# Dynamics, temperature, chemistry, and dust:

## Ingredients for a self-consistent AGB wind


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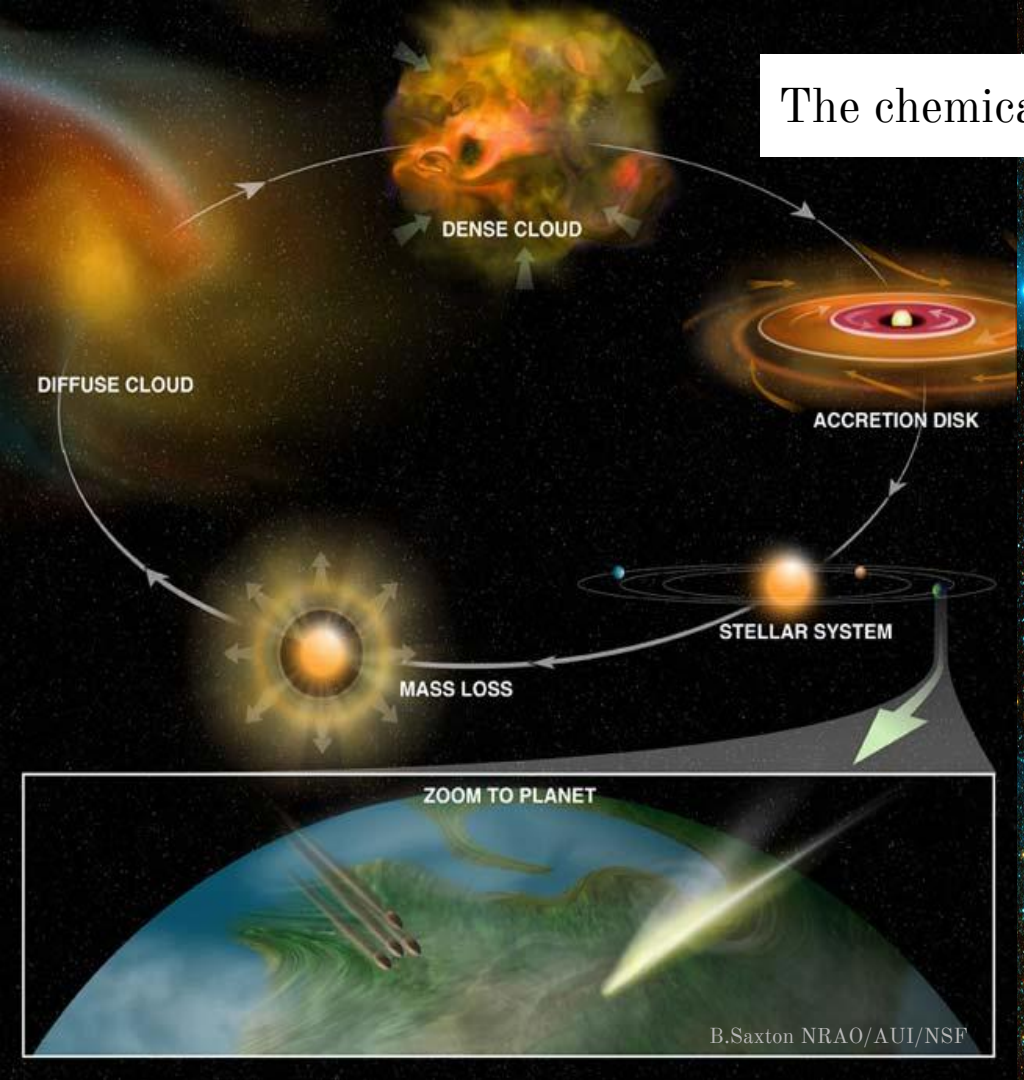
A. J. van Marle - UNIST Uslan
Sup. **L. Decin** - KU Leuven



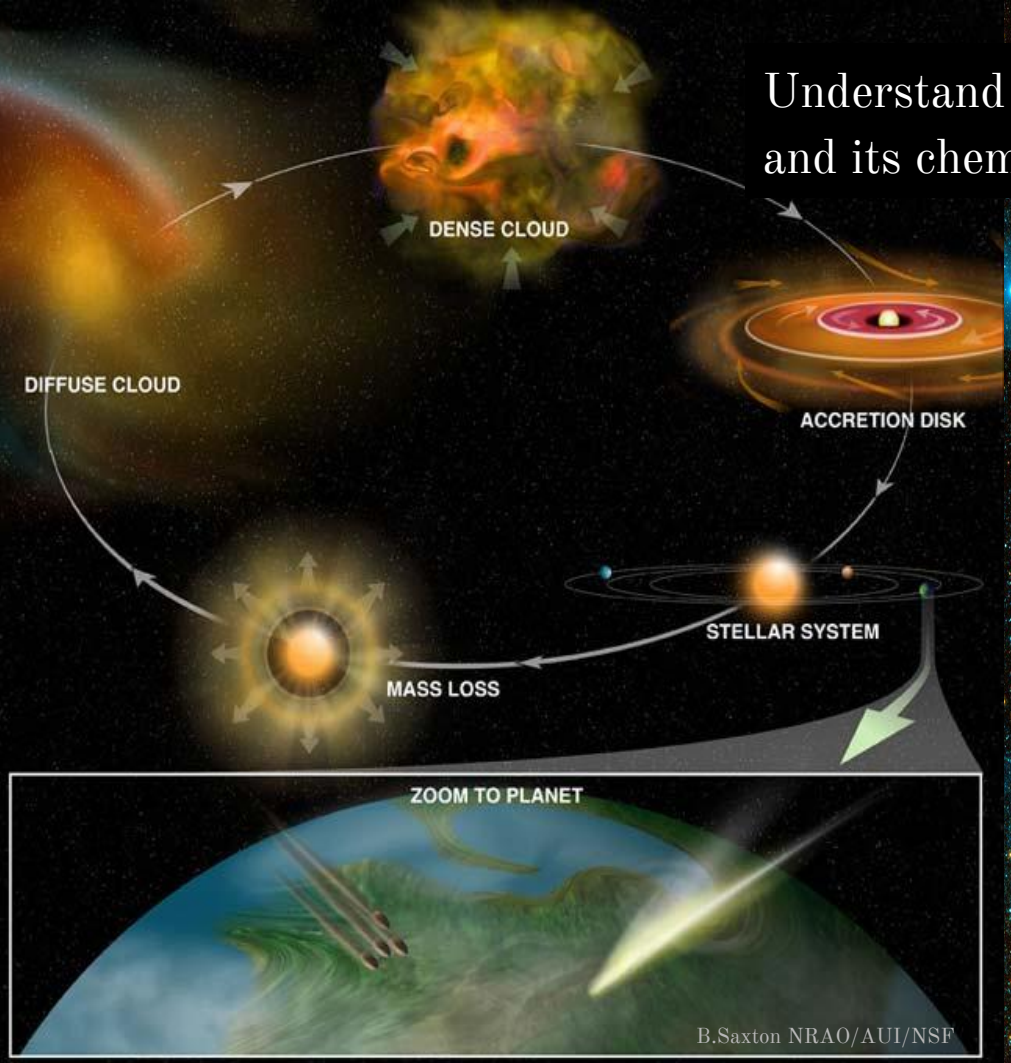
AEROSOL

erc
European Research Council
Established by the European Commission

# The chemical life cycle



Understand the onset of the AGB wind and its chemical composition

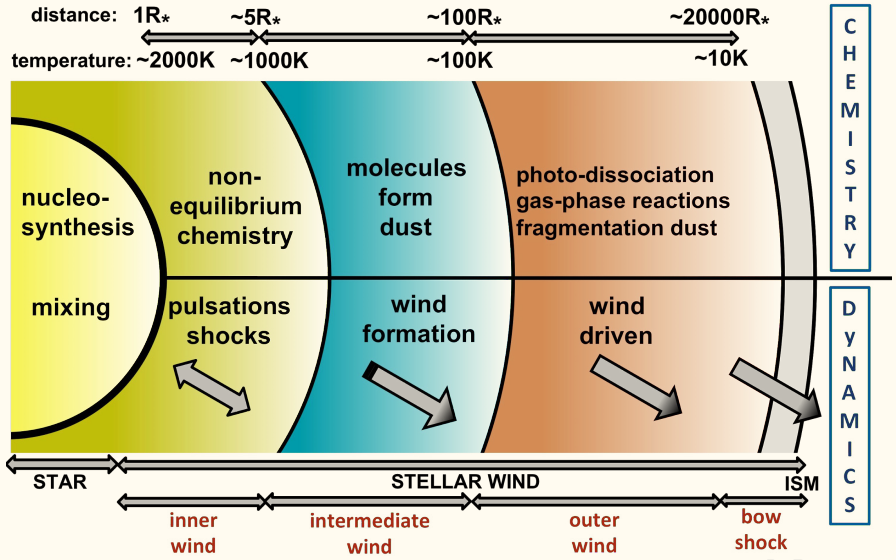



CW Leo - NASA/JPL-Caltech

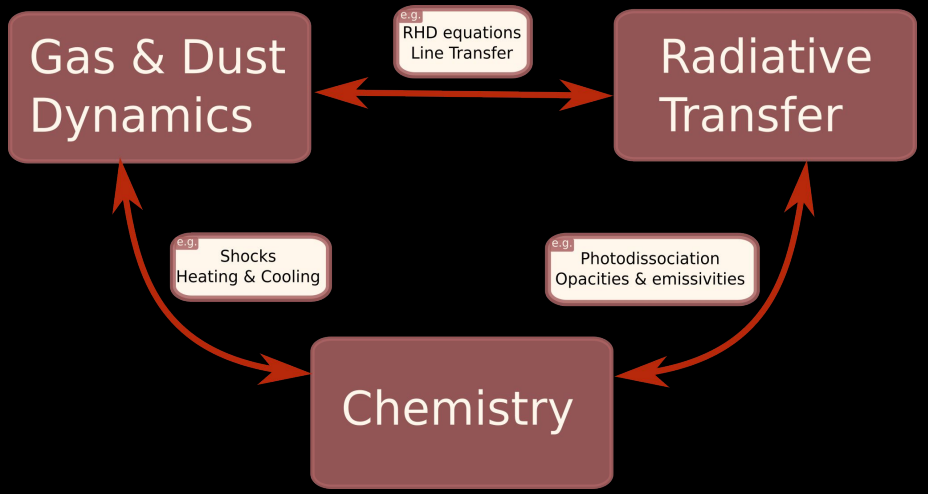
# Current limitations

1. Lack of high resolution observations
2. Simplified theoretical models
3. Lack of laboratory data

# AGB structure

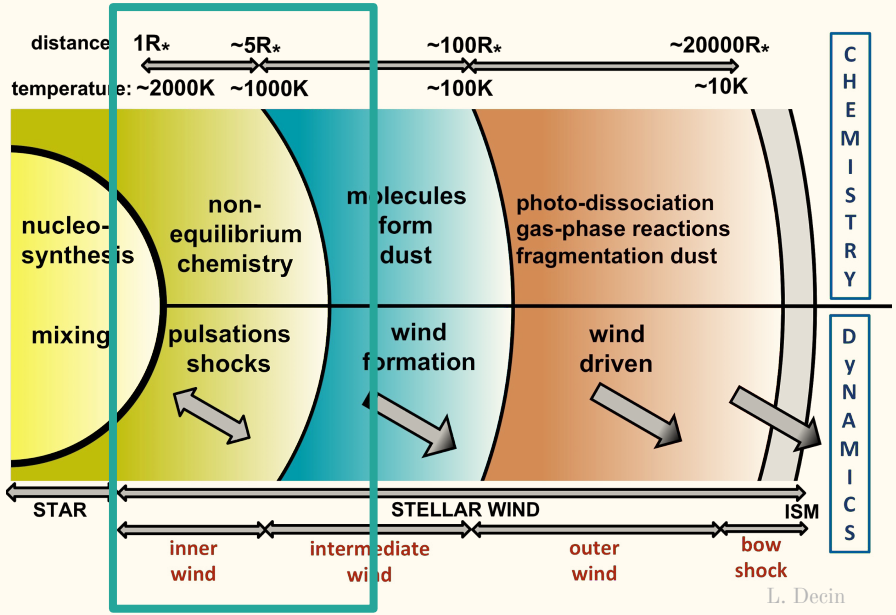




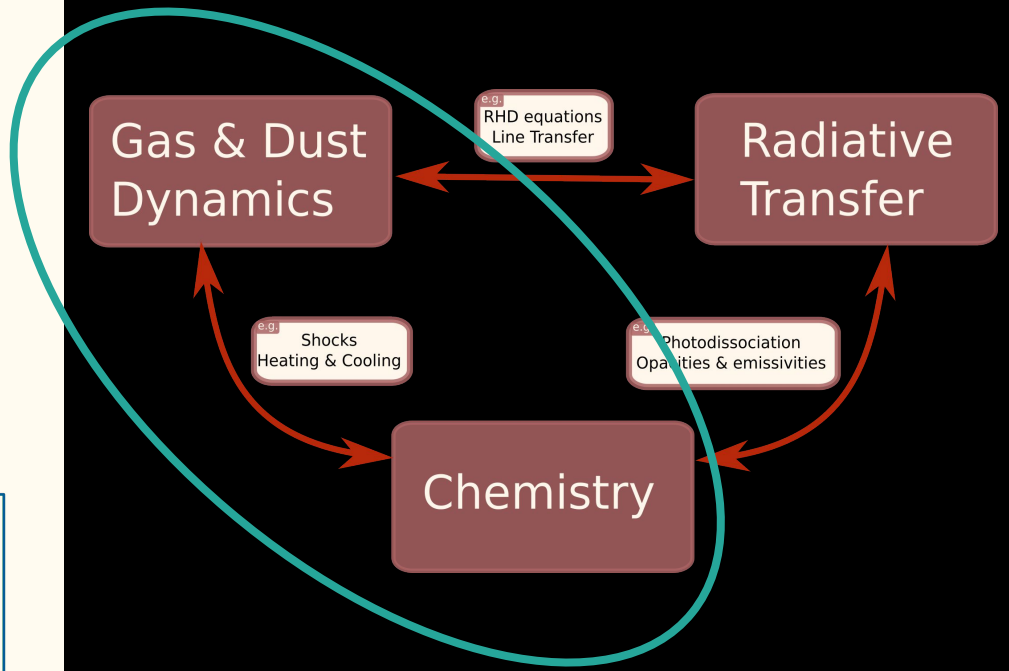




# AGB mechanisms

# AGB structure




L. Decin




# AGB mechanisms

# Hydrochemistry

# Hydrochemistry

## Nucleation theory

Hydrochemistry

Nucleation theory

Dust evolution with radiation field

# Self-consistent AGB wind

Hydrochemistry

+

Nucleation theory

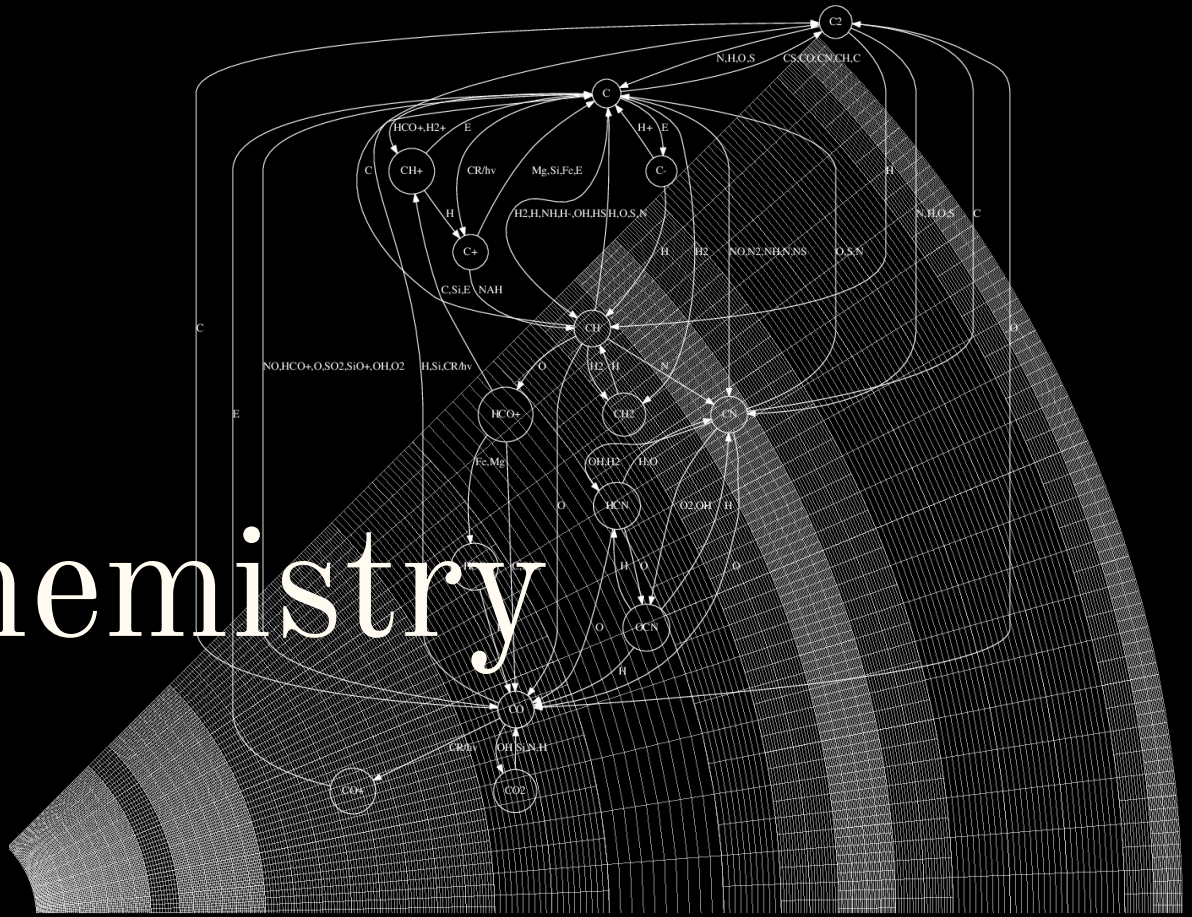
+

Dust evolution with radiation field

# Questions

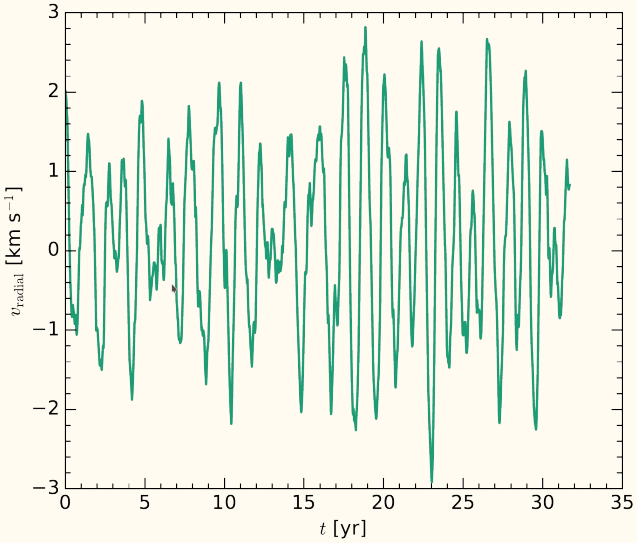
1. What is the dynamical structure in AGB winds?
2. Which chemical pathways are most dominant?
3. How important is the chemical-dynamical feedback loop?
4. Do chemical instabilities exist?
5. What types of dust are able to form?

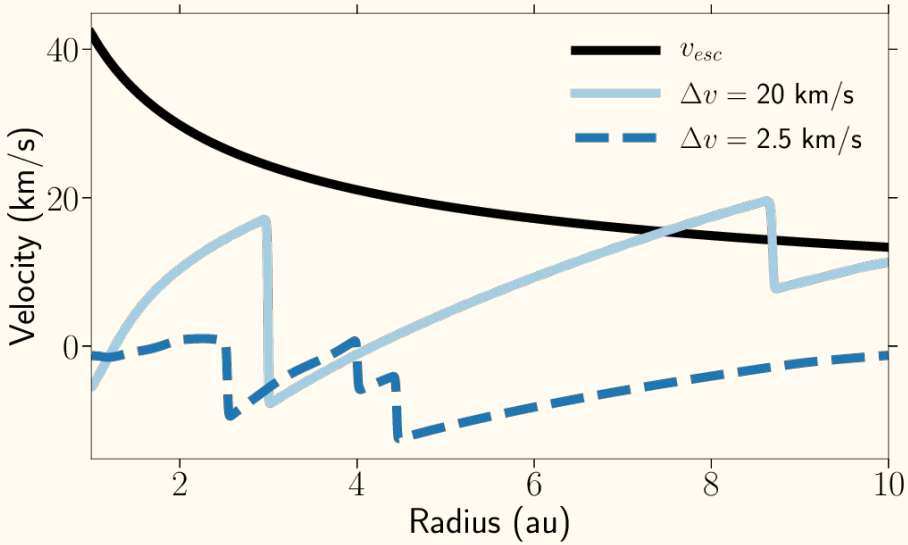
# Hydrochemistry



# Hydro alone cannot drive the wind

Radial velocity at $R_\star$ from 3D-RHD models (Freytag et al. 2017)



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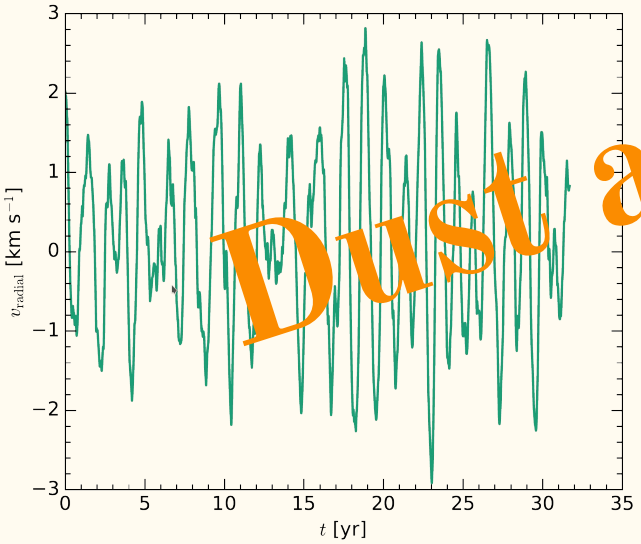
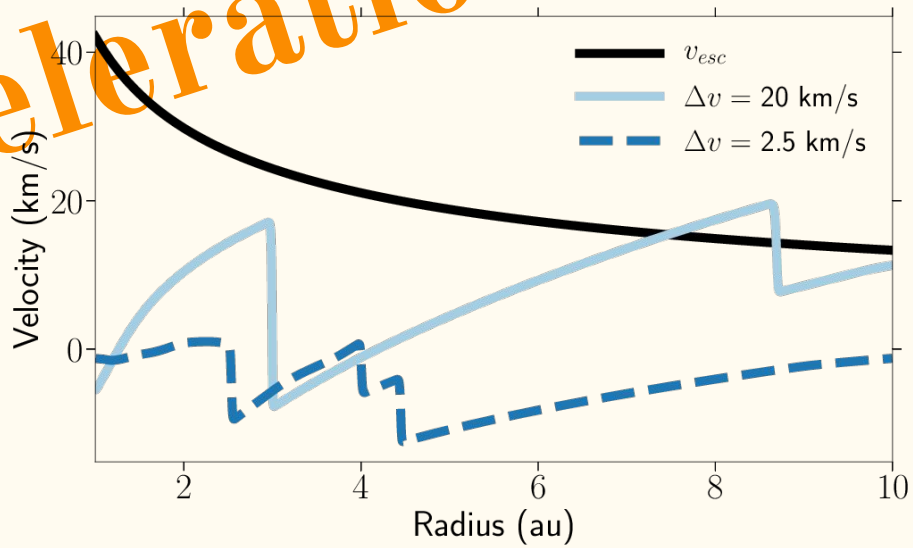



Dust acceleration



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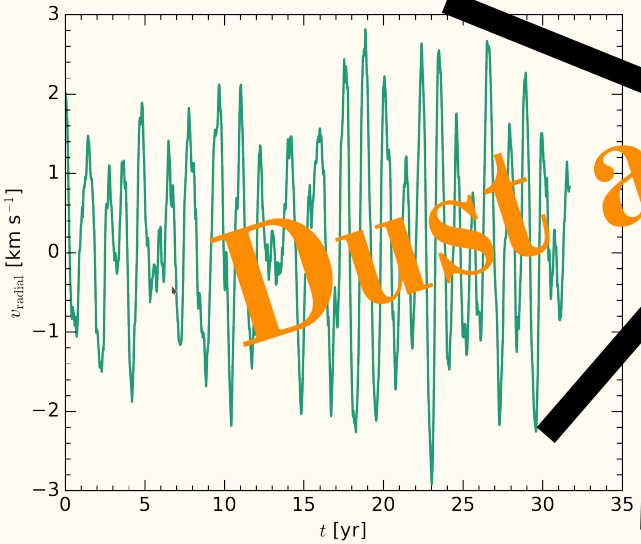
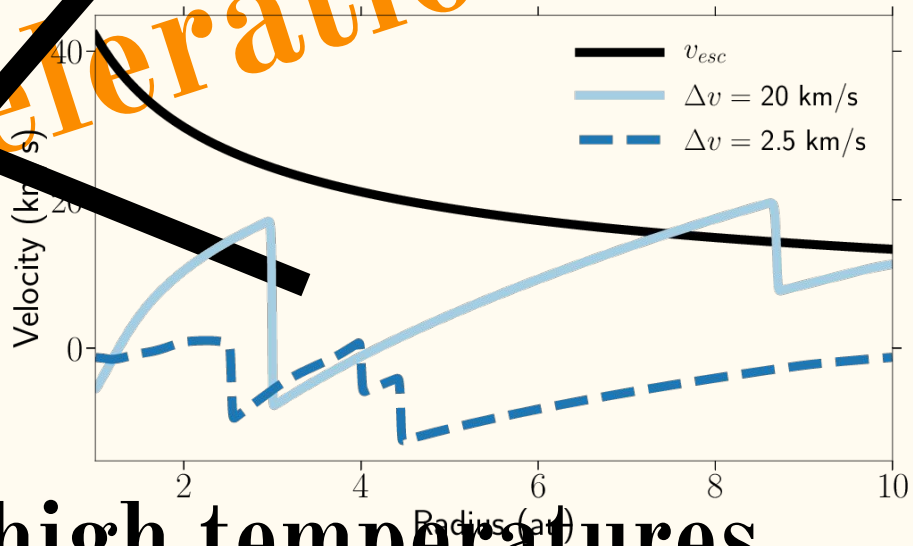



Dust acceleration




**Too high temperatures**

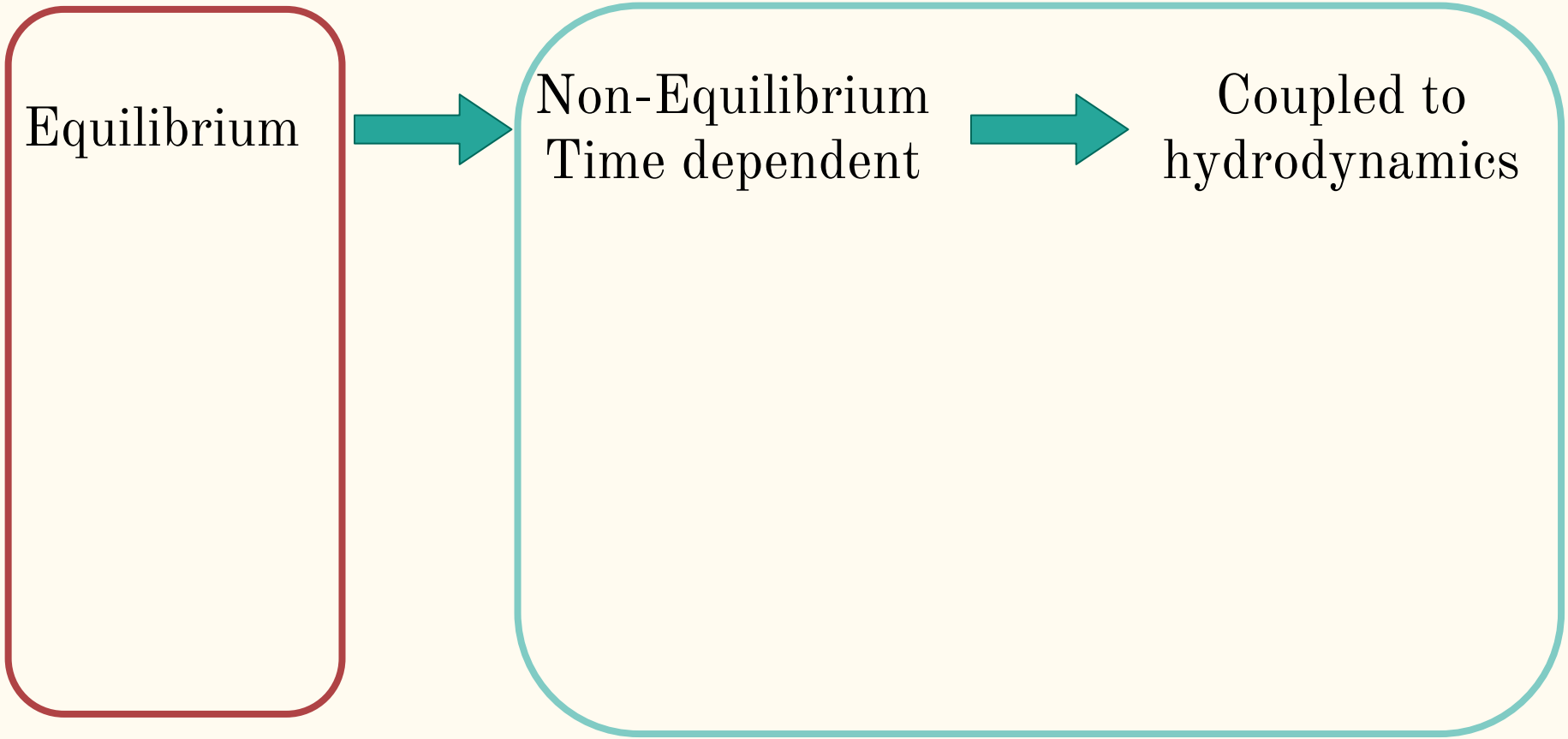
Current chemistry

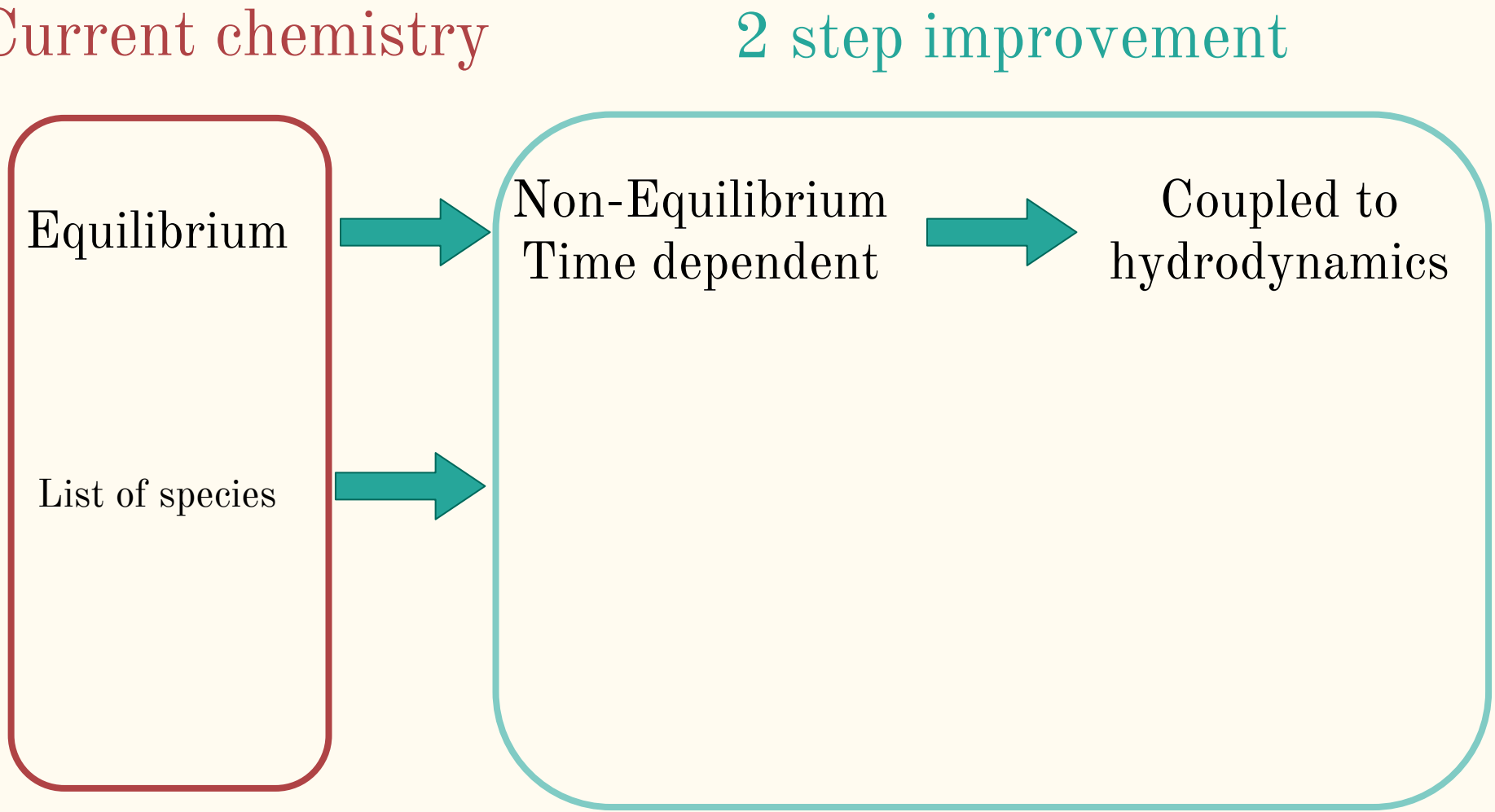
2 step improvement

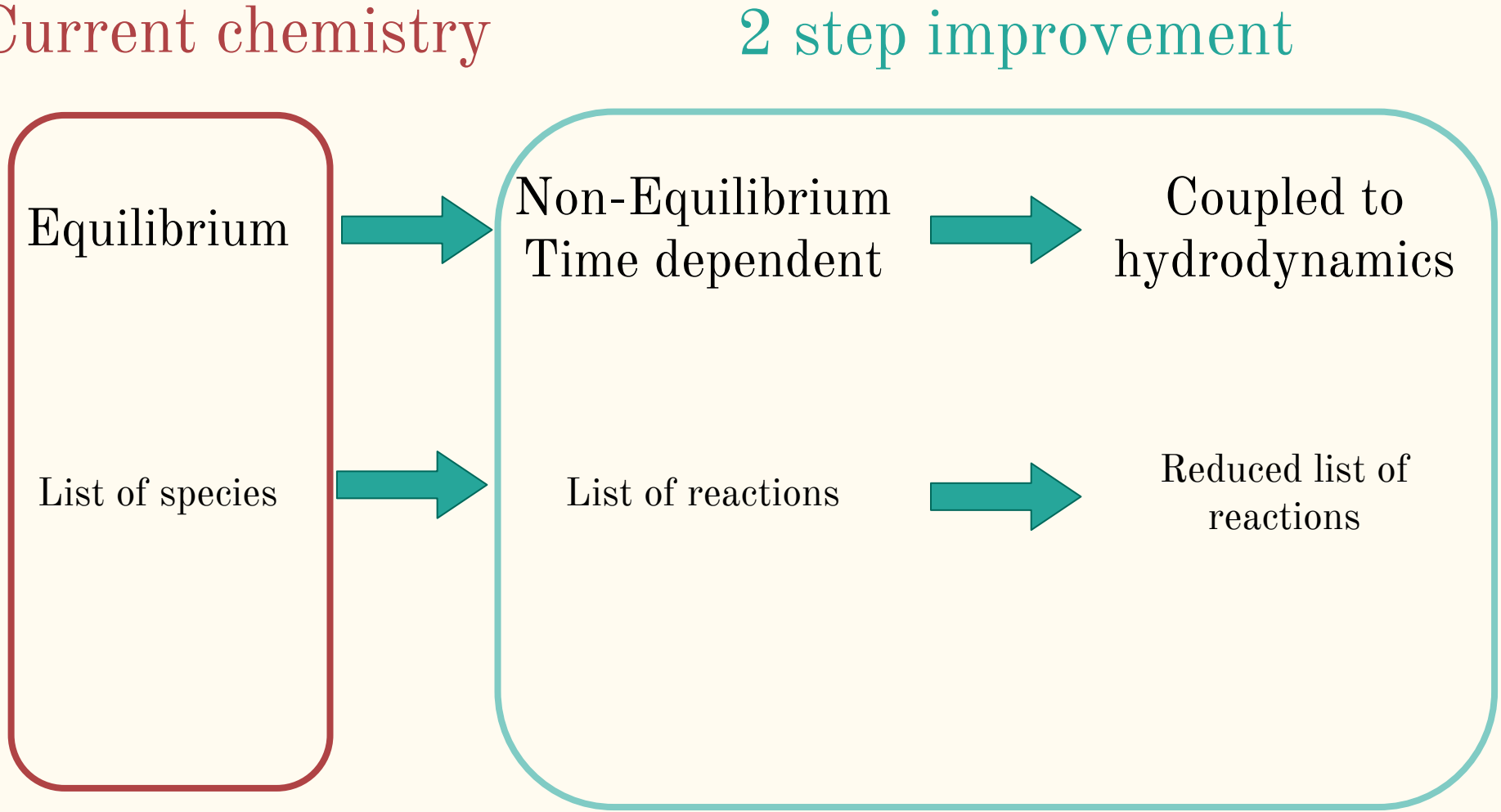
Equilibrium

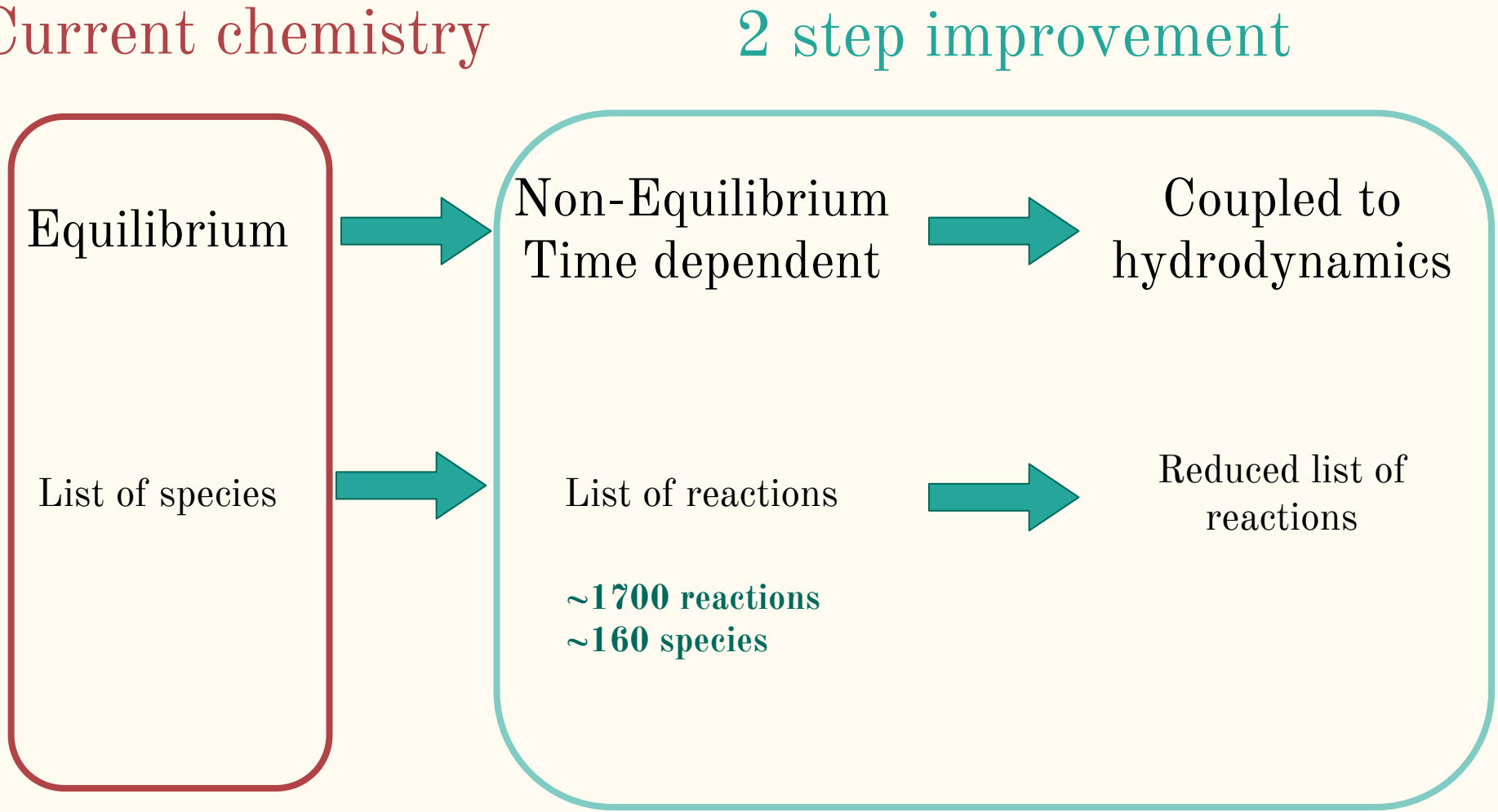
Current chemistry

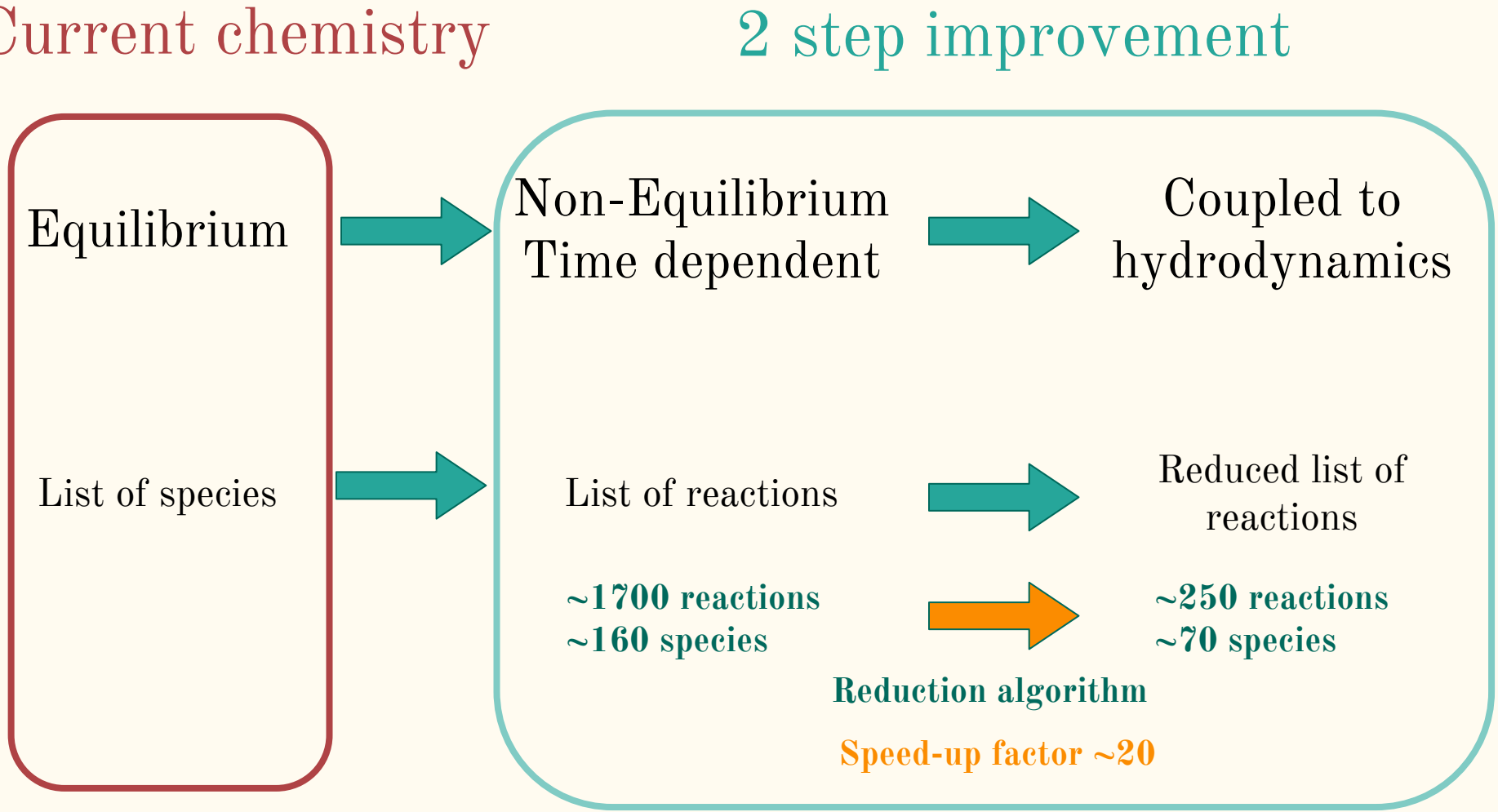
2 step improvement




Current chemistry
2 step improvement
Equilibrium
List of species
Non-Equilibrium
Time dependent
Coupled to
hydrodynamics


Current chemistry
2 step improvement
Equilibrium
List of species
Non-Equilibrium
Time dependent
List of reactions
Coupled to
hydrodynamics
Reduced list of
reactions


Current chemistry
2 step improvement
Equilibrium
List of species
Non-Equilibrium
Time dependent
List of reactions
~1700 reactions
~160 species
Coupled to
hydrodynamics
Reduced list of
reactions

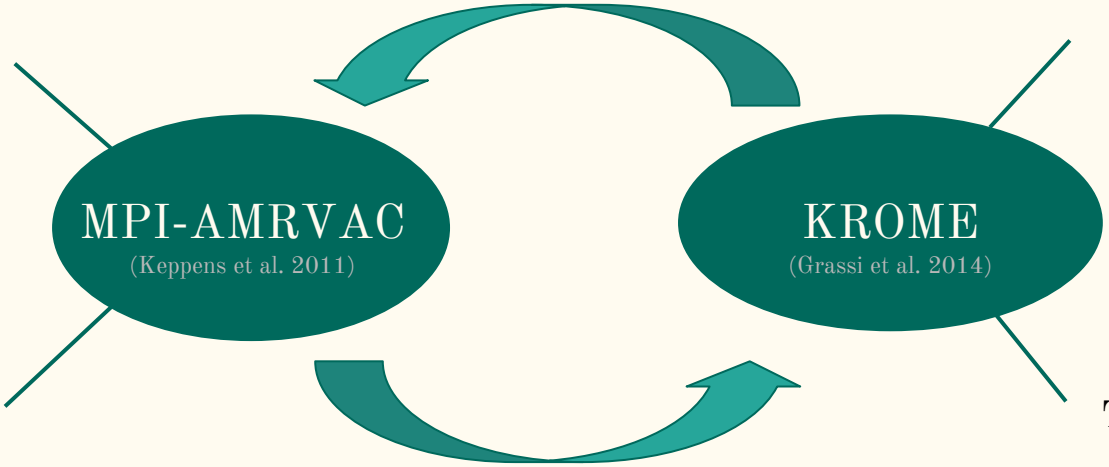

Current chemistry
2 step improvement
Equilibrium
List of species
Non-Equilibrium
Time dependent
Coupled to
hydrodynamics
List of reactions
Reduced list of
reactions
~1700 reactions
~160 species
~250 reactions
~70 species
Reduction algorithm
Speed-up factor ~20

# Computational framework

Conservation of chemical elements
(Plewa & Müller 1999, Glover et al. 2010, Grassi et al. 2017)

- Updated temperature
- Updated fractional abundances

Chemical evolution



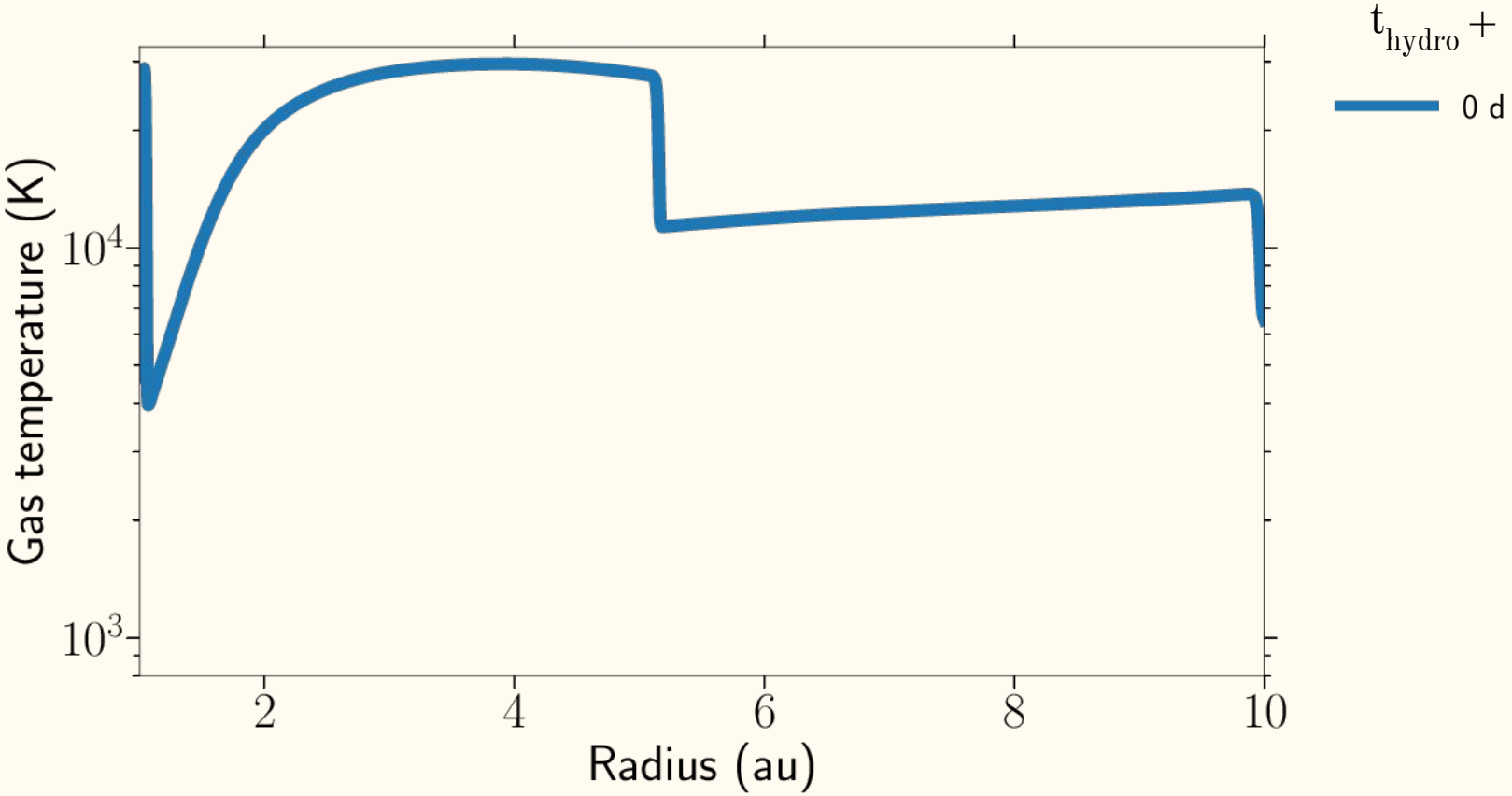

Variable adiabatic index

- Temperature
- Fractional abundances

Thermal evolution:

*H and He line, $H_2$ line, CO line, $H_2$ chemical, Metal line, CIE, Cosmic ray*

# Cooling is super efficient



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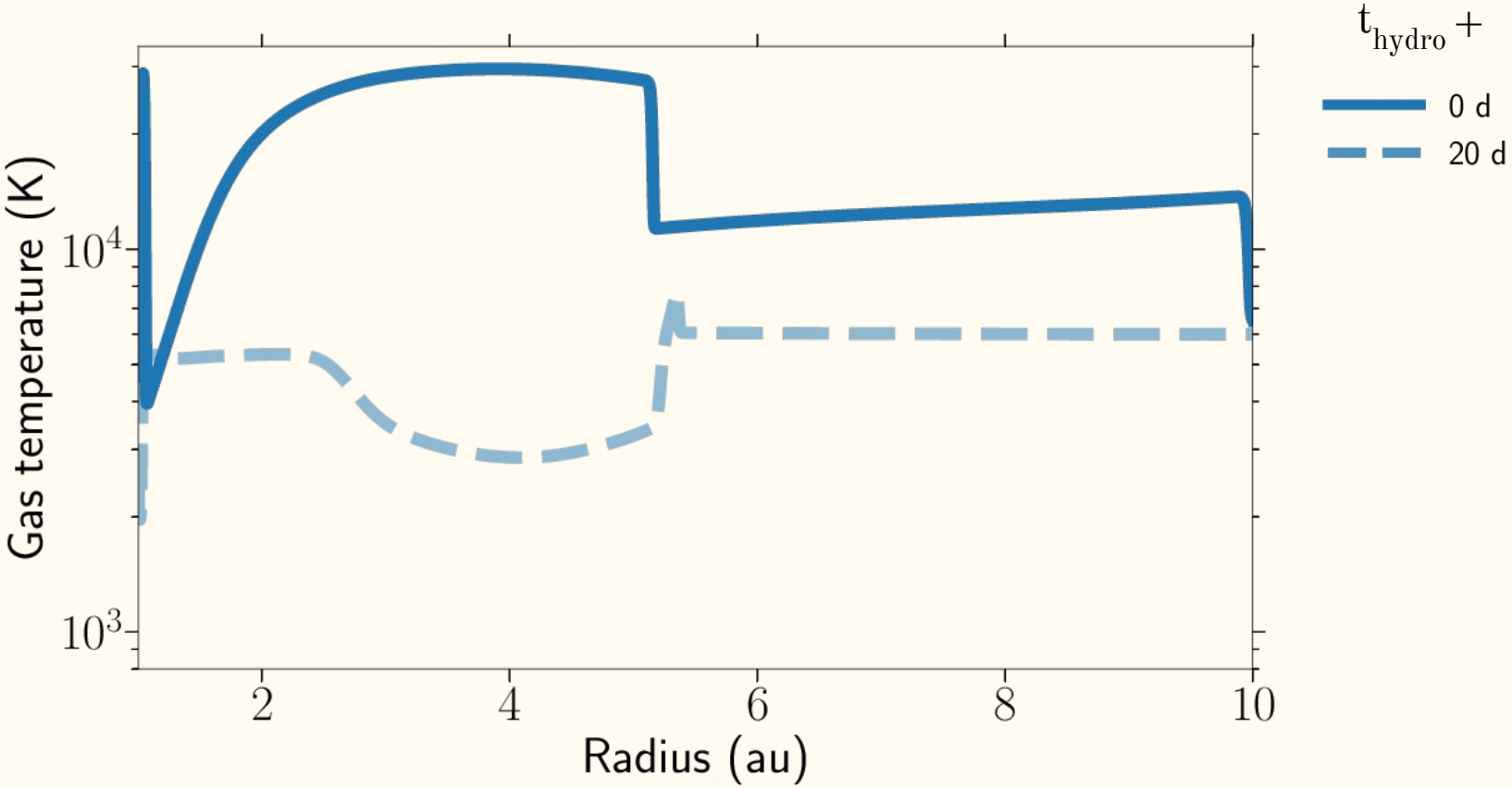

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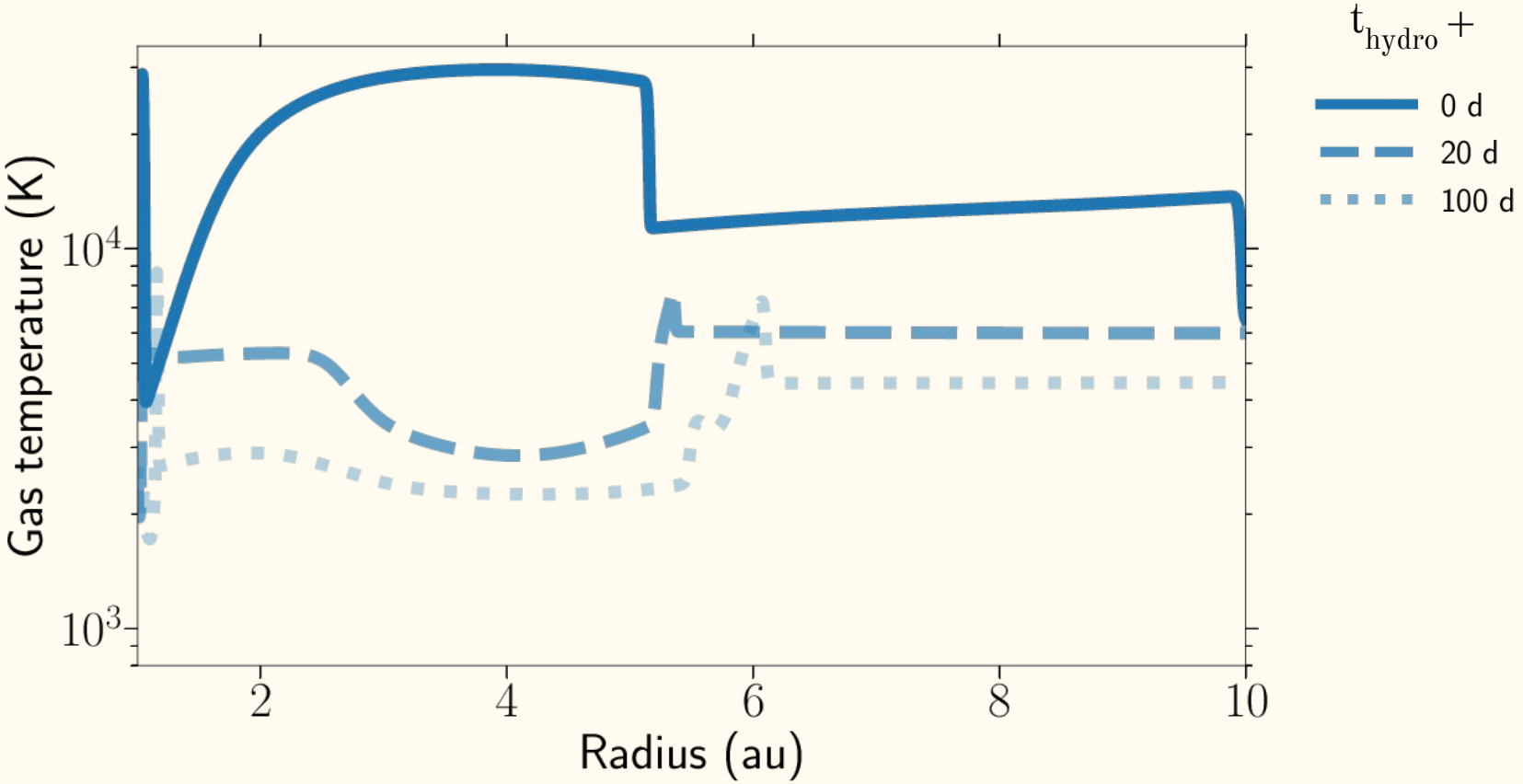

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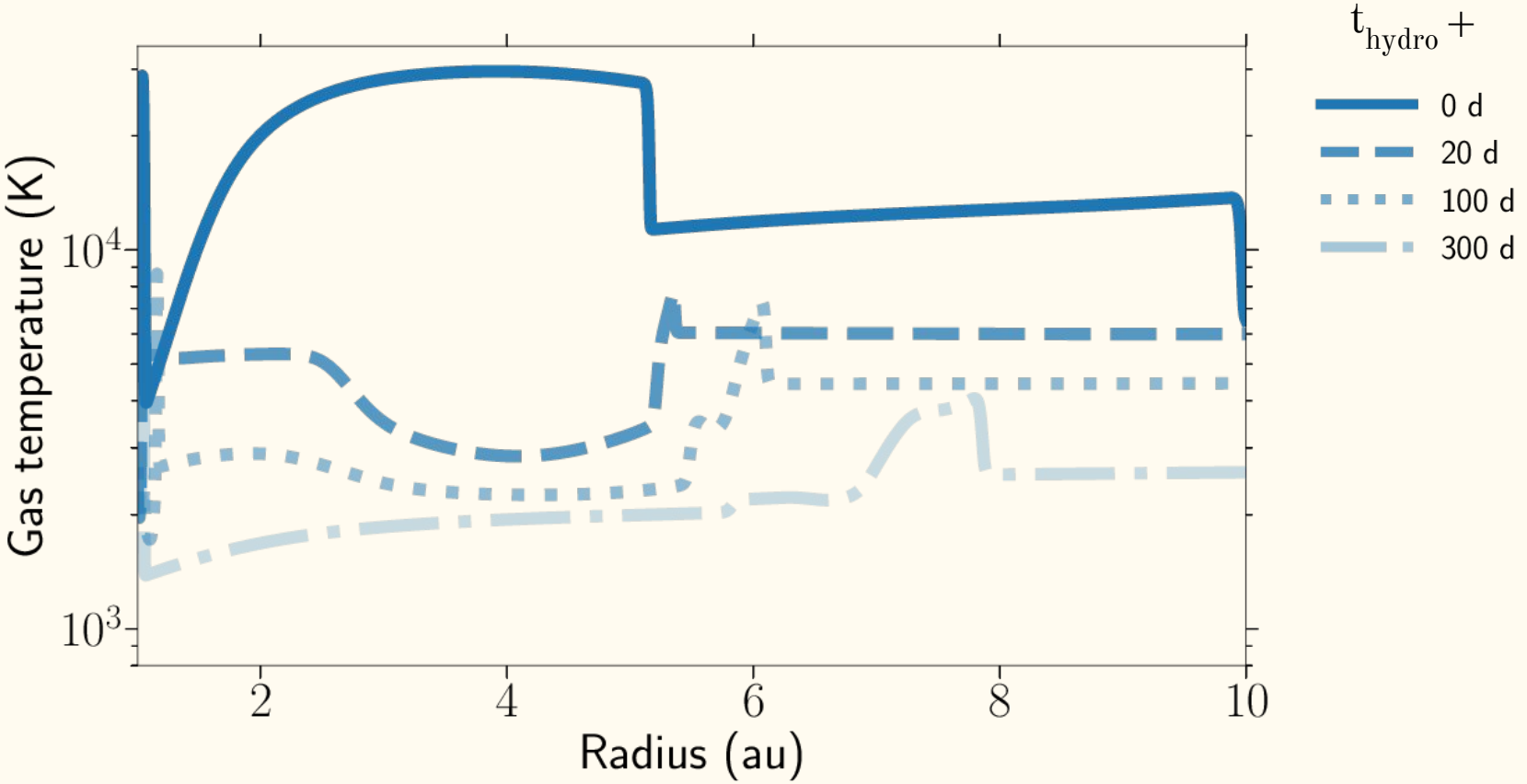

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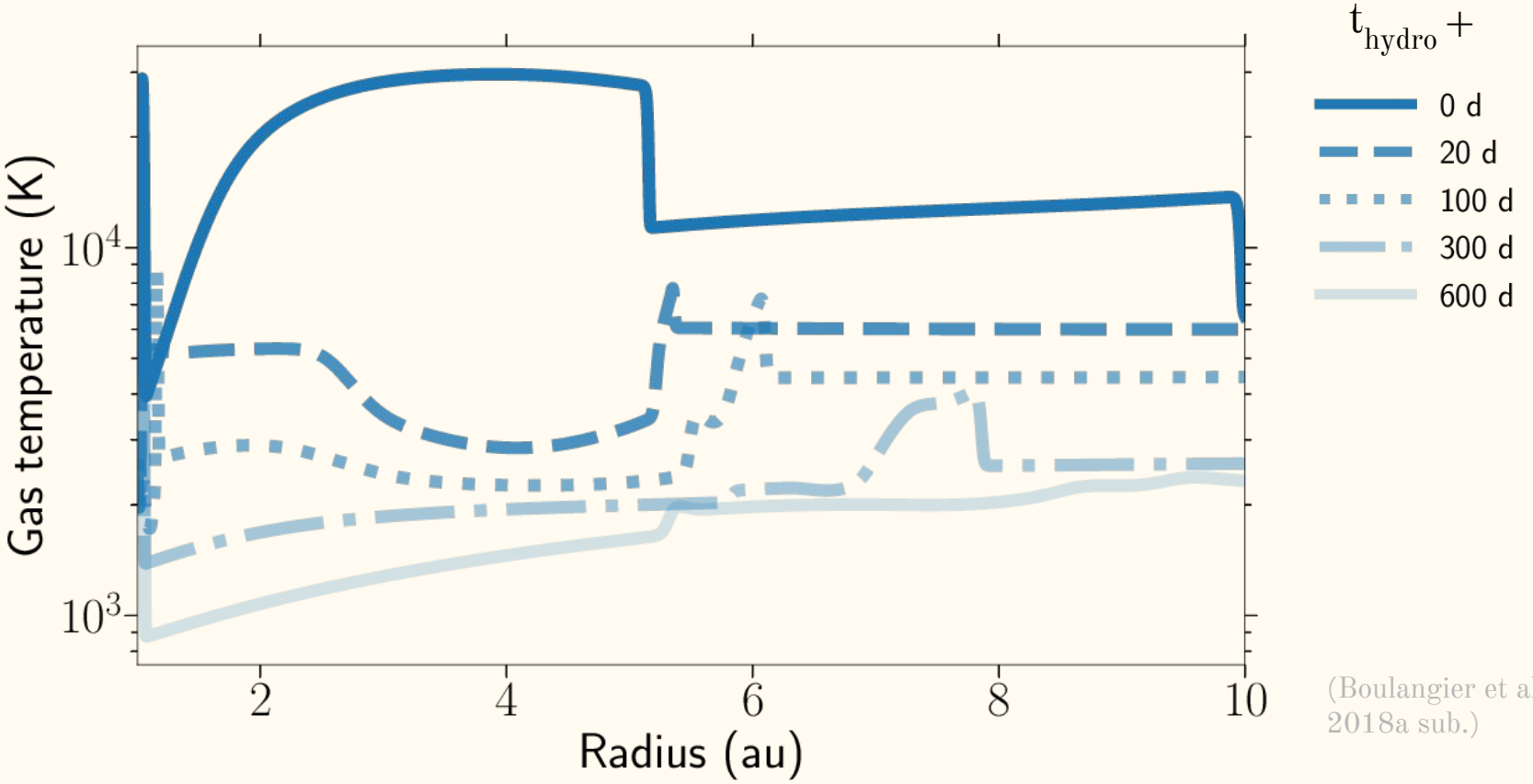


(Boulangier et al. 2018a sub.)

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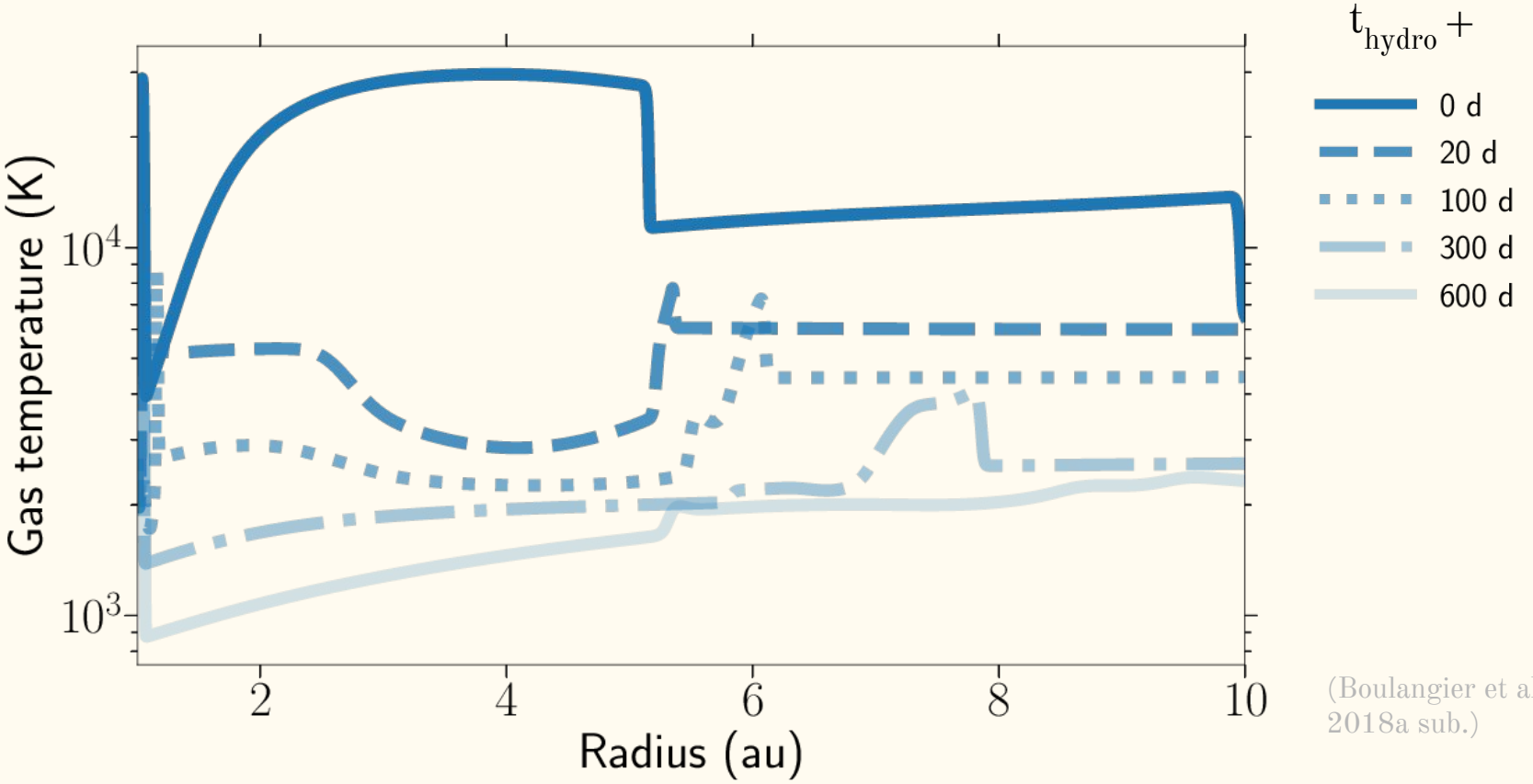


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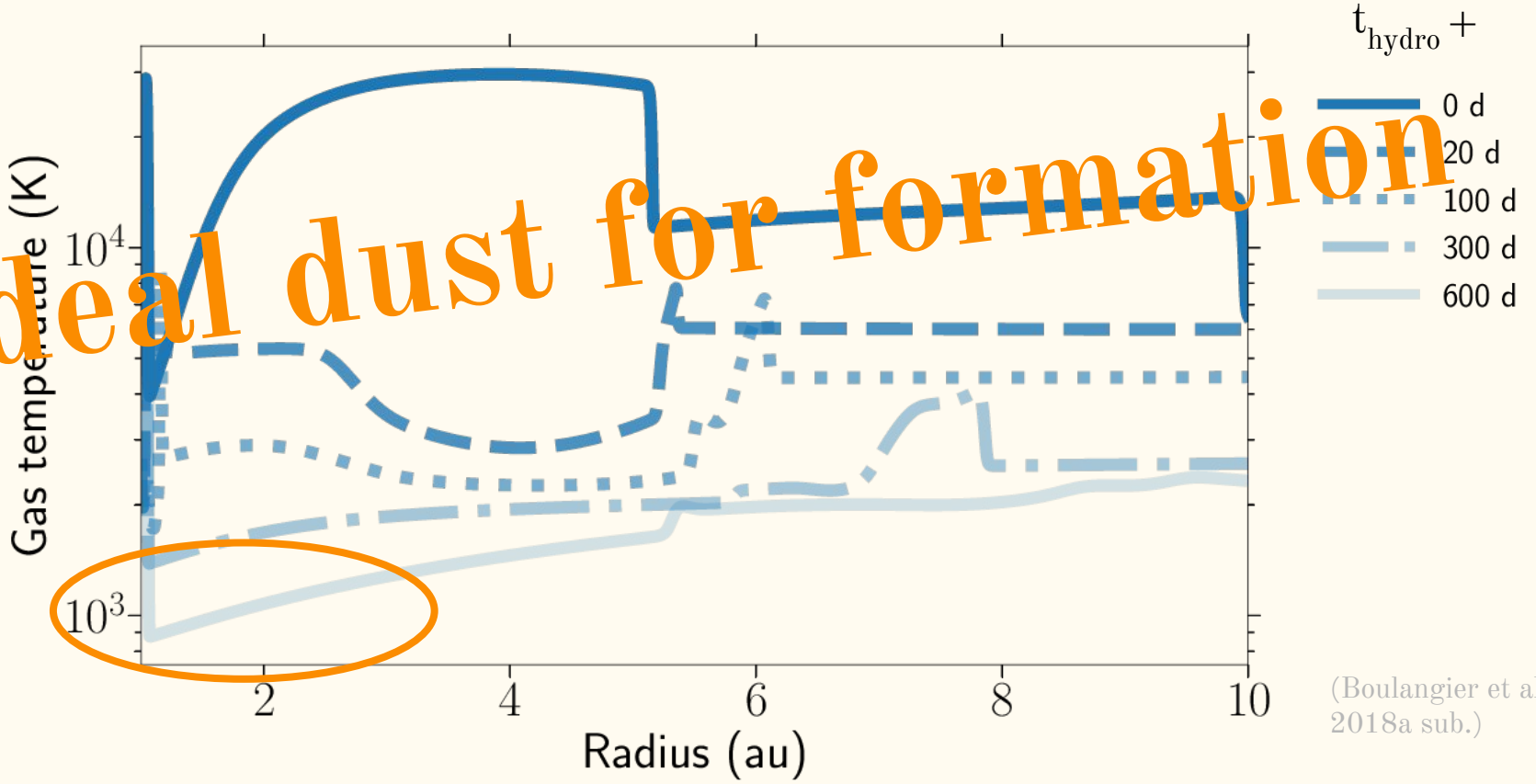
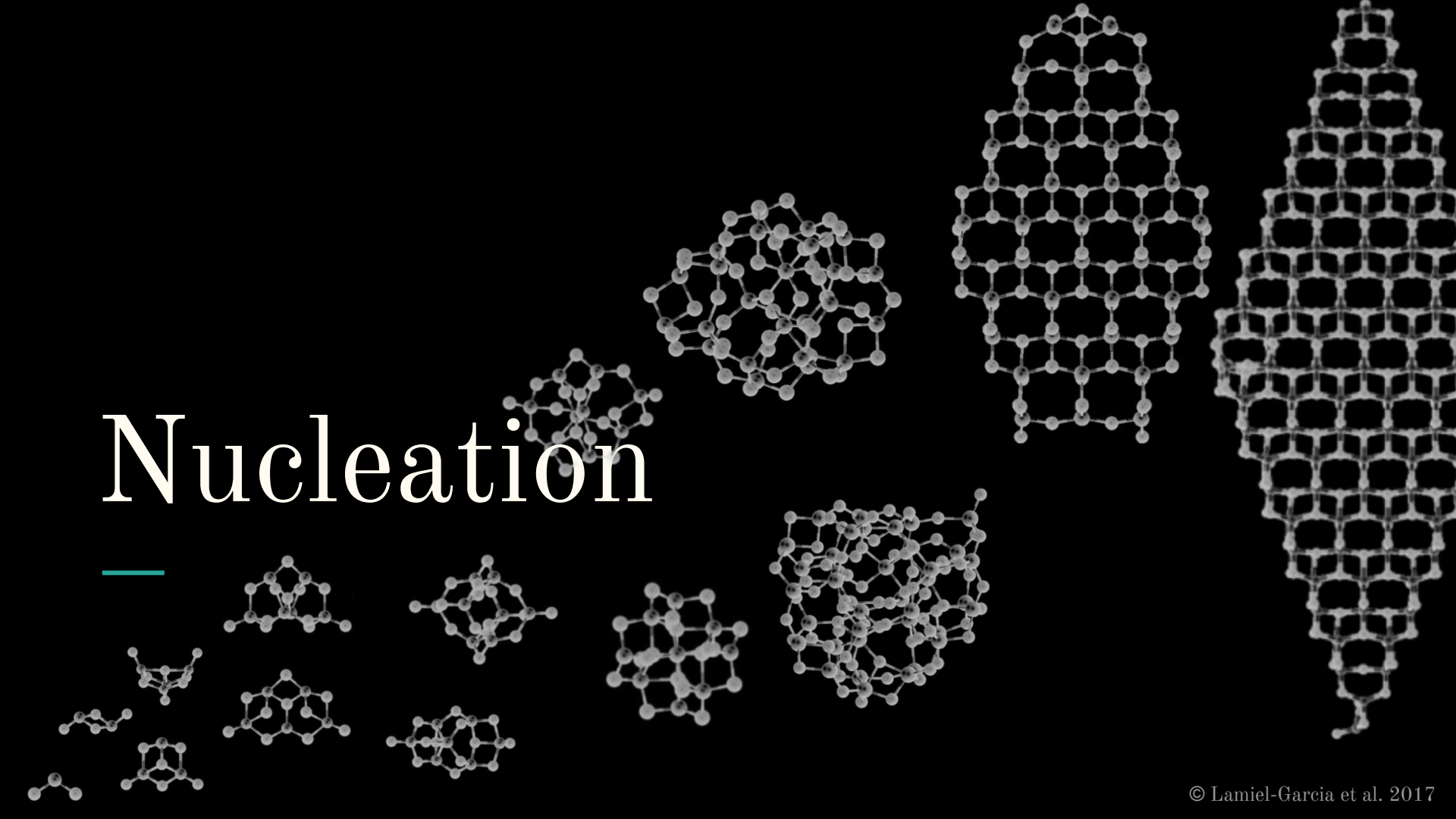



Ideal dust for formation

(Boulangier et al. 2018a sub.)

# Nucleation



© Lamiel-Garcia et al. 2017

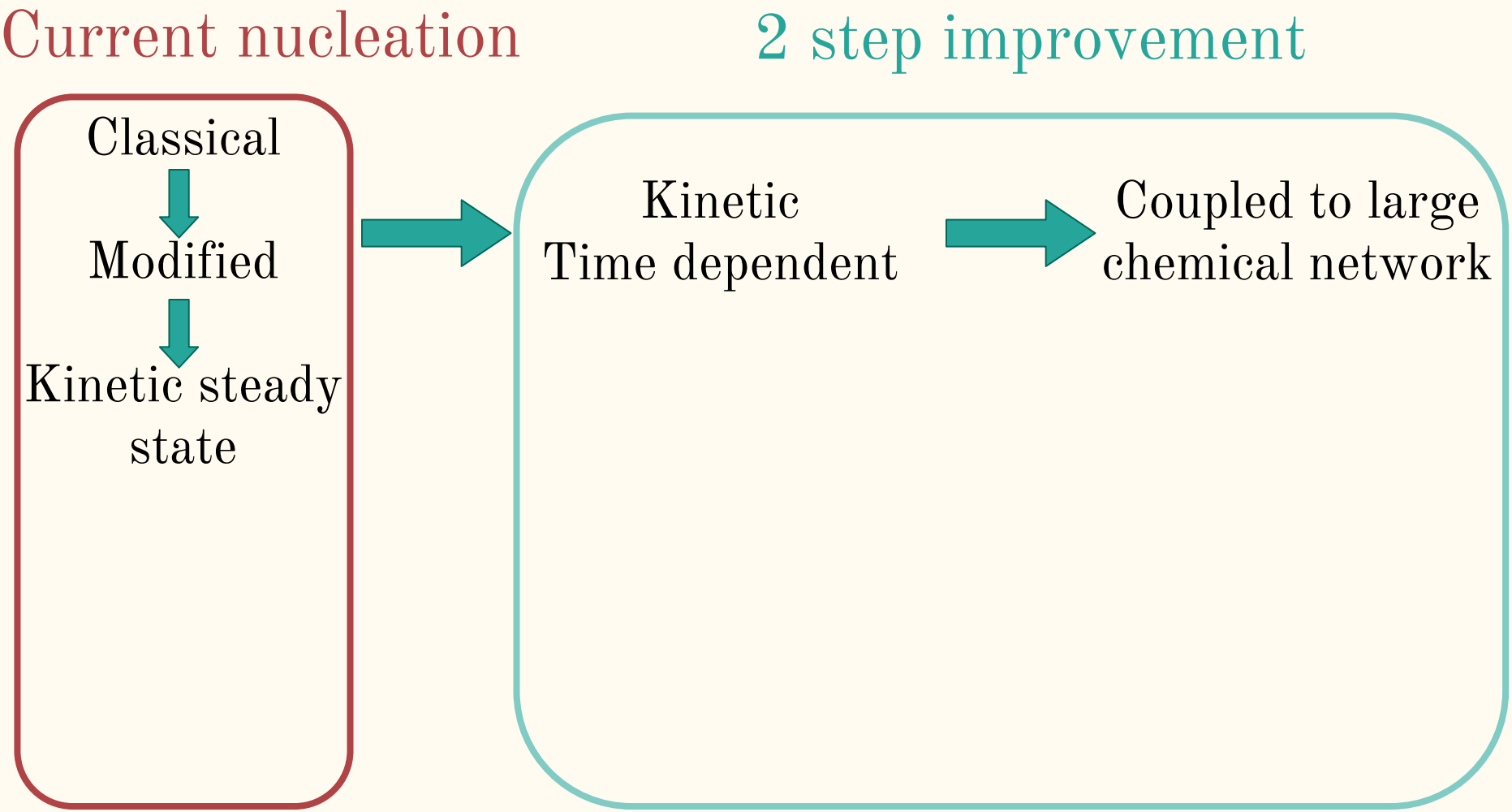
Current nucleation

Classical

Modified

Kinetic steady state

2 step improvement


Current nucleation
2 step improvement
Classical
Modified
Kinetic steady state
Kinetic
Time dependent
Coupled to large chemical network

# Current nucleation

Classical

↓

Modified

↓

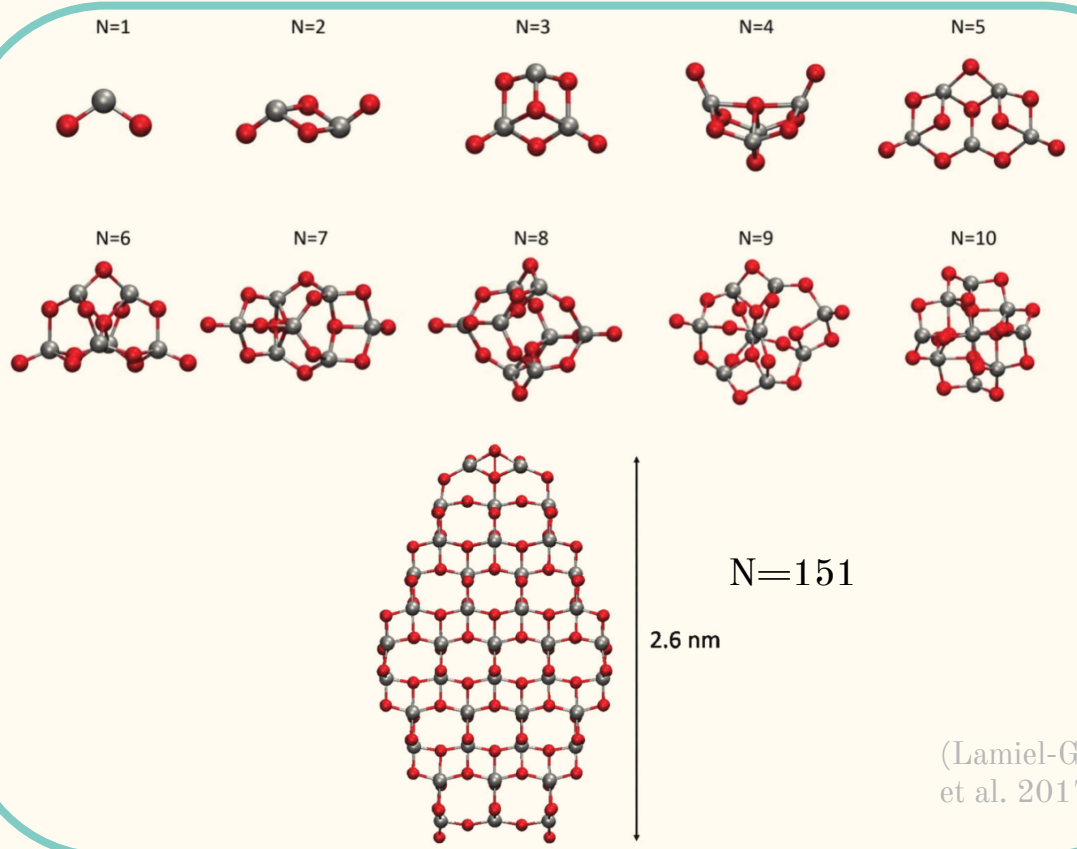
Kinetic steady state

Bulk properties

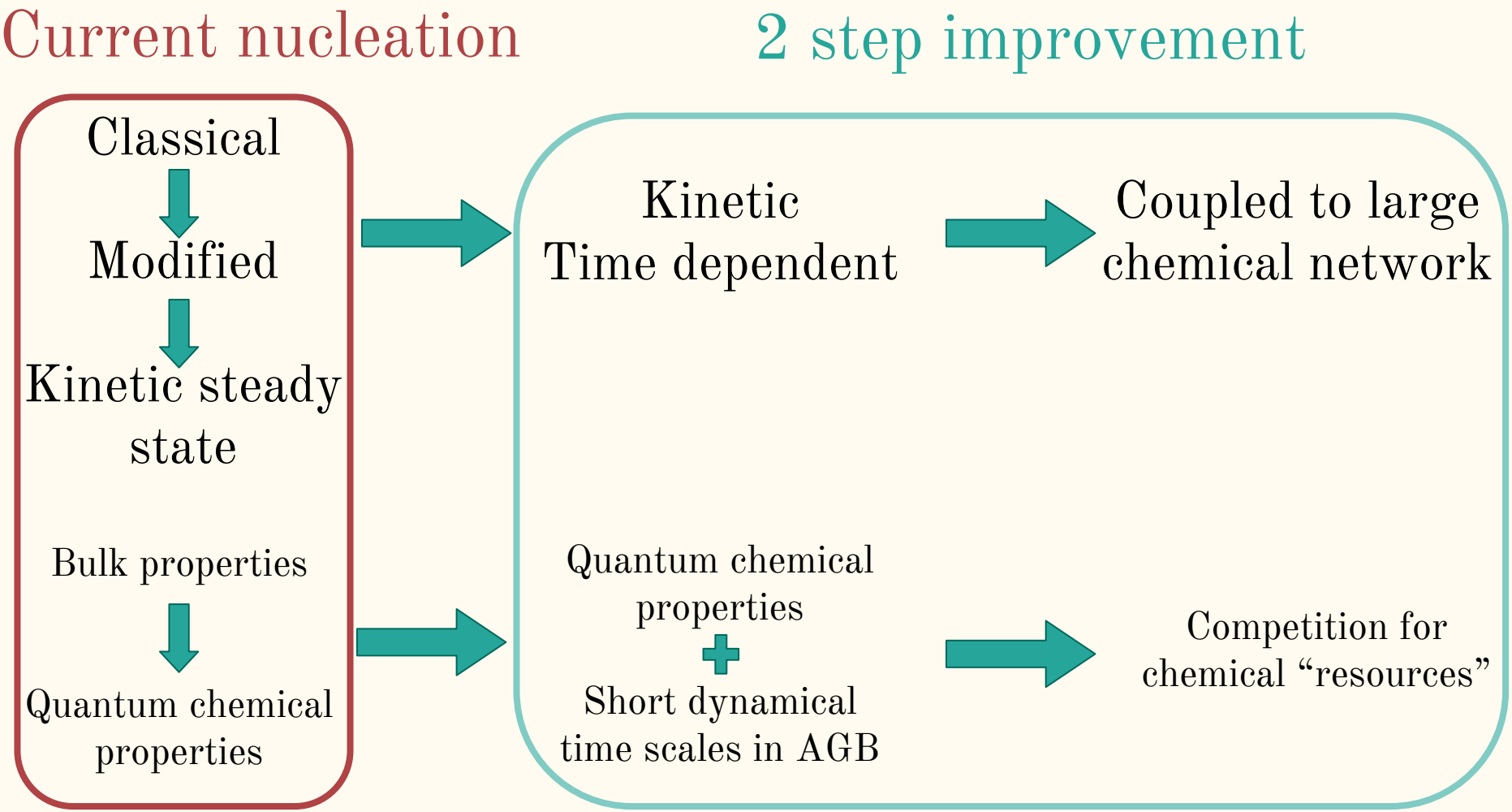
↓

Quantum chemical properties

# 2 step improvement

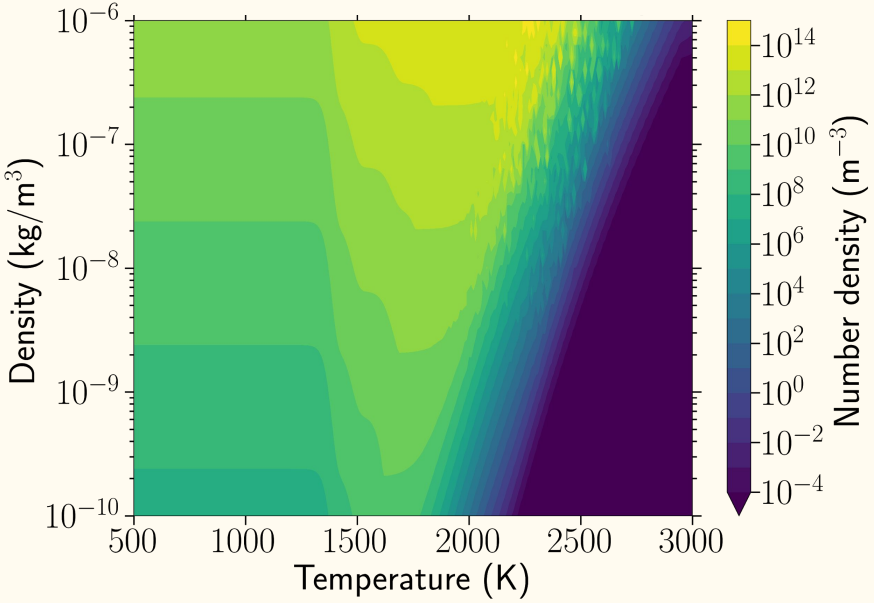



(Lamiel-Garcia et al. 2017)

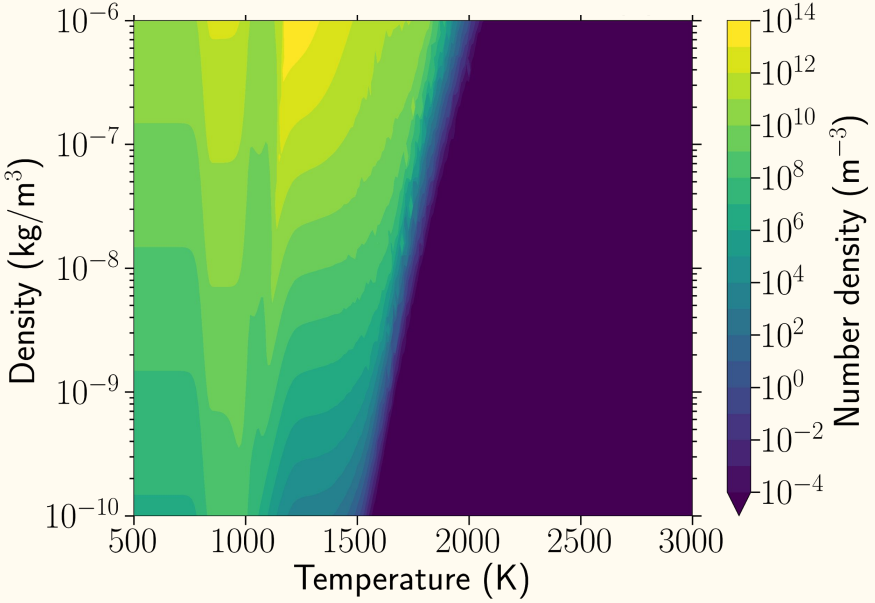

Current nucleation
2 step improvement
Classical
Modified
Kinetic steady state
Bulk properties
Quantum chemical properties
Kinetic
Time dependent
Coupled to large chemical network
Quantum chemical properties
+
Short dynamical time scales in AGB
Competition for chemical “resources”

# Different candidates, different temperatures

Absolute $(Al_2O_3)_7$ abundance



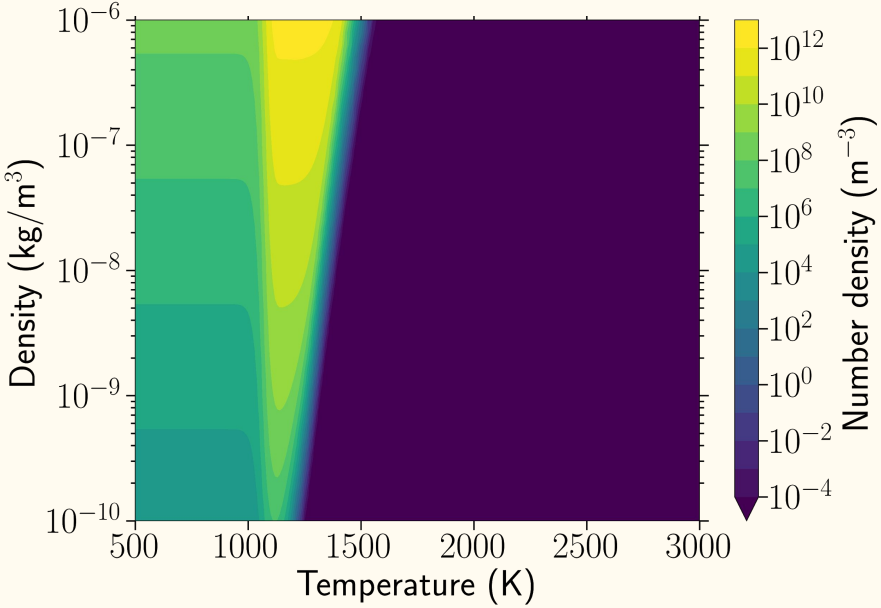

Absolute $(MgO)_{10}$ abundance



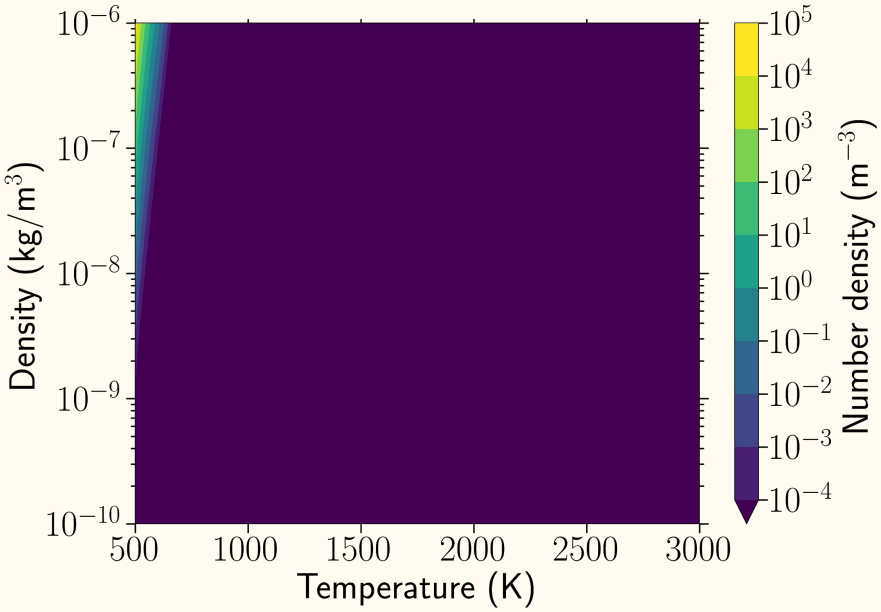

(Boulangier et al. 2018b in prep.)

# $(Al_2O_3)_7 > (MgO)_{10} > (TiO_2)_{10} > (SiO_2)_9$

Absolute $(TiO_2)_{10}$ abundance

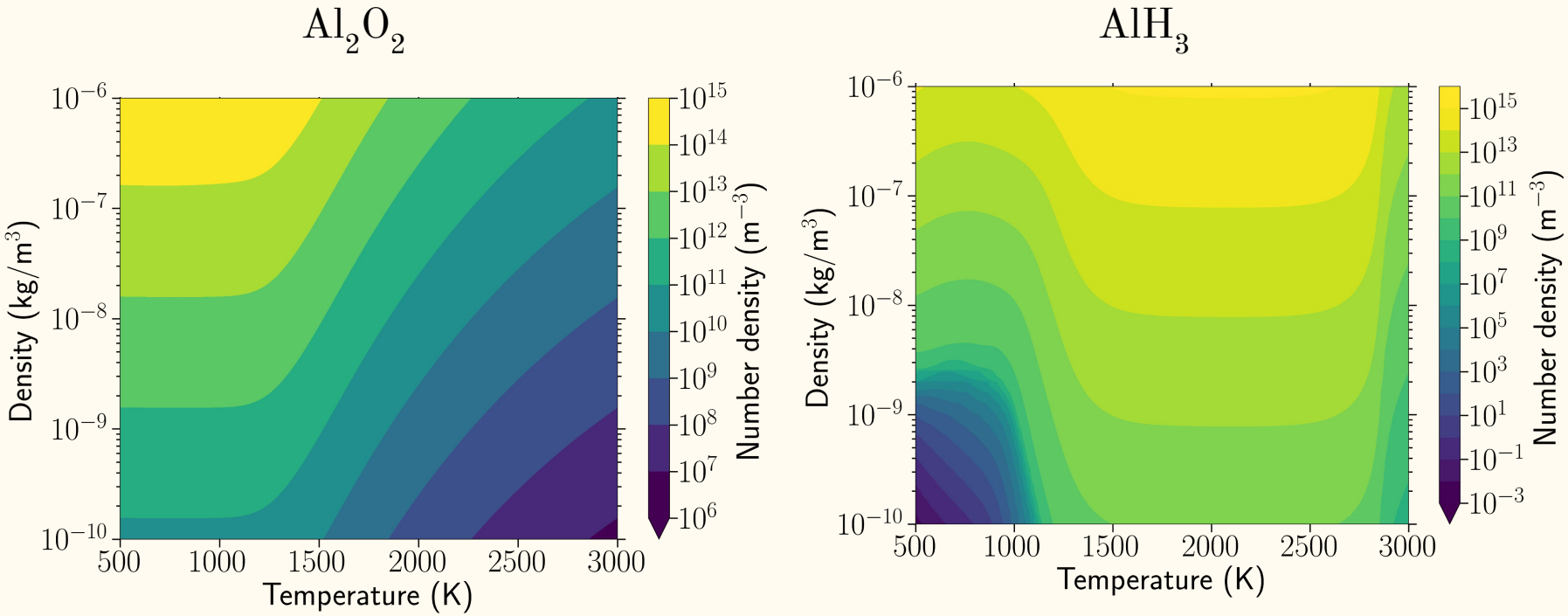



Absolute $(SiO_2)_9$ abundance



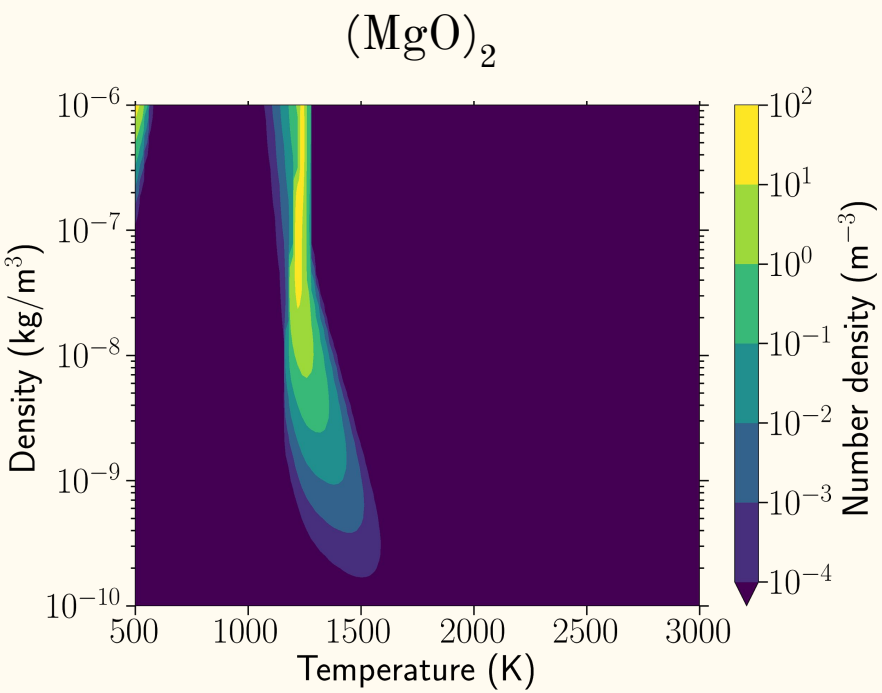

(Boulangier et al. 2018b in prep.)

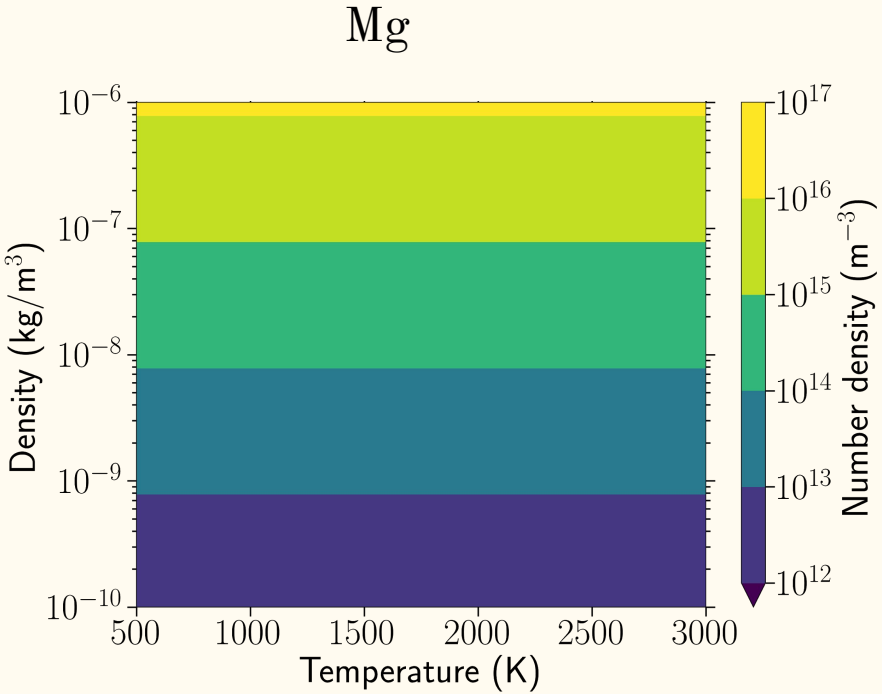
# Cannot form any $Al_2O_3$, Al in other molecules




(Boulangier et al. 2018b in prep.)

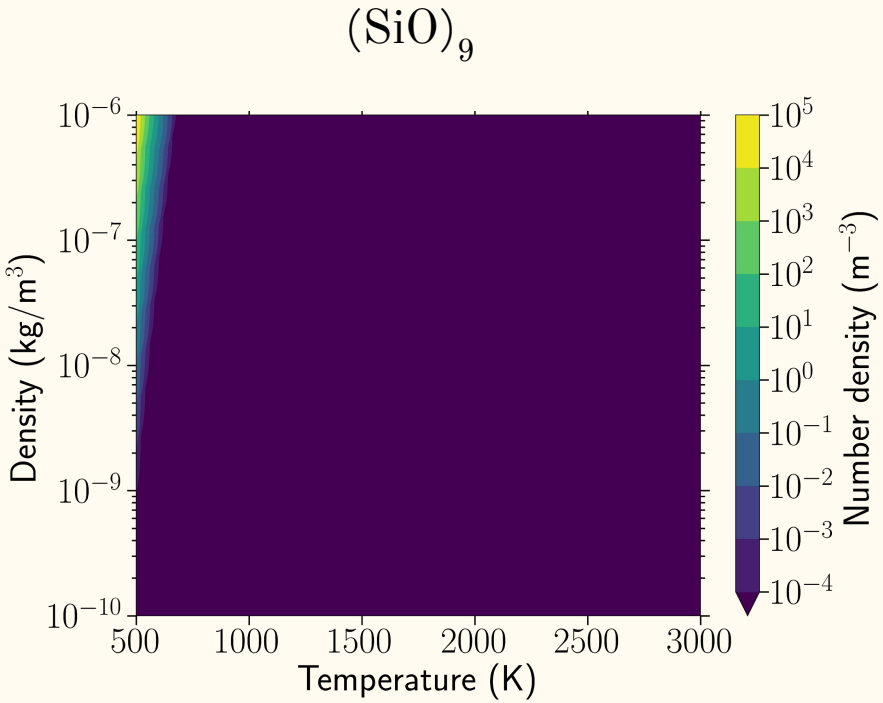
# Bottleneck at $(MgO)_3$

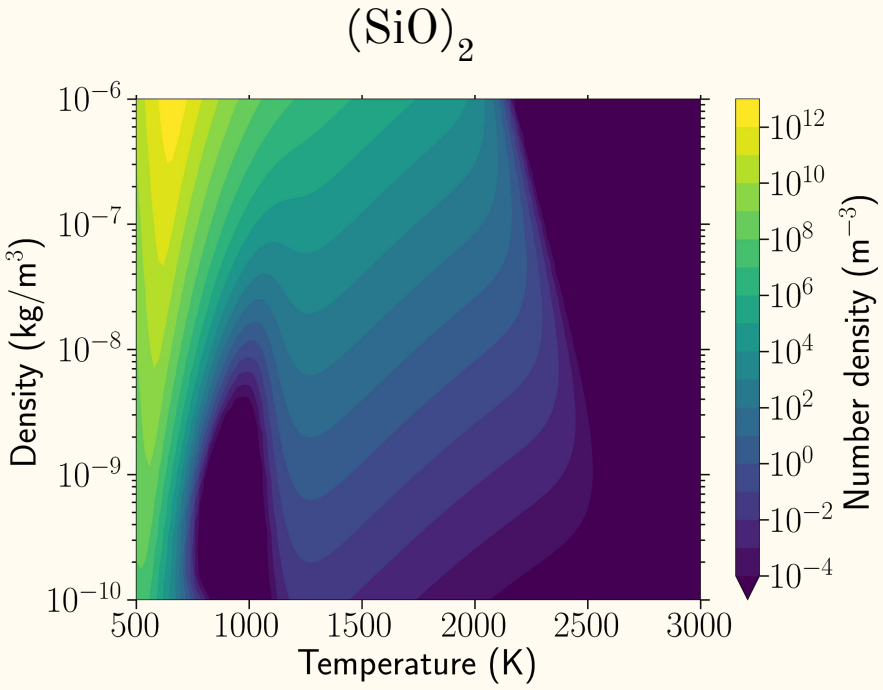



(Boulangier et al. 2018b in prep.)

# $(SiO)_N$ needs too low temperature

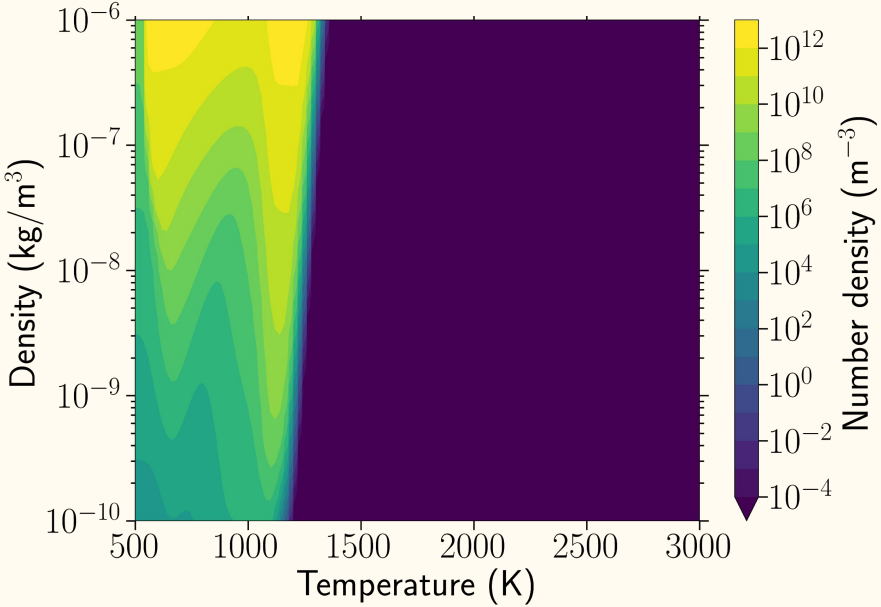


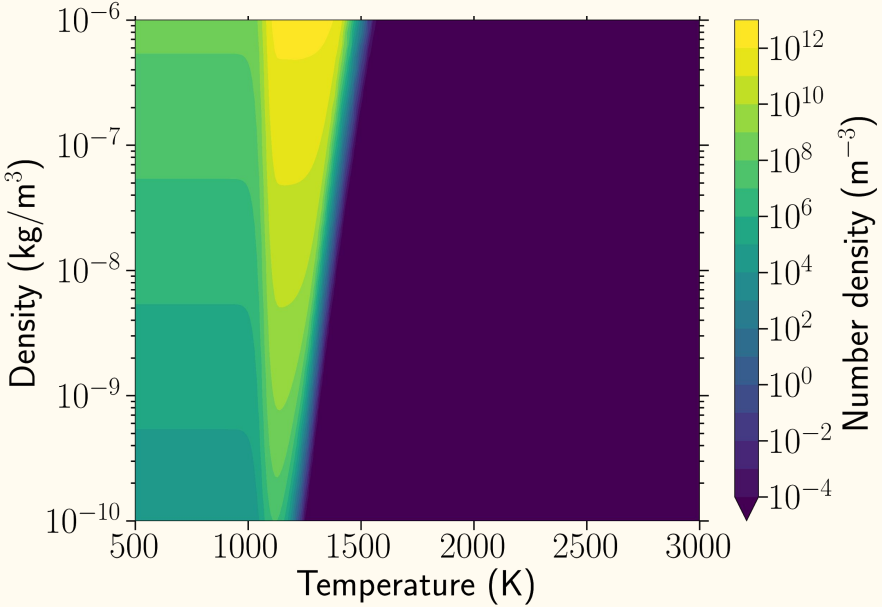

(Boulangier et al. 2018b in prep.)

# $(TiO_2)_N$ is still a good candidate

$(TiO_2)_{10}$




$(TiO_2)_{10}$ only $(TiO_2)_N$ nucleation



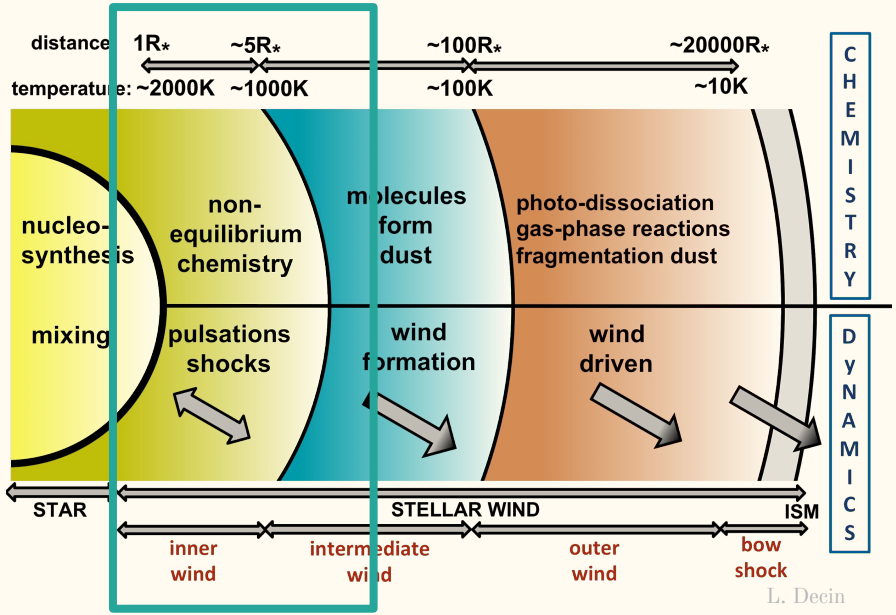

(Boulangier et al. 2018b in prep.)

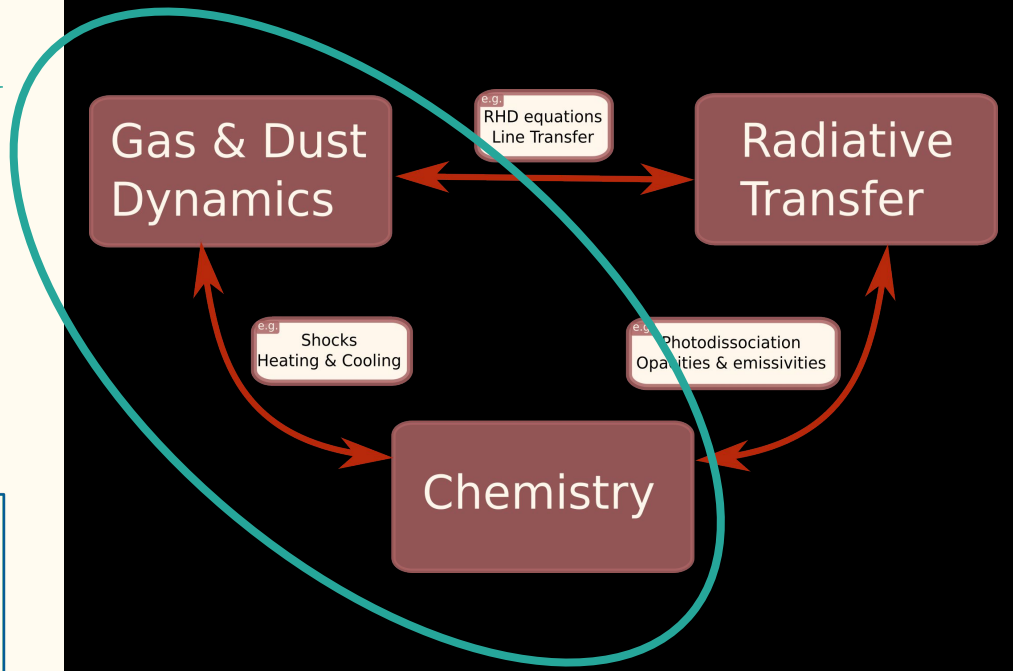
# Open questions

- Missing reactions to form $(Al_2O_3)_N$ clusters?
- Will there be enough Ti?
- Will $(TiO_2)_N$ clusters form fast enough with low temperature-limit?
- What if temperature varies?
- Need for composite clusters?

# Self-consistent hydrochemistry

More correct dynamical, temperature and chemical abundance profile

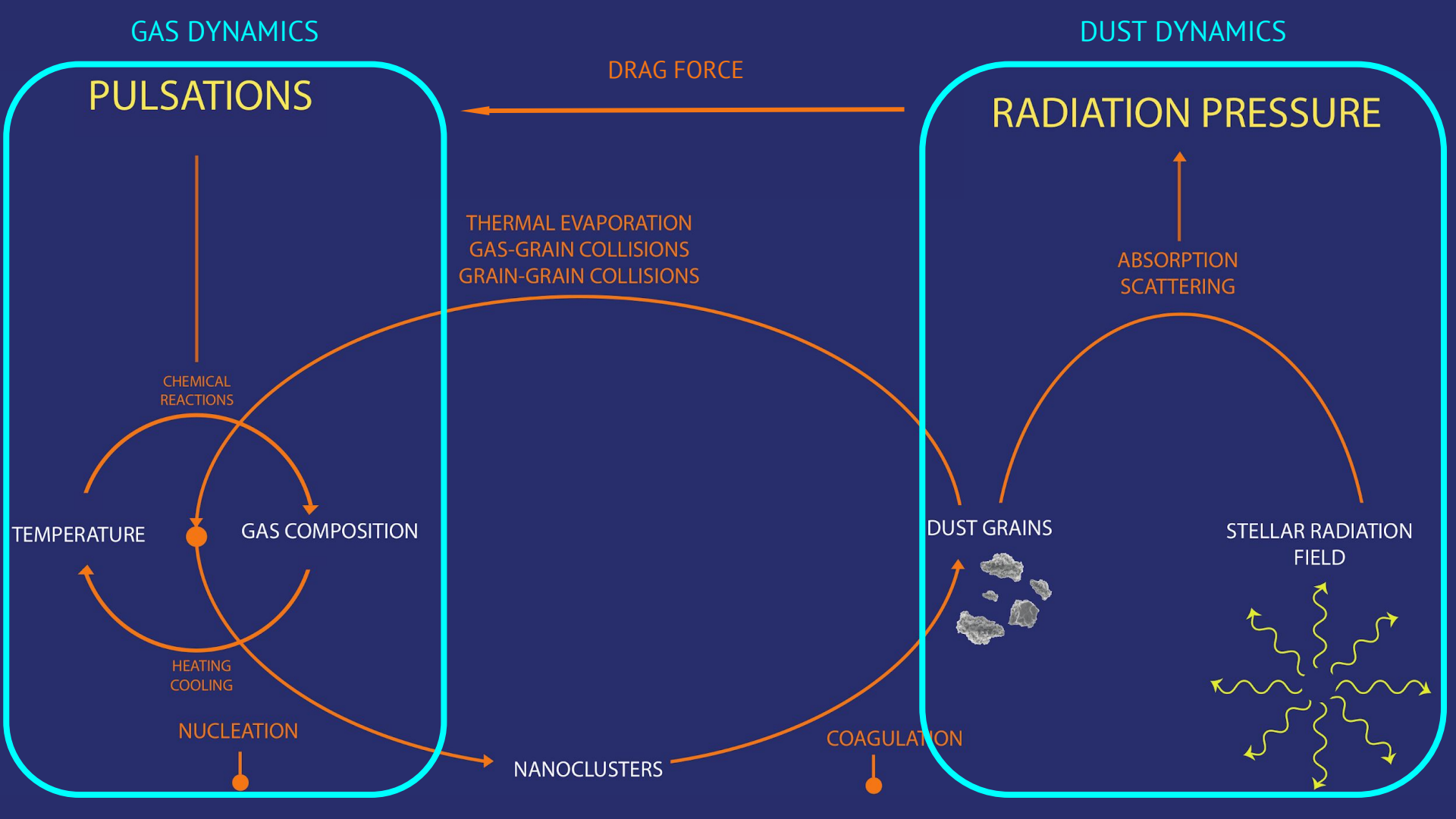



\+ Self-consistent nucleation

Removes assumptions on seed particles positions, abundances, and composition

# Extra slides


GAS DYNAMICS
DUST DYNAMICS
PULSATIONS
DRAG FORCE
RADIATION PRESSURE
THERMAL EVAPORATION
GAS-GRAIN COLLISIONS
GRAIN-GRAIN COLLISIONS
ABSORPTION
SCATTERING
CHEMICAL
REACTIONS
TEMPERATURE
GAS COMPOSITION
DUST GRAINS
STELLAR RADIATION
FIELD
HEATING
COOLING
NUCLEATION
NANOCLUSTERS
COAGULATION

# Find important reactions

1. Run chemical network in (temperature, density) - grid
2. Get flux of all reactions at different time steps during the evolution
3. Reaction is important if:

$$\frac{\textit{Flux of reaction}}{\textit{Sum of fluxes of all reactions}} > \textit{Threshold}$$

*in any given (temperature, density, time) - grid point*

**User defined**

**Compare abundance of reduced network with original network**

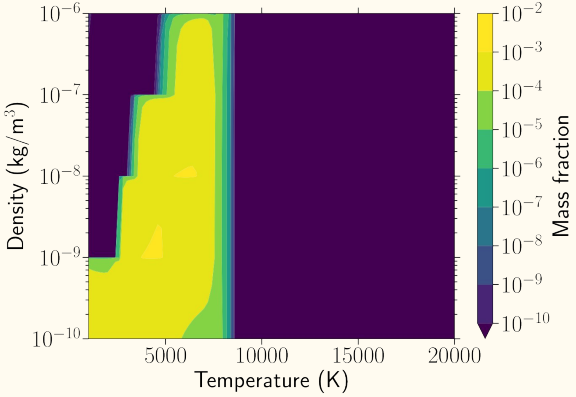
Threshold $= 10^{-7}$

**~250 reactions and ~70 species**

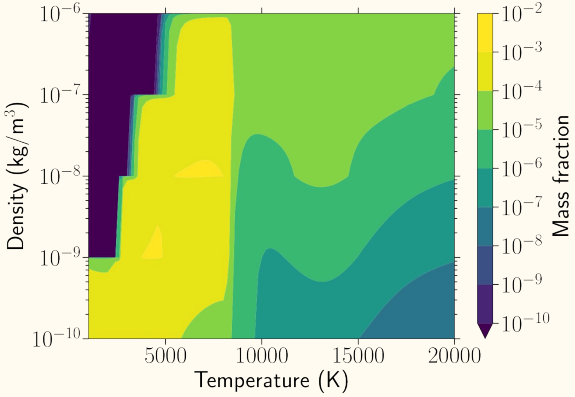
**Speed-up factor ~20**

# Reduction check example: SiO

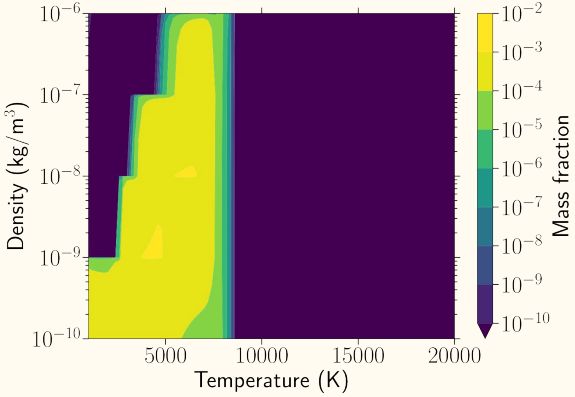
Original

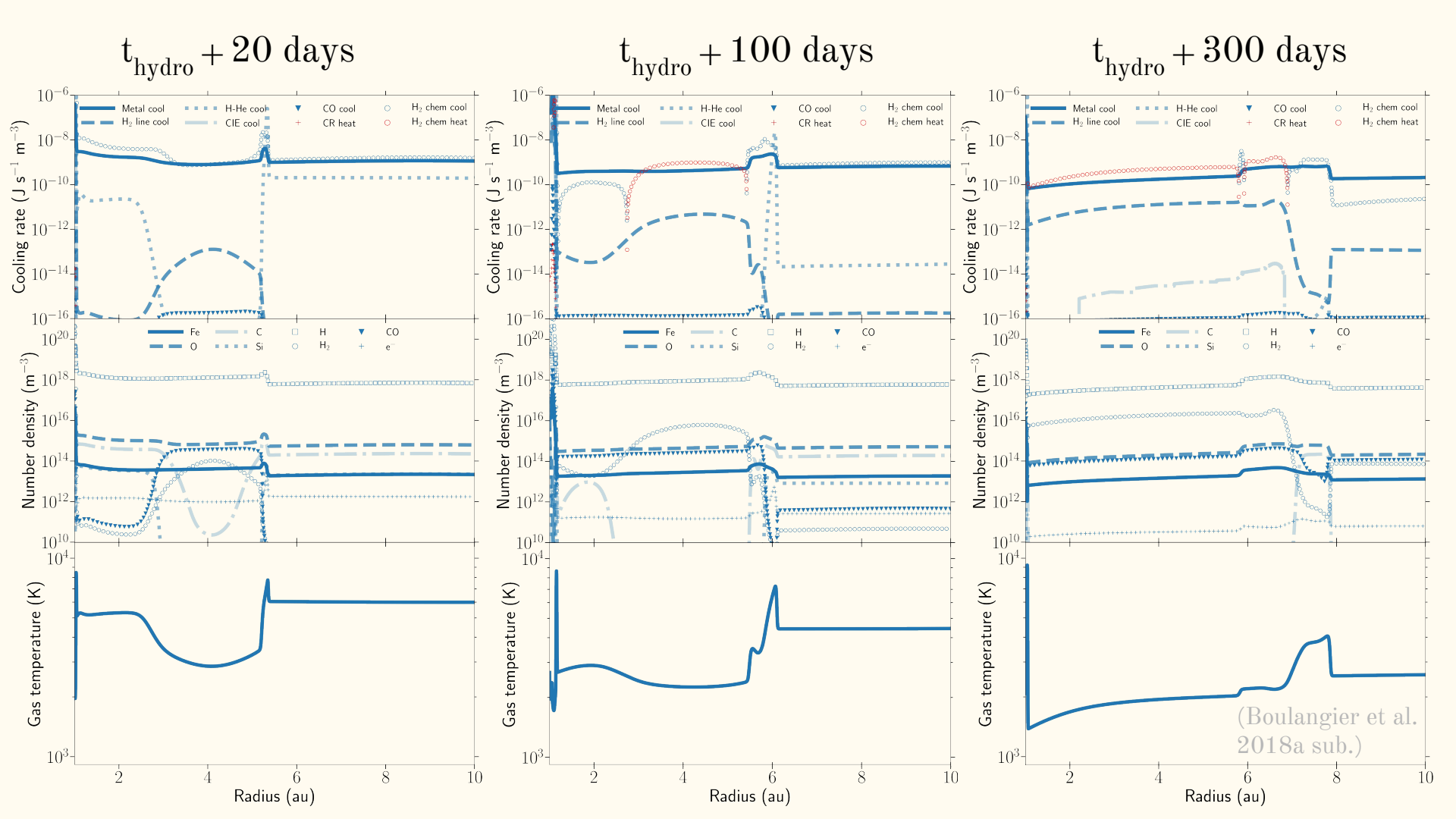



Threshold = $10^{-4}$

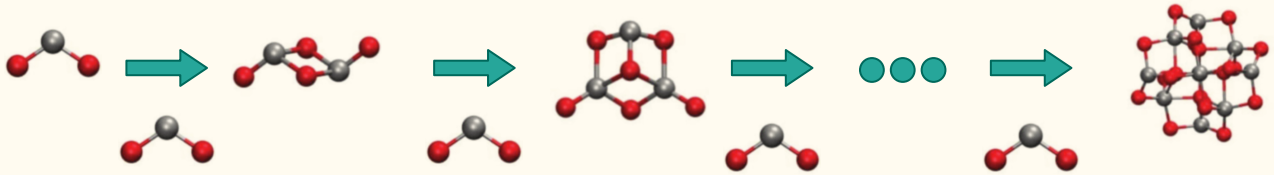



Threshold = $10^{-7}$



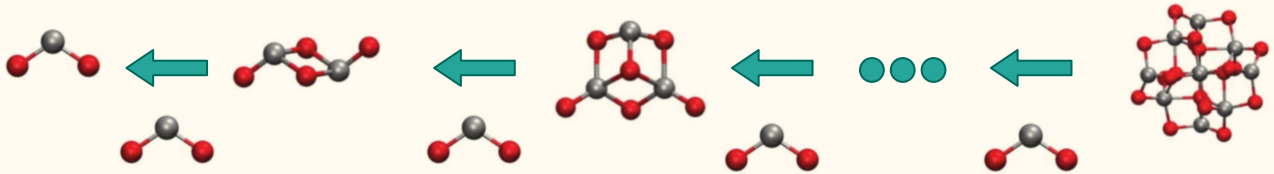

$t_{hydro} + 20$ days
$t_{hydro} + 100$ days
$t_{hydro} + 300$ days
Cooling rate (J s$^{-1}$ m$^{-3}$)
Metal cool
H$_2$ line cool
H-He cool
CIE cool
CO cool
CR heat
H$_2$ chem cool
H$_2$ chem heat
Number density (m$^{-3}$)
Fe
O
C
Si
H
H$_2$
CO
e$^-$
Gas temperature (K)
Radius (au)
(Boulangier et al. 2018a sub.)

# Cluster growth/destruction



Grow rate = $n_N * n_1 * k^+$

$k^+ = P_{meet} * P_{react}$



Destruction rate = $n_N * k^-$

$k^- \propto k^+ * \exp[-\Delta G_r/kT]$

# Gibbs free energy

(An introduction to thermal physics - D. Schroeder)

Determine minimal energy structure
via density functional theory

Identify internal degrees of freedom
via vibrational analysis

Obtain Gibbs free energy
via thermodynamics

# Nucleation candidates

| | $(TiO_2)_N$ | $(SiO)_N$ | $(MgO)_N$ | $(Al_2O_3)_N$ |
|---|---|---|---|---|
| $N_{max}$ | 10 | 9 | 10 | 7 |
| Structure | Literature | Literature | Literature | Literature |
| Vibrational analysis | Literature | **This work** | **This work** | **This work** |
| Gibbs free energy | Literature | **This work** | **This work** | **This work** |
| Extra reactions | **~20** | **0** | **~50** | **~100** |