Computational Astrophysics and Centre for ExoLife Sciences

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The role of Computational Astrophysics in general

The use of computational modeling in Astrophysics largely splits into **two categories**:

1. **Parametrized modeling**, using for example Python, or C or Fortran programs that include a number of **free parameters** (even “one” qualifies as “a number” ;-)

2. **Realistic modeling**, where the model includes essentially **all relevant physics**, and where even the remaining freedom (to choose initial and boundary conditions) can be more or less removed, by relying on observationally well-established (possibly statistical) properties. Examples:
   - Cosmic micro-wave background ⇒ **Cosmological simulations**
   - Larson’s relations for the ISM ⇒ **Star formation simulations**
   - Teff, log g, abundance (**B?**) ⇒ **3-D stellar atmospheres**

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Where does AI / Neural Networks belong here?

- In principle perhaps in the **2nd category**, since they have the potential of pinpointing "**the most likely physical conditions**" from a murky set of observational fingerprints
- But in practice it could also easily be the **1st category**, at least when AI is only used to "find the most likely parameter combination" – then it could both fail to find the correct interpretation, and even worse **appear to favor something that just "looks right"**, but isn't

Pro’s and con’s

The 2nd category may appear as the clear winner, but there are some caveats

- It can be **very costly**, easily to the point of being out-of-reach (**N^4**)
- Even when affordable, cost limitations always require *some* parametrization
- Parametrized models may allow exploring a much larger physical regime

What to conclude from this?

- No matter what the details and the costs are, **lowering the cost** is key to being the first to realistically model larger and more complex situations
- Just as the forefront of observational astrophysics relies on both better / larger instruments ***and*** on developing new observational methods, the forefront of Computational Astrophysics depends on **both hardware and software** ….. **as well as on asking the right questions**

What can we contribute to the Centre for ExoLife Sciences?

We can contribute primarily on three fronts:

1. **Planet atmosphere modeling**, which even in 1-D is a very complex affair (low-temperature, clouds) – in a wider context (super-Earths, …)

2. **Planet formation and evolution**: The overall state of a planet atmosphere at any one time is the ultimate result of history:
   - ✓ the formation of the planet, with its primordial atmosphere, and
   - ✓ the subsequent evolution (cooling, in-gassing, out-gassing, escape, …)

3. **Tools**: The DISPATCH **code framework**
   - ✓ performance and parallelization to millions of cores
   - ✓ modularity and ease of integration

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3.

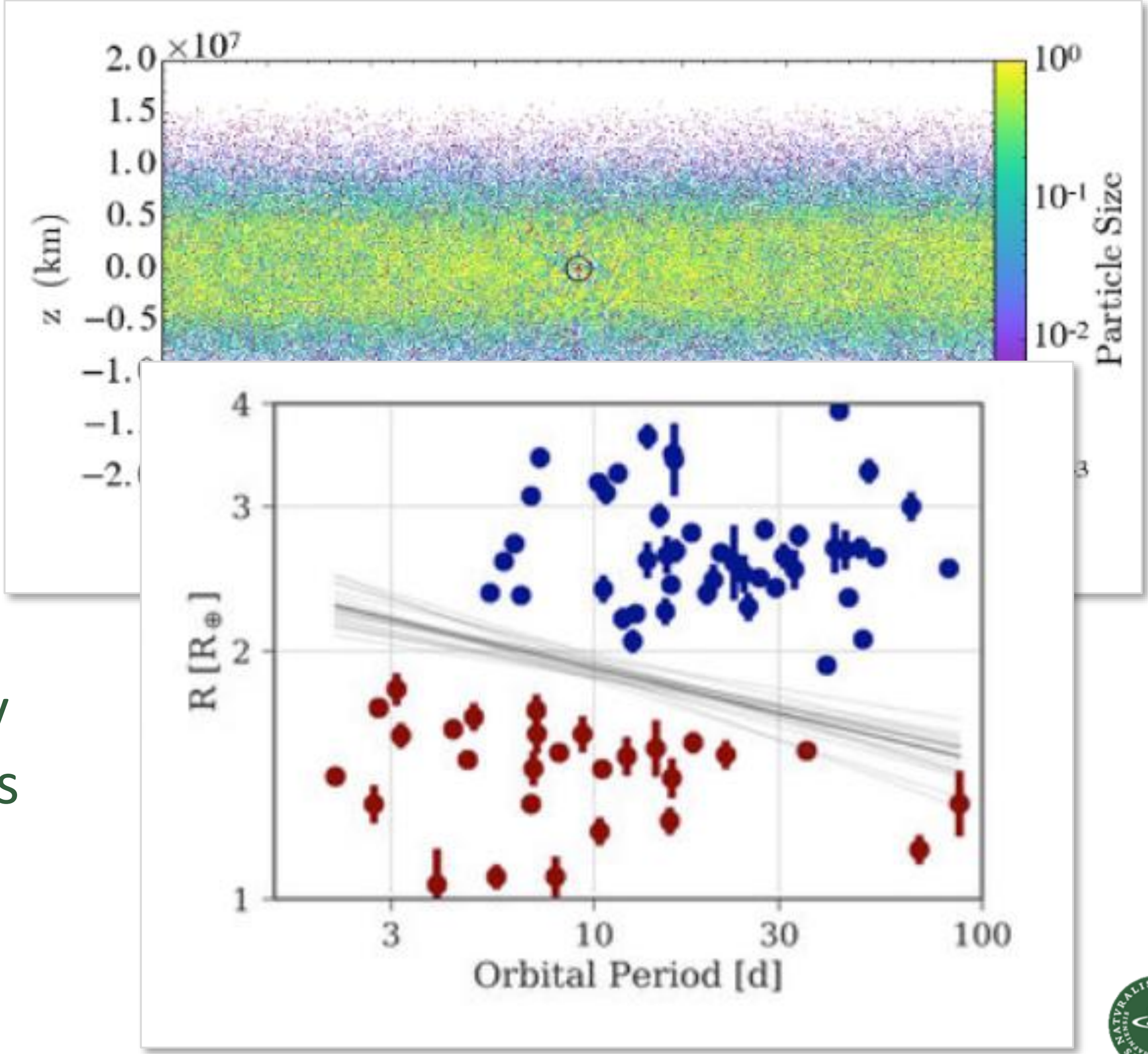
Status, prospects?

- ❖ Even 1-D atmosphere spectral modeling is a complex undertaking -- chemical fingerprints need to be strong! What would we learn from 1-D models of the Earth's atmosphere? **Need 3-D modeling: convection, vertical non-equilibrium, etc**
- ❖ While star formation is to some extent well understood, **planet formation is in many ways not well understood**! Here we will be "putting down the rails in front of the train", no-matter-what!
- ❖ **Non-LTE and non-equilibrium modeling** is being integrated into the DISPATCH code framework – more about the needs for that in Maria's talk

Some central issues in planet formation:

- **Primordial planet atmospheres:** The clear conclusion from recent progress (observational and modeling) is that planets form very early and rapidly; definitely while the PPD still has significant gas left => they have **substantial primordial atmospheres**

- **The “radius valley”**: This is the valley (in the R-period plane) that separates rocky planets from gas dwarfs (or super-Earths from sub-Neptunes if you will)



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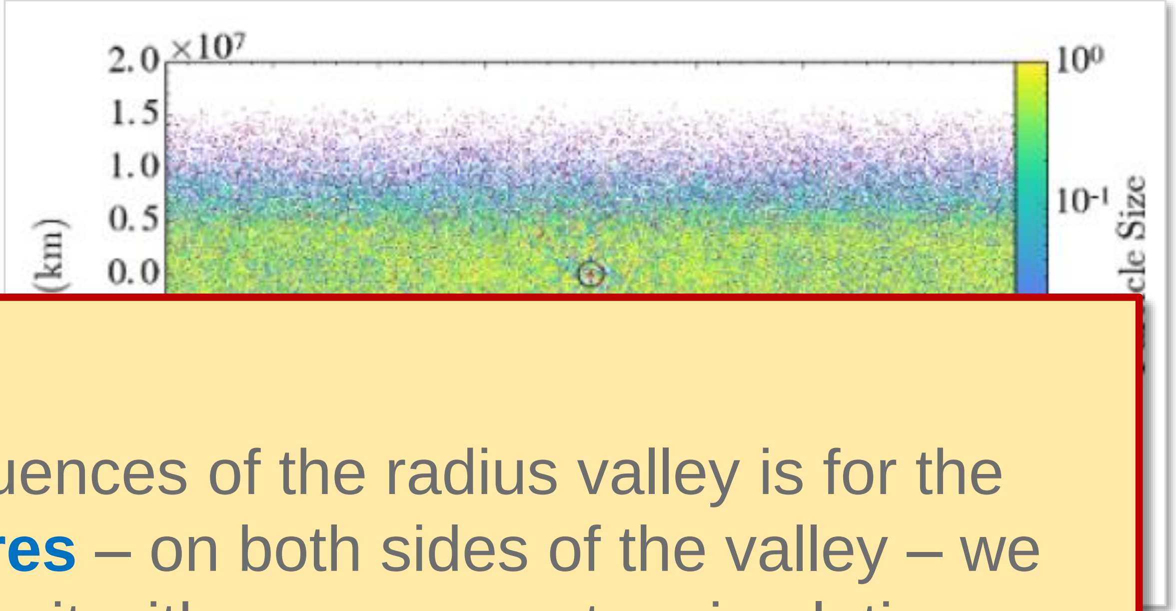

- ☐ **Th**
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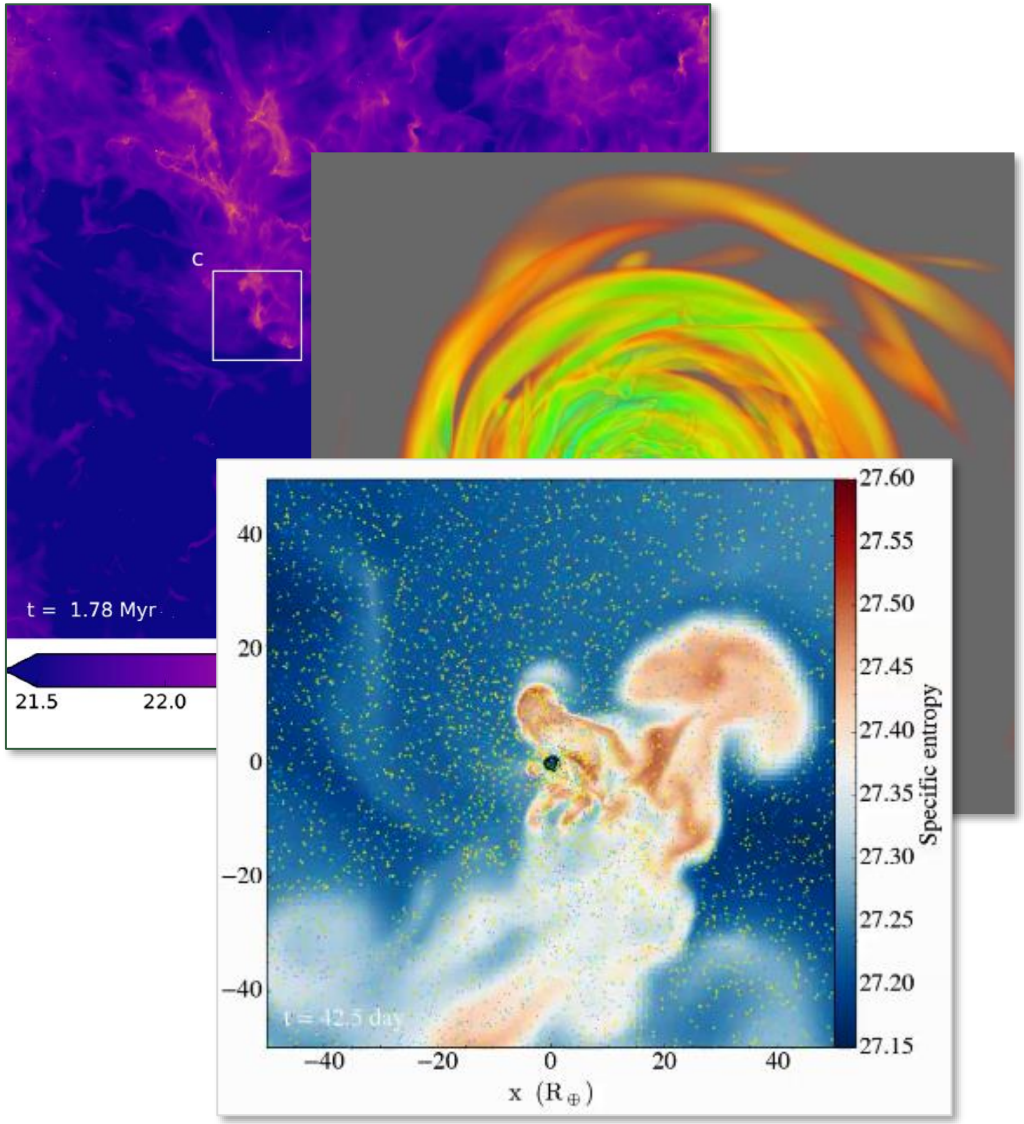
Prospects?

- ❖ To understand what the consequences of the radius valley is for the **evolution of planet atmospheres** – on both sides of the valley – we need to first be able to reproduce it with supercomputer simulations.
- ❖ Not necessarily by modeling planet formation *ab initio* – this is still a tall undertaking, but we can start by “planting” different planets inside **evolving *ab initio* proto-planetary disks** and study their atmosphere loss

Brief overview of recent results

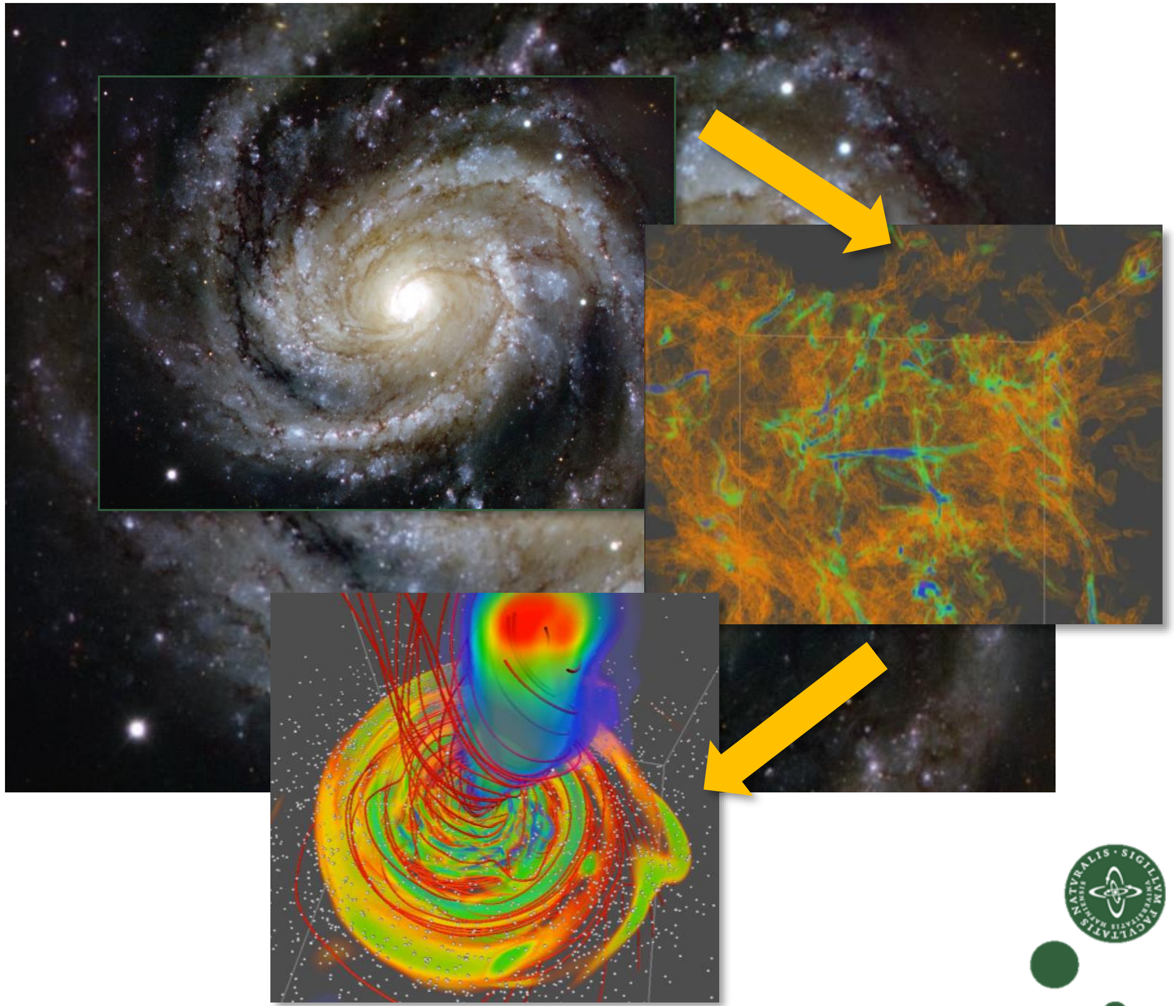
- **Star formation simulations**
  - ✓ following the formation of thousands of stars
- **Protoplanetary disk simulations**
  - ✓ revealing the very early phase
- **Planet formation simulations**
  - ✓ resolving primordial atmospheres
- **Supercomputing framework**
  - ✓ enabling unlimited scaling



Motivation for introducing task-based computing (ÅN et al 2018)

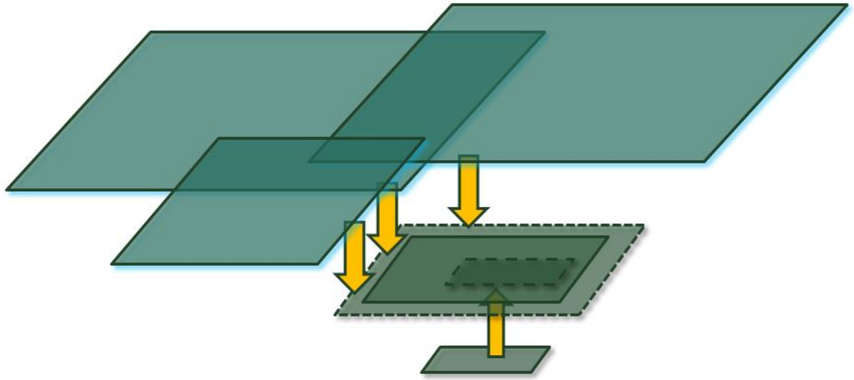
Imagine: a ***full galaxy*** simulation, down to ***individual stars and planets***

- ☐ ***Exascale ⇒ target huge systems***
  - Unavoidably: ***many semi-autonomous hierarchical regions of space***
    - ***GMCs, MCs, accretion disks, planets, …***
- ☐ This point of view has ***decisive implications*** for code design
  - A distant molecular cloud influences other molecular clouds by its **gravitation** and **light output**
  - Once a pre-stellar envelop collapses it's evolution time scale drops by orders of magnitude
  - Needs surroundings mainly as a **boundary condition in space-time**

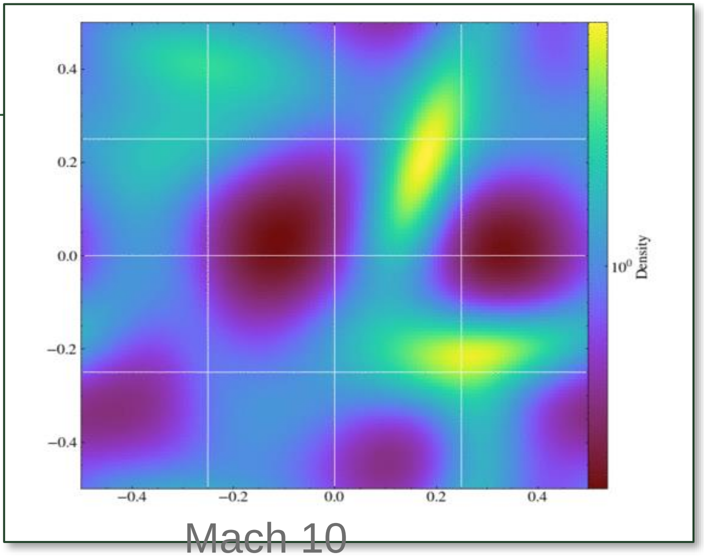


DISPATCH breaks with traditions to achieve ~unlimited scaling:

- Allows **asynchronous evolution** of sub-domains (patches)
- Allows **moving patches** – small Cartesian meshes with bulk motion
- Allows **local time steps**; determined independently for each patch
- Uses **task-based scheduling**, via OpenMP inside nodes
- Uses **neighborhood-limited MPI** between nodes
- Allows **any preferred solver inside** patches, balancing speed against quality and guard zone requirements
- Can include **Multiple-Domain-Multiple-Physics**
  - e.g. particle-in-cell codes for kinetic simulations inside MHD
  - dust+gas dynamics
  - …



Five **Key Concepts** in DISPATCH

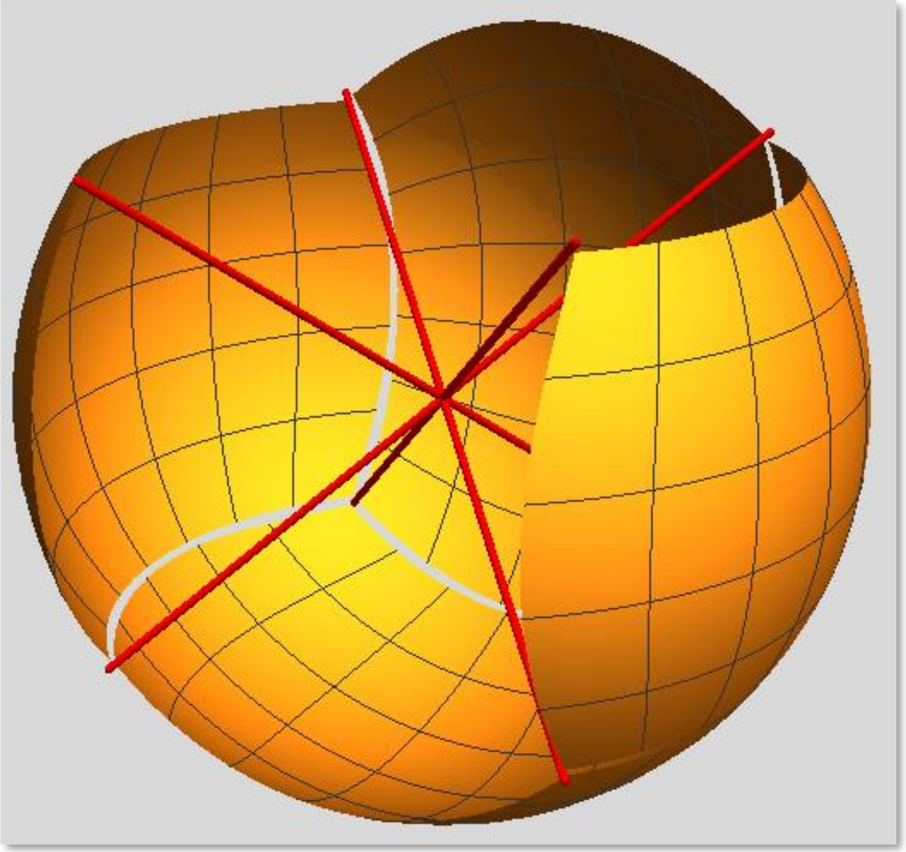


Mach 10 supersonic turbulence

- Local tasks use **local time steps**
  - A generalization of AMR: essentially ***AMR in space-time***
- "**Perfectly OMP parallel**" on sockets (MPI ranks)
  - Semi-independent OpenMP-parallel tasks inside MPI ranks
- "**Perfectly MPI parallel**" btw MPI ranks
  - Only nearest neighbor communication, load balancing is trivial
- Accepts **any solver**, which may vary btw local tasks
  - Mesh, particle, HD, MHD, RT, PIC, Vlasov, … (multiple-physics)
- Object oriented and **adaptive**: adaptive mesh, ***adaptive physics***
  - Mesh refinement, method refinement, …

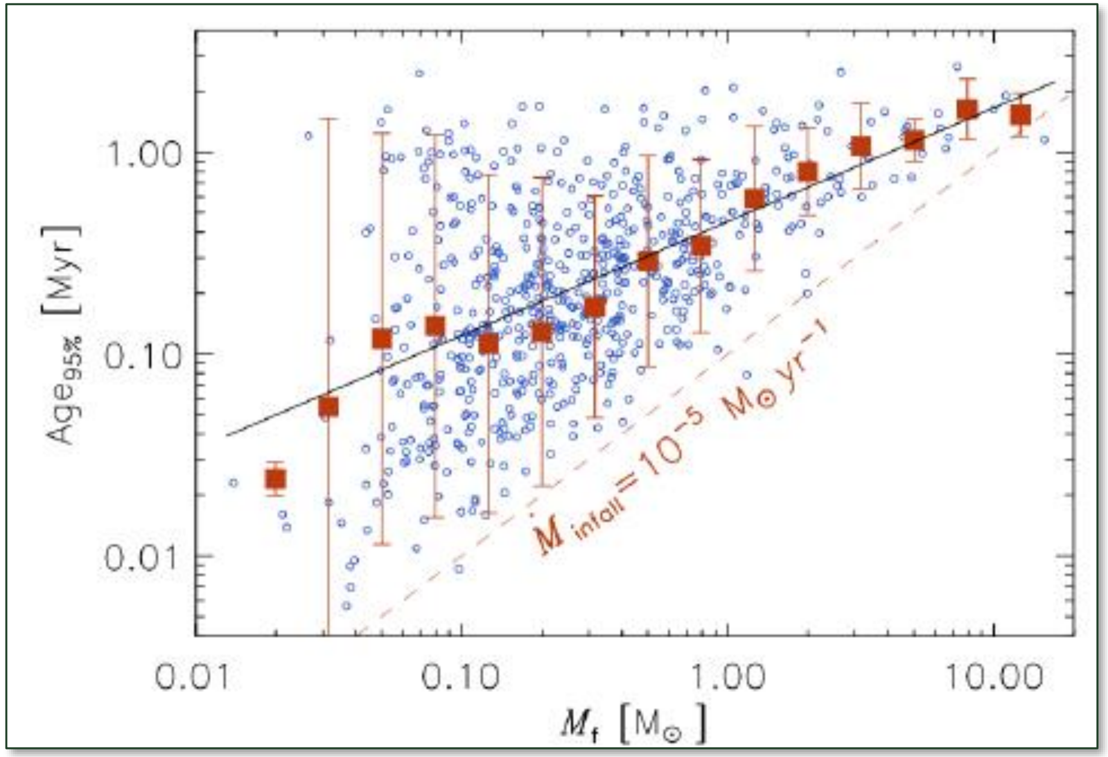
The **Volleyball Geometry** for spherical objects

Allows **covering a sphere with perfectly cubical “patches”,** with only a small amount of tilt between neigboring patches



Star formation facts from realistic simulations

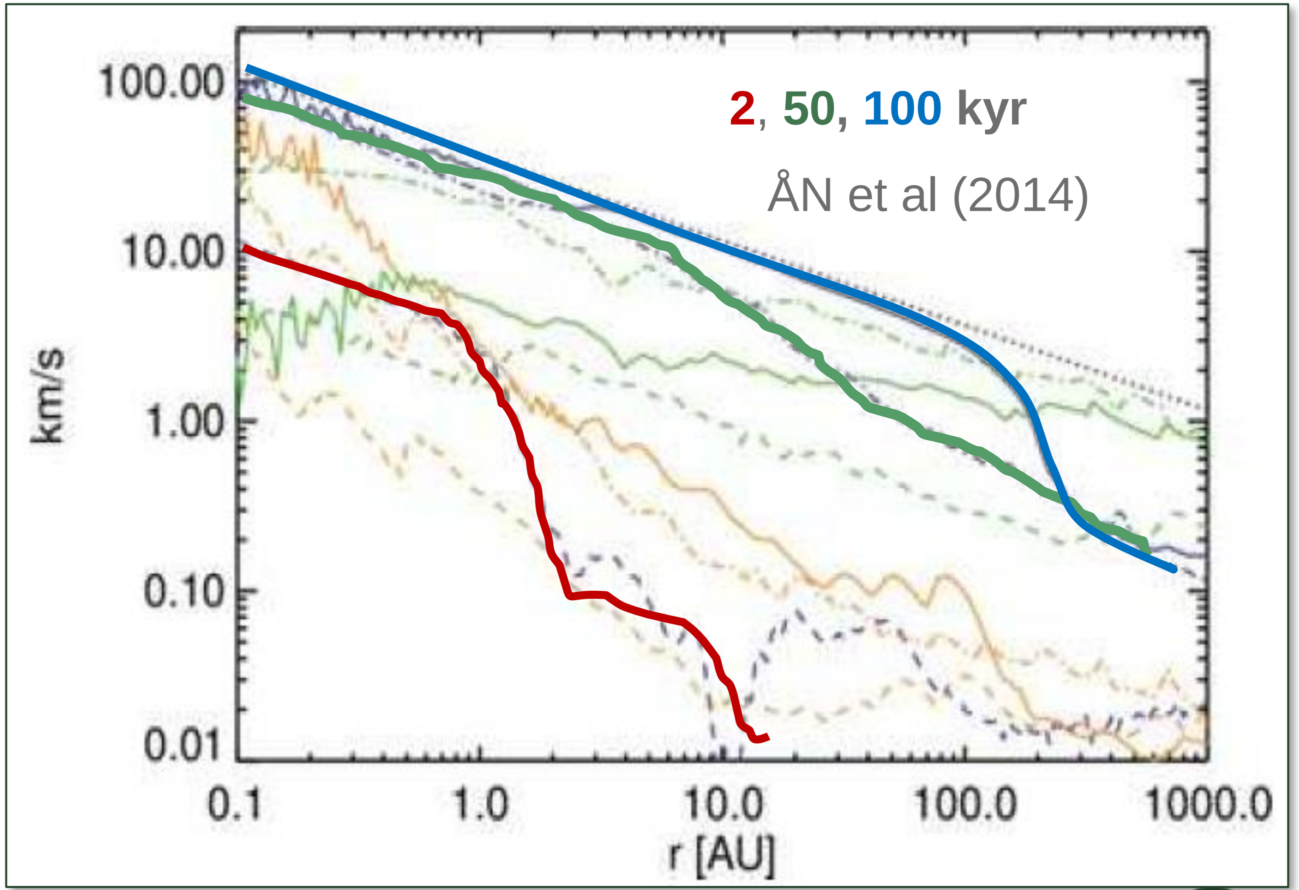
ÅN et al (2014), Padoan et al (2014-19, …), Küffmeier et al (2017-20, …)



- **Accretion** to 95% of final mass **takes considerable time**
  - Here, in Fig 13, from Padoan et al, 2014 one can see that forming 1 solar mass star can take anything from 0.1 to >1 Myr
- **Disk are accretion buffers**, not static left-overs
  - replenishment times are **shorter than life-times**
  - the **accretion rate is set by the envelope environment**, the disk is a “slave”

The formation of proto-planetary disks

- ☐ accretion to final stellar mass takes considerable time
- ☐ disk formation is (literally!) “connected” to star formation
- ☐ disks (PPDs) are accretion buffers, not static left-overs
  - See Tazzari et al (2021) for inconsistency of observations with dust drift in static disks
- ☐ **disks form inside-out**, growing in size with time
  - This is the result of the growth with time of the average angular momentum of accreting gas+dust



Küffmeier et al 2017, zoom-in simulations, 40 pc outer scale, AMR: 2 AU)

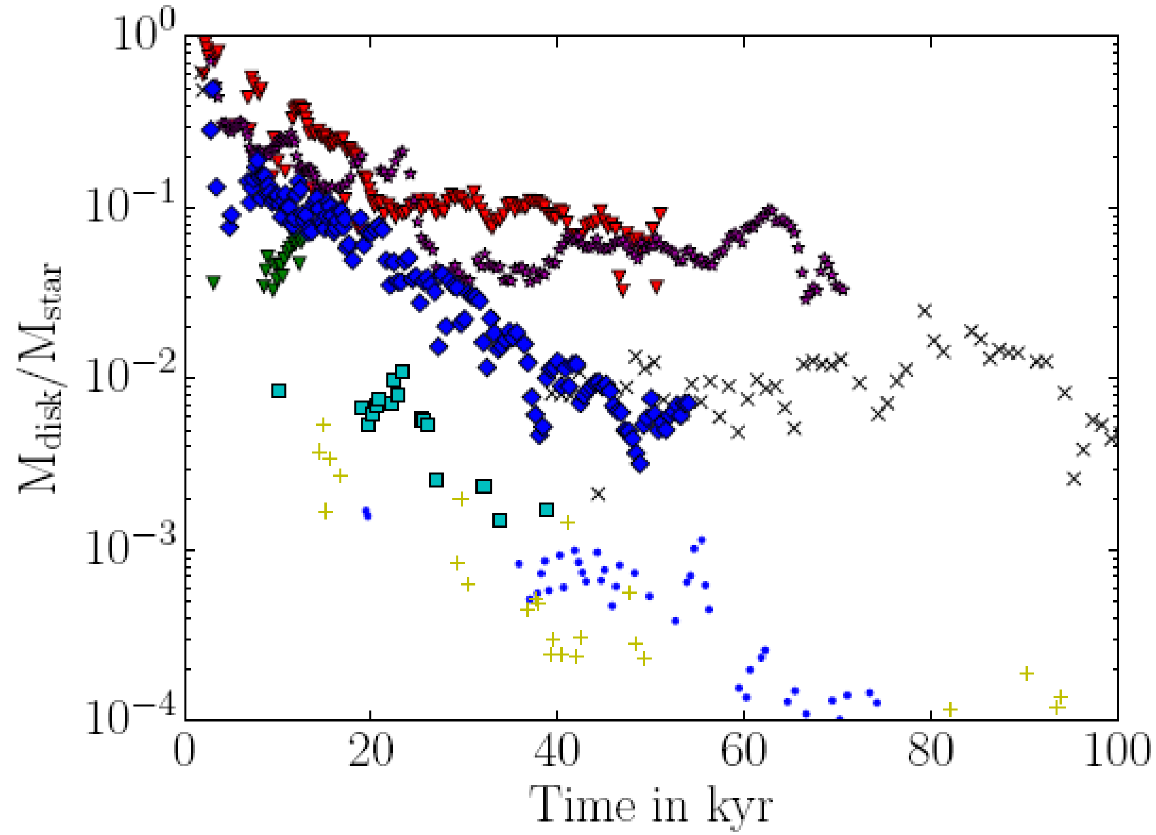
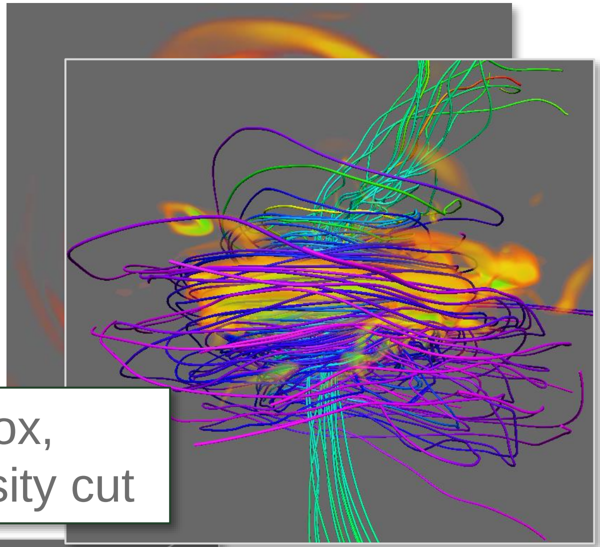
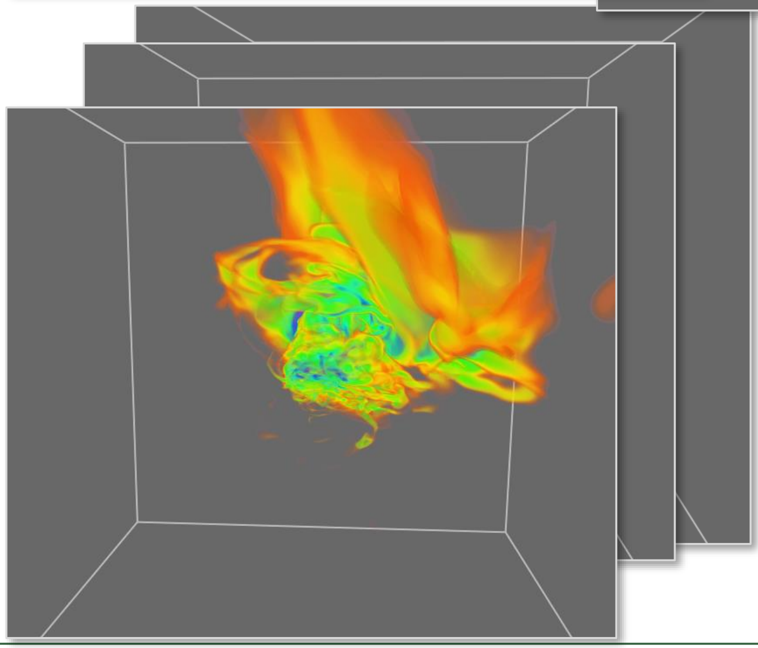


Figure 26. Time evolution of the ratio between disk and sink mass around the different protostars after sink creation. The symbols belong to the same sinks as in Fig. 10.

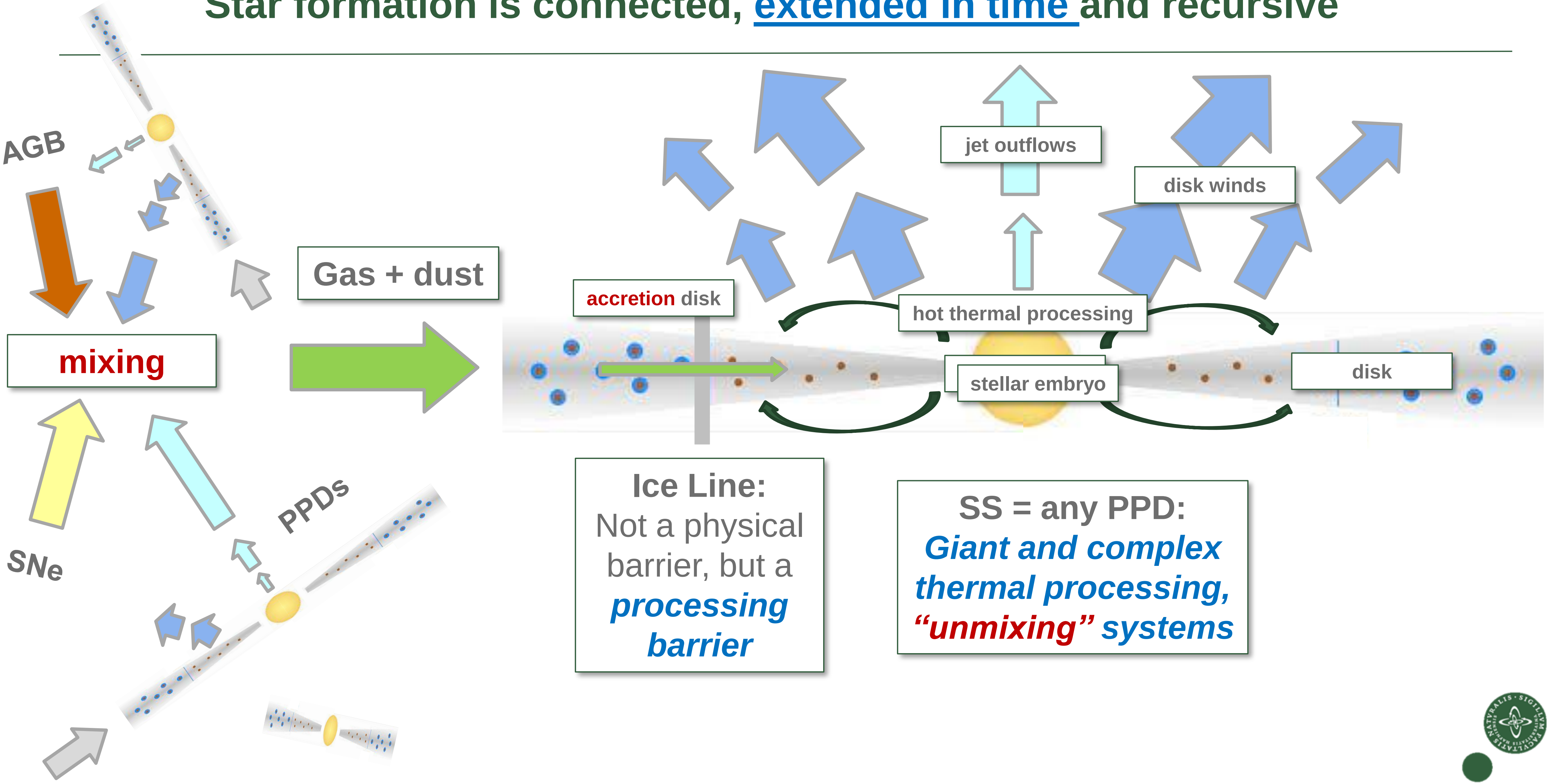


50 AU radius
@ t = 50 kyr

side views in1000 AU box,
same disk, varying density cut



Star formation is connected, extended in time and recursive



AGB

SNe

PPDs

mixing

Gas + dust

accretion disk

jet outflows

disk winds

hot thermal processing

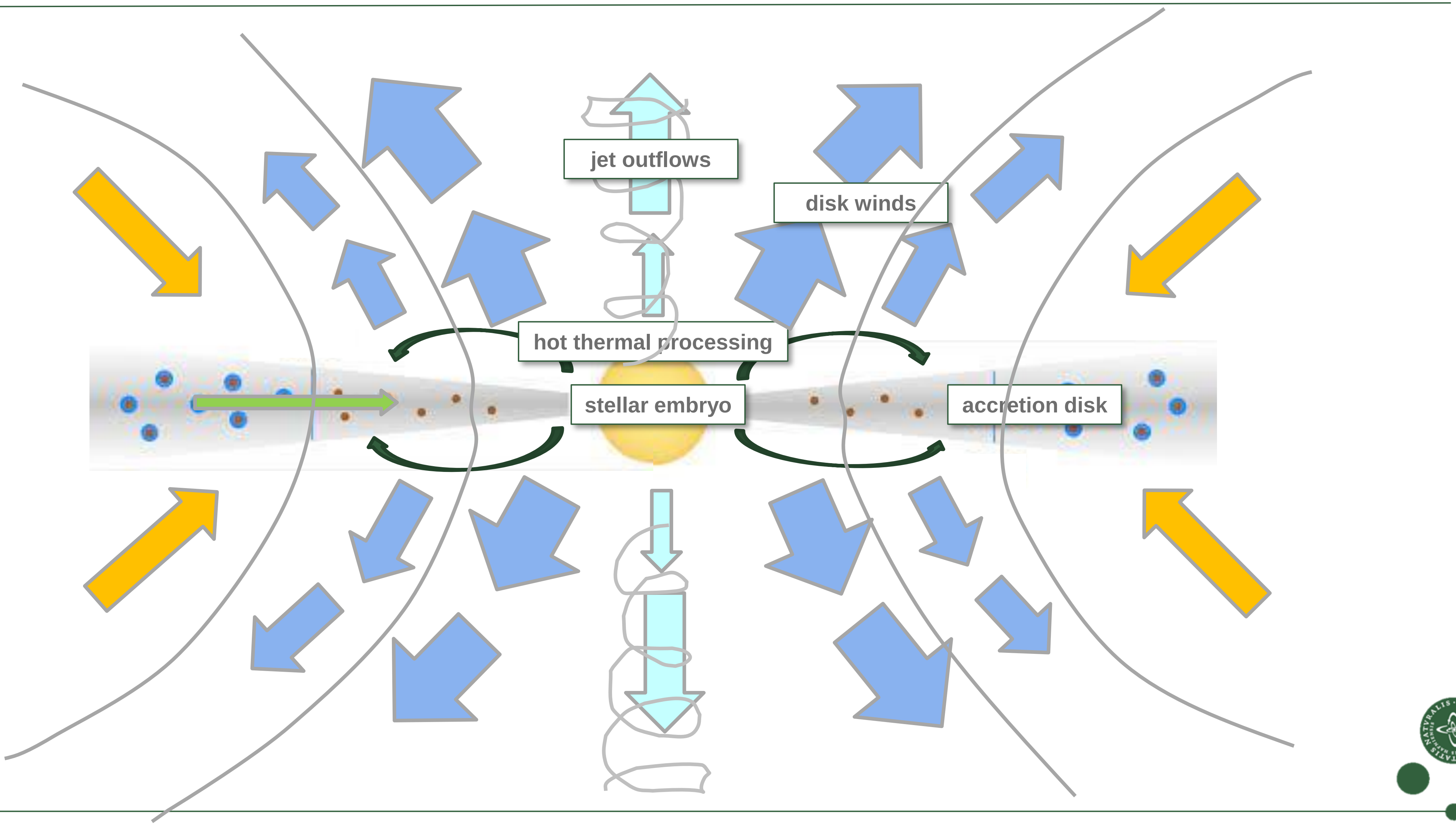
stellar embryo

disk

Ice Line:
Not a physical barrier, but a ***processing barrier***

SS = any PPD:
Giant and complex thermal processing, "unmixing" systems

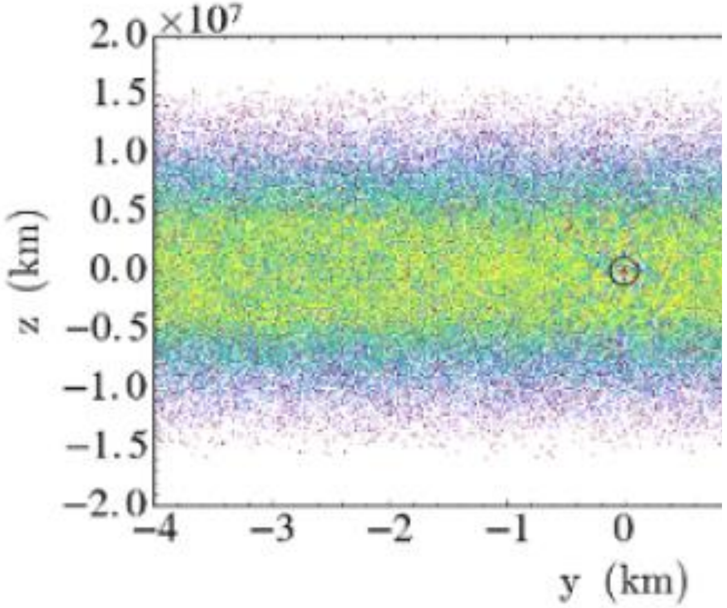
Disk formation: a consequence of accretion – the fight against angular mom

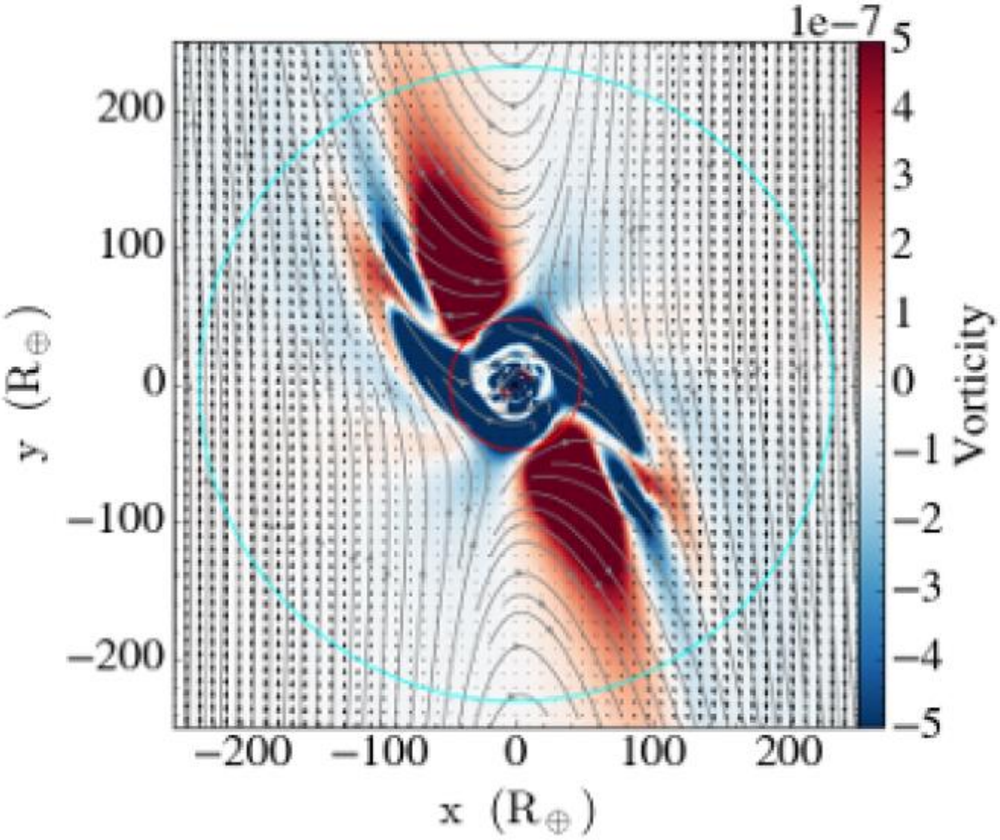


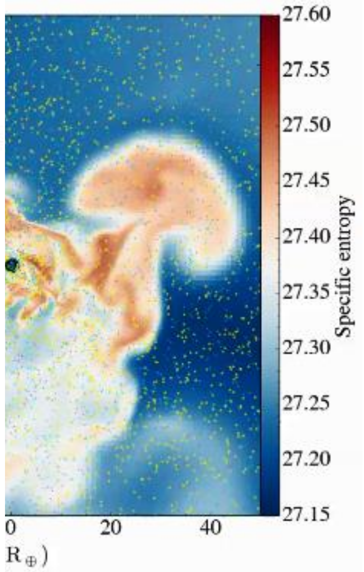
DISPATCH Applied to Planet Formation (Popovas et al, MNRAS 2018)

First 3-D simulations that begin to fully resolve the Hill sphere

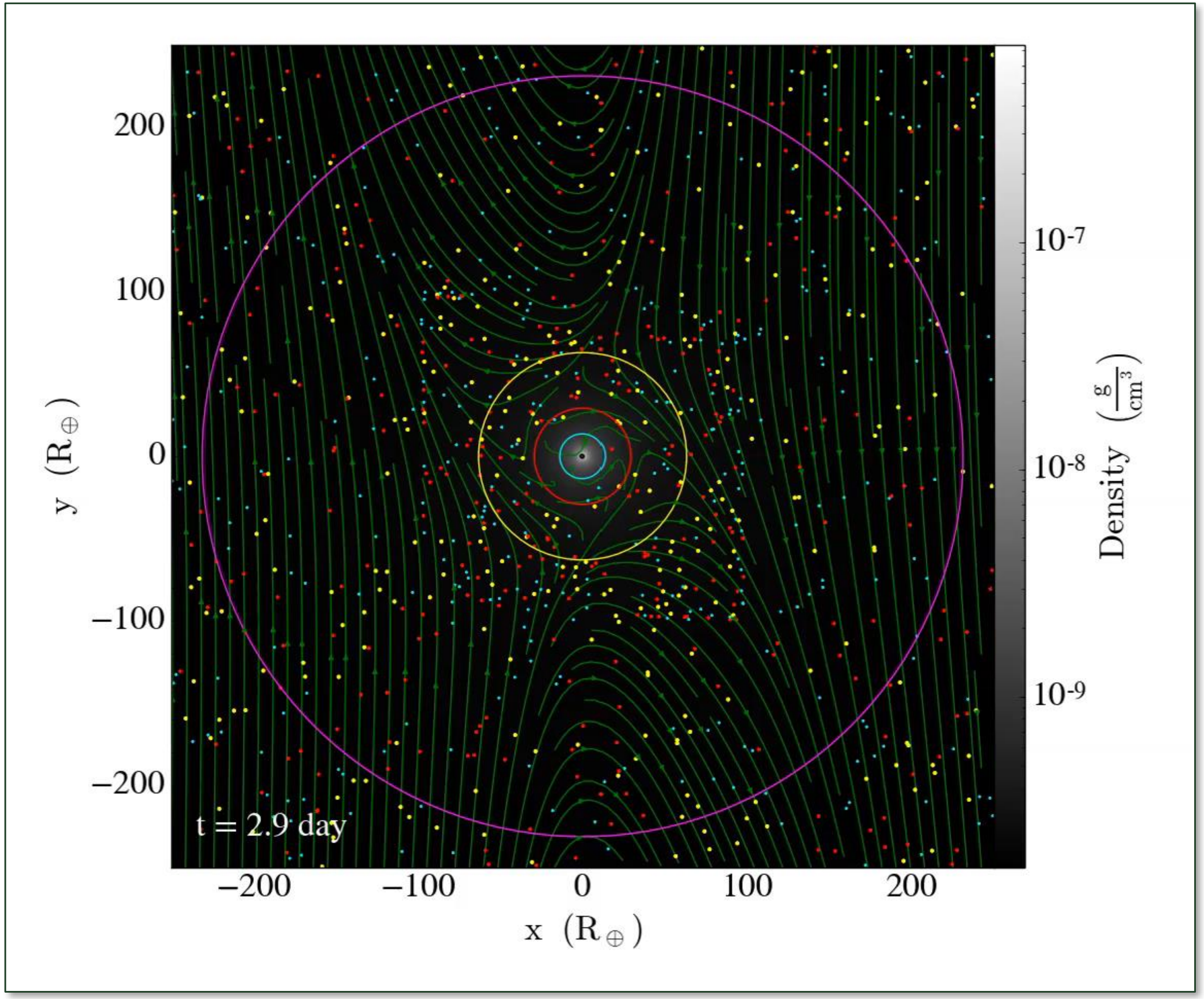
- Scenario: Chondrule accretion ***in a pressure trap*** $\Rightarrow$ no head wind, increasing Z/H
- **Scale range $L/\Delta s \sim 5\ 10^5$** ($L_y \sim 15{,}000\ R_{Earth}$, $\Delta s \sim 1/30\ R_{Earth}$)
- Shearing box, with no gravitational softening (important !)
- More than 50 million particles with drag, from 0.001 to 1 cm in size (dust:gas=1%)
- Accretion heating drives 3-D conve







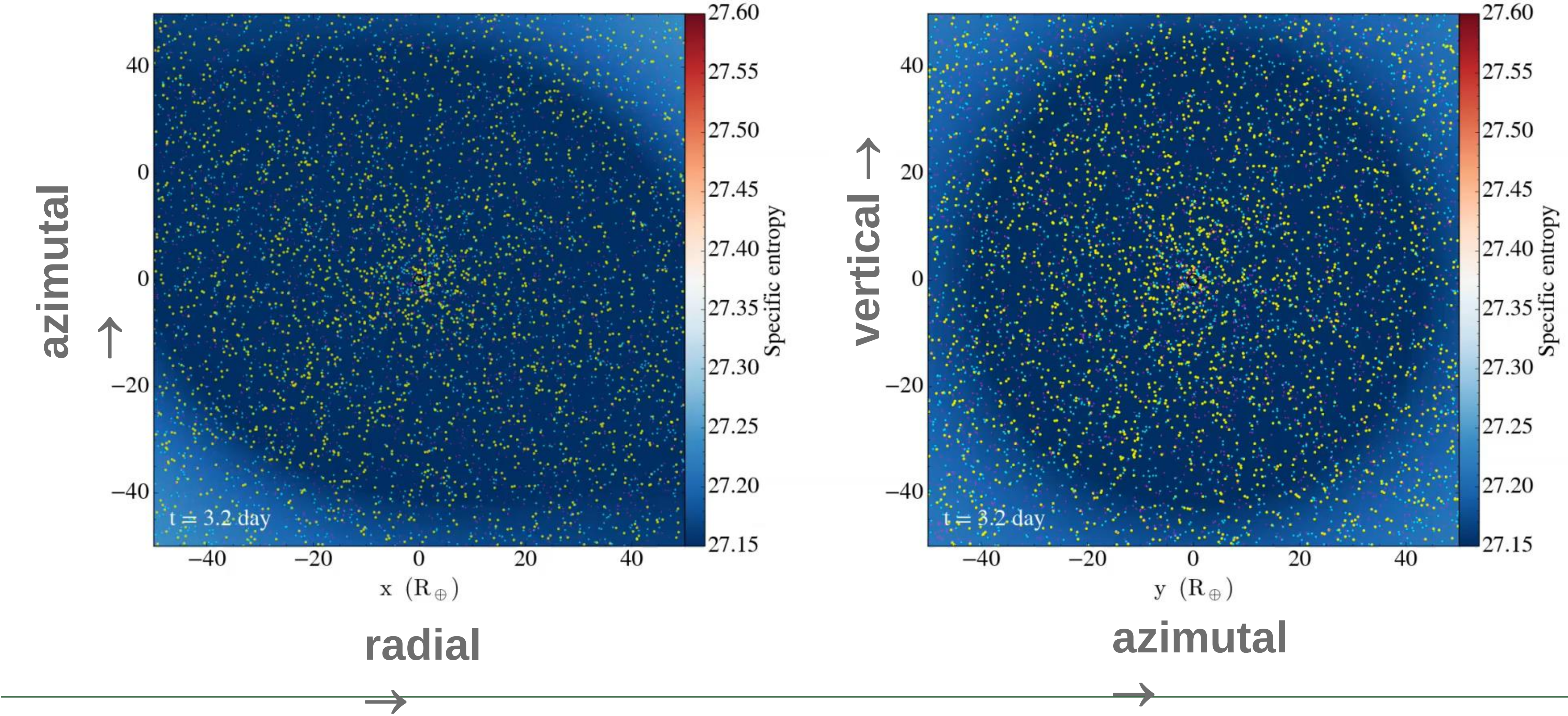
Accretion by radial drift (color encodes particle size)



yellow: 1-10 mm
red: 0.1-1 mm
blue: 0.01-0.1 mm

Planet accretion heating is crucial for near-planet dynamics

Drives **strong convective flows** (Popovas et al 2018, MNRAS)



Summary

- ☐ **Star formation simulations have shown us:**
  - ✓ **diversity** of accretion process
  - ✓ **range** of accretion time
- ☐ **Protoplanetary disk simulations**
  - ✓ the crucial **growth phase** of protoplanetary disk
- ☐ **Planet formation simulations**
  - ✓ protoplanetary disks are **boundary conditions**
- ☐ **Supercomputing framework**
  - ✓ **task based computing** ⇒ unlimited scaling and optimal performance

Serious synergy needed here ;-!