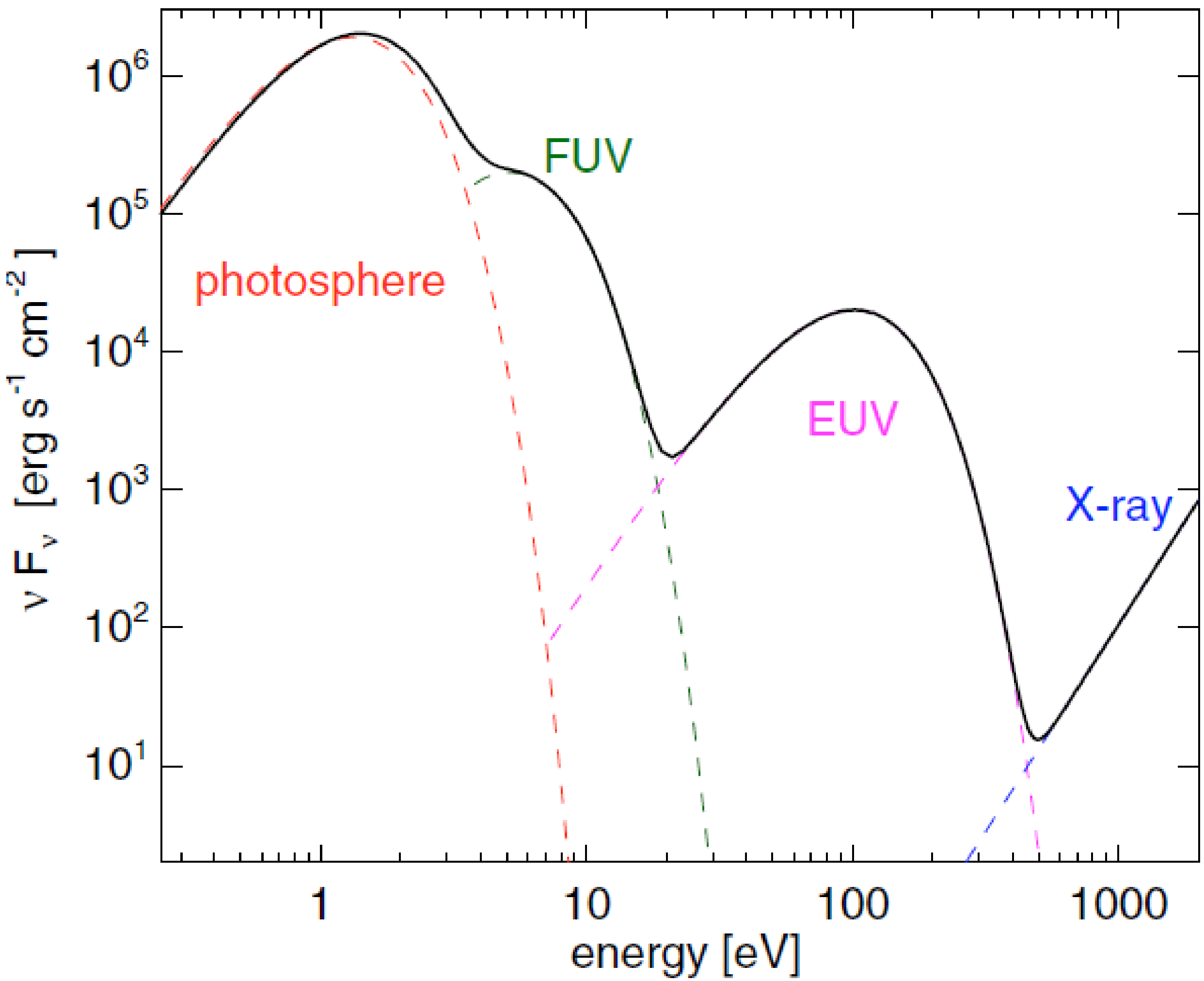
FURLAN ET AL.



PAH detection rate:

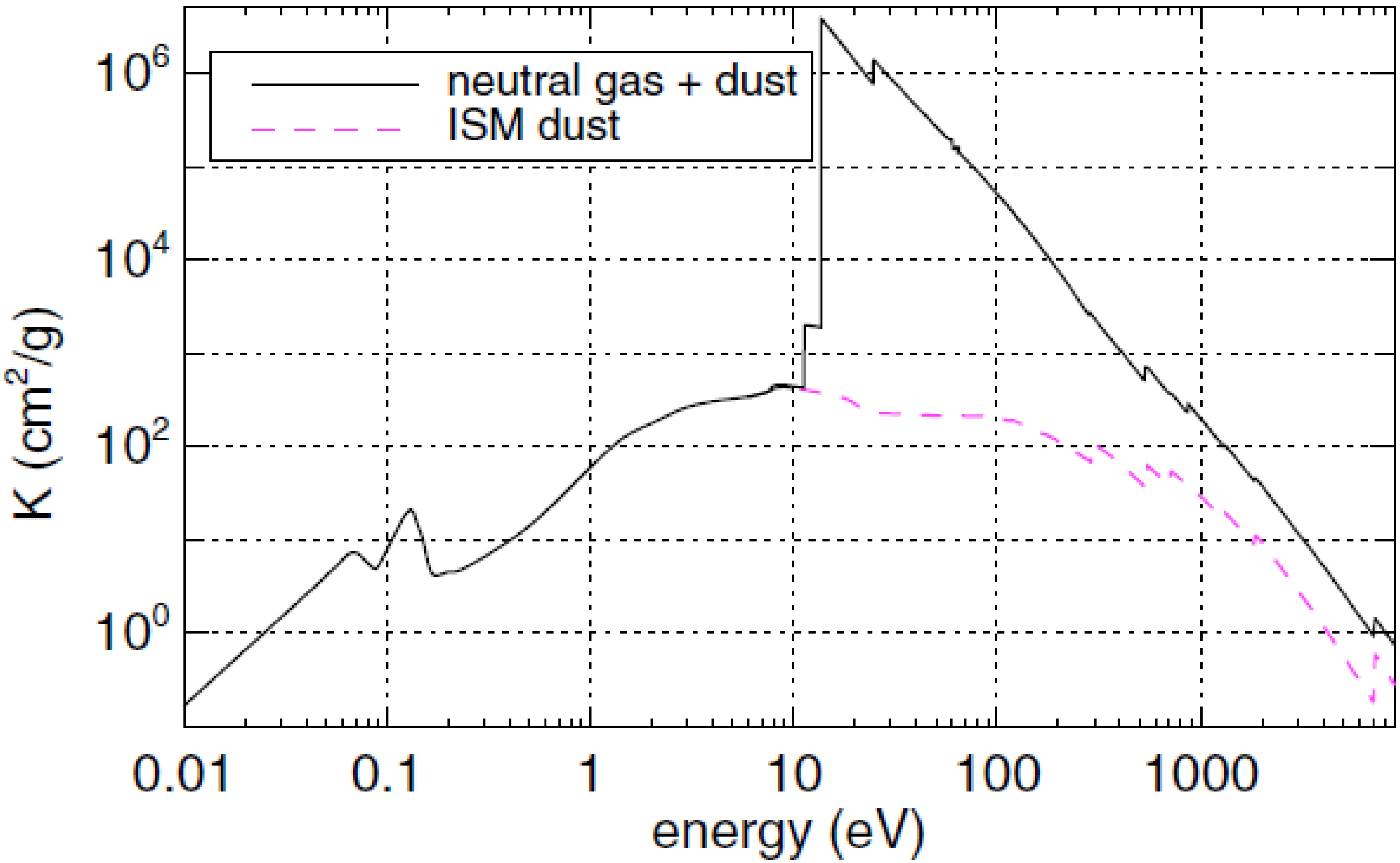
Herbig AeBe	60%
TTS	10%

T Tauri stars



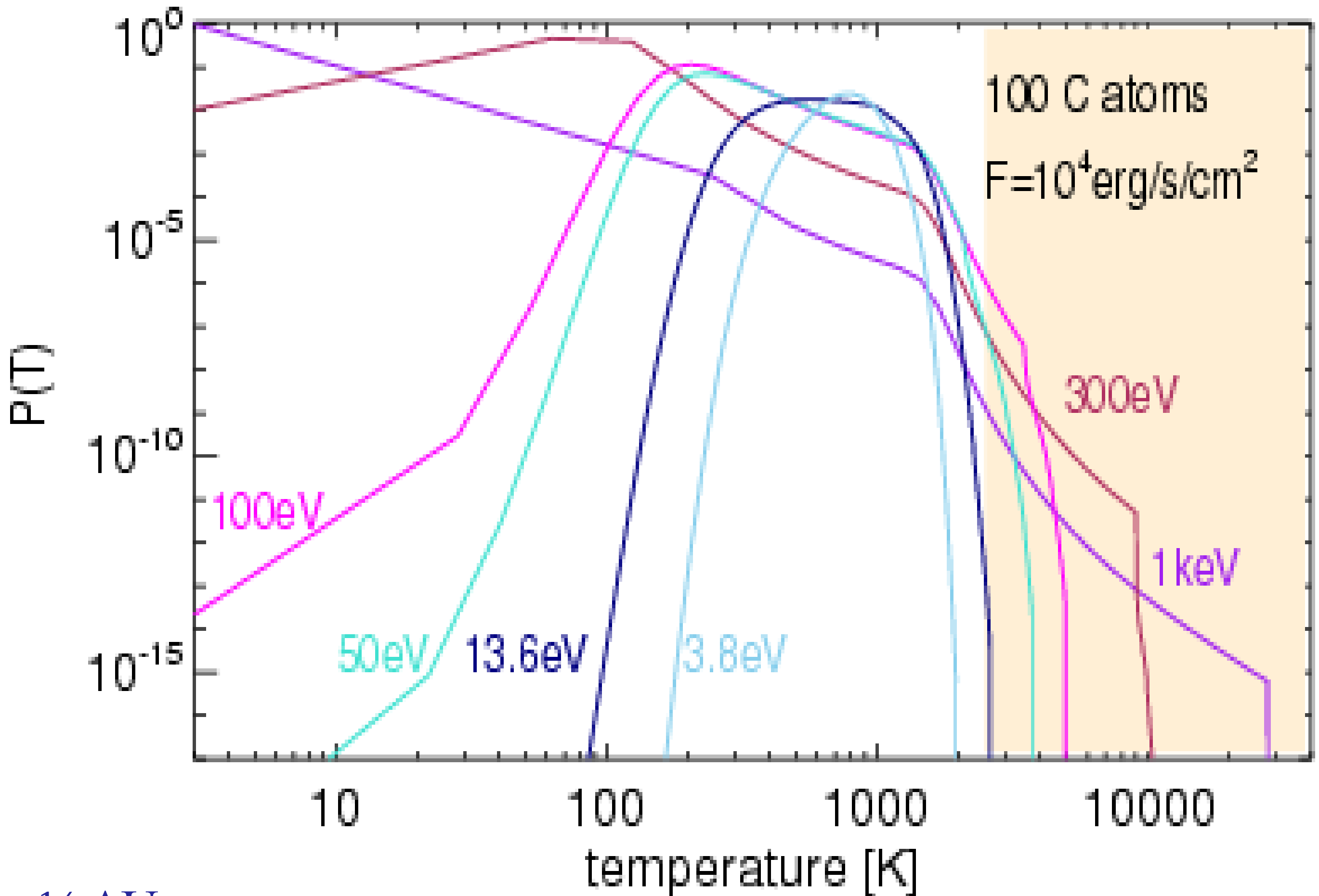
The spectral energy distribution of our T Tauri model star at 1 AU

PAH in 3D



neutral gas + dust
ISM dust
10^6
10^4
10^2
10^0
K (cm²/g)
0.01
0.1
1
10
100
1000
energy (eV)

PAH in a mono-energetic heating bath

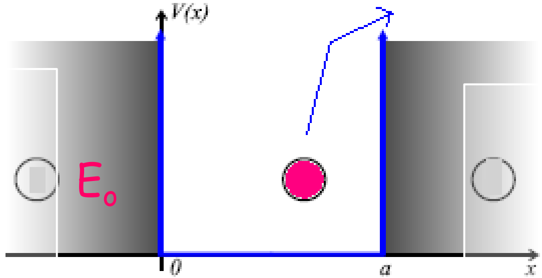


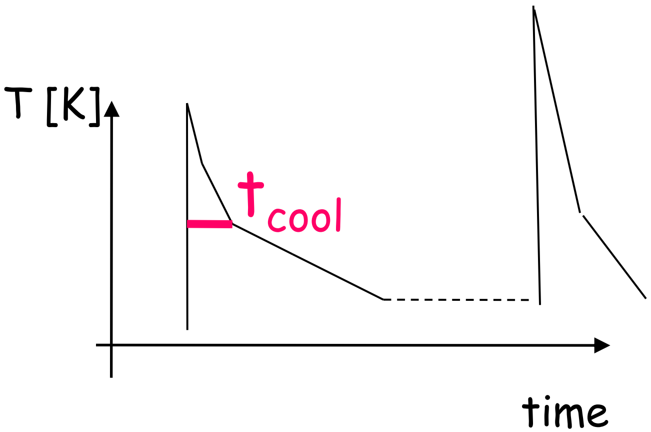
if $| U_f - U_i - h\nu | < \frac{1}{2} \Delta U_f$:

$$A_{fi} = K_\nu F_\nu / h\nu$$

Siebenmorgen & Krűgel (2010)

PAH destruction





$t_{abs} \sim 1h$

Unimolecular dissociation:

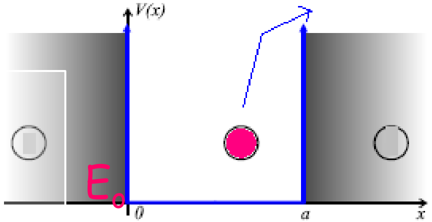
Arrhenius form:

$t_{dis} \sim \exp(E_o/kT) / \nu_0 \quad \ll t_{cool}/f \sim 1s$

$T_{min} = E_o/k \ln(\nu_0) \sim 2000K; \quad E_b \sim 5eV; \quad \nu_0 = 10^{13}Hz$

$\Delta E = 3N_c\, kT_{min} \quad \sim 0.1\, N_c \cdot E_o \quad => \quad N_c < 2\, \Delta E /[eV]$
(PAH unstable)

Omont (1986); Micedlotta et al. (2010); Tielens (2005)



PAH destruction

Unimolecular dissociation:

$t_{dis} \sim \exp(E_o/kT) / \nu_0 \quad \ll t_{cool}/f \sim 1s$

$T_{min} = E_o/k \ln(\nu_0) \sim 2000K; \quad E_o \sim 5eV$

$\Delta E = 3N_c\, kT_{min} \sim 0.1\, N_c \cdot E_o \Rightarrow N_c < 2\, \Delta E / [eV]$

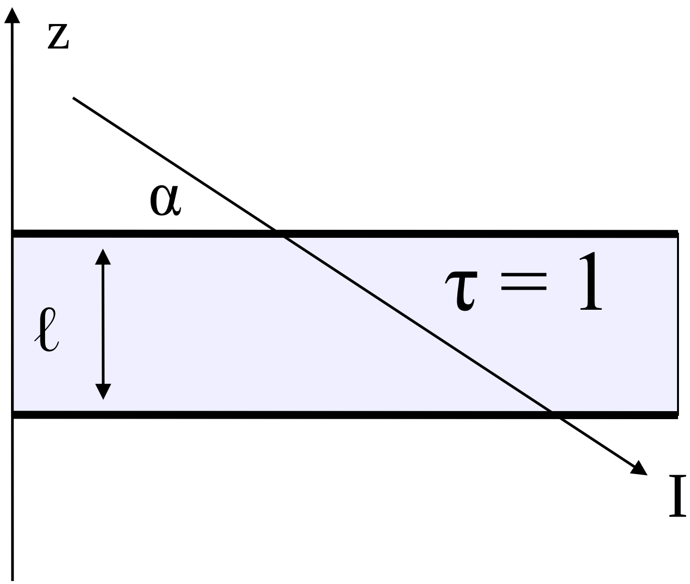
(PAH unstable)

1) single **hard** photon : independent of distance

2) many **soft** photons : ~ 1AU

Stationary disk

Sufficient X-ray photons?



} top surface layer $\Sigma_\ell = \alpha/\kappa$

$$\frac{\#\ \text{C in PAH}}{\#\ \text{hard}\ \gamma\ \text{absorption/sec}} = h\nu \cdot 4\pi r^2/L\kappa$$

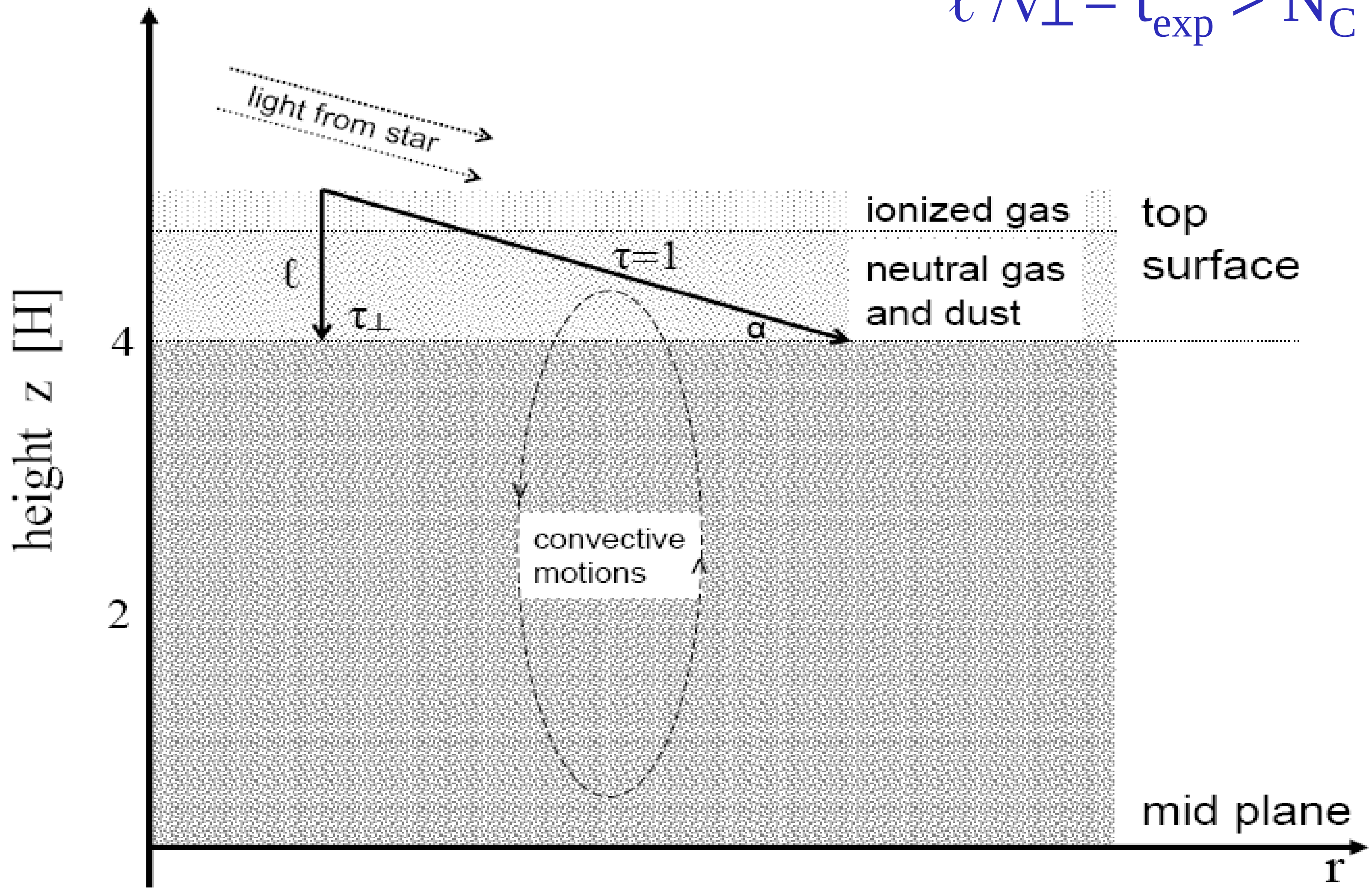
↑

'PAH removal time'   << TT phase

PAH replenishment

Vertical mixing in disk?

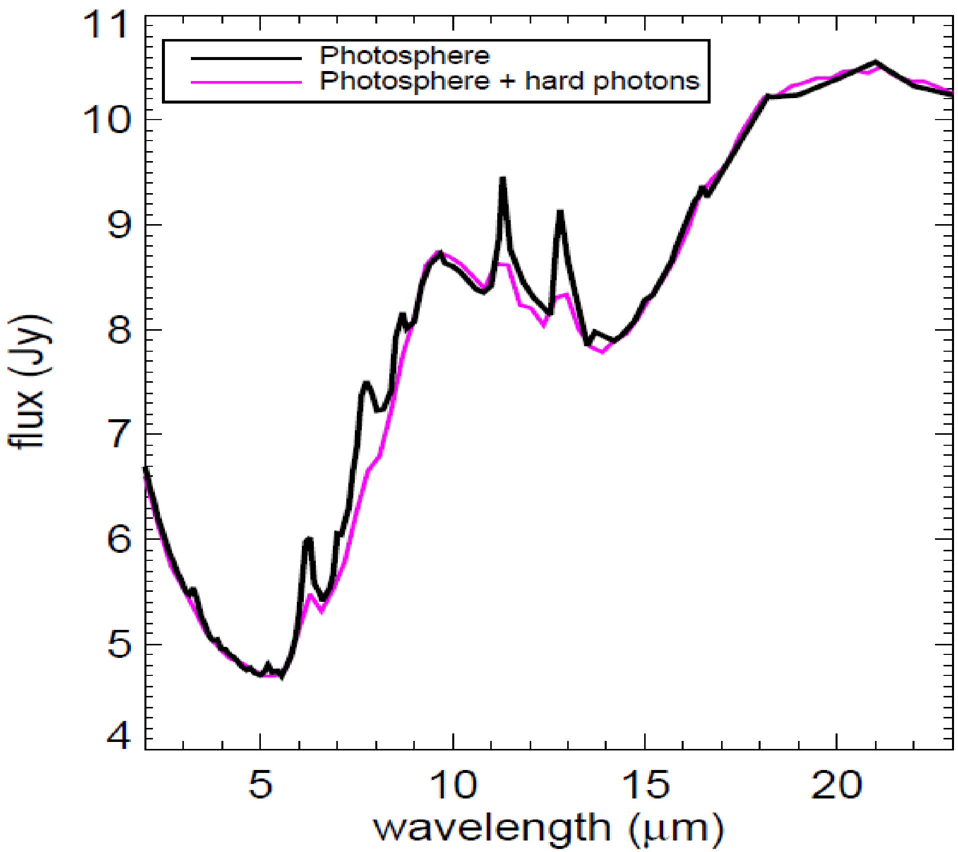
$\ell / v_{\perp} = t_{exp} > N_C \, t_{abs}$



Siebenmorgen & Krűgel (2010)

Future

MC model of T Tauri disks



- Heating:
  photosph.+FEUV + X-rays
- Dust + Gas
- Density structure
- PAH
  emission + destruction

Conclusion

?