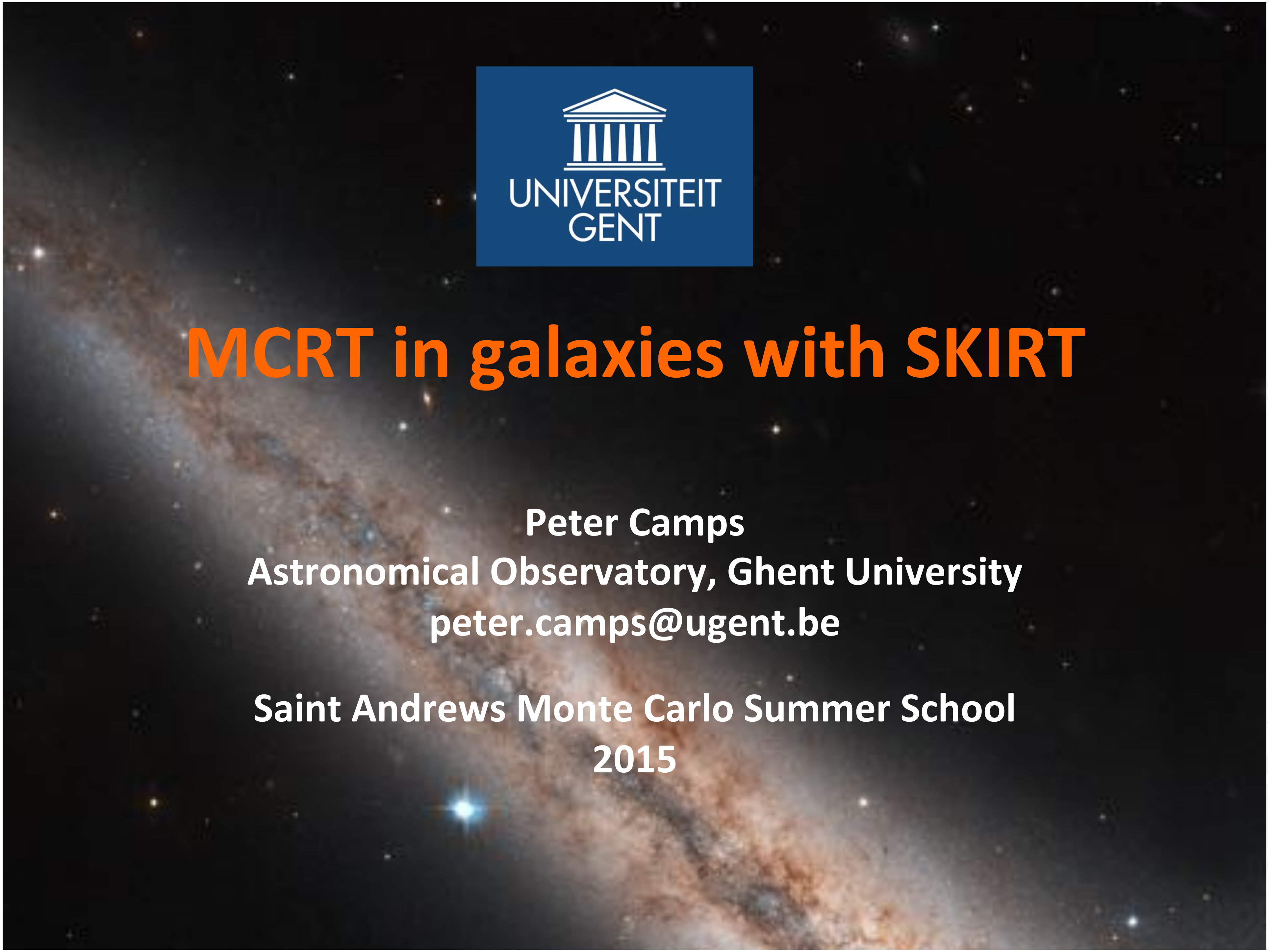

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MCRT in galaxies with SKIRT

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Saint Andrews Monte Carlo Summer School
2015

Peter Camps

Academic (Ghent University)

- 1980: Master Engineering
- 2011: Bachelor Physics & Astronomy
- 2012-current: PhD student (Maarten Baes)

Commercial (30 years in between)

- commercial software development
- international management
- technical software (e.g. PDF editing)
- small teams (1 to 20)

Overview

MCRT in galaxies with SKIRT

- Dust in galaxies
- SKIRT features and code design
- Energy balance in galaxies
- Automated galaxy modeling

MCRT post-processing of hydrodynamic snapshots

- Stochastic heating of dust grains
- Dust grids: regular, hierarchical, unstructured
- Importing hydro snapshots: AMR, SPH
- FIR properties of galaxies in a cosmological simulation

Dust in galaxies

Section A-1

Interstellar dust

Minor fraction of the interstellar medium

- Dust-to-gas ratio is usually less than 1%

But a crucial constituent

- Extinction: up to 50% of the radiation emitted by stars is absorbed or scattered by interstellar dust
- Infrared emission: absorbed energy is released as thermal radiation
- Regulates the physical and chemical conditions of the interstellar gas (e.g. formation of molecules)
- Plays a key role in the formation of stars and planetary systems

Interstellar dust

Origin

- Birth in evolved stars with extended shells; possibly also in novae and supernovae
- Accretion of gas atoms and coagulation of grains in cold clouds

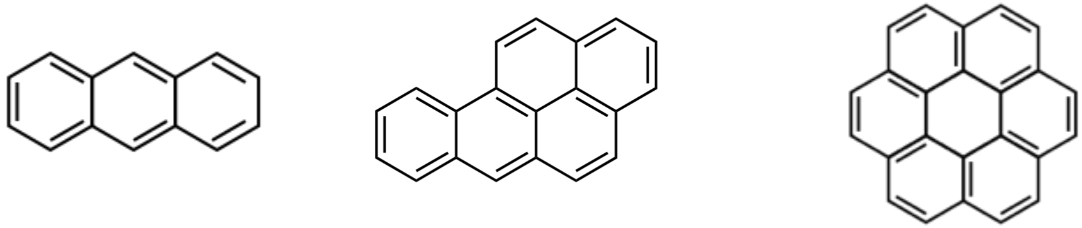
Destruction

- Star formation, hot gas, shocks
- Sputtering by high energy radiation
- Evaporation at high temperature
- Shattering in grain-grain collisions

Interstellar dust

Composition

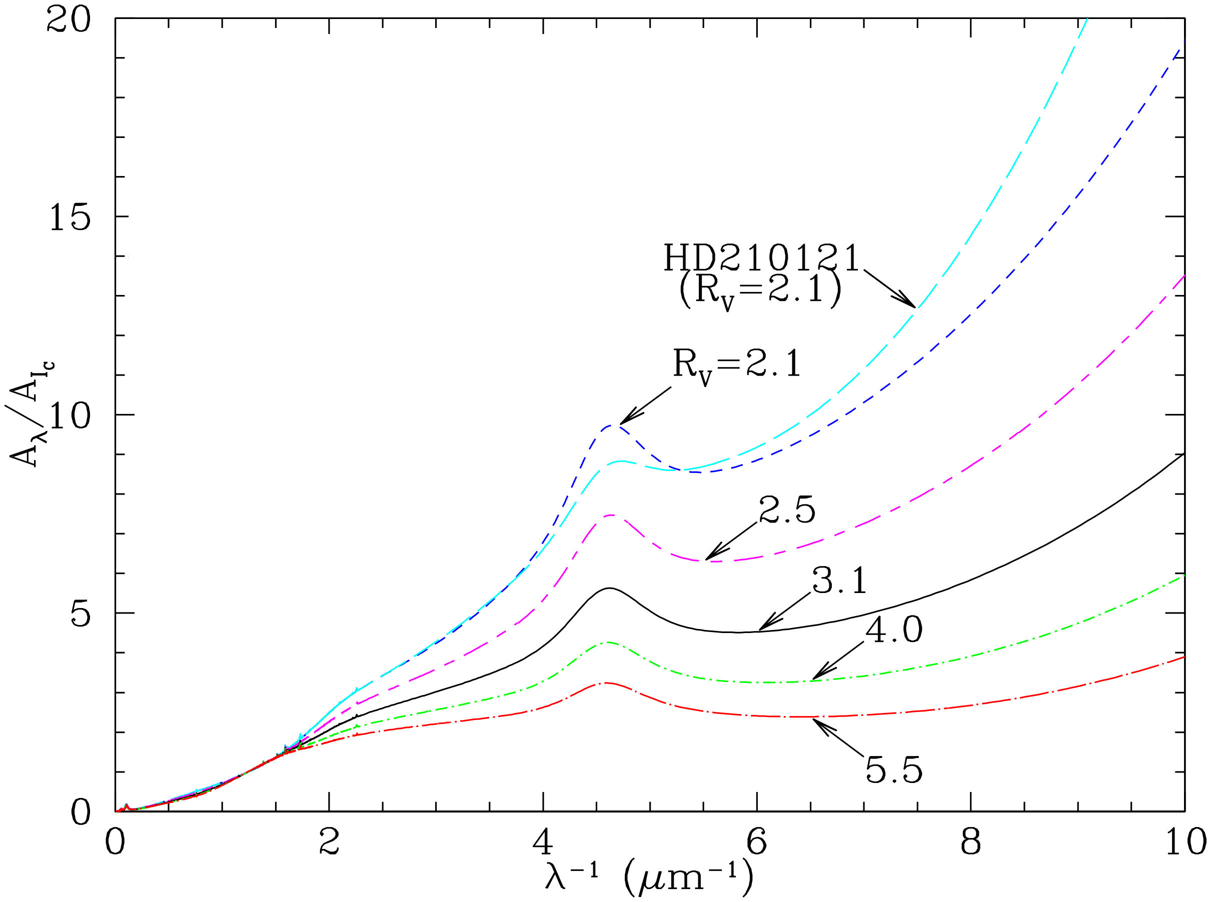
- Graphite (amorphous carbon)
- Silicates: amorphous or crystalline
  - e.g. Enstatite ($MgSiO_3$), Forsterite (Mg_2SiO_4)
- PAH molecules (polycyclic aromatic hydrocarbon)



Grain size

- 1/3 nm (a few atoms) up to 1/3 micron
- “Logarithmic” size distribution
- Irregular shapes

Extinction curve



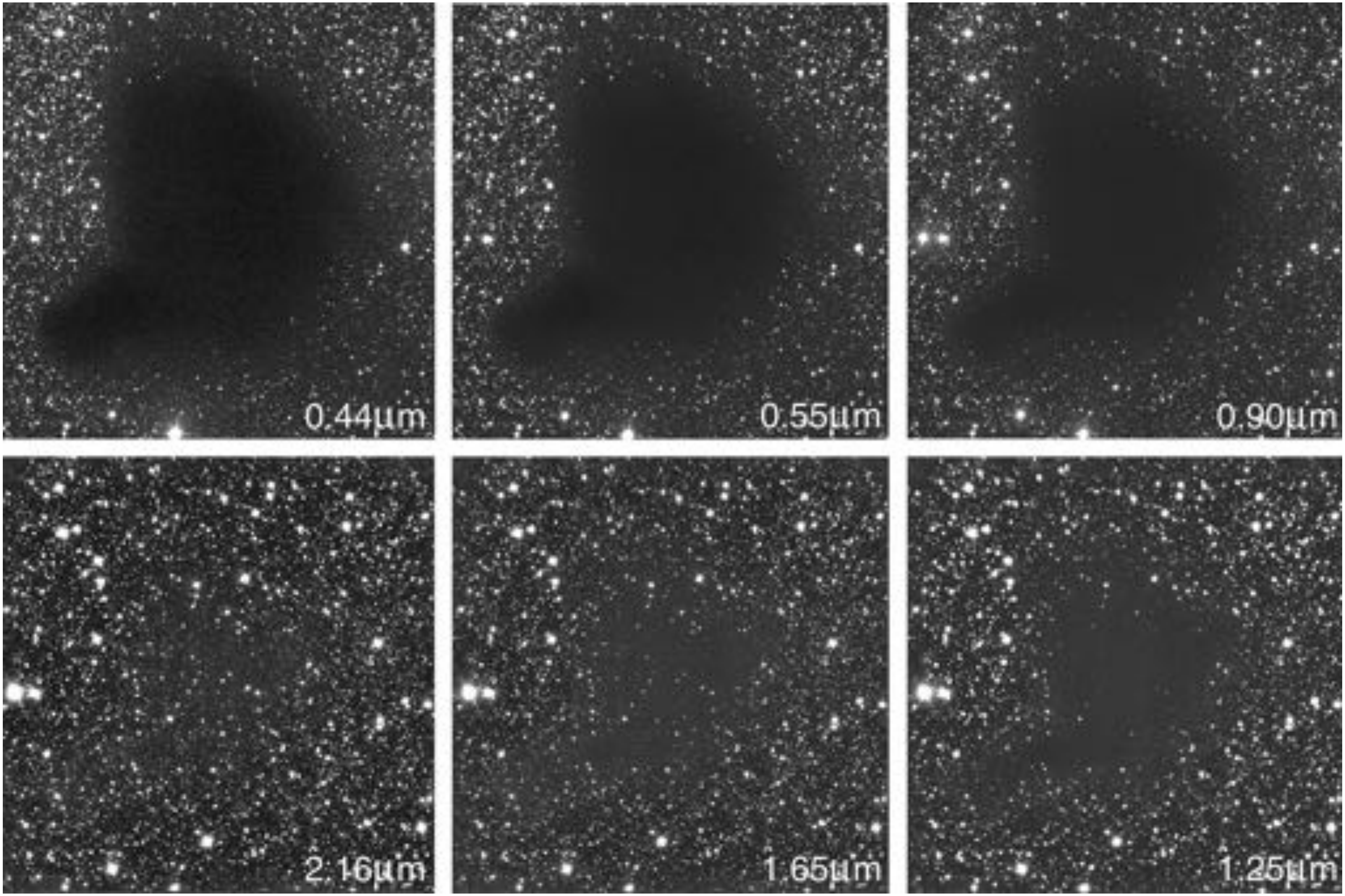
0.5 µm

0.1 µm

- Extinction rapidly decreases with wavelength
- Dependency is highly nonlinear

Draine 2003

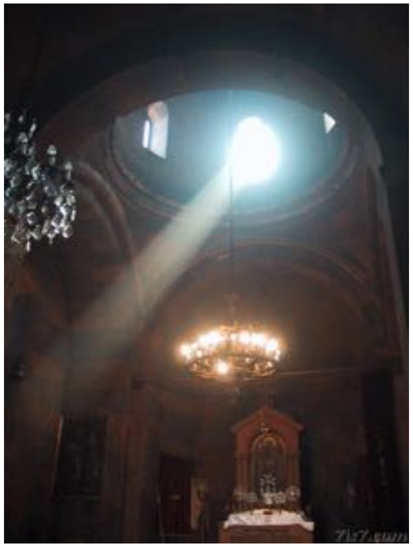
Reddening



Absorption and scattering

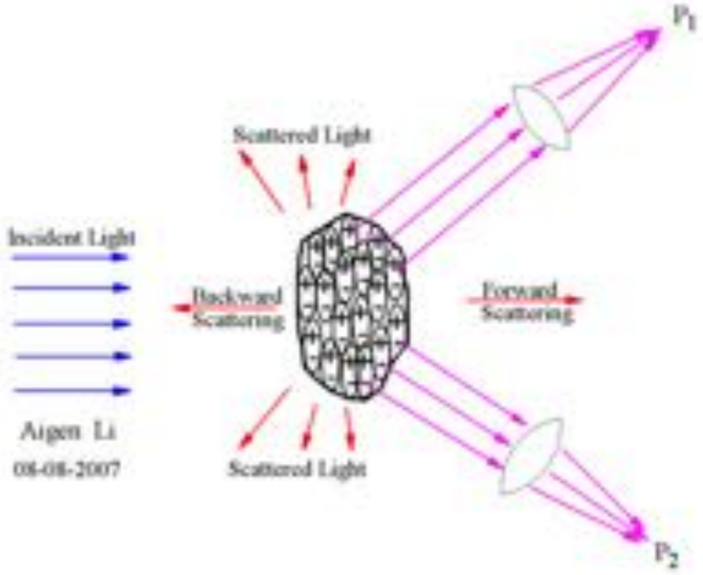
Two sink terms (extinction processes) to be considered in dust RT:

- **absorption:** dust grain absorbs the radiative energy (the photon) and converts it to internal energy
- **scattering:** dust grain changes the propagation direction of a photon



Absorption and scattering can be characterized by the absorption and scattering coefficients (depend on the size, shape and chemical composition of the dust grains)

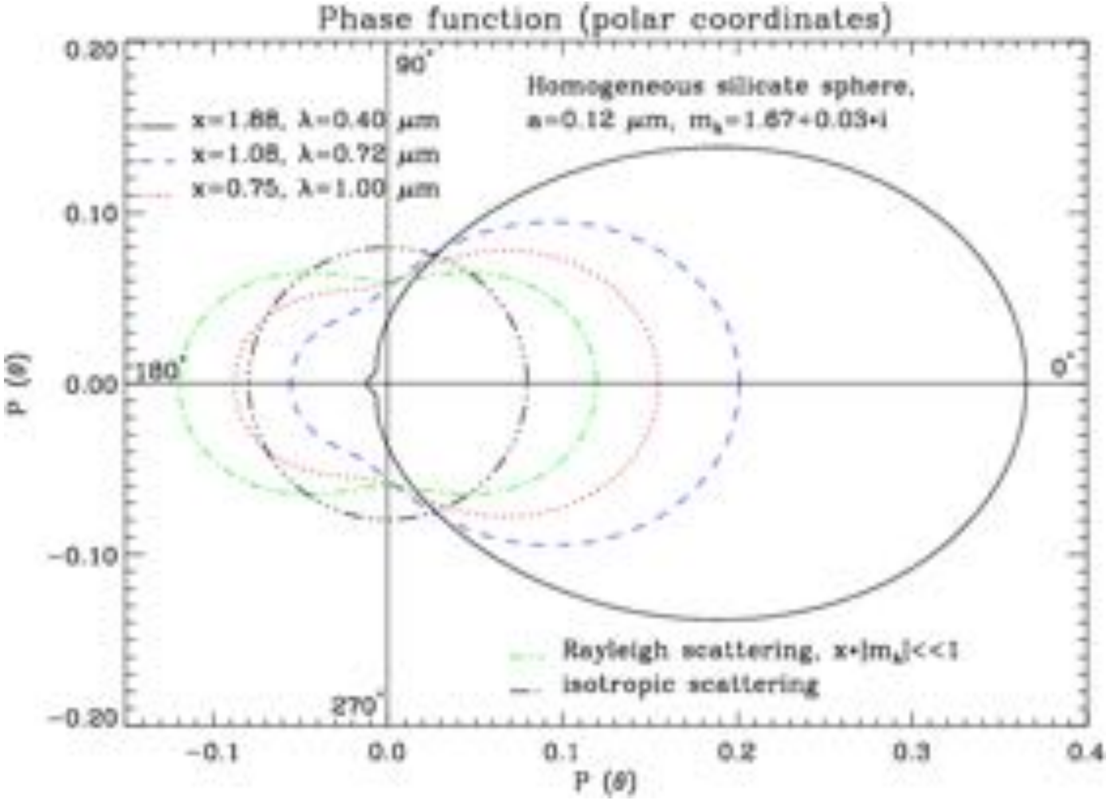
$$\kappa_\lambda = \kappa_\lambda^{\text{abs}} + \kappa_\lambda^{\text{sca}}$$



Scattering phase function

Scattering redirects photons into another direction, so it is both a sink and a source term.

The phase function $\Phi_\lambda(\boldsymbol{k},\boldsymbol{k}')$ describes the probability that a photon coming from direction $\boldsymbol{k}'$ will have $\boldsymbol{k}$ as its new propagation direction.



Scattering off dust grains is anisotropic and generally forward. The scattering function typically depends only on the angle between incoming and outgoing direction.

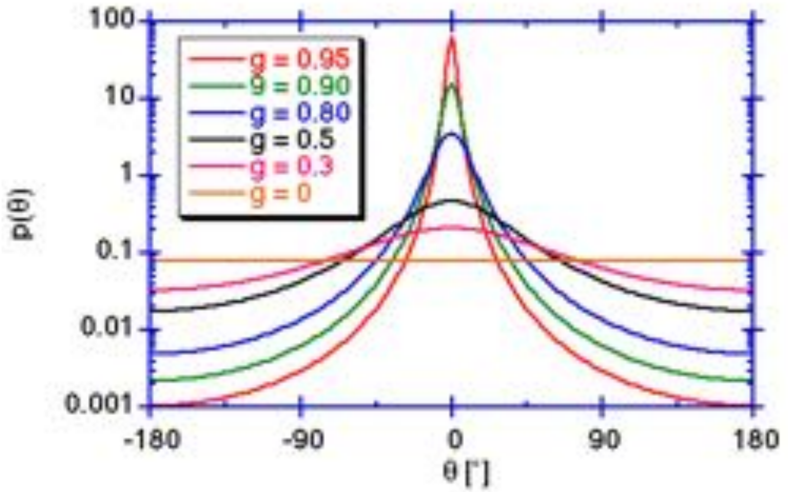
Henyey-Greenstein phase function

The most widely used phase function = Henyey-Greenstein phase function

$$\Phi_\lambda(\cos\alpha) = \frac{1}{4\pi}\frac{1-g_\lambda^2}{(1+g_\lambda^2-2g_\lambda\cos\alpha)^{3/2}}$$

Contains one free parameter: the asymmetry parameter g_λ,

$$g_\lambda = \int \Phi_\lambda(\cos\alpha)\cos\alpha\,\mathrm{d}\Omega$$



The asymmetry parameter g_λ, can be defined for any phase function, but the HG phase function contains it as an explicit parameter.

- $g_\lambda = 0$: isotropic scattering
- $g_\lambda = 1$: completely forward scattering
- $g_\lambda = -1$: completely backward scattering

How to trace interstellar dust (1)

Model the extinction

- Stellar emission
- Absorption and multiple anisotropic scattering by dust

Issues

- 6 dimensions (3 position, 2 direction, 1 wavelength) even when assuming time-independence
- Non-local
- Non-linear
- Complicated geometry (3D, inhomogeneous…)
- Optical properties of the dust are poorly known

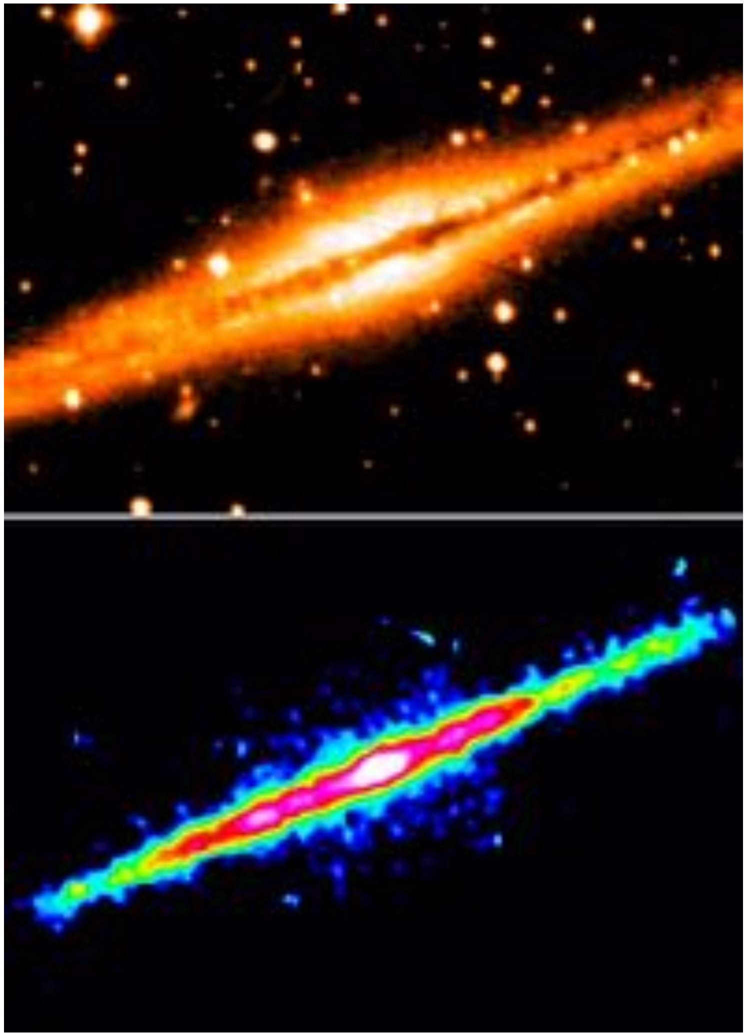
How to trace interstellar dust (2)

Energy balance: dust grains emit the energy they absorb

$$\int_0^\infty \kappa_\lambda^{\mathrm{abs}}\, J_\lambda \,\mathrm{d}\lambda = \int_0^\infty \kappa_\lambda^{\mathrm{abs}}\, B_\lambda(T_{\mathrm{d}})\,\mathrm{d}\lambda$$

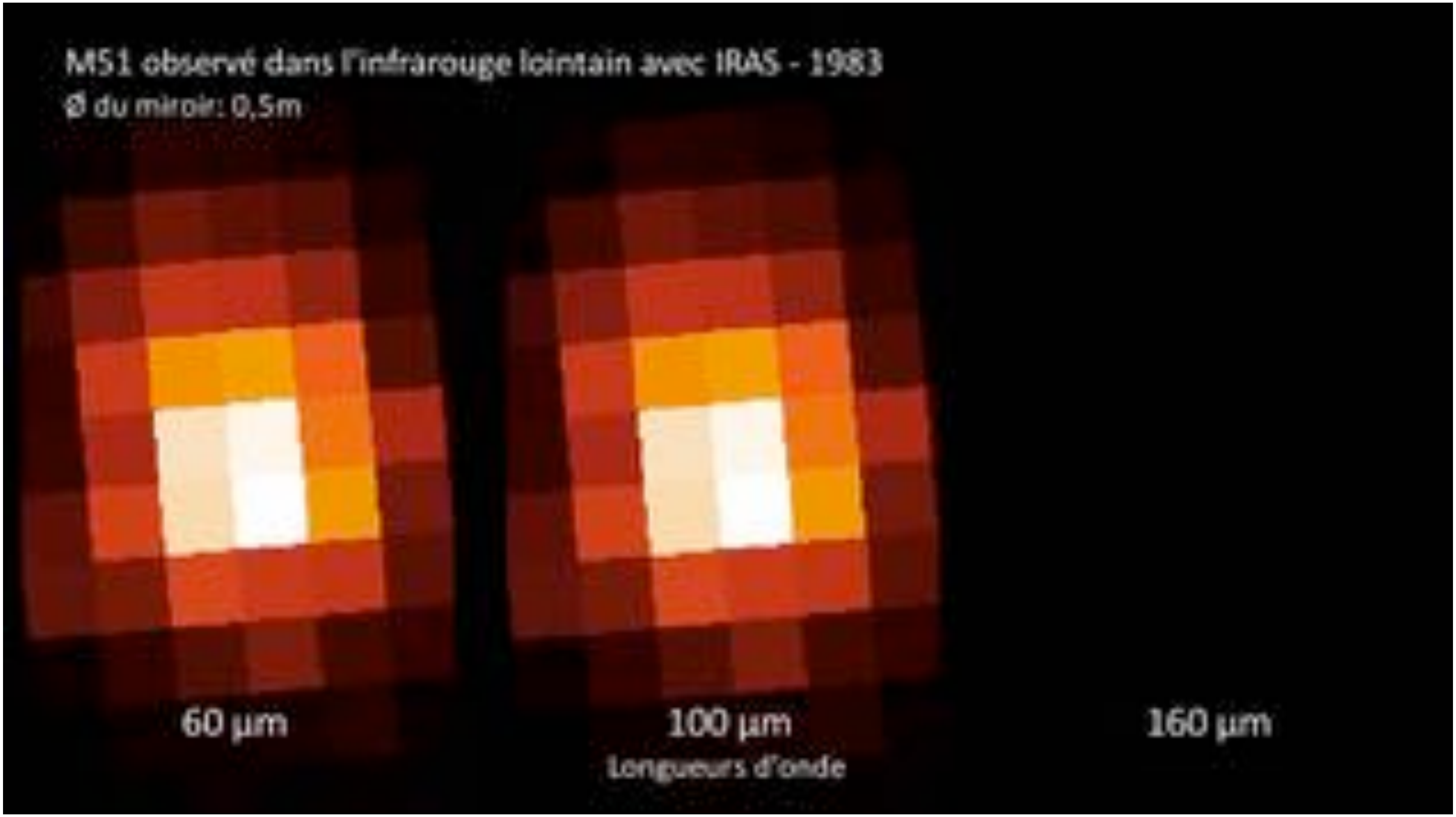
Realistic values in the interstellar medium yield temperatures of 15-30 K. The corresponding emission peaks in the far-infrared or submm range (on the order of 100 μm).

Interstellar dust effectively converts optical/UV starlight to FIR/submm emission.

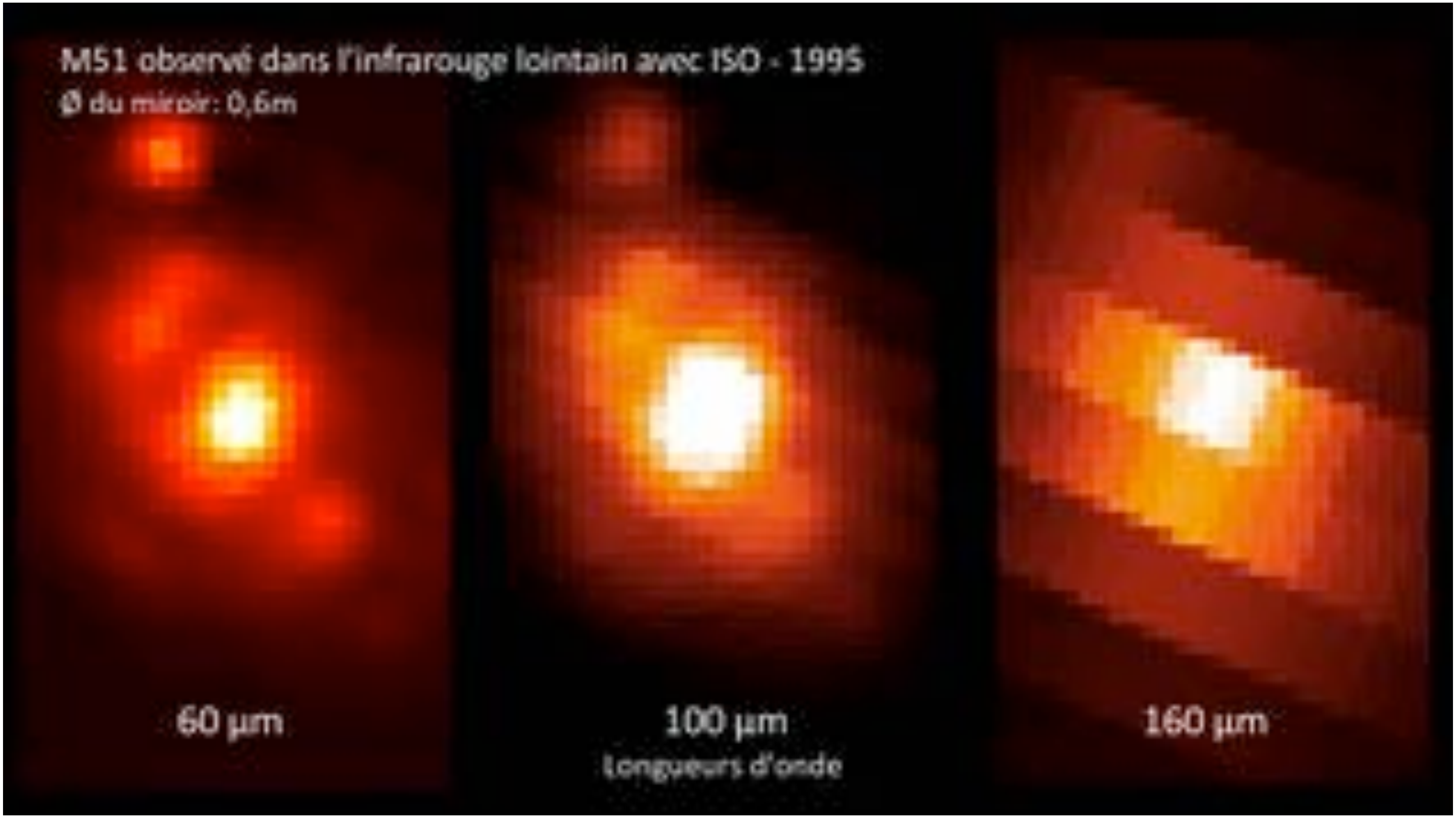


Fritz et al. 2012

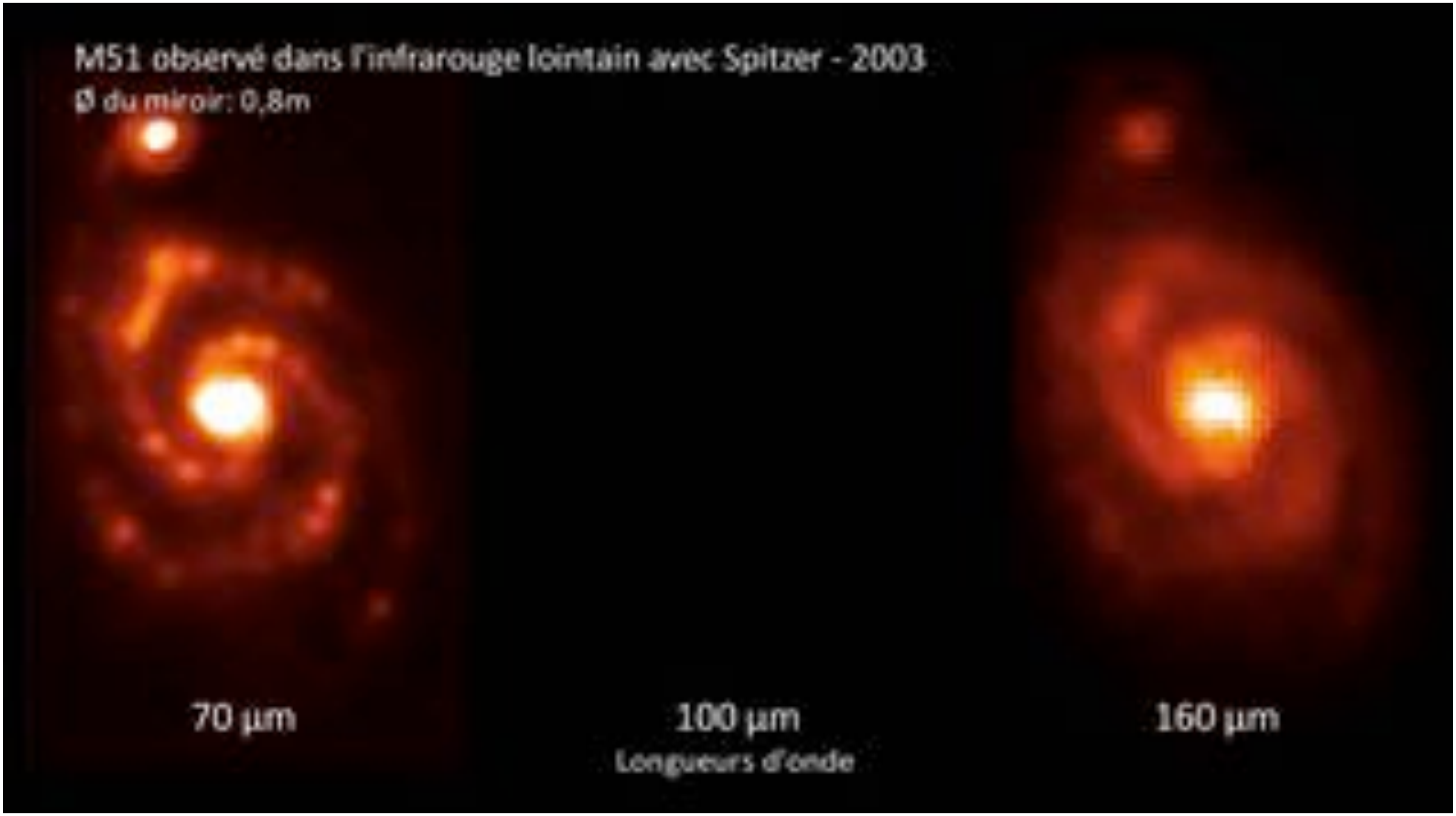
M51 with IRAS



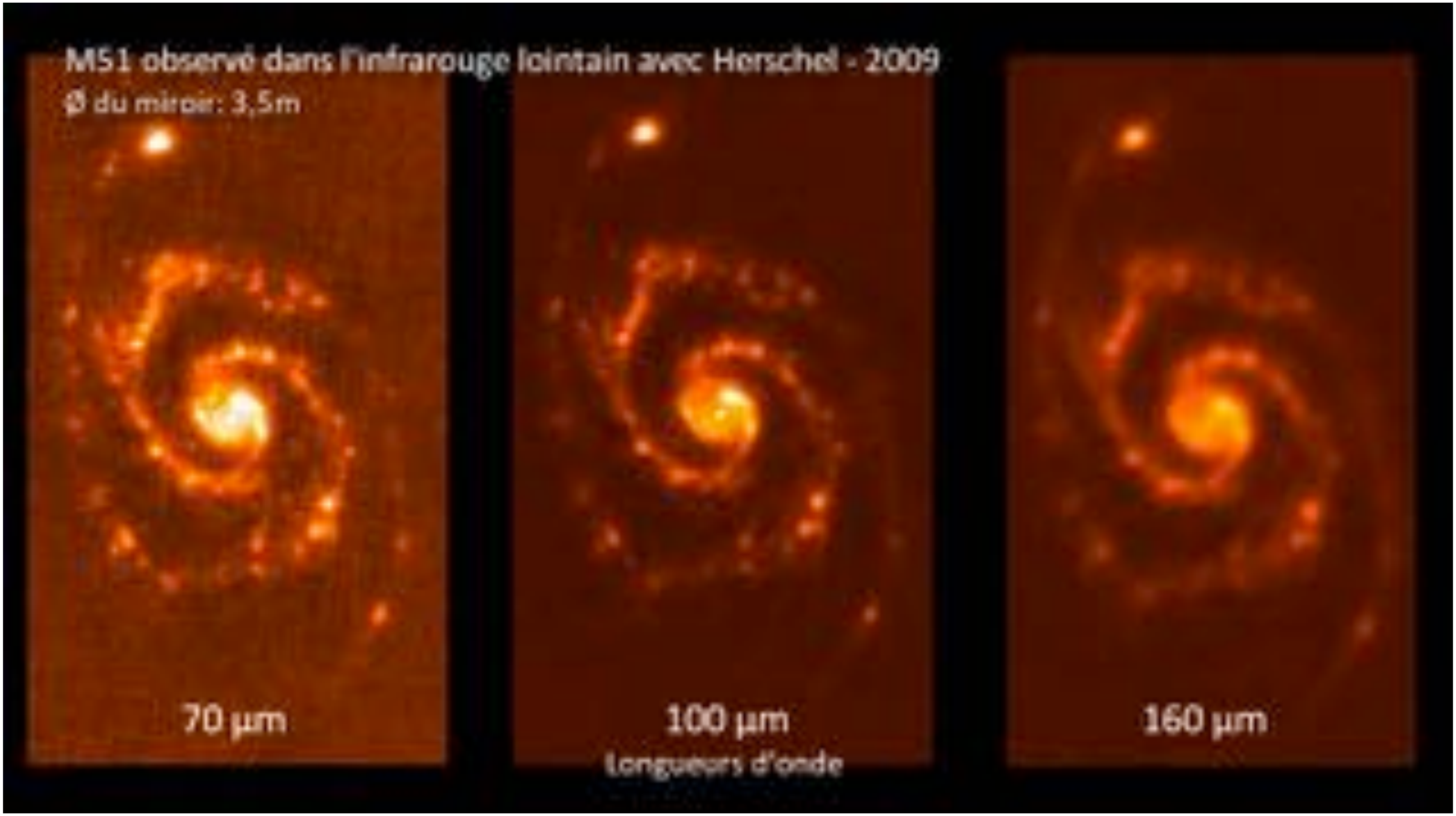
M51 with ISO


M51 observé dans l'infrarouge lointain avec ISO - 1995
Ø du miroir: 0,6m
60 µm
100 µm
Longueurs d'onde
160 µm

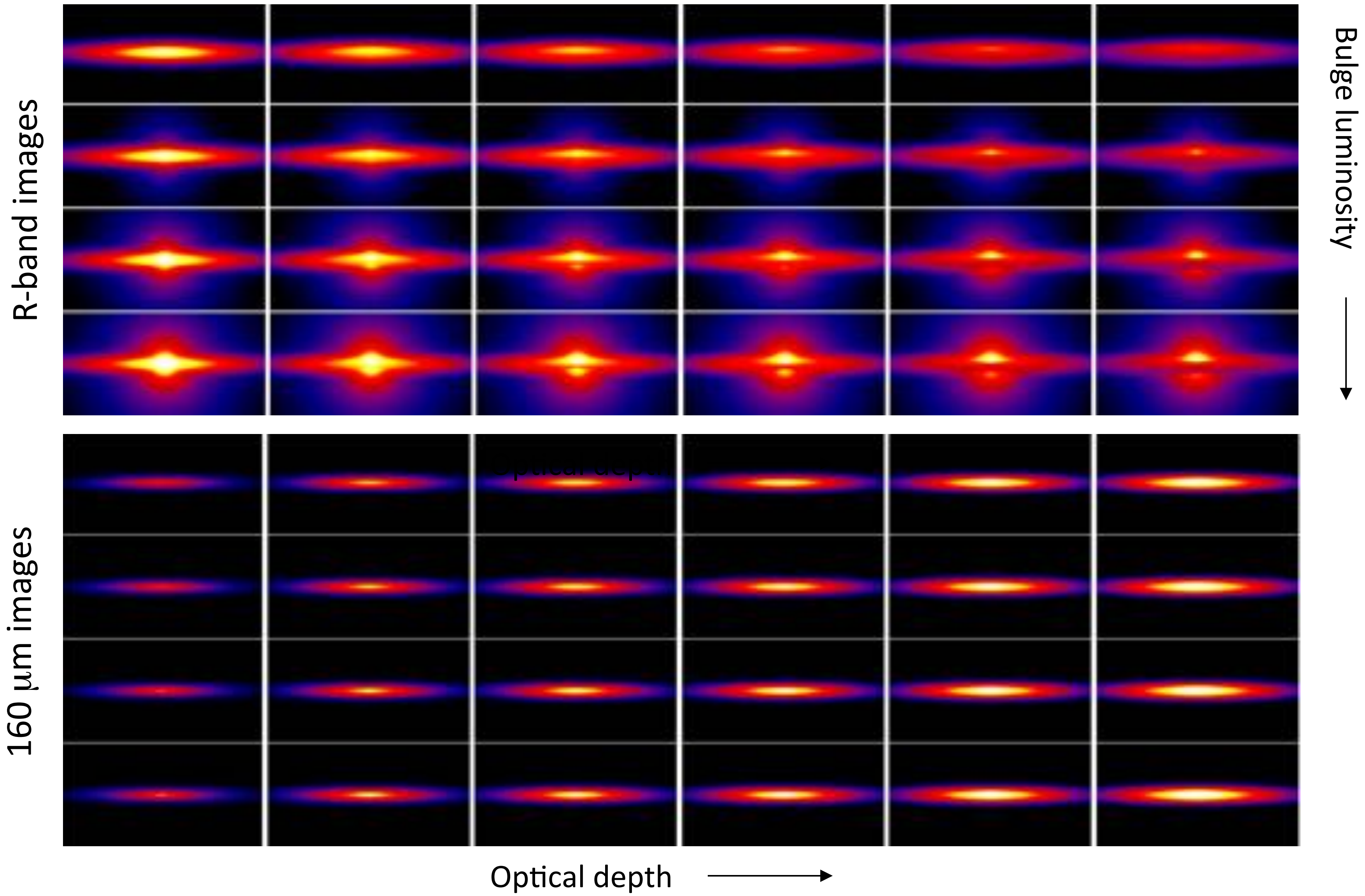
M51 with Spitzer



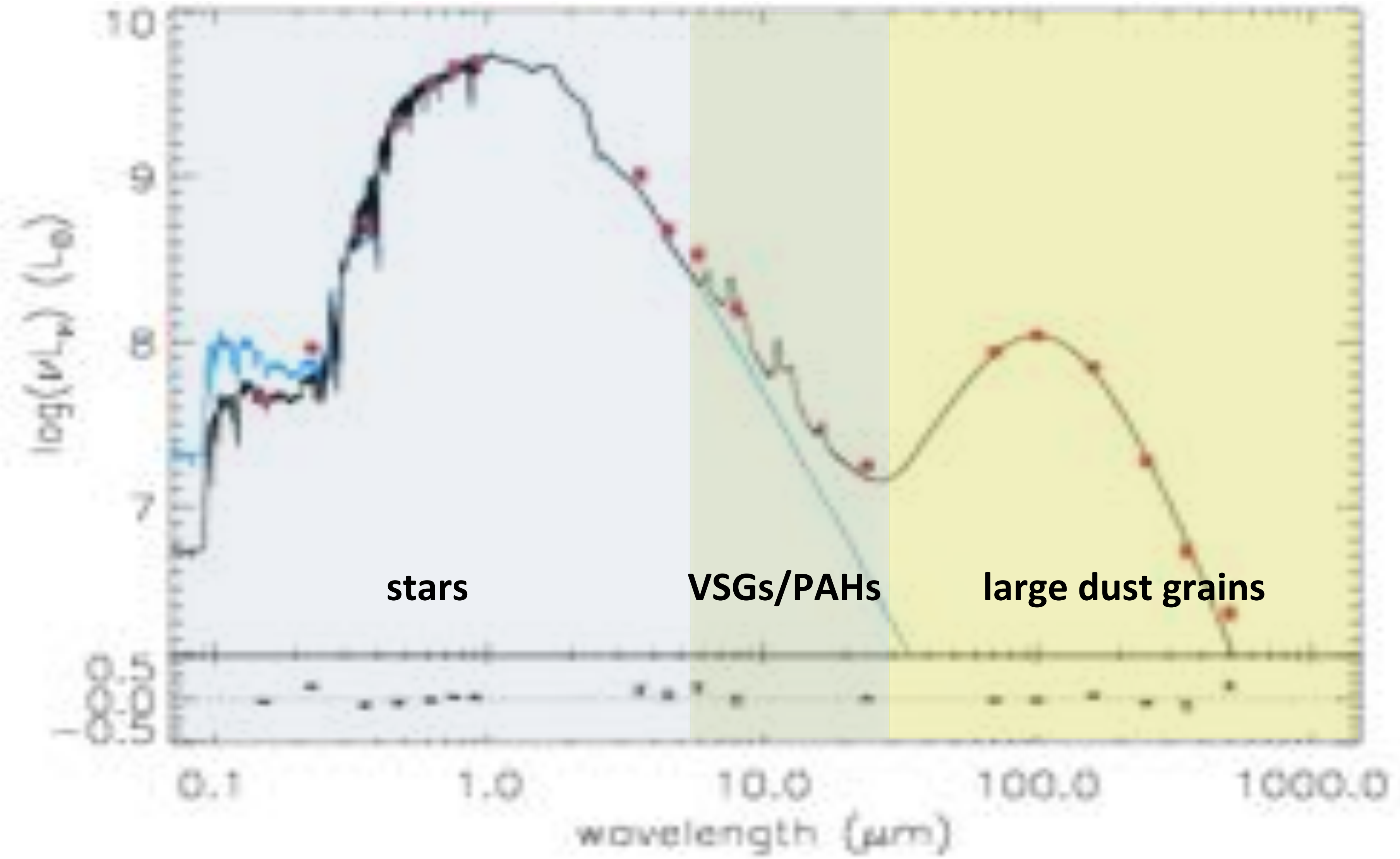
M51 with Herschel



Dust heating in spiral galaxies

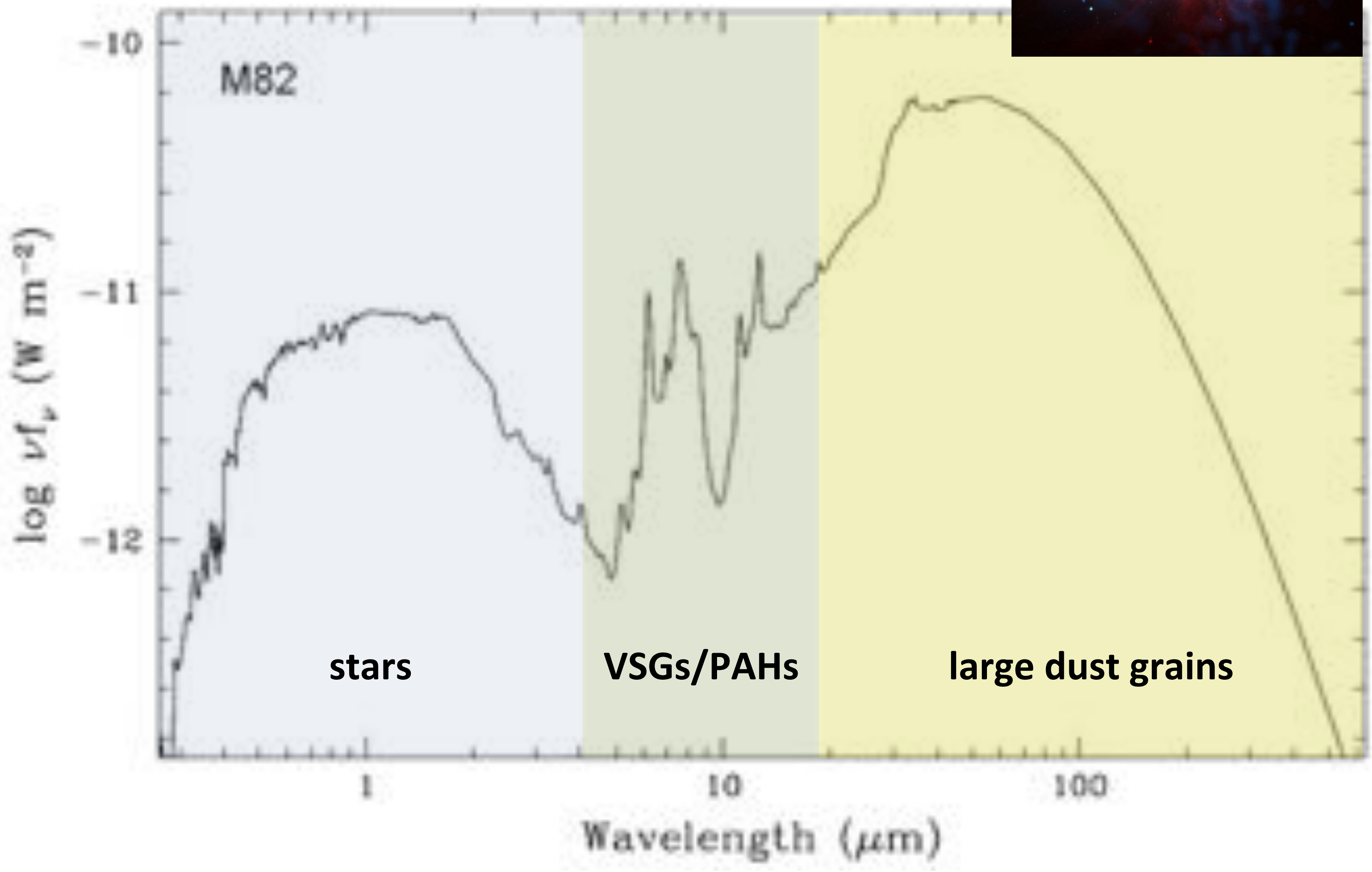


M31 SED



10
9
8
7
log(νL_ν) (L_⊙)
0.5
0.0
-0.5
0.1
1.0
10.0
100.0
1000.0
wavelength (μm)
stars
VSGs/PAHs
large dust grains

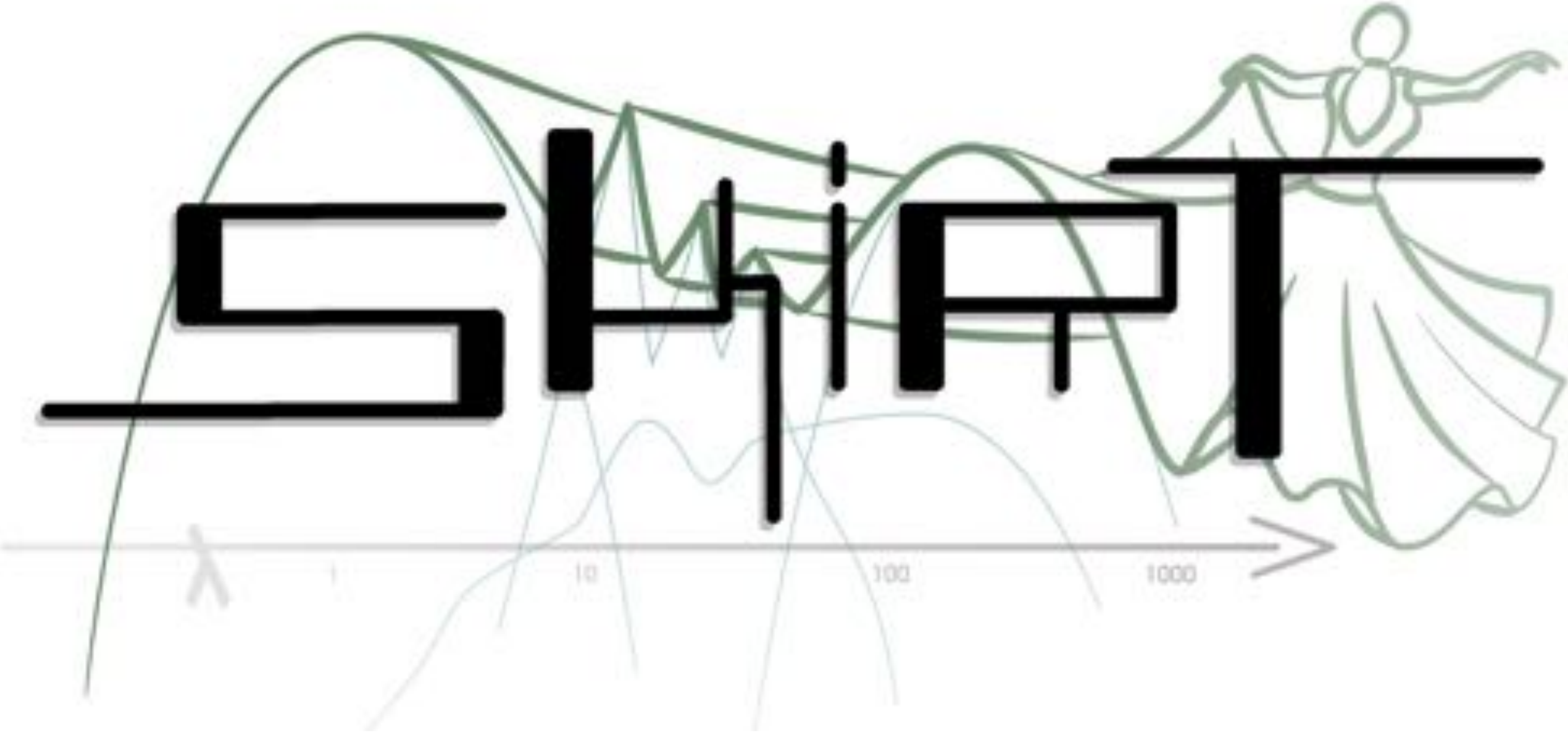
M82 SED


M82
-10
-11
-12
log νf_ν (W m⁻²)
1
10
100
Wavelength (μm)
stars
VSGs/PAHs
large dust grains

Questions ?

SKIRT features and code design

Section A-2



www.skirt.ugent.be
github.com/skirt

Key features

Monte Carlo continuum radiative transfer

- Absorption, scattering, and re-emission by dust
- Self-consistent calculation of dust temperature
- Stochastic heating of dust grains

Acceleration techniques

- Biased emission, forced scattering, continuous absorption, peel-off towards instruments
- Hybrid parallelization (shared & distributed memory)

Arbitrary geometries & properties for stars and dust

- Many built-in components, configured at run-time
- Import snapshot from hydrodynamic simulation

Application focus

Compare models to observations

- Images and emission spectrum

Dust in spiral galaxies

- Geometry and structure
- Energy balance
- Scaling relations

Other applications

- Dust torus in active galactic nuclei
- Molecular clouds
- Dusty outflows from (binary) stars

Infrastructure

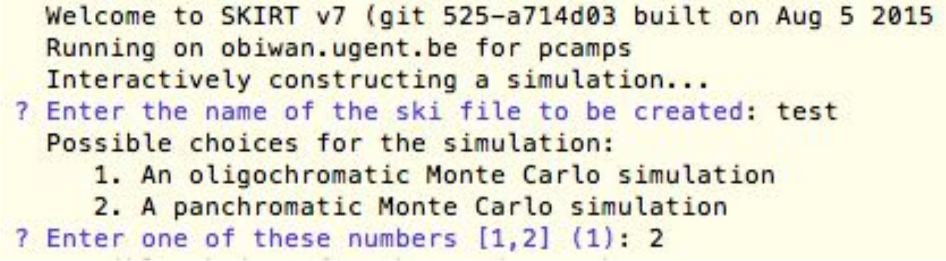
- Open source
- Published on GitHub (github.com/skirt)
- Fully documented (www.skirt.ugent.be)
- Written in C++11 (75000 lines in 300 classes)
- Uses Qt 5.x libraries and tools
- Optional use of MPI (multi-node parallelization)
- No other dependencies
- Well tested (200+ regression test cases)

Configurable built-in options

```
skirt

skirt <ski-filename>
```

- Command-line interface



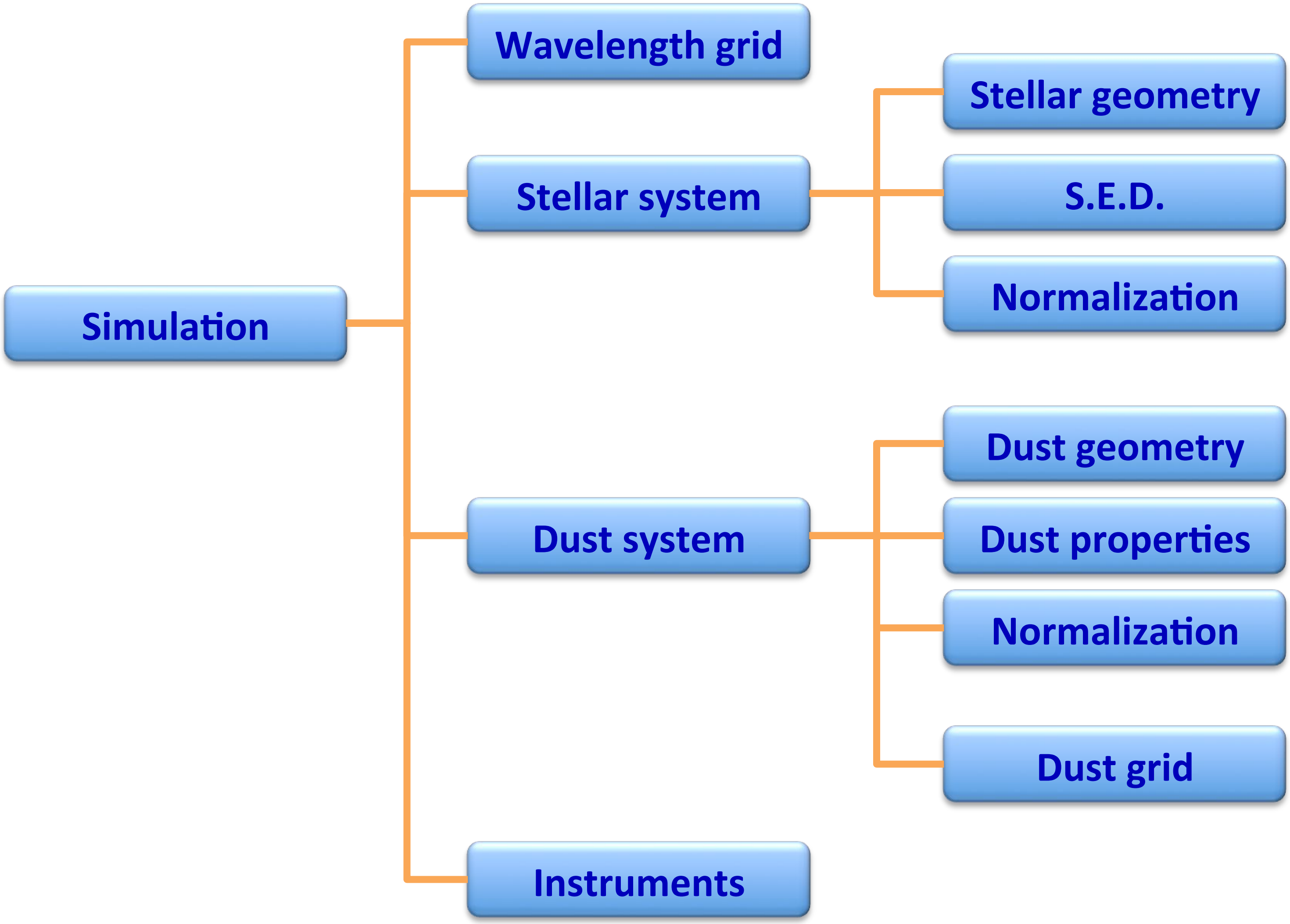
```
  Welcome to SKIRT v7 (git 525-a714d03 built on Aug 5 2015
  Running on obiwan.ugent.be for pcamps
  Interactively constructing a simulation...
? Enter the name of the ski file to be created: test
  Possible choices for the simulation:
     1. An oligochromatic Monte Carlo simulation
     2. A panchromatic Monte Carlo simulation
? Enter one of these numbers [1,2] (1): 2
```

- Q&A session to create configuration file

```
<PanDustSystem
    writeDensity="true"
    dustEmission="true"
    transient="false"
    selfAbsorption="false">
```

- XML-based configuration file
  - Easy to adjust in editor
  - Upgradable by automatic process

Simulation structure



Simulation

Wavelength grid

Stellar system

Stellar geometry

S.E.D.

Normalization

Dust system

Dust geometry

Dust properties

Normalization

Dust grid

Instruments

Instruments

Instrument name	SED	Frame	Sources Separated
DistantInstrument			
SEDInstrument	✔	--	--
FrameInstrument	--	✔	--
SimpleInstrument	✔	✔	--
FullInstrument	✔	✔	✔
PerspectiveInstrument	--	✔	--

Geometries

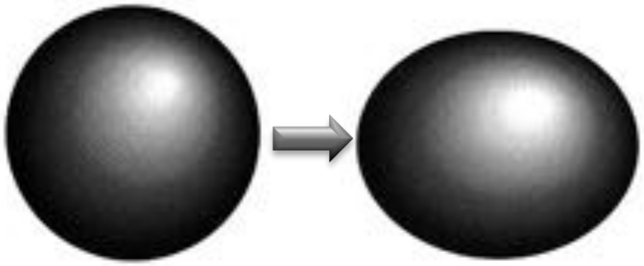
Basic (often symmetric)
Point
Plummer
Gamma
Sersic
Einasto
Shell
Ring
Torus
Exponential disk
Cuboid
Multi-Gaussian expansion

Hydro snaphots
AMR (adaptive mesh)
SPH (smoothed particles)

Decorators
Offset
Rotation
Spheroidal distortion
Triaxial distortion
Spherical cavity
Cylindrical cavity
Crop
Add spiral arms
Make clumpy
Combine

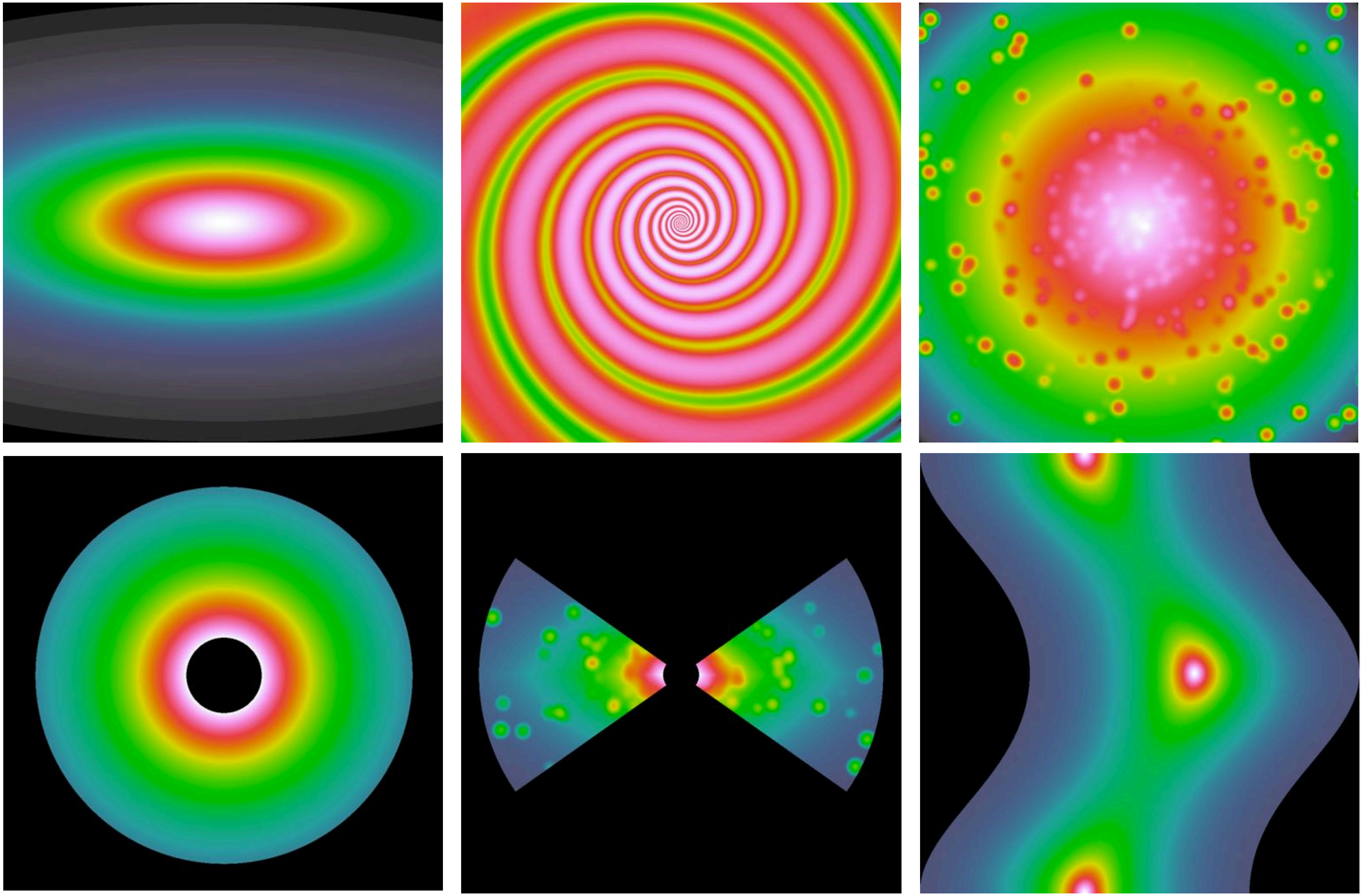
Anisotropic sources
Laser
Netzer accretion disk
Spherical surface
Spherical background

- A geometry defines a spatial density distribution
- All geometries can be used for both stellar and dust distributions
- Decorators serve to adjust and combine other geometries



- Decorators can be nested to arbitrary levels

Geometries

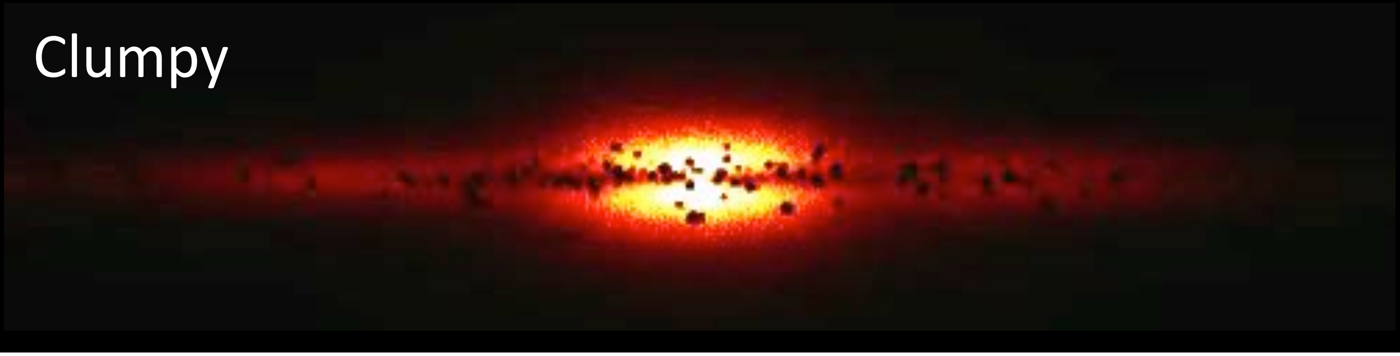


Geometries


Spiral arms


Peanut bulge

De Geyter 2015

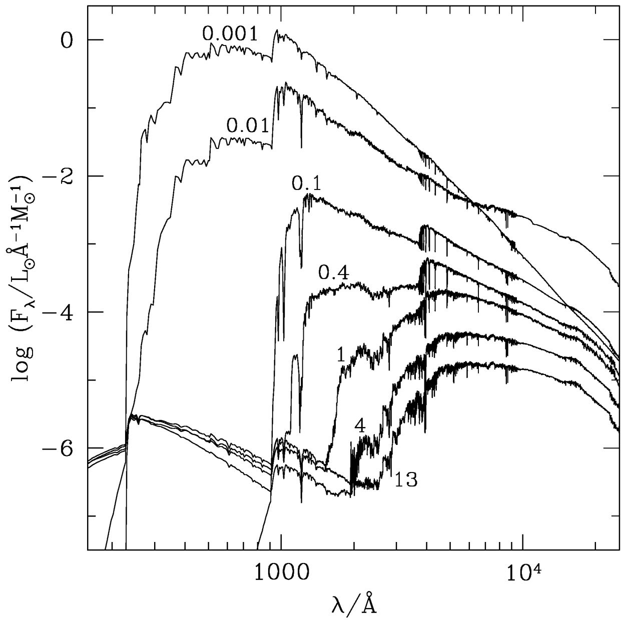

Clumpy

Stellar SEDs

SED
Black Body
Sun
Pegase
Quasar
Maraston
Kurucz
Bruzual-Charlot
Starburst (Mappings)
File

SED family
Bruzual-Charlot
Starburst (Mappings)

- An SED is assigned to each stellar geometry



Bruzual & Charlot 2003

- An SED family allows each particle/cell in an imported hydro snapshot to be assigned its own spectrum based on its properties (e.g. metallicity, age)

Dust properties

Turn-key dust mixture
Draine & Li 2007
MRN
Weingartner & Draine
Zubko et al.

Configurable dust mixture

Grain composition
Graphite
Silicate
Ionized PAH
Neutral PAH
Enstatite
Forsterite

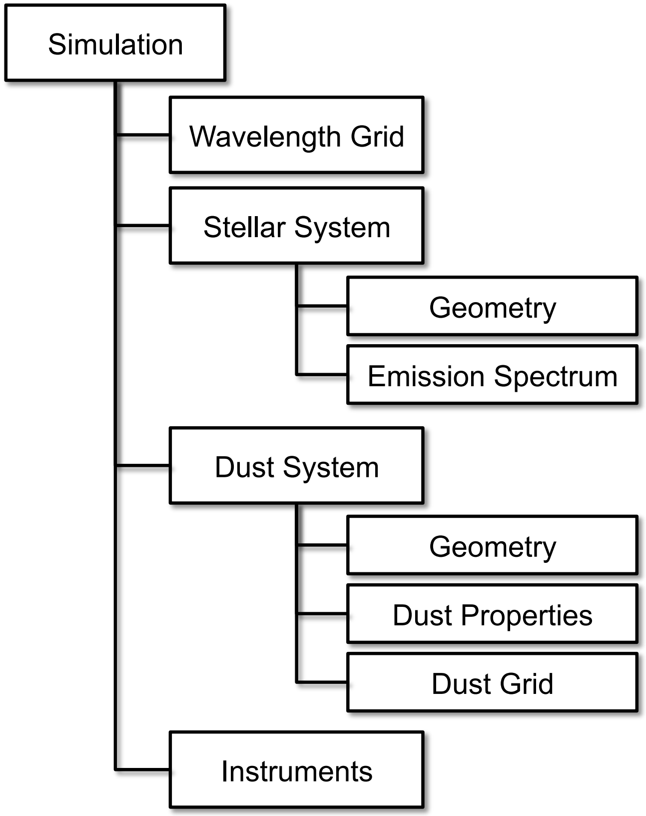
Grain size distribution
LogNormal
PowerLaw
ModifiedPowerLaw
SingleGrain
Zubko

- A dust system can have multiple dust components, each with its own geometry and dust mixture
- Turn-key dust mixtures include pre-configured properties
- The configurable dust mix allows specifying grain composition and size distribution in detail

Software architecture

Complex configuration

- Many built-in options
- Nontrivial structure (iteration, nesting)



- Simulation
  - Wavelength Grid
  - Stellar System
    - Geometry
    - Emission Spectrum
  - Dust System
    - Geometry
    - Dust Properties
    - Dust Grid
  - Instruments

How to deal with this?

Scientific codes can benefit from careful object-oriented design

A non-graphical user interface can be friendly

Design goals

Single point of definition

- Define user interface properties with the program logic

Data-driven user interface

- Have the user interface adjust automatically as new features are added

Structured parameter file

- Use human-readable self-documenting format that supports iteration and nesting

Modularity

- Minimize dependencies through appropriate interfaces and data encapsulation

Single point of definition in the code

```
class ClumpyGeometry : public Geometry
{
    Q_OBJECT
    Q_CLASSINFO("Title", "a geometry that adds clumpiness to any geometry")

    Q_CLASSINFO("Property", "geometry")
    Q_CLASSINFO("Title", "the geometry to which clumpiness is added")

    Q_CLASSINFO("Property", "clumpFraction")
    Q_CLASSINFO("Title", "the fraction of the mass locked up in clumps")
    Q_CLASSINFO("MinValue", "0")
    Q_CLASSINFO("MaxValue", "1")

public:
    Q_INVOKABLE void setGeometry(Geometry* value);
    Q_INVOKABLE Geometry* geometry() const;

    Q_INVOKABLE void setClumpFraction(double value);
    Q_INVOKABLE double clumpFraction() const;

     ...
 };
```

Property name

Human readable title

Value restrictions

Data type

Data-driven “Q&A” user interface

```
$ skirt
? Enter the name of the ski file to be created: spiralgalaxy
  Possible choices for the simulation:
     1. An oligochromatic Monte Carlo simulation
     2. A panchromatic Monte Carlo simulation
? Enter one of these numbers [1,2] (1): 1
  Possible choices for the units system:
     1. SI units
     2. Stellar units (length in AU, distance in pc)
     3. Extragalactic units (length in pc, distance in Mpc)
? Enter one of these numbers [1,3] (3):
? Enter the number of photon packages per wavelength [0,2e13] (1e6): 1e7
  Possible choices for the wavelength grid:
     1. A list of one or more distinct wavelengths
  Automatically selected the only choice: 1
? Enter the wavelengths [0.0001 micron,1e6 micron]: 0.55
  Possible choices for the stellar system:
     1. A stellar system composed of various stellar components
     2. A stellar system derived from an SPH output file
     ...
? Enter one of these numbers [1,4] (1): 1
     ...
  Possible choices for the geometry of the dust component:
     1. A point source geometry
     2. A Plummer geometry
     ...
     9. An exponential disk geometry
     ...
? Enter one of these numbers [1,26] (9): 9
```

Allowed range and default units

Choices derived from source code data

Default value

XML-based parameter file

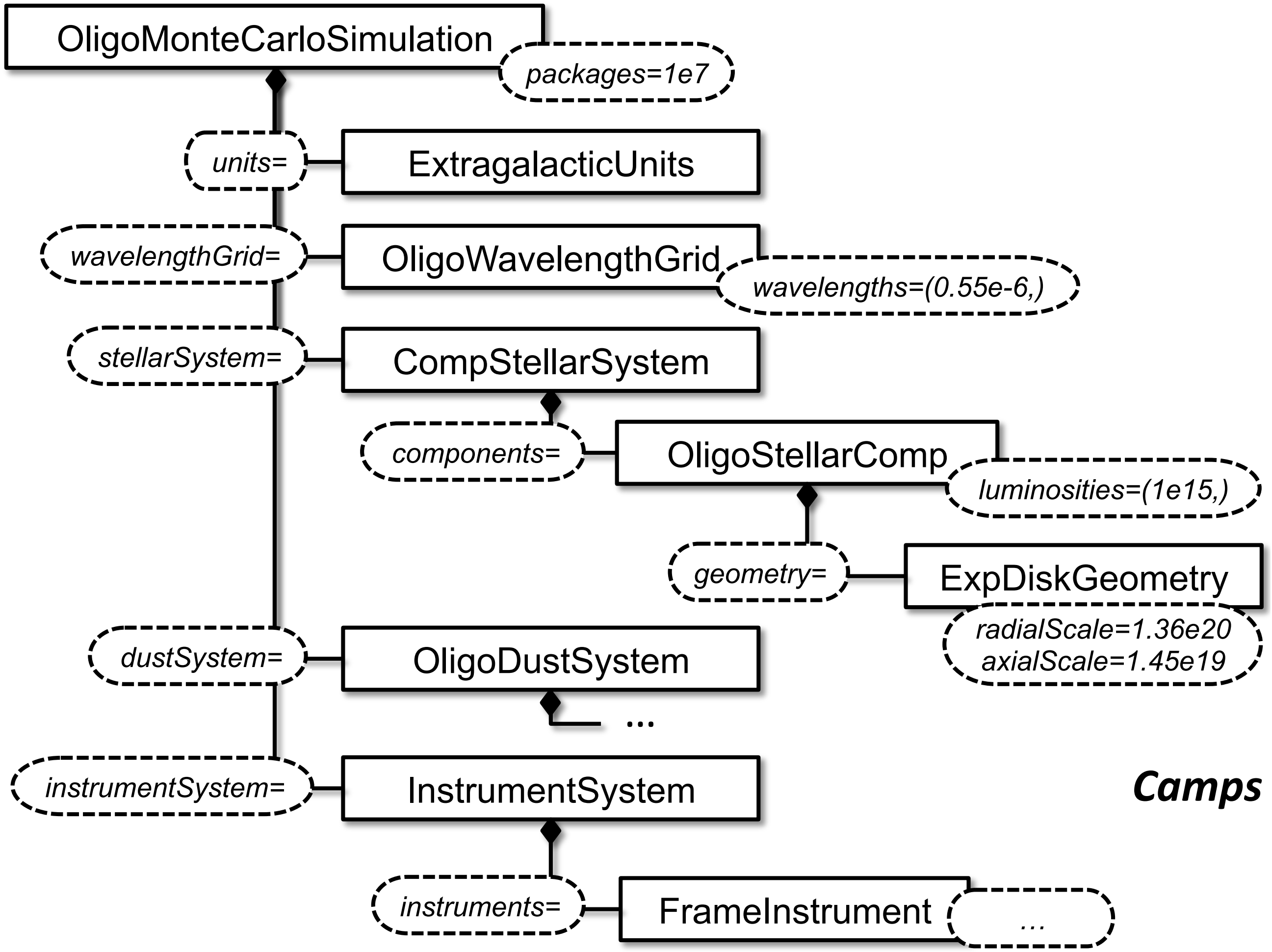
```xml
<?xml version="1.0" encoding="UTF-8"?>
<skirt-simulation-hierarchy type="MonteCarloSimulation" format="6.1">
    <OligoMonteCarloSimulation packages="1e7">
        <units type="Units">
            <ExtragalacticUnits/>
        </units>
        <wavelengthGrid type="OligoWavelengthGrid">
            <OligoWavelengthGrid wavelengths="0.55 micron"/>
        </wavelengthGrid>
        <stellarSystem type="StellarSystem">
            <CompStellarSystem>
                <components type="StellarComp">
                    <OligoStellarComp luminosities="1e11">
                        <geometry type="Geometry">
                            <ExpDiskGeometry radialScale="4400 pc" axialScale="500 pc"
                                radialTrunc="0 pc" axialTrunc="0 pc"/>
                        </geometry>
                    </OligoStellarComp>
                </components>
            </CompStellarSystem>
        </stellarSystem>
        <dustSystem type="OligoDustSystem">
            <OligoDustSystem>
                <dustDistribution type="DustDistribution">
                    <CompDustDistribution>
                        <components type="DustComp">
```

Supports iteration and nesting to any depth

Property names are documented

Values include units

Run-time structure of simulation

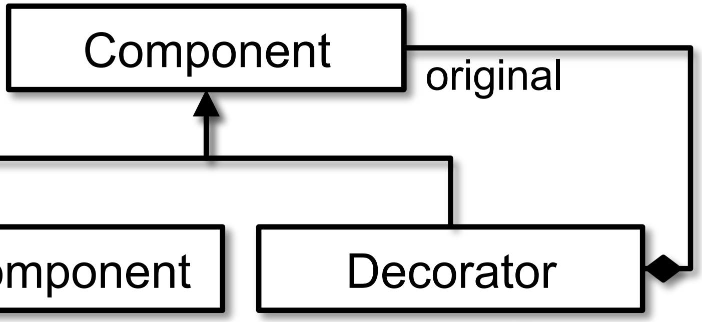


Camps & Baes 2015

Run-time hierarchy and parameter file have identical structure

Geometry decorators

```
class Geometry {
  public:
    Geometry();
    virtual ~Geometry();
    virtual double density(Position x) const = 0;
    virtual Position generatePosition() const = 0;
}
```



```
class ConcreteGeometry : public Geometry {
  public:
    ConcreteGeometry(double p) {_p=p}
    double density(Position x) const;
    Position generatePosition() const;
  private:
    double _p;
}
```

```
class OffsetGeometryDecorator : public Geometry {
  public:
    OffsetGeometryDecorator(Geometry* g, Position a)
      {_g = g; _a = a;}
    double density(Position x) const
      {return _g->density(x-a);}
    Position generatePosition() const
      {return _g->generatePosition()+a;}
  private:
    Geometry* _g;
    Position _a;
}
```

Camps & Baes 2015
Baes & Camps 2015

Conclusion

SKIRT

- Is a state-of-the art dust continuum RT code
- Offers a large suite of built-in components
- Includes a flexible configuration mechanism
- Allows easily adding new components

All (scientific) codes

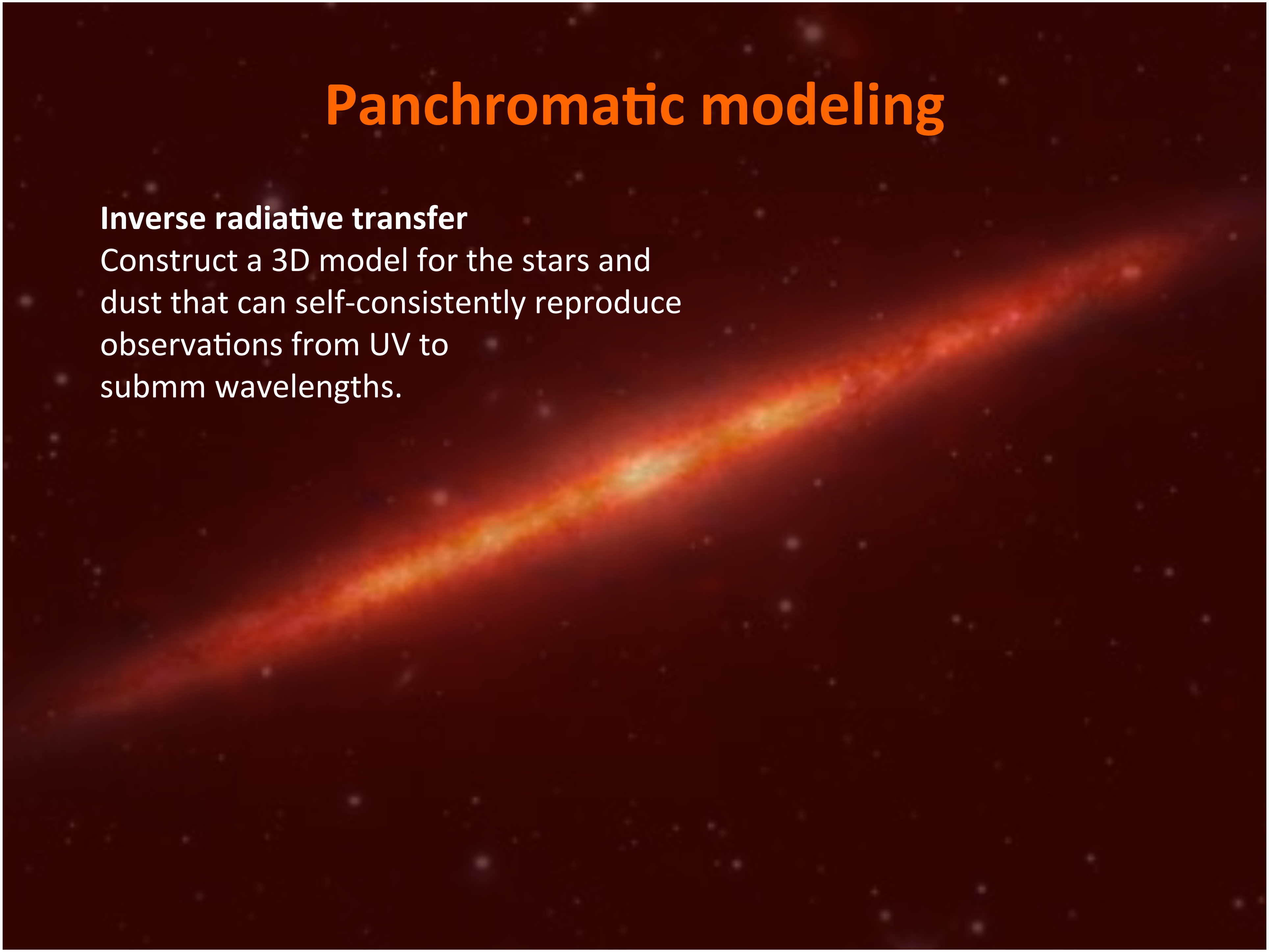
- Can benefit from careful object-oriented design
- Can offer a friendly user interface (even if not graphical)

Questions ?

Energy balance in galaxies

Section A-3

Panchromatic modeling



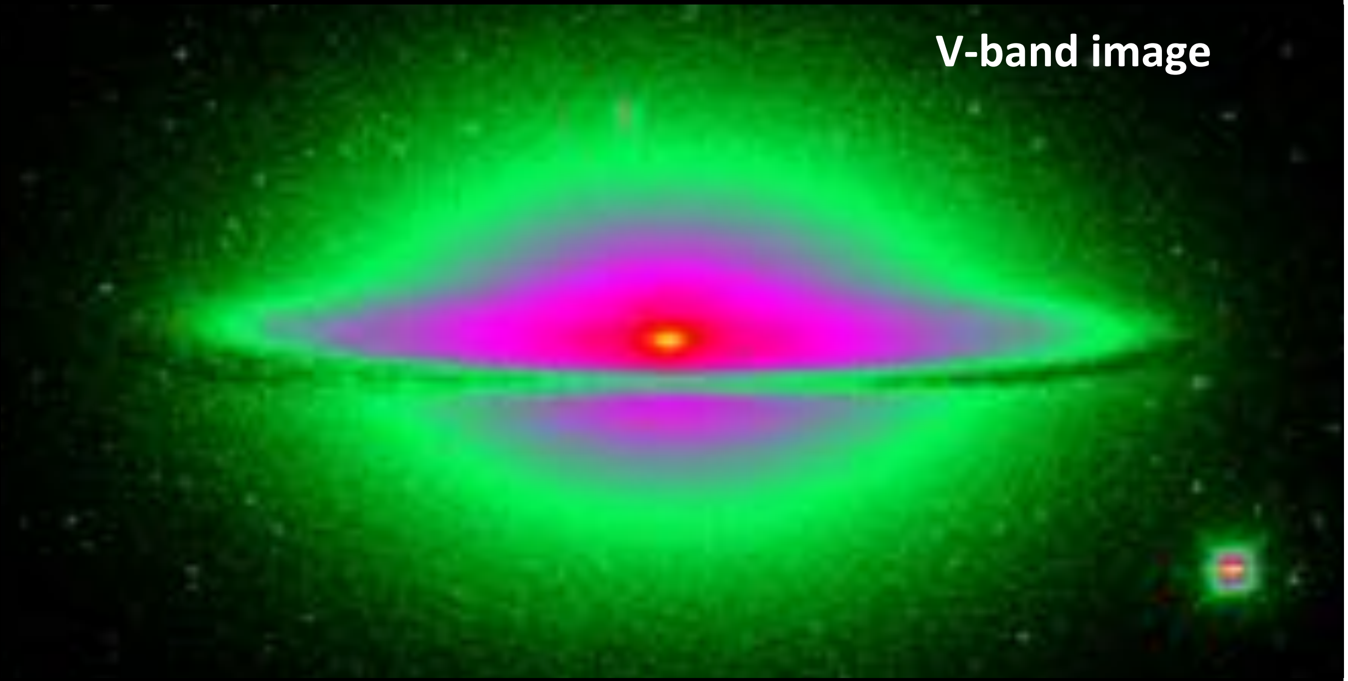
Inverse radiative transfer

Construct a 3D model for the stars and dust that can self-consistently reproduce observations from UV to submm wavelengths.

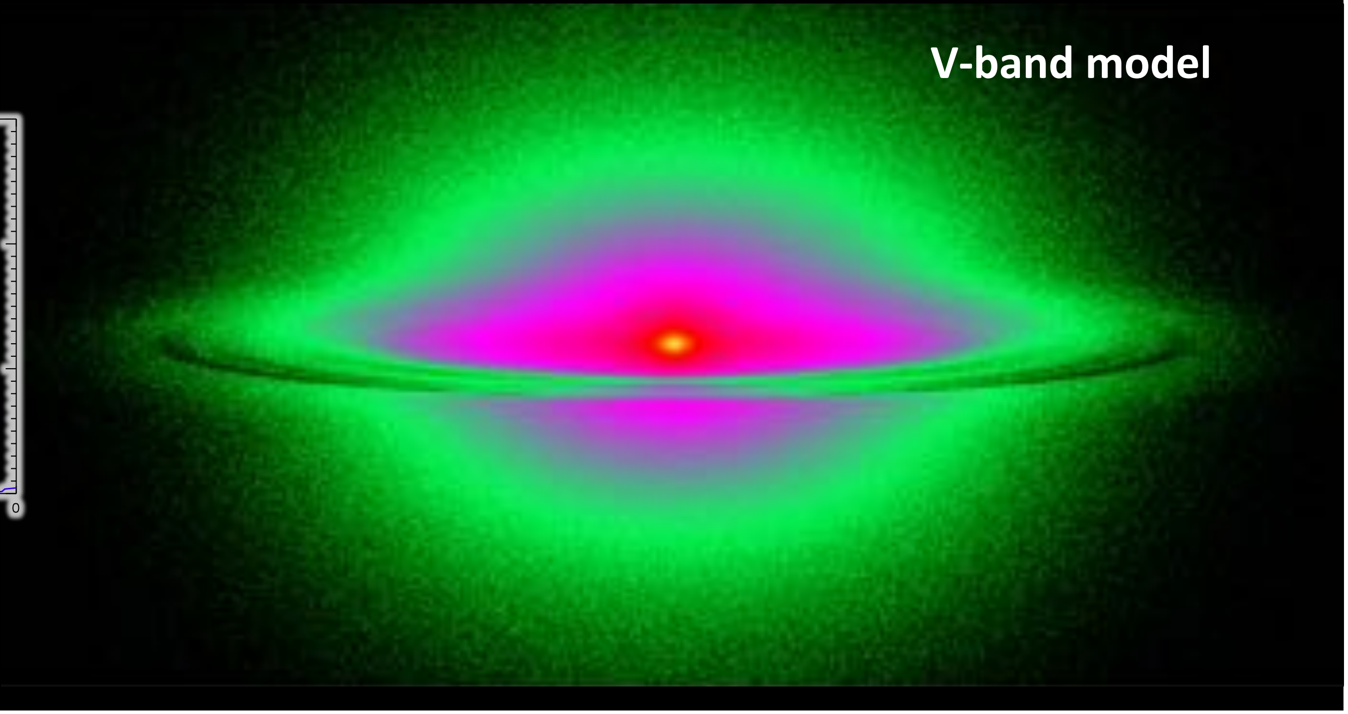
Case study: Sombrero galaxy (NGC 4594)

NGC 4594

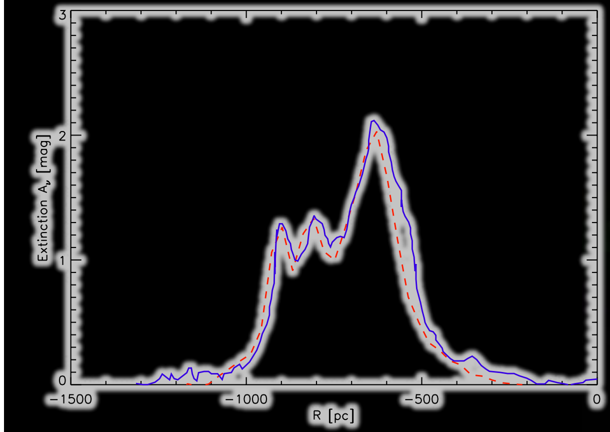
Construct a model reproducing
the optical image;
in particular the
minor axis intensity
profile



V-band image

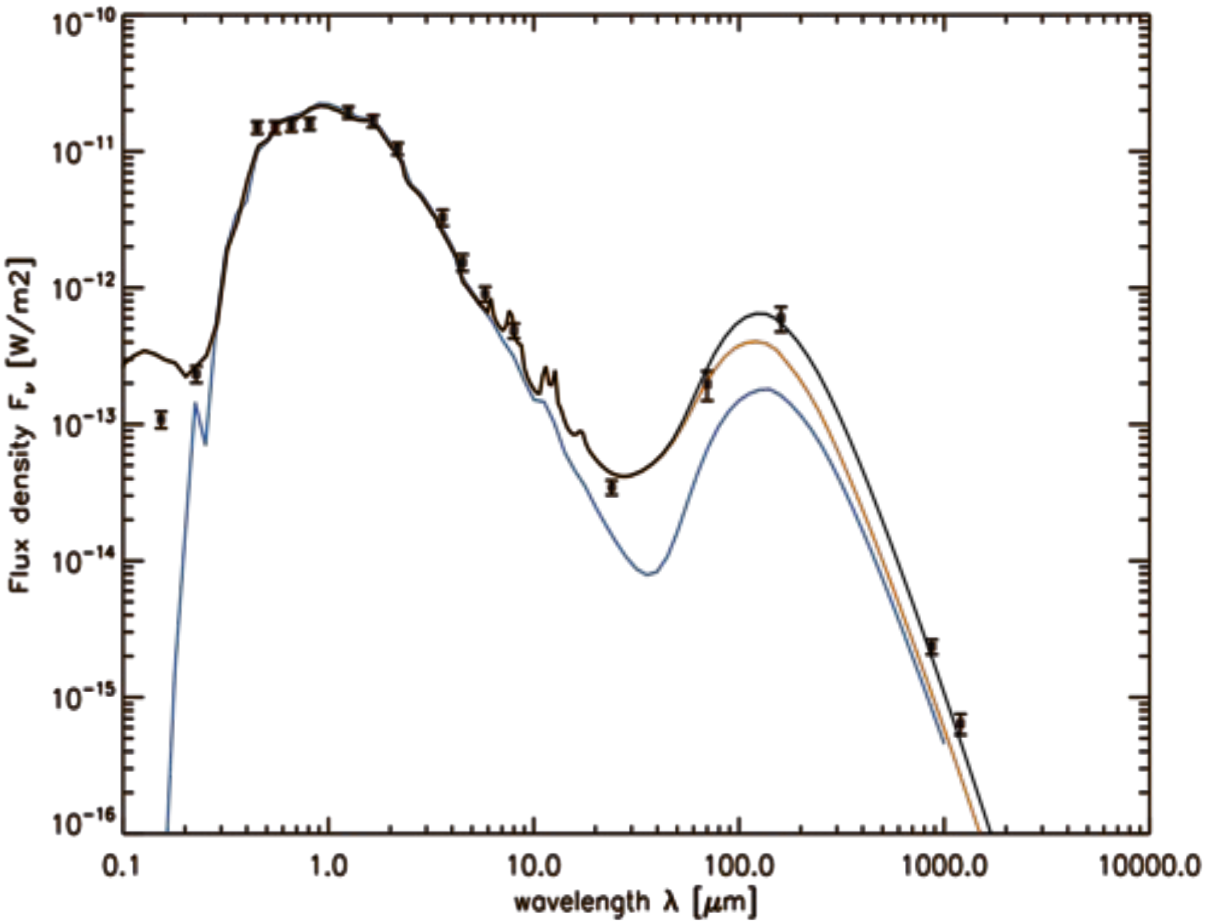


V-band model



De Looze et al. 2012

Energy balance study for NGC 4594



De Looze et al. 2012

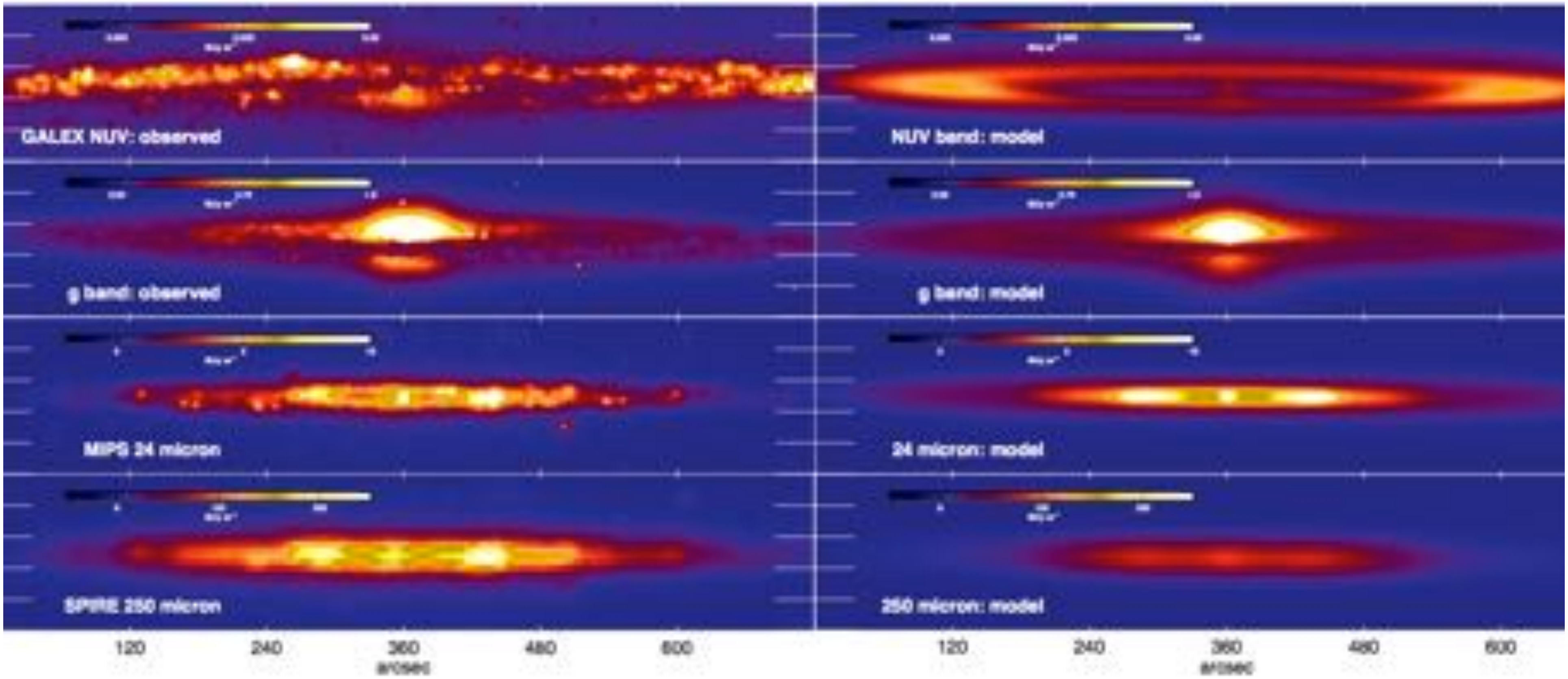
- Generate full SED from model
- Add young stars to match UV data
- We need an extra component of 17 K dust to explain the submm emission
- The dust seems to emit 3 times more energy than it absorbs

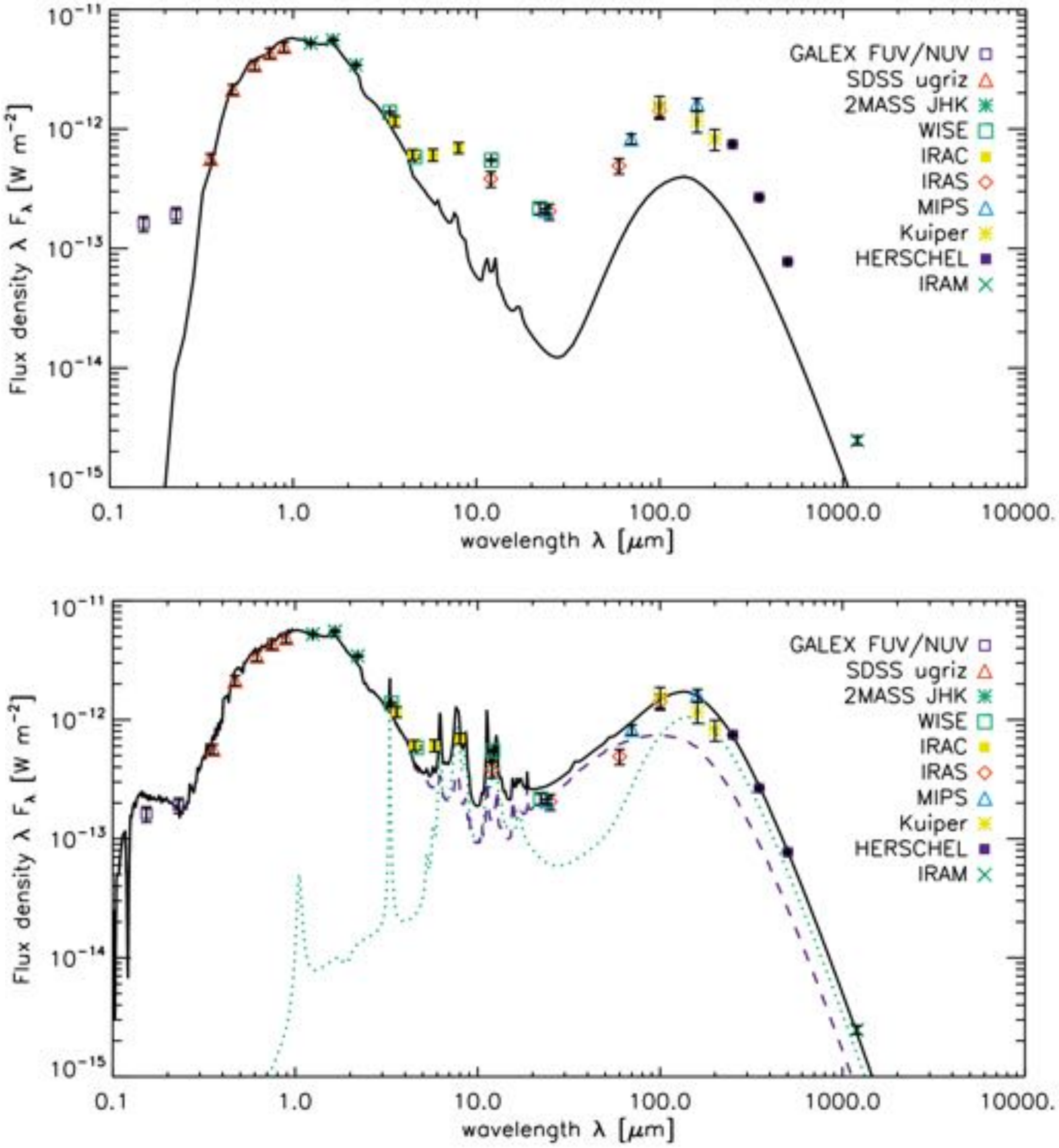
Case study: NGC 4565

Energy balance study for NGC 4565

Construct a model fitting images in multiple bands from UV to infrared

De Looze et al. 2012





NGC 4565

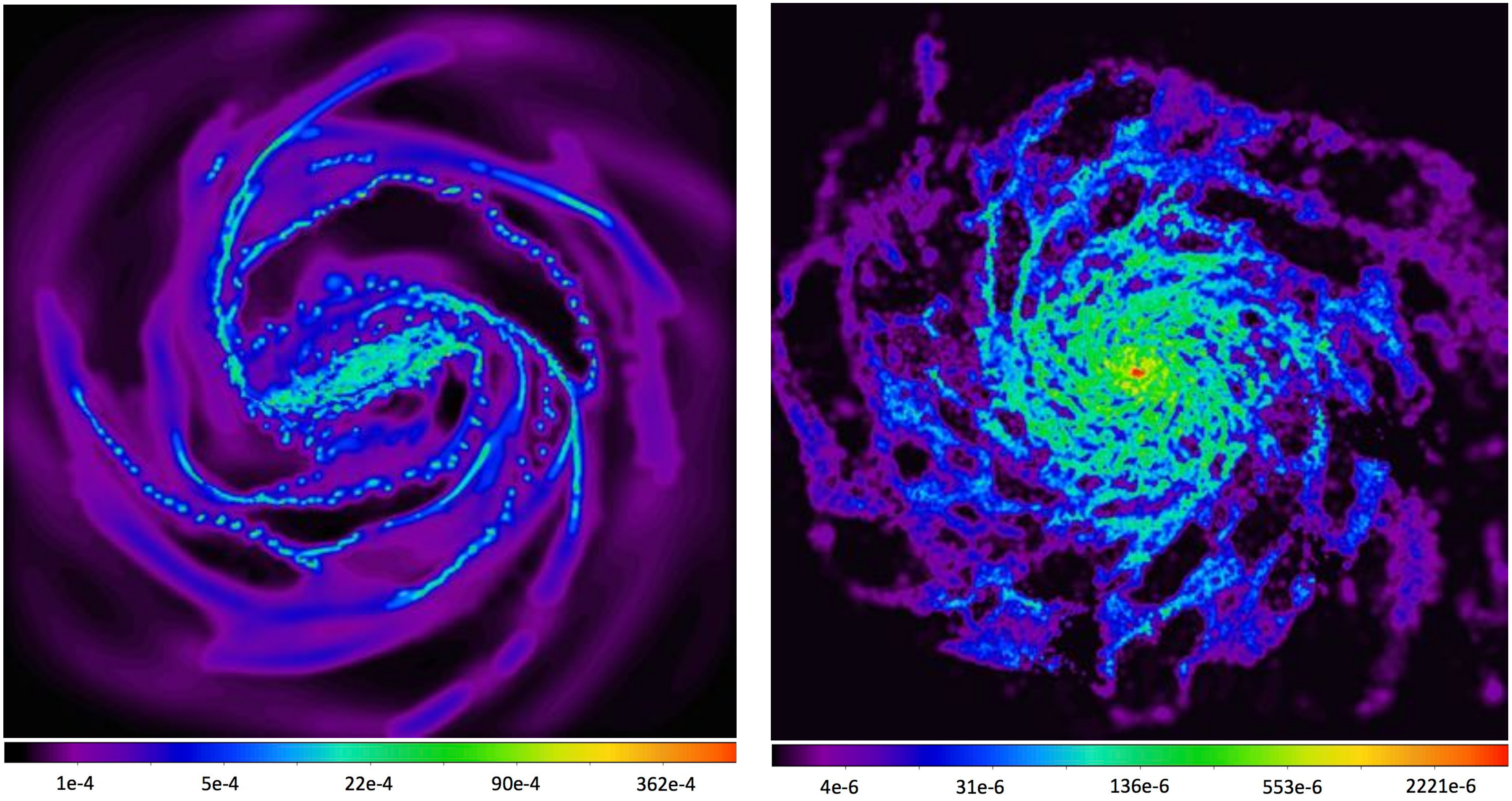
- Generate full SED from model
- Discrepancy at UV/FIR
- Add star formation constrained by NUV and MIR
- Still deficit of factor 3-4

De Looze et al. 2012

The dust energy balance problem

- For some (not all) edge-on spiral galaxies
  - the dust mass estimated from extinction is 3 or 4 times smaller
  - than the dust mass estimated from emission in FIR/submm
- However, our models are smooth, unlike real galaxies
  - Large-scale structure: bars, spiral arms
  - Small-scale structure: granularity, filaments, star forming regions, compact dust clumps
- Better models?
  - Models with large-scale structure (spiral arms, large clumps) fail to resolve the discrepancy (e.g. *Misioriotis et al. 2000, 2002*)
  - What about small-scale structure? Test this hypothesis using galaxies created in hydrodynamical simulations…

Input models from hydrodynamical simulations



R13 (*Renaud et al. 2013*)

Eris (*Guedes et al. 2011*)

Cut through the dust density distribution in the equatorial plane of each galaxy


R13


Eris

Fitting results

R13

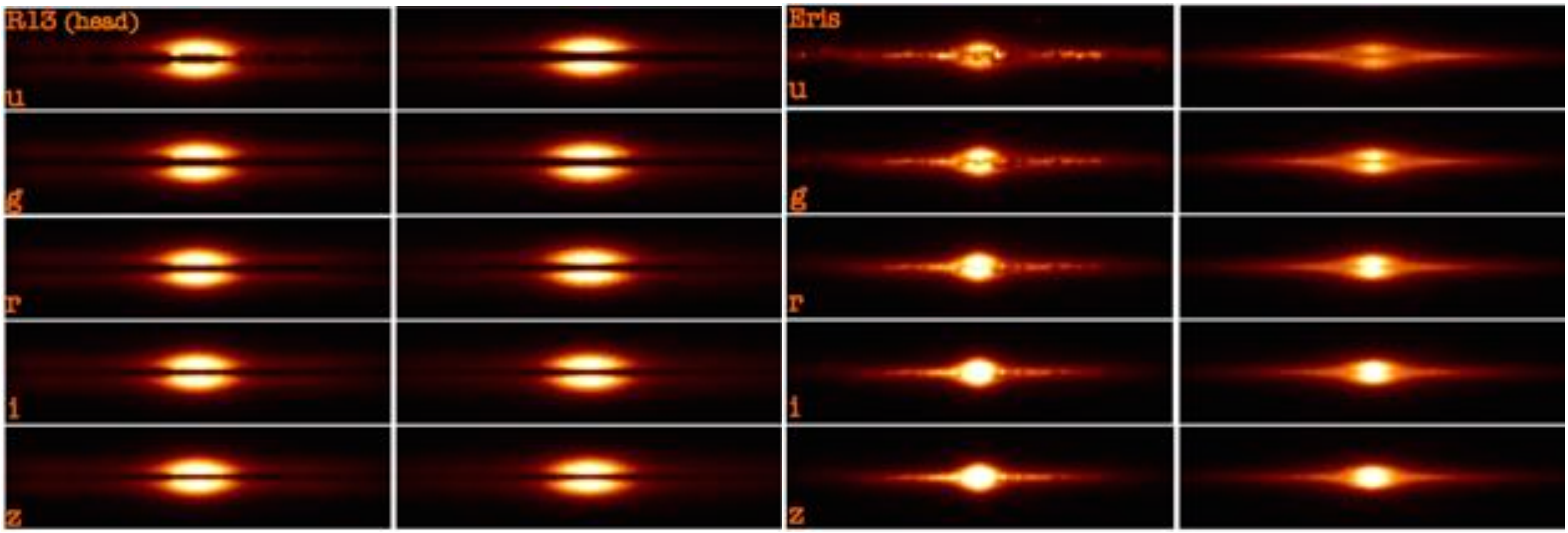
Reference images

Fitted images

Eris

Reference images

Fitted images



Par.	Units	R13 (head)	R13 (side)	Eris
M_d	$10^6\ M_\odot$	6.26 ± 0.24	7.68 ± 0.33	1.48 ± 0.18

$18.1 \times 10^6\ M_\odot$

$5.94 \times 10^6\ M_\odot$

The RT model underestimates the “true” dust mass by a factor of: 2.9 and 2.4 for R13, and by a factor of 4 for Eris.

Saftly et al. 2015

Conclusion

Fitting a smooth galaxy model to realistic input models from hydrodynamic simulations underestimates the total dust mass by a factor of about 3.

This suggests that the inhomogeneous small-scale structure of galaxies may be the source of the dust energy balance problem.

In other words, it suggests that the clumpy structure keeps a large amount of dust from being observed through extinction in the optical wavelength range.

Questions ?

Automated galaxy modeling

Section A-4

Automated inverse radiative transfer

Objective

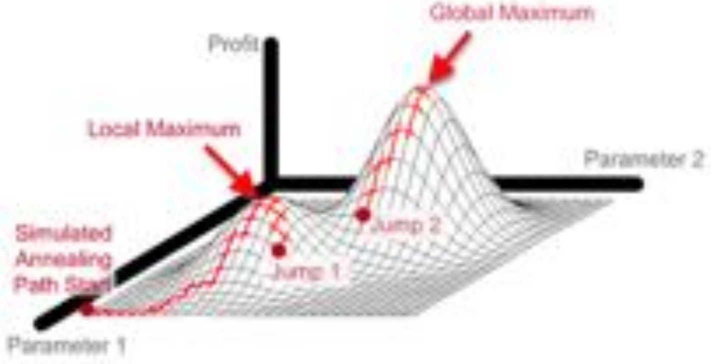
- Automatically find optimal model parameters by coupling a radiative transfer code to an optimization process

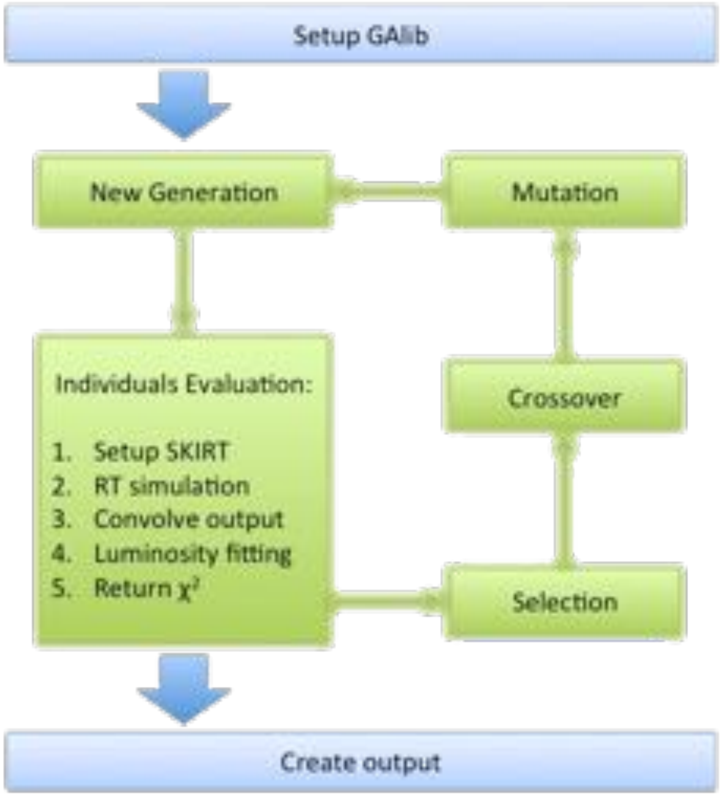
Complications

- Large number of model parameters to be fitted
  - Intrinsic star & dust geometry
  - Orientation
  - Dust properties
- Run-time for a single RT simulation (i.e. a single point in the multi-dimensional parameter space) is considerable
- Monte Carlo noise makes fitting more complicated

Automated parameter fitting

Poisson noise on Monte Carlo simulations prevents standard fitting and complicates simulated annealing





Setup GAlib

New Generation

Mutation

Individuals Evaluation:

1. Setup SKIRT
2. RT simulation
3. Convolve output
4. Luminosity fitting
5. Return χ^2

Crossover

Selection

Create output

Genetic algorithm:

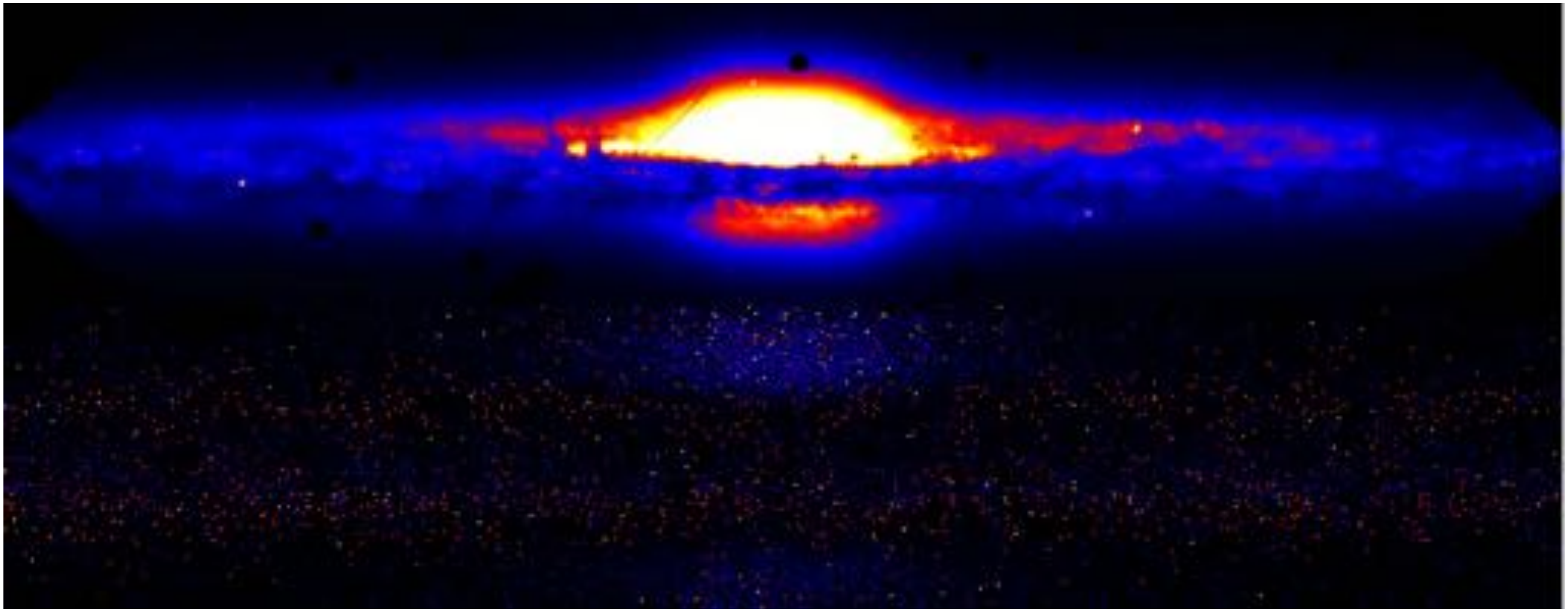
- Poisson noise averages out over population
- Uniformly samples parameter space
- More easily tests distant global maximum

De Geyter et al. 2012

FitSKIRT

- Automatically fits parametric 3D models to a set of UV/optical/NIR images
- Searches the parameter space using a genetic algorithm
- Uses SKIRT to evaluate each individual against the data

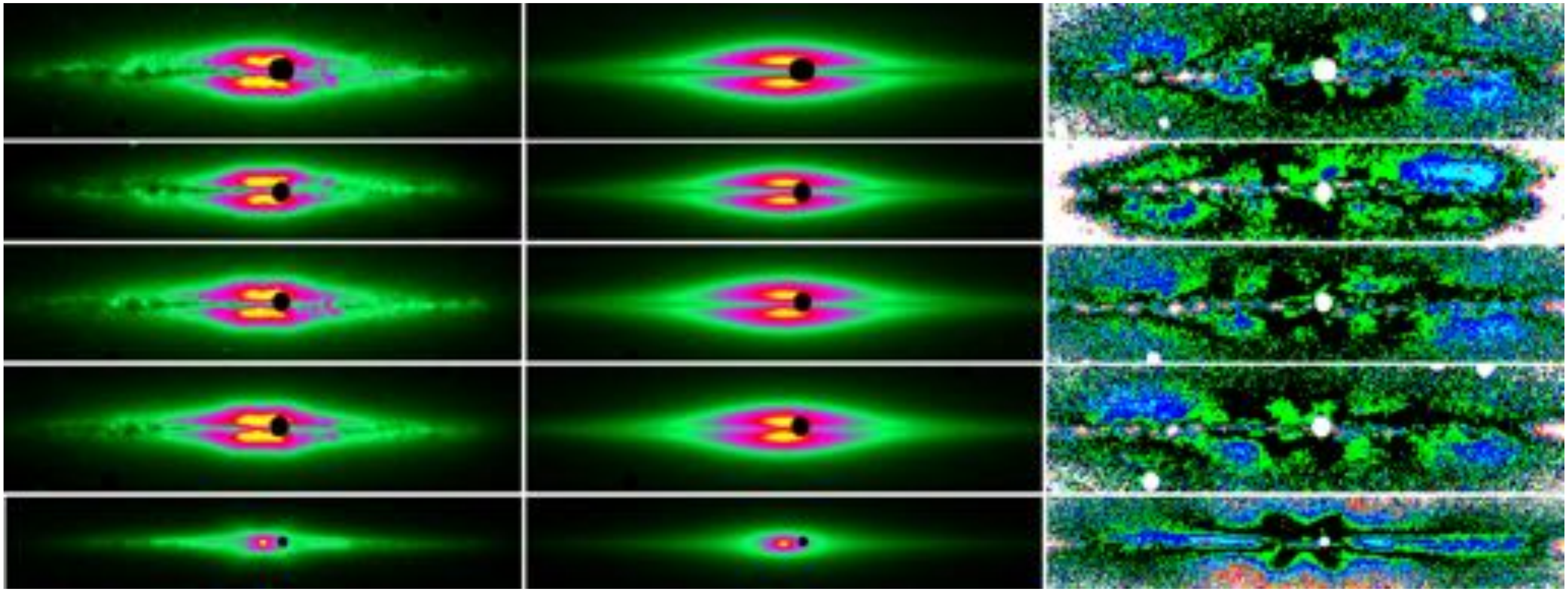
De Geyter et al. 2012

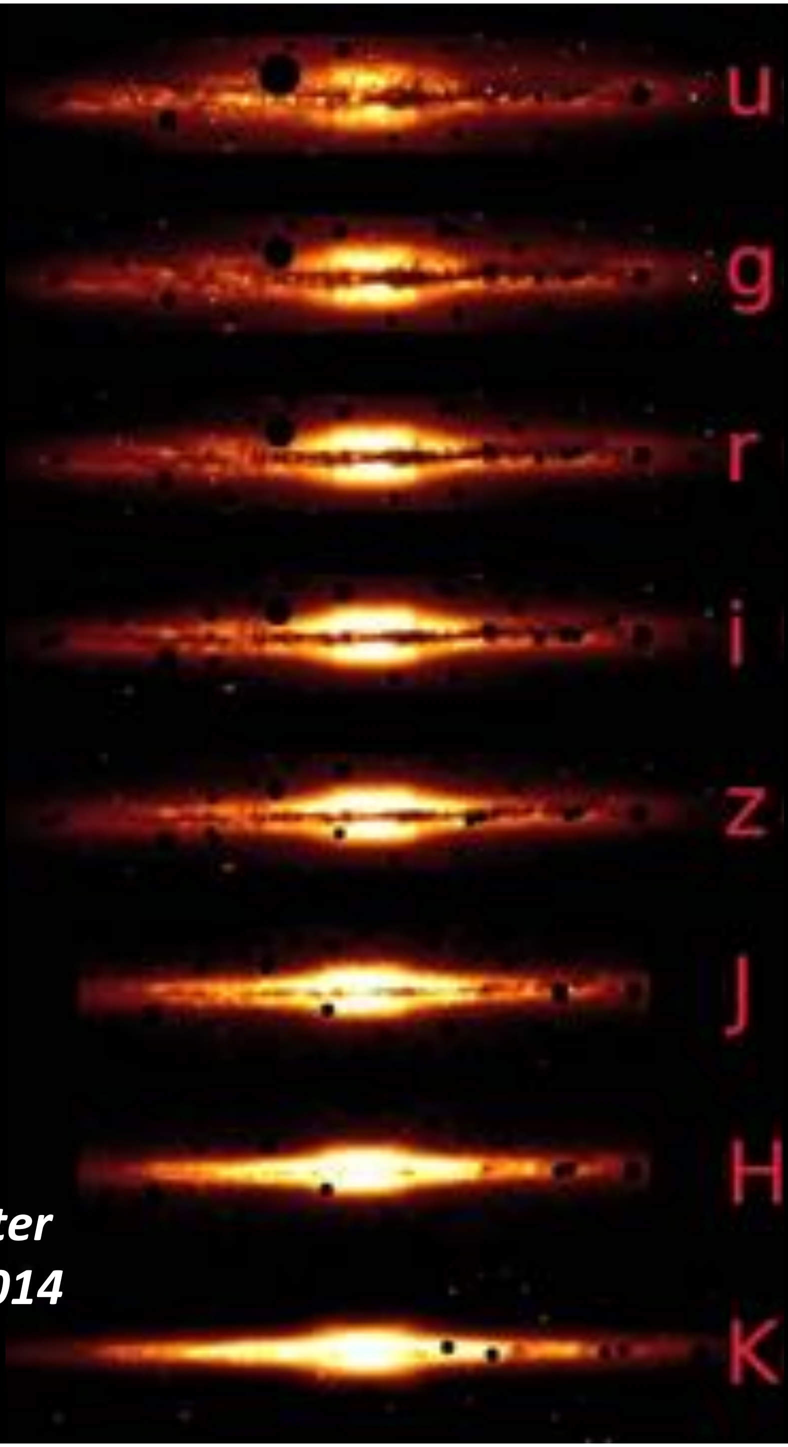


Automated oligochromatic fit of NGC 4013

- Monochromatic fitting (single-wavelength) shows degeneracy in dust properties
- Improved by oligochromatic fitting (multiple wavelengths)
  - Simultaneous fit in multiple bands (5 in this case)
  - 11 parameters: stellar disk & bulge, dust disk

De Geyter et al. 2013





De Geyter et al. 2014

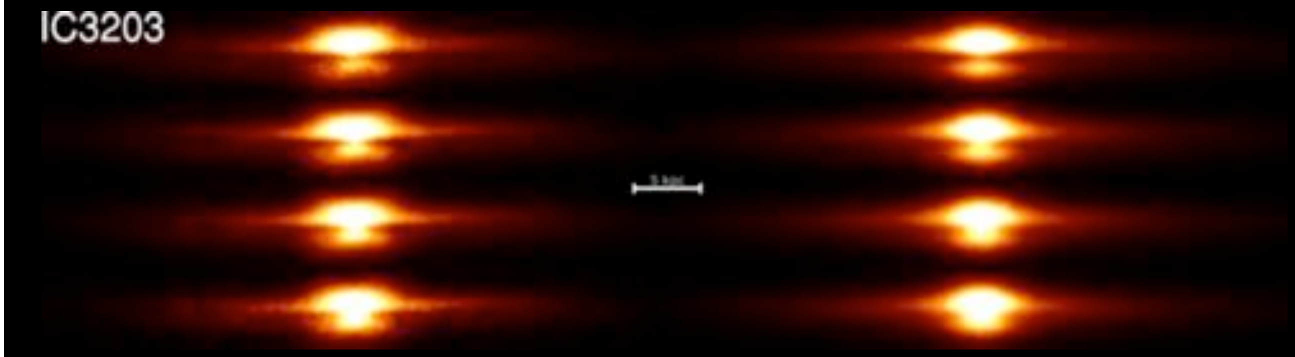
Case study: CALIFA edge-on spiral galaxies

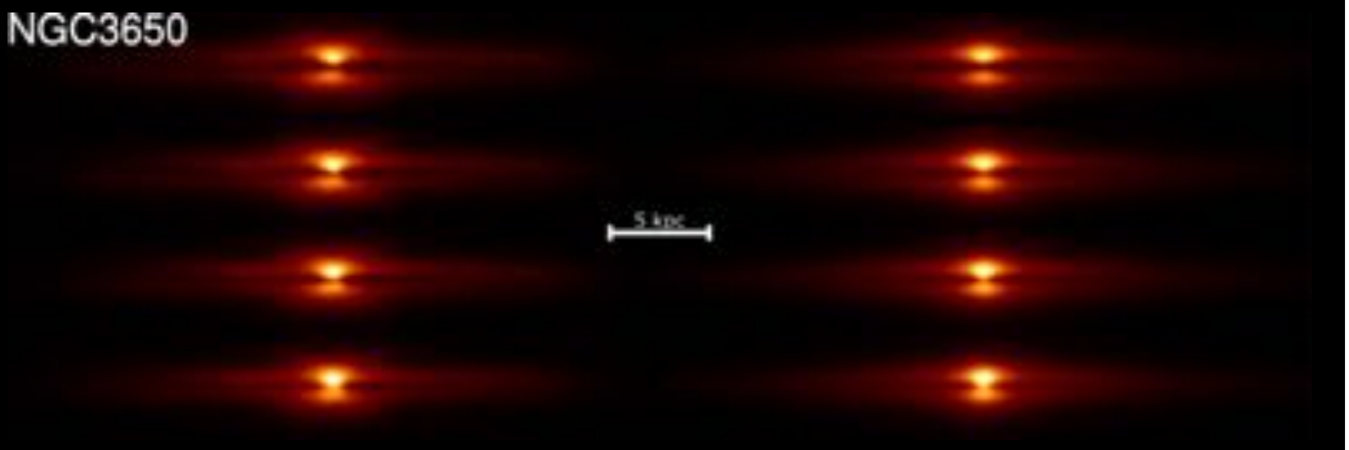
- 12 edge-on spiral galaxies selected from the CALIFA sample
- Oligochromatic g, r, i and z-band fitting
- Star and dust geometry?
- Face-on optical depth?

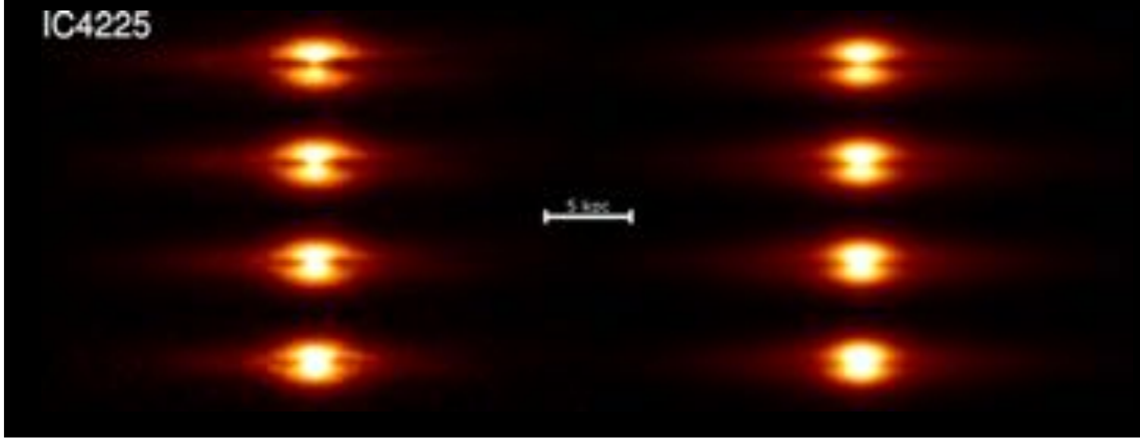
De Geyter et al. 2014

CALIFA

Some
fitting
results

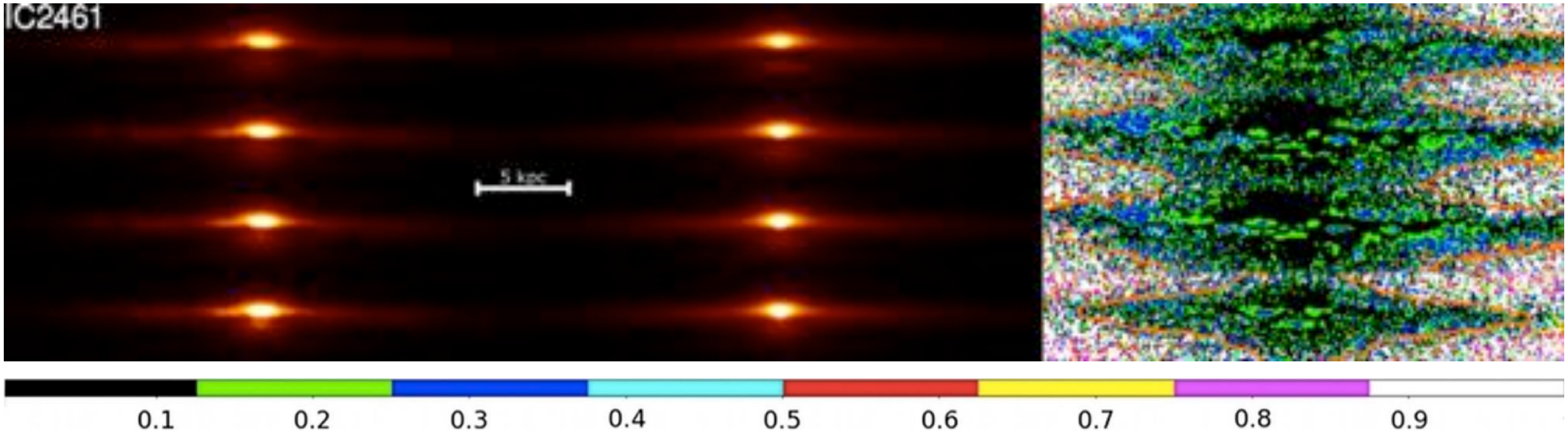


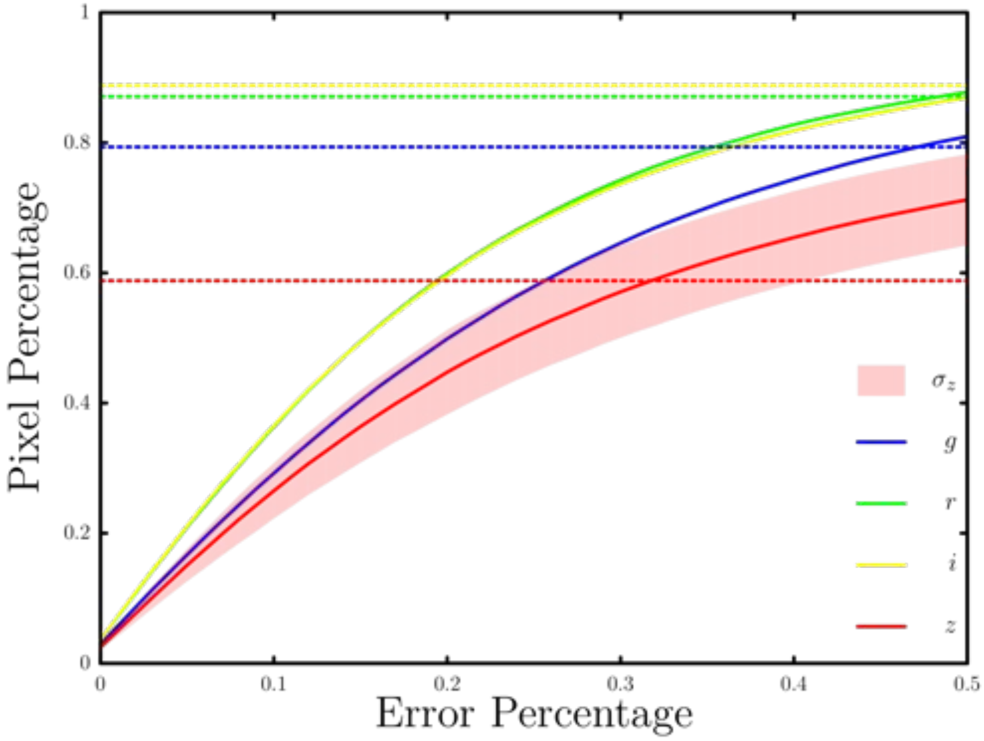


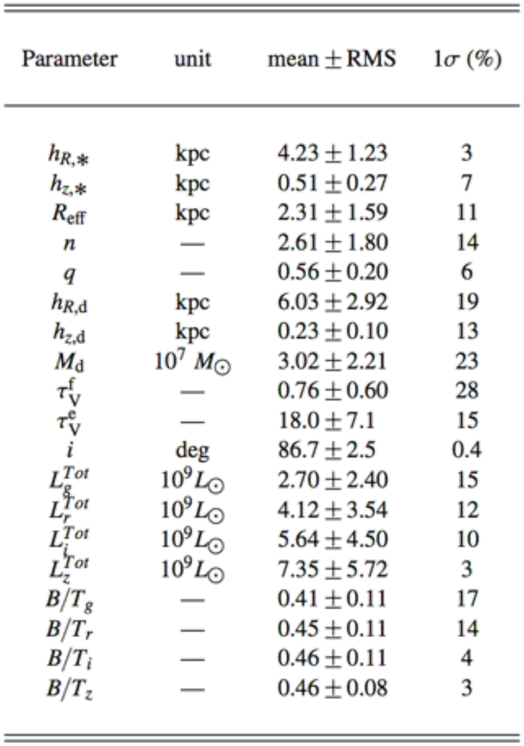


De Geyter et al. 2014

CALIFA - fitting accuracy







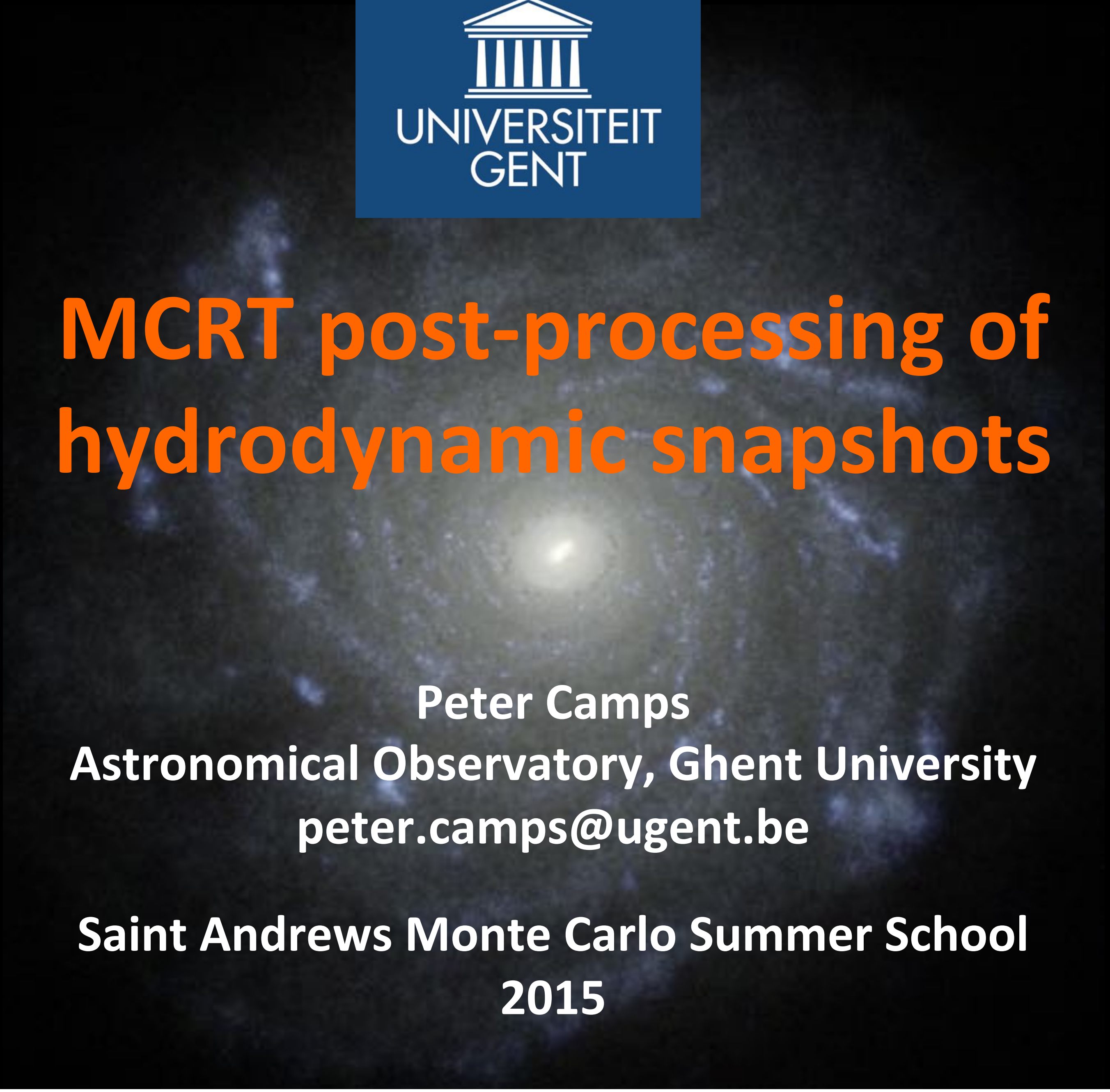
Parameter	unit	mean ± RMS	1σ (%)
$h_{R,*}$	kpc	4.23 ± 1.23	3
$h_{z,*}$	kpc	0.51 ± 0.27	7
$R_{\rm eff}$	kpc	2.31 ± 1.59	11
n	—	2.61 ± 1.80	14
q	—	0.56 ± 0.20	6
$h_{R,\rm d}$	kpc	6.03 ± 2.92	19
$h_{z,\rm d}$	kpc	0.23 ± 0.10	13
$M_{\rm d}$	$10^7\ M_\odot$	3.02 ± 2.21	23
$\tau_{\rm V}^{\rm f}$	—	0.76 ± 0.60	28
$\tau_{\rm V}^{\rm e}$	—	18.0 ± 7.1	15
i	deg	86.7 ± 2.5	0.4
L_g^{Tot}	$10^9 L_\odot$	2.70 ± 2.40	15
L_r^{Tot}	$10^9 L_\odot$	4.12 ± 3.54	12
L_i^{Tot}	$10^9 L_\odot$	5.64 ± 4.50	10
L_z^{Tot}	$10^9 L_\odot$	7.35 ± 5.72	3
B/T_g	—	0.41 ± 0.11	17
B/T_r	—	0.45 ± 0.11	14
B/T_i	—	0.46 ± 0.11	4
B/T_z	—	0.46 ± 0.08	3

CALIFA case study conclusions

- Sample of 12 edge-on spiral galaxies from CALIFA survey
- Reasonable accuracy on frame reproduction and parameter determination
- Values for stellar parameters and dust properties similar to those found by others

- Dust disks about 70% more extended than stellar disks, and about half as thick
- Large spread within sample for face-on optical depth, up to τ=3 i.e. fairly opaque!

Questions ?



MCRT post-processing of hydrodynamic snapshots

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Saint Andrews Monte Carlo Summer School
2015

Overview

MCRT in galaxies with SKIRT

- Dust in galaxies
- SKIRT features and code design
- Energy balance in galaxies
- Automated galaxy modeling

MCRT post-processing of hydrodynamic snapshots

- Stochastic heating of dust grains
- Dust grids: regular, hierarchical, unstructured
- Importing hydro snapshots: AMR, SPH
- FIR properties of galaxies in a cosmological simulation

Stochastic heating of dust grains

Section B-1

Emission from a dust mixture

- Thermal emission depends nonlinearly on grain size *a*
    - For each dust type *k*, split the grain size range into *b* bins
- Emissivity when exposed to radiation field *J*(λ):

  (according to Kirchhoff's law of thermal radiation)

$$\varepsilon(\lambda) = \sum_{k,b} \varsigma^{\mathrm{abs}}_{k,b}(\lambda) \int_0^\infty P_{k,b,J}(T)\, B(\lambda, T)\, \mathrm{d}T$$

Absorption cross section for representative grain in each bin

Planck function describing Black Body radiation

Probability of finding the representative grain of bin *k*,*b* at temperature *T* when exposed to field *J*(λ)

Emission in LTE conditions

$$\varepsilon(\lambda) = \sum_{k,b} \varsigma_{k,b}^{\text{abs}}(\lambda) \int_0^\infty P_{k,b,J}(T)\, B(\lambda, T)\, \mathrm{d}T$$

- If representative grain is in local thermal equilibrium (LTE) with the surrounding radiation, we have:

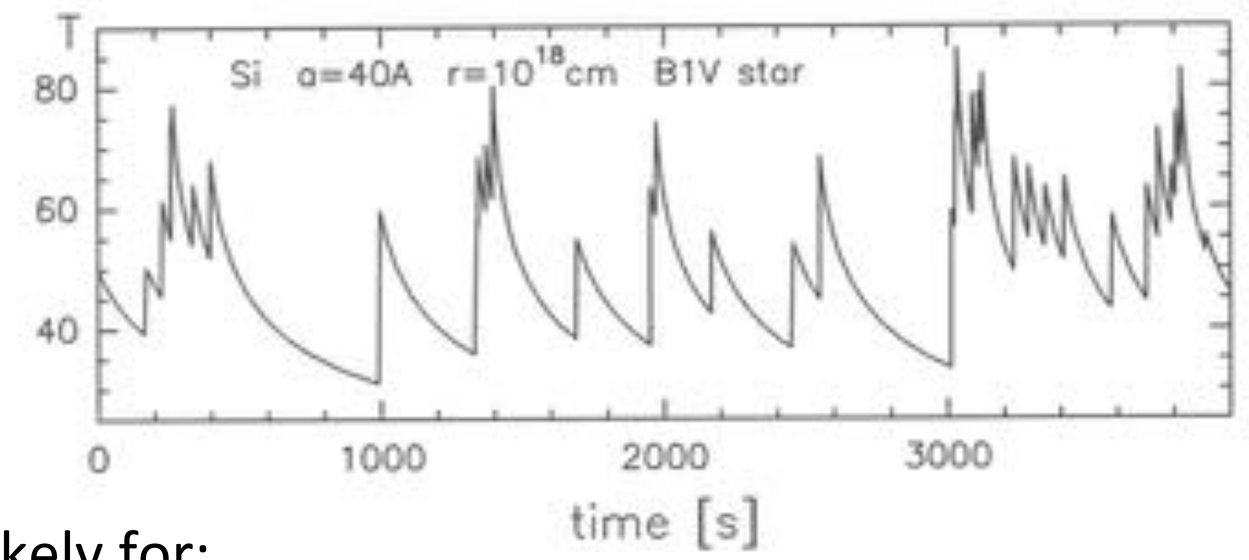
$$P_{k,b,J}(T) = \delta(T - T_{k,b,J}^{\text{eq}})$$

- where the equilibrium temperature is determined from the energy balance equation

$$\underbrace{\int_0^\infty \varsigma_{k,b}^{\text{abs}}(\lambda)\, J(\lambda)\, \mathrm{d}\lambda}_{\text{Absorbed energy}} = \underbrace{\int_0^\infty \varsigma_{k,b}^{\text{abs}}(\lambda)\, B(\lambda, T_{k,b,J}^{\text{eq}})\, \mathrm{d}\lambda}_{\text{Emitted energy}}$$

Non-LTE conditions

- If a single photon can significantly change the internal energy of a representative grain, the grain is not in local thermal equilibrium (LTE) with the surrounding radiation
  - » The grain is stochastically heated



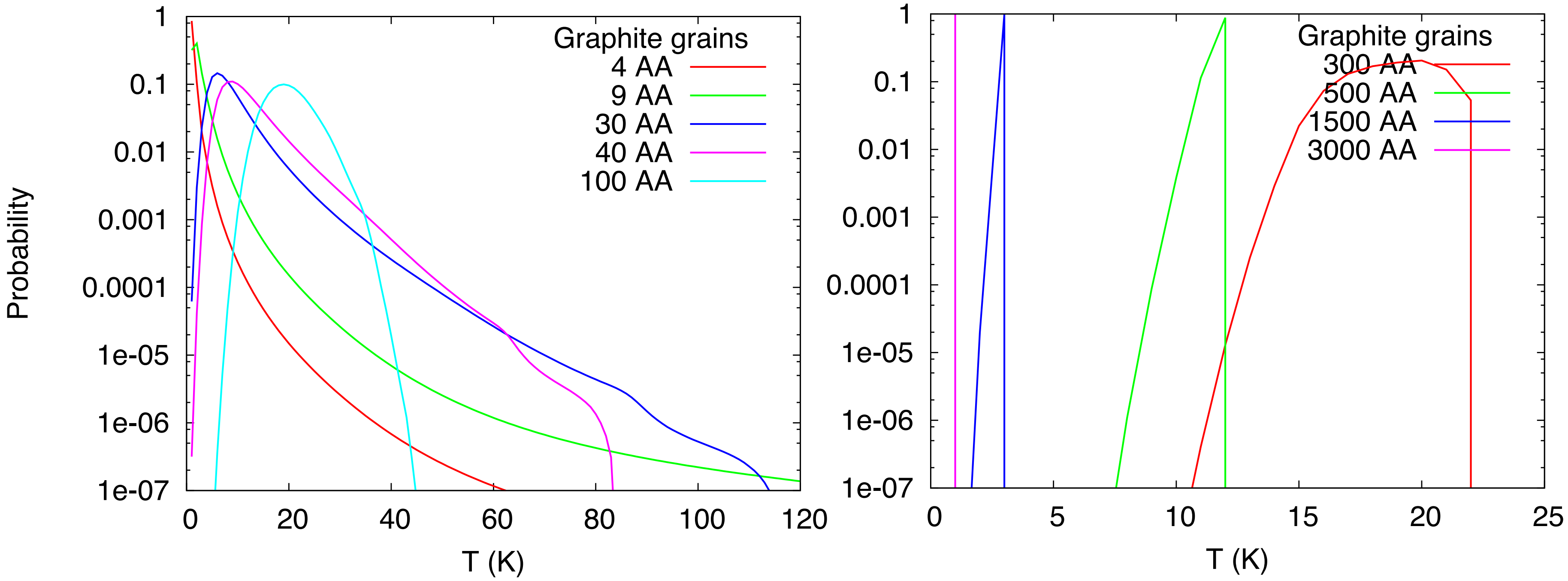
- This is more likely for:
  - » Small grains or molecules
  - » Hard radiation (high-energy photons)
  - » Weak fields (fewer photons)

Emission in non-LTE conditions

$$\varepsilon(\lambda) = \sum_{k,b} \varsigma_{k,b}^{\text{abs}}(\lambda) \int_0^\infty P_{k,b,J}(T)\, B(\lambda,T)\, \mathrm{d}T$$

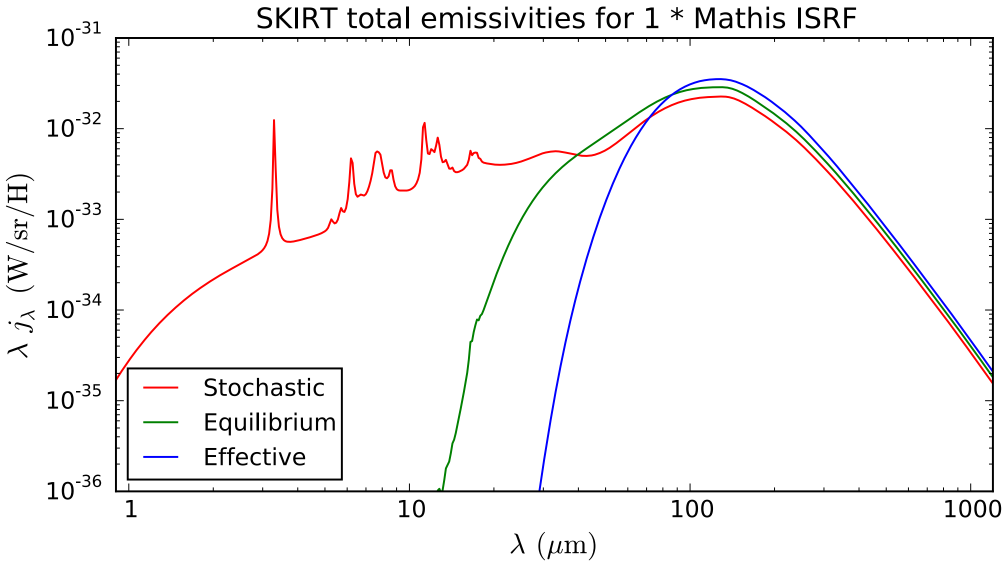
- We need to solve for the temperature probability distribution $P_{k,b,J}(T)$, which depends on the radiation field $J(\lambda)$ in addition to the properties of the representative grain of bin *k*,*b*
- This is computationally very demanding
  - » RT codes routinely need to calculate many millions of dust emission spectra so performing a full statistical treatment would be prohibitive
  - » We assume that a dust grain cools by radiating photons with an energy that is very small compared to the internal energy of the grain
  - » Using this continuous cooling assumption, the complexity can be reduced to $O(N^2)$ where N is the number of temperature grid points
  - » Still challenging in near-equilibrium regimes where the probability distribution approaches a delta function (requiring a very fine grid)

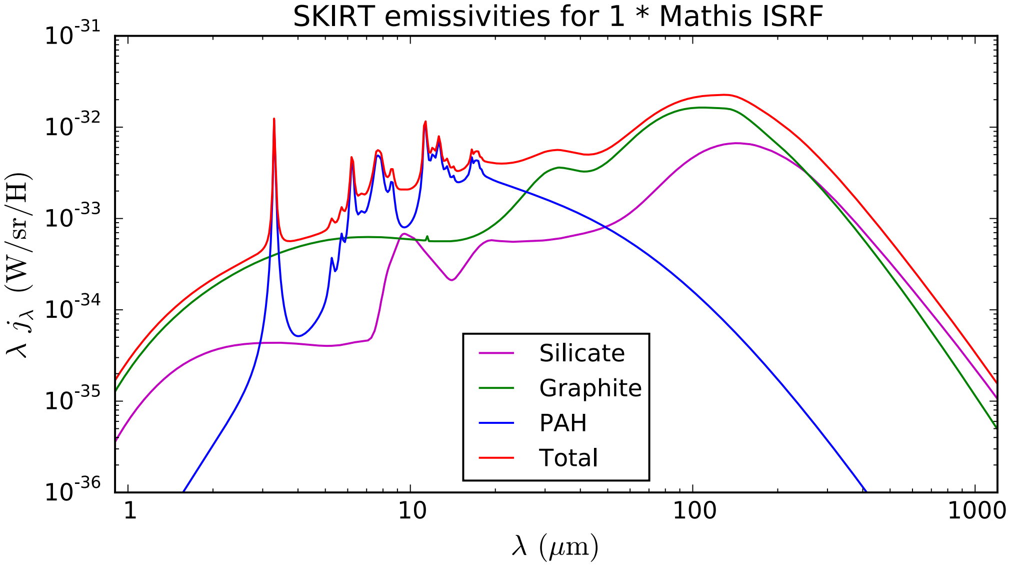
Temperature probability functions



- For large grains, P(T) → $\delta(T_{eq})$, so calculation becomes unstable
- Cutoff point for switching to equilibrium calculation is subject to debate

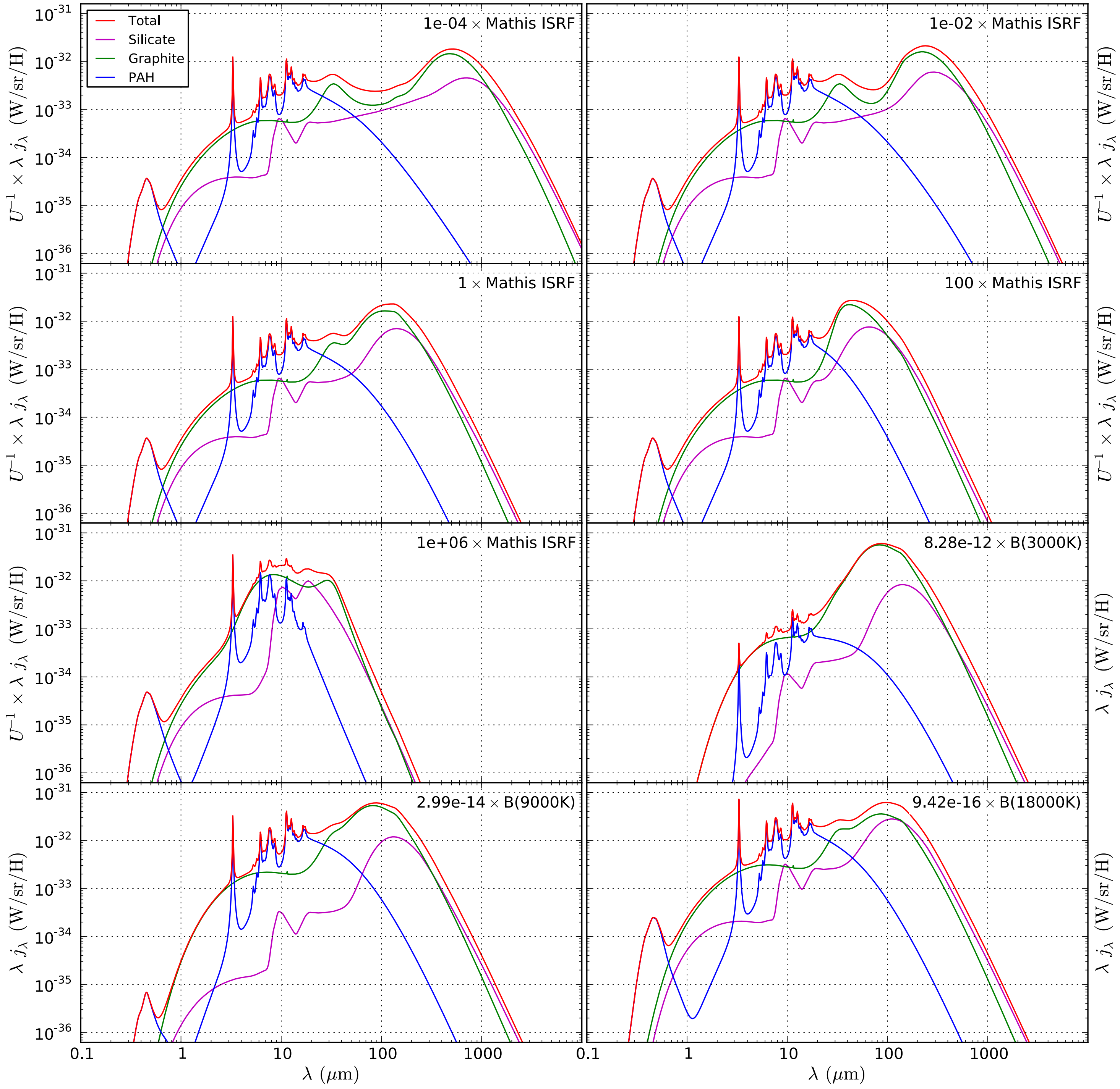
Dust emission in typical ISRF





- Assumptions
  - » Interstellar radiation field (ISRF) as observed in solar neighborhood (*Mathis et al. 1983*)
  - » Simple dust model approximating Milky Way observations
- We see that
  - » SHGs shift emission to shorter wavelengths (up to factor 10 or more)
  - » PAH emission features sharp peaks in wavelength range 3-20 µm

Dust emission for a range of embedding fields



- weak to strong
  - continuum peak shifts
- soft to hard
  - SHG emission increases

Camps et al. 2015

Stochastically heated grains benchmark

- Compare SHG emission calculations in the context of RT
  - Reference solution by non-RT code + 6 RT codes
  - Precisely defined dust model
  - 17 input fields ranging from weak to strong, soft to hard
- Explain differences and provide guidelines for implementation
  - For all but the most extreme input fields, we find agreement within 10% across the important wavelength range 3 µm ≤ λ ≤ 1000 µm
  - A lot of algorithmic and discretization details must be handled with care to achieve this level of accuracy with acceptable performance
    - Transition from stochastic to equilibrium
    - Grids for temperature, wavelength, grain size
  - Can calculate several hundred spectra per second per core → a few hours for 5 million cells on a regular desktop computer

Questions ?

Dust grids

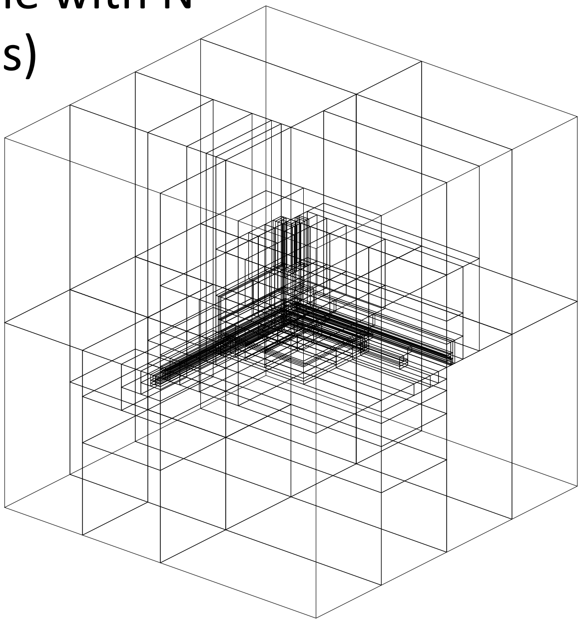
Section B-2

Dust grids in (SKI)RT

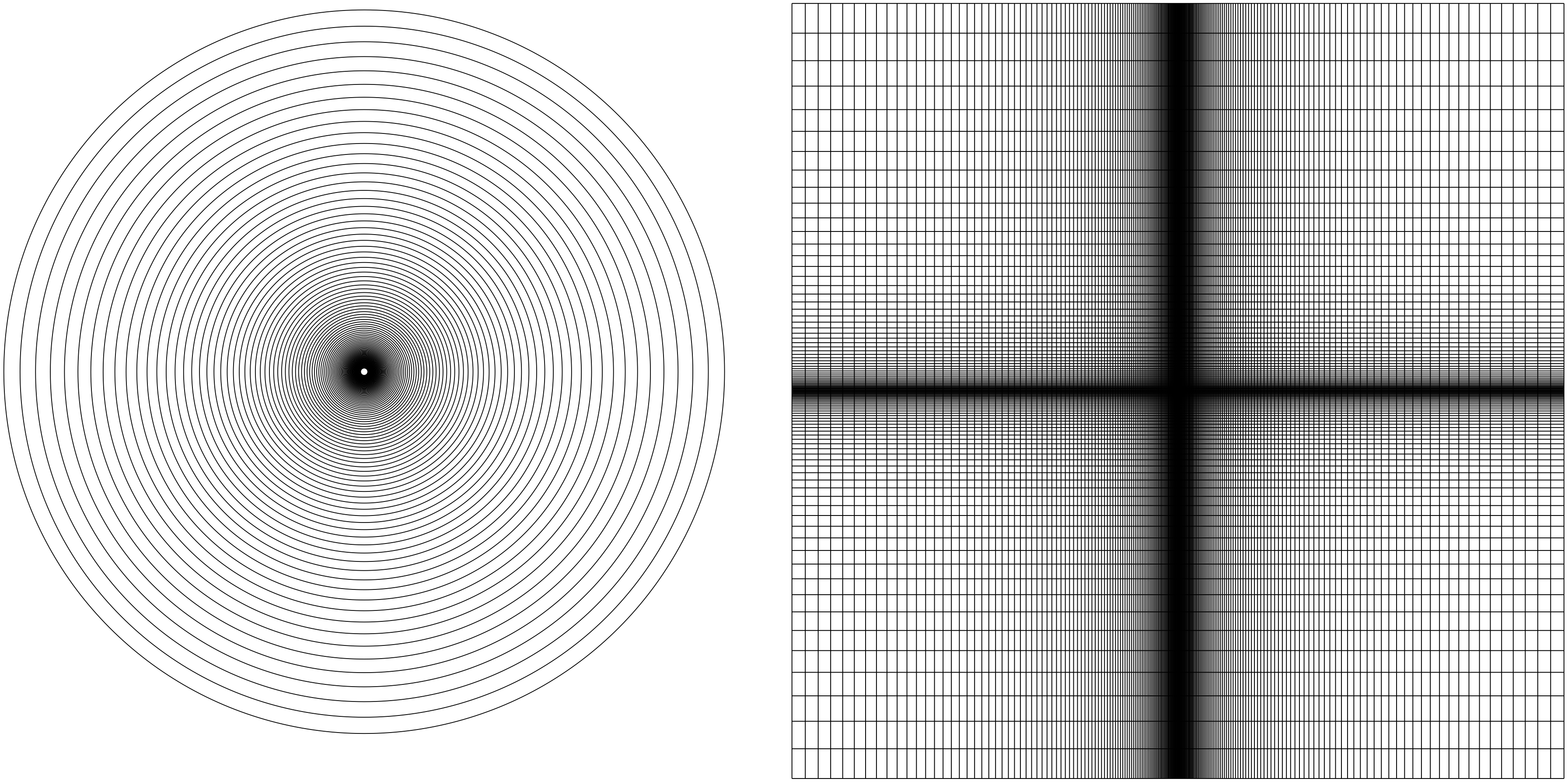
- Dust grid = spatial discretization of dust medium
- Physical quantities are assumed constant in each cell
  - Radiation field
  - Dust density, optical properties, temperature
- Need small cells to properly resolve the physics
- Number of cells N determines resource requirements
  - Memory needs and execution time roughly scale with N (need more photons to properly sample all cells)

➡

- Quest for schemes that place many small cells where needed and fewer large cells elsewhere



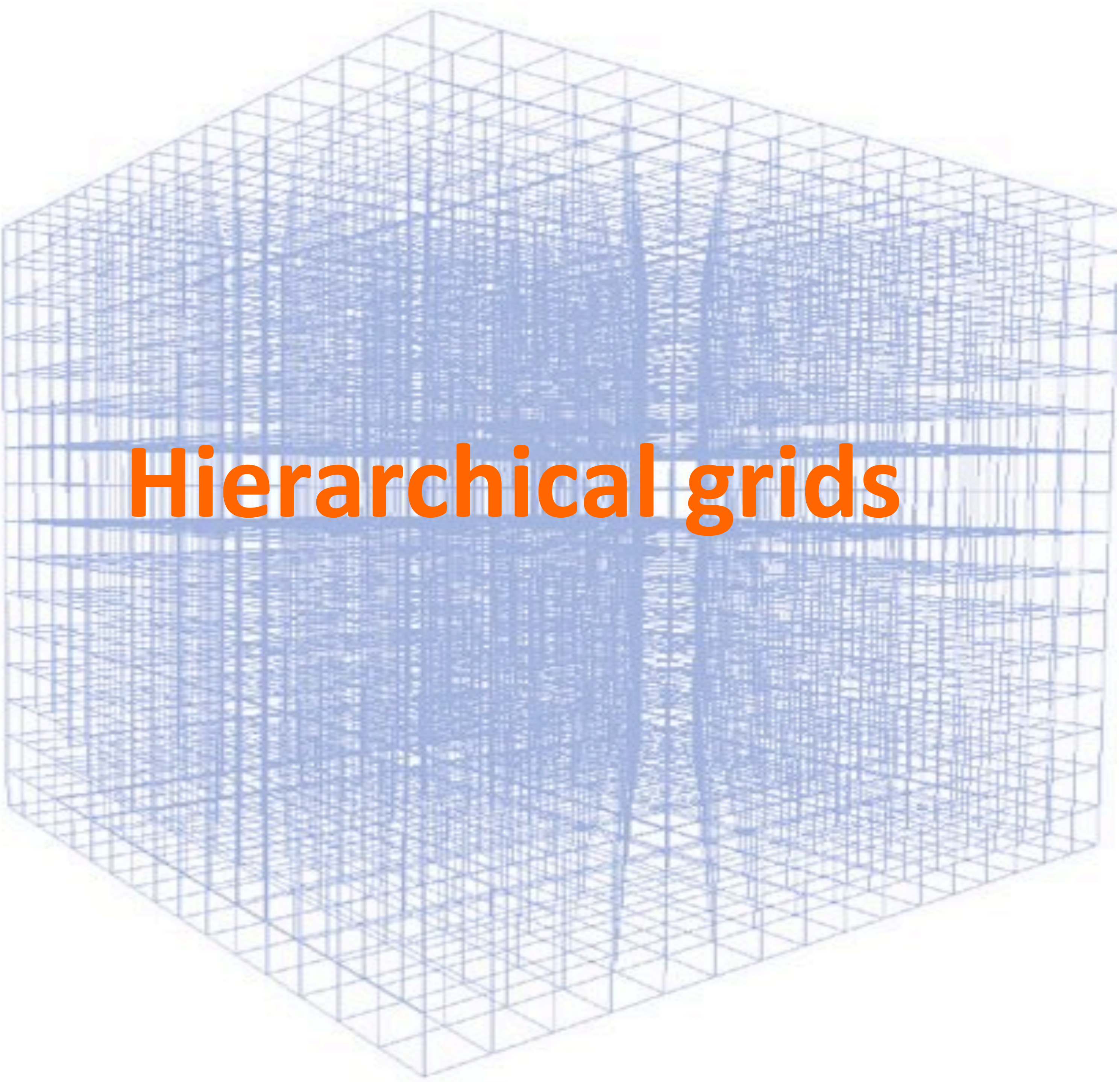
Fixed dust grids

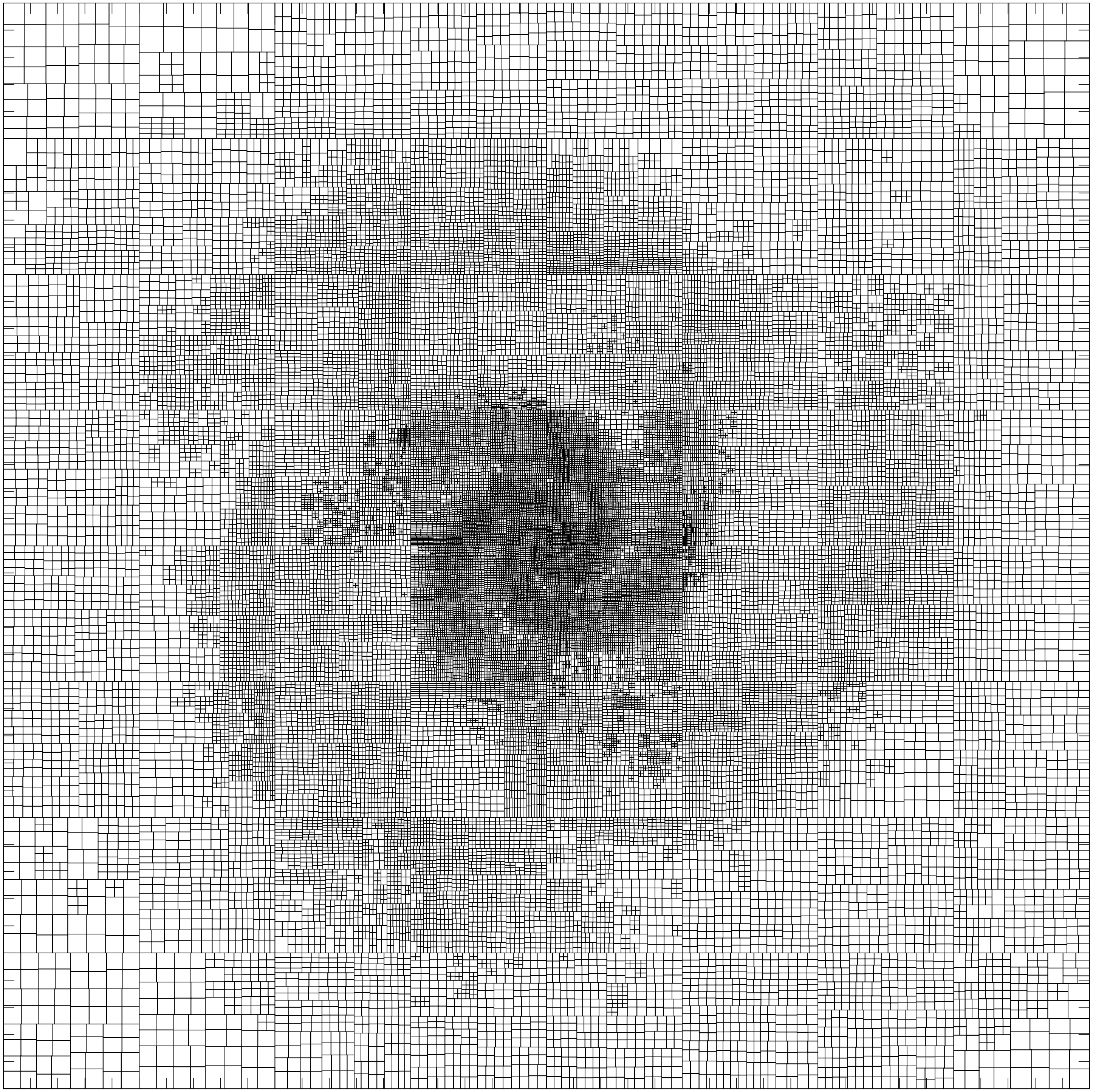


1D, 2D, 3D

regular, log, power law

Hierarchical grids





Hierarchical dust grids

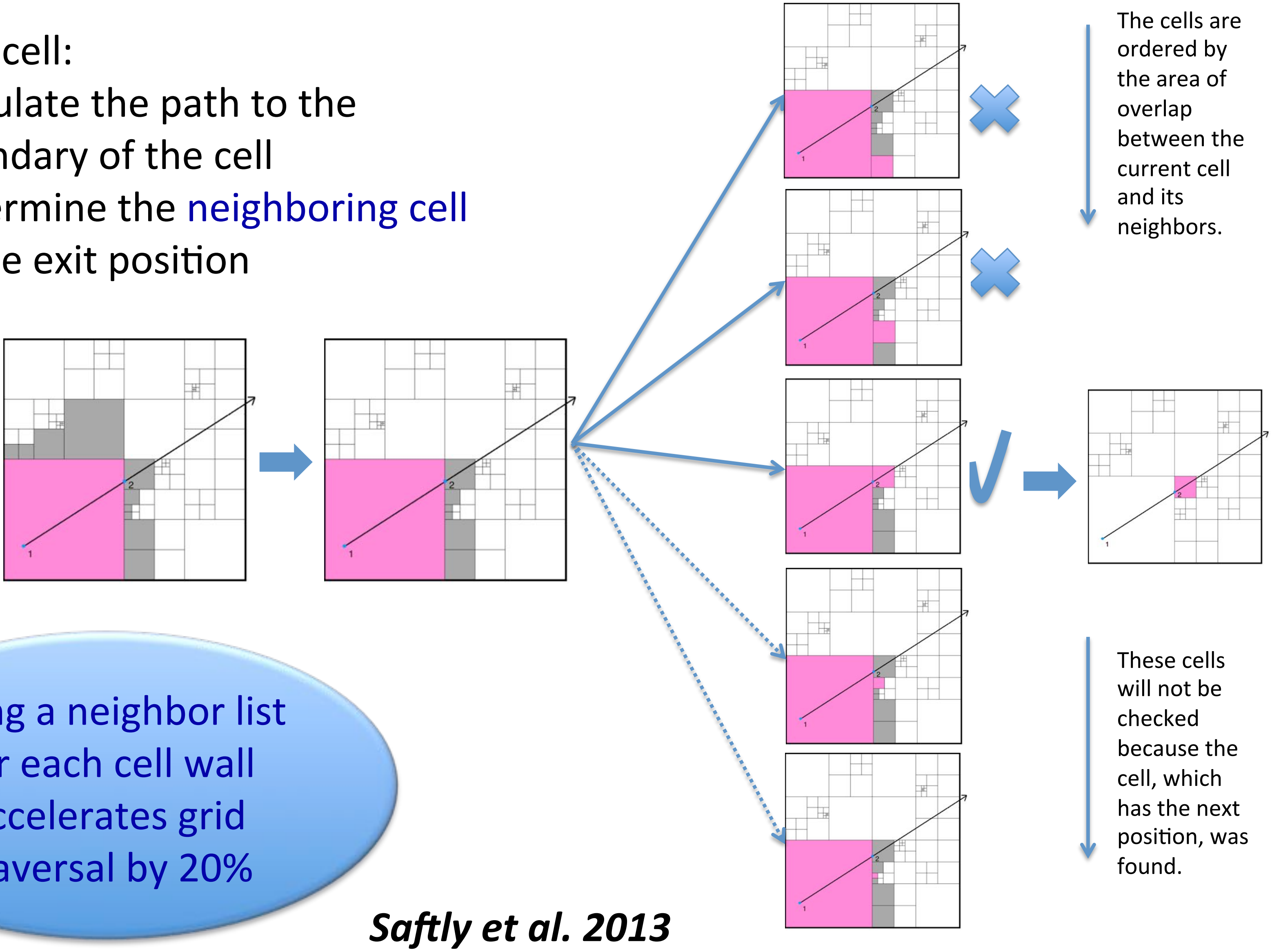
Cut through octree with recursive barycentric subdivision based on dust density distribution of a spiral galaxy

Saftly et al. 2013

Grid traversal

For each cell:

1. Calculate the path to the boundary of the cell
2. Determine the neighboring cell at the exit position



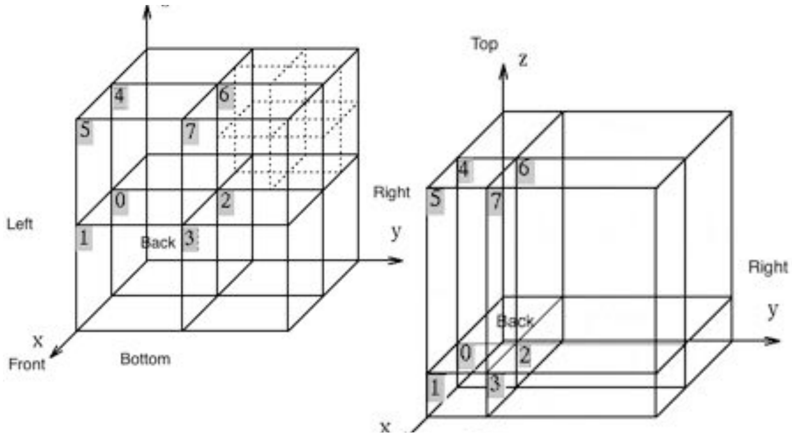
The cells are ordered by the area of overlap between the current cell and its neighbors.

These cells will not be checked because the cell, which has the next position, was found.

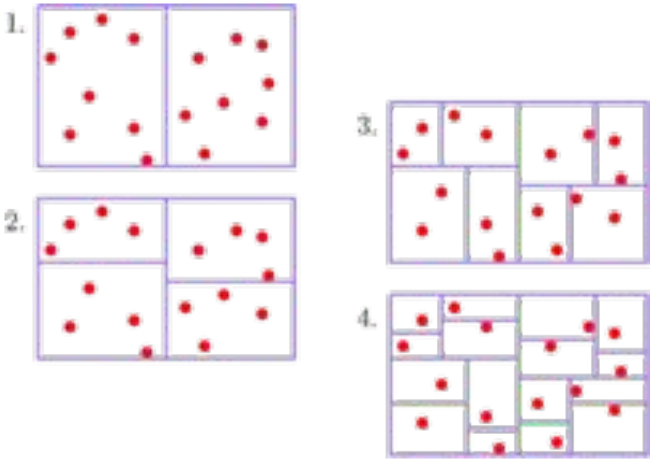
Using a neighbor list for each cell wall accelerates grid traversal by 20%

Saftly et al. 2013

Octree versus *k*-d tree



Octree subdivides a node into eight subnodes



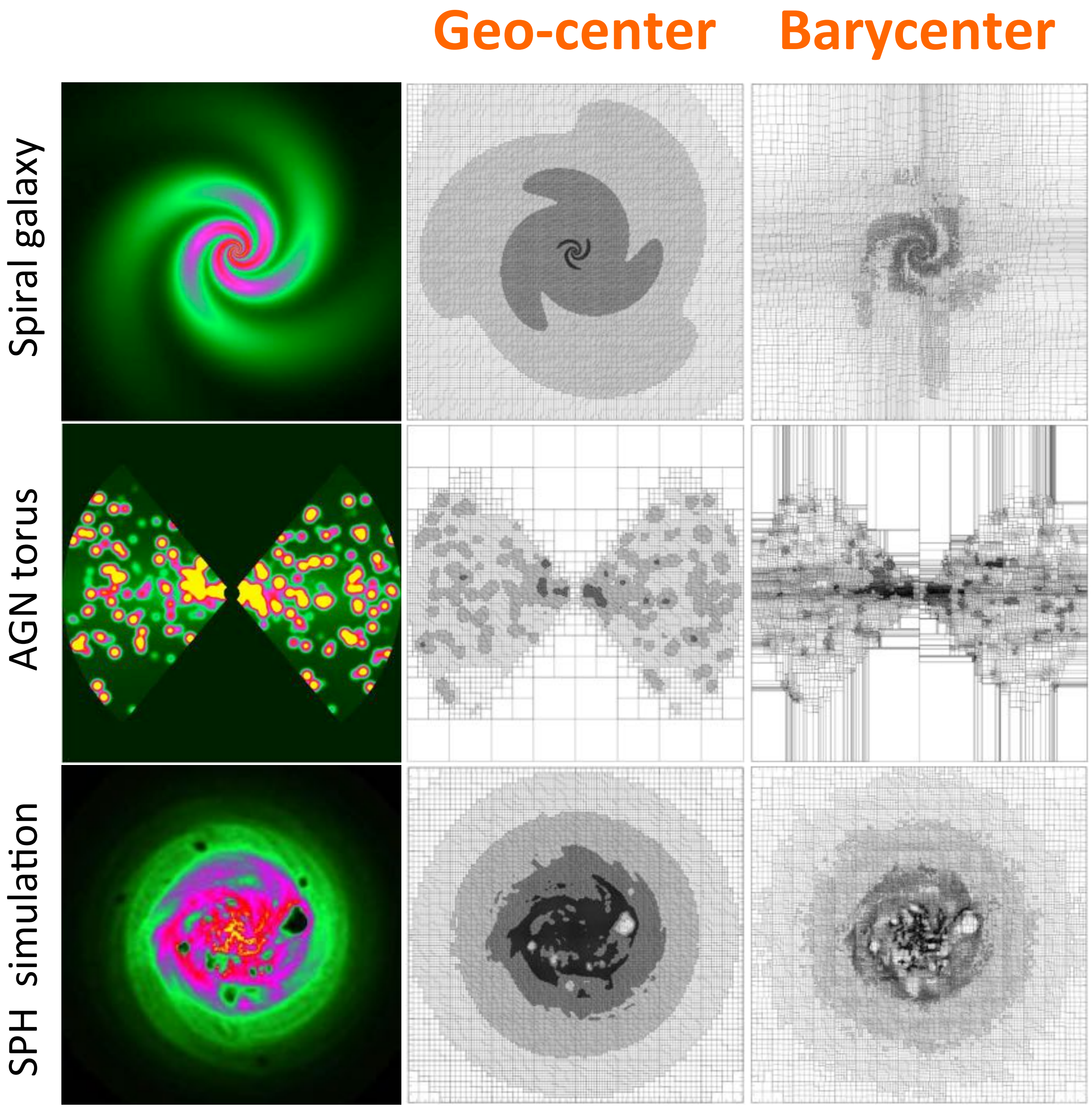
k-d tree subdivides a node into two subnodes

Quality measure
standard deviation of
randomly sampled
density error

k-d tree needs 20%
fewer cells to
achieve the same
quality

Saftly et al. 2013

Subdivision point



Geo-centric grids are more accurate and more efficient

Saftly et al. 2013

Grid resolution criteria

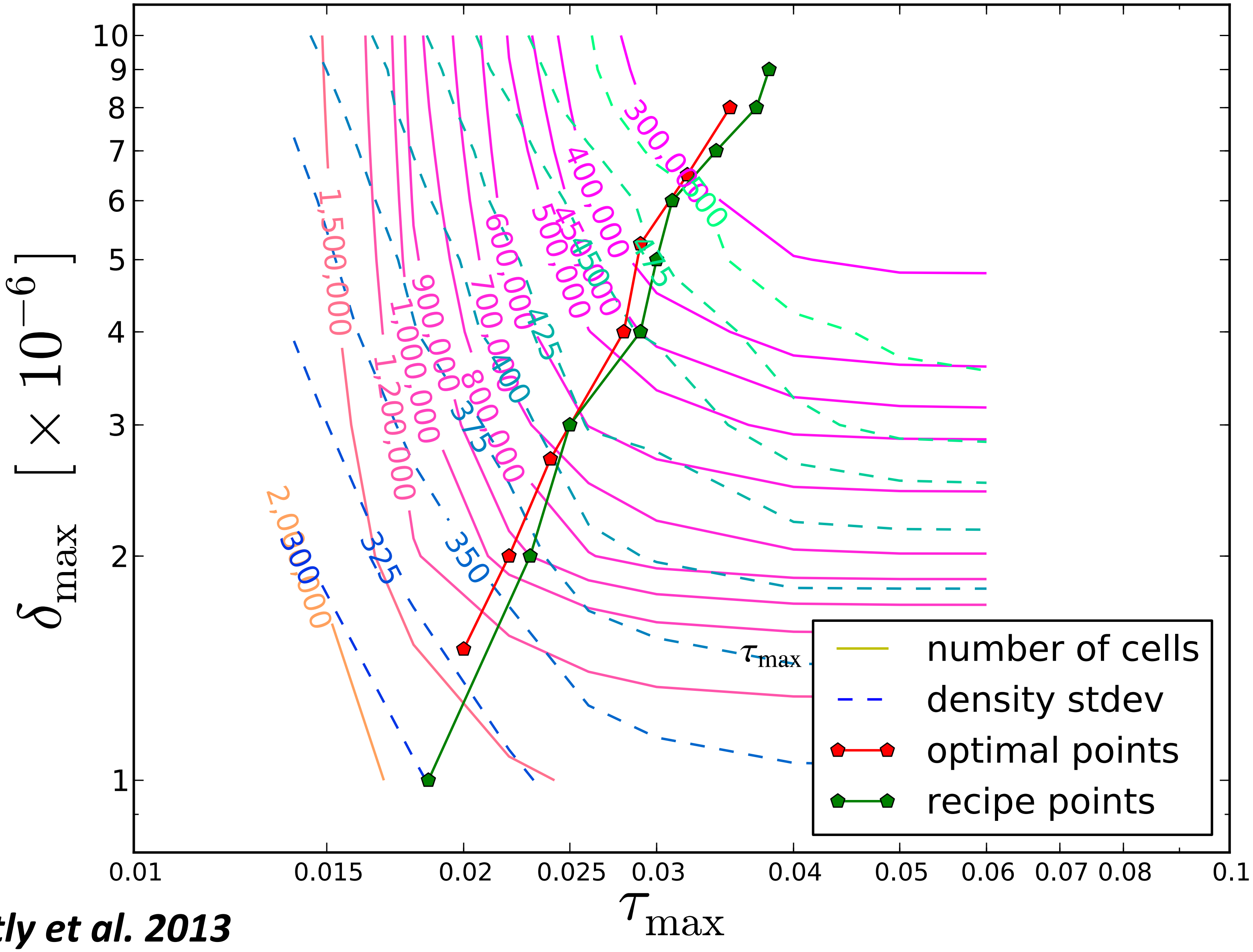
How to determine subdivision depth?

- The objective is to properly resolve the radiation field
- But… we don't know this until we run a RT simulation
- For now: criteria based on the dust density distribution
- Future: adjust grid during the simulation based on the radiation field calculated so far

Criteria implemented in SKIRT

- Nesting level: $L < L_{max}$ (overrides other criteria)
- Dust mass fraction: $M_{cell} / M_{tot} = \delta < \delta_{max}$
- Optical depth: $\tau_{cell} < \tau_{max}$
- Density dispersion: $(\rho_{max} - \rho_{min})/\rho_{max} = q < q_{max}$

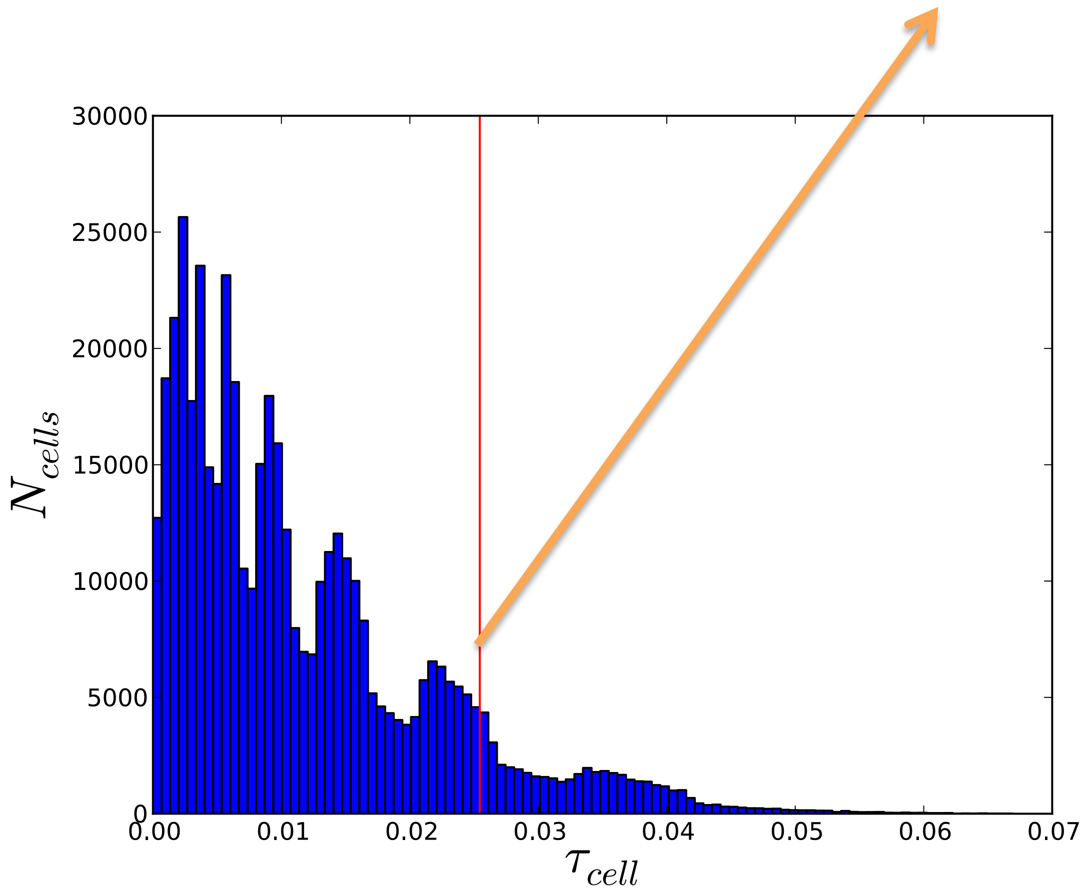
Dust mass fraction and optical depth criteria



Saftly et al. 2013

Optimal scheme combining δ_{max} and τ_{max}

- Dust mass fraction: $\delta < \delta_{max}$ “sets number of cells”
- Optical depth: $\tau_{cell} < \tau_{max} = \tau_{90}$ “improves quality”

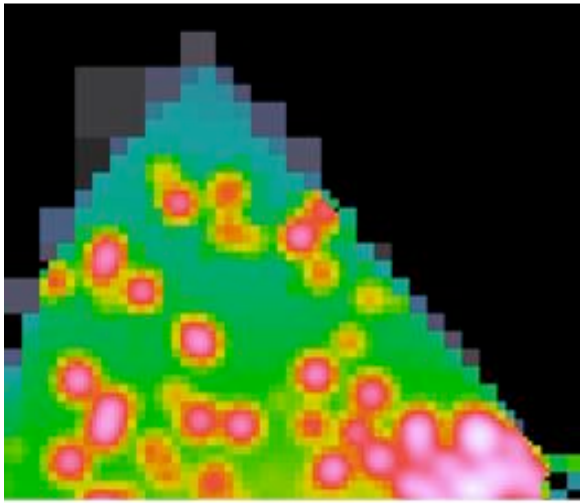


Using τ_{90}
to cutoff the 10% tail
of the δ_{max}-only result
produces optimal grids

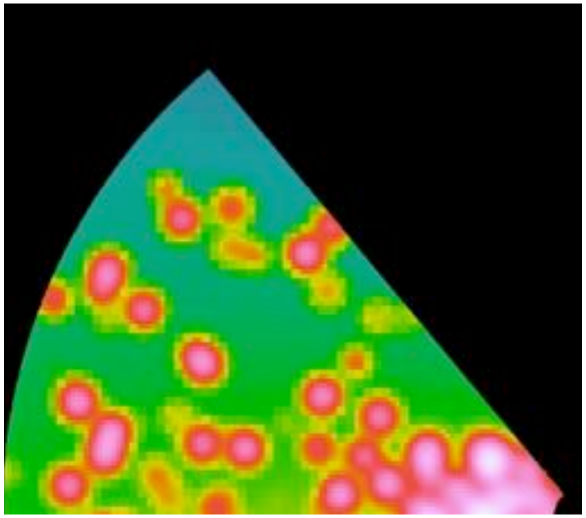
Saftly et al. 2013

Strong gradients and sharp edges

- Using just the mass fraction criterion, sharp edges can still have large cells with a tiny and compact dusty corner

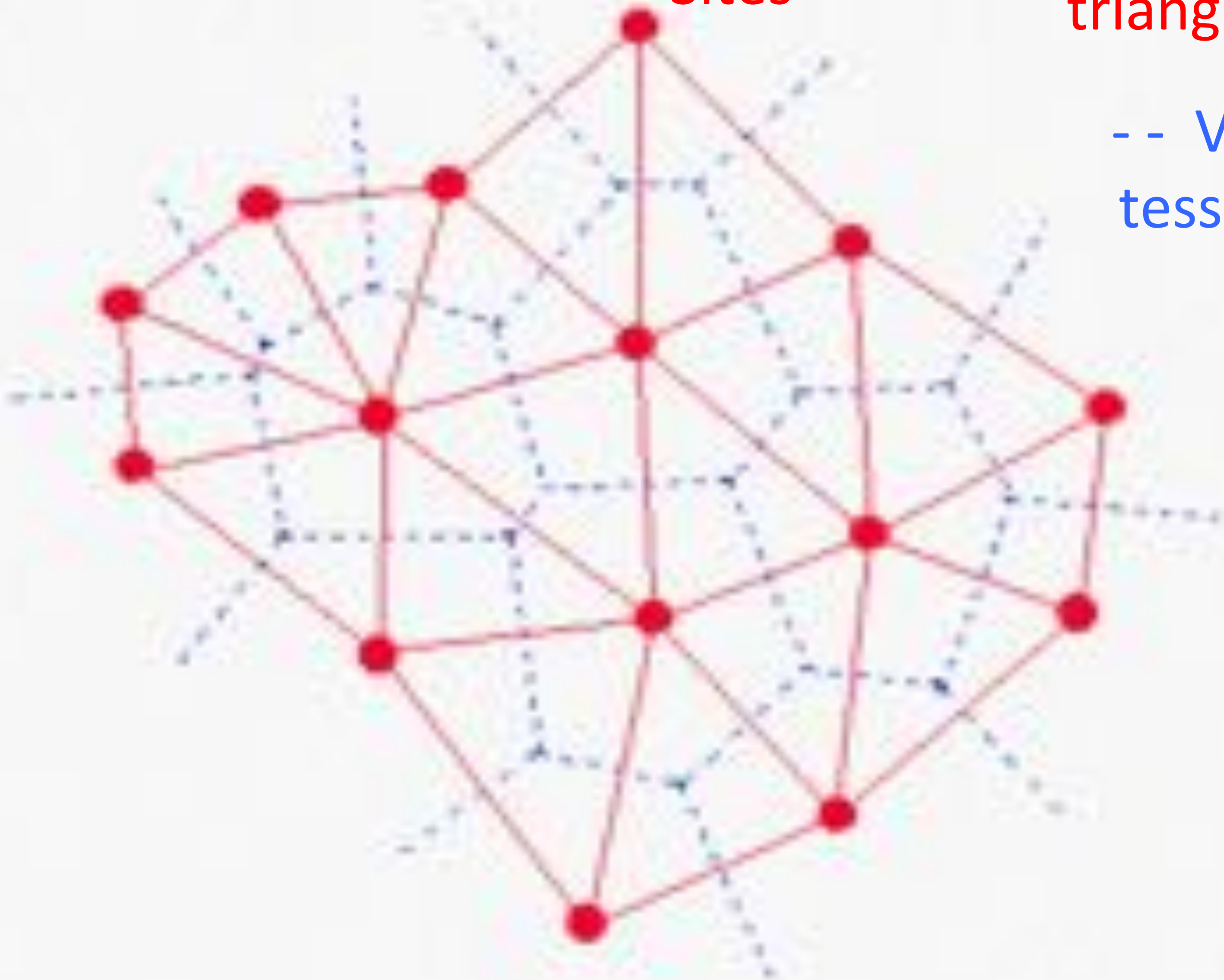


- The density dispersion criterion further subdivides these cells



Unstructured grids

Voronoi cells in 2D

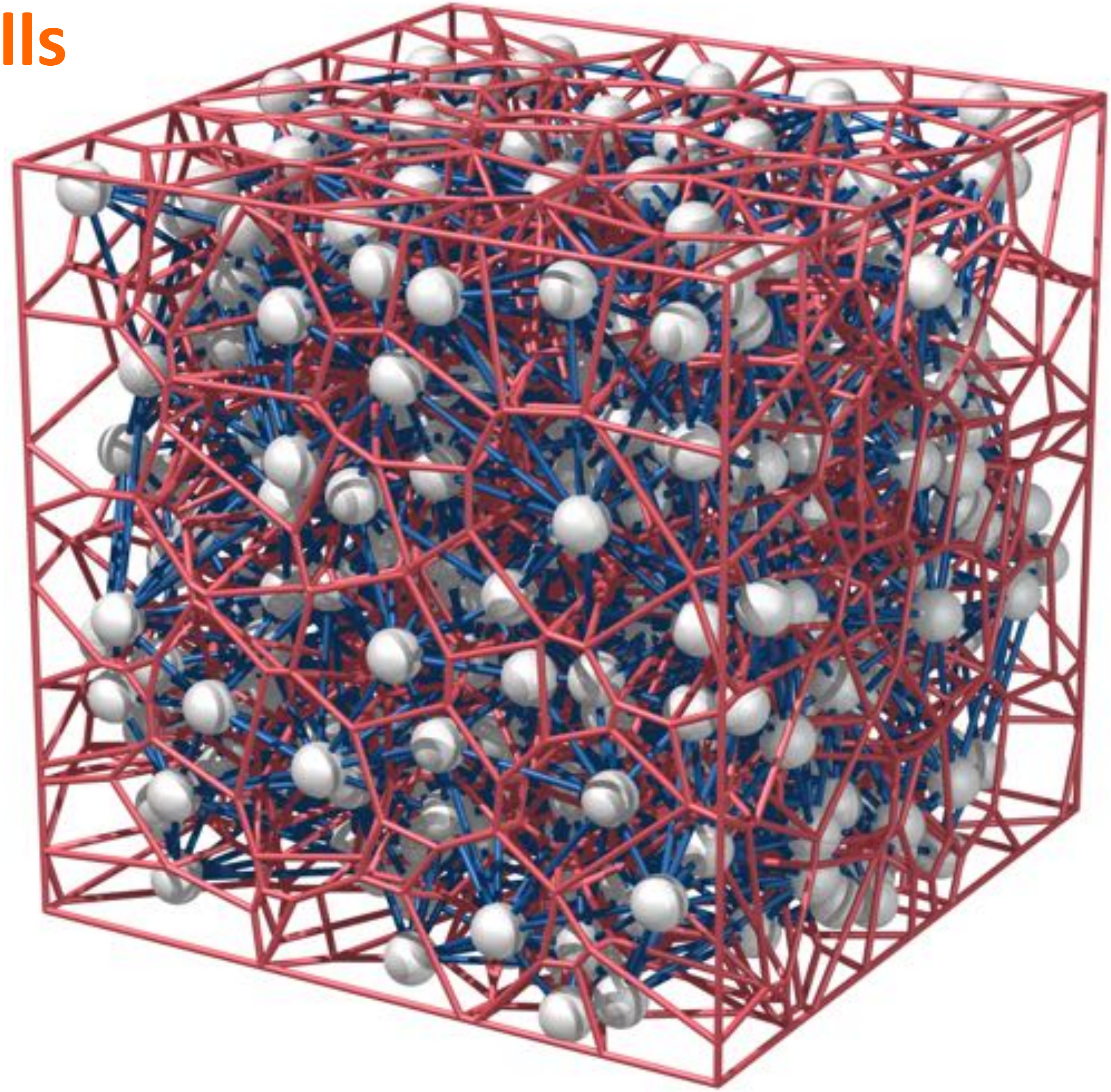


Sites

—— Delaunay triangulation

- - Voronoi tesselation

Voronoi cells in 3D



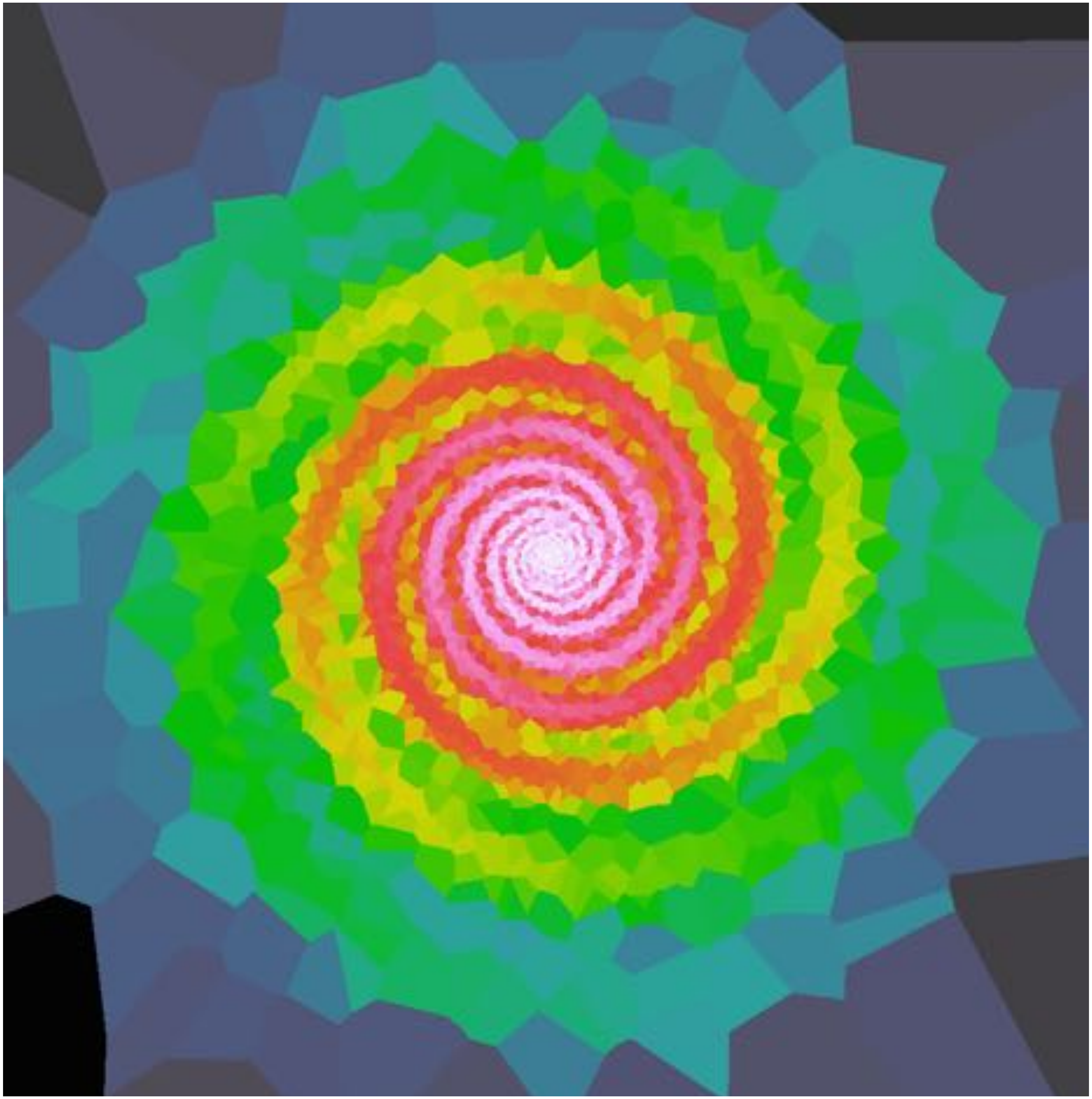
— Delaunay edges

— Voronoi cell edges

(400 sites)

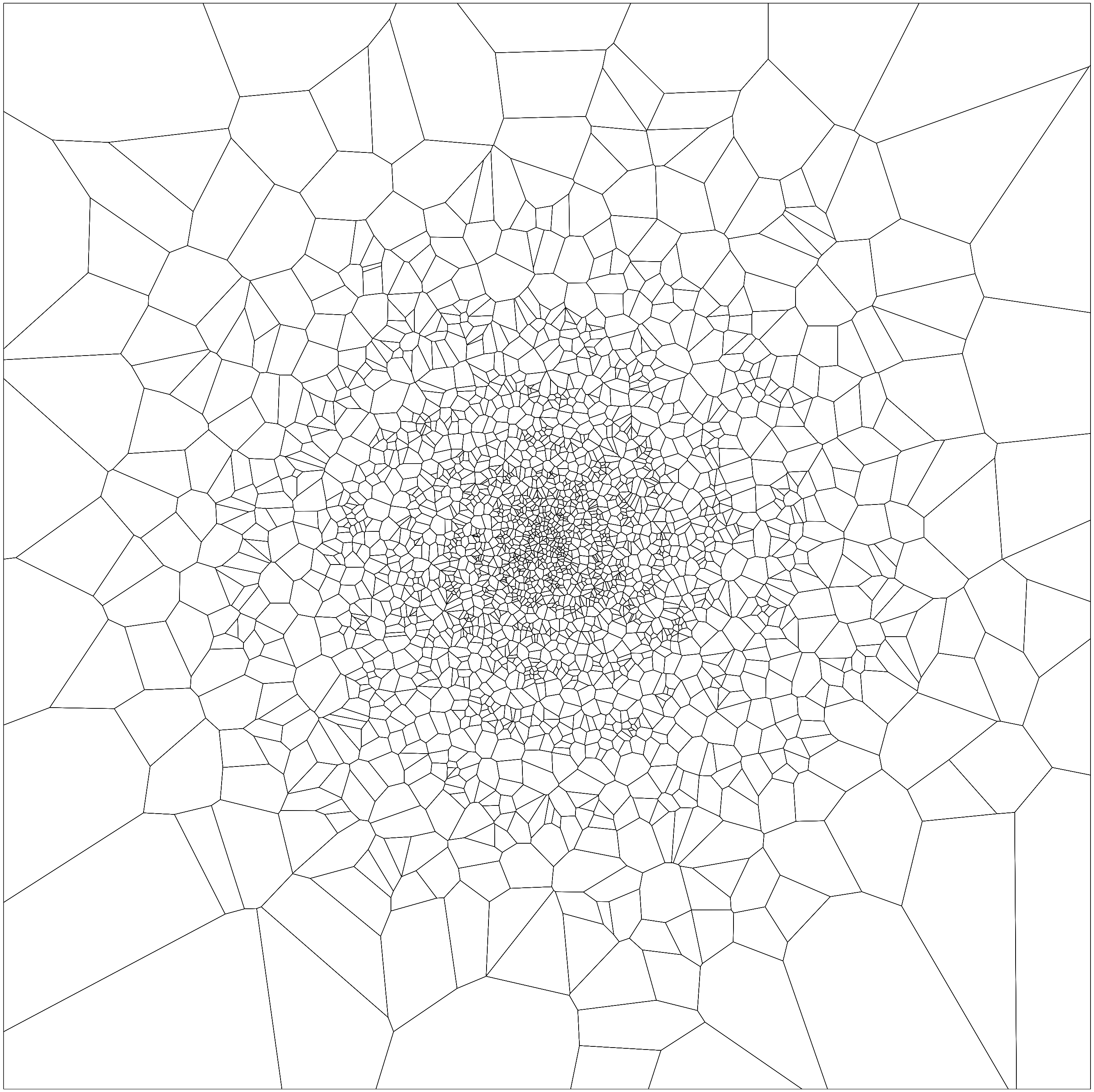
Planar cut

Sites placed according to density distribution of dust in a spiral galaxy



Planar cut

Sites placed according to density distribution of dust in a spiral galaxy

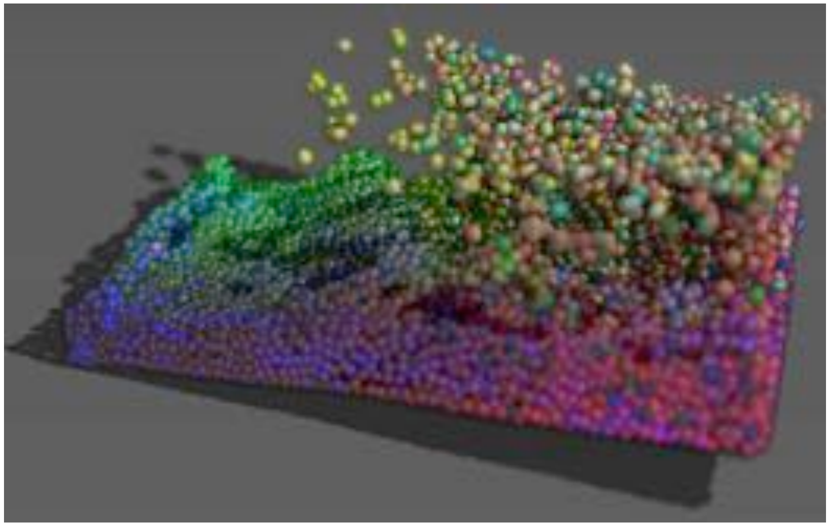


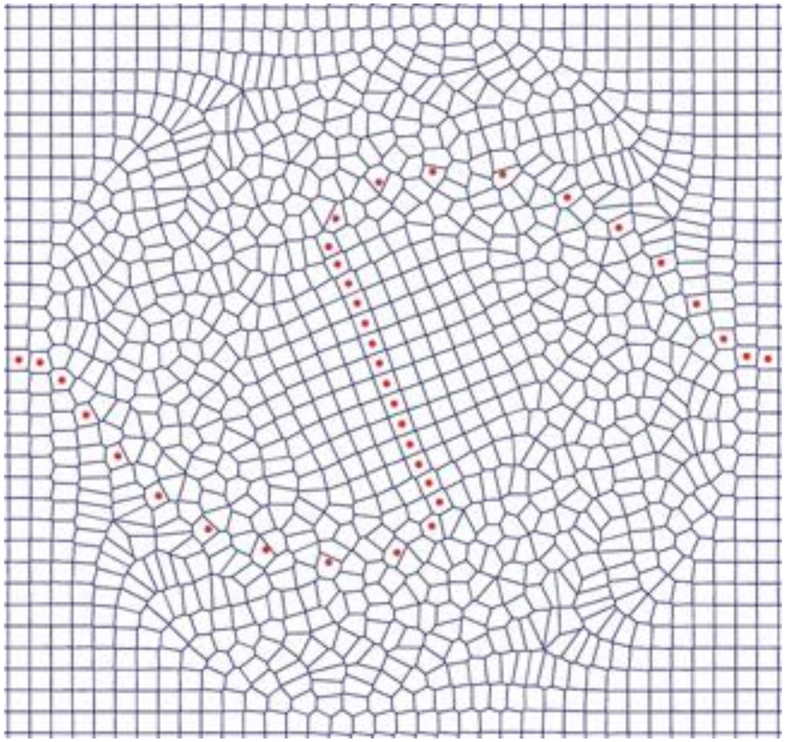
Why consider Voronoi grids?

Minimize the number of cells

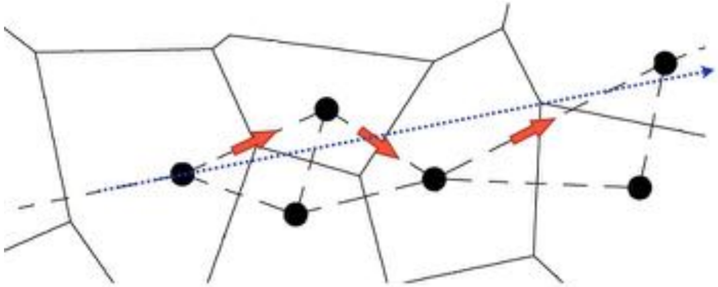
Place cell boundaries according to gradients

Natural grid for hydro input models (SPH, moving mesh)



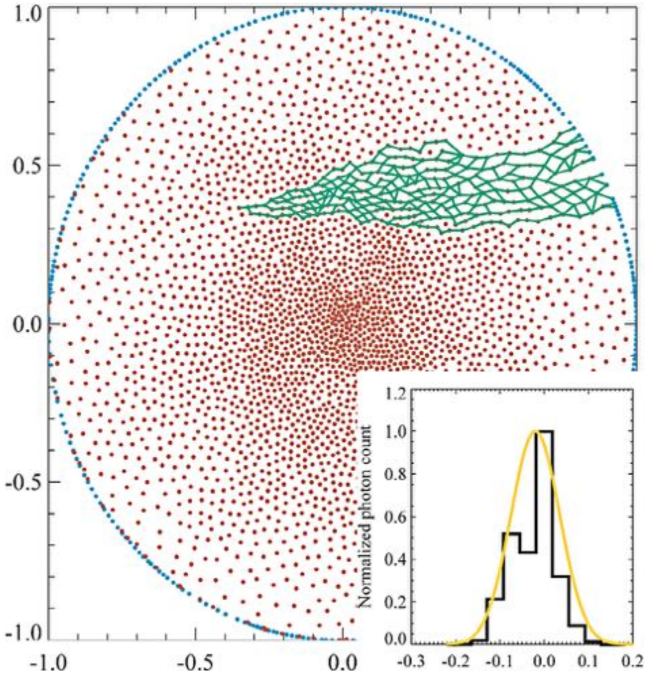


Paths along Delaunay edges



SimpleX

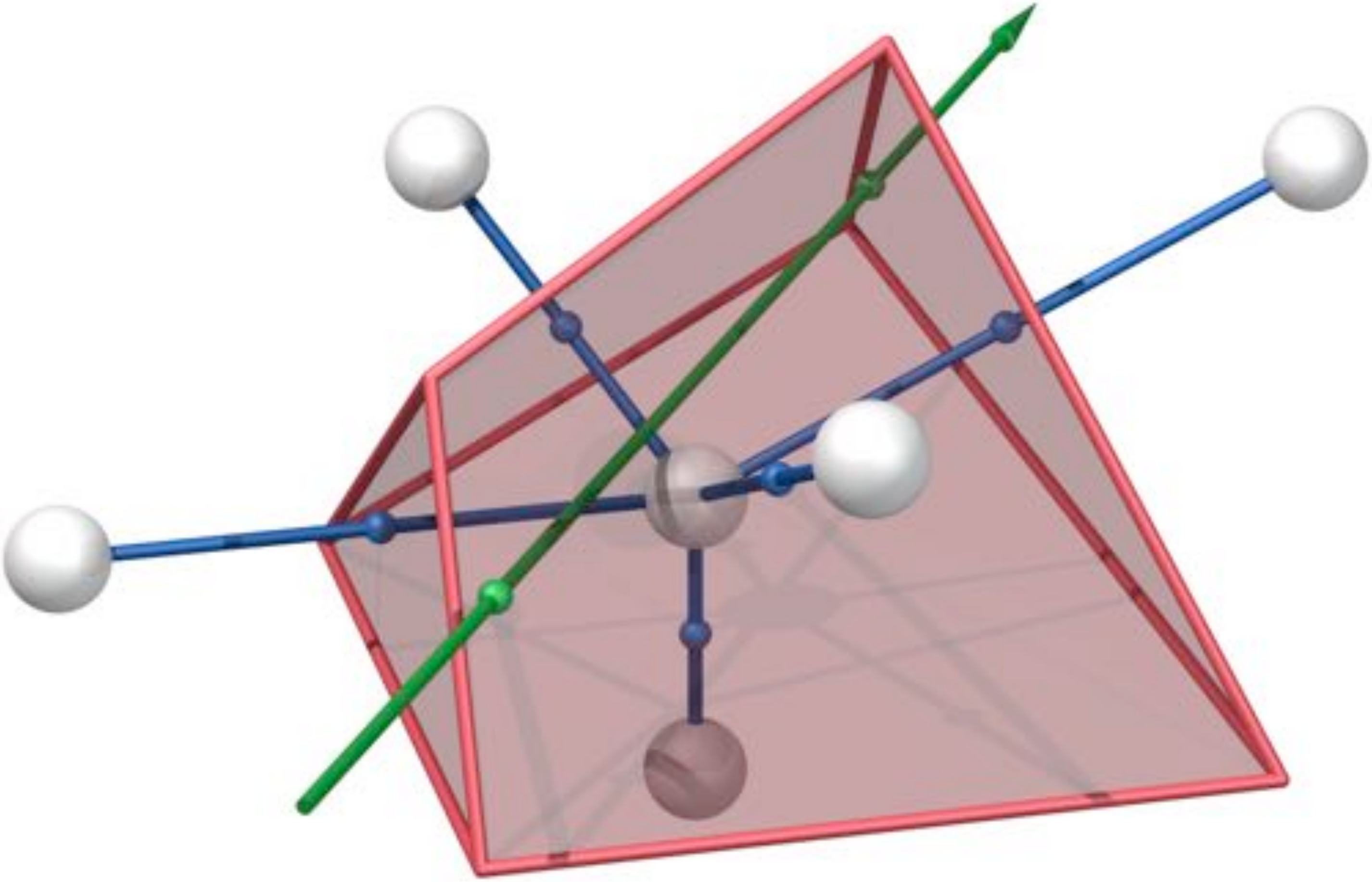
Paardekooper et al 2010



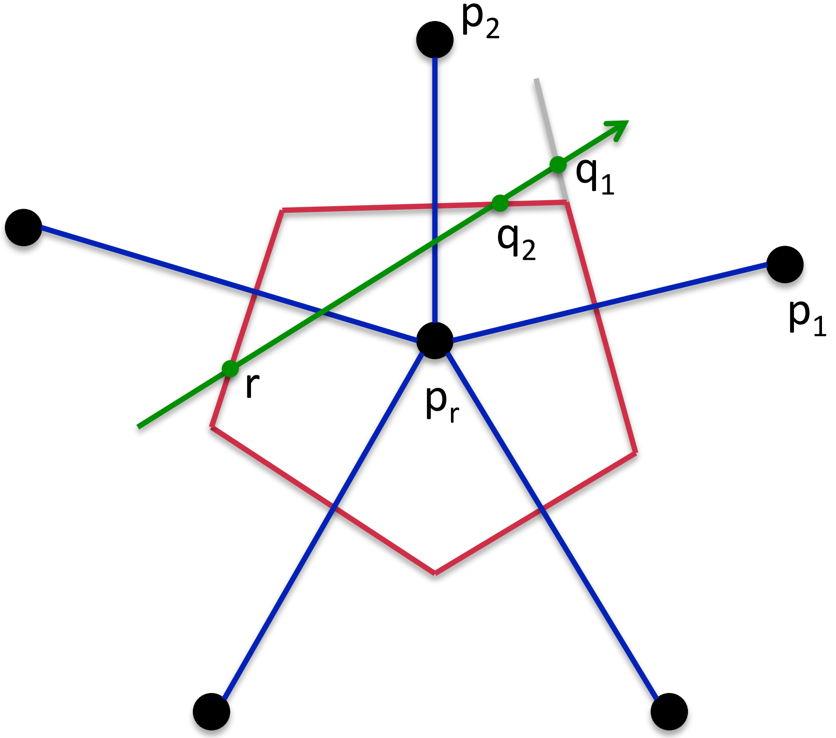
LIME

Brinch & Hogerheijde 2010

Straight path through a Voronoi grid



Straight path through a Voronoi grid



Camps et al. 2013

$$\mathbf{n} = \mathbf{p}_i - \mathbf{p}_r$$

$$\mathbf{p} = \frac{\mathbf{p}_i + \mathbf{p}_r}{2}$$

Equation of the plane

$$\mathbf{n} \cdot (\mathbf{x} - \mathbf{p}) = 0$$

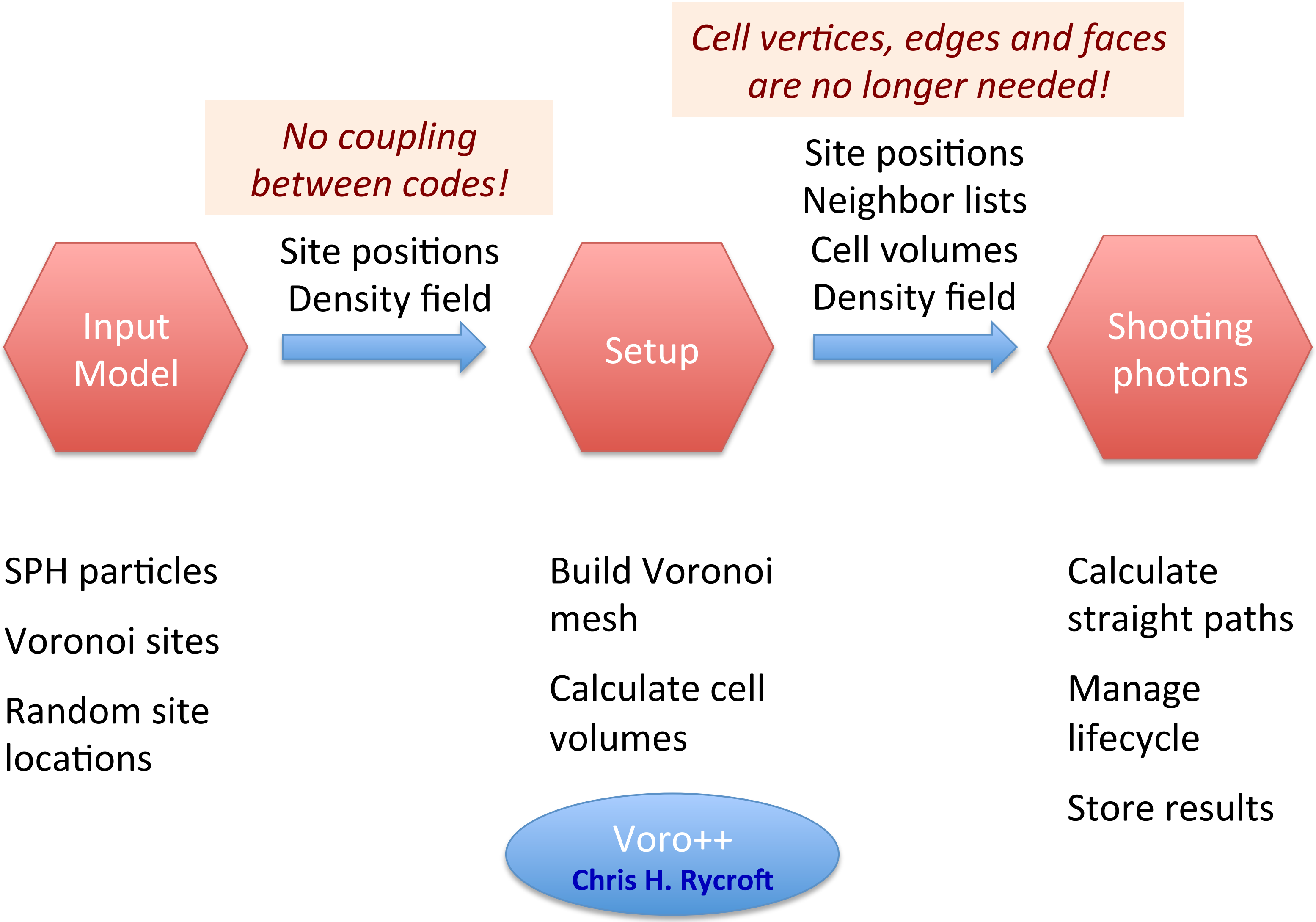
Equation of the path

$$\mathbf{x} = \mathbf{r} + s\,\mathbf{k}$$

Intersection, solved for s

$$s = \frac{\mathbf{n} \cdot (\mathbf{p} - \mathbf{r})}{\mathbf{n} \cdot \mathbf{k}}$$

Thin interfaces



No coupling between codes!

Cell vertices, edges and faces are no longer needed!

Input Model

Site positions
Density field

Setup

Site positions
Neighbor lists
Cell volumes
Density field

Shooting photons

SPH particles

Voronoi sites

Random site locations

Build Voronoi mesh

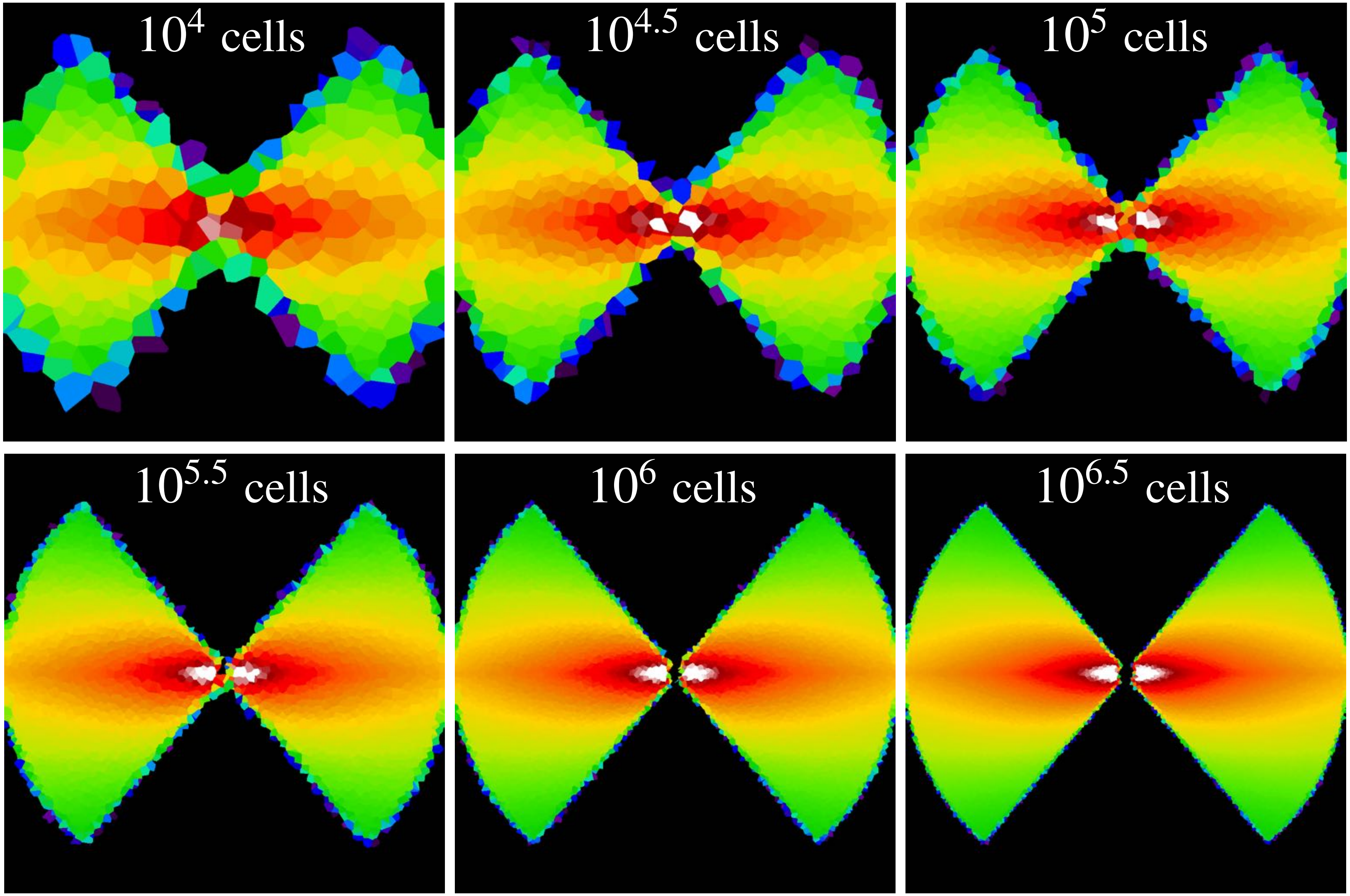
Calculate cell volumes

Voro++
Chris H. Rycroft

Calculate straight paths

Manage lifecycle

Store results

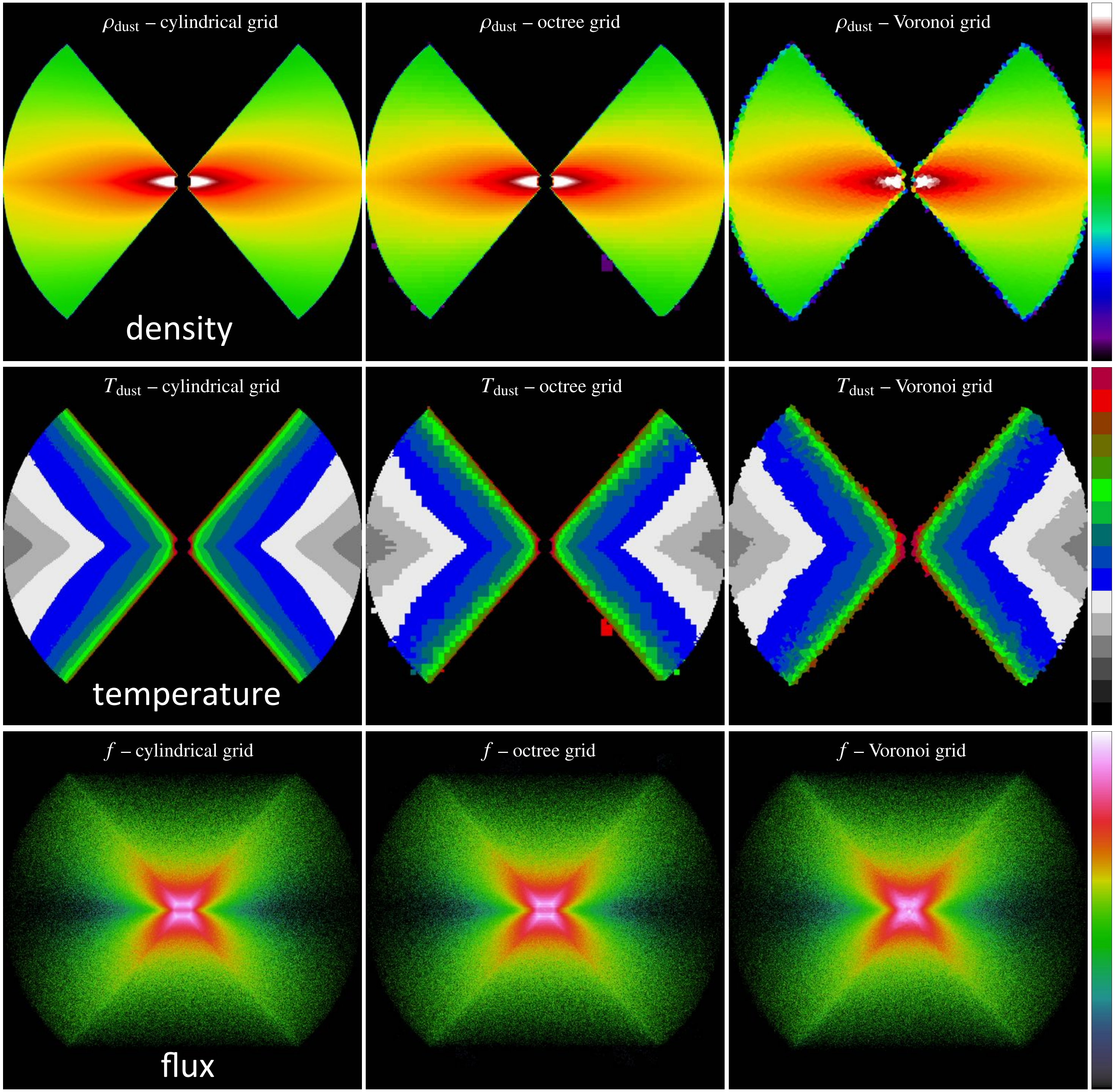


Cuts through grid with increasing number of cells

Torus model

Octree &
Voronoi grids
have
950 000 cells

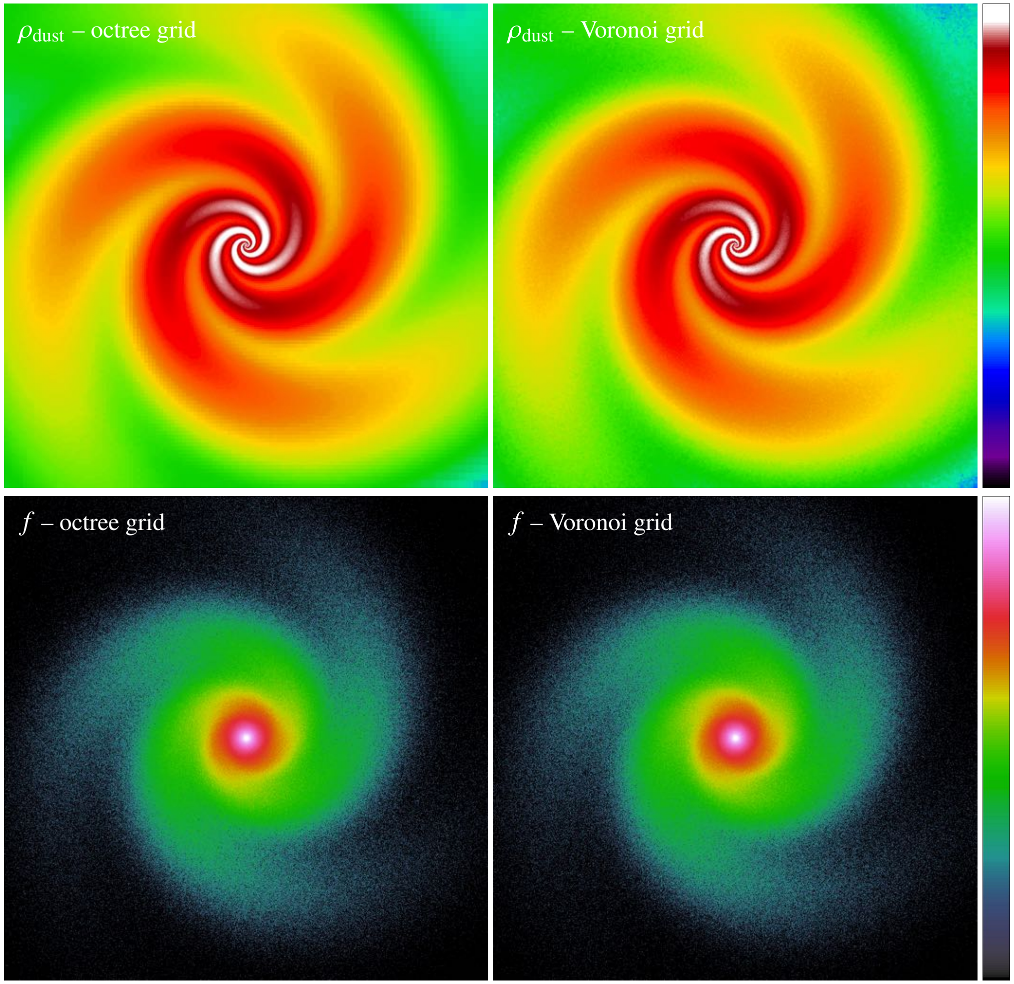
Voronoi sites
are distributed
uniformly

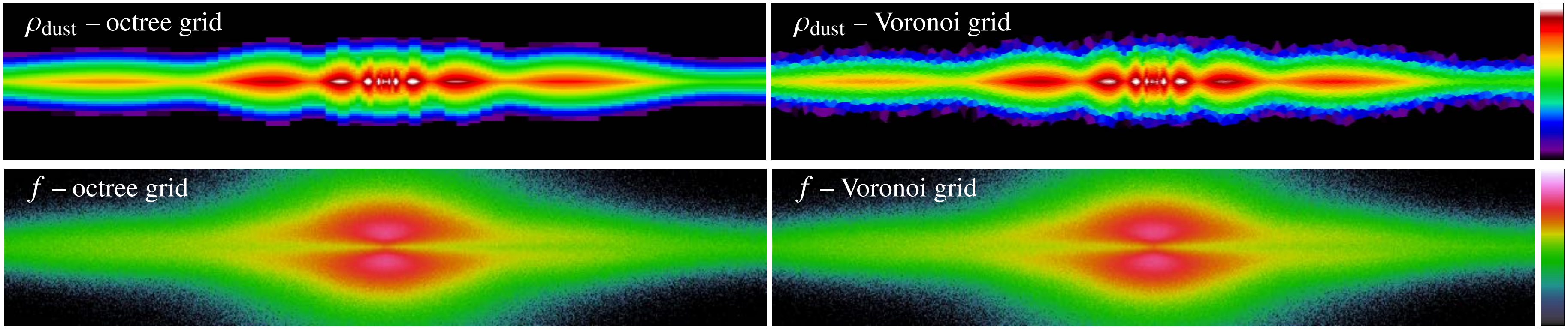


Spiral model

Both grids have
1 350 000 cells

Voronoi sites are
distributed according
to dust density





Grid quality

(std.dev. of $\rho_t - \rho_g$)

Model	Cylindrical	Octree	Voronoi
Torus	0.82	1	1.75
Spiral	–	1	1.68

Run time

(including overhead)

		Time per cell crossing (ns)		
Model	Simulation type	Octree	Voronoi	Vor./Oct.
Torus	monochromatic	219	693	3.2
Torus	panchromatic	400	1006	2.5
Spiral	monochromatic	309	903	2.9
Spiral	panchromatic	442	1095	2.5

Conclusions – 3D dust grids

Hierarchical grids with cuboidal cells

- Use neighbor lists to traverse the grid
- k-d tree grids are about 20% “better” than octree grids
- Combination of mass and optical depth criteria is optimal

Unstructured Voronoi grids

- Rather straightforward to implement in radiative transfer
- Only 3 times slower per cell crossing
- Promise to have fewer and more optimally placed cells (to be confirmed)

Questions ?

Importing hydro snapshots

Section B-3

Observables for simulated galaxies

Properties deduced directly from simulation results:

- Size, mass, age, chemical composition
- Kinematics (central dispersion, rotation curve)
- Intrinsic 3D morphology (concentration, flattening, bulge to disk)
- Total bolometric luminosity

Properties calculated through dust radiative transfer:

- 2D morphologies from various viewing angles
- SEDs from UV to FIR wavelengths
- Luminosity in specific band, color

Importing SPH and AMR data

SPH = Smoothed Particle Hydrodynamics
AMR = Adaptive Mesh Refinement

Data format

- Read native snapshot data (in various formats), or define intermediate format containing just the required data

Stars

- Assign SED based on particle/cell properties
- Launch random photons with appropriate distribution

Dust

- Derive dust distribution from gas distribution (most hydro simulations do not trace the dust)
- Sample the dust density distribution defined by a large number of smoothed particles (can be very slow)
- Build adaptive grid that adjusts to dust density distribution

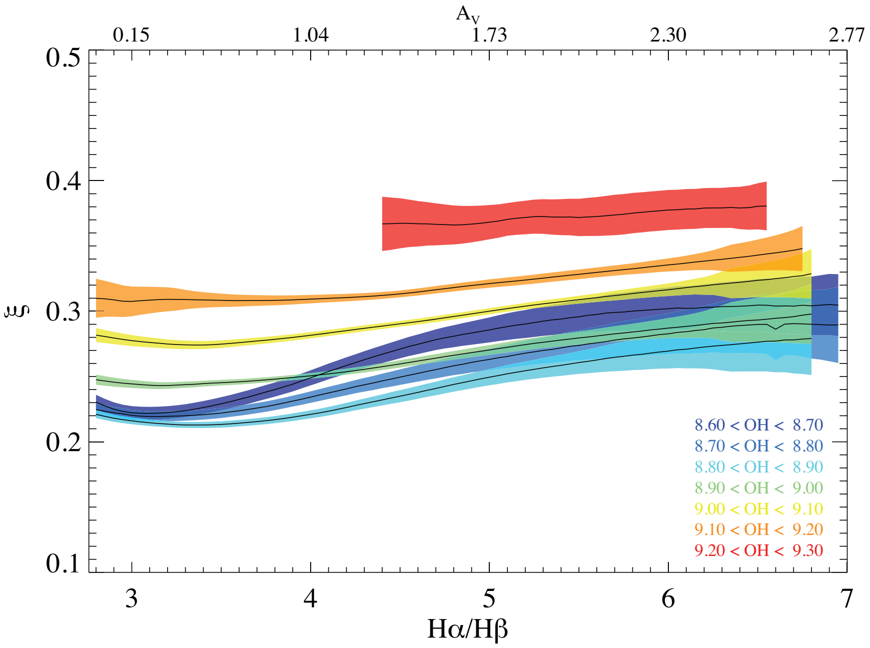
The gas-to-dust relation

We use a (too) simple heuristic to determine the amount of dust contained in each gas particle/cell:

$$M_{\rm dust} = \begin{cases} f_{\rm dust}\, Z\, M & \text{if } T < T_{\rm max} \\ 0 & \text{otherwise,} \end{cases}$$

Gas properties:
 Z: metallicity
 T: temperature

Parameters:
 $f_{\rm dust}$: fraction of metals locked in dust
 $T_{\rm max}$: gas temperature above which all dust is destroyed



The dust-to-metal ratio as a function of the Balmer decrement (SDSS sample, ***Brinchmann et al. 2013***)

Density sampling on SPH particles

Organize particles in a smart search grid

- List of particles that overlap each cell in a regular grid

Optimize density interpolation on each particle

$$\rho(\mathbf{r}) = f_{\text{dust}} \sum_i Z_i M_i W(h_i, |\mathbf{r}-\mathbf{r}_i|)$$

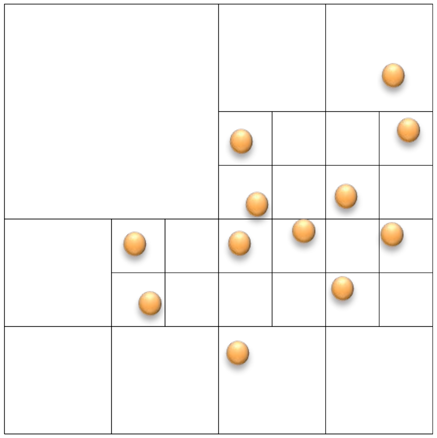
standard spline kernel: $$W(h,r) = \frac{8}{\pi h^3} \times \begin{cases} 1-6u^2(1-u) & \text{for } 0<u<\frac{1}{2}, \\ 2(1-u)^3 & \text{for } \frac{1}{2}<u<1, \\ 0 & \text{else.} \end{cases}$$

$$M_{\text{box}} = f_{\text{dust}} \sum_i Z_i M_i \int_{x_{\text{min}}}^{x_{\text{max}}} \int_{y_{\text{min}}}^{y_{\text{max}}} \int_{z_{\text{min}}}^{z_{\text{max}}} W(h_i, |\mathbf{r}-\mathbf{r}_i|)\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z$$

scaled Gaussian kernel: $$W(h,r) = \frac{a^3}{\pi^{3/2} h^3} \exp\left(-\frac{a^2 r^2}{h^2}\right) \qquad a = 2.42$$

6 error function evaluations per integral -> tabulate error function

Specialty dust grids for hydro snapshots

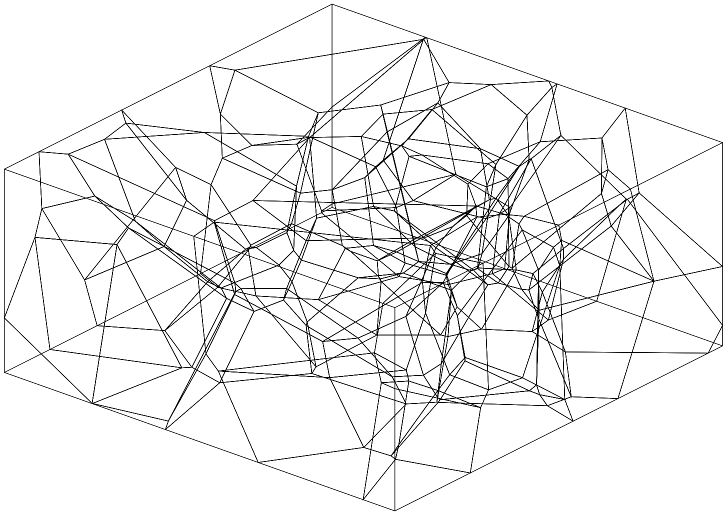


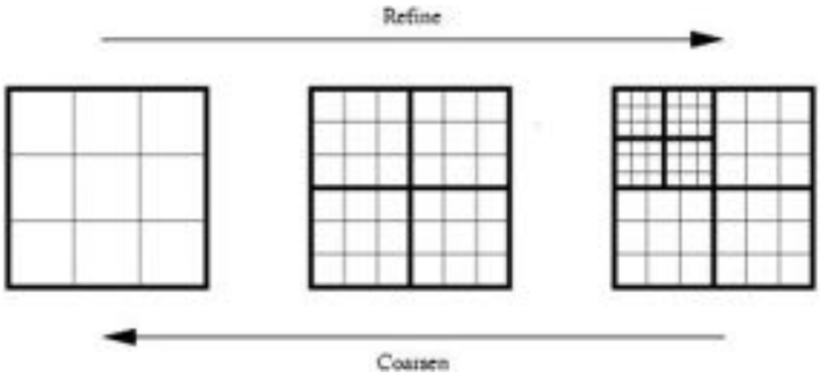
Octree or *k*-d tree

- Subdivide until there is at most one particle in each cell
- Then subdivide further with usual stopping criteria

Voronoi grid

- Use particle positions as seeds (one cell per particle)

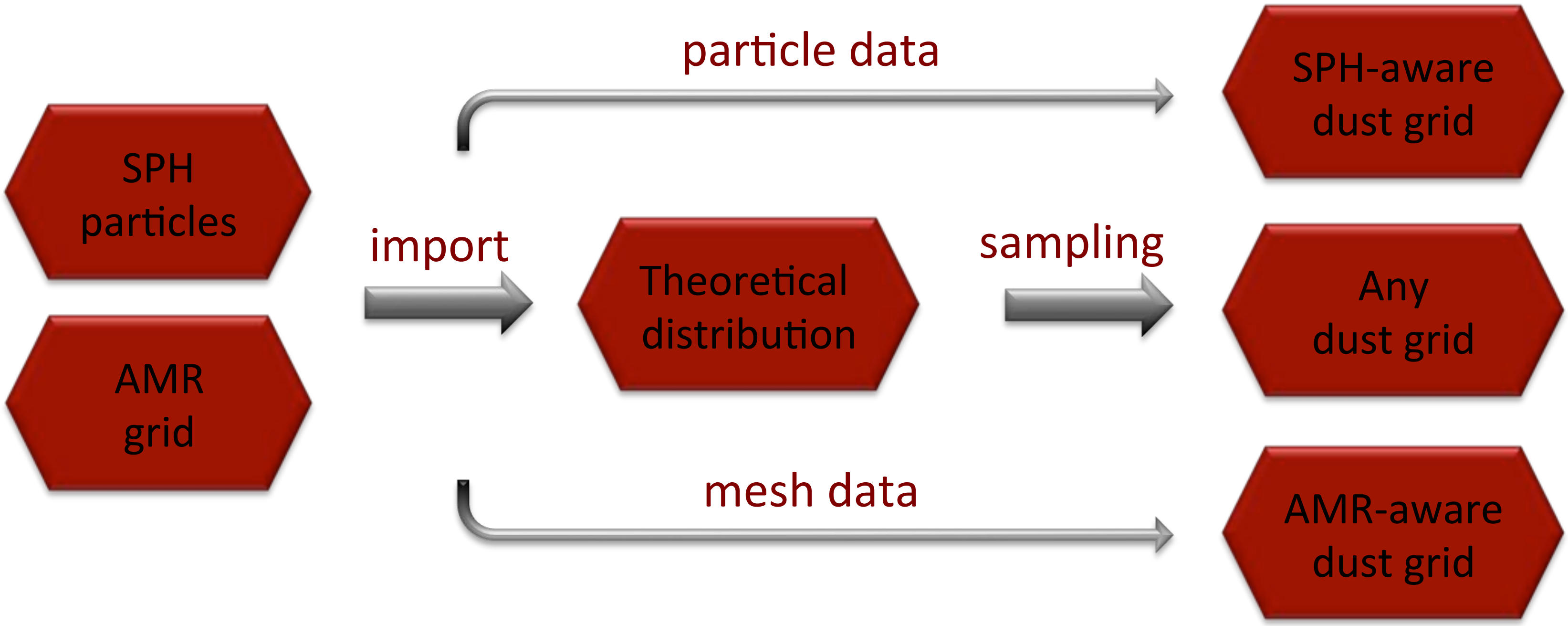




AMR grid

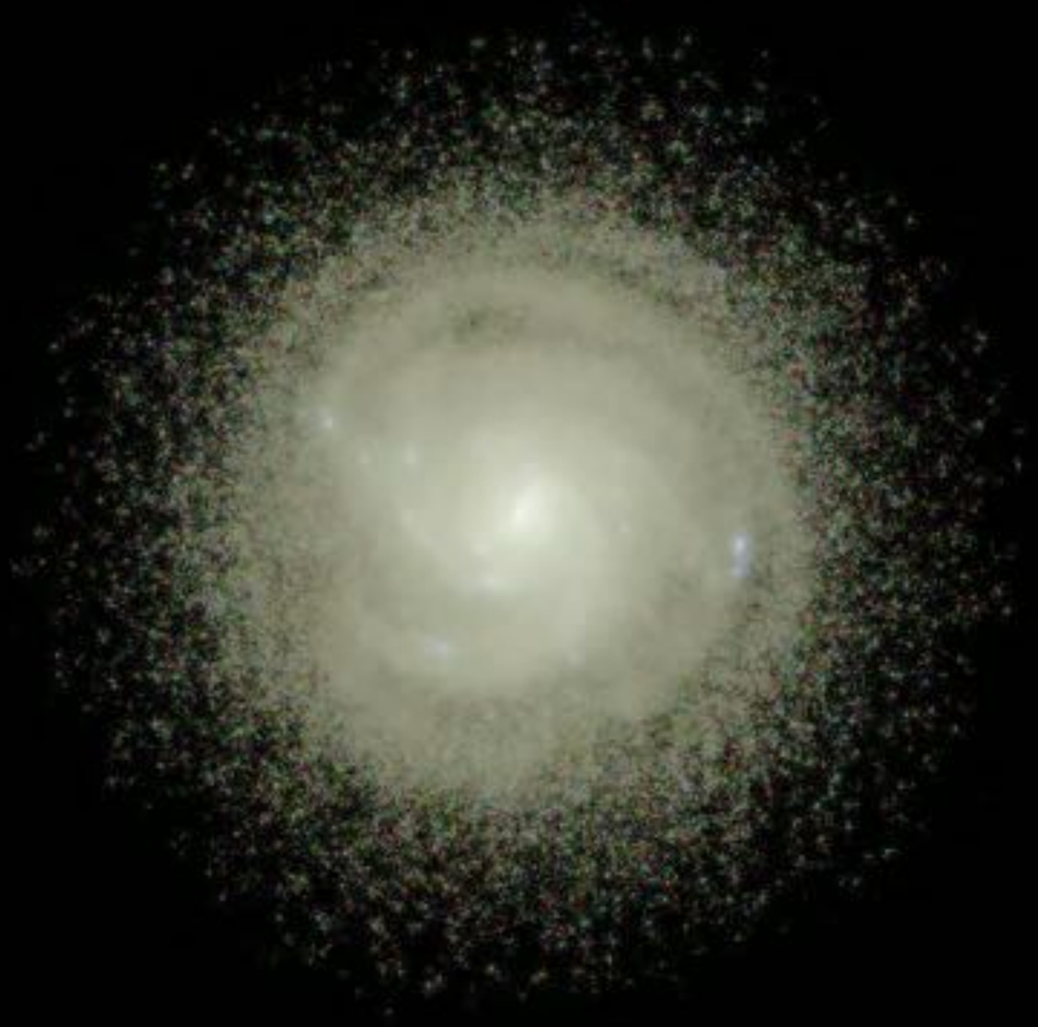
- Identical to imported grid

Code structure in SKIRT



- Bypass interfaces operate only when both parties support it
- Input-format-aware dust grids can be smarter
    - Use particle positions or mesh cells to setup grid structure
    - Analytically calculate density in cuboid

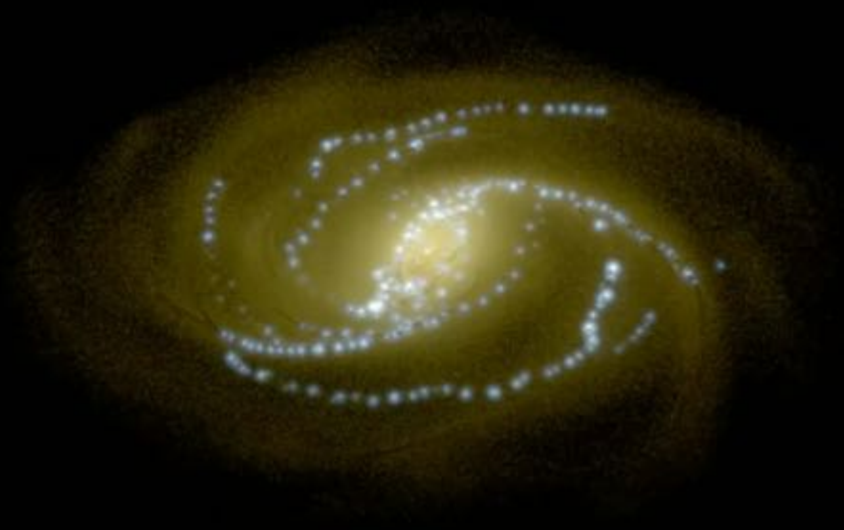
→ Faster import, and conceivably also higher-quality grid

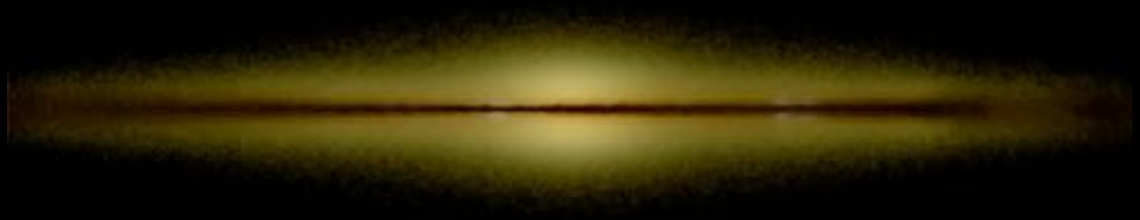


SPH Data:
Rahimi & Kawata 2012

Eris

R13



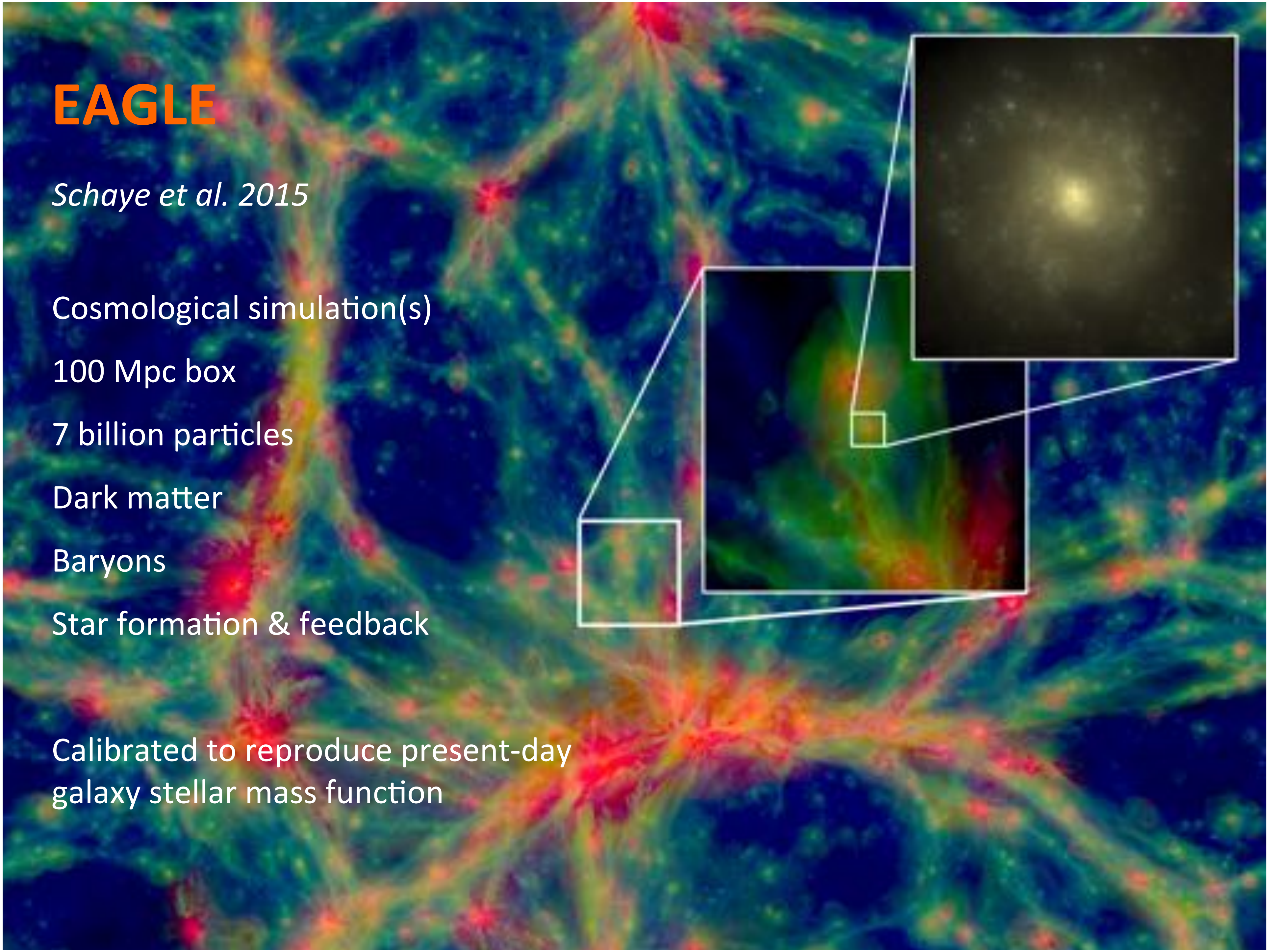


Questions ?

FIR properties of galaxies in a cosmological simulation

Section B-4

EAGLE



Schaye et al. 2015

Cosmological simulation(s)

100 Mpc box

7 billion particles

Dark matter

Baryons

Star formation & feedback

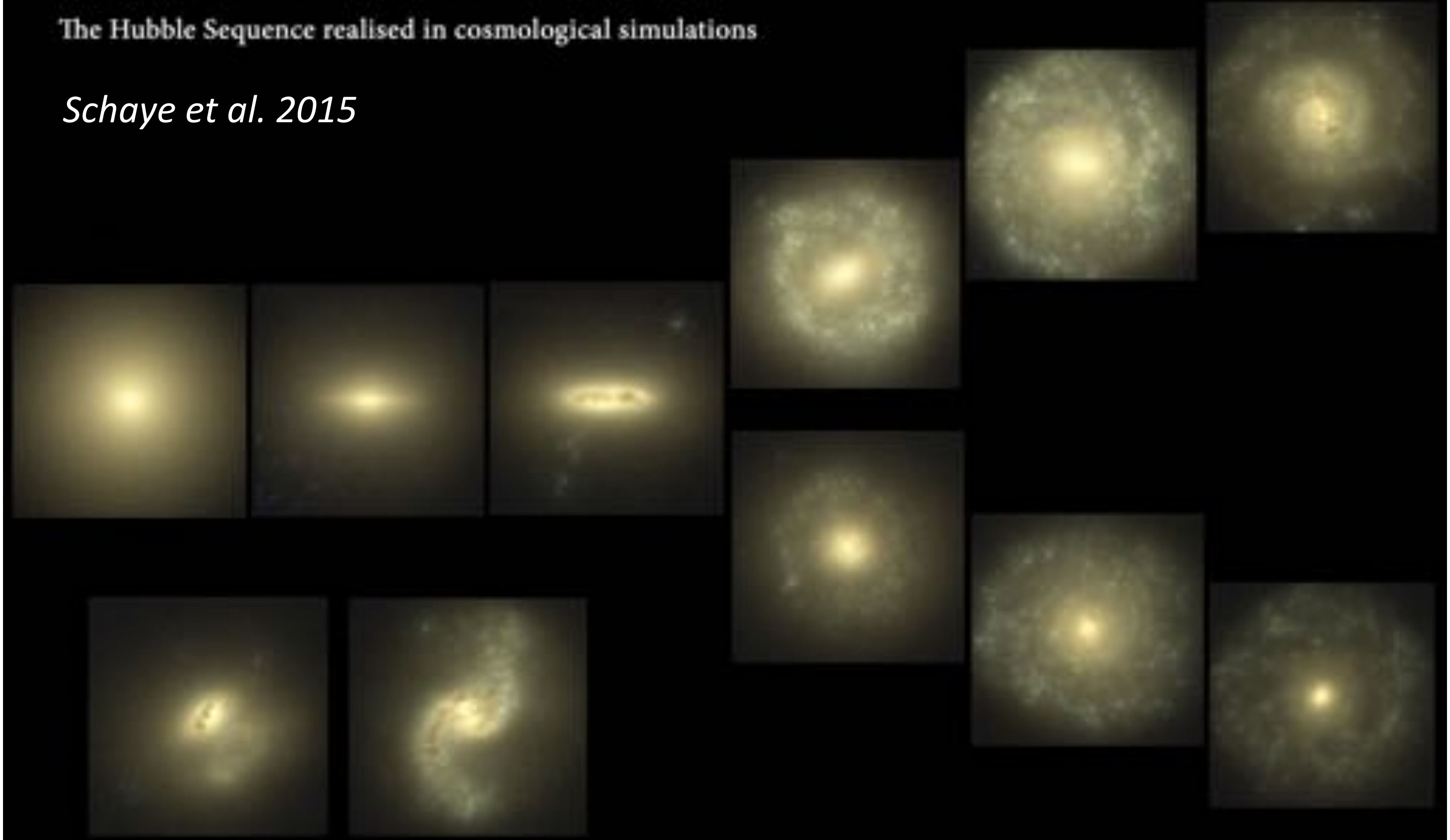
Calibrated to reproduce present-day galaxy stellar mass function

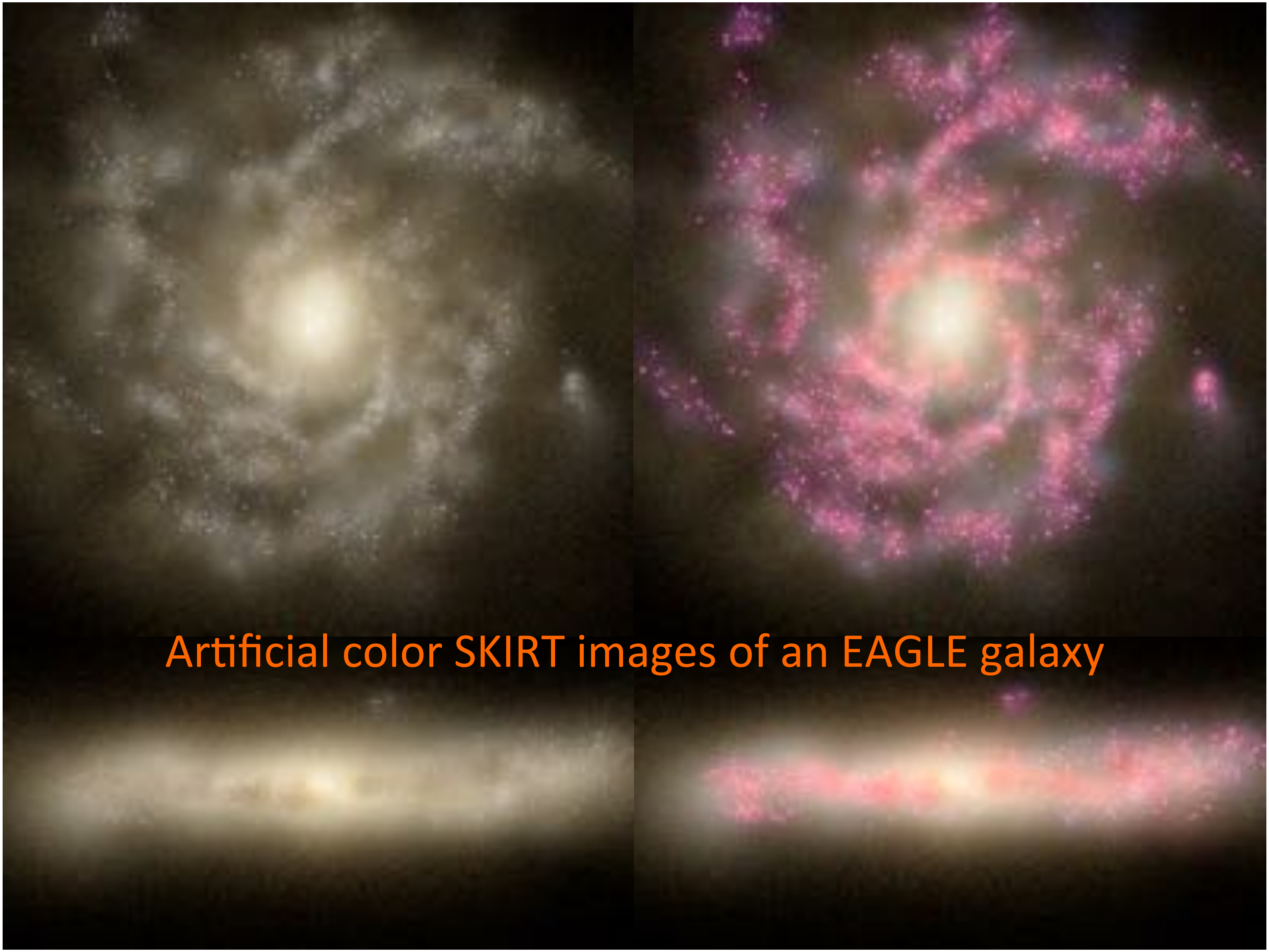
The Eagle Simulations

EVOLUTION AND ASSEMBLY OF GALAXIES AND THEIR ENVIRONMENTS

The Hubble Sequence realised in cosmological simulations

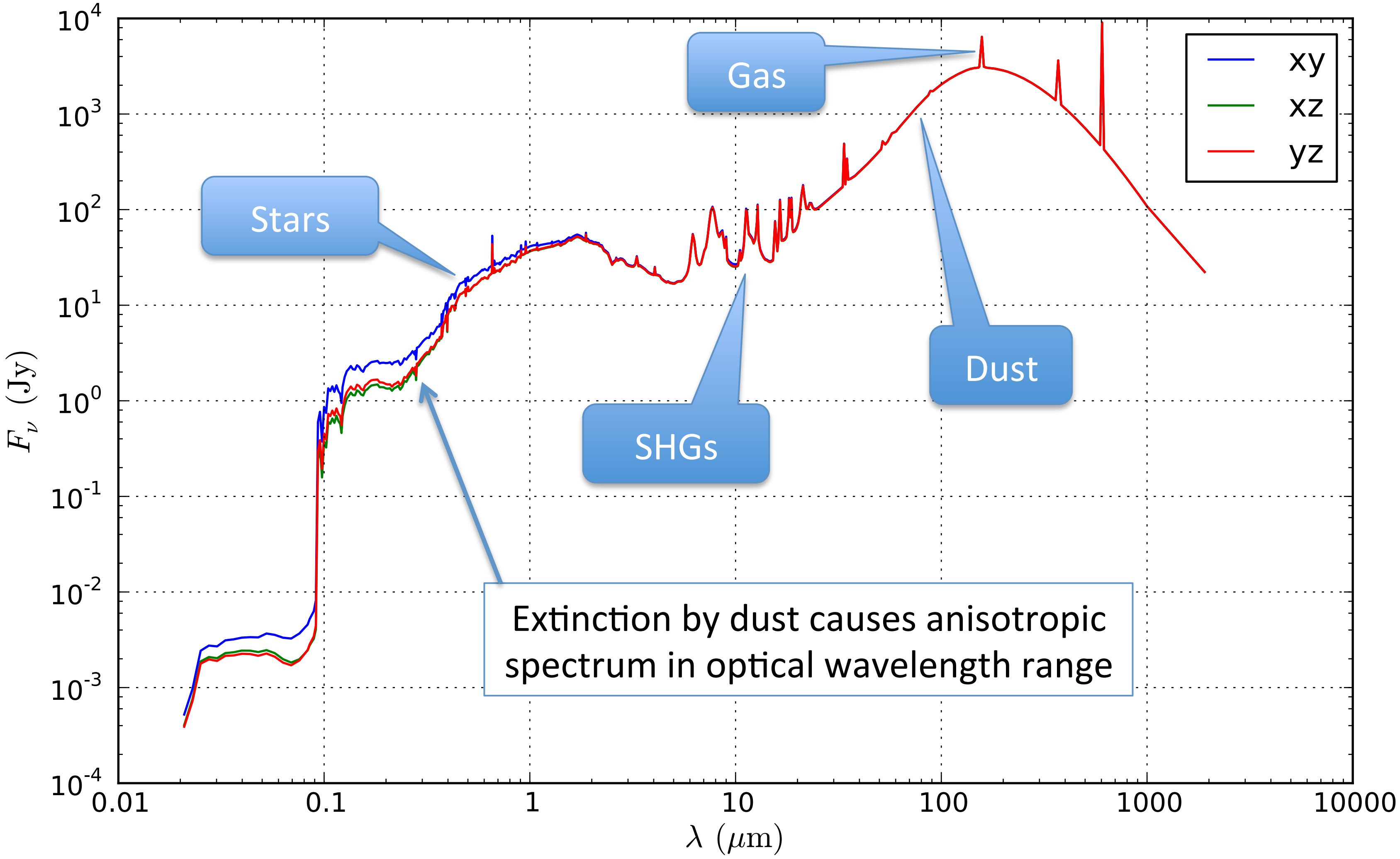
Schaye et al. 2015



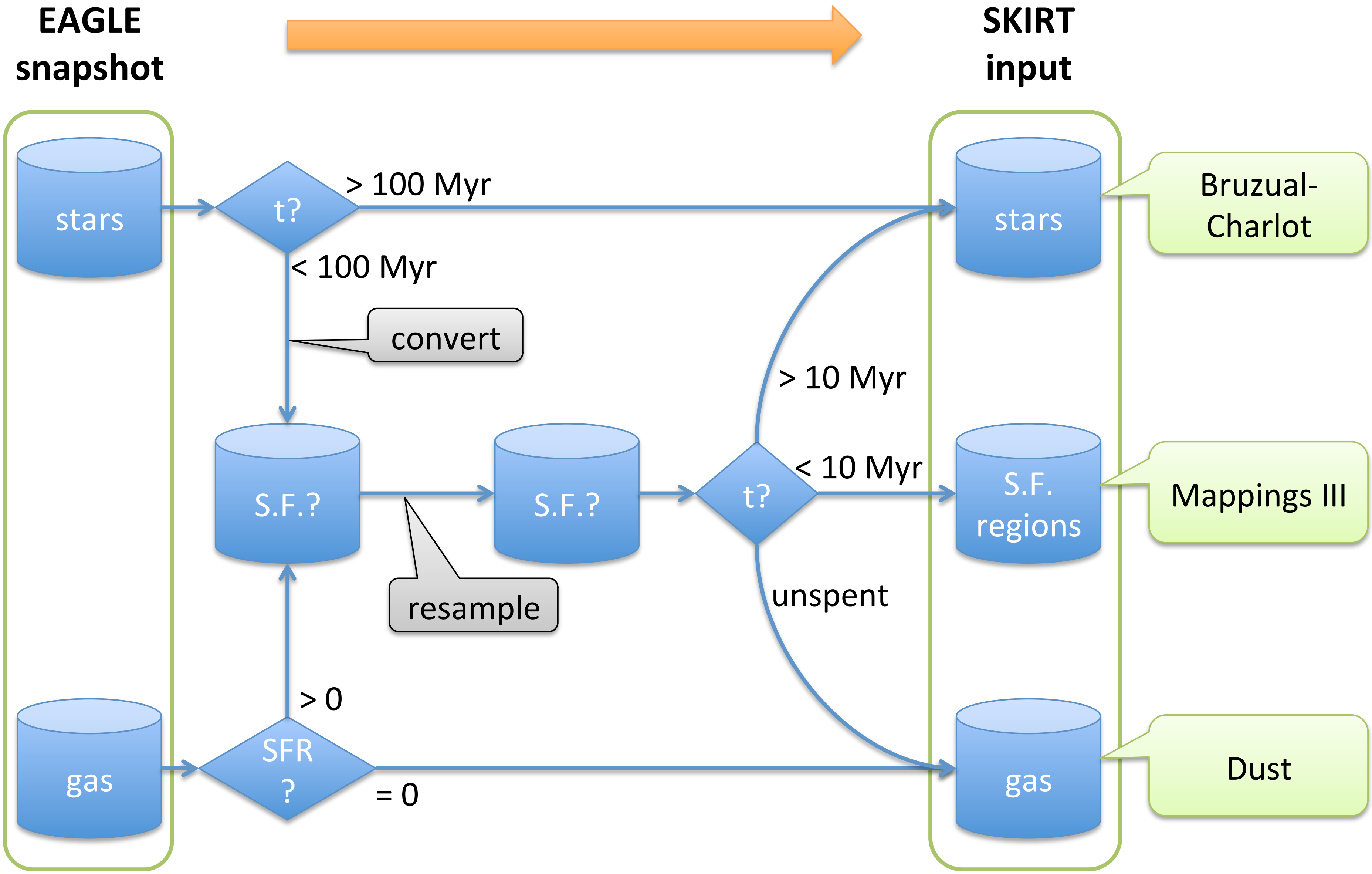


Artificial color SKIRT images of an EAGLE galaxy

Full SED from UV to sub-mm produced by SKIRT



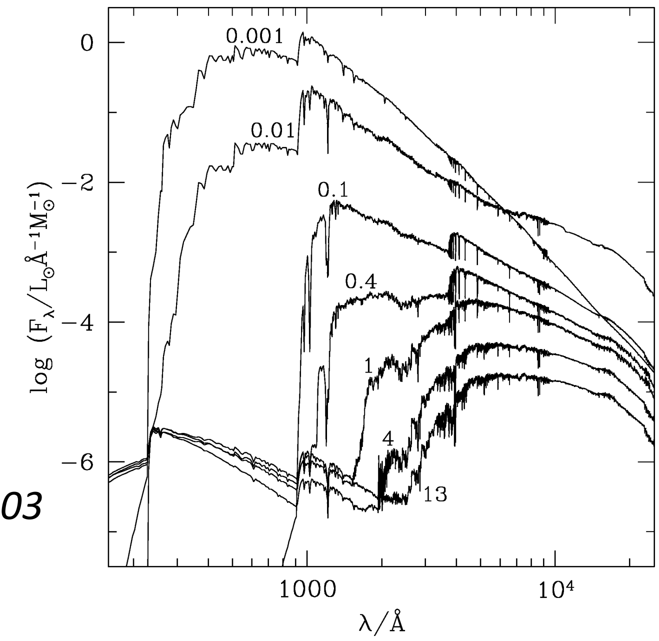
Extinction by dust causes anisotropic spectrum in optical wavelength range


EAGLE snapshot
SKIRT input
stars
gas
t?
> 100 Myr
< 100 Myr
convert
S.F.?
resample
S.F.?
t?
> 10 Myr
< 10 Myr
unspent
SFR ?
> 0
= 0
stars
S.F. regions
gas
Bruzual-Charlot
Mappings III
Dust

SKIRT assigns SEDs to input particles

Star

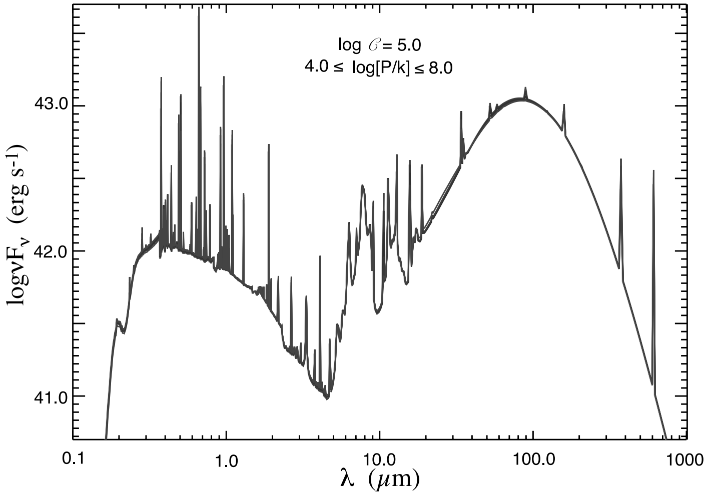
→ Bruzual-Charlot stellar population SED
depending on age and metallicity



Bruzual & Charlot 2003

Star forming region

→ MAPPINGS III starburst SED
(HII region around cluster of young stars)
depending on metallicity, compactness,
pressure, PDR covering factor

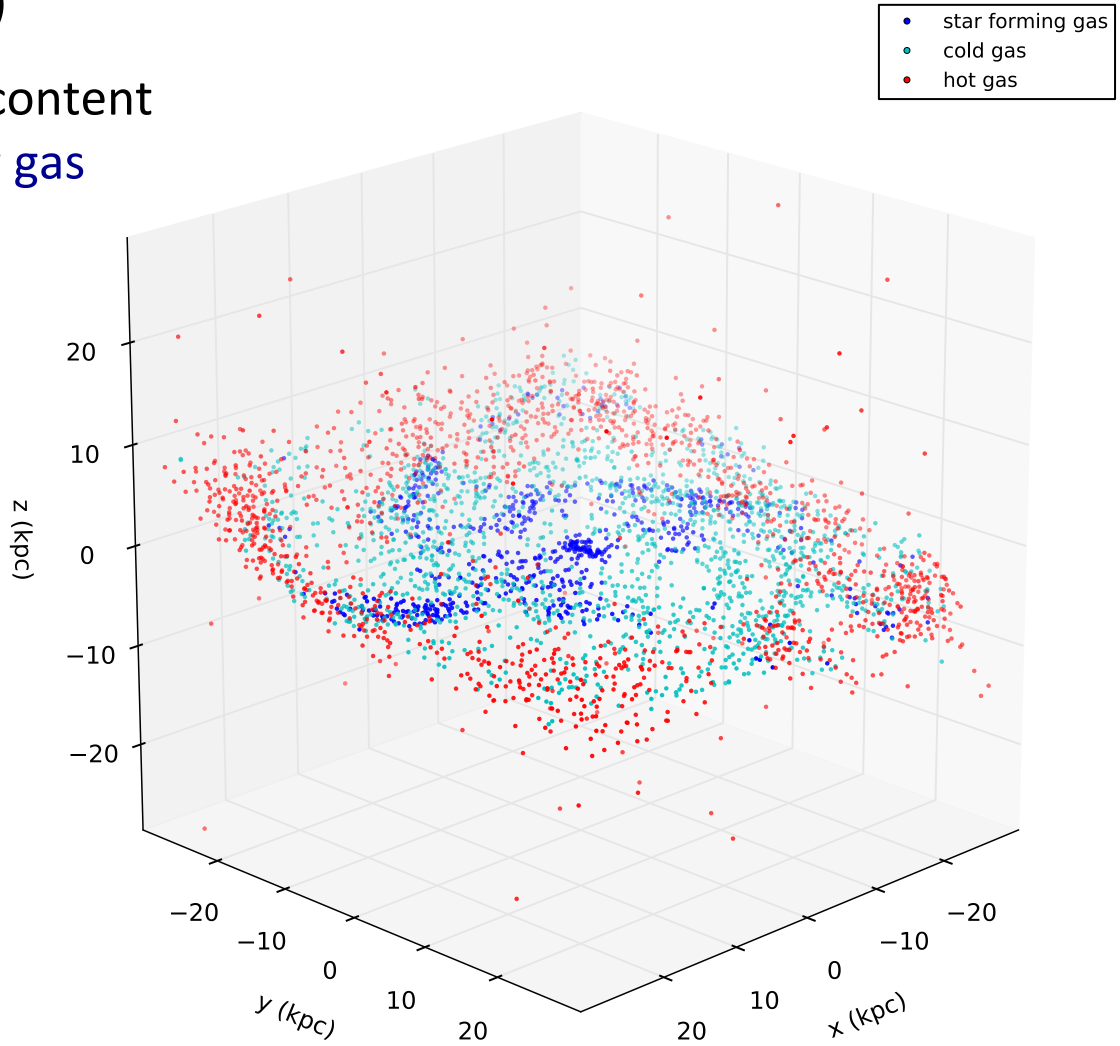


Groves et al. 2008

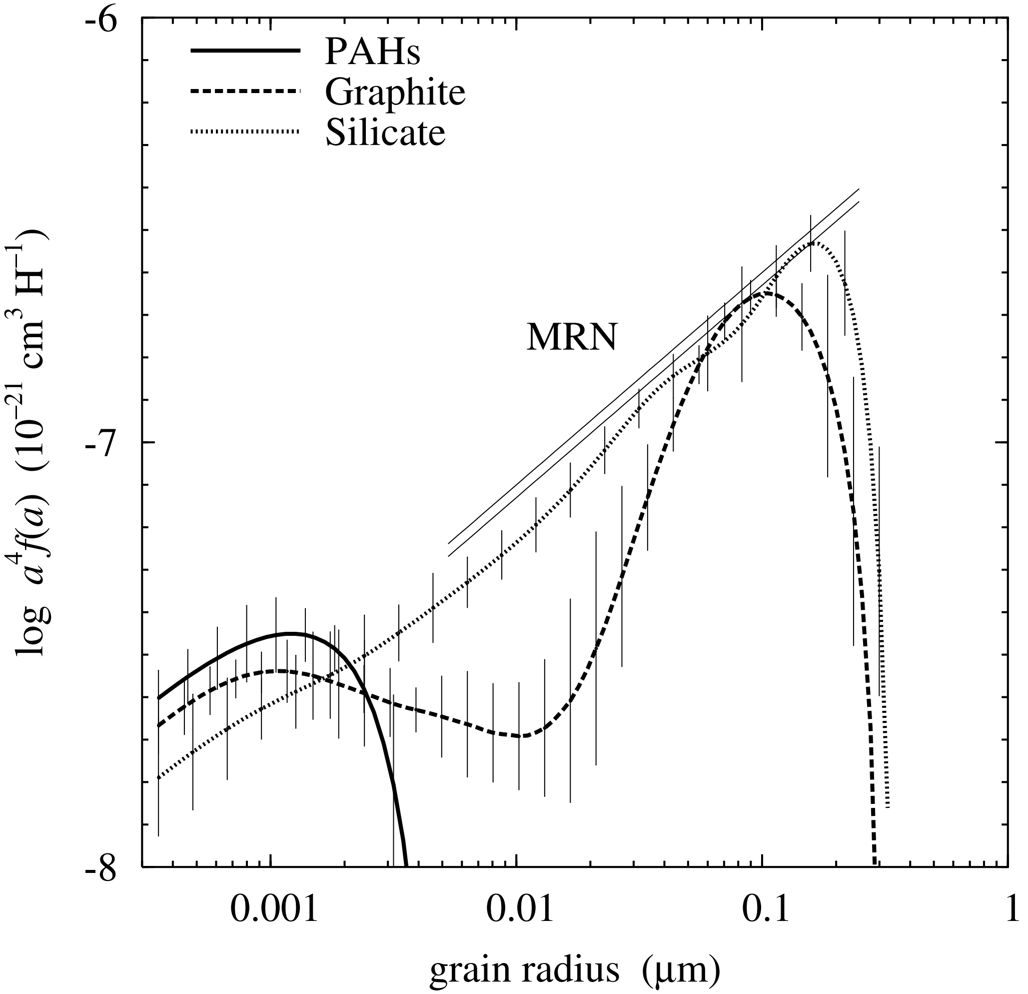
SKIRT assigns dust content to input gas particles

No dust in hot gas (T > 8000 K)

Fixed fraction (40%) of metal content in cold gas and in star-forming gas



Dust model used for EAGLE galaxies

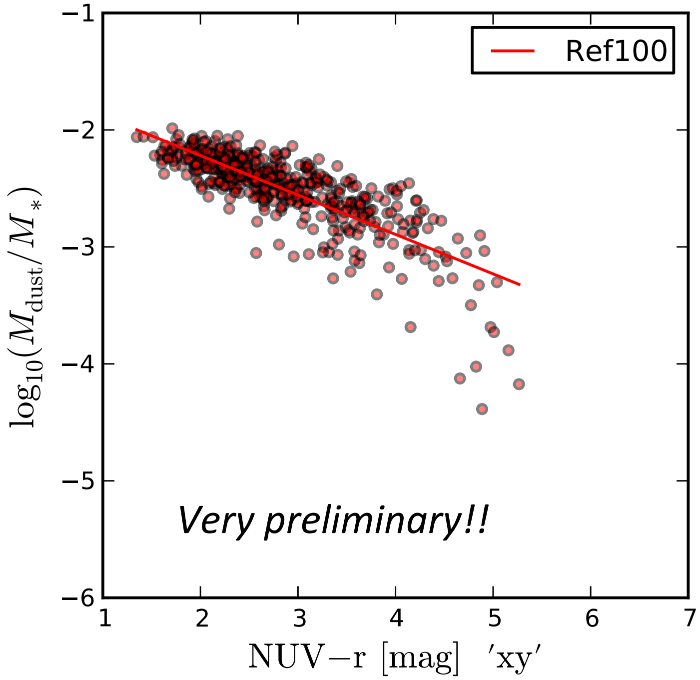


Size distribution for BARE_GR_S model from *Zubko, Dwek & Arendt 2004*

- Realistic mixture
  - 33% graphite grains
  - 62% silicate grains
  - 5% neutral and ionized PAHs
- Fine-tuned to accurately reproduce the extinction, emission and abundance constraints on the Milky Way

Objective: compare far-infrared and dust properties of EAGLE galaxies to observations

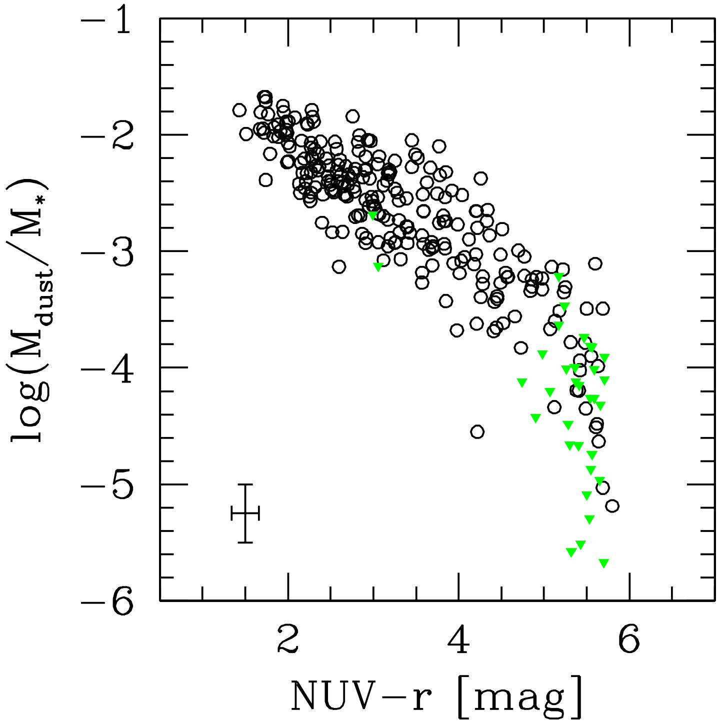
SKIRT results for EAGLE galaxies



Very preliminary!!

Cortese et al. 2012

Herschel Reference Survey



TO DO

- → mimic observational selection effect
- → use mock observational quantities for M_{dust} en M_{star}
- → fine-tune parameters such as dust fraction, PDR coverage factor, …

Questions ?