Computational Cost Optimization via Stochastic Kernel Sampling for the Numerical Integration of the Smoluchovski Coagulation Equation

Vincent C. Mader

June 20, 2023

Contents

1	Pre		
	1.1	Ackno	wledgements
	1.2	Abstra	act
	т,	1 4	
2		roducti	
	2.1		Planetary Disks & their Formation
		2.1.1	Material Composition of the Interstellar Medium
		2.1.2	Collapse of Interstellar Gas Clouds into a Disk
		2.1.3	Star Formation at the Disk Center
		2.1.4	Spatial Structure of Proto-Planetary Disks
		2.1.5	Material Composition of Proto-Planetary Disks
	2.2	Gas &	Dust Particles inside PPDs
		2.2.1	QUES How to model the gas inside the disk?
		2.2.2	QUES What characterizes a dust particle?
		2.2.3	QUES How does the central star influence the disk around it?
		2.2.4	QUES How does the gas affect the dust?
		2.2.5	QUES What other effects are there?
		2.2.6	Gas Kinematics inside PPDs
		2.2.7	Dust Kinematics inside PPDs
	2.3		Formation inside Proto-Planetary Disks
		2.3.1	Particle-Particle Collisions
		2.3.2	Particle Coagulation
		2.3.3	Formation of Planetary Cores
	2.4		on the Structure of this Thesis
		1.000	
3	Def	inition	of a simplified Radial Model for the Proto-Planetary Disk
	3.1	Introd	uction, Overview, & Goals for this Section
		3.1.1	QUES How to formulate a model for the PPD, its contents, & the planet formation
			processes?
		3.1.2	QUES How to model the central star?
		3.1.3	QUES How to model the gas?
		3.1.4	QUES How to model the dust?
		3.1.5	
			Necessary Simplifications
	3.9	3.1.6	Necessary Simplifications
	3.2	3.1.6 Prope	Necessary Simplifications
	3.2	3.1.6 Prope 3.2.1	Necessary Simplifications
		3.1.6 Prope 3.2.1 3.2.2	Necessary Simplifications
	3.2	3.1.6 Prope 3.2.1 3.2.2 Prope	Necessary Simplifications 1 What do we need to define? 1 rties of the Star at the Center of the PPD 1 Age 1 Mass 1 rties of the PPD 1
		3.1.6 Prope 3.2.1 3.2.2 Prope 3.3.1	Necessary Simplifications What do we need to define? Integration of the Star at the Center of the PPD Age Mass Introduction Introduction
		3.1.6 Prope 3.2.1 3.2.2 Prope 3.3.1 3.3.2	Necessary Simplifications What do we need to define? Ities of the Star at the Center of the PPD Age Mass Ities of the PPD Introduction Disk Scale Height
		3.1.6 Prope 3.2.1 3.2.2 Prope 3.3.1 3.3.2 3.3.3	Necessary Simplifications What do we need to define? Interior of the Star at the Center of the PPD Age Mass Introduction Disk Scale Height Midplane Temperature
	3.3	3.1.6 Prope 3.2.1 3.2.2 Prope 3.3.1 3.3.2 3.3.3 3.3.4	Necessary Simplifications What do we need to define? Inties of the Star at the Center of the PPD Age Mass Introduction Disk Scale Height Midplane Temperature Kepler Frequency
		3.1.6 Prope 3.2.1 3.2.2 Prope 3.3.1 3.3.2 3.3.3 3.3.4 Prope	Necessary Simplifications What do we need to define? It is of the Star at the Center of the PPD Age Mass It is of the PPD Introduction Disk Scale Height Midplane Temperature Kepler Frequency It is of the Gas inside the PPD Start Start Simplifications Age Age Age Age Age Age Age Ag
	3.3	3.1.6 Prope 3.2.1 3.2.2 Prope 3.3.1 3.3.2 3.3.3 4 Prope 3.4.1	Necessary Simplifications What do we need to define? Inties of the Star at the Center of the PPD Age Mass Introduction Disk Scale Height Midplane Temperature Kepler Frequency Interest of the Gas inside the PPD Radial Profile of Gas Density
	3.3	3.1.6 Prope 3.2.1 3.2.2 Prope 3.3.1 3.3.2 3.3.3 3.3.4 Prope	Necessary Simplifications What do we need to define? It is of the Star at the Center of the PPD Age Mass It is of the PPD Introduction Disk Scale Height Midplane Temperature Kepler Frequency It is of the Gas inside the PPD Start Start Simplifications Age Age Age Age Age Age Age Ag
	3.3	3.1.6 Prope 3.2.1 3.2.2 Prope 3.3.1 3.3.2 3.3.3 4 Prope 3.4.1	Necessary Simplifications What do we need to define? Inties of the Star at the Center of the PPD Age Mass Introduction Disk Scale Height Midplane Temperature Kepler Frequency Interest of the Gas inside the PPD Radial Profile of Gas Density
	3.3	3.1.6 Prope 3.2.1 3.2.2 Prope 3.3.1 3.3.2 3.3.3 3.3.4 Prope 3.4.1 3.4.2	Necessary Simplifications What do we need to define? Inties of the Star at the Center of the PPD Age Mass Ties of the PPD Introduction Disk Scale Height Midplane Temperature Kepler Frequency Ties of the Gas inside the PPD Radial Profile of Gas Pressure

	3.5	Properties of the Dust inside the PPD	30
		3.5.1 Stokes Number	30
		3.5.2 Reynold's Number	31
		3.5.3 Stopping Time	32
	3.6	Location in Disk	33
	3.7	Total Disk Mass Calculation	33
4	Def	finition of a simplified Model for Dust Coagulation	34
	4.1	Ensemble Approach	34
		4.1.1 QUES How can particle collisions be modeled?	34
		4.1.2 QUES What is a particle distribution function?	35
		4.1.3 QUES What is the dust particle distribution function?	35
		4.1.4 QUES Assumptions needed for the (naive/simple) particle mass distribution	35
		4.1.5 QUES What is the dust particle mass distribution function?	36
		4.1.6 QUES What happens when particles collide? (from standpoint of particle mass distr.)	37
	4.2	The Dust Particle Mass Distribution Function	37
		4.2.1 Initialization	38
		4.2.2 Normalization	39
	4.3	The Smoluchovski Coagulation Equation	40
		4.3.1 QUES What is the Smoluchovski coagulation equation?	40
		4.3.2 QUES What is the coagulation kernel?	40
		4.3.3 Smoluchovski Coagulation Equation	41
5	Disc	cretization of the Dust Coagulation Model	42
	5.1	Introduction, Overview, & Goals for this Section	42
	5.2	Discretization of the Mass Axis	43
		5.2.1 QUES Why do we even need to discretize at all?	43
		5.2.2 QUES How to discretize the mass axis in a linear fashion?	43
		5.2.3 Discretization of the Mass Axis	44
	5.3	Discretization of the Particle Mass Distribution Function	50
		5.3.1 QUES How to discretize the dust particle mass distribution function?	50
		5.3.2 Discretization	51
	5.4	Discretization of the Smoluchovski Coagulation Equation	51
		5.4.1 QUES How to discretize the Smoluchovski equation?	51
	5.5	Initialization of the Particle Mass Distribution Function	52
		5.5.1 QUES How to initialize the particle mass distribution function?	52
	5.6	Integration of the Smoluchovski Equation	53
		5.6.1 QUES How to discretize the time axis in a linear fashion?	53
		5.6.2 QUES What is the difference between additive/multiplicative incrementation of time	53
		5.6.3 QUES How to integrate the Smoluchovski equation using an explicit Euler scheme?	53
		5.6.4 QUES How to discretize the time axis in a logarithmic fashion?	54
		5.6.5 QUES How to integrate the Smoluchovski equation using implicit schemes?	54
6	Con	nstruction of the Kernel for Simple Hit-and-Stick Coagulation	5 5
	6.1	Introduction, Overview, & Goals for this Section	55
		6.1.1 Construction of a Kernel for Hit-and-Stick Coagulation	55
	6.2	Definition of the Kernel for simple Stick-and-Hit Coagulation	56
		6.2.1 QUES How to implement stick-and-hit coagulation on a linear mass axis?	56
	6.3	Numerical Integration with the Explicit Euler Scheme	57
		6.3.1 QUES Why does the mass error increase over time? -> "Mass Outflow"	57

		6.3.2 6.3.3	Hit-and-Stick Collision on Linear Mass Grid	58 58		
7	Imp	Implementation of a Logarithmic Mass Axis Representation				
	7.1	Introd	uction, Overview, & Goals for this Section	59		
	7.2		ns for Making Use of a Logarithmic Representation	59		
	7.3		nges Associated with a Logarithmic Representation	59		
	7.4	Defini	tion of the Logarithmic Mass Axis	59		
		7.4.1	QUES How to discretize the mass axis in a logarithmic fashion?	59		
	7.5		mentation of the Kovetz-Olund algortihm	60		
		7.5.1	Reasons for the Necessity of the Kovetz-Olund Algorithm	60		
		7.5.2	Implementation of the Kovetz-Olund Algorithm	60		
	7.6	_	mentation of Near-Zero-Cancellation Handling for Coagulation	62		
		7.6.1	QUES What is Near-Zero-Cancellation and where can it occur in general?	62		
		7.6.2	QUES Where can Near-Zero-Cancellation occur in our model?	62		
		7.6.3	Handling Near-Zero-Cancellation for Stick-and-Hit Coagulation	62		
8			of Fragmentation Processes into the Kernel	63		
	8.1	,	Simple/Naive Attempt"	63		
	0.0	8.1.1	QUES How to implement naive fragmentation?	63		
	8.2		IRN Distribution	64 64		
		8.2.1 8.2.2	QUES How to implement MRN distribution (for initialization):	64		
		8.2.3	QUES Test integration speed with MRN distribution enabled. Is there a slowdown?	65		
	8.3		ementation of Near-Zero-Cancellation Handling for Fragmentation" (?)	65		
9	Defi	Definition of a the Dust Particle Reaction Rates				
•	9.1		tion of the Dust Particle Reaction Rates	66		
	9.2		tion of the Dust Particle Collision Rates	67		
		9.2.1	QUES How to define the particle collision rate?	67		
	9.3	Defini	tion of the Collision Cross Section	68		
		9.3.1	QUES How to implement realistic collision cross sections?	68		
	9.4	Defini	tion of the Relative Particle Velocity	69		
		9.4.1	QUES How to implement realistic relative velocities between dust particles?	69		
10	Calo	culatio	n of the Relative Dust Particle Velocities	7 0		
			tion of the Relative Velocity due to Radial Drift	70		
			tion of the Relative Velocity due to Differential Settling	72		
			tion of the Relative Velocity due to Brownian Motion	73		
			tion of the Relative Velocity due to Turbulence	74		
			tion of the Azimuthal Relative Velocity	75		
	10.6	Total	Relative Velocity	76		
11	Imp	lemen	tion of Stochastic Kernel Sampling	77		
12	Sun	nmary	of Results	7 8		
13	The	sis Dis	scussion & Outlook	7 9		
14		endix		80		
	14.1	Glossa	TV	80		

14	4.2 Testing: Can I use <i>subfigures</i> for "multicol" LATEX plots in Emacs org-mode?	80						
15 References								
List	of Figures							
1	plots of	80						
List	of Tables							

- 1 Preface
- 1.1 Acknowledgements

1.2 Abstract

What is the topic of this thesis?

- We want to test whether the numerical integration of the Smoluchovski coagulation equation can be sped up via stochastic sampling of the kernel.
- Depending on how accurate one wants to model the involved processes, the integration of the coagulation equation can become quite costly (from a computational standpoint).
- This is due to the "high dimensionality" of the problem.
 - 3 dimensions of space (in principle)
 - 3 dimensions of mass (explain why -> fragmentation)
 - X dimensions of porosity
 - + maybe other attributes of the dust particles
- Therefore, the idea is that a big gain in computational performance could be gained by only including the "relevant" parts of the kernel into the integration. ("relevant" according to what criterion?)
- Finding out whether this works (and by how much the computational cost can be reduced) is the big goal of this thesis.

2 Introduction

2.1 Proto-Planetary Disks & their Formation

2.1.1 Material Composition of the Interstellar Medium

The interstellar medium consists mainly of low-mass particles, which can be categorized into

- 1. atomic gas (mostly atomic hydrogen & helium), and (to a lesser extent)
- 2. larger dust particles (characterized mainly by their mass & porosity) [citations needed]

2.1.2 Collapse of Interstellar Gas Clouds into a Disk

- Why does it even happen?
 - A cloud of gas/dust collapses under its own gravity.
- What happens?
 - The cloud flattens out into a disk.
- Why does the cloud flatten out?
 - Angular momentum is conserved.
 - There is a most likely a non-zero *total* angular momentum. When an object is hit, and it's not hit *exactly* in the center, it starts to spin.
 - Gravity pulls the particles inwards, but rotation (centrifugal/centripetal forces) opposes gravity.
 - Thus, a disk is formed.

2.1.3 Star Formation at the Disk Center

- gravity \rightarrow high pressure \rightarrow nuclear fusion

2.1.4 Spatial Structure of Proto-Planetary Disks

QUES: Talk about

- approximately (first-order) circular shape of a PPD,

- disk flaring, midplane, ...

- ...

QUES: Include pictures: observations.

QUES: Include pictures: diagrams/graphs of simplified disk.

2.1.5 Material Composition of Proto-Planetary Disks

- It's made of the same material that made up the original cloud.
- This is mostly gas, and a little bit of dust.

Most of the mass inside PPDs is concentrated inside the star at its center. [citation needed]

- We can take a (kind of random) look at our own solar system, where [how much? I believe about 99] percent of the mass is concentrated inside the Sun.

QUES: Find data/sources about mass distribution inside PPDs.

The model used in this thesis will be based on the assumption that this is the case. Let M_* label the stellar mass, and M_{disk} label the disk mass.

Then, we can define a "disk-to-star" mass ratio, which we label $q_{\rm dts}$. If not otherwise stated, the value of this ratio will be assumed to be...

QUES: Choose value of "disk-to-star" mass ratio.

Let us now turn our attention to the mass not concentrated inside the star, but spread across the protoplanetary disk. It is comprised mostly [citation needed] of atomic/molecular gas (mostly hydrogen & helium) [citation needed] and larger (but still very small [how small?]) dust particles [citation needed].

QUES: Talk about element composition of interstellar medium, and how that translates into the composition of the disk. QUES: Talk about approximate scale of dust particles.

Analogously to before, we can define a "dust-to-gas" mass ratio, which we label $q_{\rm dtr}$.

If not stated otherwise, a value of ... will we used throughout this thesis.

QUES: Talk about how to choose the "dust-to-gas" ratio, cite others.

2.2 Gas & Dust Particles inside PPDs

2.2.1 QUES How to model the gas inside the disk?

What are the most relevant properties of the gas?

- density
- viscosity
- velocity
- ... [QUES]

QUES Write this section

- Give broad overview
 - More detail can be given later.

2.2.2 QUES What characterizes a dust particle?

A dust particle has the following attributes:

Particle position:

- This can be given either
 - in cartesian coordinates (x, y, z), or
 - in cylindrical coordinates (r, φ, z) .
- Due to the (approximately) circular shape of the disk, cylindrical coordinates are the more fitting choice here.

Particle velocity:

- Analogously to the particle position, the preferred system of coordinates is a cylindrical one here.
- Thus, we write the particle velocity as (v_r, v_{φ}, v_z) .

Particle mass:

- In a very naive/simple model, the particles are assumed to
 - be perfectly spherical (with radius a), and
 - share a common solid density ρ_s .
- This is of course not the case in reality, but we will make this assumption throughout the thesis (if not otherwise stated.)
- Thus, the particle mass m can be calculated directly from the particle radius. The two quantities are related by the equation

$$m = \frac{4}{3}\pi a^3 \cdot \rho_s$$

Time:

- With the exception of the particle mass, all of the quantities discussed above can not assumed to be constant with time (in this model -> in reality, none of them are constant).
- Thus, the temporal parameter t is included into the model as well.

Porosity:

- (not included in the model)
 - Particles have "fractal-like" shape, not spherical.

QUES:

- Think re:
 - Only list attributes & their labels/symbols here.
 - Make model assumptions elsewhere?

2.2.3 QUES How does the central star influence the disk around it?

- The star exerts its gravitational influence onto the disk.
 - As a first order approxmiation, the matter in the disk moves around the star on Keplerian trajectories.
- The lighter particles in the disk move on sub-Keplerian trajectories though.
 - "This is due to the radiation pressure".

2.2.4 QUES How does the gas affect the dust?

- The sub-Keplerian motion of the gas leads to a non-zero relative velocity between gas and dust particles.
 - This results in a drag force acting on the dust particles.
 - Therefore, the dust particles are "slowed down" and spiral inwards.

2.2.5 QUES What other effects are there?

TODO: Talk about (relative) velocity components.

2.2.6 Gas Kinematics inside PPDs

2.2.7 Dust Kinematics inside PPDs

2.3 Planet Formation inside Proto-Planetary Disks

2.3.1 Particle-Particle Collisions

In a PPD, dust particles move around at

- partly systematic, and
- partly random

velocities.

This includes [QUES: sort this out]

- Keplerian motion
- drag from interaction with gas
- Brownian motion
- radial drift
- turbulence

- ...

This causes the dust particles to occasionally collide with each other.

```
[\dots coagulation\dots] [\dots fragmentation\dots]
```

2.3.2 Particle Coagulation

Coagulation is

- the process of particles sticking together and forming larger bodies
- the most-likely origin of planetary cores [citation needed]
- a complex process
 - coagulation + fragmentation

- ...

How can you model coagulation?

- Smoluchovski equation
- ... [other ansatz?]

2.3.3 Formation of Planetary Cores

2.4 Notes on the Structure of this Thesis

3 Definition of a simplified Radial Model for the Proto-Planetary Disk

3.1 Introduction, Overview, & Goals for this Section

3.1.1 QUES How to formulate a model for the PPD, its contents, & the planet formation processes?

The choice of a model is not at all trivial, and a lot of assumptions will have to be made (in order to not complicate things too much).

This can not be assumed to be a comprehensive and/or physically accurate model. The attempt is to formulate a model that is *good enough* to capture the "behavior [...]" qualitatively, "and even quantitatively in an approximate way".

We assume:

A protoplanetary disk is essentially made up of... [citations needed]

- the star at its center, (We assume it to already have formed.)
- the atomic/molecular gas, and
- the dust.

The disk can be assumed to be (approximately) symmetrical. [citation needed]

- This simplifies the treatment by "not including" the azimuthal direction. [except for rel. vel., there it is included!]
- The [later introduced] particle distribution function does not depend on φ .

We have to think about...

- 1. how the mass is distributed inside the disk, i.e.
 - the ratio between stellar mass & gas/dust mass,
 - the ratio between gas & dust mass.
- 2. how to model the gas, i.e.
 - its relevant properties (and how their are distributed radially)
 - densities, viscosities, sound speed, [...]
 - kinematics (velocities, relative velocities -> collisions -> coagulation)
 - . . .
- 3. how to model the dust.
 - interaction with the gas
 - interaction with other dust [-> coagulation]

QUES:

- Talk more about the central star. If it has already formed...
 - then when are we?
 - how old is the disk already?

3.1.2 QUES How to model the central star?

What do we need to define?

- Stellar mass
 - Default:

$$M_{\rm star} = 1 \cdot M_{\odot}$$

- Stellar luminosity
 - Default:

$$L_{\rm star} = 1 \cdot L_{\odot}$$

- 3.1.3 QUES How to model the gas?
- 3.1.4 QUES How to model the dust?

3.1.5 Necessary Simplifications

- PPD is a 3D object.
 - This is too complex to model fully.
 - We will take advantage of symmetries.
 - This is of course a big simplification.
 - It is assumed that the model is still sophisticated enough to arrive at realistic results. (TODO: Argue why this is possible.)
- In reality, disk properties are functions
 - f(x, y, z) of the three cartesian coordinates, or
 - $f(r, \phi, z)$ in cylindrical coordinates. (TODO: Elaborate on meaning of variables.)
- Simplifications
 - 1. Assume radial symmetry.

$$f(r,\phi,z) \rightarrow f(r,z)$$

(TODO: Explain why one can do this.)

2. Integrate vertically.

$$f(r,z) \rightarrow f(r)$$

(TODO: Explain why one can do this.)

- As such, the disk model used in this thesis depends only on the radial coordinate r. This is of course a very simplified model making use of a rather big assumption. (TODO: Explain for what this is good enough, and where it may fall short.)

3.1.6 What do we need to define?

- Properties of central star
- Properties of disk
- Location inside the disk (loc. of "measurement")

3.2 Properties of the Star at the Center of the PPD

- 3.2.1 Age
- 3.2.2 Mass

3.3 Properties of the PPD

3.3.1 Introduction

What do we need to define?

- Disk mass
 - Default:

$$M_{\rm disk} = q_{m, \rm disk} \cdot M_{\rm star}$$

- Ratio of disk mass to stellar mass
 - Default:

$$q_{m,\text{disk-to-star}} = 0.01$$

- Ratio of dust to gas
 - Default:

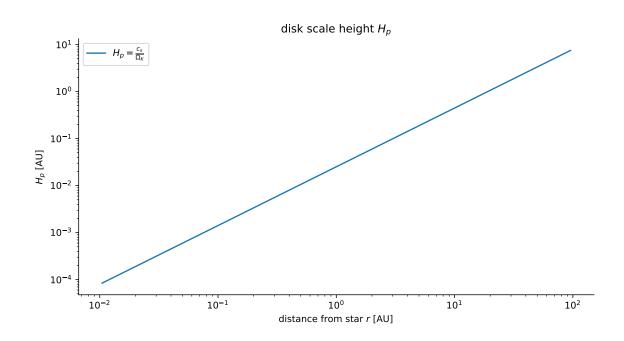
$$q_{m,\text{dust-to-gas}} = 0.01$$

- Flaring Angle of Disk
 - Default:

$$\alpha_{\rm fl} = 0.05 \text{ rad}$$

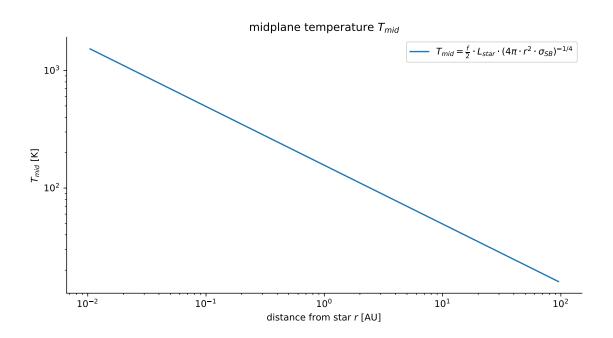
3.3.2 Disk Scale Height

$$H_p = \frac{c_s}{\Omega_K}$$



3.3.3 Midplane Temperature

$$\sigma_{\rm SB} \cdot T^4 = \frac{\alpha_{\rm fl}}{2} \cdot L_{\rm star}$$



1. Derivation Flux at distance r from star:

$$B(r) = \frac{\alpha_{\rm fl}}{2} \frac{L_{\rm star}}{4\pi r^2}$$

Now use Stefan-Boltzmann law:

$$B(T) = \sigma_{\rm SB} \cdot T^4$$

Midplane temperature at distance r from star:

$$T_{\text{mid}} = \left[\frac{B(r)}{\sigma_{SB}}\right]^{1/4}$$
$$= \left[\frac{\alpha_{\text{fl}}}{2} \cdot \frac{L_{\text{star}}}{4\pi r^2 \cdot \sigma_{\text{SB}}}\right]^{1/4}$$

Rearrange for $T_{\rm mid}$ to arrive at the above definition.

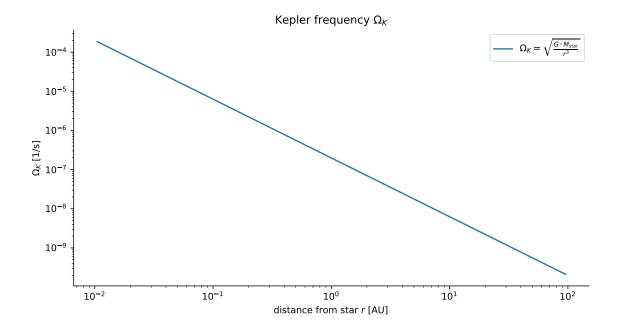
3.3.4 Kepler Frequency

Kepler velocity:

$$v_K = \sqrt{\frac{GM_*}{r}}$$

Kepler frequency:

$$\Omega_K = \sqrt{\frac{GM_*}{r^3}}$$



3.4 Properties of the Gas inside the PPD

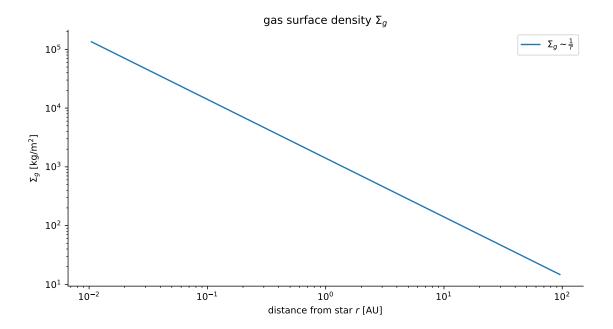
3.4.1 Radial Profile of Gas Density

1. Gas Surface Density How is it defined?

$$\Sigma_g = \int_{-\infty}^{\infty} \rho_g(z) \, \mathrm{d}z$$

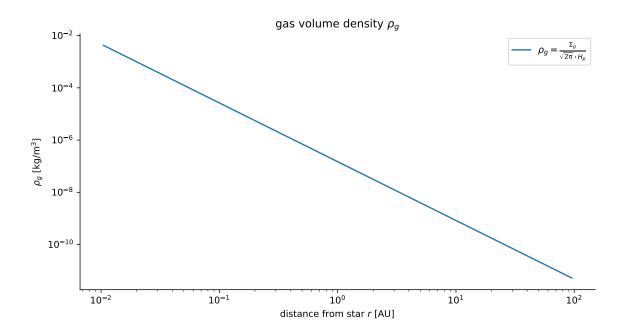
How can it be written as a function of the distance to the star? Ansatz: Use a power law, such that

$$\Sigma_g \sim \frac{1}{r^k}$$



2. Gas Volume Density

$$\rho_g = \frac{1}{\sqrt{2\pi}} \frac{\Sigma_g}{H_p}$$



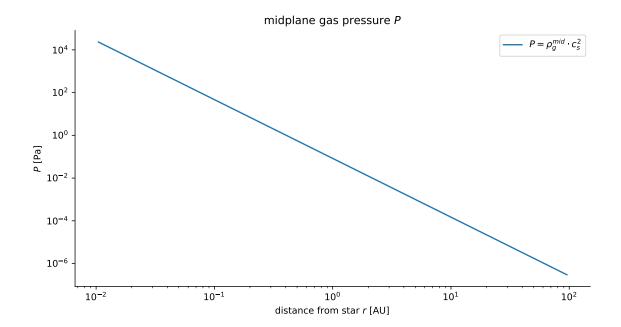
3. Gas Volume Number Density

$$n_g = \frac{\rho_g}{2.3 \cdot m_{\rm p}}$$

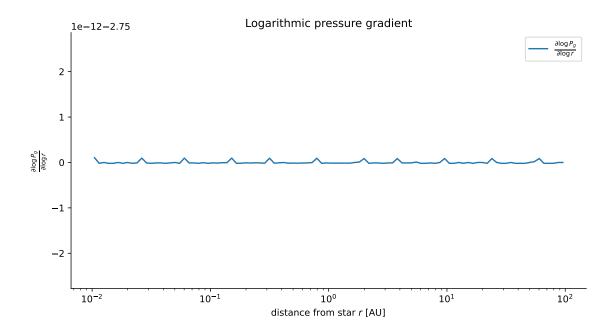
3.4.2 Radial Profile of Gas Pressure

1. Midplane Gas Pressure

$$P_g = \rho_g \cdot c_s^2$$



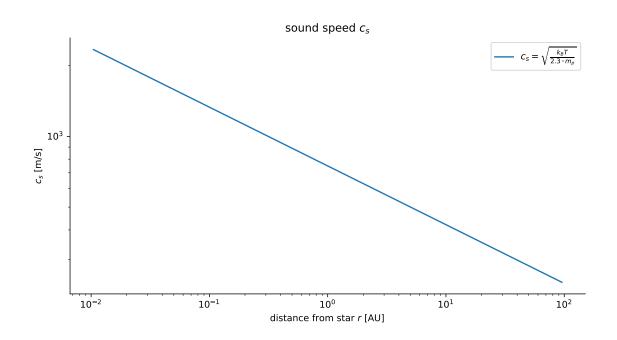
2. Gas Pressure Gradient



3.4.3 Thermal Speed & Sound Speed

1. Sound Speed

$$c_s = \sqrt{\frac{k_B \cdot T_{\text{mid}}}{2.3 \cdot m_{\text{p}}}}$$



(a) Derivation

$$2.3 \cdot m_{\rm p} \cdot c_s^2 = k_B \cdot T_{\rm mid}$$

Why though?

2. Mean Thermal Velocity of Gas Particles

$$u_{\rm th}\bar{v} = \sqrt{\frac{8}{\pi}} \cdot c_s$$

3.4.4 Gas Molecular Viscosity

$$\nu_{\rm mol} = \frac{\bar{u} \cdot \lambda_{\rm mfp}}{2}$$

3.4.5 Mean Free Path

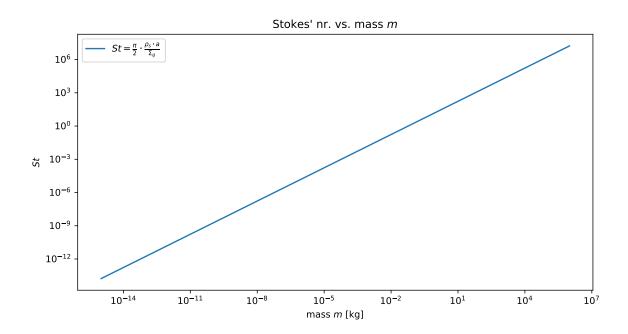
$$\lambda_{\rm mfp} = \frac{1}{n_g \cdot \sigma_{\rm H_2}}$$

with

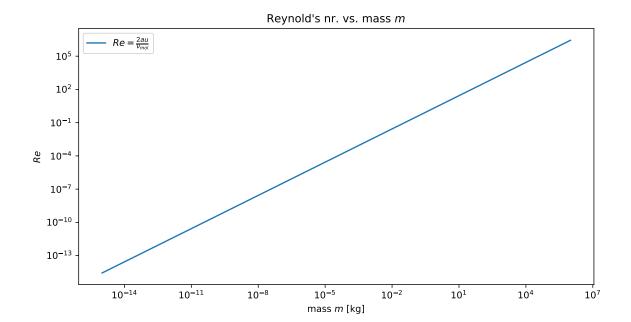
- (volume) particle number density

3.5 Properties of the Dust inside the PPD

3.5.1 Stokes Number



3.5.2 Reynold's Number



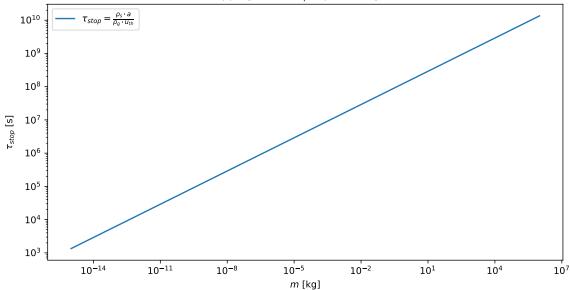
3.5.3 Stopping Time

= the ratio of the momentum of a particle divided by the drag force acting on it.

$$\tau_{\rm s} = \frac{mv}{F_d}$$

$$\tau_s = \begin{cases} \frac{\rho_s a}{\rho_g \overline{u}} & \text{for } \lambda_{\text{mfp}}/a \gtrsim \frac{4}{9} \\ \frac{2\rho_s a^2}{9\nu_{\text{mol}}\rho_g} & \text{for Re} < 1 \\ \\ \frac{2^{0.6}\rho_s a^{1.6}}{9\nu_{\text{mol}}^{0.6}\rho_g^{1.4}u^{0.4}} & \text{for } 1 < \text{Re} < 800 \\ \\ \frac{6\rho_s a}{\rho_g u} & \text{for Re} > 800 \end{cases}$$





3.6 Location in Disk

What do we need to define?

- Coordinate system: Cylindrical.
- Radial distance to star r
 - Default:

r=10 au

- Vertical distance above midplane
 - TODO
- Azimuthal angle
 - Assume radial symmetry \rightarrow no dependence on azimuthal angle.

3.7 Total Disk Mass Calculation

4 Definition of a simplified Model for Dust Coagulation

4.1 Ensemble Approach

4.1.1 QUES How can particle collisions be modeled?

["ensemble approach"]

[...]

- Particle collisions can be modeled using the Smoluchovski equation.

[...]

4.1.2 QUES What is a particle distribution function?

- Consider a distribution of particles.
- Let the particles have various different properties, e.g. position, velocity, and mass.
- Assume these properties to *not* be distributed homogenously among the particles.
- The distribution can then be described by a fitting particle distribution function

$$f(...) = ...$$

QUES: Continue writing this section.

- What is a particle distribution function *generally*?

4.1.3 QUES What is the dust particle distribution function?

QUES: Apply the definition of a general particle distribution function (from above) to the (special) case of a protoplanetary disk.

- We assumed the relevant properties to be
 - radial position in the disk (radial distance from star)
 - height above the midplane
 - particles mass
- These properties (in general) depend on time.

Therefore, we can write the distribution function for dust particles inside the modeled PPD as

- NOTE:
 - After this section, focus (for now) on naive/simple particle mass distribution function.

4.1.4 QUES Assumptions needed for the (naive/simple) particle mass distribution.

Consider a distribution of dust particles with different masses m.

- Let them all have the same material density ρ_s (and other properties).
- Also, (for now) assume that their shape is always spherical.

Then, each dust particle is characterized solely by its mass, and hence its radius a:

$$m = \frac{4\pi}{3}\rho_s a^3$$

4.1.5 QUES What is the dust particle mass distribution function?

The particle mass distribution function n(m) is defined in such a way that the integral

$$N = \int_0^\infty n(m) \, \mathrm{d}m$$

is the total number of dust particles per unit volume.

Following from that, the integral

$$\rho = \int_0^\infty m \cdot n(m) \, \, \mathrm{d}m$$

gives the total dust mass per unit volume, i.e. the dust density.

4.1.6 QUES What happens when particles collide? (from standpoint of particle mass distr.)

Collisions can be regarded as two-body collisions:

- The occurrence of three-body interactions is so tiny that it can be neglected entirely (negligible).

Outcomes:

- 1. bouncing
- 2. merging
- 3. fragmentation

Bouncing:

- Here: The only property we trace is the particle mass.
- Therefore, "nothing happens".

Merging:

- The two original particles with masses m_1 and m_2 "disappear".
- A single new particle with mass $m_{\text{tot}} = m_1 + m_2$ "appears".

Fragmentation:

- The two original particles with masses m_1 and m_2 also "disappear".
- But: A whole series/range of particles can appear, with a total mass of $m_{\rm tot}=m_1+m_2$

The input to a collision event are therefore always two bodies, but the output can be any number of particles.

4.2 The Dust Particle Mass Distribution Function

- Continuous
- Let n(m) be the particle mass distribution function, i.e. the number of particles per unit volume that possess a mass m.
- Total number of particles per unit volume:

$$N = \int_0^\infty n(m) \, \mathrm{d}m$$

- Total mass per unit volume: (mass density)

$$\rho = \int_0^\infty m \cdot n(m) \, \mathrm{d}m$$

- Total disk mass: (correct?)

$$m_D = \int_0^{2\pi} \int_0^{\infty} \int_{-\infty}^{\infty} \rho \, d\phi \, dr \, dz$$

4.2.1 Initialization

1. Dirac-delta Together with the normalization criterion from above, the Dirac-delta distribution δ_D is defined by the condition

$$\delta_D(x) = 0 \ \forall x \neq 0$$

Assuming all particles have a starting mass m_0 , we can write the initial discrete mass distribution function as

$$N_i = \delta_D(m_i - m_0)$$

2. Gaussian The Gaussian distribution f_{Gauss} is given by

$$f_{\text{Gauss}}(x) = \frac{1}{\sigma\sqrt{2\pi}} \cdot \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right)$$

Here, μ labels the "expectation value" around which the distribution is centered, and σ^2 is the variance distribution's variance ("width").

Assuming a Gaussian state in the beginning of the simulation, the initial discrete mass distribution function can then be written as

$$N_i = f_{\text{Gauss}}(m_i)$$

3. Flat (homogenous) Choose N_i in such a way that

$$N_i = C \quad \forall i$$

with a constant C.

The normalization condition leads to

$$C = \frac{1}{\mathcal{N}_m}$$

and thus also

$$N_i = \frac{1}{\mathcal{N}_m}$$

4. "True Flat" Choose N_i in such a way that

$$m_i \cdot N_i = C \quad \forall i \in [0, \mathcal{N}_m - 1) \cap \mathbb{N}$$

with a constant $C \in \mathbb{R}$.

This leads to

$$N_i = \frac{C}{m_i}$$

Before we can construct the discretized initial particle density distribution function though, we need to find out what C is. A constraint for this is given by the normalization condition

$$1 = \sum_{i=0}^{N_m - 1} N_i$$

Plugging in and rearranging for C leads to

$$C = \frac{1}{\sum_{i=0}^{N_m - 1} \frac{1}{m_i}}$$

4.2.2 Normalization

All of the following distributions (here labeled f) are normalized in such a way that the condition

$$\int_{-\infty}^{\infty} f(x) \, \mathrm{d}x = 1$$

holds. This then assures that the total disk mass

$$\sum_{i=0}^{\mathcal{N}_m - 1} N_i = 1$$

is equal to unity (bounded, not too large, easy conservation-checking). [Is this correct?]

- 1. NOTE (delete later)
 - x labels the values m_i of the discretized mass grid.
 - f(x) labels the discretized particle mass distribution function

$$N_i = \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} n(m) \, \mathrm{d}m$$

4.3 The Smoluchovski Coagulation Equation

4.3.1 QUES What is the Smoluchovski coagulation equation?

The general time evolution of the particle mass distribution function due to collision can (by virtue of the two-body nature) be expressed using the Smoluchovski coagulation equation.

... background ... [1916 Smoluchovski]

The coagulation equation reads

$$\frac{\mathrm{d}n}{\mathrm{d}t}(m,t) = \int_0^\infty \int_0^\infty K(m,m',m'') \cdot n(m',t) \cdot n(m'',t) \, \mathrm{d}m' \, \mathrm{d}m''$$

Here, K(m, m', m'') labels the "so-called" coagulation kernel.

This general form of the (temporal) evolution equation of the particle mass distribution function encompasses all possible collision outcomes (bouncing, merging, fragmentation).

The Smoluchowski coagulation equation is a (nonlinear?) integro-differential equation. It is used to model the evolution of system in which particles undergo aggregation.

4.3.2 QUES What is the coagulation kernel?

- NOTE:
 - Stay very general/"vague" here.
 - Details will follow in sections on stick-and-hit / fragmentation.
- First problem to look at:
 - simple case of Stick-and-Hit coagulation
- But before we do that, we need to talk about discretization...
 - discretization of mass axis
 - discretization of dust particle (mass) distribution function
 - discretization of kernel
 - discretization of time axis
- ... and about numerical integration of the Smoluchovski equation
 - for that, we need to talk about discretization of the time axis

4.3.3 Smoluchovski Coagulation Equation

A commonly-used method of formulating a general description for the temporal evolution of a protoplanetary disk's particle mass distribution is given by the Smoluchovski coagulation equation:

$$\frac{\partial n(m,t)}{\partial t} = \int_0^\infty \int_0^\infty K(m,m_1,m_2) \cdot n(m_1,t) \cdot n(m_2,t) \, dm_1 \, dm_2$$

Here, $K(m, m_1, m_2)$ labels the *coagulation kernel*, into which all information on the collisional dynamics is encoded. It summarizes all aspects of the collisions.

- integro-differential equation, population balance equation
- introduced by M.V. Smoluchovski in 1916
- can be used to determine the temporal evolution of the number density per mass n(m) of particles as they coagulate.

- 5 Discretization of the Dust Coagulation Model
- 5.1 Introduction, Overview, & Goals for this Section

5.2 Discretization of the Mass Axis

5.2.1 QUES Why do we even need to discretize at all?

Due to the discrete nature of number representation on computers, for numerical treatment it is necessary to move away from the continuous representation of the mass grid, the evolution equations, and the coagulation kernel. Instead, a discrete analogon has to be constructed.

5.2.2 QUES How to discretize the mass axis in a linear fashion?

- Here: The relevant dimension is that of mass.
 - We look at the distribution of differently-sized particles in the disk, and how that distribution (defined on the mass axis) changes with time.
- In reality, the involved scales for the masses of particles in the disk range from those of individual atoms up to those of planets.
 - I.e., approximately from 1 proton mass to 1 Jupiter mass. That's quite the range!
 - In this thesis, we will limit this range, since we're specifically interested in the evolution of the distribution of dust particles.
 - Let m_{\min} and m_{\max} label the minimum and maximum masses "relevant to our discussion", respectively. TODO: Define minimum & maximum mass relevant for dust.
 - Therefore it will not make sense to use a linear representation of the mass axis, since "small masses will be under-, and large masses overrepresented". TODO: Is the sentence about overrepresentation correct?
- Let's not get ahead of ourselves & start with a very simple/basic model:
 - We will start off by discretizing the mass axis in a linear fashion.
 - Therefore, we will "split" the axis into a number of "grid points" / "bins".
- Let \mathcal{N}_m label the number of grid points.
 - TODO: Decide: Is N_m the number of grid points, or the number of bins? Be consistent here!
- TODO: Define the grid spacing.

5.2.3 Discretization of the Mass Axis

1. Introduction

- The continuous range of masses inside the disk is partitioned into $\mathcal{N}_m \in \mathbb{N}$ "bins".
- Change in notation: Use indices to label the mass grid bins:

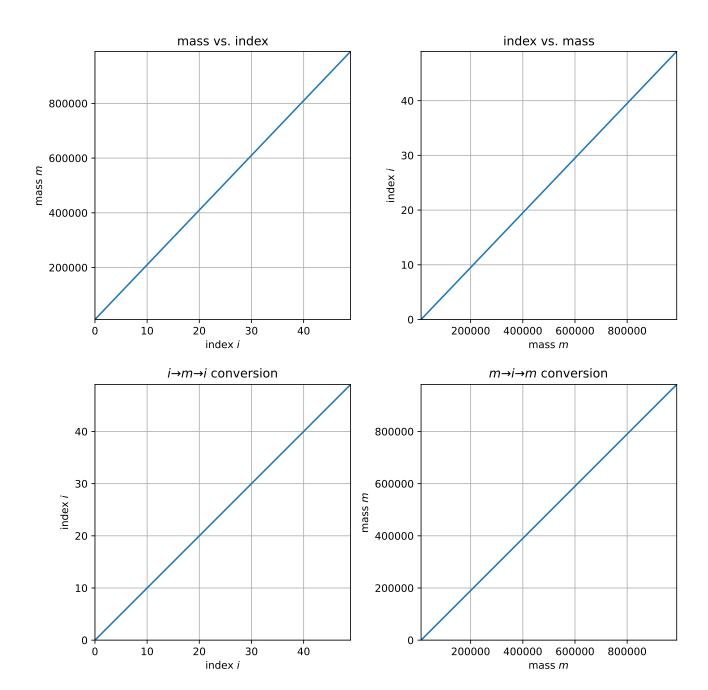
$$m \to m_i$$
 with $i \in \mathbb{N} \cap [0, \mathcal{N}_m)$

- For the lower & upper boundaries of the resulting mass grid, an appropriate choice of a minimum mass value m_{\min} and maximum mass value m_{\max} has to be made.

- 2. Discretization of the Mass Axis on a Linear Scale
 - Pro: Simpler to implement than logarithmic grid.
 - Con: Under-representation of small, over-representation of large masses.
 - Later: Logarithmic, better representation of all orders of magnitude.
 - The bins are defined in such a way that the boundaries are centered around the mass m_i . The lower and upper boundaries of a bin with index i are then given by the masses $m_{i-1/2}$ and $m_{i+1/2}$.
 - In the linear case, the "width" of each bin is given by

$$m_{i+1/2} - m_{i-1/2} = \frac{m_{\text{max}} - m_{\text{min}}}{\mathcal{N}_m}$$

- Note that this width is constant across all bins, independent of their labeling indices. This will change once the switch to a logarithmic grid is made. [...]
- 3. Mass-Index Conversion on Linear Scale



- 4. Discretization of the Mass Axis on a Logarithmic Scale
 - As above, \mathcal{N}_m is used to label the number of bins, and the grid boundaries are labeled m_{\min} and m_{\max} to signify the lower and upper bound of the grid, respectively,
 - In contrast to the linear grid, the "width", i.e. additive offset from one bin to the next is not the same for all bins in the logarithmic grid.
 - Instead, the relative mass increase from one mass grid point to the next is what stays the same for all bins i.
 - The factor describing this relative mass increase is labeld q_m . It has to be chosen in such a way as to satisfy the conditions

$$m_{i+1} = q_m \cdot m_i$$

$$m_{\max} = m_{\min} \cdot (q_m)^{\mathcal{N}_m}$$

- This leads to the expression

$$q_m = \sqrt[N_{
m grid}]{rac{m_{
m max}}{m_{
m min}}}$$

- 5. Mass-Index Conversion on Logarithmic Scale
 - (a) Index to Mass With the above definition of the relative mass increase q_m from one grid point to the next, the conversion from index to mass becomes trivial. It can be described by

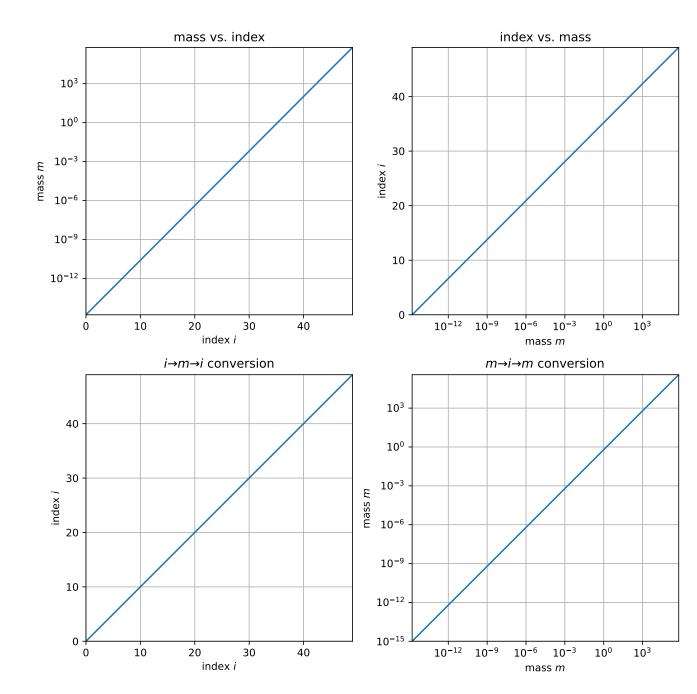
$$m(i) = m_{\min} \cdot q_m^i$$

(b) Mass to Index To arrive at a description for the inverse conversion from mass to index, we simply rearange the above for *i*. The resulting law can then be written as

$$i(m) = \frac{1}{\log(q_m)} \cdot \log\left(\frac{m_i}{m_{\min}}\right)$$

Here, attention needs to be given to one additional step: Since the resulting i is not necessarily an integer, the right-hand side of the above equation needs to be "floored" (integer division).

[explain: why nearest-lower index, not upper? just convention?]



6. "Things to Watch out for" When switching from a linear representation of the mass grid to a logarithmic representation one, several points need to be addressed to guarantee both stability and accuracy of the algorithm.

For hit-and-stick collisions:

- (a) Mass conservation [rename section?] In a merge event, the masses corresponding to the two colliding particles have to be removed from the mass distribution, and exactly one new particle has to be added. It is important that this particle's mass is exactly equal to the sum of the two colliding particles' masses, to ensure conservation of mass.
- (b) "Non-integer indices of resulting mass" [rename section] In a merge event between two masses m_i and m_j , the resulting mass

$$m_{\rm res} = m_i + m_j$$

does not necessarily correspond exactly to any of the mass grid points.

Instead, m_{res} typically lies somewhere in between two grid points. In this case, the mass thus has to be divided between the nearest neighboring grid points in some sensible way.

Let the nearest neighbors in the grid be labeled by the indices k and k+1, with m_k being the mass point just below the mass resulting from the merge event, and m_{k+1} the mass point just above, such that

$$m_{\bar{k}} < m_{\rm res} < m_{\bar{k}+1}$$

i.e.

$$m_{\bar{k}} \le m_i + m_j < m_{\bar{k}+1}$$

5.3 Discretization of the Particle Mass Distribution Function

5.3.1 QUES How to discretize the dust particle mass distribution function?

$$n_i := n(m_i)$$

To be more specific, the current time value should be included into the notation as well. We define:

$$n_{i,\xi} := n(m_i, t_{\xi})$$

5.3.2 Discretization

Just as we discretized the range of masses, so we also have to discretize the particle mass distribution function. For this, we define:

$$n_i := n(m_i)$$

The number of particles per unit unit volume in bin i is then calculated by integration over the particle mass distribution function from the lower to the upper bin boundary:

$$N_i = \int_{m_{i-1/2}}^{m_{i+1/2}} n(m) \, \mathrm{d}m$$

The mass density ρ_i in the bin i is given by

$$\rho_i = \int_{m_{i-1/2}}^{m_{i+1/2}} m \cdot n(m) \, dm$$

To arrive at the total mass density independent of particle mass, one has to sum over all bins:

$$\rho = \sum_{i=0}^{\mathcal{N}_m - 1} \rho_i$$

5.4 Discretization of the Smoluchovski Coagulation Equation

5.4.1 QUES How to discretize the Smoluchovski equation?

With $i, j \in \mathbb{N}$ "being indices":

$$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \sum_{i=1}^{N_m} \sum_{j=1}^{N_m} K_{kij} \cdot n_i \cdot n_j$$

Equivalent formulation: [which one to use? I like the lower one <3]

$$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \sum_{i=0}^{N_m - 1} \sum_{j=0}^{N_m - 1} K_{kij} \cdot n_i \cdot n_j$$

5.5 Initialization of the Particle Mass Distribution Function

5.5.1 QUES How to initialize the particle mass distribution function?

Now, let us turn our attention to the initialization of the particle mass distribution function.

Options:

- 1. Dirac-delta distribution
- 2. MRN distribution

What would be best?

- MRN is more physical than Dirac-delta. (see later chapter)
- It does not *really* make that much of a difference though.
- The information about the initialization is quickly lost anyways.
- Both 1. & 2. qualitatively lead to the same results (even if not quantitatively).

Observation:

- Using the MRN distribution leads to a significant slowdown of the integration. (minutes, instead of seconds)
- This might be because I chose $m_{\rm max}$ to be the largest mass grid bin.
 - Do not do this!
 - This is unphysical!
 - Instead use $\approx 0.5 \mu \mathrm{m}$
- Test whether this problem persists!

5.6 Integration of the Smoluchovski Equation

5.6.1 QUES How to discretize the time axis in a linear fashion?

Let the temporal domain be divided into \mathcal{N}_t discrete "bins". Then, let ξ be the index used to uniquely identify each time step, i.e.

$$\xi \in \mathbb{N} \cap [0, \mathcal{N}_m - 1]$$

When discretizing the time axis in a linear way, this leads to

$$t_{\xi} = t_0 + \xi \cdot \Delta t$$

Here, t_0 labels the time value at the start of the simulation (can be set to $t_0 = 0$ without loss of generality), and Δt labels the size of each time step.

The step size needs to be chosen sufficiently small as to assure stability of the integration scheme.

[...CFL criterion...] [...implicit integration...]

5.6.2 QUES What is the difference between additive/multiplicative incrementation of time

- TODO: Move?
- 1. Additive time-steps
 - straightforward approach
 - incrementation of time via

$$t_{n+1} = t_n + \Delta t$$

- 2. Multiplicative time-steps
 - more appropriate here [explain why]

$$t_{n+1} = t_n \cdot q_t$$

5.6.3 QUES How to integrate the Smoluchovski equation using an explicit Euler scheme?

As above, we use the notation $n_{i,\xi}$ to label the dust particle mass distribution function evaluated for the mass m_i at a point in time t_{ξ} .

The goal now is to compute the distribution function's value after one additional step in time, i.e. at the time

$$t_{\xi+1} = t_{\xi} + \Delta t$$

This can be done by making use of an explicit Euler integration scheme [when?]. For a sufficiently small time step Δt , we can thus arrive at an approximate expression for the distribution function's updated value via the transformation

$$n_{k,\xi} \to n_{k,\xi} + \Delta t \cdot \frac{\mathrm{d}n_{k,\xi}}{\mathrm{d}t}$$
$$= n_{k,\xi} + \Delta t \cdot \sum_{i=0}^{N_m - 1} \sum_{j=0}^{N_m - 1} K_{kij} \cdot n_i \cdot n_j$$

If the step size is chosen too large, the method will break down due to the insufficient stability properties of the explicit Euler integration scheme.

Instead, [...implicit Euler/Radau...] [see above]

5.6.4 QUES How to discretize the time axis in a logarithmic fashion?

As the temporal domain spans over multiple orders of magnitude for the processes involved in planet formation, it makes sense to discretize the time axis in a logarithmic fashion. [write this differently?]

[...]

5.6.5 QUES How to integrate the Smoluchovski equation using implicit schemes?

6 Construction of the Kernel for Simple Hit-and-Stick Coagulation

6.1 Introduction, Overview, & Goals for this Section

- Here, we only take a look at the simple case of...
 - ... simple *linear* mass axis discretization.
 - ... simple *Dirac-delta* initialization.
 - ... simple explicit Euler integration.

6.1.1 Construction of a Kernel for Hit-and-Stick Coagulation

Assuming simple hit-and-stick coagulation, the kernel can be written as

$$K(m, m_1, m_2) = \frac{1}{2} \left[\delta(m - m_1 - m_2) - \delta(m - m_1) - \delta(m - m_2) \right] \cdot R(m_1, m_2)$$

Here, the coefficient $R(m_1,m_2)$ labels the collision-and-merging rate.

6.2 Definition of the Kernel for simple Stick-and-Hit Coagulation

6.2.1 QUES How to implement stick-and-hit coagulation on a linear mass axis?

Let us first turn our attention to the simple case of stick-and-hit coagulation: Here, two particles with masses m_1 and m_2 collide, and subsequently merge into a single particle with combined mass $m_{\text{tot}} = m_1 + m_2$.

Let $C(m_1, m_2)$ be the rate at which collisions occur between such a pair of particles. Then, let

$$R(m_1, m_2)$$

label the rate of collision events that lead to a merging of the two particles into a single new one.

Of course, in actuality not every collision leads to a merge event. For simplicity, we will for now will assume that it does. As such, we can write

$$R(m_1, m_2) = C(m_1, m_2)$$

Later on, we will more carefully examine how the collision+sticking rate can be calculated.

[... also talk about definition of collision rate...] [... also talk about "reaction rates"...] [... difference between "collision", "collision+merge", "reaction" rates (fragmentation?)...]

[... collision+sticking rate, sticking probability, "Dust evolution w/ binning methods" eq.1.6-1.11...]

[... move the above elsewhere? \rightarrow "collisions" section?] [...]

A kernel describing the stick-and-hit coagulation process can be written as

$$K(m, m_1, m_2) = \frac{1}{2} \left[\delta_D(m - m_1 - m_2) - \delta_D(m - m_1) - \delta_D(m - m_2) \right] \cdot R(m_1, m_2)$$

Here, δ_D labels the Dirac delta function.

[...]

- 6.3 Numerical Integration with the Explicit Euler Scheme
- 6.3.1 QUES Why does the mass error increase over time? -> "Mass Outflow"

- 6.3.2 Hit-and-Stick Collision on Linear Mass Grid
- 6.3.3 Hit-and-Stick Collision on Logarithmic Mass Grid

- 7 Implementation of a Logarithmic Mass Axis Representation
- 7.1 Introduction, Overview, & Goals for this Section
- 7.2 Reasons for Making Use of a Logarithmic Representation
- 7.3 Challenges Associated with a Logarithmic Representation
- 7.4 Definition of the Logarithmic Mass Axis
- 7.4.1 QUES How to discretize the mass axis in a logarithmic fashion?

7.5 Implementation of the Kovetz-Olund algorithm

7.5.1 Reasons for the Necessity of the Kovetz-Olund Algorithm

Even in a highly simplified scenario, where only hit-and-stick coagulation is included, the definition of the kernel K_{kij} is not at all trivial. To assure both the consistency and accuracy of the algorithm, one has to take care of two separate problems, namely:

- 1. The conservation of mass has to be assured, otherwise the numerical solution can not be assumed to remain stable for long. In the case of stick-and-hit coagulation, this means that for every pair of colliding particles, a single new particle has to be created. At the same time, the two initial particles have to be removed from the distribution. During this process, the total mass should remain unaffected down to machine precision.
- 2. When using a logarithmically spaced grid for the discretized mass axis, it can not be assumed that after a collision of two dust particles with masses m_i and m_j the resulting particle will carry a mass $m_k = m_i + m_j$ whose value can be mapped trivially onto the grid. In general, the corresponding index will not be an integer, and instead lie between somewhere between the two neighboring grid points with indices k and k+1. Therefore, the result of the merging of m_i and m_j has to be divided in some sensible way between these two neighboring bins.

7.5.2 Implementation of the Kovetz-Olund Algorithm

An elegant way for solving the two problems listed above is given in the paper by [Kovetz & Olund, 1969], where they used the following procedure:

1. The stick-and-hit coagulation kernel is split into two parts. The first is the gain of particles in bin k due to the collision of particles from the bins i and j. The second is the loss of particles from bin k due to collisions of particles in bin k with particles from any other bin j.

Using this separation into gain & loss, the dust particle mass distribution's temporal derivative can be expressed in the following form:

$$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \sum_{i,j} K_{kij}^{\mathrm{gain}} n_i n_j - \sum_j K_{kj}^{\mathrm{loss}} n_k n_j$$

In other words, the total kernel [from above, cite eq.] can be written as

$$K_{kij} = K_{kij}^{\text{gain}} - K_{ij}^{\text{loss}} \delta_{ki}$$

Splitting the kernel like this into a gain & a loss term is a quite general approach, and can be used in more complex scenarios as well (including e.g. particle fragmentation processes).

2. For the scenario of pure hit-and-stick coagulation, a unique discretization of the kernel can be defined such that both the number of particles and the conservation of total mass are handled correctly. To do this, consider a pair of colliding particles with indices i and j. Then, let the index \bar{k} be chosen in such a way that the condition

$$m_{\bar{k}} \le m_i + m_j < m_{\bar{k}+1}$$

is satisfied.

3. As stated before, in hit-and-stick coagulation, a single new particle emerges for each pair of colliding particles. Using the definitions from above, this condition can be expressed as follows:

$$K_{\bar{k},ij}^{\text{gain}} + K_{\bar{k}+1,ij}^{\text{gain}} \stackrel{!}{=} K_{ij}^{\text{loss}}$$

4. The second condition is that of mass conservation, which can be written as:

$$m_{\bar{k}} K_{\bar{k},ij}^{\text{gain}} + m_{\bar{k}+1} K_{\bar{k}+1,ij}^{\text{gain}} \stackrel{!}{=} (m_i + m_j) K_{ij}^{\text{loss}}$$

5. Now, for the mapping of the resulting particle's mass onto two neighboring bins, let us define a parameter ε such that

$$\begin{split} K_{\bar{k},ij}^{\text{gain}} &= K_{ij}^{\text{loss}} \cdot (1 - \varepsilon), \text{ and} \\ K_{\bar{k}+1,ij}^{\text{gain}} &= K_{ij}^{\text{loss}} \cdot \varepsilon \end{split}$$

This assures that [equation from pt 3] is satisfied. If we now plug this definition into [equation from pt 4] and solve for ε , we arrive at

$$\varepsilon := \frac{m_i + m_j - m_{\bar{k}}}{m_{\bar{k}+1} - m_{\bar{k}}}$$

This is the algorithm of [Kovetz & Olund (1969)], and it was also used in subsequent papers like [Brauer et al. (2008)] and [Birnstiel et al. (2010)].

7.6 Implementation of Near-Zero-Cancellation Handling for Coagulation

7.6.1 QUES What is Near-Zero-Cancellation and where can it occur in general?

When using floating-point numbers following the representation defined by the IEEE-754 standard, it can occur that

$$a + b = a$$
 for $b \neq 0$

Typically, this happens when

$$|b| < \varepsilon_m \cdot |a|$$

Here, ε_m labels the machine precision.

[Add: How big is ε_m for an f32, how big for an f64?]

7.6.2 QUES Where can Near-Zero-Cancellation occur in our model?

Let i and j once again be the indices used to label two colliding particles. Additionally, assume now that particle i is $much \ smaller$ than particle j.

The detailed balance approach from above requires the removal of both the big and the small particle from the mass distribution, followed by the re-insertion of a new particle carrying the initial pair's combined mass. This new particle would then have a mass which is nearly identical to that of the bigger one of the original two particles, it would be only a tiny bit heavier.

In the approach defined above this would mean that $\bar{k} = j$, i.e. the resulting particle will reside in the same bin as the larger original one. Also, it would follow that $\varepsilon \ll 1$.

Let us now take a look at the particle mass distribution in the bin \bar{k} and, more specifically, by how much it changes from one timestep to the next. For this particular pair of i and $\bar{k} = j$, we can write:

$$\frac{\mathrm{d}n_{\bar{k}}}{\mathrm{d}t} = K_{\bar{k},i\bar{k}}^{\mathrm{gain}} n_i n_{\bar{k}} - K_{\bar{k}i}^{\mathrm{loss}} n_i n_{\bar{k}}$$

Plugging in [equation from above] leads to

$$\frac{\mathrm{d}n_{\bar{k}}}{\mathrm{d}t} = (1 - \varepsilon)K_{\bar{k}i}^{\mathrm{loss}}n_i n_{\bar{k}} - K_{\bar{k}i}^{\mathrm{loss}}n_i n_{\bar{k}}$$

Here, the two terms alsomst cancel each other out. What remains is a contribution which is proportional to ε .

If ε is small enough, the double-precision accuracy of the floating point representation will lead to break-down of the method. [rewrite this sentence, copied almost exactly from Kees]

7.6.3 Handling Near-Zero-Cancellation for Stick-and-Hit Coagulation

It is relatively easy to identify the particle pairs (i, j) for which the scenario detailed above will occur. Let i (without loss of generality) be the index of the larger one of the two colliding masses. Cancellation may then occur when the resulting k is equal to j.

In that case, we carry out the subtraction in [previous equation] analytically, and write:

$$\frac{\mathrm{d}n_{\bar{k}}}{\mathrm{d}t} = -\varepsilon K_{\bar{k}i}^{\mathrm{loss}} n_i n_{\bar{k}}$$

[Elaborate on this, see "Dust Evolution with Binning Methods"]

- 8 Inclusion of Fragmentation Processes into the Kernel
- 8.1 "First/Simple/Naive Attempt"
- 8.1.1 QUES How to implement naive fragmentation?
 - "Pulverization"

8.2 The MRN Distribution

- introduced by Mathis-Rumpl-Nordsieck, 1977

8.2.1 QUES How to implement MRN distribution (for initialization)?

Particle mass distribution function is defined by the condition:

$$\rho = \int_{m_{\min}}^{m_{\max}} n(m) \cdot m \, \, \mathrm{d}m$$

Ansatz: power law with q = -11/6 (see 'sizedistributions.pdf')

$$n(m) \sim m^q$$

Choose constant A such that

$$n(m) = A \cdot m^q$$

Plug into the integral from above

$$\begin{split} \rho &= \int A \cdot m^q \cdot m \, \, \mathrm{d}m \\ &= \int A \cdot m^{q+1} \, \, \mathrm{d}m \\ &= \frac{A}{q+2} \, \left. m^{q+2} \right|_{m_{\min}}^{m_{\max}} \\ &= \frac{A}{q+2} \, \left. \left(m_{\max}^{q+2} - m_{\min}^{q+2} \right) \right. \end{split}$$

Rearanging for A leads to

$$A = \frac{(q+2) \cdot \rho}{m_{\text{max}}^{q+2} - m_{\text{min}}^{q+2}}$$

Now we only need to choose values for m_{\min} and m_{\max} .

- For the minimum mass, no lower limit exists. For it, the value corresponding to the smallest bin can be chosen [citation needed].
- For the maximum mass, an upper limit has to be chosen. It can be left as a free parameter to be set in 'config.toml', or set to something approximating 0.5 μ m. [see 2004 Dullemond & Dominik] ^ max. in interstellar medium (use for m_{min}?)

8.2.2 QUES How to implement MRN distribution for fragmentation?

Let m_i and m_j be the masses of two particles that are involved in a collision leading to fragmentation.

How do we model this?

- Distribute the mass $m_{\text{tot}} = m_i + m_j$ onto bins with $m < m_{\text{tot}}$.

- For this, use the MRN distribution $n(m) = Am^q$.
- For this, find the value of A.
- For this, use the formula from [Summarize: How to implement MRN distri].
- For this, find a value for m_{max} .

How do we choose a value for m_{max} ?

- Can it be larger than $\max(m_i, m_i)$?
 - "Some merging, some fragmenting"
 - "1 + 1 \rightarrow 1.5 + 0.1 + 0.1 + 0.1 + 0.1 + 0.1"
- If...
 - ... yes: It can at most be equal to $m_i + m_j$
 - ... no: It can at most be equal to $\max(m_i, m_i)$
- In either case, it can't really be equal to either of the two values.
 - That would be stick-and-hit in case "yes", and bouncing in case "no".
 - It can at most be equal to the mass corresponding to the next-lower bin.

Answer:

- We don't really know.
- It doesn't really matter that much anyhow.
- One could specify the method in 'config.toml', or just use one of the methods.
- 8.2.3 QUES Test integration speed with MRN distribution enabled. Is there a slow-down?
- 8.3 "Implementation of Near-Zero-Cancellation Handling for Fragmentation" (?)

- 9 Definition of a the Dust Particle Reaction Rates
- 9.1 Definition of the Dust Particle Reaction Rates

9.2 Definition of the Dust Particle Collision Rates

9.2.1 QUES How to define the particle collision rate?

The collision rate for a pair of masses m_1 and m_2 can be written as

$$C(m_1, m_2, \Delta v) = \sigma(m_1, m_2) \cdot \langle |\vec{v}_1 - \vec{v}_2 \rangle$$

Here, $\sigma(m_1, m_2)$ labels the cross section for a collision event. The relative velocity between such two particles is given by the difference $\vec{v}_1 - \vec{v}_2$, its absolute value is $|\vec{v}_1 - \vec{v}_2|$, and $\langle |\vec{v}_1 - \vec{v}_2| \rangle$ is the expectation value of that quantity.

[Simplification was done here] [Elaborate: Give more precise formula]

In our notation:

$$C_{ij} = \sigma_{ij} \cdot \langle \Delta v_{ij} \rangle$$

9.3 Definition of the Collision Cross Section

9.3.1 QUES How to implement realistic collision cross sections?

The cross section for a collision of two particles i and j with radii a_i and a_j can be written as

$$\sigma_{ij} = \pi \cdot (a_i + a_j)^2$$

Here, the radii can be computed from the corresponding masses m_i and m_j from equation [Summarize: Assumptions needed for the (naive/simple) particle mass distribution.].

[Add plot here]

- 9.4 Definition of the Relative Particle Velocity
- 9.4.1 QUES How to implement realistic relative velocities between dust particles?

10 Calculation of the Relative Dust Particle Velocities

10.1 Definition of the Relative Velocity due to Radial Drift

$$\Delta u_{\rm RD} = \left| u_r(m_1) - u_r(m_2) \right|$$

dust radial velocity:

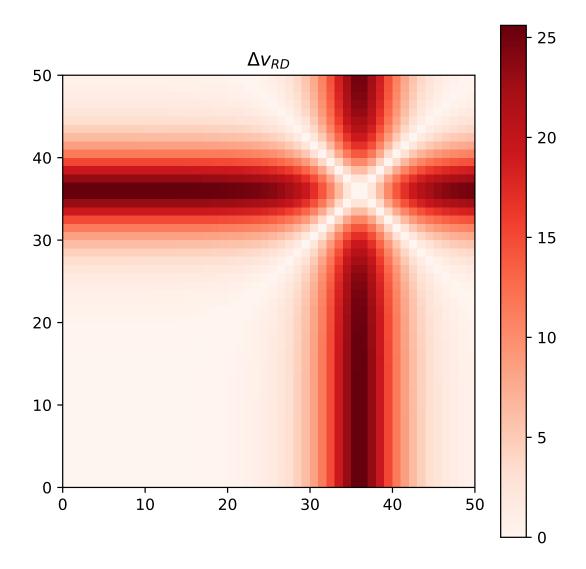
$$u_r = \frac{u_g}{1 + \operatorname{St}^2} - \frac{2u_n}{\operatorname{St} + \operatorname{St}^{-1}}$$

gas radial velocity:

$$u_g = -\frac{3}{\Sigma_g \sqrt{r}} \cdot \partial_r \left(\Sigma_g \nu_g \sqrt{r} \right)$$

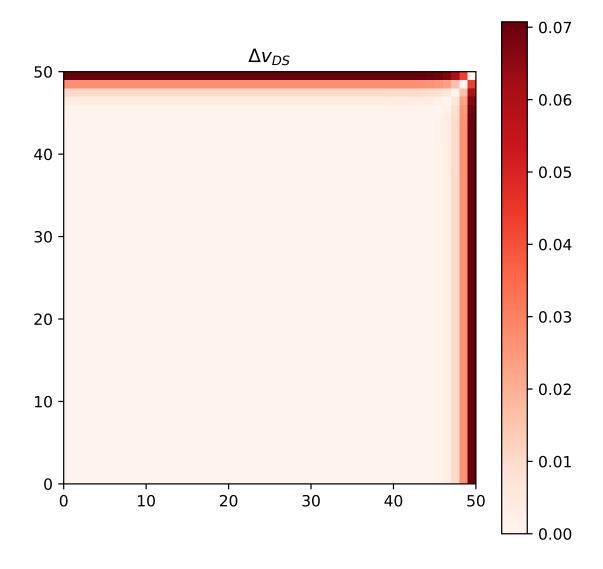
particle maximum drift velocity:

$$u_n = -\frac{E_d}{2\rho_g \ \Omega_K} \cdot \frac{\partial P_g}{\partial r}$$



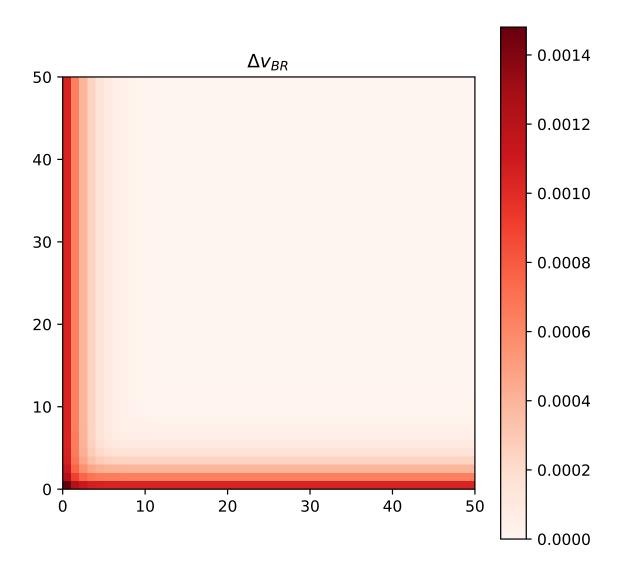
10.2 Definition of the Relative Velocity due to Differential Settling

$$\Delta u_{\rm DS} = \left| u_i - u_j \right|$$
$$u_i = ts \cdot \Omega_K^2 \cdot z$$
$$St = \Omega_K \cdot t_s$$

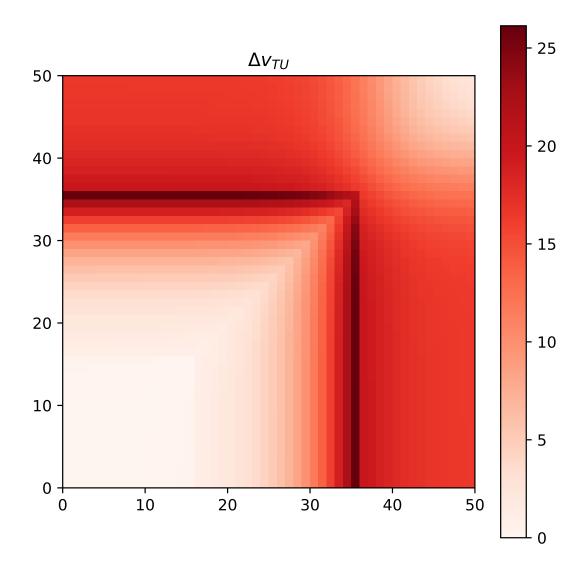


10.3 Definition of the Relative Velocity due to Brownian Motion

$$\Delta u_{ij}^{\text{BR}} = \sqrt{\frac{8k_B T}{\pi} \cdot \frac{m_i + m_j}{m_i \cdot m_j}}$$
$$= \sqrt{\frac{8}{\pi \beta \mu_{ij}}}$$

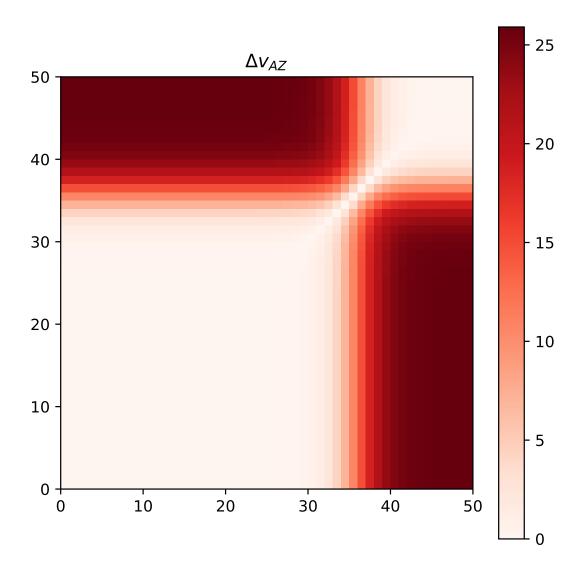


10.4 Definition of the Relative Velocity due to Turbulence



10.5 Definition of the Azimuthal Relative Velocity

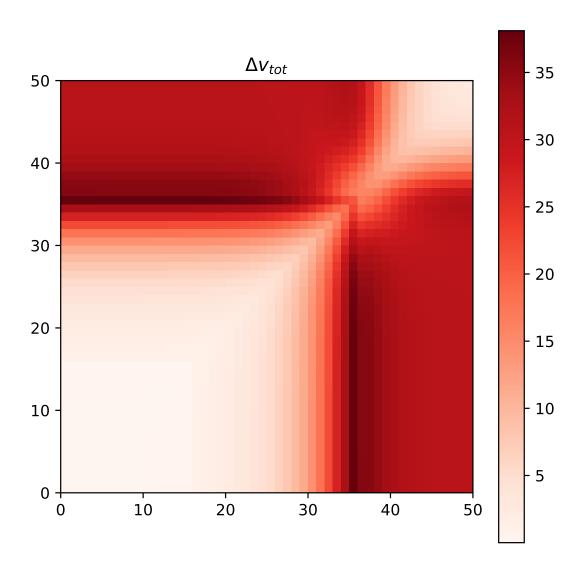
$$\Delta u_{ij} = \left| u_n \cdot \left(\frac{1}{1 + \operatorname{St}_i^2} - \frac{1}{1 + \operatorname{St}_j^2} \right) \right|$$



10.6 Total Relative Velocity

$$\Delta u_{ij} = \Delta u_{\mathrm{BR}} + \Delta u_{\mathrm{RD}} + \Delta u_{\mathrm{AZ}} + \Delta u_{\mathrm{TU}} + \Delta u_{\mathrm{DS}}$$

$$\Delta u_{ij} = \sqrt{\Delta u_{\rm BR}^2 + \Delta u_{\rm RD}^2 + \Delta u_{\rm AZ}^2 + \Delta u_{\rm TU}^2 + \Delta u_{\rm DS}^2}$$



11	Implemention of Stochastic Kernel Sampling

12 Summary of Results

13 Thesis Discussion & Outlook

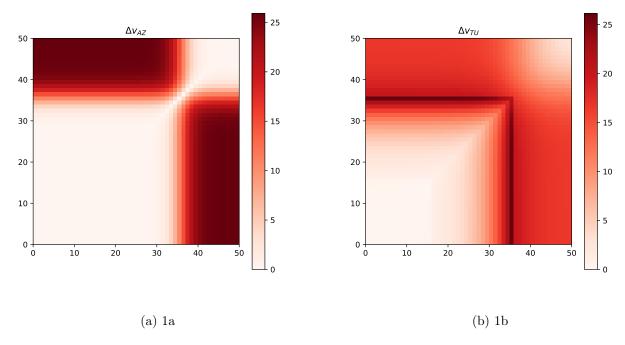


Figure 1: plots of....

14 Appendix

14.1 Glossary

14.2 Testing: Can I use subfigures for "multicol" LATEX plots in Emacs org-mode?

- Yes! See below:

15 References