Radiative Transfer

Lecture 02

The Physics of Star Formation

Les Houches School of Physics February 21, 2024

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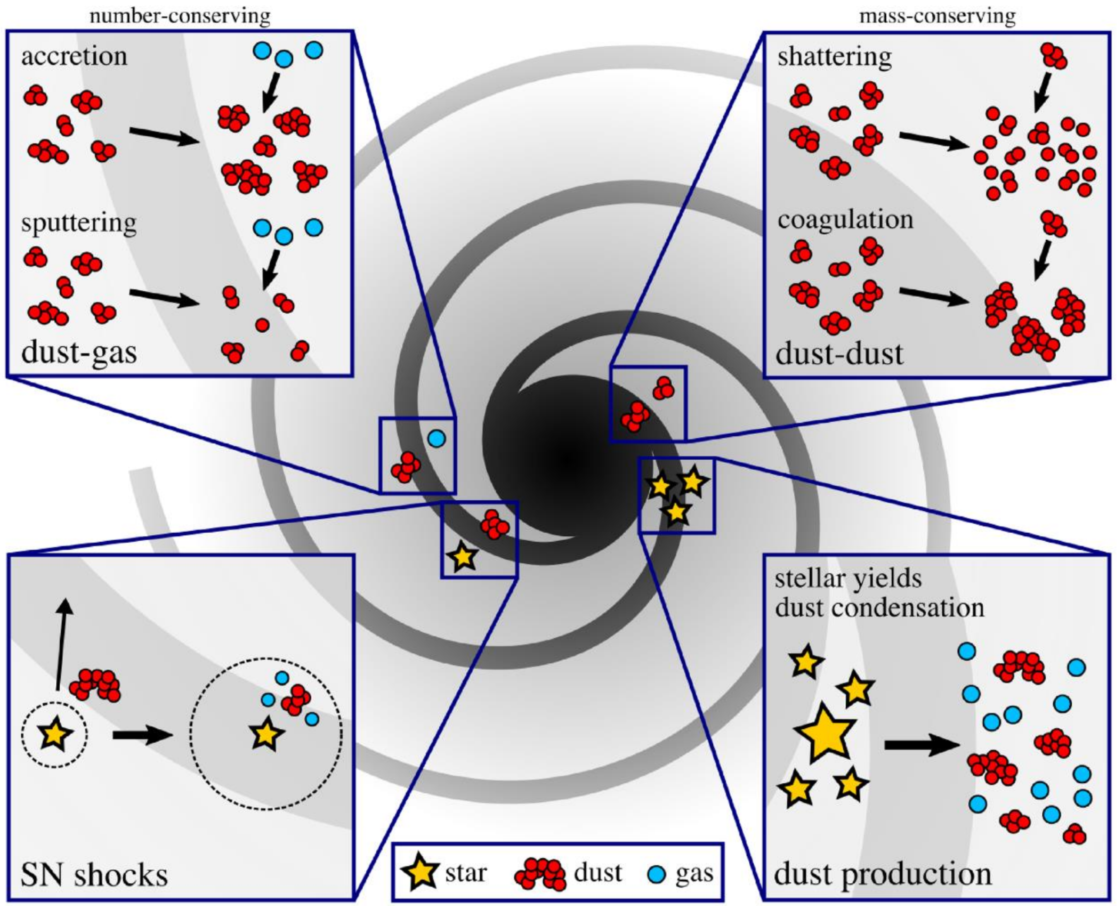
Zentrum für Astronomie der Universität Heidelberg

Optical properties of dust

Lifecycle of dust

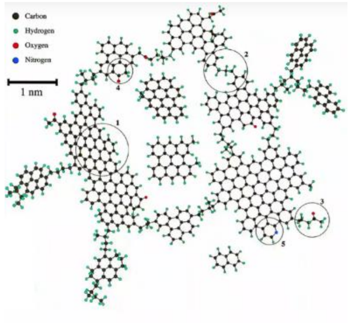


McKinnon+ 2018

⇒ Dust is omnipresent and comes in different shapes sizes and compositions

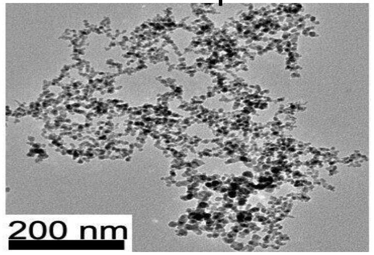
Dust sizes and shapes

Polycyclic aromatic hydrocarbons (PAH)

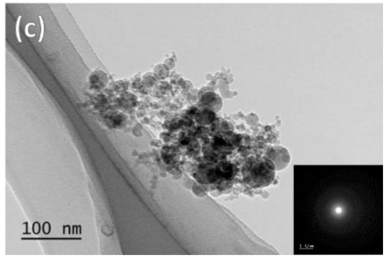


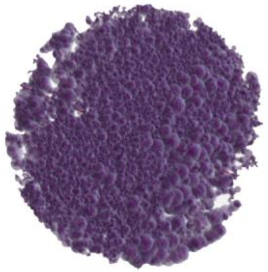
1 nm

Sooth in the earth athmosphere



Theoretical model



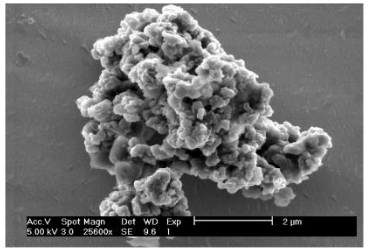


Laboratory experiment

100 nm

"typical" dust

Interplanetary dust



1 µm

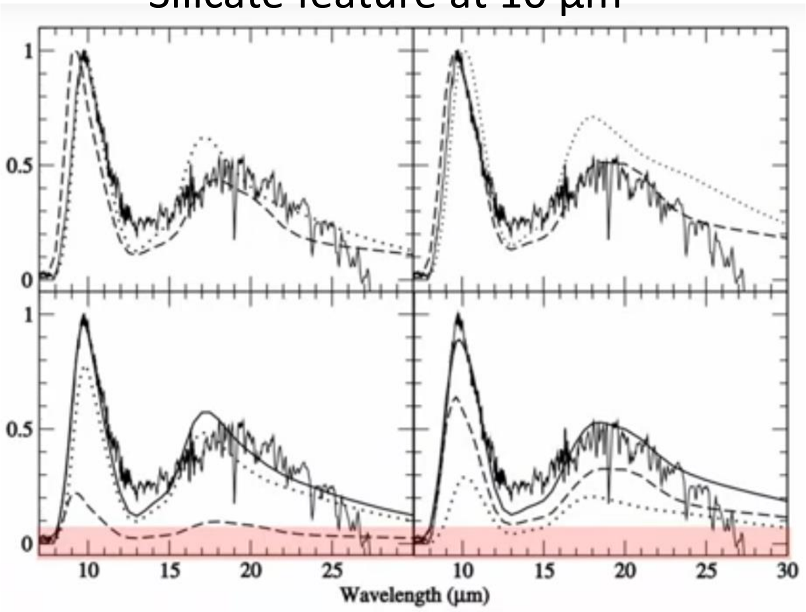
meteor

1 cm

(effective) grain size: $a_{\mathrm{eff}} = \sqrt[3]{\frac{3}{4\pi} V_{\mathrm{grain}}}$

Dust ingredients

Silicate feature at 10 µm



Chiar & Tielens 2006

~100 % Si, Mg, Ca, Al, Fe, and Ni is in grains

- Almost all Si and Mg is in silicates
- 30 % of Fe is in silicates (rest is missing)
- 20 % of O is in silicates and oxides

Possible candidates

- Forsterite (Mg_2SiO_4) (astrosilicate)
- Fayalite (Fe_2SiO_4)
- Enstatite ($Mg\ SiO_3$)
- Ferrosilite ($Fe\ SiO_3$)

~40 % of C is in grains

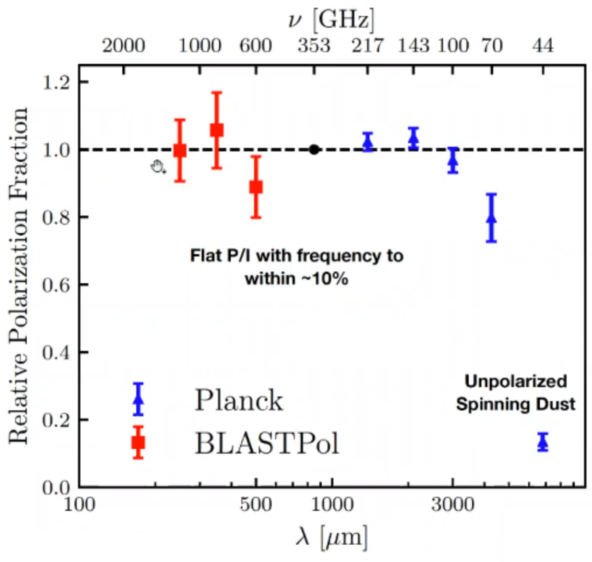
- ~15 % is in PAHs
- 5 – 10 % is in hydroyarbons
- 20 % is unknown

Dust material

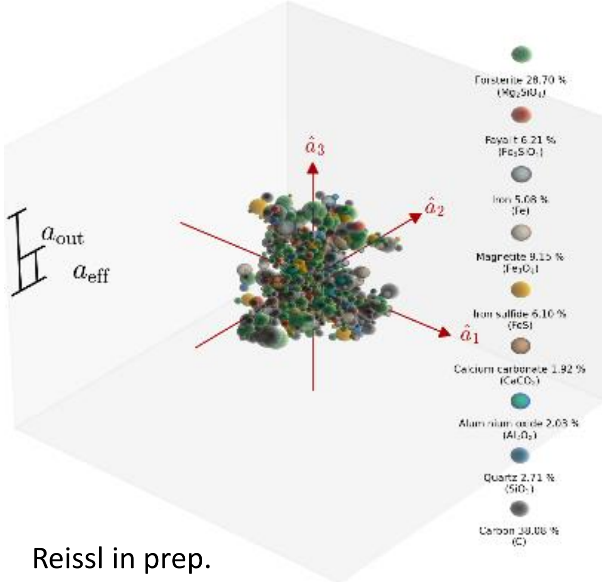
Silicates + Graphite + PAH

“Classic” Dust:
Silicates and graphite are separate components

“Astrodust” model:
Amorphous silicates + carbon material + other ($\mathrm{Fe_XO_Y}$ + $\mathrm{Al_2O_2}$ + $\mathrm{CaCo_3}$ + …)



Draine+ 2021



Reissl in prep.

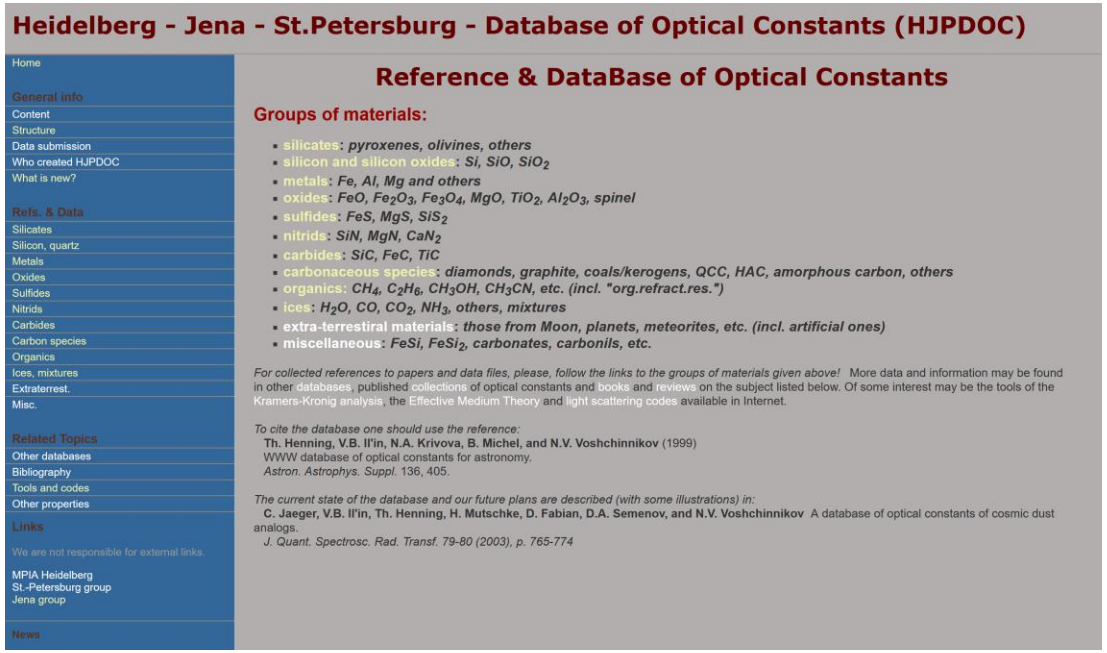
Optical properties are quantified by the complex refractive index:

$$m = n + ik$$

- Real part n (refraction)
- Imaginary part k (attenuation)

Material constants

https://www2.mpia-hd.mpg.de/HJPDOC/



Heidelberg - Jena - St.Petersburg - Database of Optical Constants (HJPDOC)

- Home
- General info
- Content
- Structure
- Data submission
- Who created HJPDOC
- What is new?
- Refs. & Data
- Silicates
- Silicon, quartz
- Metals
- Oxides
- Sulfides
- Nitrids
- Carbides
- Carbon species
- Organics
- Ices, mixtures
- Extraterrest.
- Misc.
- Related Topics
- Other databases
- Bibliography
- Tools and codes
- Other properties
- Links

We are not responsible for external links.

MPIA Heidelberg
St.-Petersburg group
Jena group

News

Reference & DataBase of Optical Constants

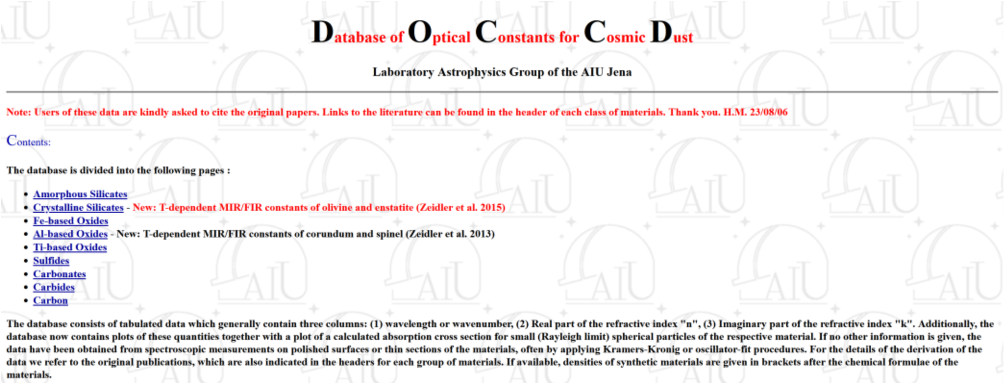
Groups of materials:

- silicates: *pyroxenes, olivines, others*
- silicon and silicon oxides: *Si, SiO, SiO_2*
- metals: *Fe, Al, Mg and others*
- oxides: *FeO, Fe_2O_3, Fe_3O_4, MgO, TiO_2, Al_2O_3, spinel*
- sulfides: *FeS, MgS, SiS_2*
- nitrids: *SiN, MgN, CaN_2*
- carbides: *SiC, FeC, TiC*
- carbonaceous species: *diamonds, graphite, coals/kerogens, QCC, HAC, amorphous carbon, others*
- organics: *CH_4, C_2H_6, CH_3OH, CH_3CN, etc. (incl. "org.refract.res.")*
- ices: *H_2O, CO, CO_2, NH_3, others, mixtures*
- extra-terrestiral materials: *those from Moon, planets, meteorites, etc. (incl. artificial ones)*
- miscellaneous: *FeSi, $FeSi_2$, carbonates, carbonils, etc.*

For collected references to papers and data files, please, follow the links to the groups of materials given above! More data and information may be found in other databases, published collections of optical constants and books and reviews on the subject listed below. Of some interest may be the tools of the Kramers-Kronig analysis, the Effective Medium Theory and light scattering codes available in Internet.

To cite the database one should use the reference:
Th. Henning, V.B. Il'in, N.A. Krivova, B. Michel, and N.V. Voshchinnikov (1999)
WWW database of optical constants for astronomy.
Astron. Astrophys. Suppl. 136, 405.

The current state of the database and our future plans are described (with some illustrations) in:
C. Jaeger, V.B. Il'in, Th. Henning, H. Mutschke, D. Fabian, D.A. Semenov, and N.V. Voshchinnikov A database of optical constants of cosmic dust analogs.
J. Quant. Spectrosc. Rad. Transf. 79-80 (2003), p. 765-774



Database of Optical Constants for Cosmic Dust

Laboratory Astrophysics Group of the AIU Jena

Note: Users of these data are kindly asked to cite the original papers. Links to the literature can be found in the header of each class of materials. Thank you. H.M. 23/08/06

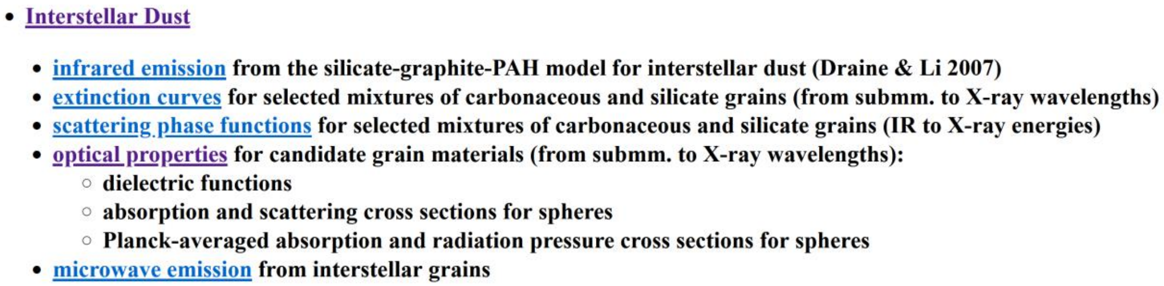
Contents:

The database is divided into the following pages :

- Amorphous Silicates
- Crystalline Silicates - New: T-dependent MIR/FIR constants of olivine and enstatite (Zeidler et al. 2015)
- Fe-based Oxides
- Al-based Oxides - New: T-dependent MIR/FIR constants of corundum and spinel (Zeidler et al. 2013)
- Ti-based Oxides
- Sulfides
- Carbonates
- Carbides
- Carbon

The database consists of tabulated data which generally contain three columns: (1) wavelength or wavenumber, (2) Real part of the refractive index "n", (3) Imaginary part of the refractive index "k". Additionally, the database now contains plots of these quantities together with a plot of a calculated absorption cross section for small (Rayleigh limit) spherical particles of the respective material. If no other information is given, the data have been obtained from spectroscopic measurements on polished surfaces or thin sections of the materials, often by applying Kramers-Kronig or oscillator-fit procedures. For the details of the derivation of the data we refer to the original publications, which are also indicated in the headers for each group of materials. If available, densities of synthetic materials are given in brackets after the chemical formulae of the materials.

https://www.astro.uni-jena.de/Laboratory/OCDB/



- **Interstellar Dust**
  - **infrared emission from the silicate-graphite-PAH model for interstellar dust (Draine & Li 2007)**
  - **extinction curves for selected mixtures of carbonaceous and silicate grains (from submm. to X-ray wavelengths)**
  - **scattering phase functions for selected mixtures of carbonaceous and silicate grains (IR to X-ray energies)**
  - **optical properties for candidate grain materials (from submm. to X-ray wavelengths):**
    - **dielectric functions**
    - **absorption and scattering cross sections for spheres**
    - **Planck-averaged absorption and radiation pressure cross sections for spheres**
  - **microwave emission from interstellar grains**

https://www.astro.princeton.edu/~draine/

Optical properties of dust

geometric cross section

$$\sigma = \pi\, a_{\text{eff}}{}^2 \quad [cm^2]$$

cross section

$$C = \sigma\, Q \quad [cm^2]$$

opacity

$$\kappa = \frac{\sigma\, Q}{m} \quad [cm^2 kg^{-1}]$$

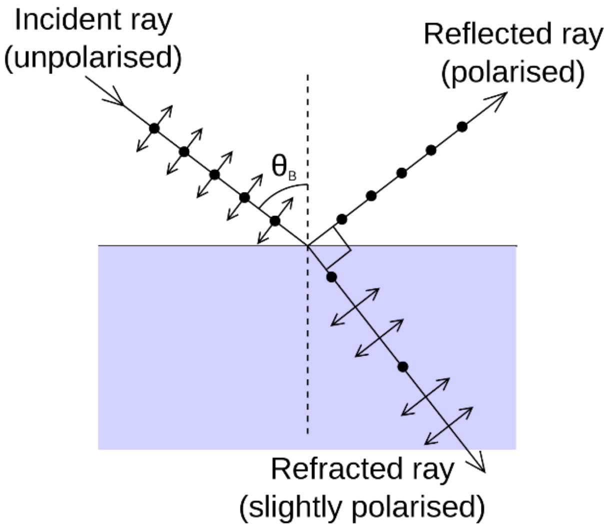
Dimensionless parameter Q quantifies:

- grain shape
- material composition
- wavelength
- grain orientation
- polarization
- temperature

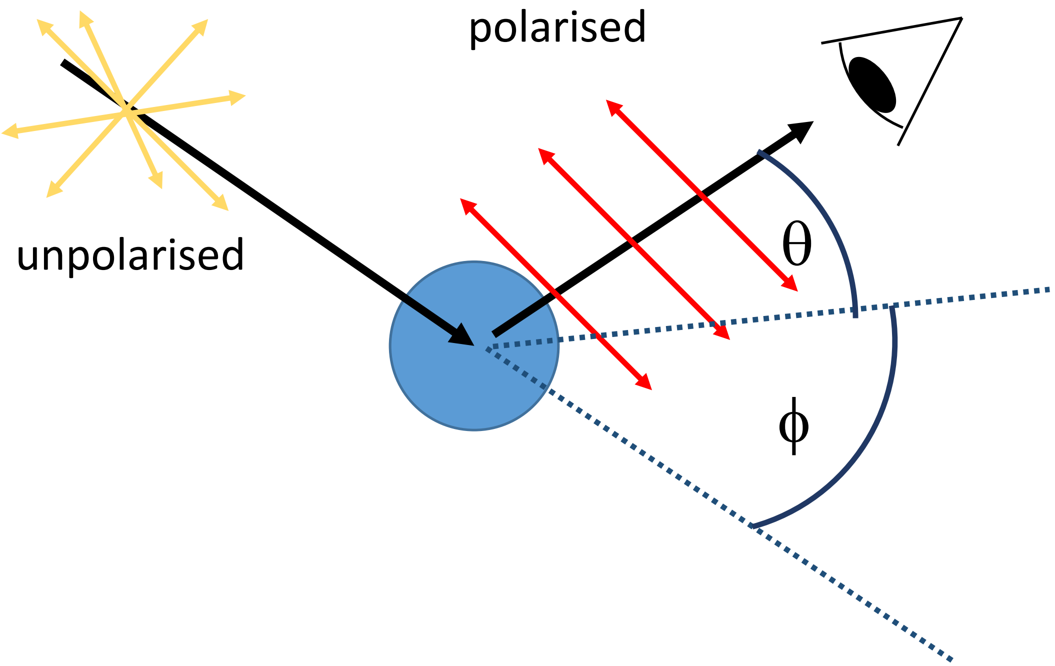
RT with dust grains

Dust scattering

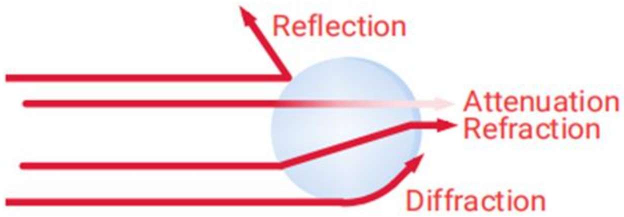
Reflection and transmission e.g. on a water surface

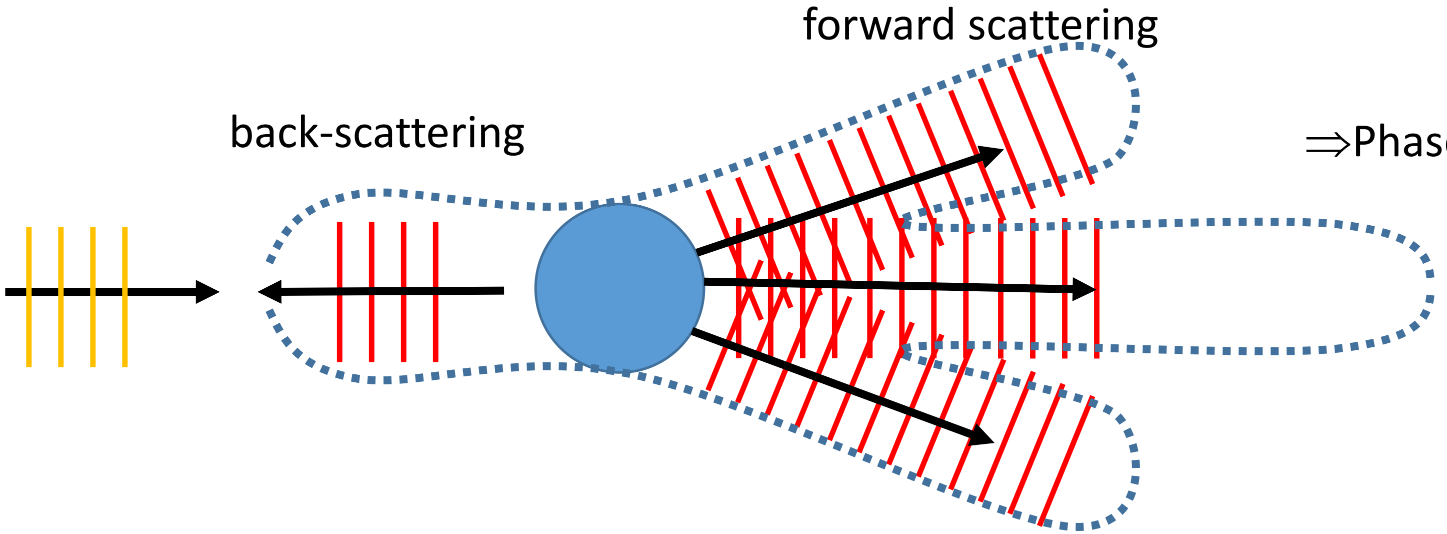


Scattering on a dust grain



Scattering phase function





$\Rightarrow$Phase function $\Psi(\theta, \phi)$ normalized such that

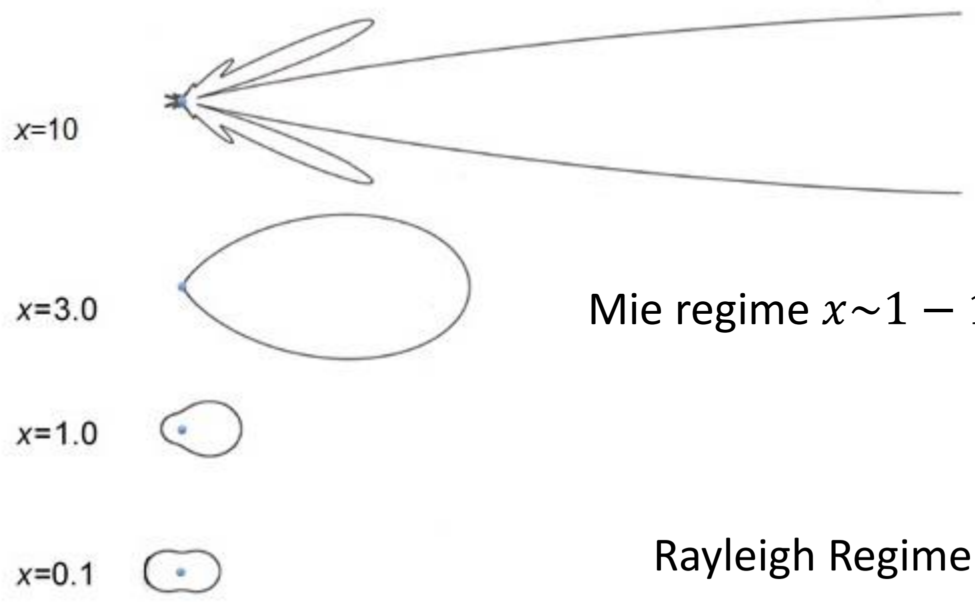
$$\int_{4\pi} \Psi(\theta, \phi)\, d\Omega = 1$$

Scattering source term: $j_{sca} = \kappa_{sca} \int_{4\pi} I \Psi(\theta, \phi) d\Omega$

Wavelengths regime

Size parameter $\mathrm{x} = \frac{2\pi\, a_{\mathrm{eff}}}{\lambda}$

Geometrical optics



Mie regime $x \sim 1 - 1000$

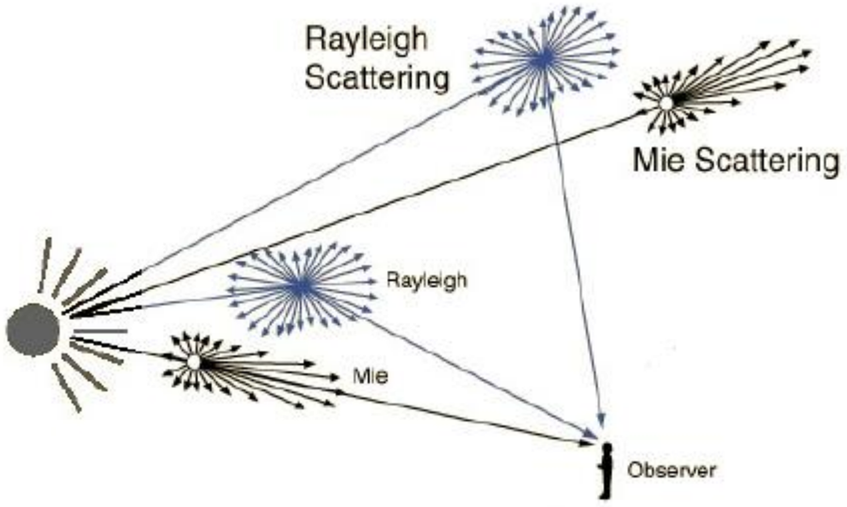
Rayleigh Regime

Rayleigh regime

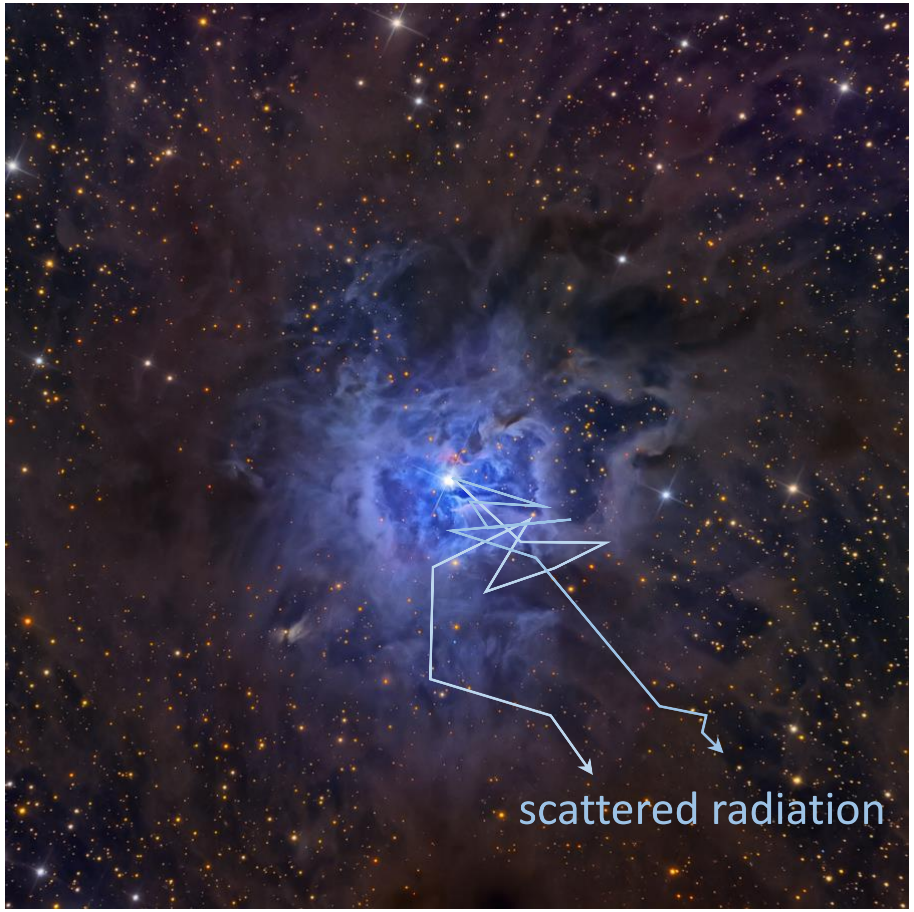
scattering: $Q_{sca} \approx \frac{8}{3} x^4 \left| \frac{m^2-1}{m^2+1} \right|^2$

Absorption: $Q_{abs} \approx 4x \,\mathrm{Im}\left(\frac{m^2-1}{m^2+1} \right)$

Phase function: $\Psi(\theta) \approx \frac{3}{4}\left(1 + \cos\theta^2\right)$



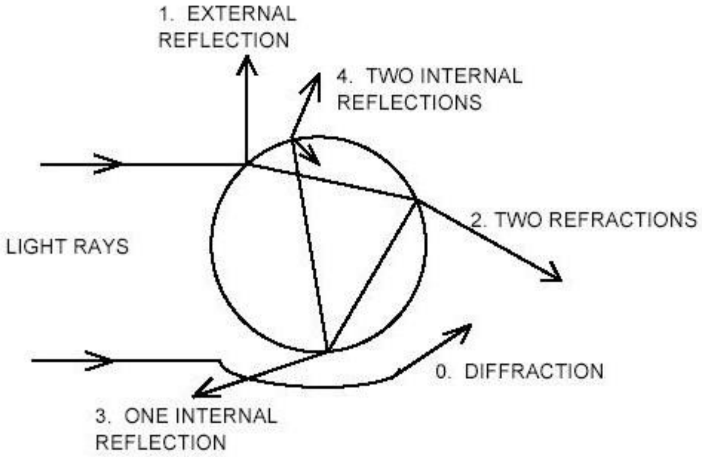
NGC 7023 Iris Nebula



Mie Theory

The Mie theory is a complete mathematical–physical theory of the scattering of electromagnetic wave by homogeneous spherical particles

Solution for each direction Θ can be calculated as a sum of Ricati – Bessel functions $\psi_k(x)$ and $\xi_k(x)$ and the recursive angular functions



$$\pi_k(\theta) = \frac{2k-1}{2k+1}\pi_{k-1}(\theta) \cos\theta - \frac{k}{k-1}\pi_{k-2}(\theta)$$

with $\pi_0(\theta) = 0, \pi_1(\theta) = 1$

and

$$\tau_k(\theta) = k \cos\theta\, \pi_k(\theta) - (k+1)\, \pi_{k-1}(\theta)$$

Amplitude function

Defines amplitude functions

$$S_1(\theta) = \sum_{k=1}^{\infty} \frac{2k+1}{k(k+1)} \left(a_k \pi_k(\theta) + b_k \tau_k(\theta) \right)$$

and

$$S_2(\Theta) = \sum_{k=1}^{\infty} \frac{2k+1}{k(k+1)} \left(a_k \tau_k(\theta) + b_k \pi_k(\theta) \right)$$

where coefficients a_k and b_k are a combination of $\psi_k(x)$ and $\xi_k(x)$ and the refractive index $m = n + ik$ as well as the derivatives $\psi'_k(x)$ and $\xi'_k(x)$

$$a_k = \frac{\psi'_k(mx)\psi_k(x) - m\psi_k(mx)\psi'_k(x)}{\psi'_k(mx)\psi_k(x) - m\psi_k(mx)\xi'_k(x)}$$

$$b_k = \frac{m\psi'_k(mx)\psi_k(x) - \psi_k(mx)\psi'_k(x)}{m\psi'_k(mx)\xi_k(x) - \psi_k(mx)\xi'_k(x)'}$$

Scattering matrix

Scattering of the Stokes vector $\overrightarrow{S'} = \hat{M}\,\vec{S}$

Scattering matrix $\hat{M} = \begin{pmatrix} m_{11} & m_{12} & 0 & 0 \\ m_{12} & m_{11} & 0 & 0 \\ 0 & 0 & m_{33} & m_{34} \\ 0 & 0 & -m_{34} & m_{33} \end{pmatrix}$

(only 4 independent components for spherical grains)

Note: For irregular grains the matrix may be full and components need to be calculated by other means than Mie Theory!

Components:

- $m_{11} = \frac{1}{2}\left(|S_1(\theta)|^2 + |S_2(\theta)|^2\right)$
- $m_{12} = \frac{1}{2}\left(|S_1(\theta)|^2 - |S_2(\theta)|^2\right)$
- $m_{33} = \frac{1}{2}\left(S_1(\theta)S_2(\theta)^* + S_1(\theta)S_2(\theta)^*\right)$
- $m_{34} = \frac{1}{2}\left(S_1(\theta)S_2(\theta)^* - S_1(\theta)S_2(\theta)^*\right)$

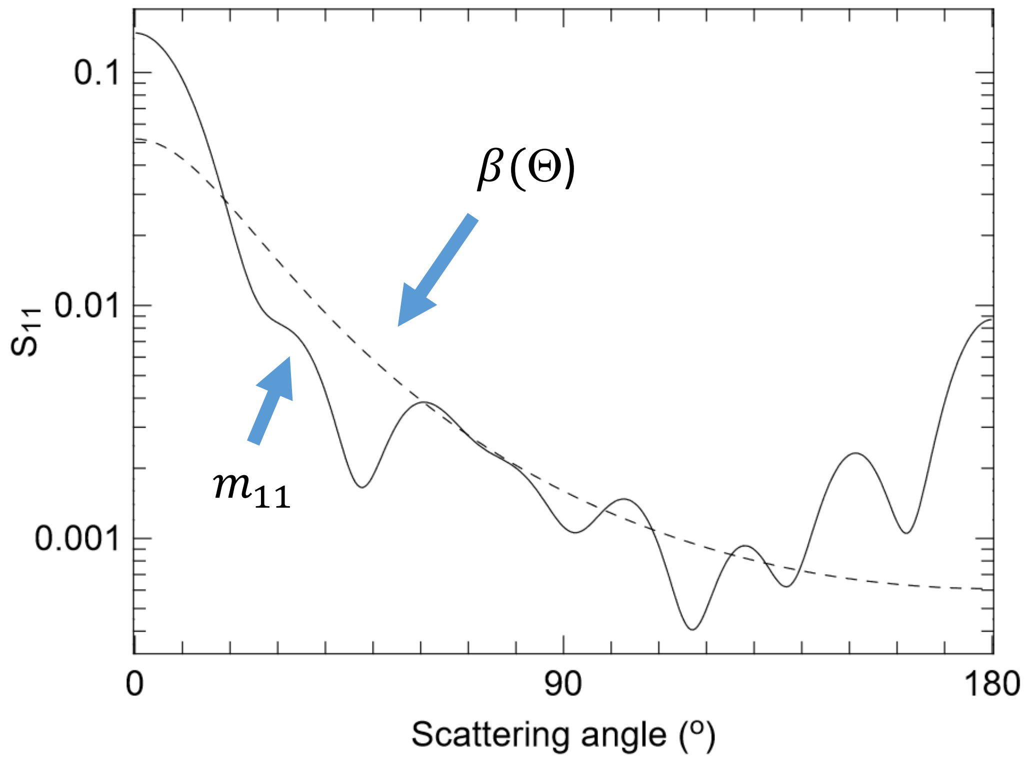
Scattering phase function

Note: The component m_{11} is the exact phase function and

$$g = \langle \cos \theta \rangle = \frac{\int m_{11} \cos \theta \, \mathrm{d}\,\Omega}{\int m_{11} \, \mathrm{d}\,\Omega}$$

is the Henye – Greenstein parameter for the approximation

$$\beta(\theta) = \frac{1}{4\pi} \frac{1-g^2}{(1-g^2-2g\cos\theta)^{3/2}}$$



Efficiencies

- Extinction: $Q_{ext} = \frac{1}{x^2}\sum_{k=1}^{\infty}(2k+1)\mathrm{Re}(a_k + b_k)$
- Scattring: $Q_{sca} = \frac{1}{x^2}\sum_{k=1}^{\infty}(2k+1)\mathrm{Re}\left(|a_k|^2 + |b_k|^2\right)$
- Absorption: $Q_{abs} = Q_{ext} - Q_{sca}$
- Pressure: $Q_{pr} = Q_{ext} - gQ_{sca}$

Note: These calculations are only valid for spherical grains!

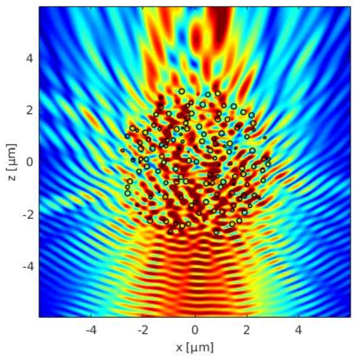
(Scattering) codes

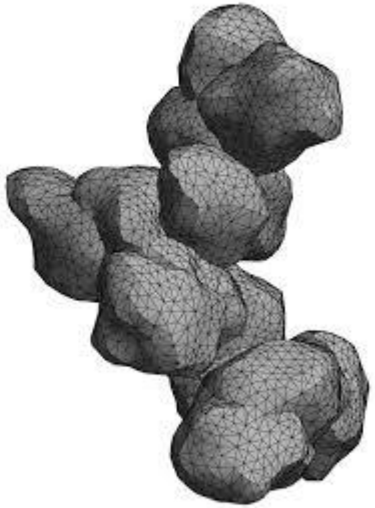
MIEX (Spherical grains, Mie Theory)
https://ui.adsabs.harvard.edu/abs/2018ascl.soft10019W/abstract

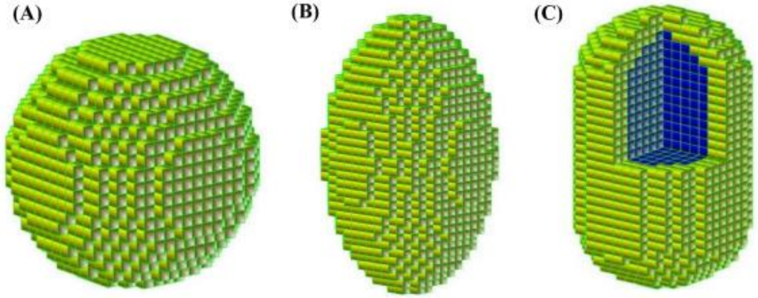
MSTM (dust aggregates, T-Matrix method)
https://pypi.org/project/mstm-studio/

SCADYN (arbitrary shapes, T-Matrix method)
$\rightarrow$ Radiative torque Q_{RAT}
https://github.com/jherrane/scadyn

DDSCAT (arbitrary shapes, discrete dipole approximation)
$\rightarrow$ Circular polarization Q_{circ} & Radiative torque Q_{RAT}
https://www.astro.princeton.edu/~draine/DDSCAT.7.3.html







RT with a dust mixture

- Grain size: a_{eff}
- Grain size distribution: $\frac{dn}{da_{\text{eff}}}$
- Weight per size bin da_{eff}: $W_k = \frac{a_k \frac{dn}{da_{\text{eff}}}}{\int_{a_{\min}}^{a_{max}} \frac{dn}{da_{\text{eff}}} da}$
- Material ratio: ζ_i with $\sum_i \zeta_i = 1$

Typical MRN (Mathis, J.S., Rumpel, W., and Nordsiek, K. H. 1977) dust model for the interstellar medium :

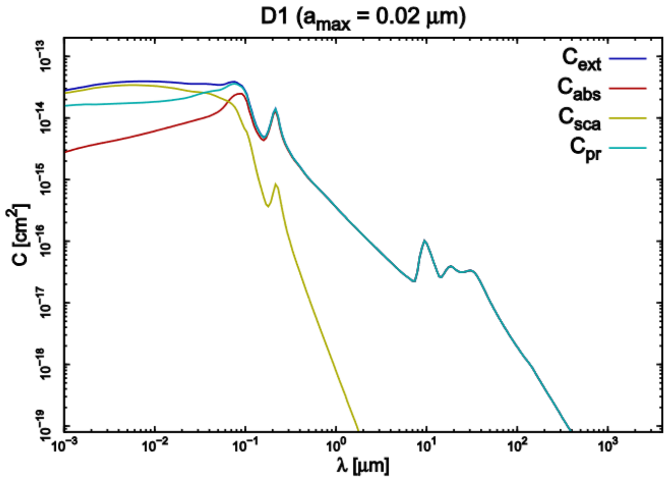
- Grain size distribution: $\frac{dn}{da_{\text{eff}}} \propto {a_{\text{eff}}}^{-3.5}$
- Size range: $a_{\min} = 5\ nm, a_{max}$ = 250 nm
- Materials
  - Silicate: $\zeta_i = 0.375$
  - Graphite: $\zeta_i = 0.625$

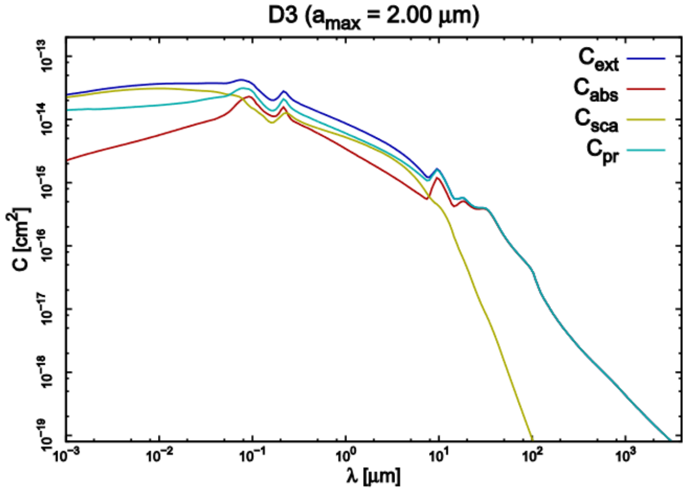
e.g. average cross section of absorption becomes

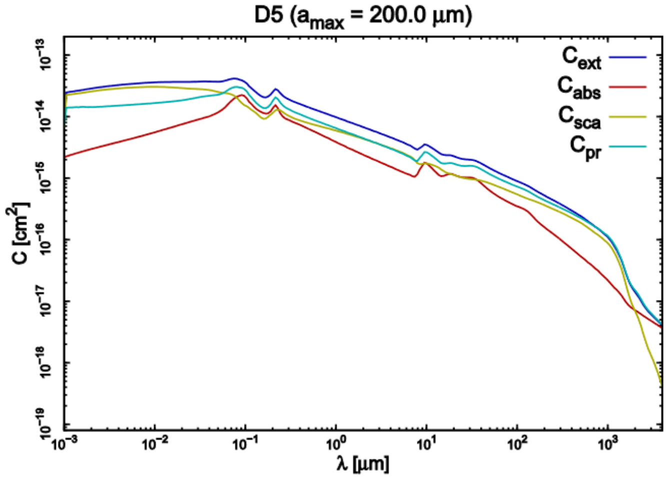
$$\bar{C}_{\text{abs}} = \sum_i \zeta_i \sum_k W_k \pi a_k^2 Q_{\text{abs,i},k}$$

Scattering probability

- average cross section: $\bar{C} = \sum_i \zeta_i \sum_k W_k \pi a_k^2 Q_{\mathrm{i},k}$
- albedo: $\alpha = \dfrac{C_{\mathrm{sca}}}{C_{\mathrm{abs}} + C_{\mathrm{sca}}}$

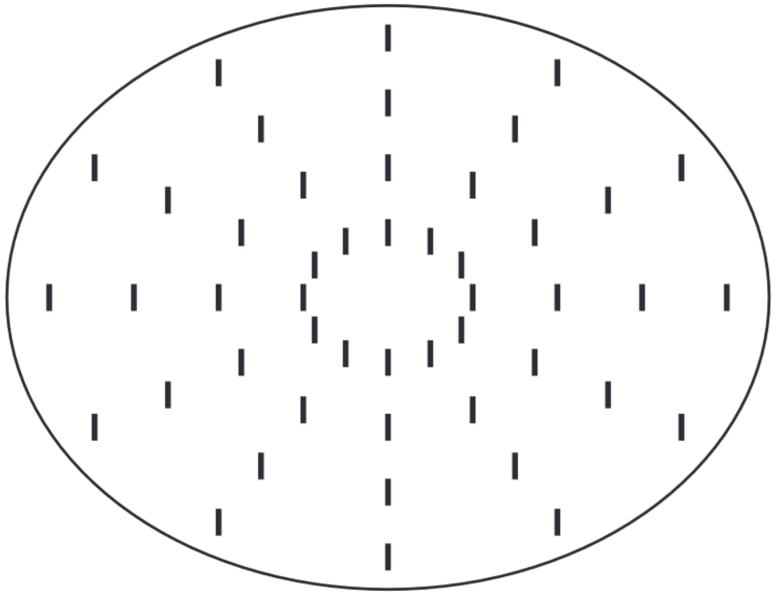




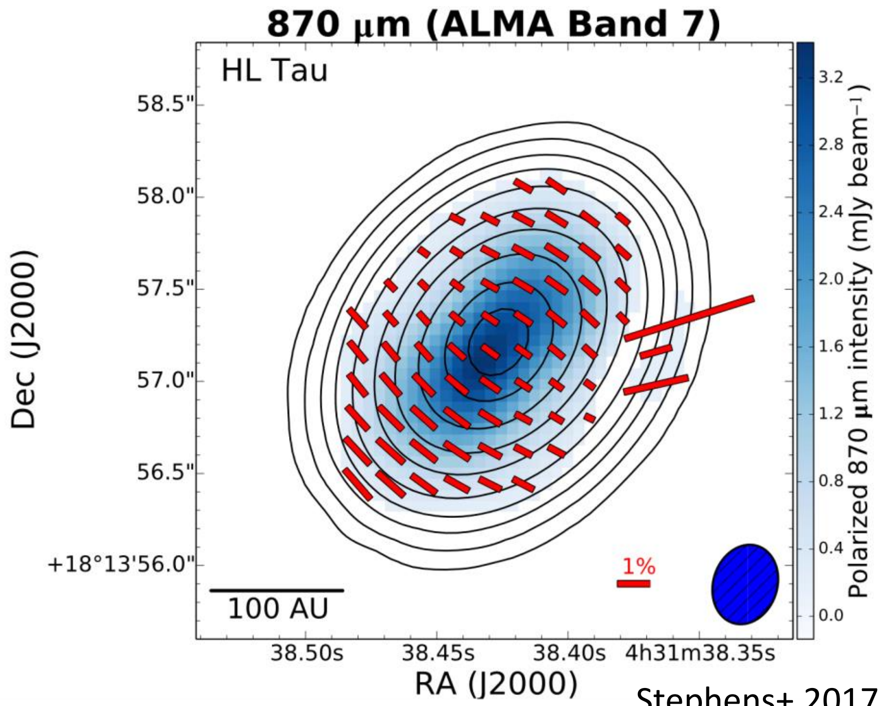


$\Rightarrow$ Scattering becomes dominant for a mixture with more larger grains

Observed dust scattering



Kataoka+ 2017



Stephens+ 2017

Grains with similar size as wavelength are present

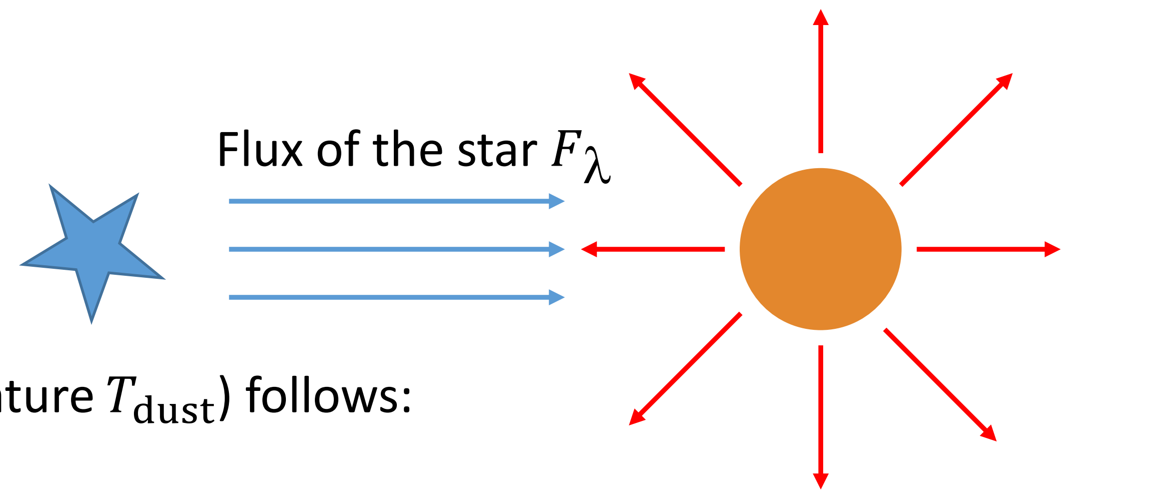
Dust heating

Dust heating

Assume the dust is in local thermodynamic equilibrium (LTE)
$\Rightarrow$ re-emission follows the Planck function $B_\lambda(T_{\rm dust})$ and $C_{\rm abs} = C_{\rm em}$

Absorbed energy per time: $\dot{E}_{\rm abs} = \int C_{\rm abs,\lambda}\, F_\lambda d\lambda$

Re-emitted energy per time: $\dot{E}_{\rm em} = 4\pi \int C_{\rm abs,\lambda}\, B_\lambda(T_{\rm dust})\, d\lambda$



In thermal balance (when grain reached its equilibrium temperature $T_{\rm dust}$) follows:

$$\dot{E}_{\rm abs} = \dot{E}_{\rm em}$$

i.e.

$$\int C_{\rm abs,\lambda} F_\lambda d\lambda = 4\pi \int C_{\rm abs,\lambda} B_\lambda(T_{\rm dust})\, d\lambda$$

(implicit solution e.g. via look-up table)

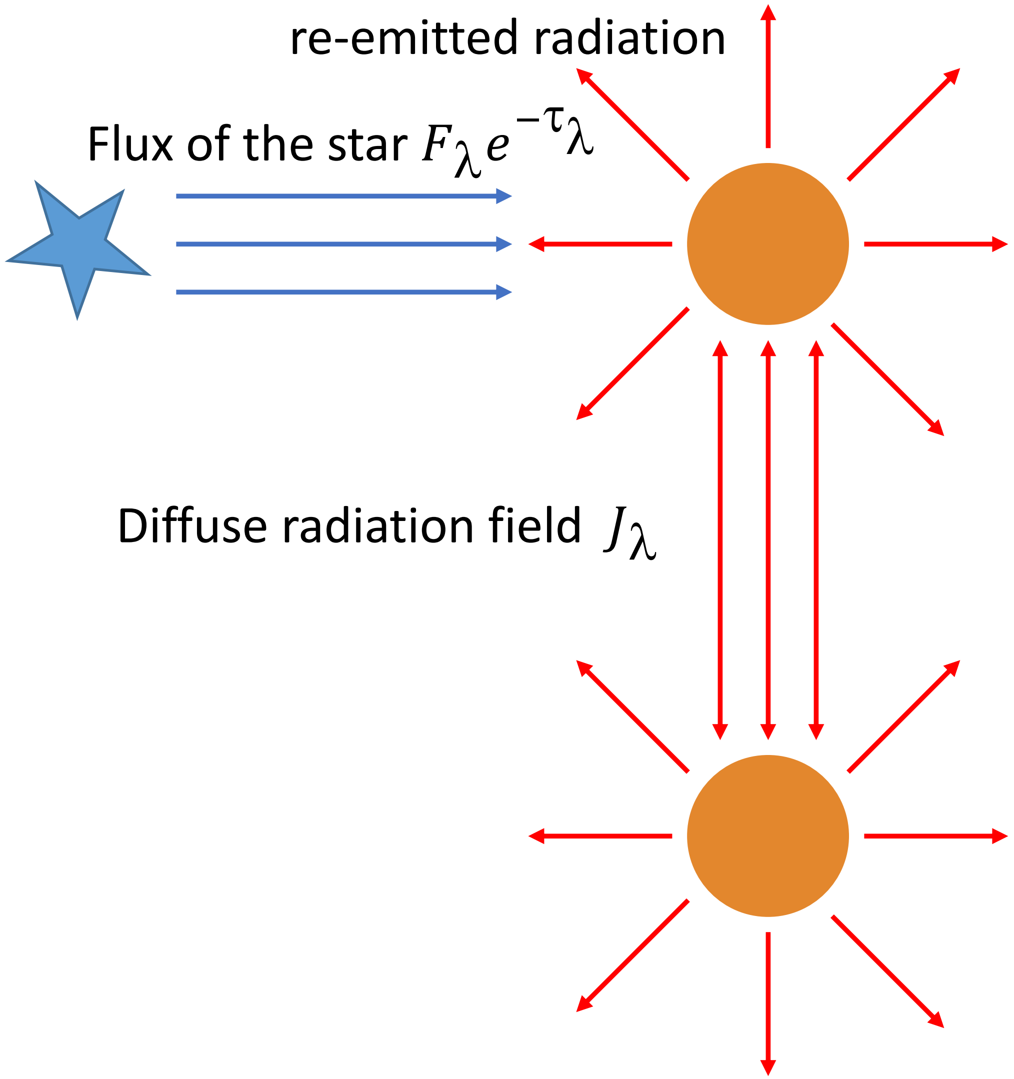
Dust heating

Thermal balance for optically thick case:

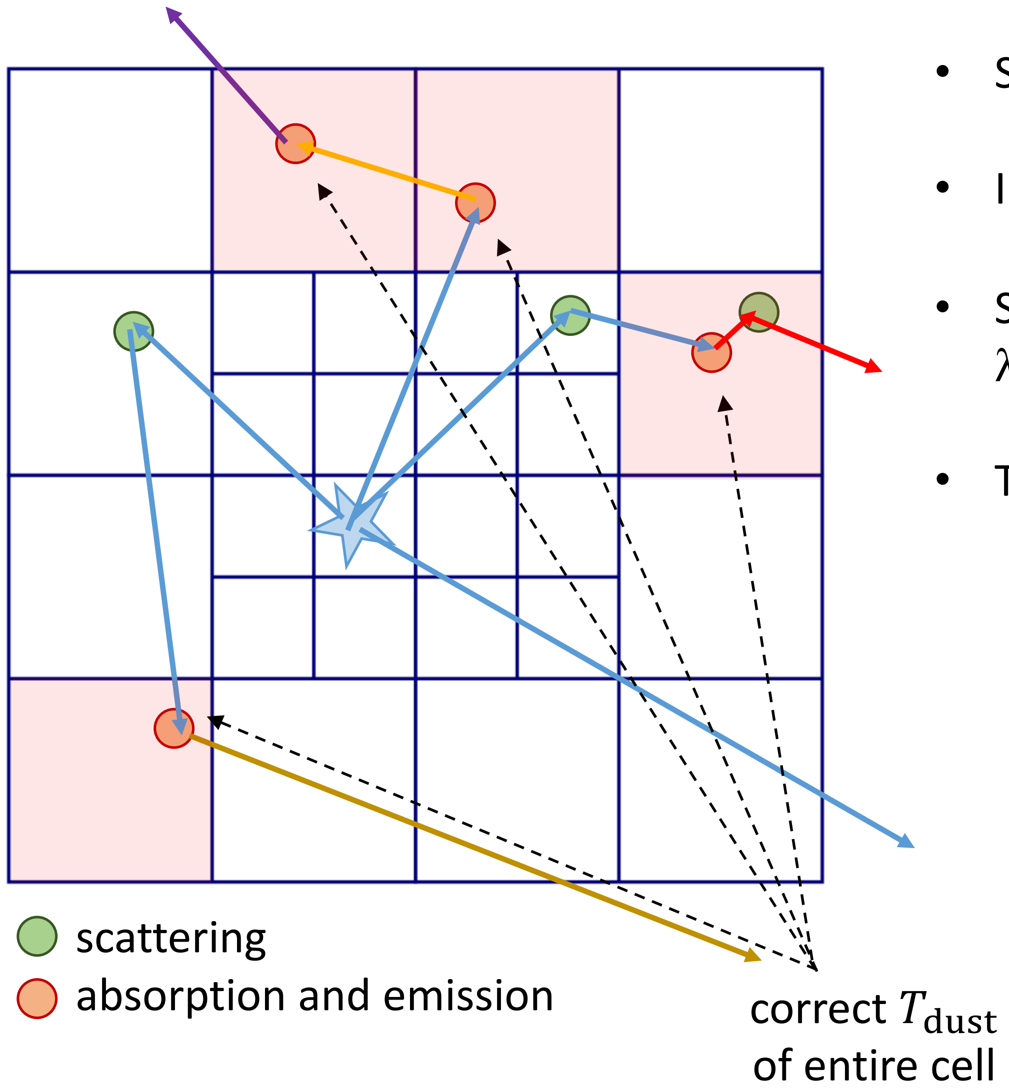
$$\int C_{\mathrm{abs}} \left(F_\lambda e^{-\tau_\lambda} + J_\lambda\right) d\lambda = 4\pi \int C_{\mathrm{abs}} B_\lambda(T_{\mathrm{dust}})\, d\lambda$$

BUT: Radiation field $F_\lambda e^{-\tau_\lambda} + J_\lambda$ is not known at the beginning

$\Rightarrow$ Monte Carlo techniques



MC dust heating



- Start with an initial dust temperature T_0
- Inject N_{ph} photons (photon packages) from each source into the grid
- Sample a new direction $\hat{n}$ (s. points on a sphere) and a new wavelength λ for each absorption event
- Temperature correction techniques:
  - Correct only in cells with an absorption event (memory efficient, some cells may not have T_{dust} in the end)
  - Store the entire radiation field (continuous absorption) in each cell and correct for each absorption and once at the end of the run (memory demanding).
  - Split photon into an absorbed and a scattered photon (time demanding)

Iterative approach

- Start with an initial dust temperature T_0
- Correct temperature $T_{\mathrm{new}} \rightarrow T_{\mathrm{old}} + \Delta T$
- Sample new wavelength from Planck function
- $z_i = \dfrac{\int_{\lambda_i}^{\lambda_i+\Delta\lambda} C_{\mathrm{abs}} B_\lambda(T_{\mathrm{new}})\, d\lambda}{\int_0^\infty C_{\mathrm{abs}} B_\lambda\, d\lambda}$
- Repeat MC run until convergence criterion is fulfilled e.g. $T_{\mathrm{new}} - T_{\mathrm{old}} < \varepsilon$ in each cell

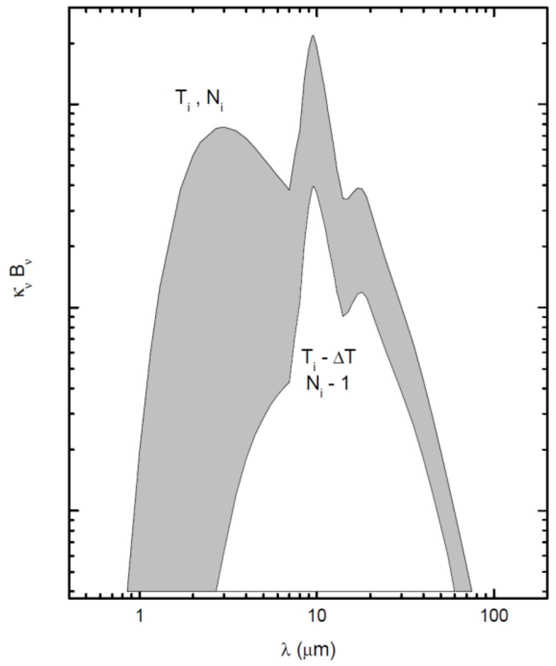
- Full control of convergence
- Very time consuming!

Spontaneous emission

- Start with an initial dust temperature T_0
- Correct temperature $T_{\text{new}} \rightarrow T_{\text{old}} + \Delta T$
- Sample new wavelength from partial temperature derivative of Planck function $B'_\lambda(T)=\frac{\partial B_\lambda(T)}{\partial T}$

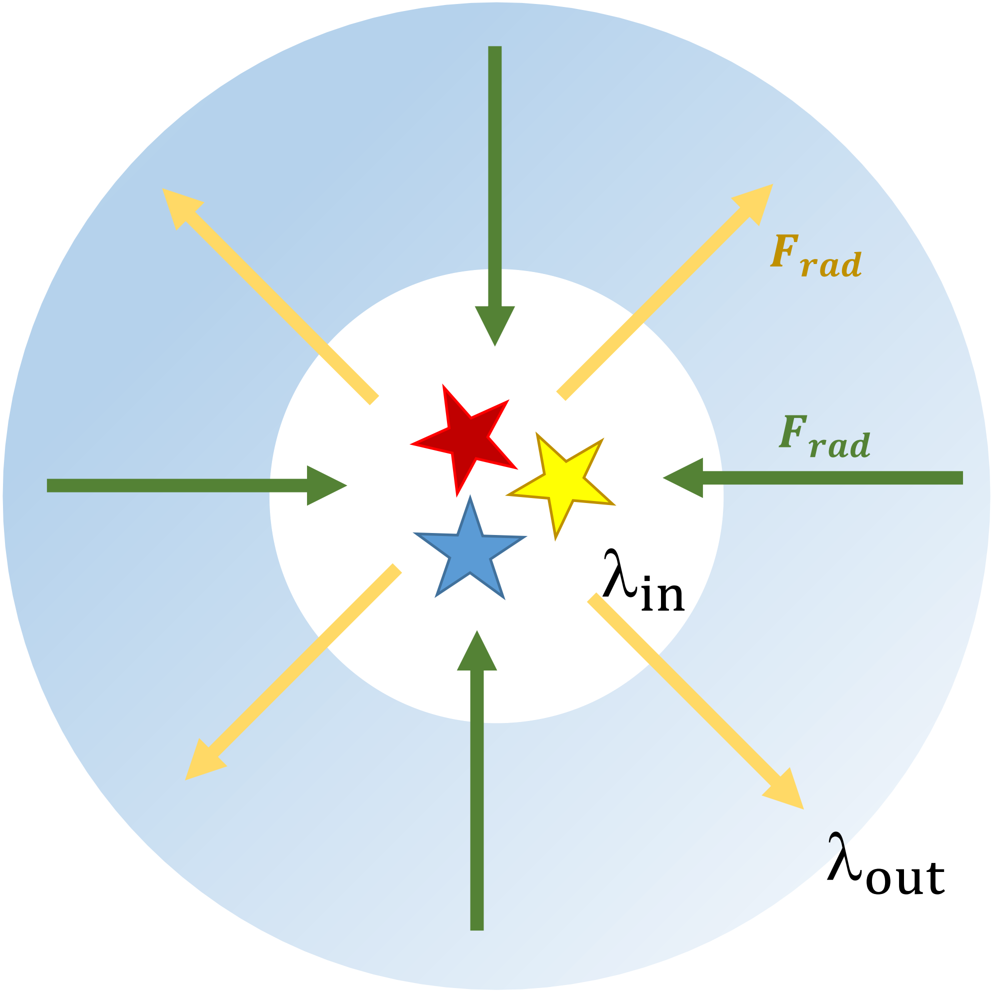
$$z_i = \frac{\int_{\lambda_i}^{\lambda_i+\Delta\lambda} C_{\text{abs}} \; B'_\lambda(T_{\text{new}}) d\lambda}{\int_0^\infty C_{\text{abs}} \, B'_\lambda(T_{\text{new}}) \; d\lambda}$$

- Only one MC run is required
- No convergence control of temperature
- The spectrum of the radiation field J_λ is always correct.



Bjorkman & Wood 2001

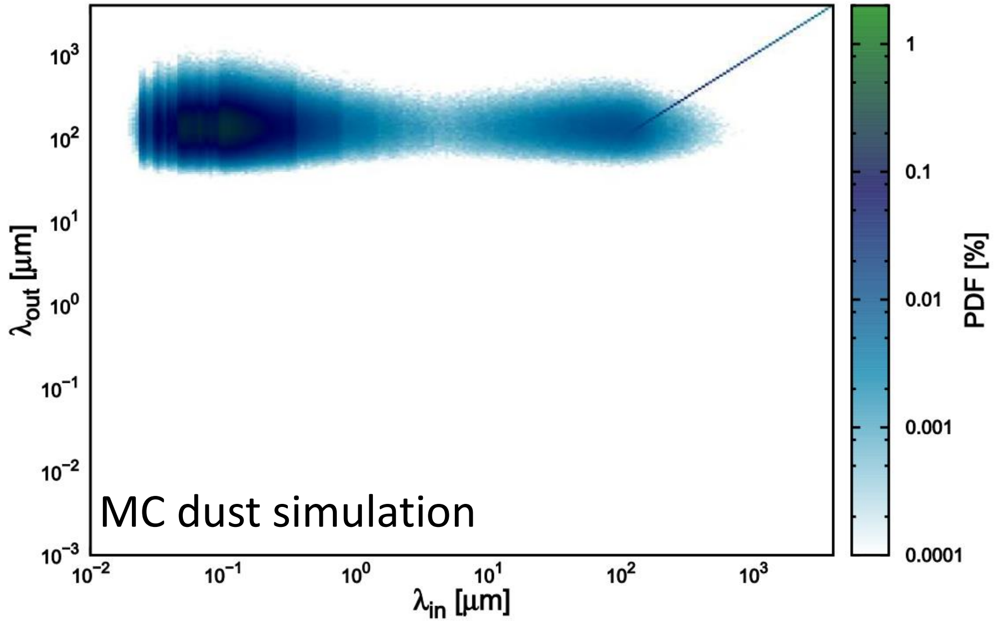
What regulates star formation?



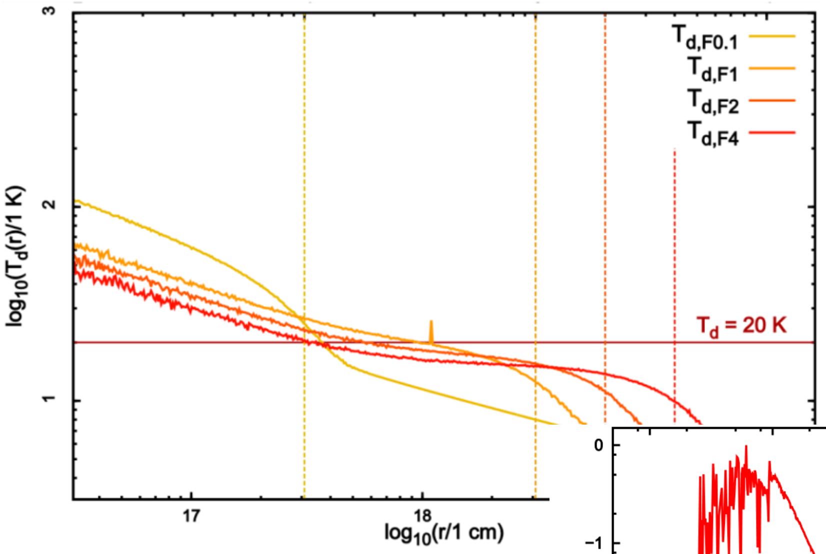
Radiative feedback

radiation $\xrightarrow[\text{pressure}]{}$ dust $\xrightarrow[\text{collision}]{}$ gas

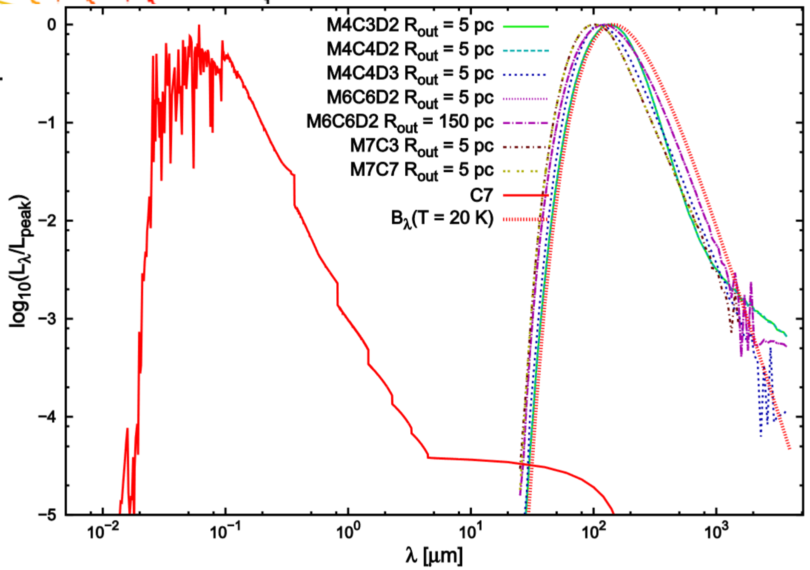
$$F_{\rm rad}(r) = \frac{f_{abs}(1+\tau_{IR})}{4\pi c\, r^2}\int C_{pr} L_\lambda \, d\lambda$$

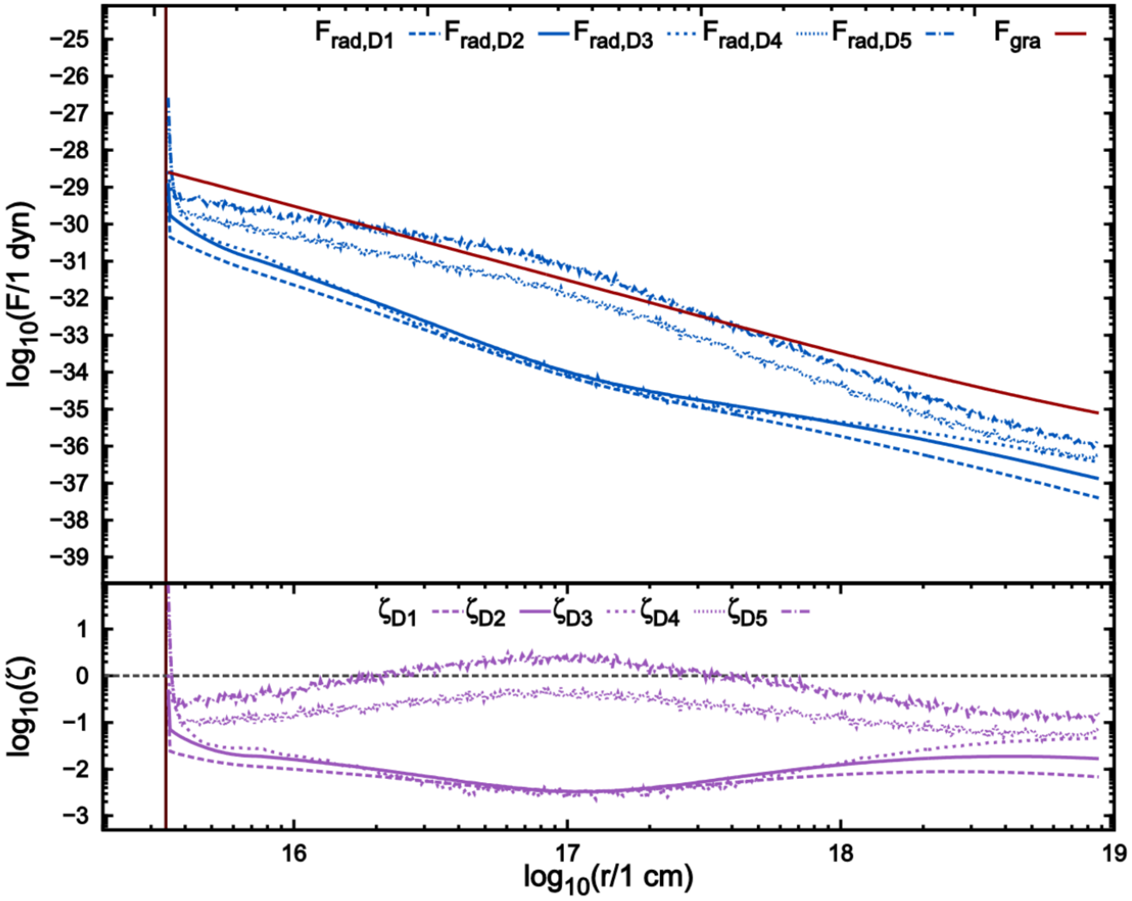


What regulates star formation?



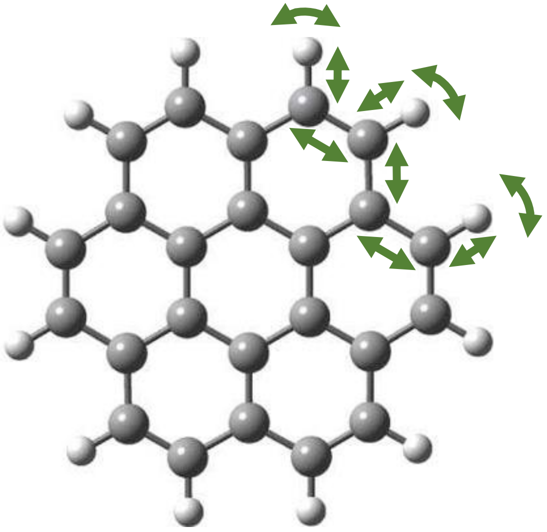
Reissl+ 2018





⇒ Dust shifts the initial SED of the cluster effectively into the IR and sub-mm where the cloud is optically thin!

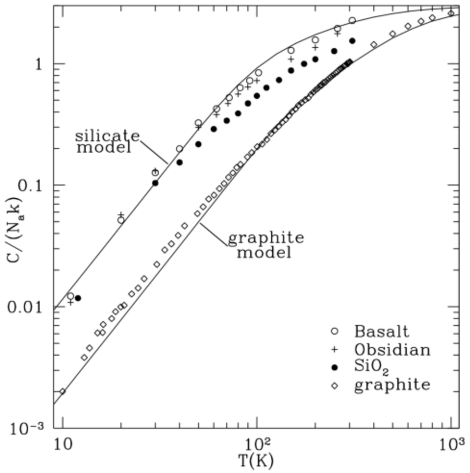
Stochastic heating



In contrast to “large” grains PAHs with N_a atoms have internally “limited” degree freedom to absorb energy:

- Rotational: 3
- vibrational: $3N_a - 6$

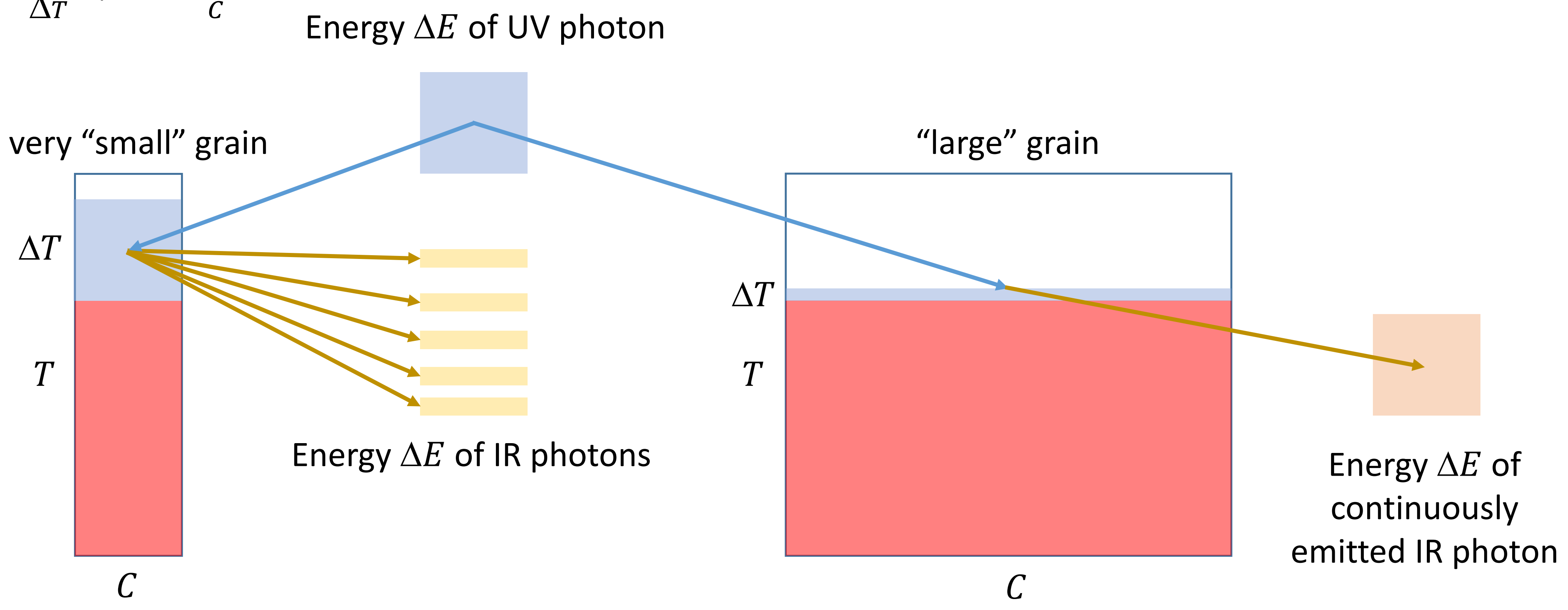
$\Rightarrow$ Smaller heat capacity: $C = \frac{\partial U}{\partial T}$



Draine & Li 2001

Stochastic heating

Heat capacity: $C \approx \frac{\Delta U}{\Delta T} \Rightarrow \Delta T \approx \frac{\Delta U}{C}$



“small” grains:

- spend a significant amount of time at much higher temperatures
- emit at shorter wavelengths, which can have a strong effect on the observed spectrum

Stochastic heating algorithm

- RT for each grain size k separately
- define temperature range $T_{dust} \in [T_{\min}, T_{\max}]$ in N bins
- enthalpy $H_k(a,T) = \frac{4}{3}\pi\, a^3 \rho \int_0^T C(T')dT'$ (pre-calculated)

Probability for heating from initial state i to final state f (f>i)

$$A_{ij} = 4\pi\lambda_{ij}\, C_{\text{abs}}(\lambda_{ij})\, J(\lambda_{ij})[H_k(T_{\max}) - H_k(T_{min})] \text{ with } \lambda_{ij} = \frac{hc}{H_k(T_{\text{f}}) - H_k(T_{\text{i}})}$$

Assume cooling occurs only to the next lower level

$$A_{i,i-1} = \frac{4\pi}{H_k(T_{\text{i}}) - H_k(T_{\text{i}-1})} \int_0^{\infty} C_{\text{abs}}\, B'_{\lambda}(T_{\text{i}})\; d\lambda$$

Diagonal elements $A_{i,i} = -\sum_{f \neq i} A_{f,i}$

Otherwise $A_{i,j} = 0$

$\Rightarrow$ Matrix A_{ij} is determined by the material specific quantities $C(T)$ and C_{abs} as well as the radiation field J_{λ}

Stochastic heating probability

Probability $P_k(T_i)dT$ of finding the k-th grain size at temperature T_i

$$\sum_{i=1}^{N-1} P_k(T_i) A_{f,i} = 0$$

(steady state condition)

with $f = 0, \ldots, N-1$ and

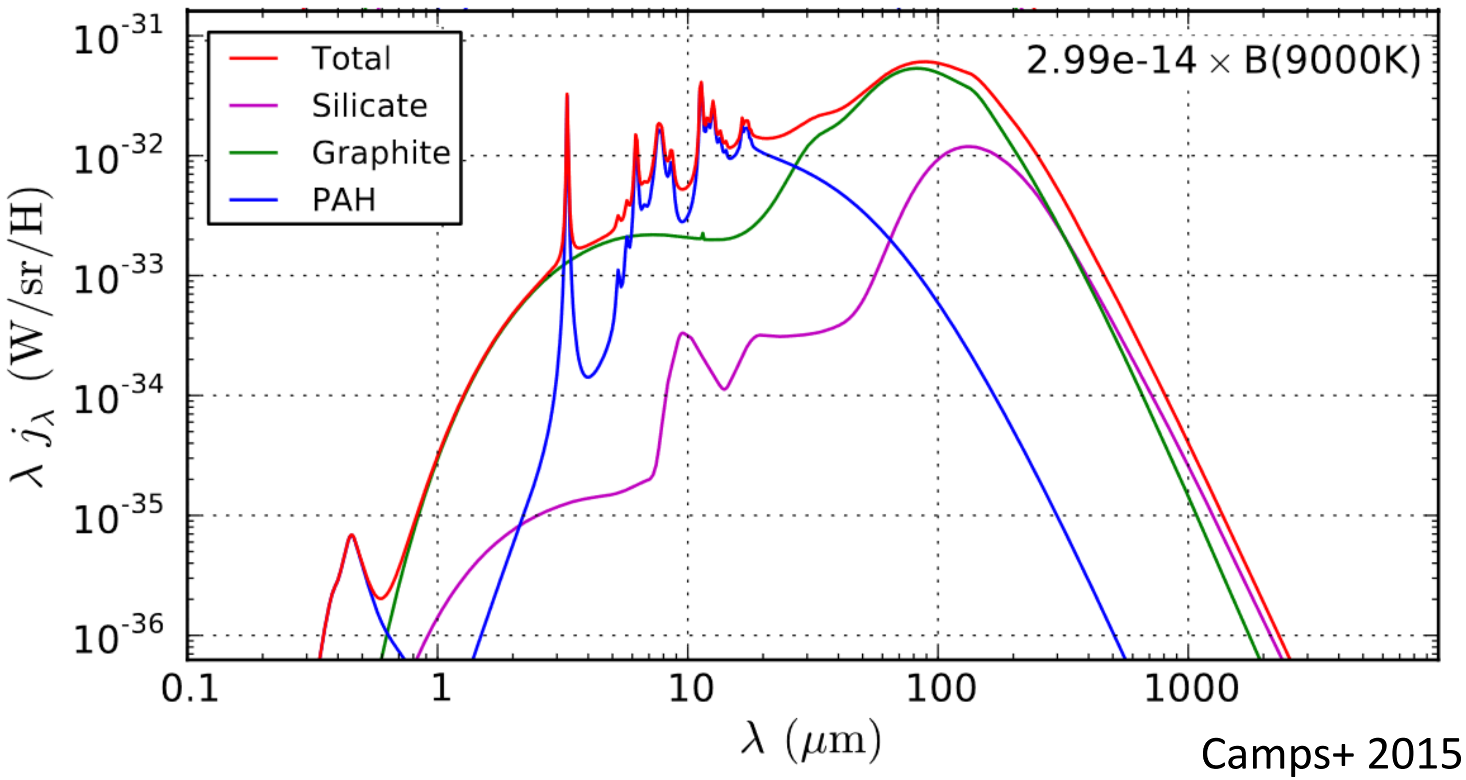
$$\sum_{i=1}^{N-1} P_k(T_i) = 0$$

(normalizing condition)

PAH emission

Finally, the emissivity over all grains of the same size is

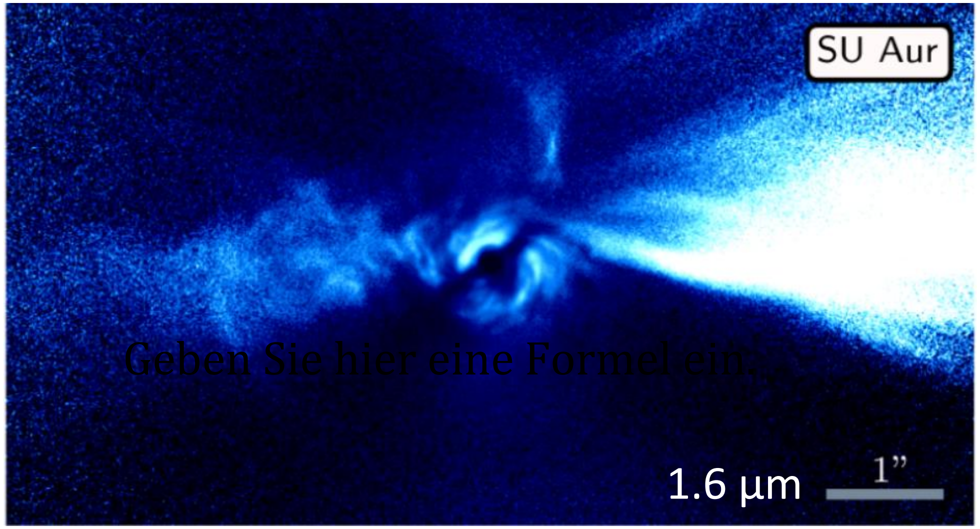
$$j_\lambda = \sum_k C_{\mathrm{abs},k} \int P_k B_\lambda(T) d\mathrm{T}$$

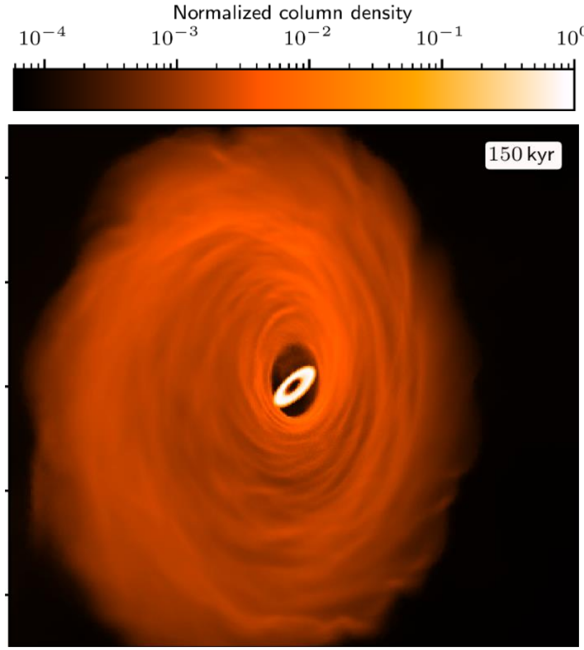


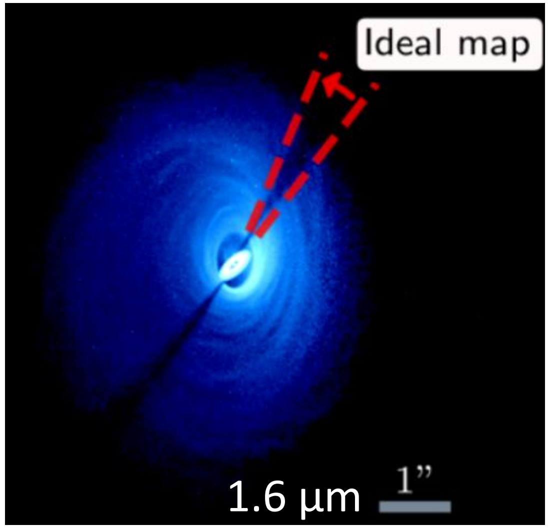
Camps+ 2015

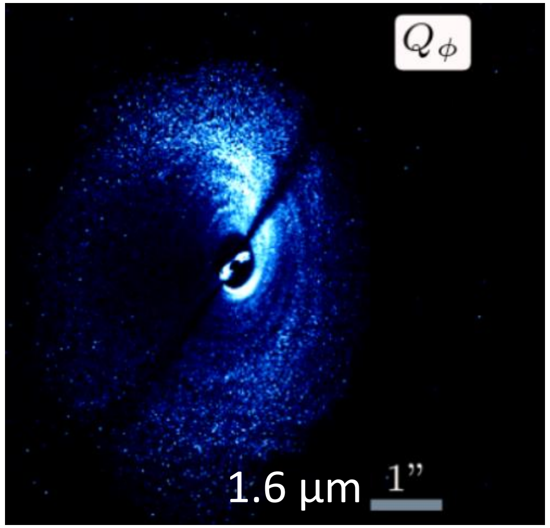
The origin of disk shadows

Ginsk+ 2021





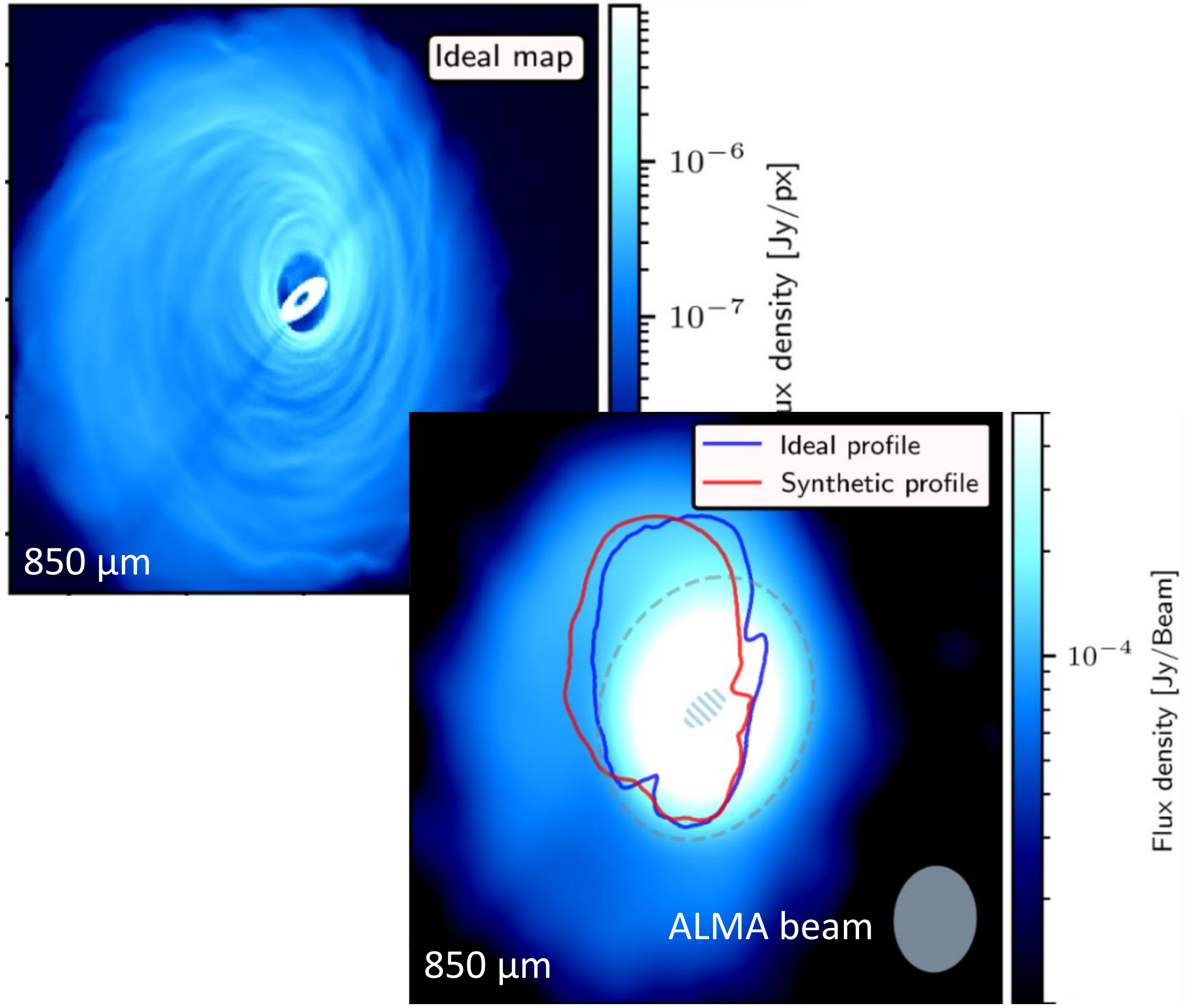




Küffmeier+ 2021

Krieger+ 2024

Disk shadows in emission



Krieger+ 2024

Dust cooling by emission

$$\frac{dT_d}{dt} = \frac{\overline{\kappa}_{abs}(T_d)}{C(T_d)} \left(T_{min}^4 - T_d^4\right)$$