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Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

The *OPAL* KSP: status update

[1,4]D. Polychroni, [2,4]P. Simonetti, [3,4]R. Politi, [1,2]D. Turrini,
[3]S. Fonte, and the OPAL team

1. INAF- OATo; 2. INAF-OATs; 3. INAF-IAPS; 4. ICSC

Spoke 3, II Technical Meeting, Bologna 17-19/12/2024

OPAL is:

- **A PNRR Key Science Project** with two goals:

  - produce a *library of detailed synthetic atmospheric models of giant planets* for the Ariel space mission (Turrini+2018; Edwards+2019)

  - port the *Arχes* planet formation suite of codes to *HPC*

Takes advantage of allocated time in:
Leonardo (4 million core hours)
Pleiadi (2.5 million core hours)

as well as the dedicated cluster GENESIS+.

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Check P. Simonetti's talk tomorrow!

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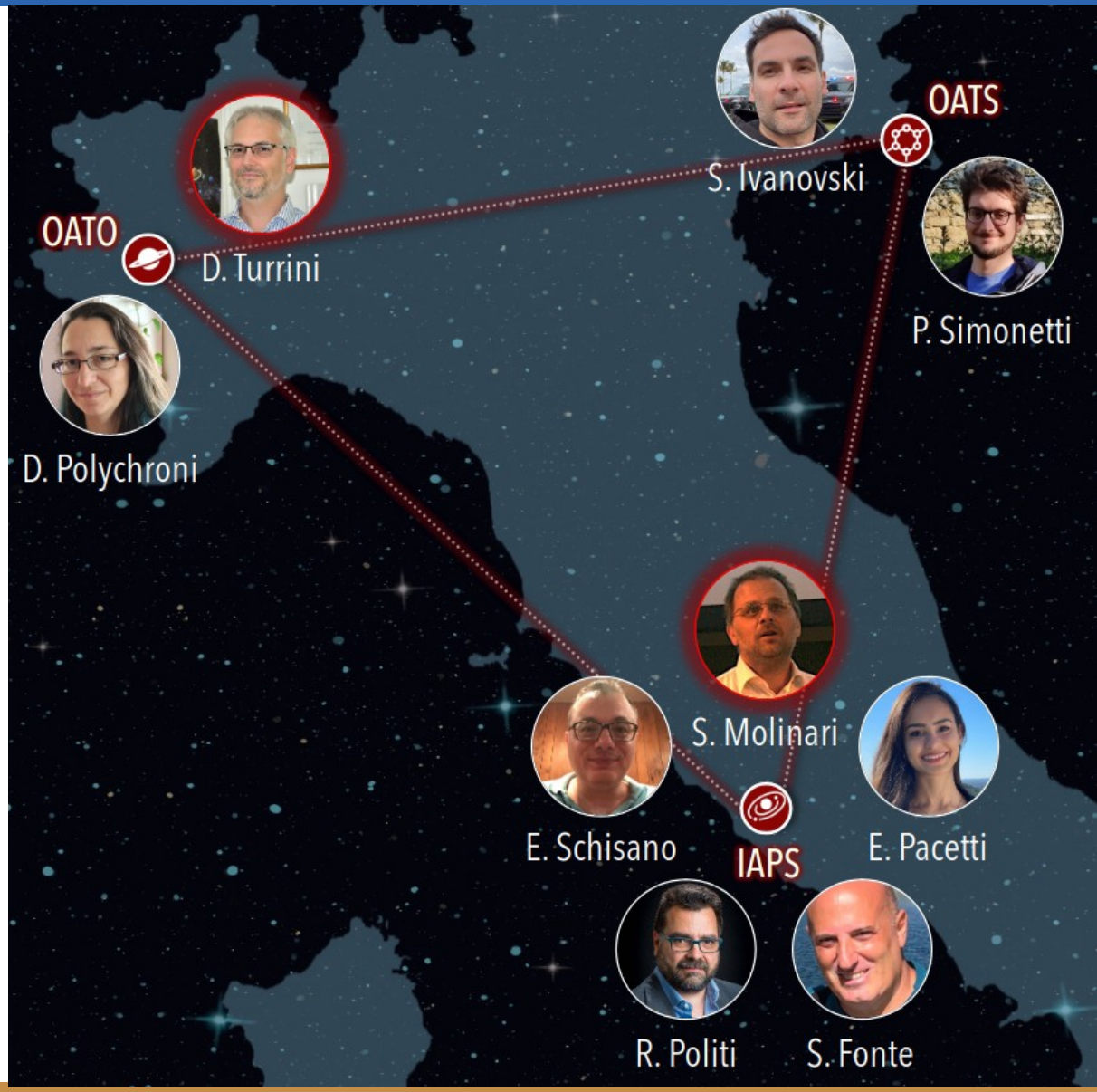
Meet the OPAL Team!

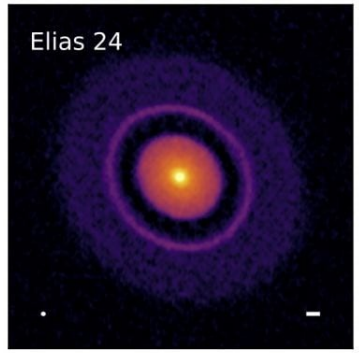
We do:
- Modelling
- Observations
- Computational science

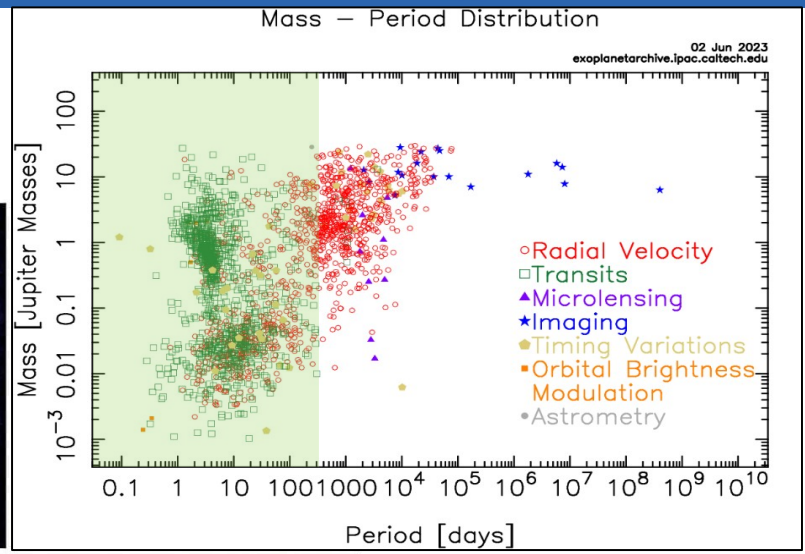
We focus on:
- Star formation
- Planet formation
- Solar system
- Exoplanets

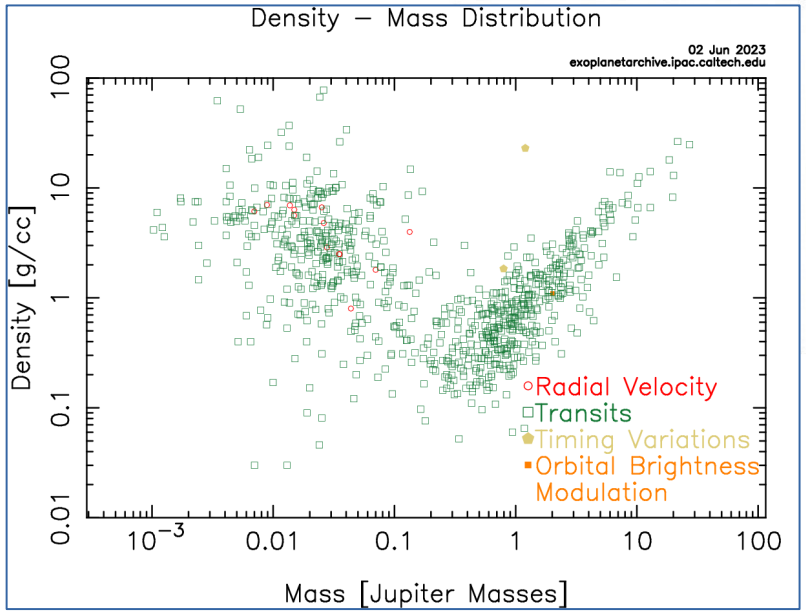


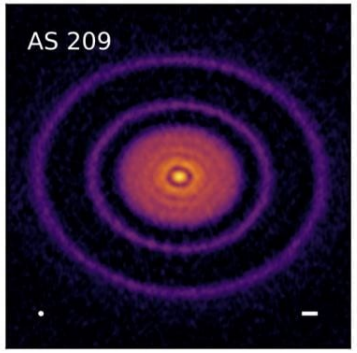
Why do we need the OPAL project?

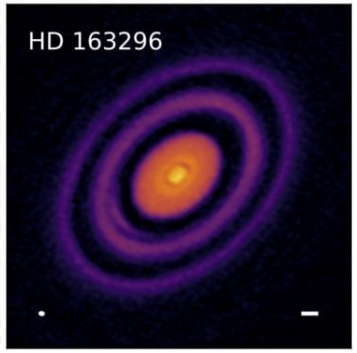
- New observational data highlight our limited understanding of where planets form in disks











- Planets form and evolve under a wider range of conditions than previously thought.

Modern Challenges in Planetary Formation

Which **processes in disks** shape the **observable properties of planets**?

- **Planet formation**
  accretion (gas/solid)
  orbital migration
- **Planet Composition**
  disk evolution
  disk chemistry

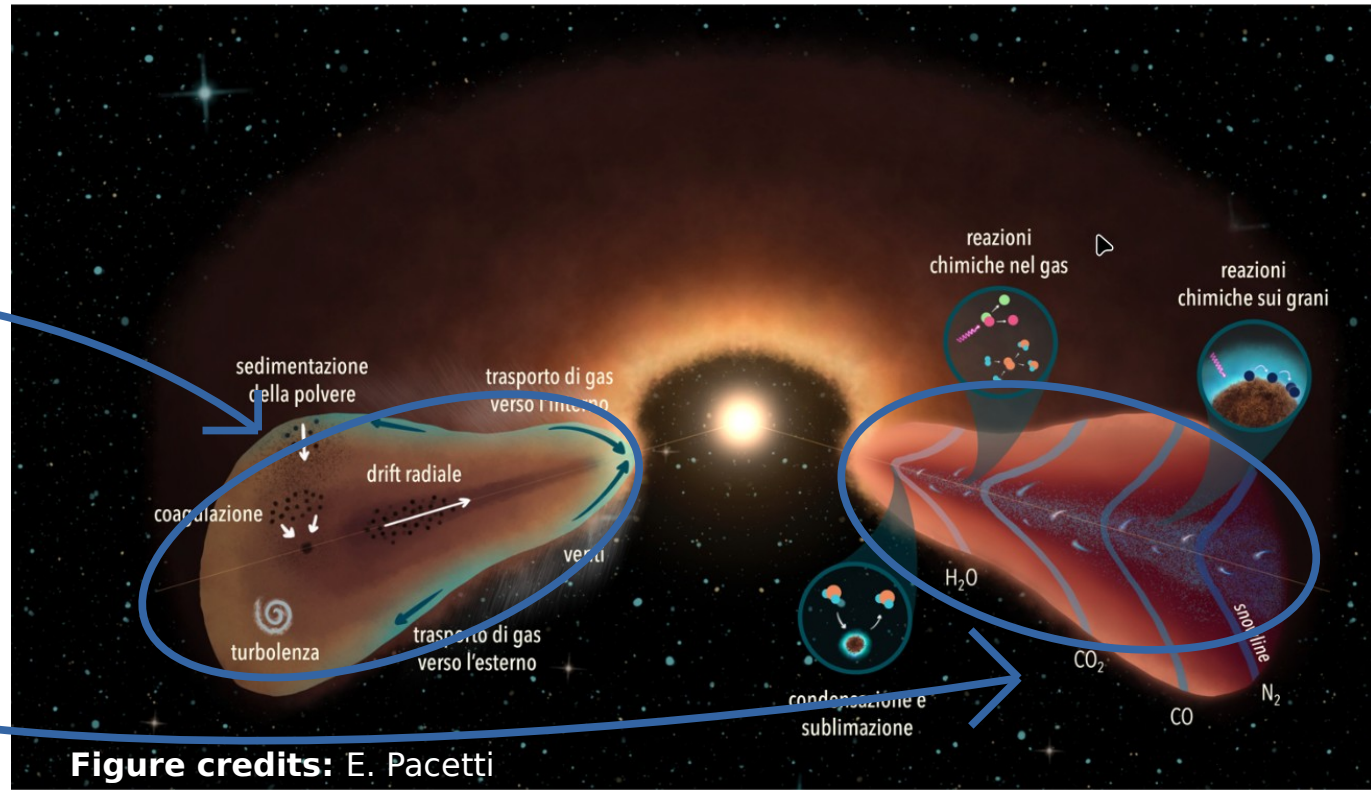


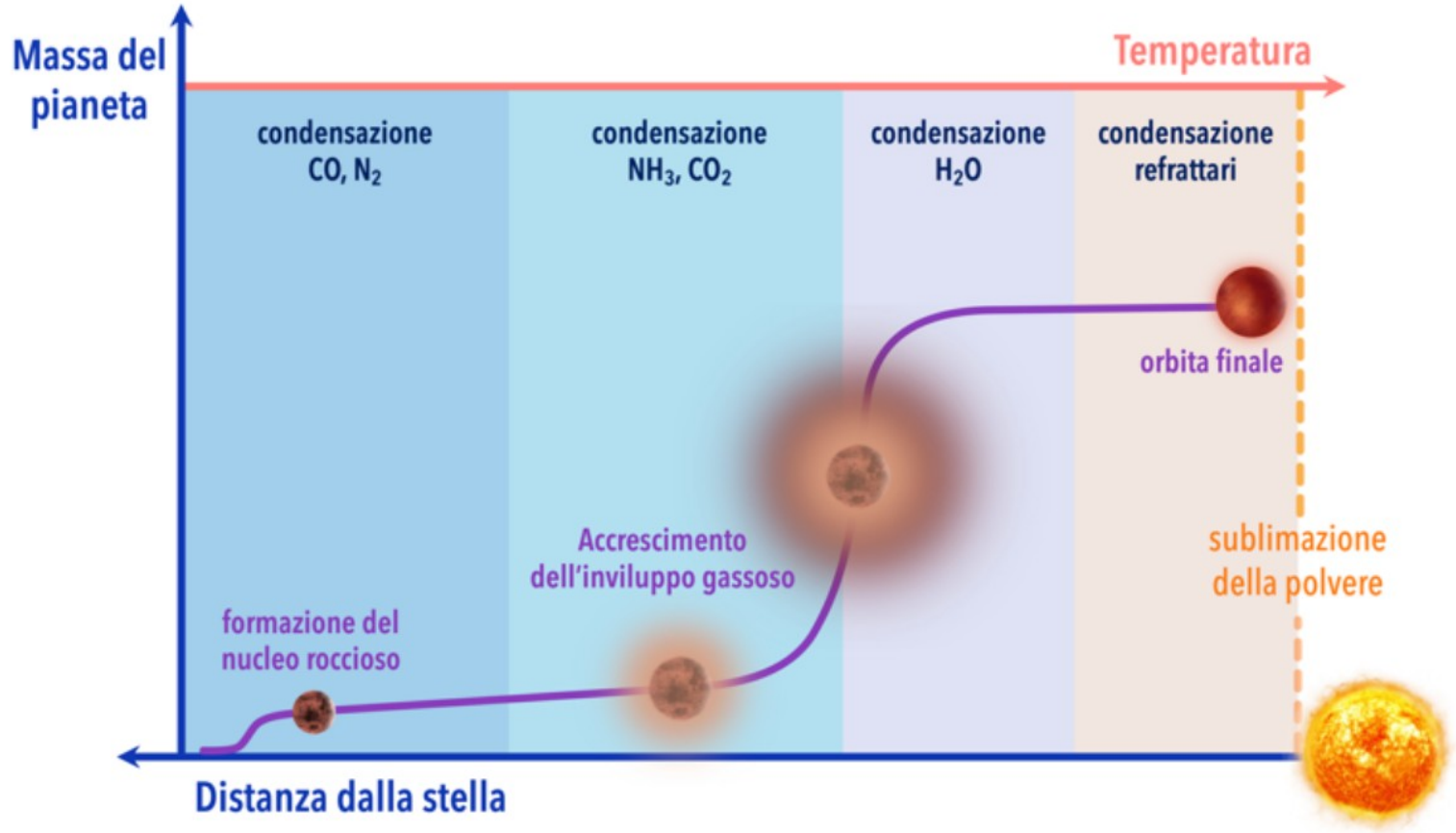
Figure credits: E. Pacetti

Modern Challenges in Planetary Formation

Which **processes in disks** shape the **observable properties of planets**?

But the you also have:

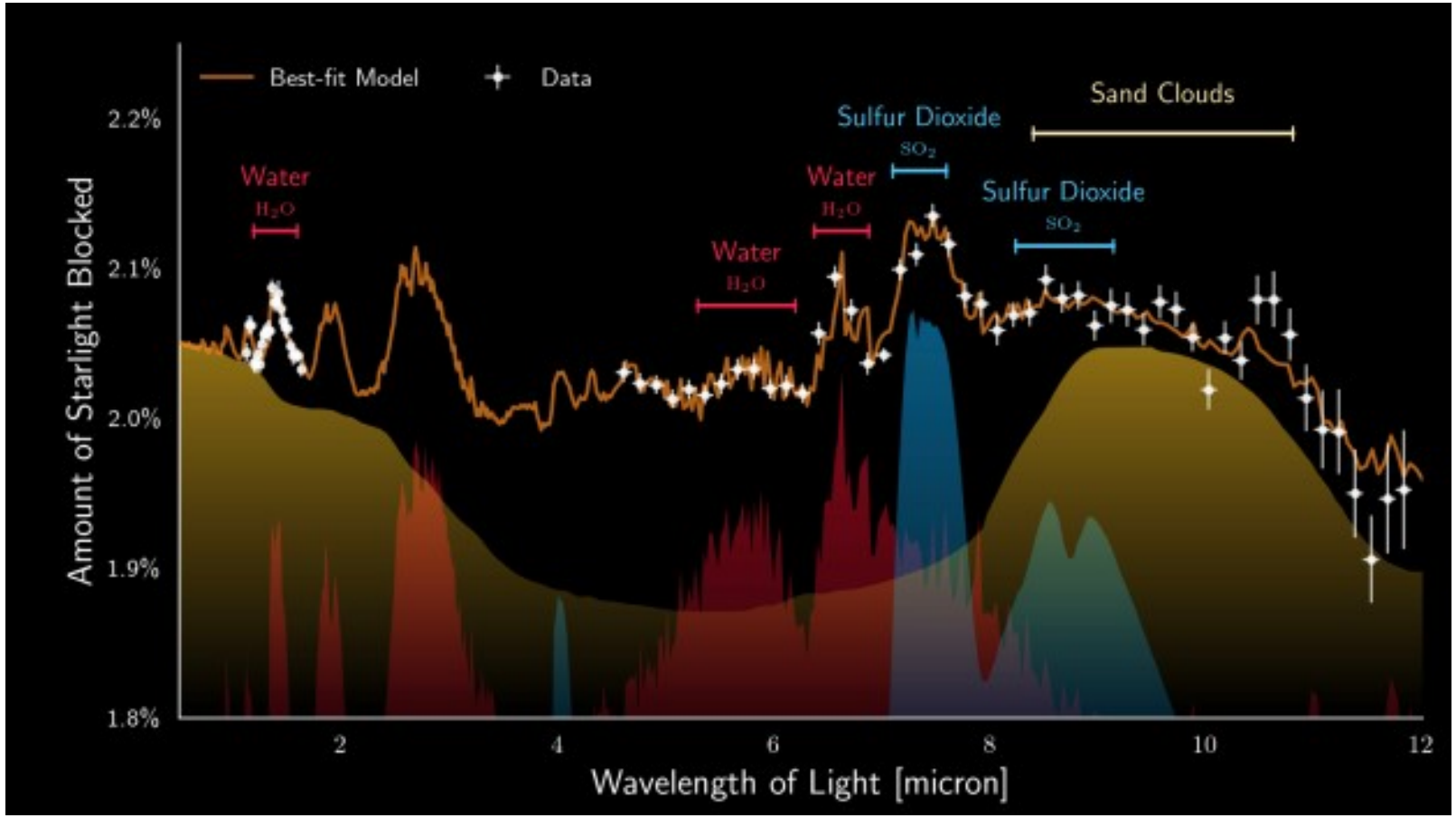
Evolution and Migration and Stochastic Events (collisions/expulsion of planets)



Modern Challenges in Planetary Formation

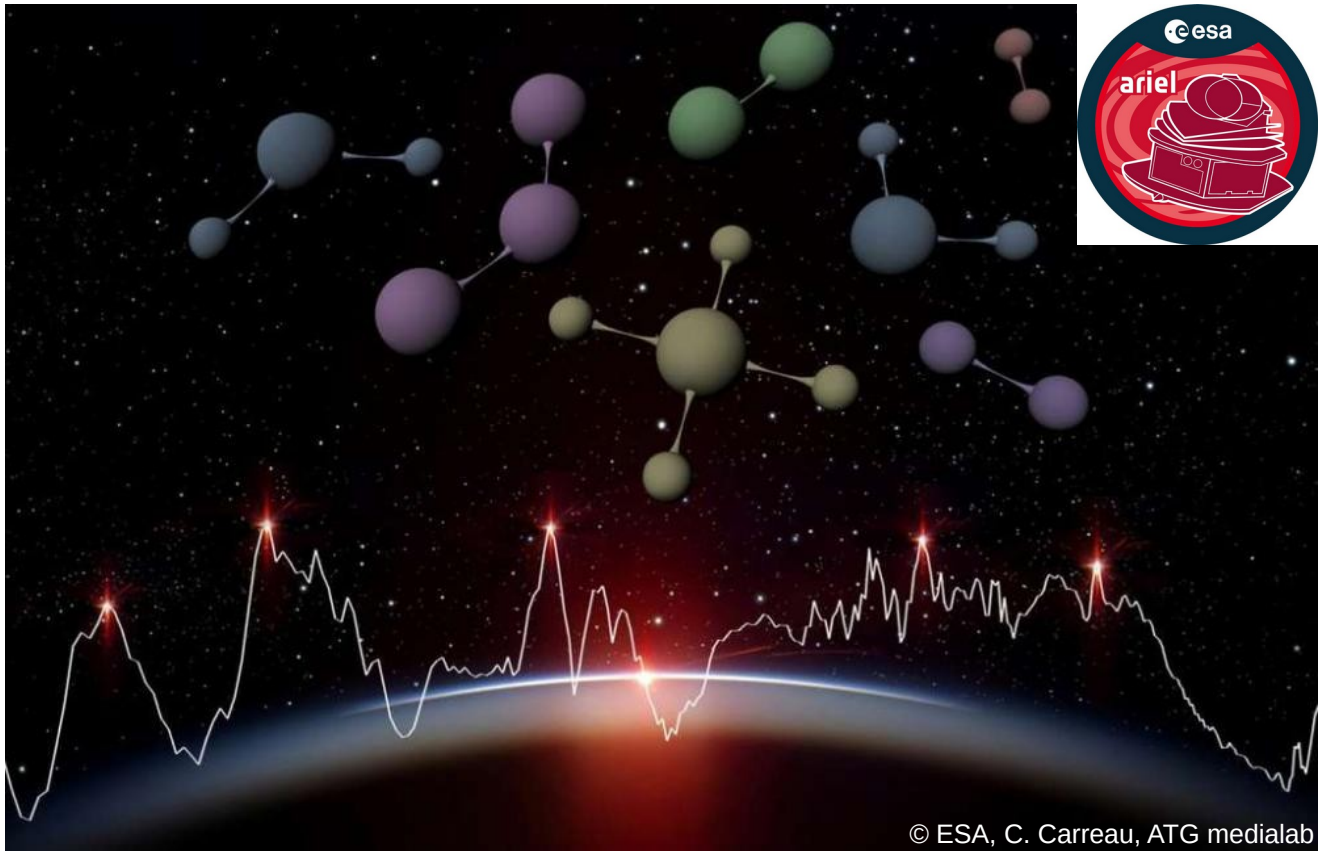
What ***can*** we observe?

Atmospheres Basically

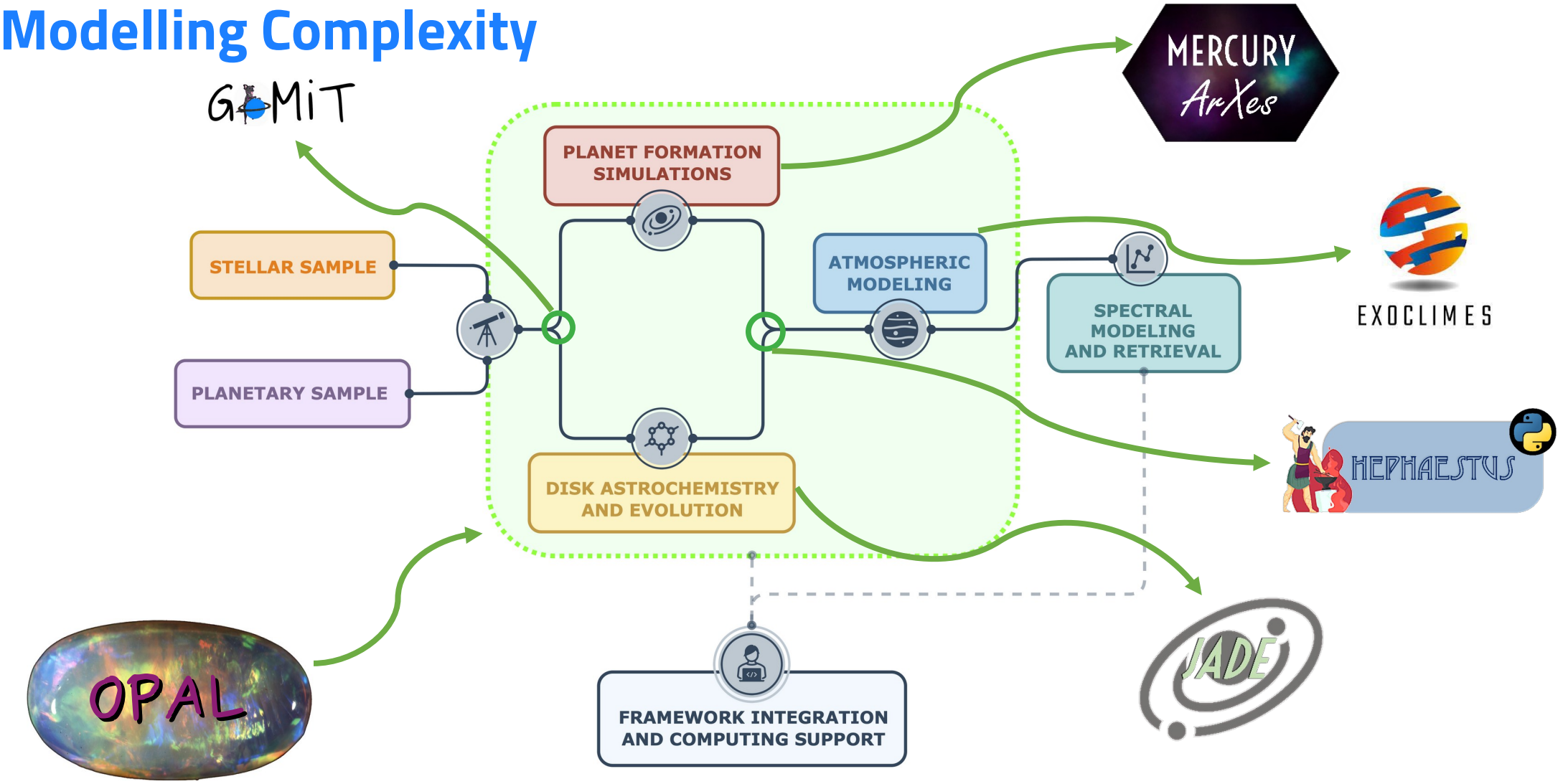


A Library of Synthetic Planetary Atmospheres

OPAL is the ongoing program to create an unprecedented library of end-to-end synthetic (exo)-planetary atmospheres, informed by actual data, using the **Arχes** suite of codes, to predict and consolidate what molecules can be detected in the planetary atmospheres that the ***Ariel Space mission*** will observe



OPAL: Modelling Complexity



Where we are now

- Design Phase is finished:
  - First systems to simulate chosen, their physical parameters 'frozen'
  - Initial conditions are set

- 1st batch of simulations with Mercury-Arχes are done

- Jade simulations on the way

- The next batch of Mercury-Arχes are going to be launched these days

- **Vulcan synthetic atmospheres will be launched once Jade simulations are ready**

We should have the first complete synthetic atmospheres ready to be released in March/Arpril 2025

OPAL: Modelling Complexity

JADE (Pacetti et al. in prep.) is the multi-language (Python + Fortran) data-parallel code to jointly simulate the ***physical and chemical evolution of protoplanetary disks*** of the *Arxes* suite.

Mercury-Arχes (Turrini+2019,2021) is the parallel n-body code of the *Arxes* suite incorporating physical libraries to simulate ***planet formation in protoplanetary disks*** (see tomorrow's presentation).

HEPHAESTUS (Turrini+2021; Pacetti+2022) is the Python compositional post-processing tool of the *Arxes* suite that resolves planetary compositions across 20+ elements.

FastChem and **Vulcan** are atmospheric modelling codes from the University of Bern's *ExoClimes* suite that convert Hephaestus' elemental compositions into atmospheric molecular compositior (e.g. Fonte+2023).

OPAL: Modelling Complexity

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Arxes

Mercury-
physical l
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sitional

An extra word on Vulcan:

We (*Paolo Simonetti*) are expanding the chemical network of Vulcan to also include the condensation and sedimentation of iron!

(and soon also the silicates!)

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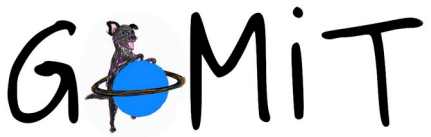
EXOCLIMES

GroMiT: The new kid in town!

GroMiT, the *Gro*wth and *Mi*gration *T*rack code, tracks how a forming planet accretes pebbles and gas as well as how it migrates depending on the local environment of its native circumstellar disk (e.g. Johansen+2019, Ida+2016, Tanaka+2020).

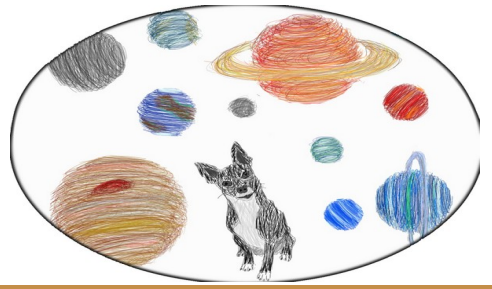
Born as a plug in for *Mercury-Arχes* to make it self consistent it found plenty of applications also a stand alone in exploring the formation histories of ***observed planets***.

Used in **OPAL** to consolidate the initial conditions of the simulations run with *Mercury-Arχes* and *Jade*

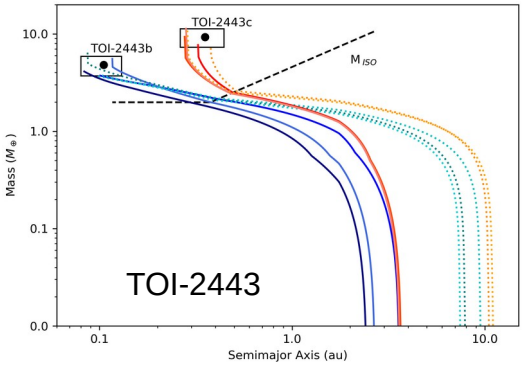


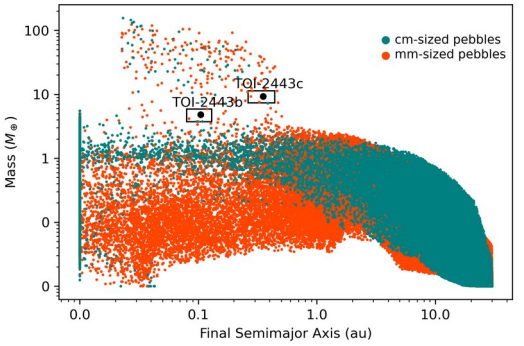
It comes in two flavours!

→ Single Planet Mode
(Polychroni+2023)



→ Population Synthesis Mode
(Polychroni+ in prep)





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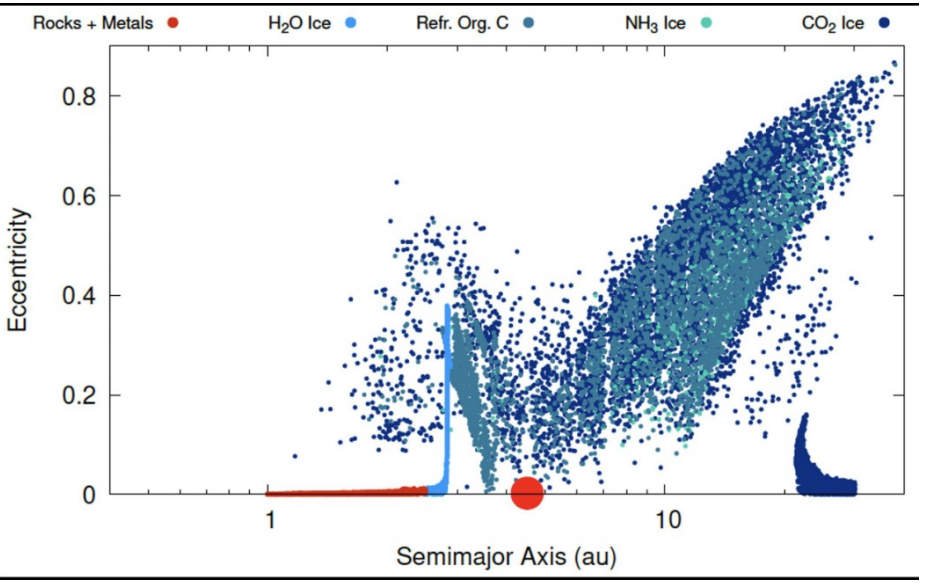
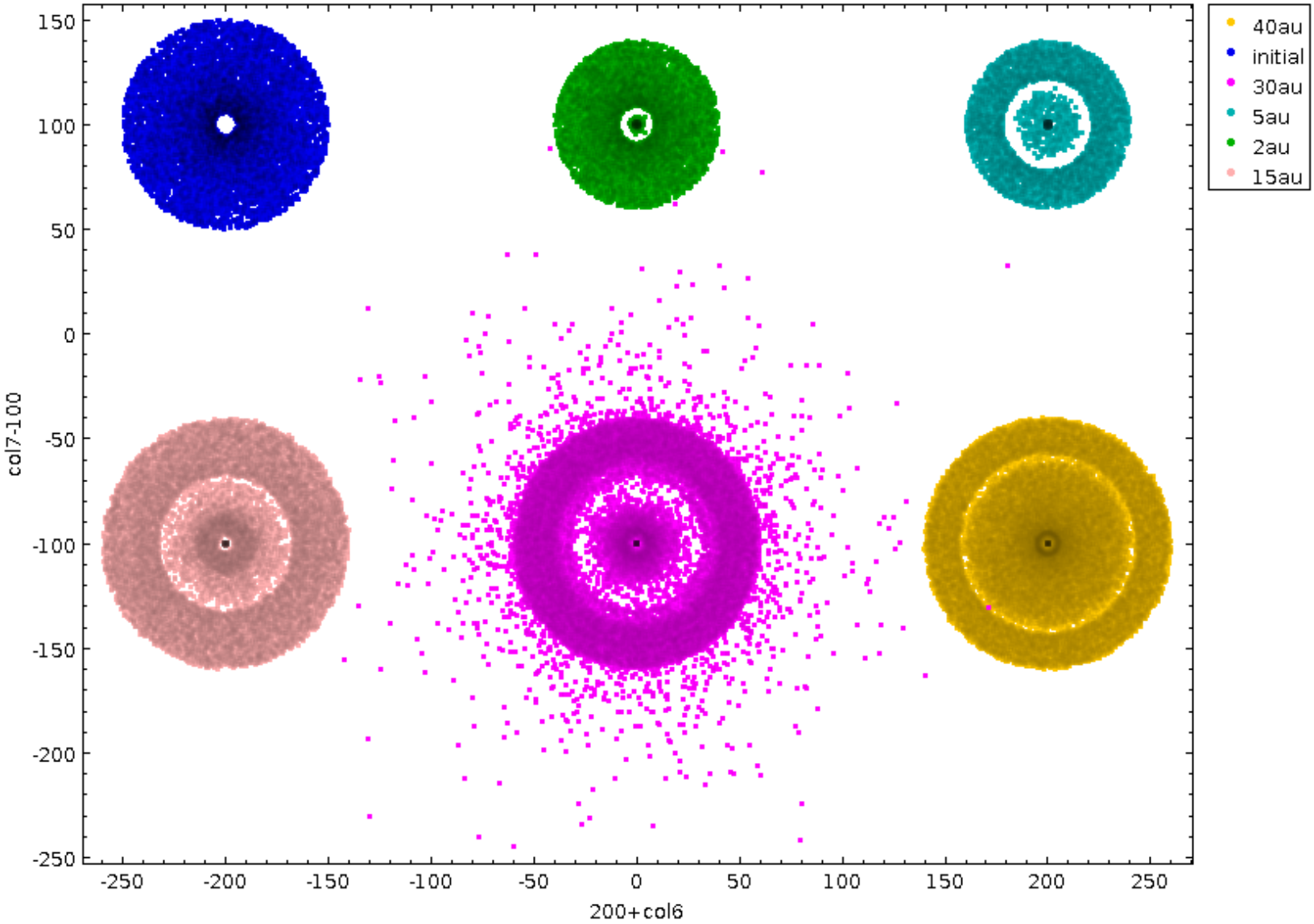
Where we are now

- First results with Mercury-Arχes

For **one** stellar system (Ariel defined) with **one** set of initial parameters **TEN possible** formation paths





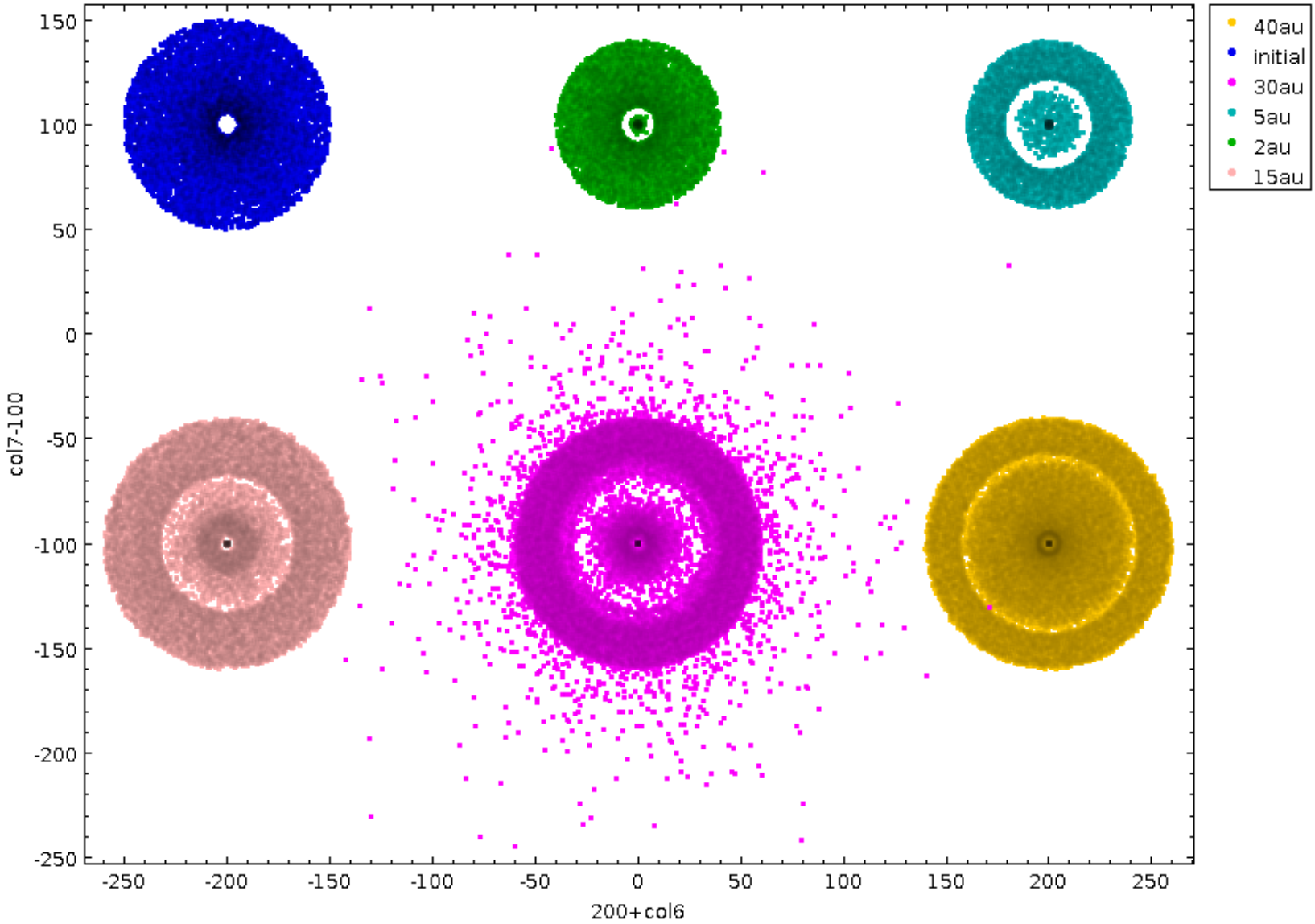
Where we are now

- First results with Mercury-Arχes

For **one** stellar system (Ariel defined)
with **one** set of initial parameters
TEN possible formation paths

(Historic overview)
one such simulation *before parallelisation* Mercury-Arχes:
Duration: ~3-4 months on GENESIS
after parallelisation:
Duration: ~3-4 weeks on GENESIS
~3-4 DAYS(!!) on Leonardo

Remains to be seen the GPU version



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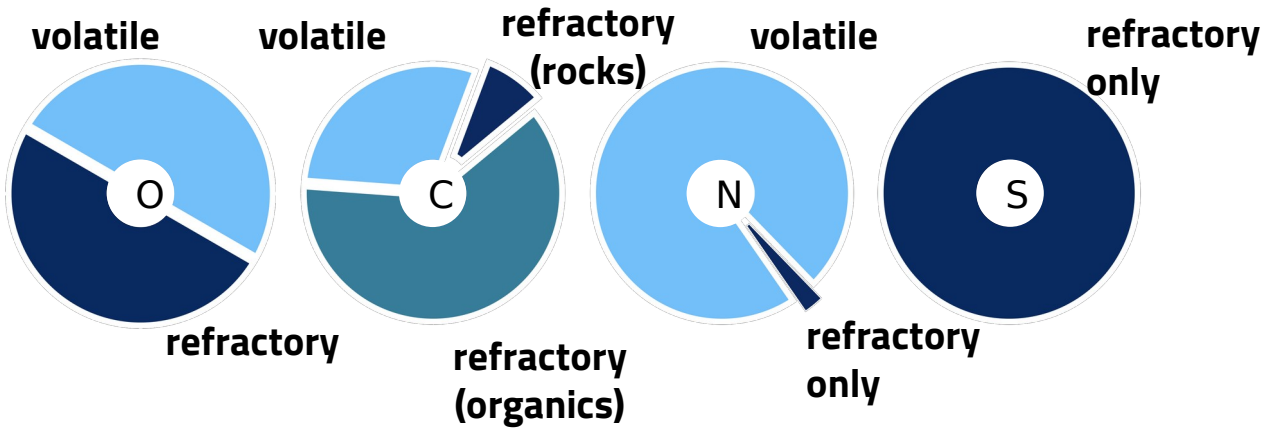
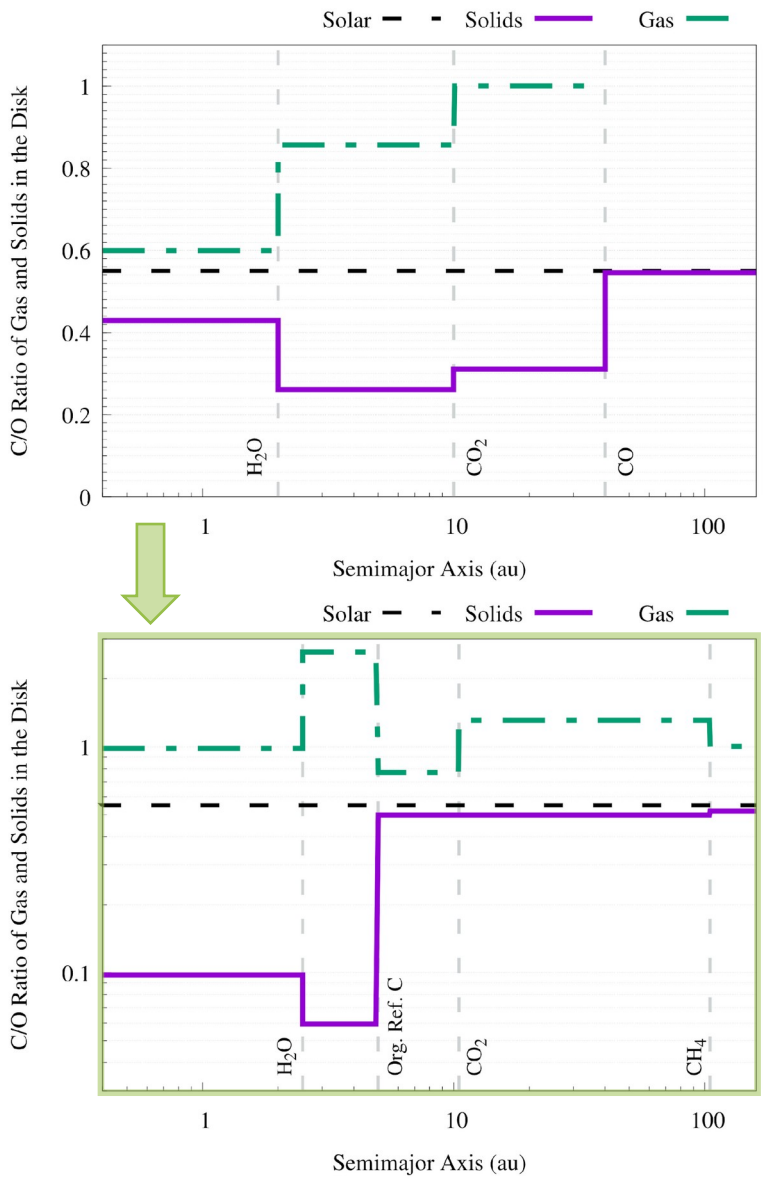
Where we are now

Jade Input for Circumstellar Disks

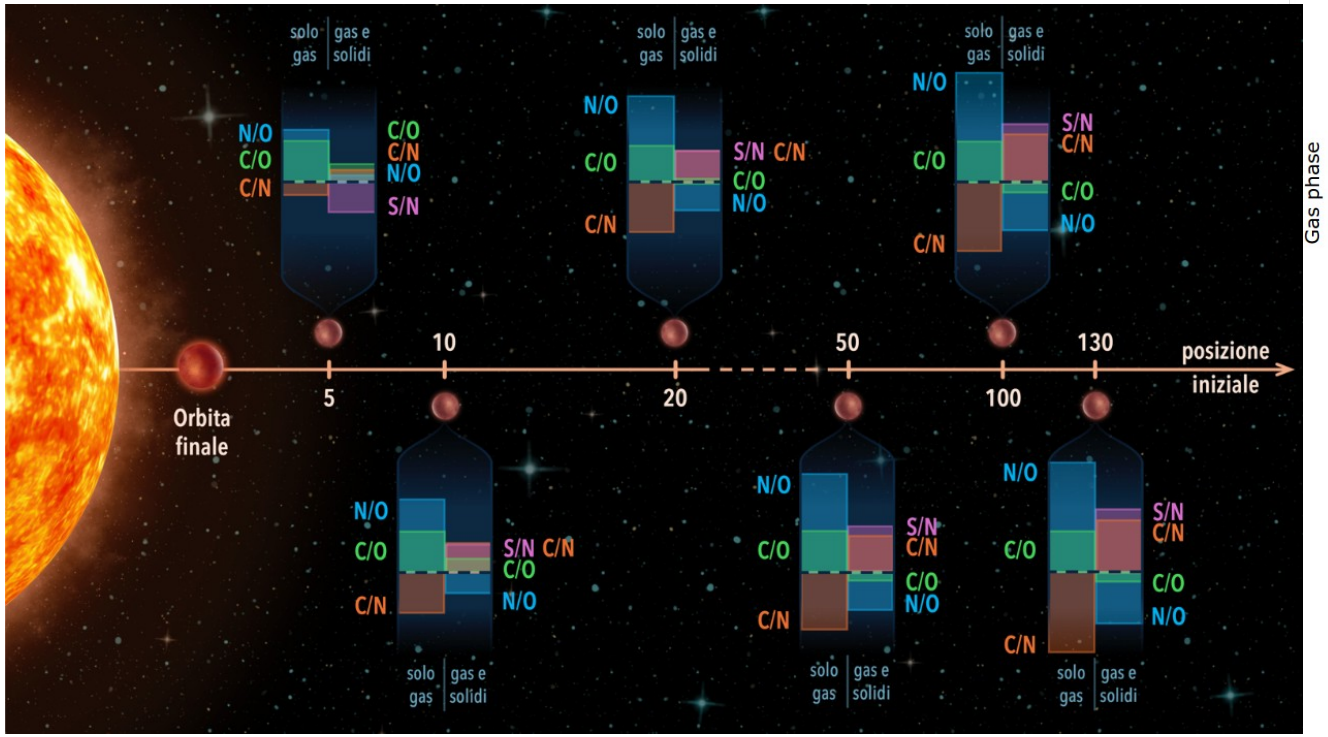


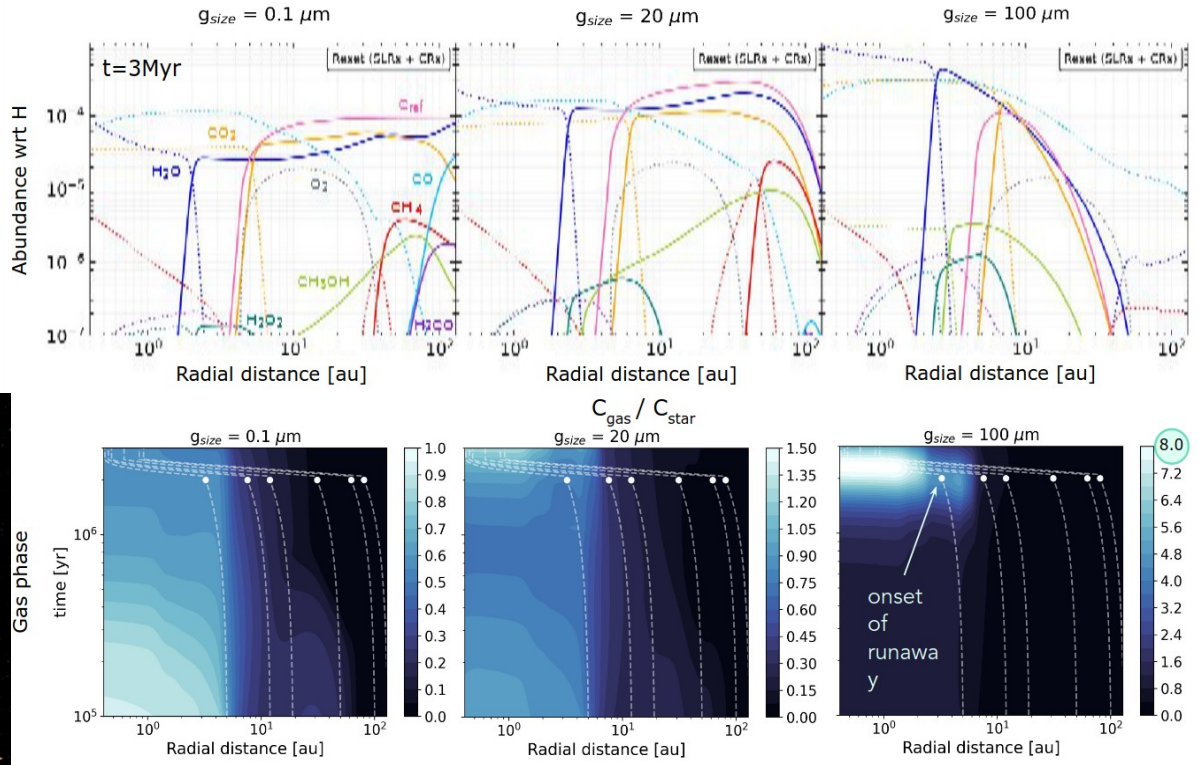


Where we are now

Jade Output:

Gas + Solids output





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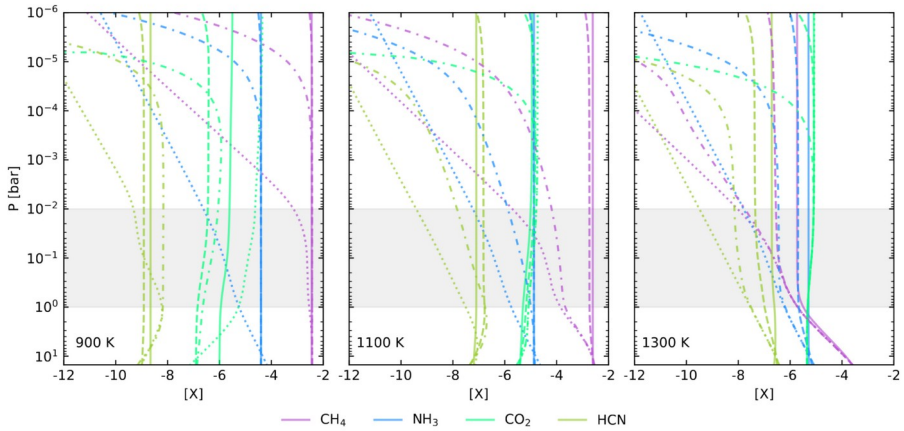
Where we are now

Chemical disequilibrium model with mixing, condensation/sedimentation & photochemistry

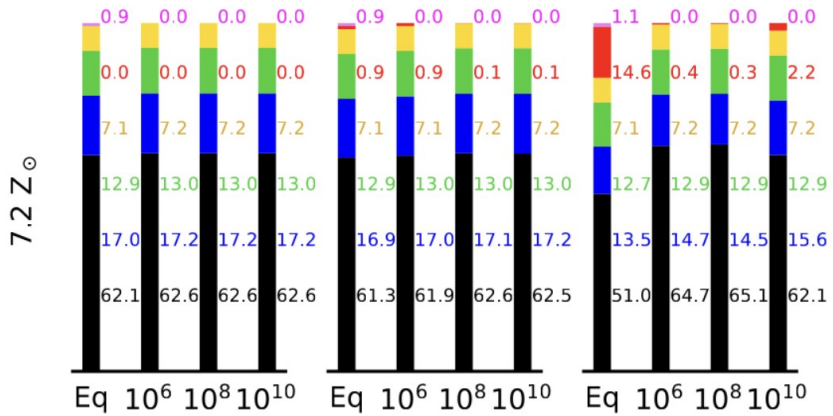
- chemical network expanded to include Mg, Si and Fe species
- recipes for the condensation and sedimentation of these refractories

Used to expand investigation of oxygen deficit (Fonte+23) & abundances of S-bearing species

Vertical atmospheric profiles



Integrated abundances



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Where we are now

OPAL progress:

GroMiT: completion: ~70%; Code operational, needs to be parallelised & optimised (in progress)

Mercury-Arχes GPU porting: ~75% ; check P. Simonetti's presentation tomorrow

Simulation Campaign: ~10% ; so much more to come.

Still need to define: Repository and database for the completed simulations

OPAL as a Key Science Project

- The **seed of OPAL** is part of the Ariel-IT 2025's activities: its scope and planetary sample are widening as support from ***INAF Pleiadi*** and ***Leonardo*** became available.

- OPAL is the **next frontier in computational planetary science**: combining multi-domain and multi-physics *ab initio* simulations to fully understand the information encoded into planetary atmospheres.

- **Our community is currently the most advanced** in this integration of expertise and code in a unified scientific and computational ecosystem in disk-planet-atmosphere formation.

OPAL is a coordinated effort between the ARIEL, INAF and the PNRR