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ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

From Planet Formation to Bio-signatures: An OPAL for the Habitable Worlds Observatory

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

Shapping the Italian Contribution to HWO
Università La Sapienza, Rome, 10-11/07/2027

Goals

- Create a library of realistic young planetary atmospheres taking into consideration multiple possible planet formation scenarios and disk chemistry combinations, in the ambit of the **ESA Ariel space mission.**
- Identify and fix any 'kinks' in the pipeline (coordination between 6 codes.)

An OPAL For HWO

Observing planets down to Earth size in the habitable zone will be ground breaking.

Spectrally characterising them and getting an idea of potential atmospheres and possible bio-signatures will be even better.

But you might want to know a priori what these spectra might look like (i.e. potential atmospheric composition of atmospheres due to their formation path). Before and after you include the instrumentation noise.

And what molecules are the most reliable and informative tracers to go for.
(bonus: once observed we can use OPAL to understand their potential formation paths!)

One slight issue: **we don't** actually **know** exactly **how planets form** (Burn & Mordasini 2025). The initial parameter space is huge!

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

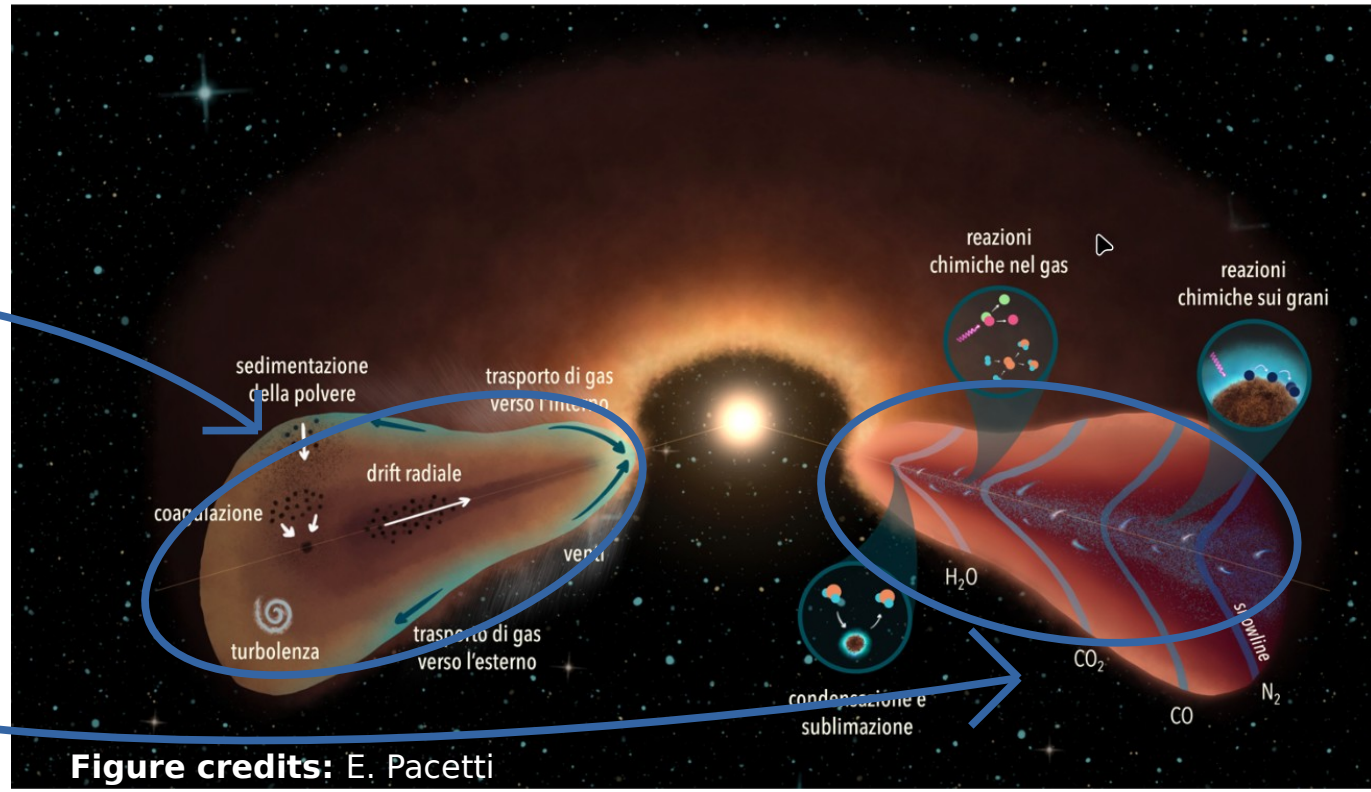


Figure credits: E. Pacetti

Modern Challenges in Planetary Formation

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

But you also have:

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

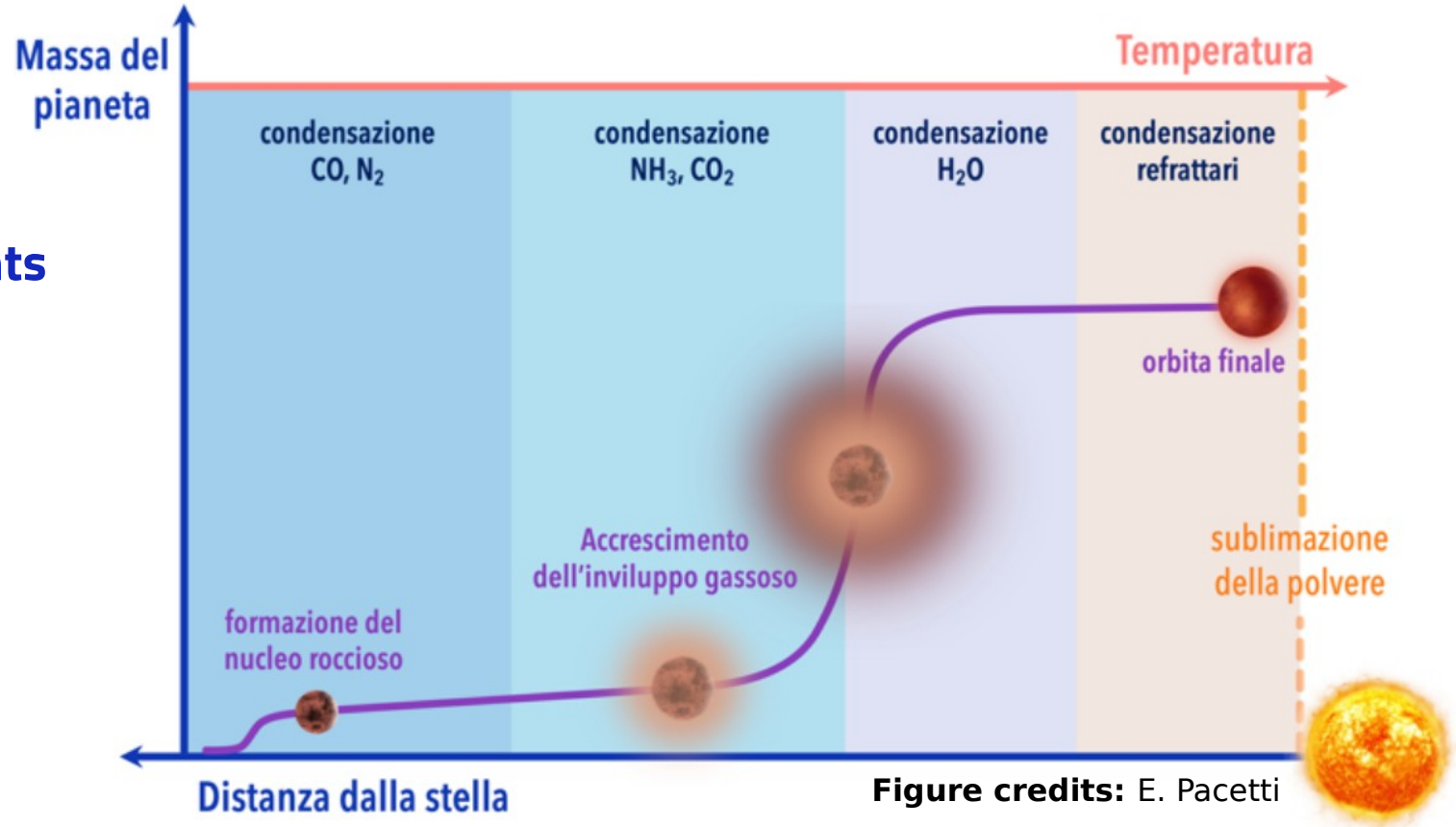


Figure credits: E. Pacetti

OPAL is the combination of two large computing programs at ICSC Leonardo (4 Mcore-hours) and INAF Pleiadi (2.5 Mcore-hours) and leverages on the Arxes and Exoclimes modeling suites to **simulate the atmospheric diversity of giant exoplanets arising from their formation environments and histories,** building on the pathfinder Ariel Synergy study.

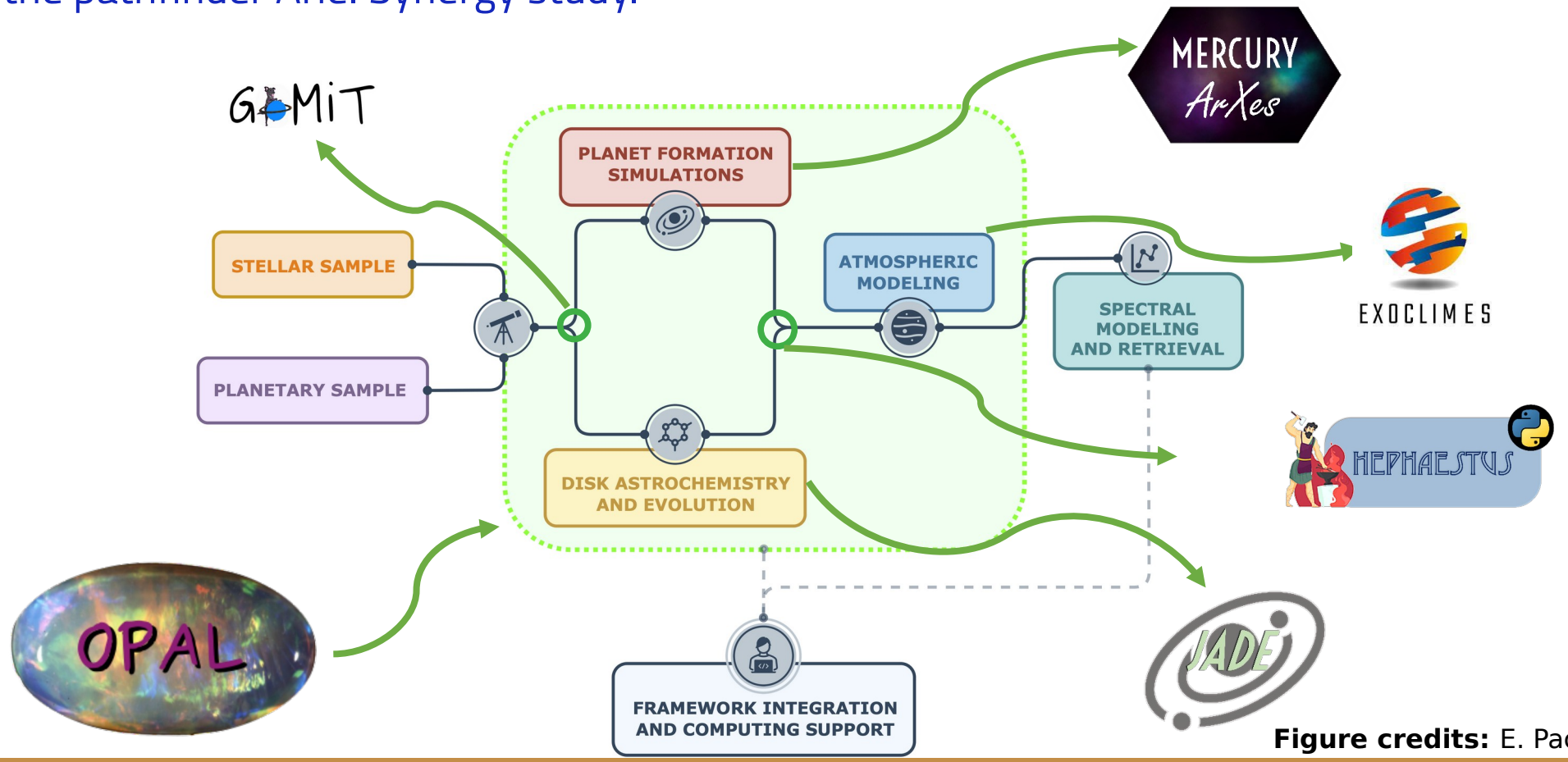
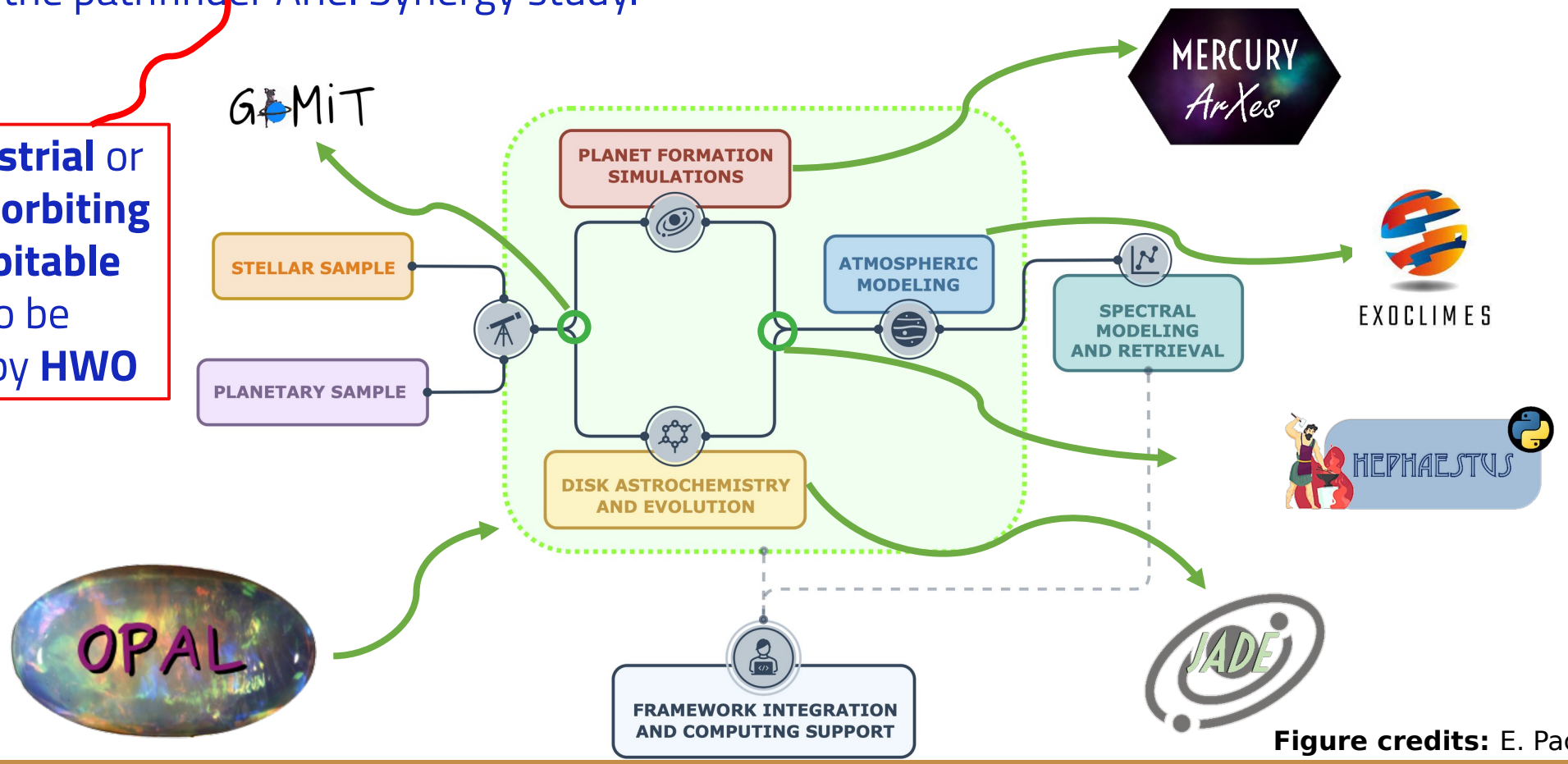


Figure credits: E. Pacetti & D. Polychroni

OPAL is the combination of two large computing programs at ICSC Leonardo (4 Mcore-hours) and INAF Pleiadi (2.5 Mcore-hours) and leverages on the Arxes and Exoclimes modeling suites to **simulate the atmospheric diversity of giant exoplanets arising from their formation environments and histories,** building on the pathfinder Ariel Synergy study.

Read **terrestrial** or any **planet orbiting** in the **Habitable Zone** to be observed by **HWO**



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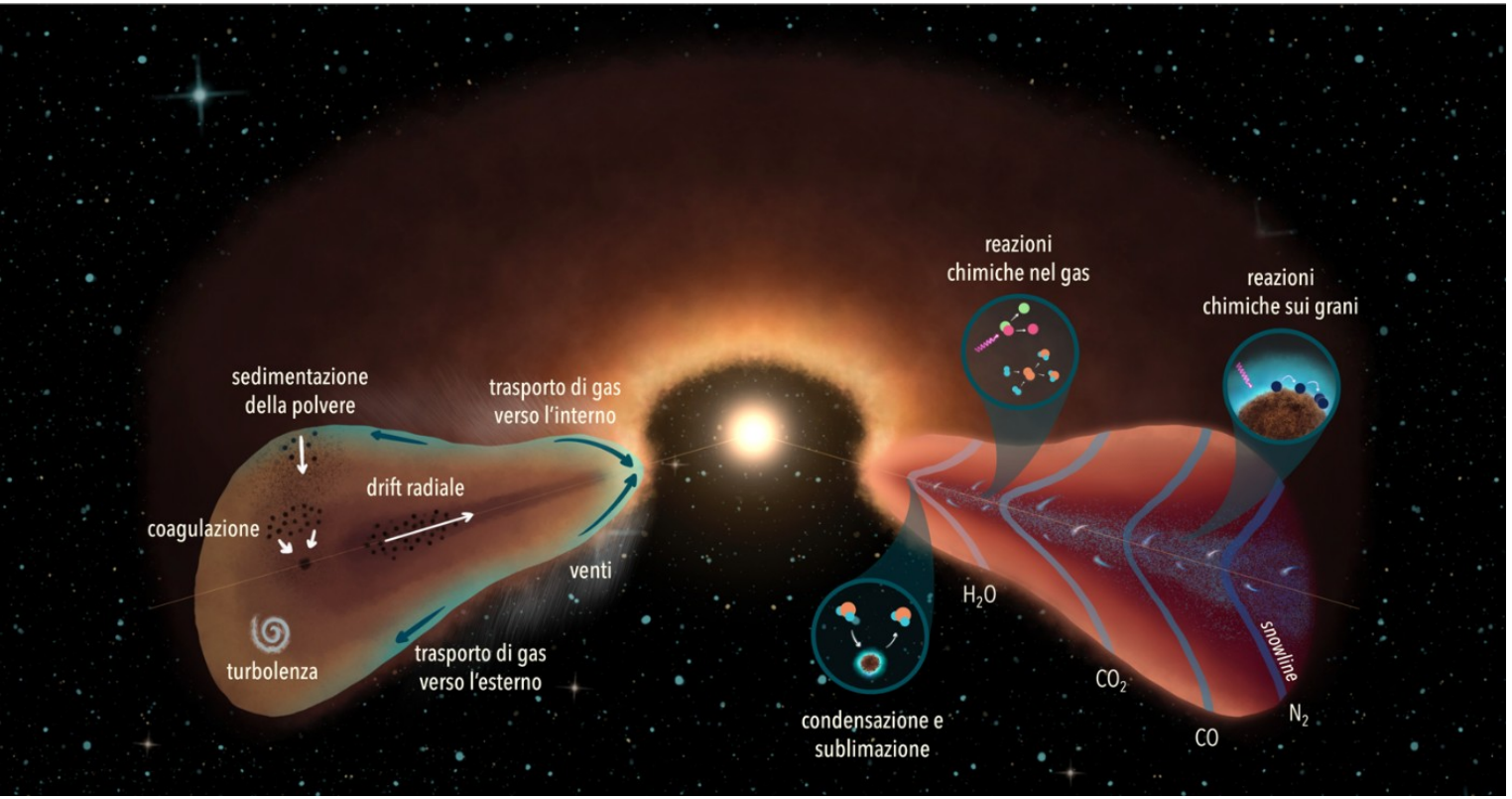
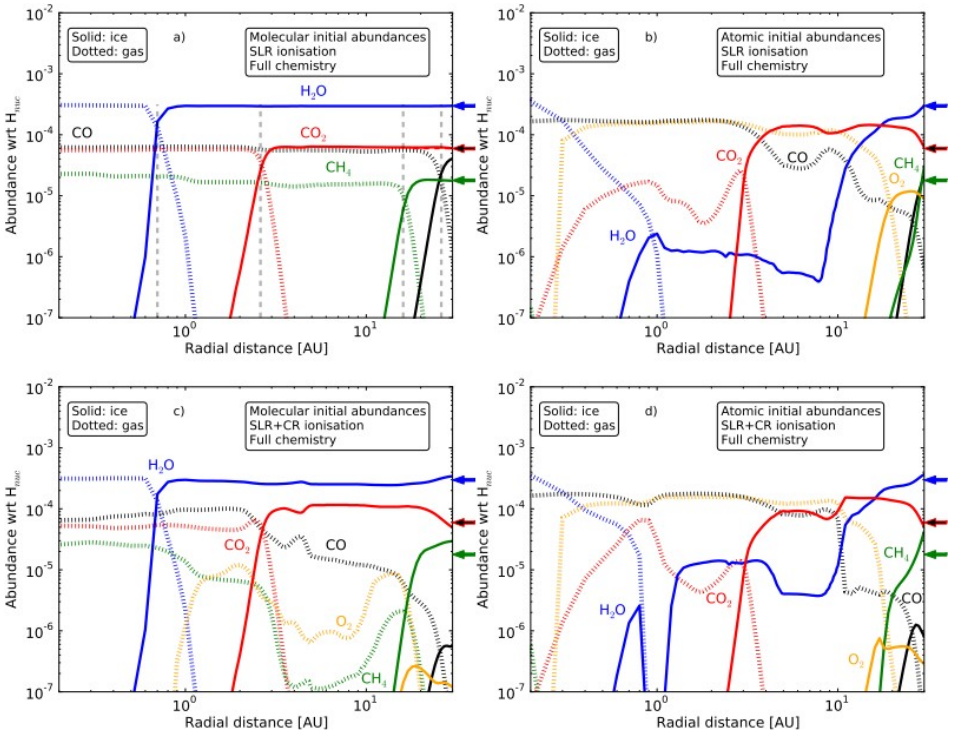
Star – Disk Link





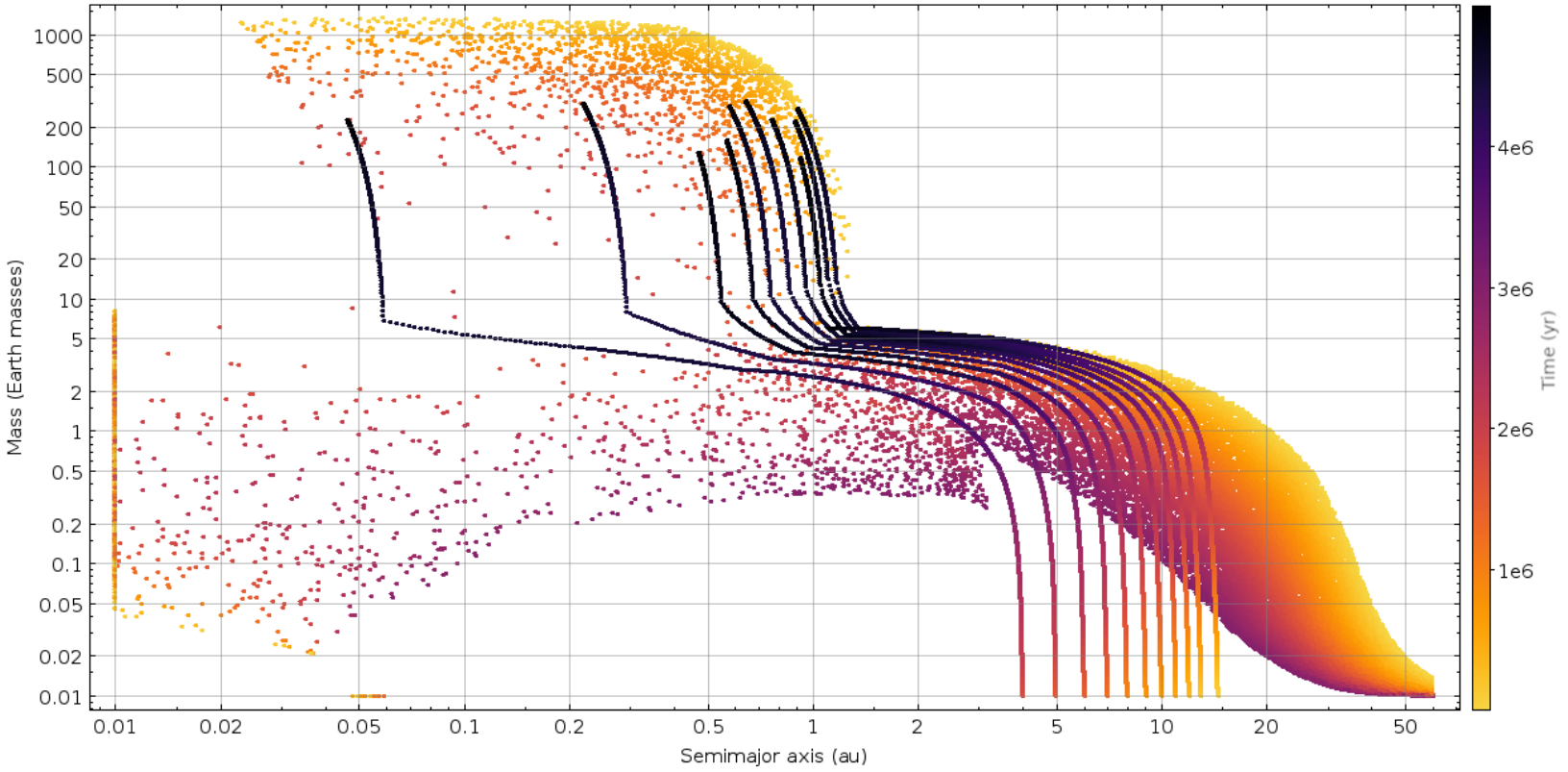
JADE (Pacetti+2025) is the multi-language (Python + Fortran) data-parallel code to jointly simulate the physical and chemical evolution of protoplanetary disks of the Arxes suite.

Disk – Planet Physical Link

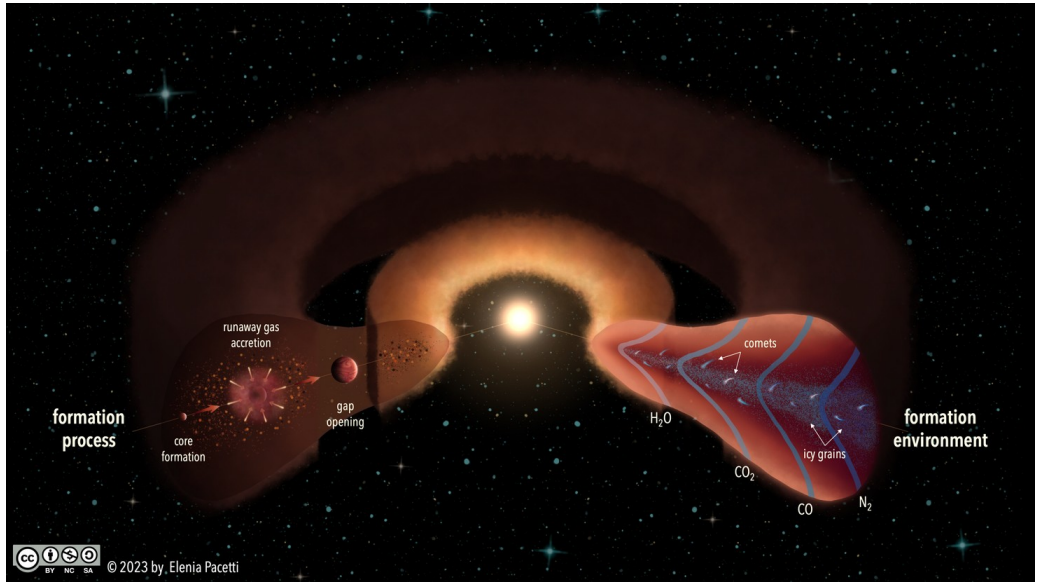
MGroMiT is a population synthesis code that tracks how forming planets accrete pebbles and gas and migrate depending on their native disk environment assuming the ***pebble accretion model***

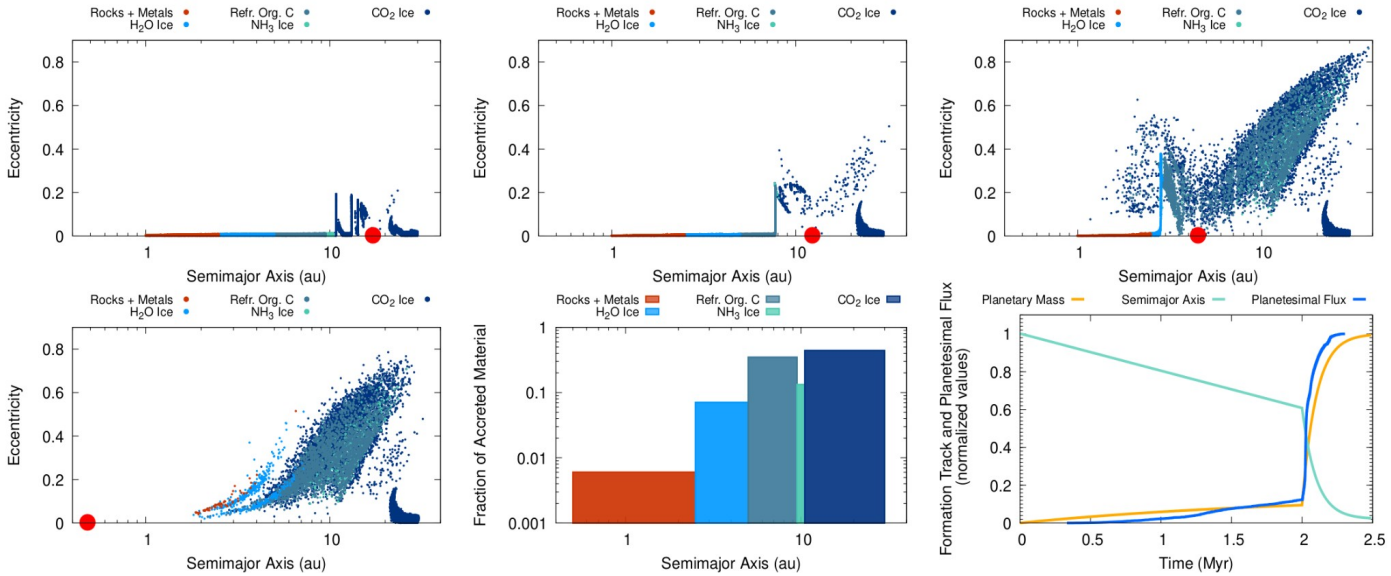
(Polychroni+2023; Mantovan+2024; Damasso+2024; Filomeno+2024; Naponielo+2025; Zingales+2025).

MGroMiT



Disk – Planet Compositional Disk





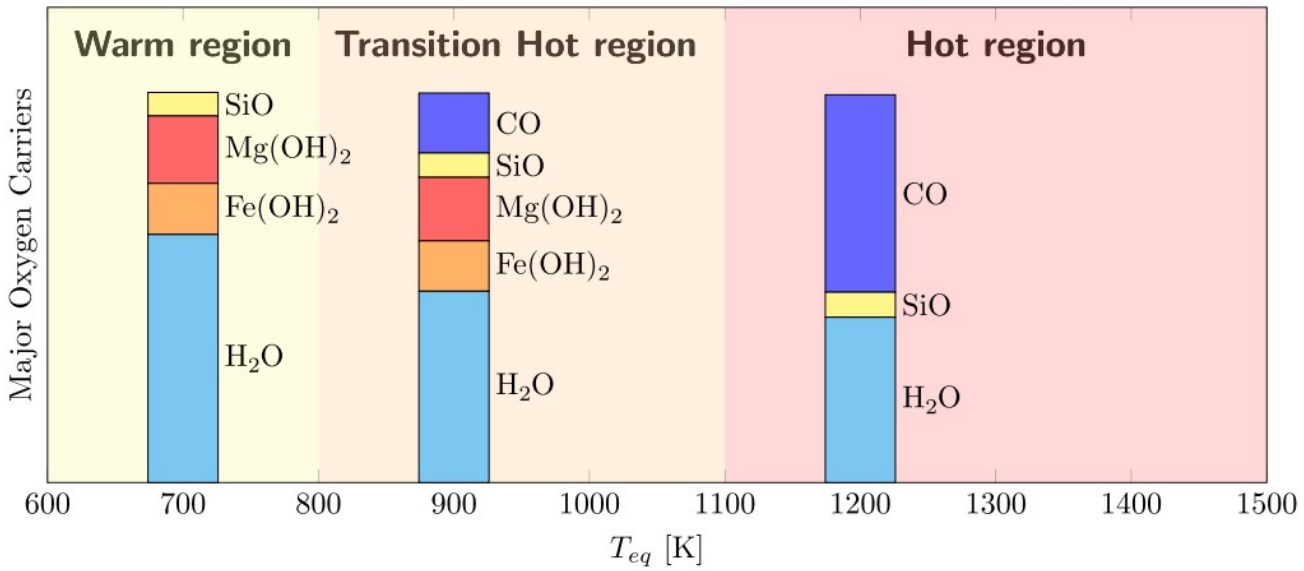
Mercury-Arχes (Turrini+2019,2021) is the parallel n-body code of the Arxes suite incorporating physical libraries to simulate planet formation in protoplanetary disks.

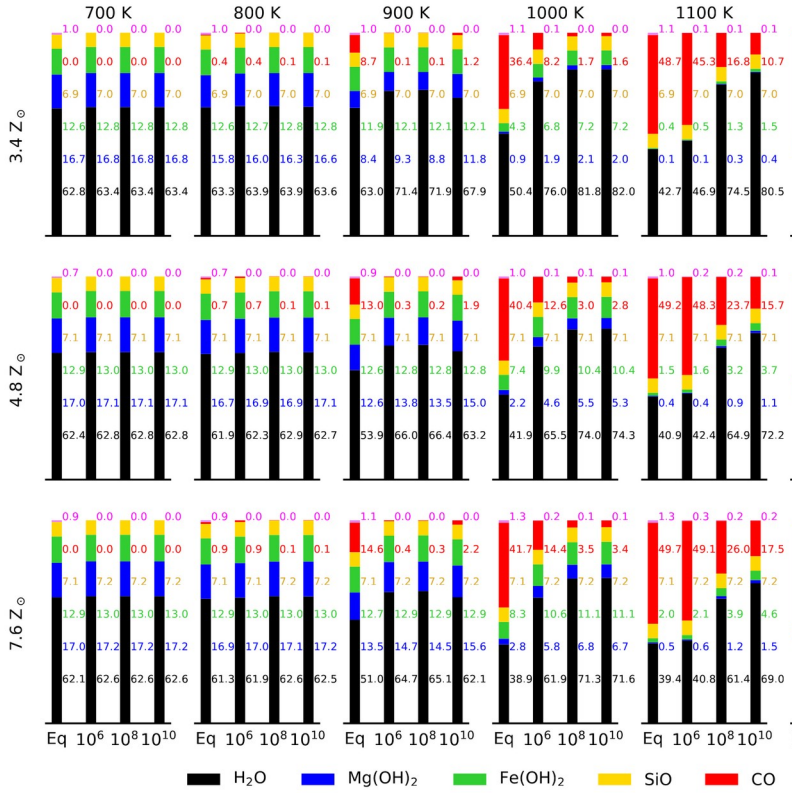
HEPHAESTUS (Turrini+2021; Pacetti+2022) is the Python compositional post-processing tool of the Arxes suite that resolves planetary compositions across 20+ elements.

Planet – Atmosphere Link

The previous steps provide the planetary elemental compositions. The use of the atmospheric modelling codes **FastChem** (Stock+2018, 2022) and **Vulcan** (Tsai+2017, 2021) from the *ExoClimes suite* allows us to convert Hephaestus' elemental compositions into *atmospheric molecular compositions* (e.g. Fonte+2023, Simonetti+ under revision).

EXOCLIMES

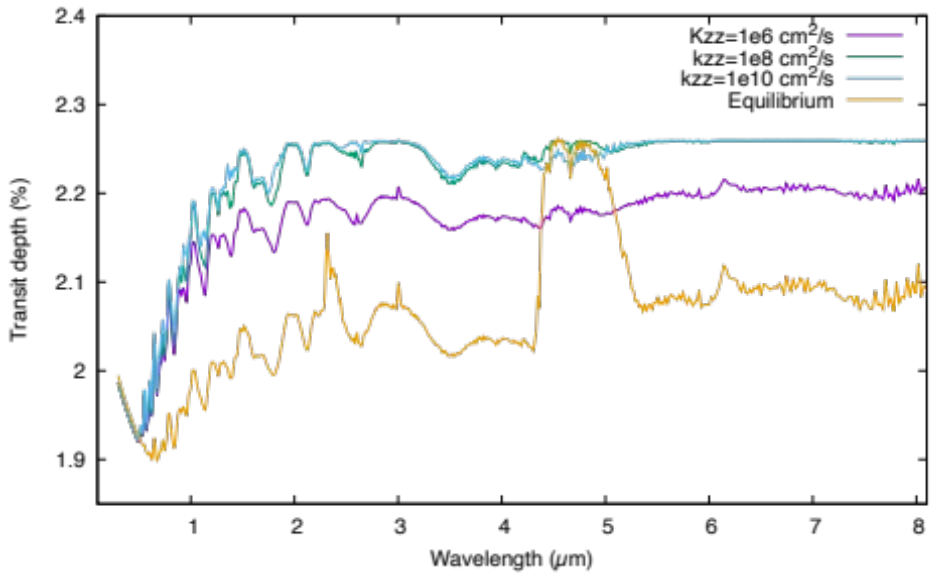




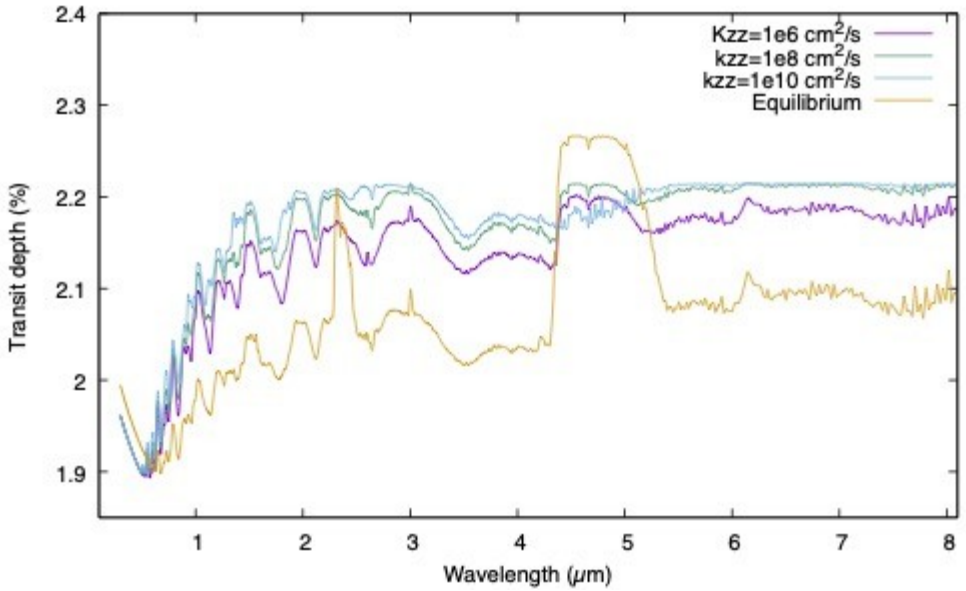
Top: partition of O among its different carriers as function of T in equilibrium chemistry (Fonte+2023). Right: example of how vertical transport affects the partition of O for different eddy diffusion coefficients (Simonetti+under revision).

Put it all together...

...and you get a **simulated planetary atmospheric spectrum** (courtesy of Daniele Locci)!



Gaseous



Gas + Solids

status in numbers:

	WASP69	HD209458
Mercury Simulations:	84	57
Jade Simulations:	62	30
Hephaestus Processing:	36	24
FastChem Simulations:	608	1428
Vulcan Simulations:	126	0

Finished: **2455!**
Running: something is always running
Queued: A heck of a lot more!

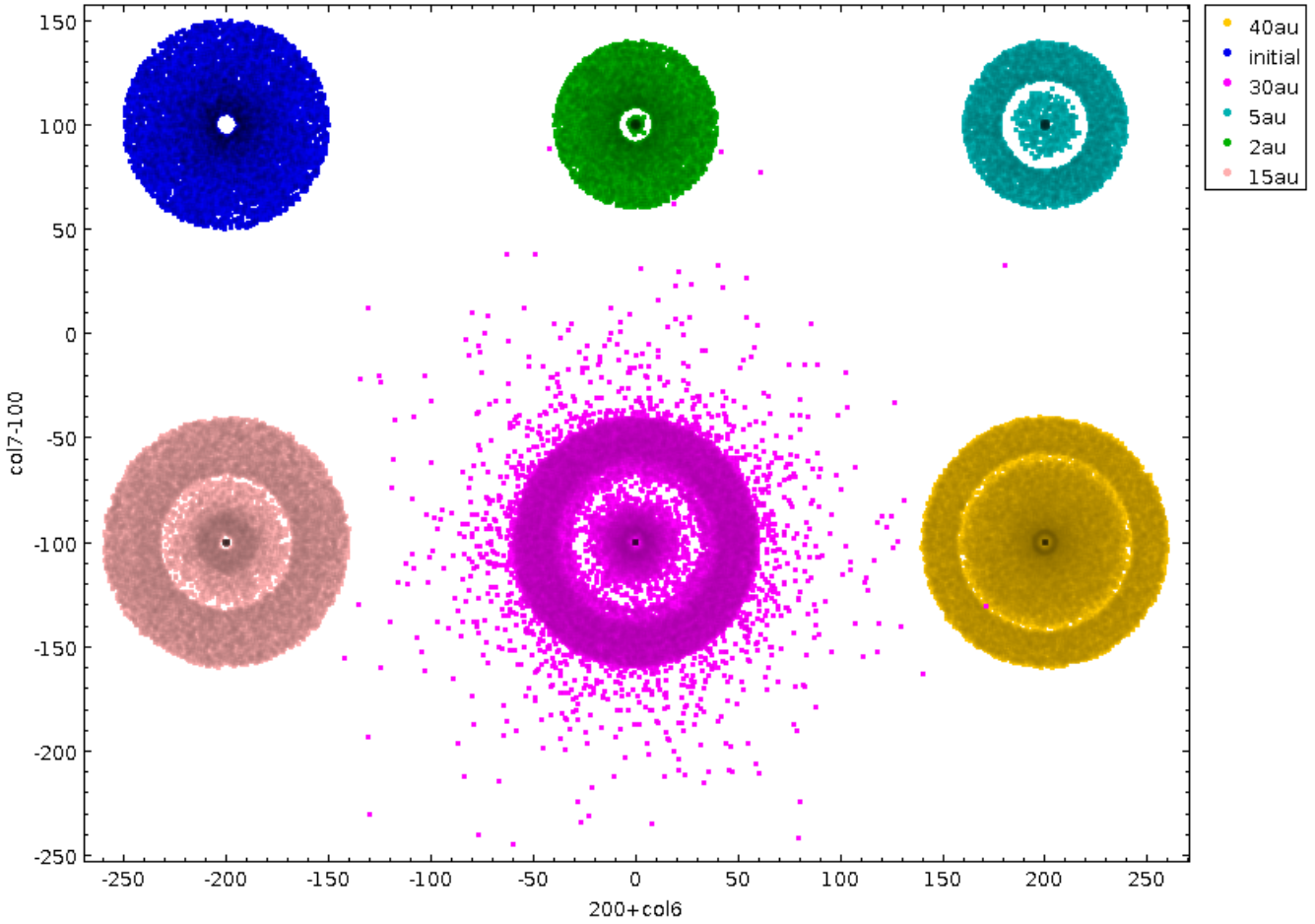
The resulting planetary elemental compositions arising from different formation environments and histories are:

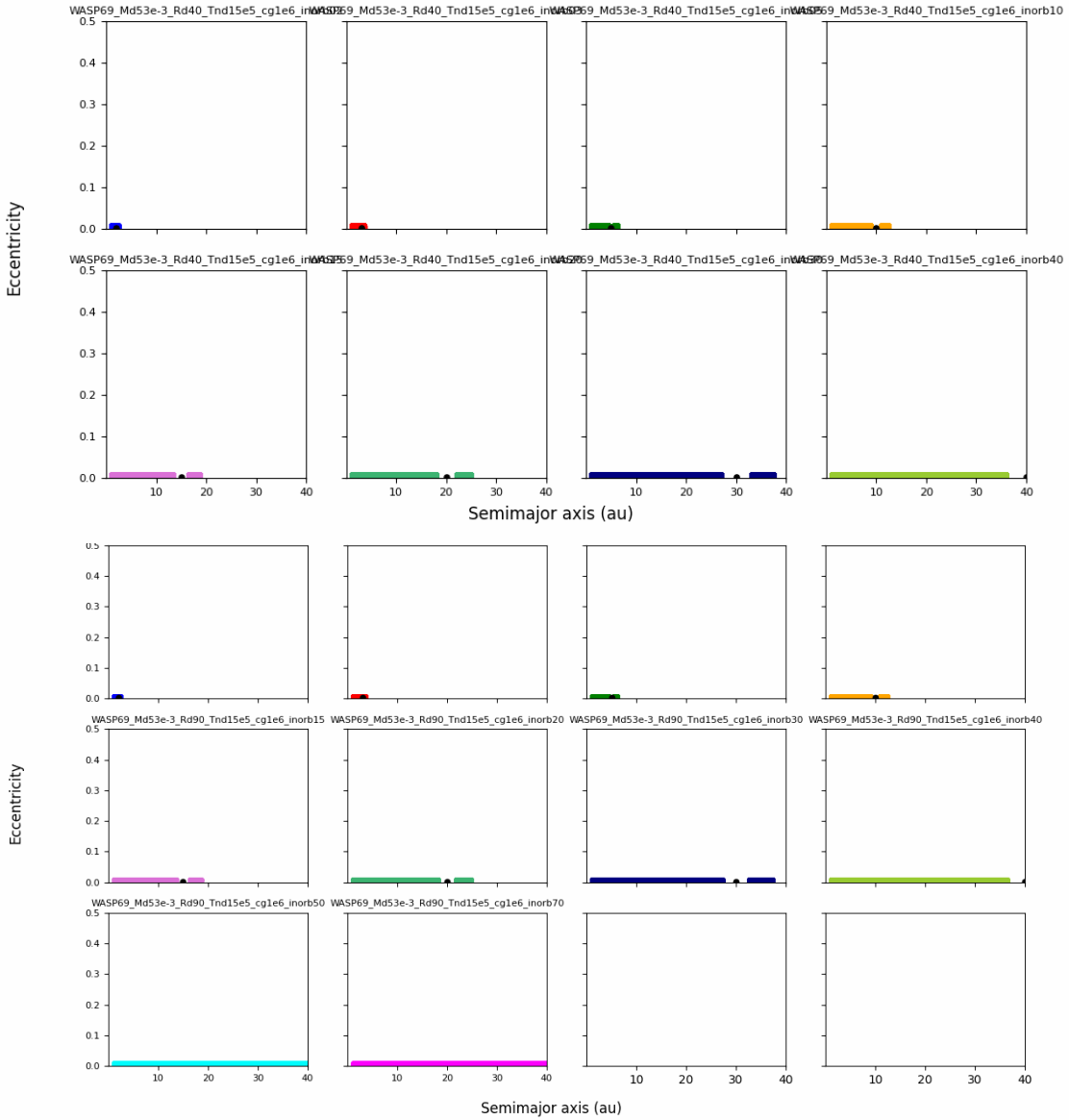
$$N_{Hep} = N_{Jade} \times N_{Merc} \times 2$$ (only gas or gas+solids)

From these, the **minimum** number of planetary atmospheric compositions is

$$N_{Hep} * 8$$ (eqiuilibrium vs disequilibrium, with and without condensation)

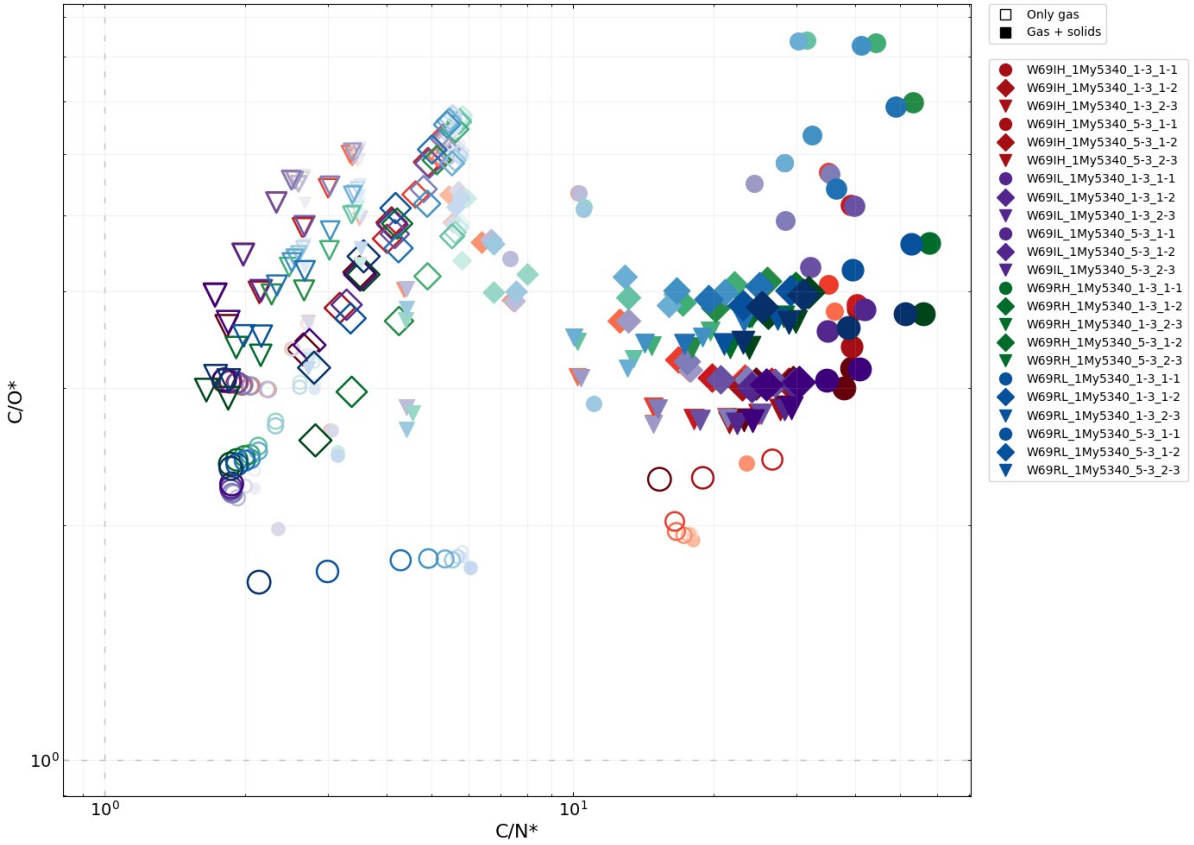
A few preliminary results:

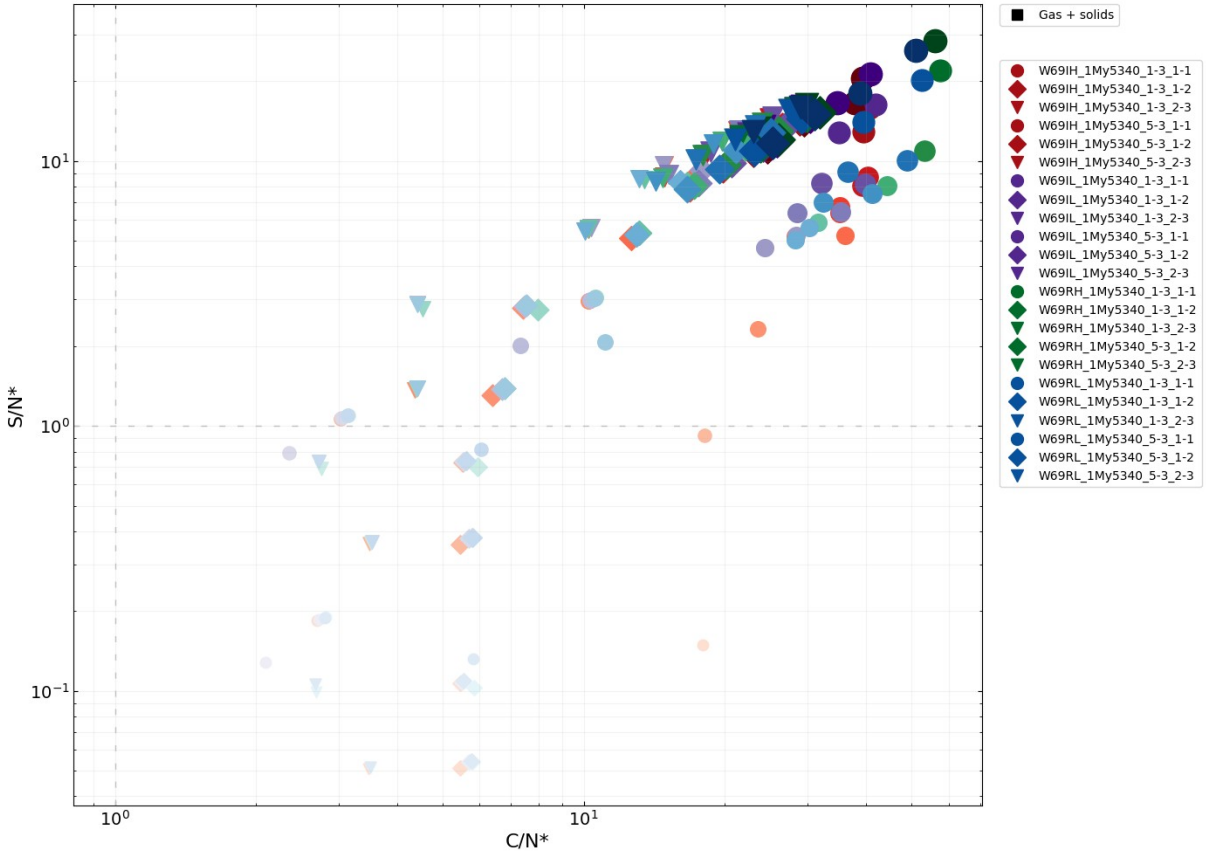




A few initial results:

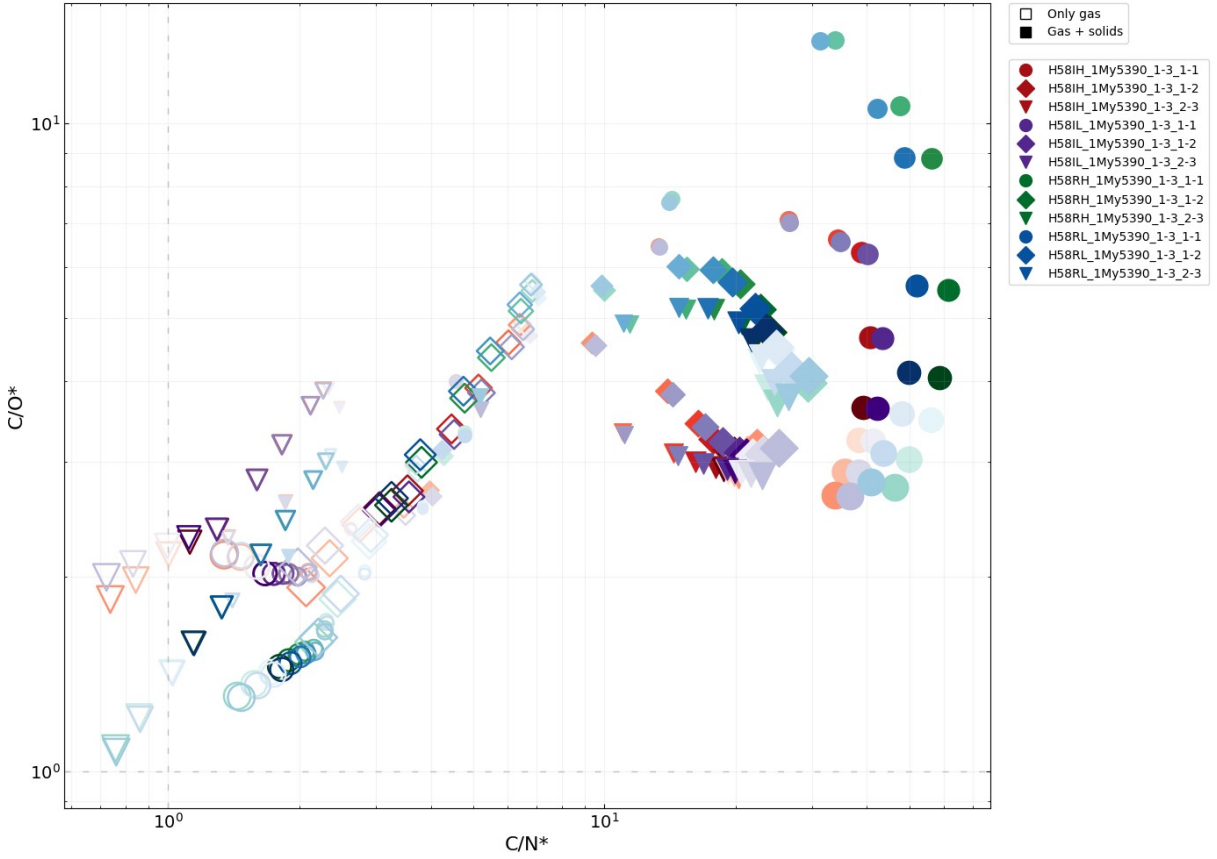
Planetary diversity - WASP69

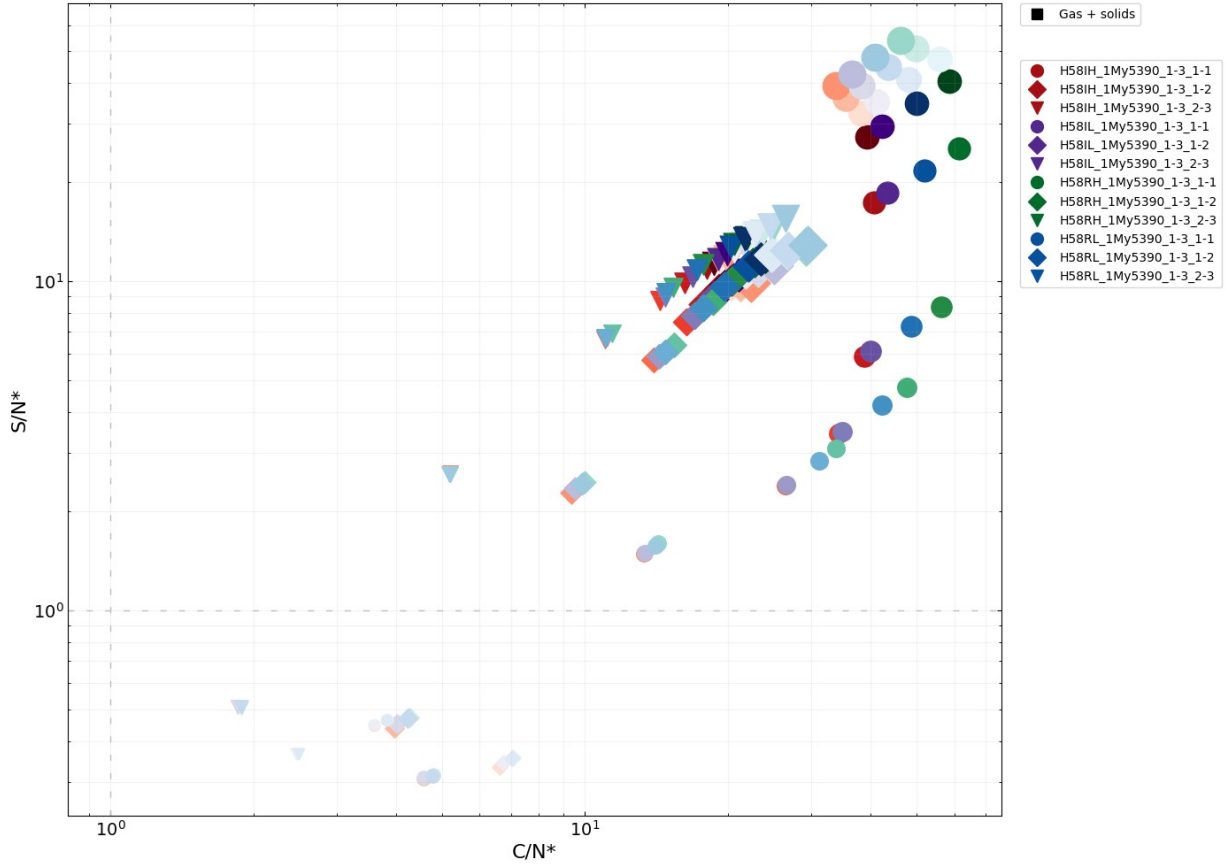




A few initial results:

Planetary diversity - HD209458





An  to support future (exoplanetary) space missions

- 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.

- **Expanding to support the preparatory HWO phase is very much possible**

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

Meet the OPAL Team!

Coordinators:

Diego Turrini, Eugenio Schisano, Romolo Politi

Grunt Workers:

Danae Polychroni (campaign coord., planet formation)
Elenia Pacetti, Michele Zusi (protoplanetary disks)
Sergio Fonte (e. atmopsheres, protoplanetary disks)
Paolo Simonetti, Stavro Ivansvski (d. atmospheres)

New Entries:

Sebastiano Ledda, (population synthesis)
Alberto Vecchiato, (pipeline optimisazion)
Giovanni Musmeci (database)

Advisor:

Sergio Molinari