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Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing
INAF ISTITUTO NAZIONALE DI ASTROFISICA
Ariel
erc
ECOGAL
asi Agenzia Spaziale Italiana

OPAL: The Origins of Planets with ArieL (ICSC - LEONARDO)
&: The Origins of Primordial Atmospheres for arieL (INAF - Pleiadi)

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and the OPAL team

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

What is OPAL?

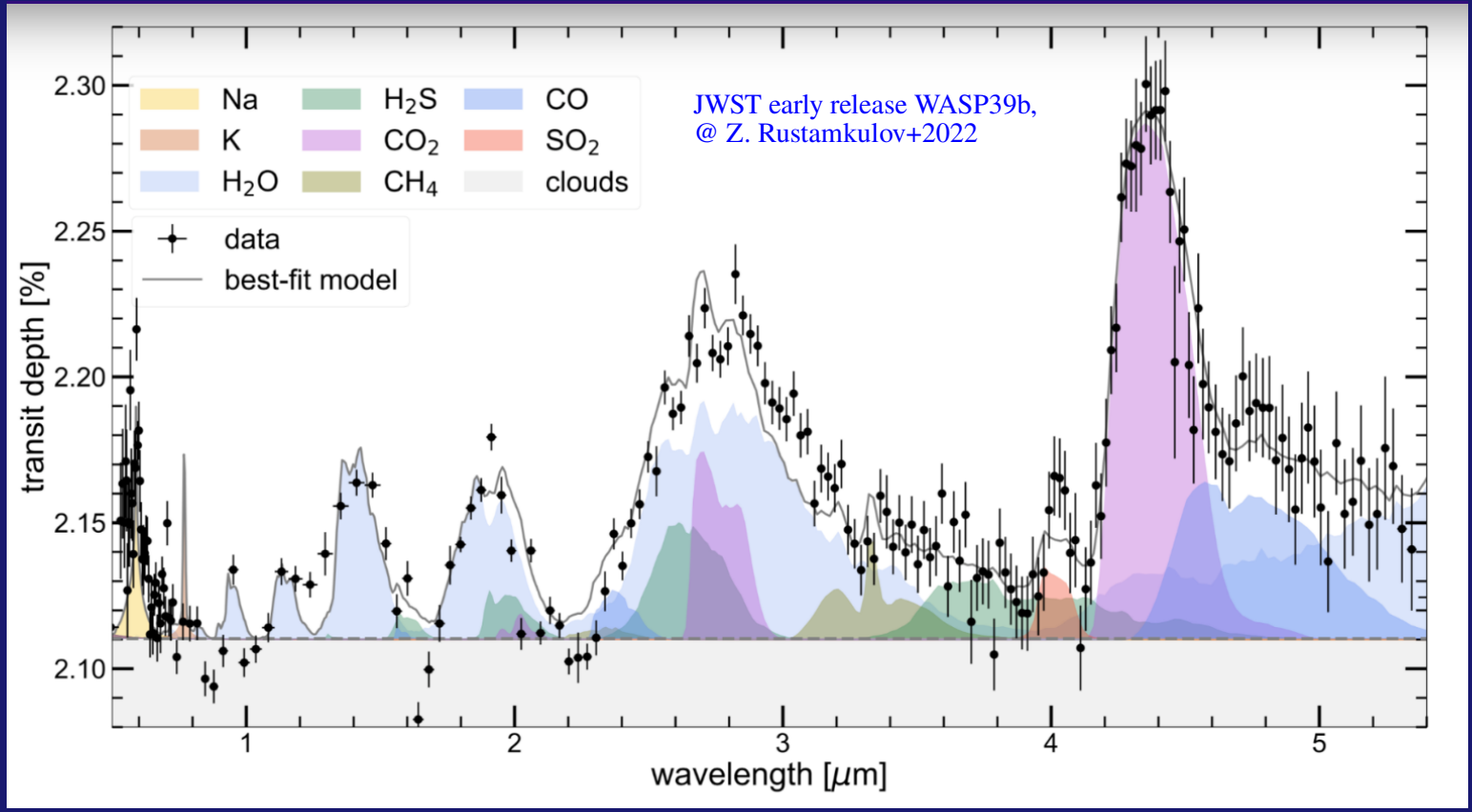
- A project dedicated to creating libraries of detailed synthetic exoplanetary spectra and atmospheric models – with JWST-like complexity.
- A planet formation **pipeline**
- A test of the capabilities of the Ariel data reduction tools
- A framework to maximize the scientific output of the Ariel mission (any facility doing exoplanetary spectroscopy, really)

Why do we need OPAL ?

- Lots of ground- & space-based facilities dedicating time to exoplanetary studies, ***rapidly evolving observational landscape***
- ***JWST's*** observations of exoplanetary atmospheres challenge our understanding with their detail and complexity… and ***ELT*** and ***Ariel*** are on the way
- We have ***no consolidated interpretation*** framework to tackle these challenges
- We need ***realistic synthetic datasets*** to inform our studies of the real observational data

Why do we need OPAL ?

What we hope to achieve

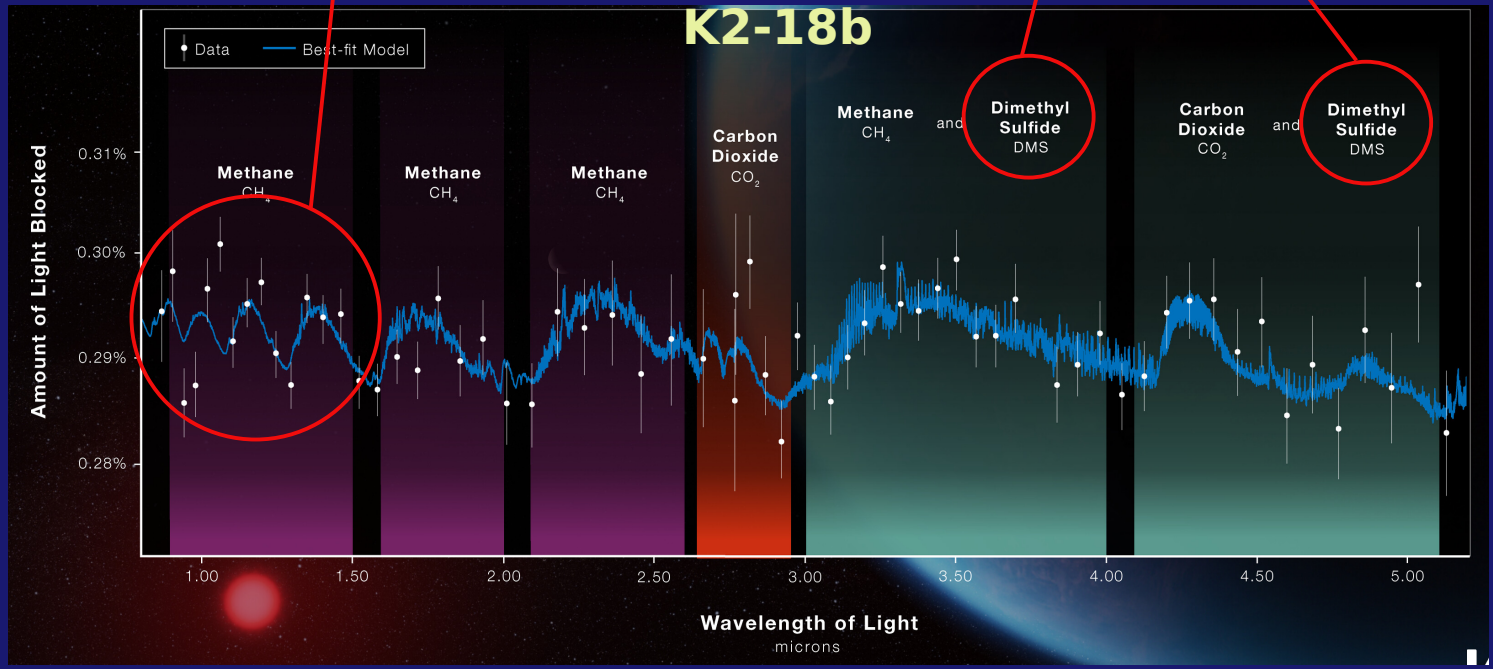


Why do we need OPAL ?

Without meaningful priors this is **what you get** instead:

Plausible molecule but bad fit

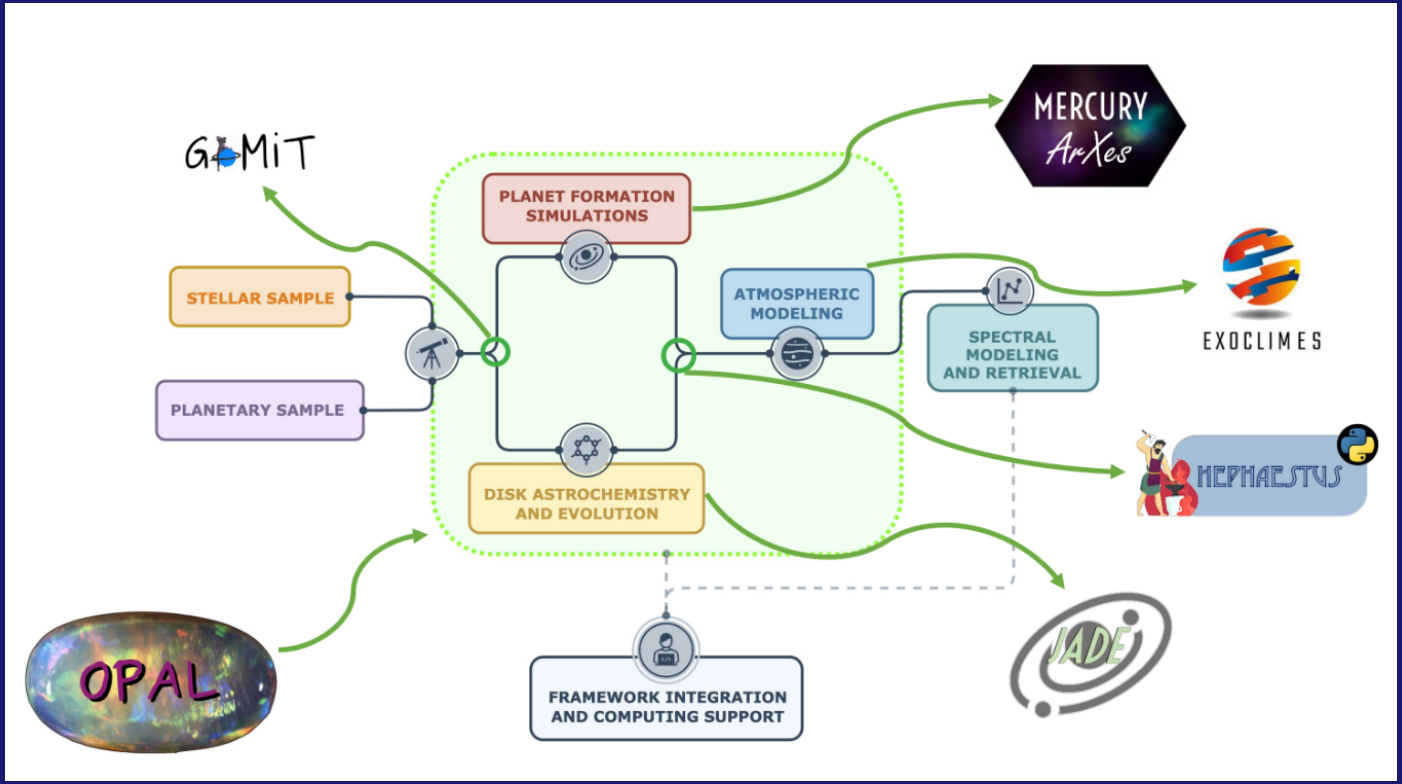
Sensational but unjustified molecule (no atmosphere modeling)



@ NASA, CSA, ESA, J. Olmstead (STScI), N. Madhusudhan (Cambridge University)

What does OPAL contain?

- Developed in-house:
  - **JADE** (Pacetti+2025)
  - **GROMIT** (Polychroni+2023)
  - **HEPHAESTUS** (Turrini+2021, Pacetti+2022)
- Extensively modified:
  - **MERCURY – ArχES** (Turrini+2019, 2021, 2026)
  - **MERCURY – OPAL** (Simonetti+2026)
  - **VULCAN – COND** (Simonetti+ submitted)
- Other codes:
  - **FASTCHEM3** (Stock+2018, 2022)
  - **GGCHEM** (Woitke+2018)

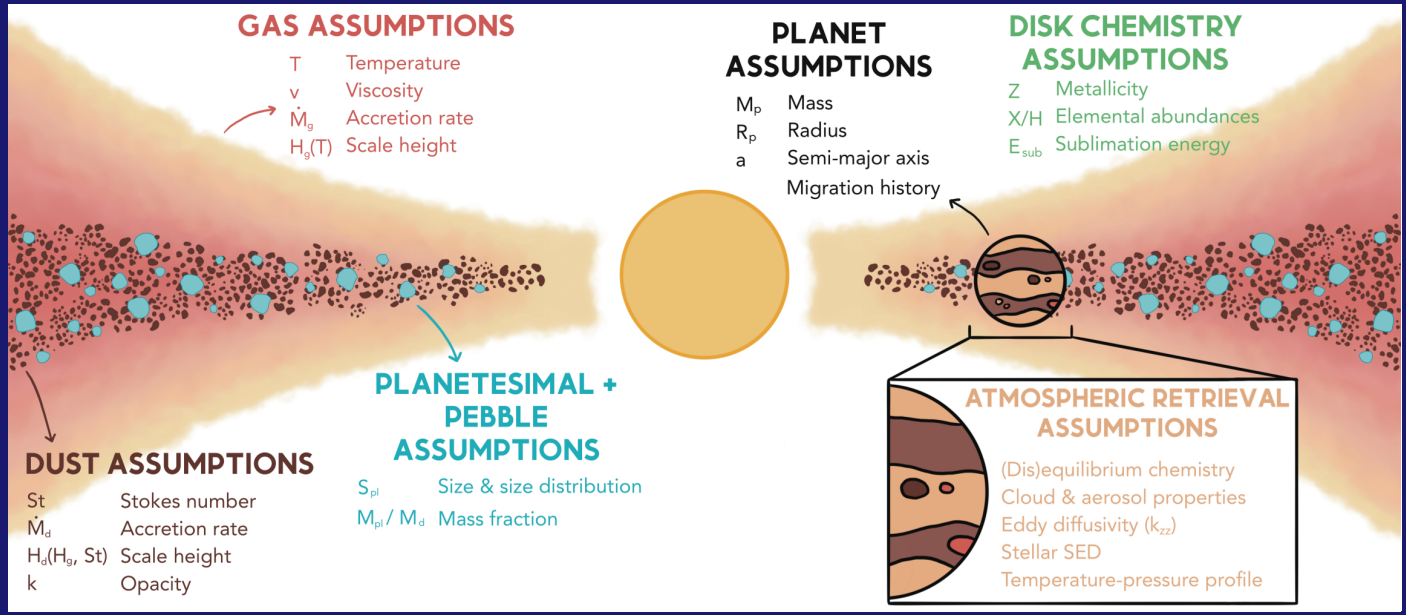


What does OPAL require?

- A lot of patience
- Code development, automatization and plenty of HPC resources
    - 1.4 million core hours on LEONARDO, CINECA
    - 2.5 million core hours on INAF – Pleiadi
    - Unlimited time on our own GENESIS+ cluster
- Storage space (in the future)
- Dedicated database (w.i.p.)
- Double-checking the input files!!!

Planet Formation with OPAL

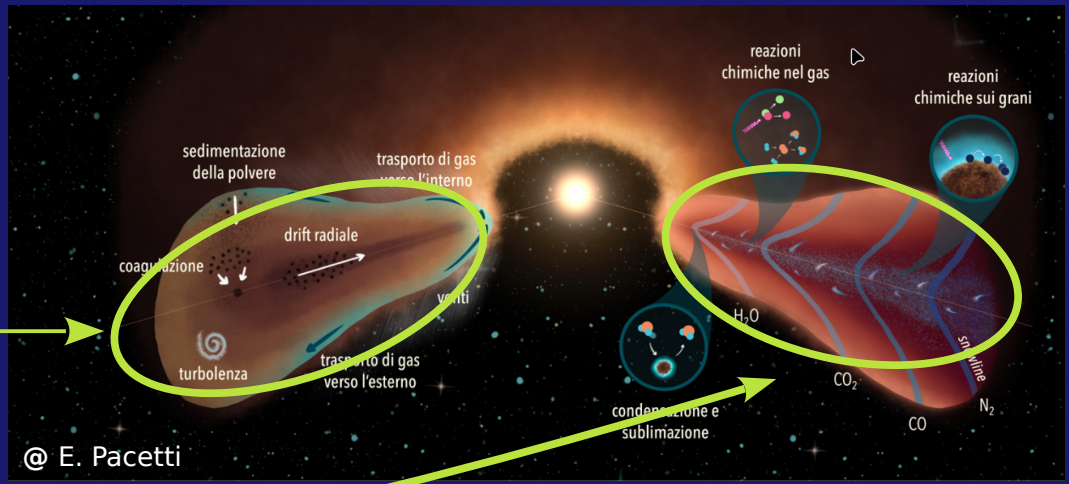
- Planet formation is a complex process shaped by Star-Disc-Planet whose initial conditions are largely unknown.
- To capture the diversity of giant exoplanets, OPAL codes need to take into consideration multiple processes, usually studied autonomously:
  - Stellar metallicity and mass
  - Disc evolution, chemistry and mass
  - Planet growth (gas/solids accretion) and migration, planet-to-disc feedback
  - Stochastic events

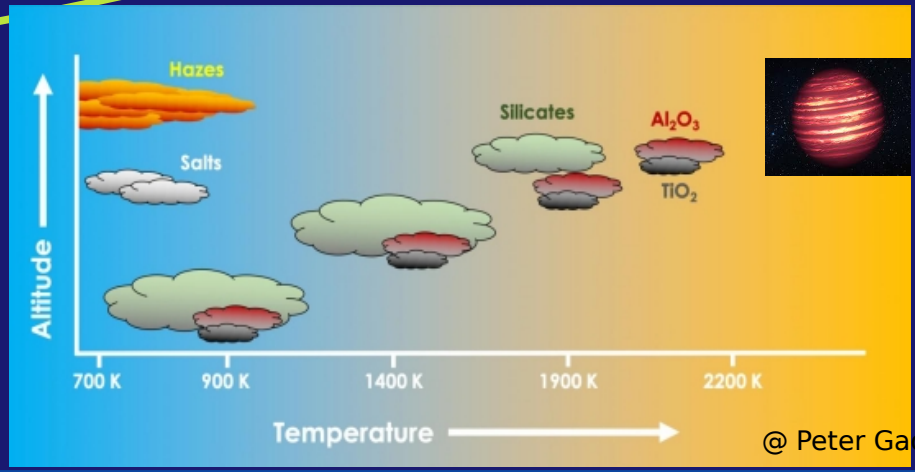


Planet Formation with OPAL

Which **key factors** shape the observable properties of planets?

- **Planet formation**
  - accretion (gas/solid)
  - orbital migration
- **Planet-forming environment**
  - stellar composition
  - disk evolution
  - disk chemistry
- **Planetary Atmosphere**
  - pressure, clouds
  - convection, evolution



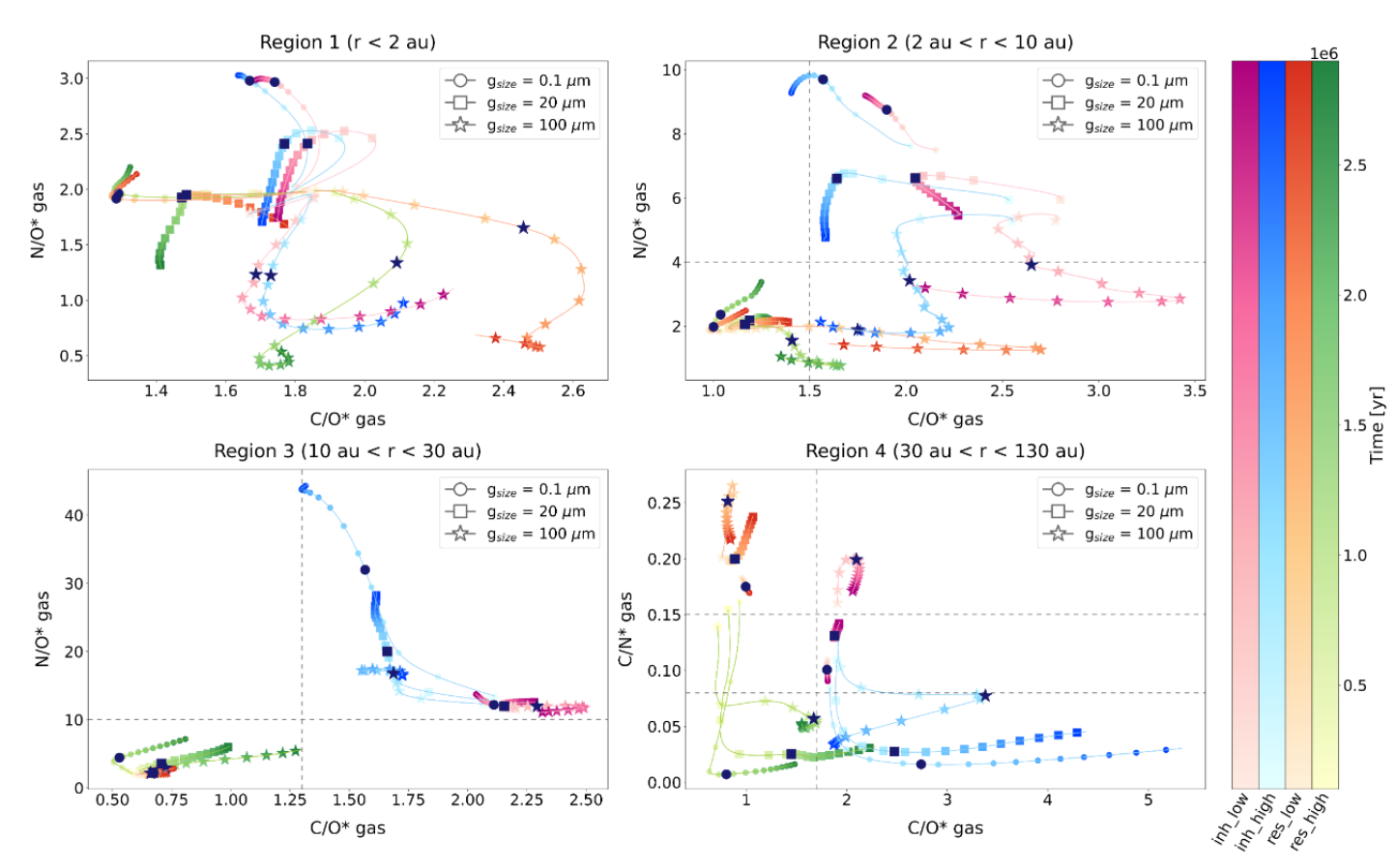


Planet Formation with OPAL

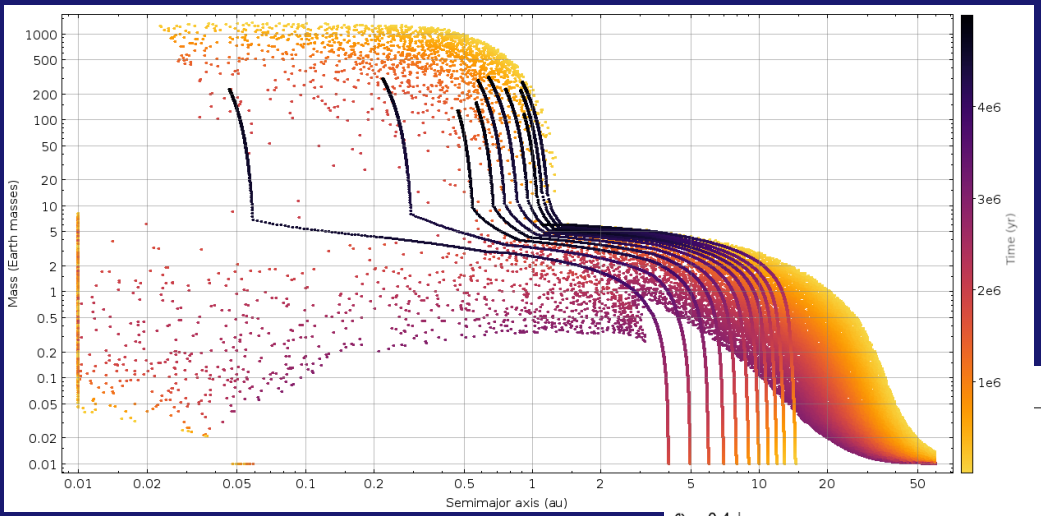
Disc variability in space & time with JADE

Evolution of the composition of different regions of the same disc

=> different atmospheric composition!



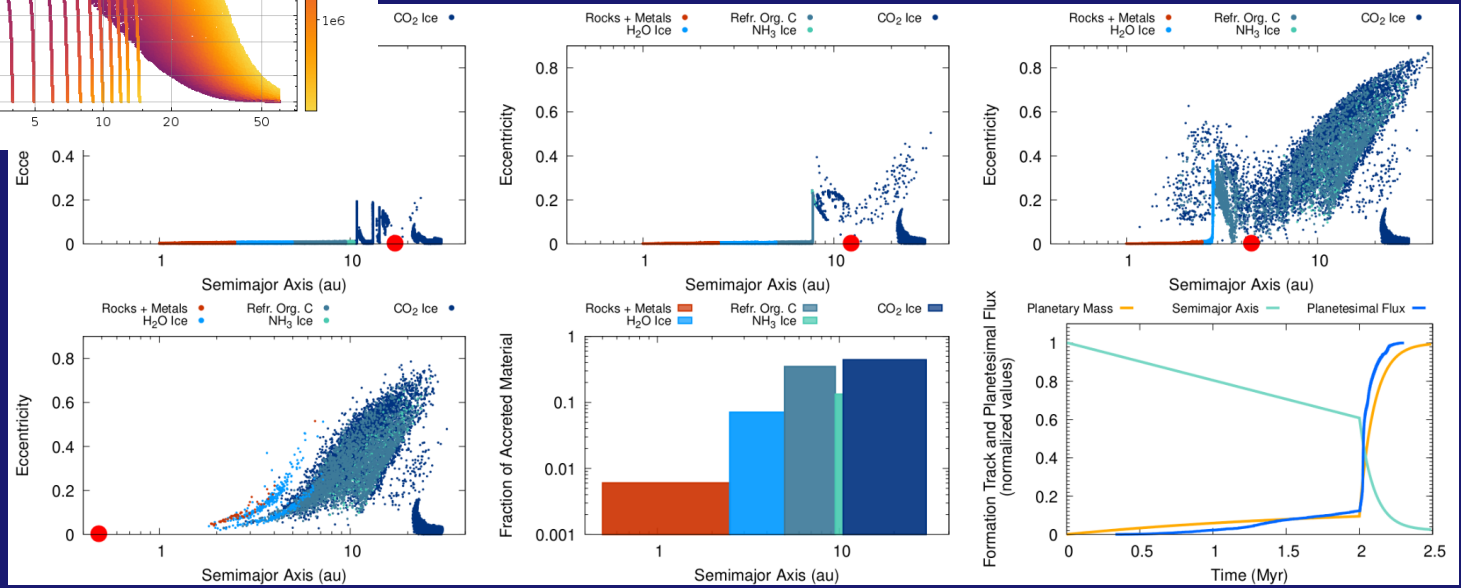
Planet Formation with OPAL



The Disc – Planet Link
with GROMIT & MERCURY – ARχES

Tracing planet growth and migration in the native disc...

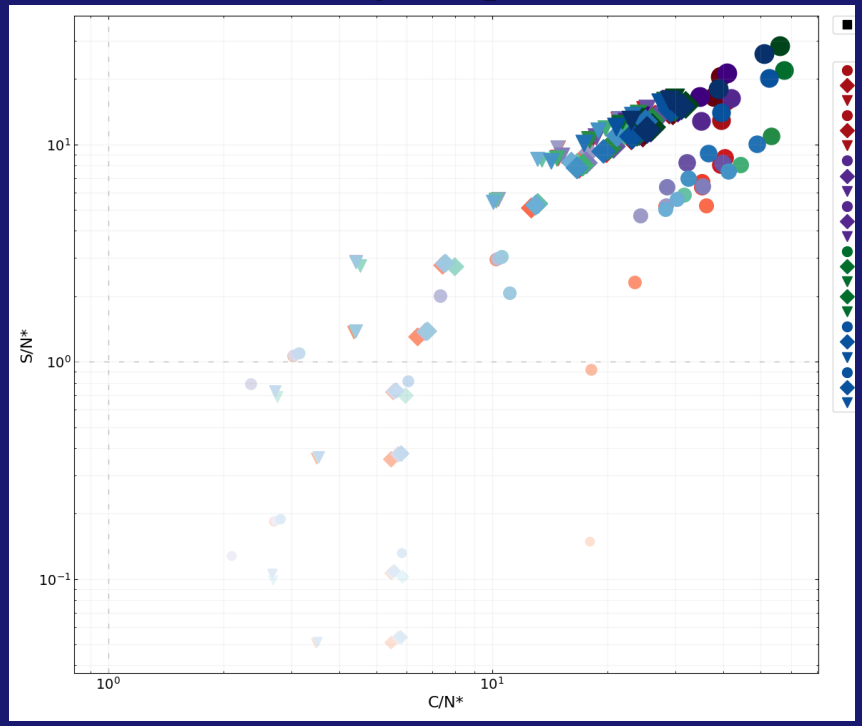
… and what they accrete along their path



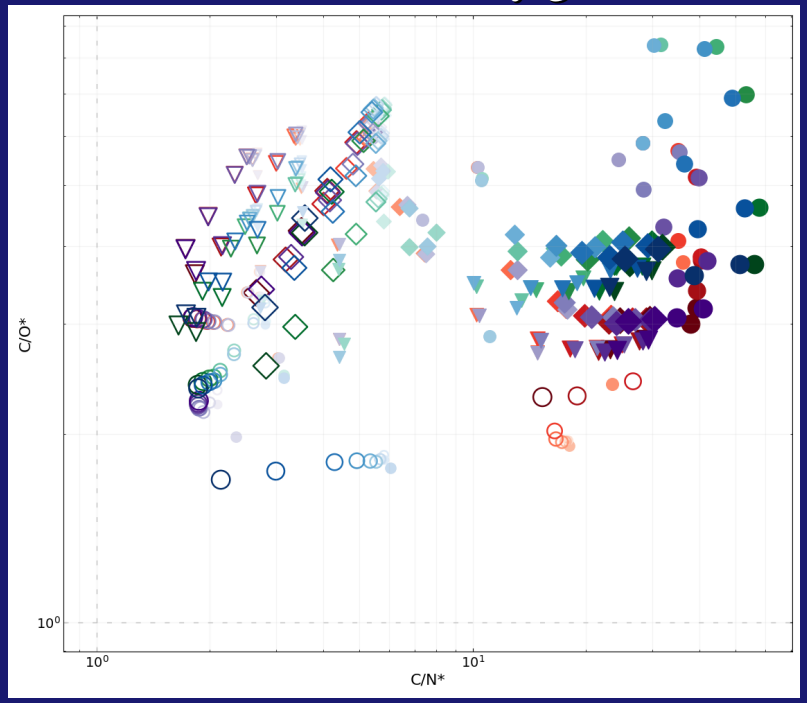
Planet Formation with OPAL

Planetary composition diversity with HEPHAESTUS

Planet accretes gas + planetesimals



Planet accretes only gas



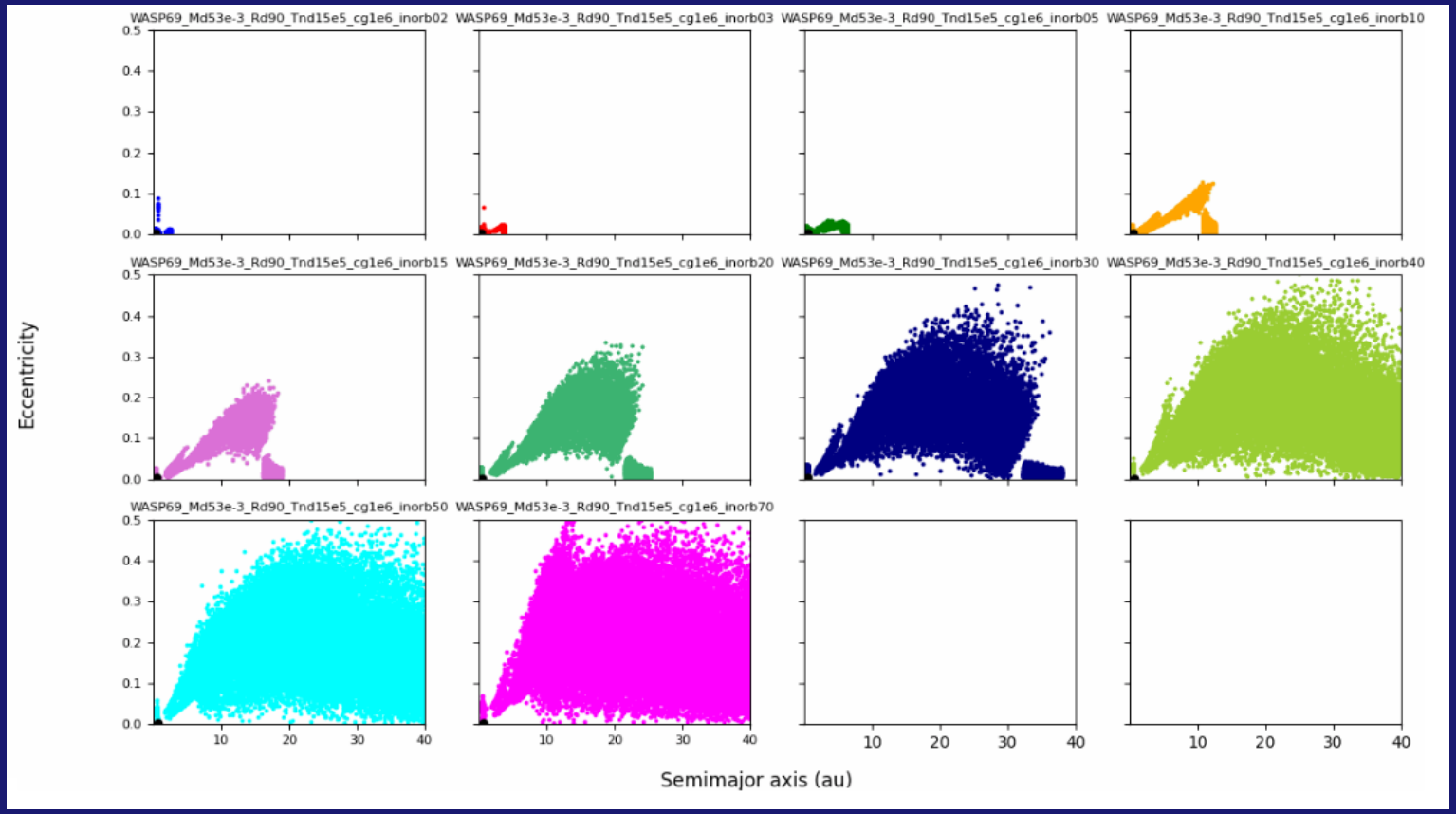
Planet Formation with OPAL

Planet migration diversity

- Same star

- Different migration path

=> different atmospheric composition!

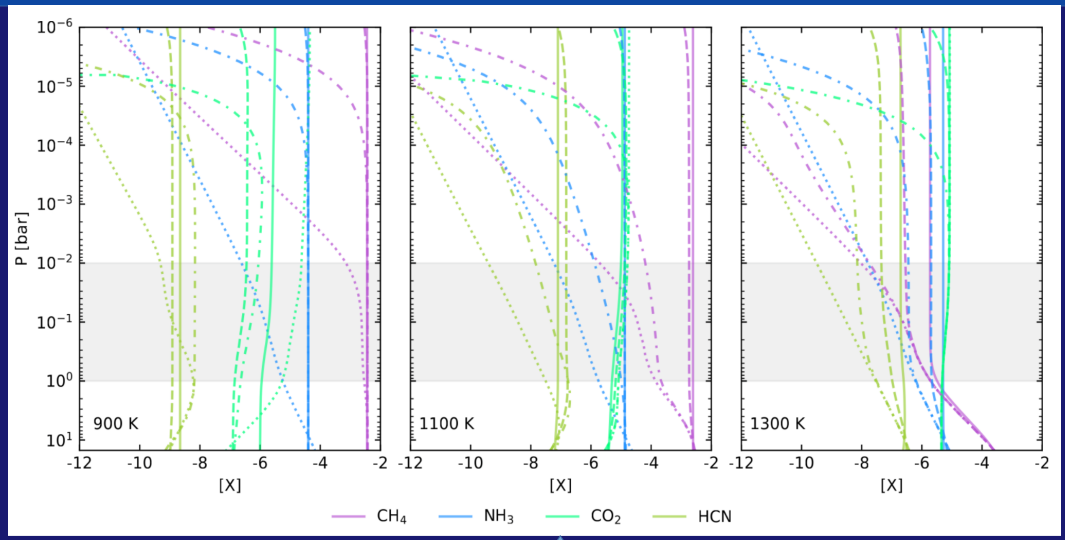


Planet Formation with OPAL

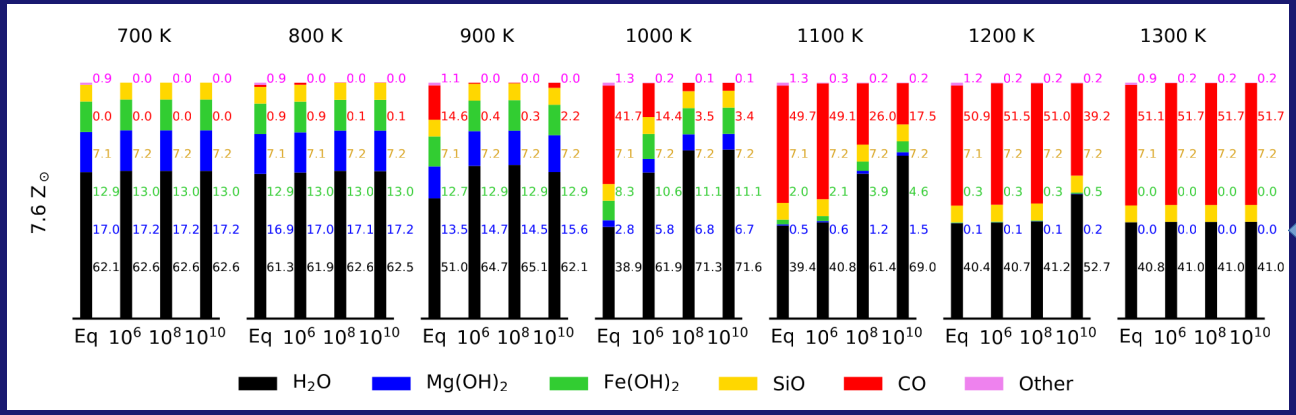
Atmospheric diversity with VULCAN – COND

- Same planet & composition
- Different vertical dynamics

=> different observed atmosphere!



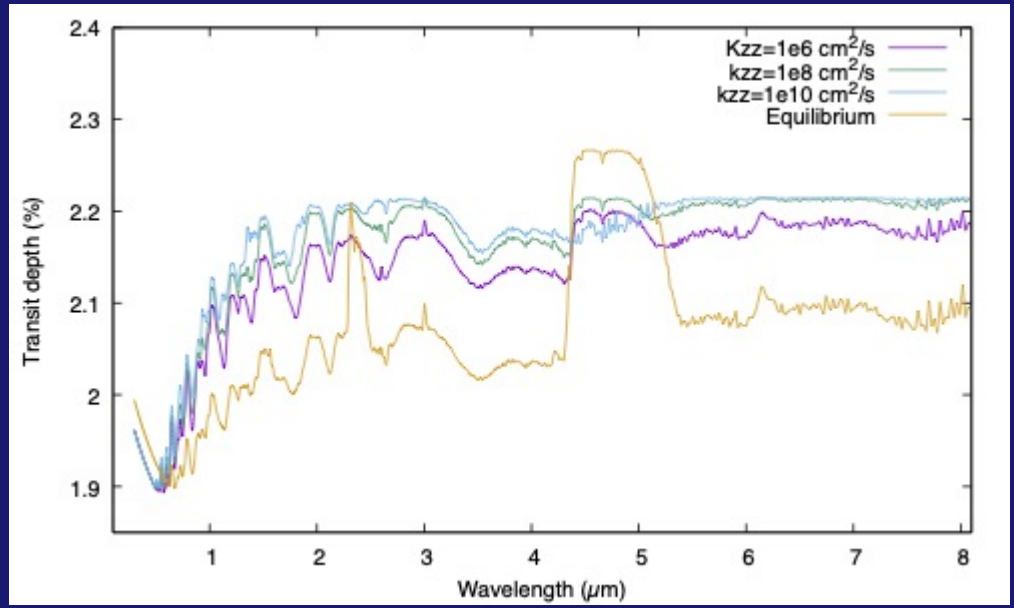
Vertical compositional profiles



Partition of oxygen in the region observed by Ariel

Put it all together...

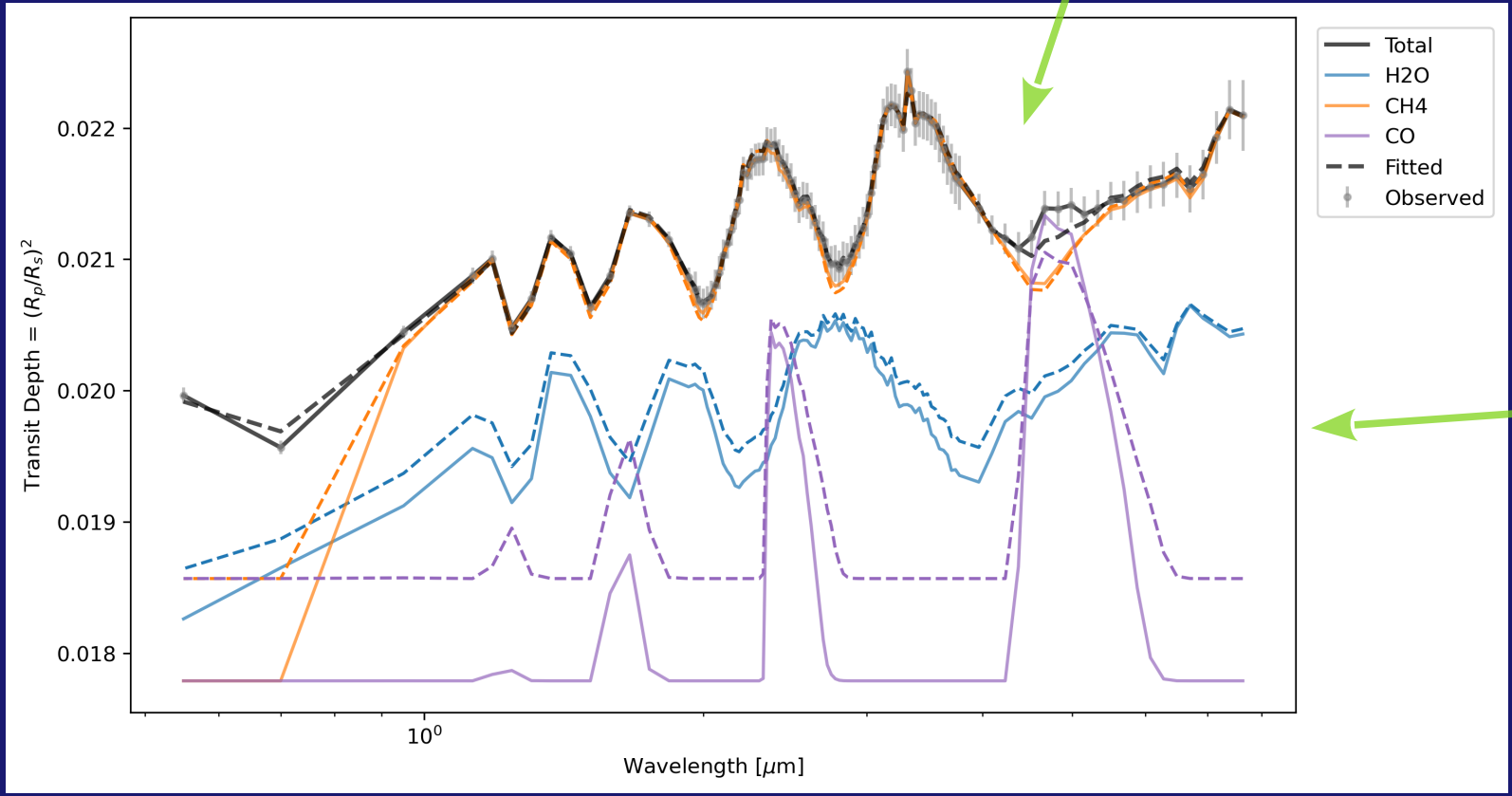
At the end you get ‘a’ **simulated planetary atmospheric spectrum** (courtesy of Daniele Locci)!



Bulk compositions of: **Gas** **Gas + Solid**

An OPAL spectrum seen through Ariel

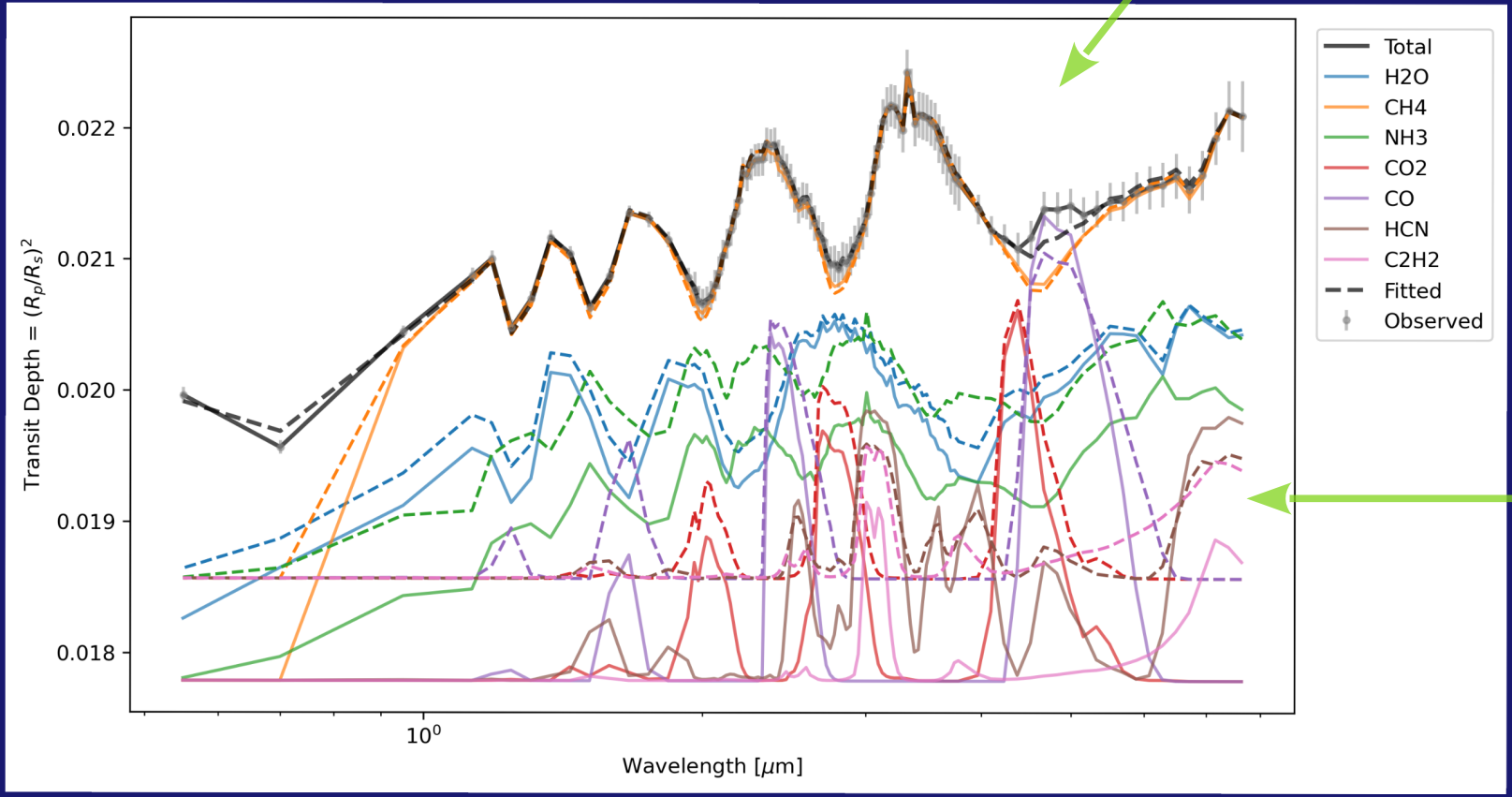
OPAL generated synthetic spectrum (WASP69b)



Modeled using only major molecules (like everyone does...)

An OPAL spectrum seen through Ariel

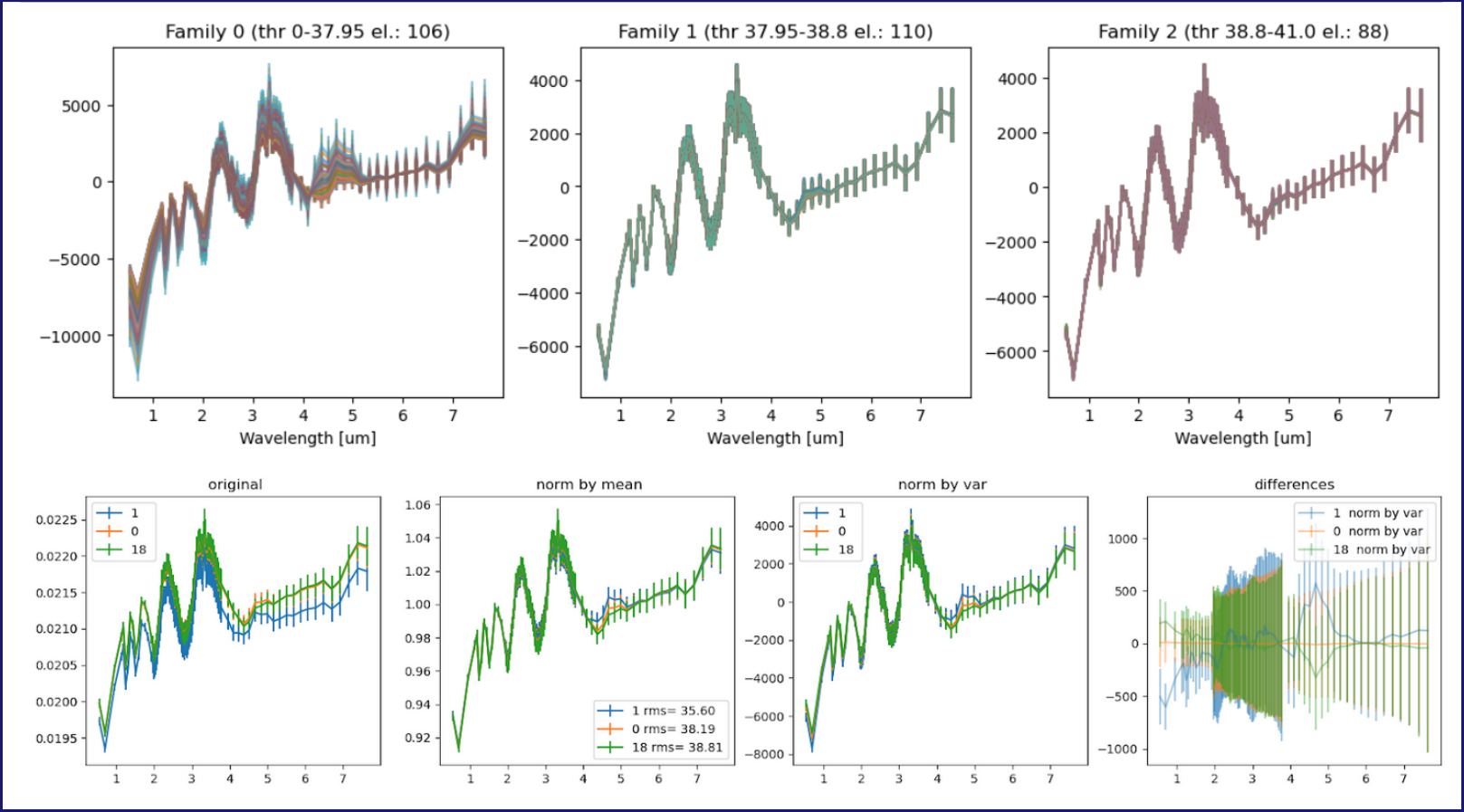
OPAL generated synthetic spectrum (WASP69b)



Capturing the atmospheric complexity (… how it should be done)

Planet diversity

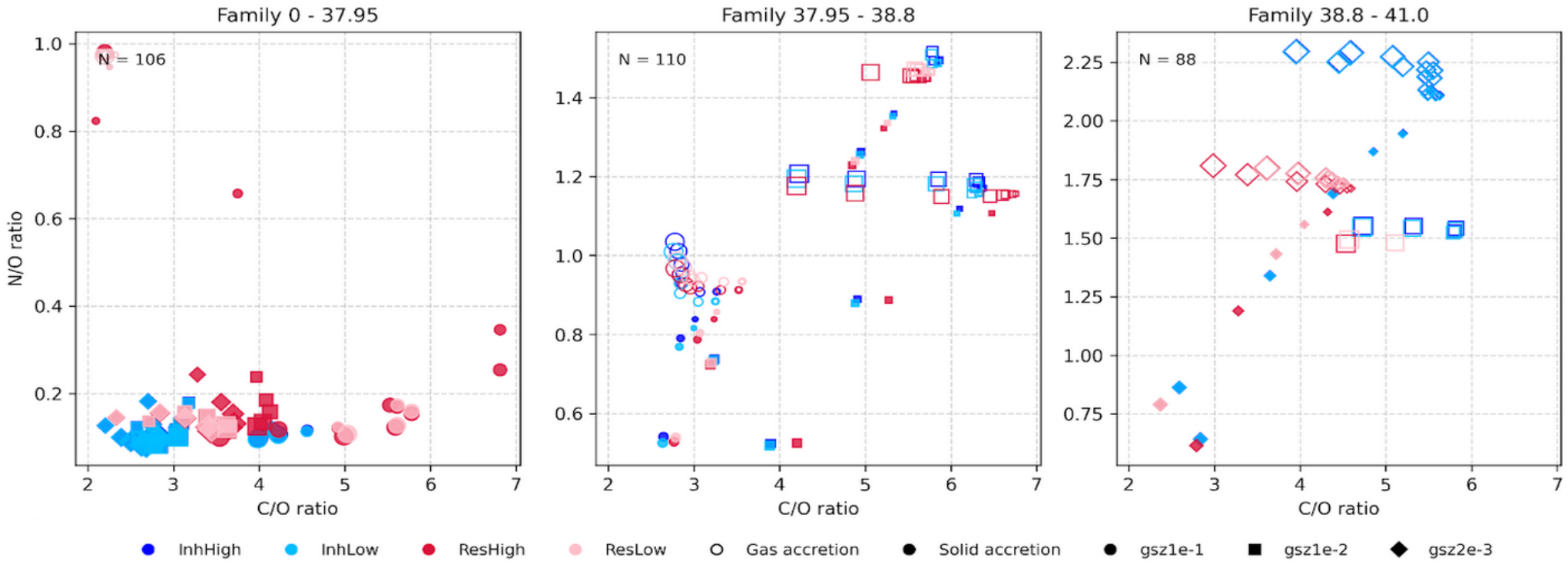
→ Synthetic spectra diversity



Synthetic spectra diversity

→ **Different formation mechanisms!**

Planetesimal accretion | Pebble accretion | Gas accretion



status in numbers:

Simulations finished: ~3000! (for 3 planets at different completion stages)
Atm. compositions: ~2000
CPU hours used: >1,260,000 (LEONARDO – 53%, Pleiadi -47%)
+ ¯_(ツ)_/¯ (GENESIS+ cluster)
Storage space: ~ 6 TB
Running: something is always running
Potential: Still a heck of a lot more
Process: Iterative between making models, making spectra and understanding the produced spectra

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)

Meet the OPAL Team!

Coordinators:

Diego Turrini, Romolo Politi, Eugenio Schisano

Grunt Workers:

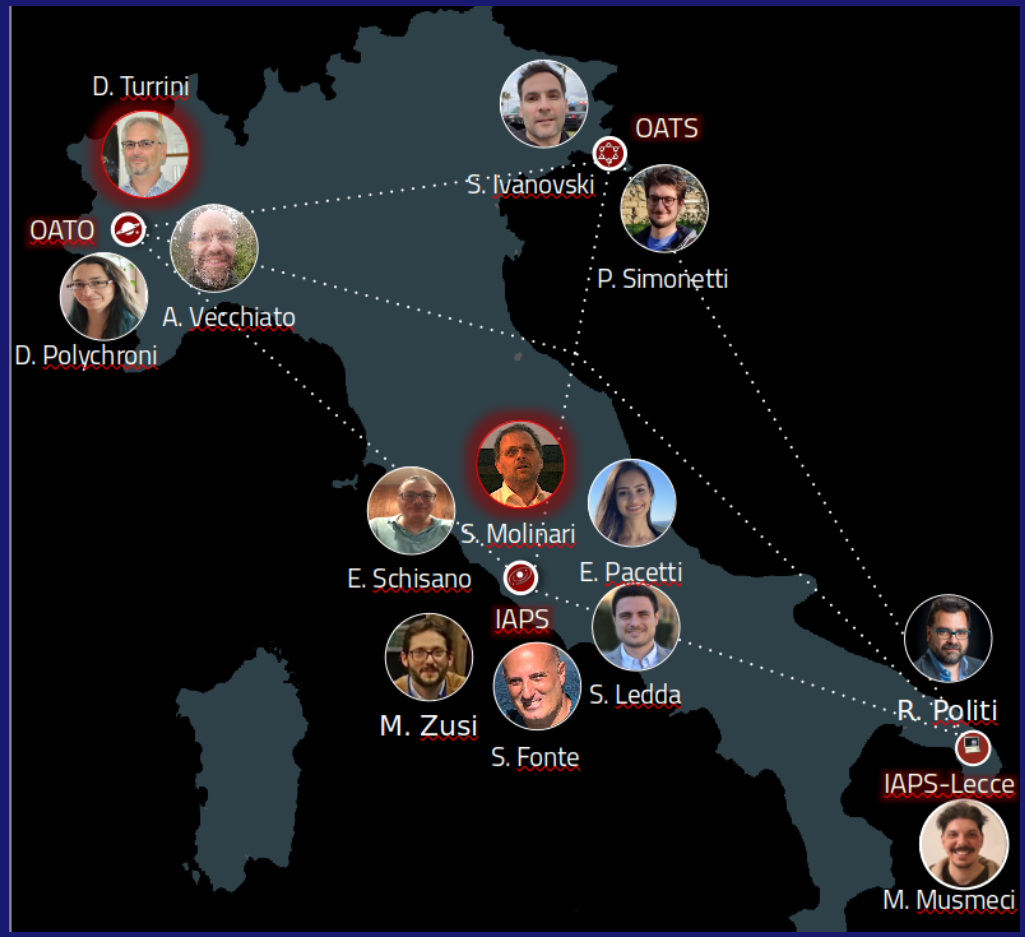
Danae Polychroni (campaign coord., planet formation)
Elenia Pacetti, Michele Zusi (protoplanetary discs)
Sergio Fonte (atmospheres, protoplanetary discs)
Paolo Simonetti, Stavro Ivansvski (atmospheres)

New Entries:

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

Senior Advisor:

Sergio Molinari



The legacy of  for INAF

OPAL is made of the **most comprehensive** planet formation algorithms and expanded atmospheric networks **internationally**, developed @INAF.

Upon its completion OPAL will serve as:

- a **unique in the world** library of exoplanetary astmospheric spectra open to all researchers through a dedicated database

- A **fundamental framework** for interpreting the new generation of observational spectra