Using machine learning to predict 1D steady-state temperature profiles from compressible mantle convection simulations

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Using machine learning to predict 1-D steady-state temperature profiles from compressible mantle convection simulations

(Towards 1D surrogate modelling)

Siddhant Agarwal, APS DFD 2019

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Agenda

- **Introduction** (Mantle Convection and need for Machine Learning)
- **Data and Results I** (using steady-state simulations)
- **Data and Results II** (using evolution simulations)
- **Conclusion**

Introduction

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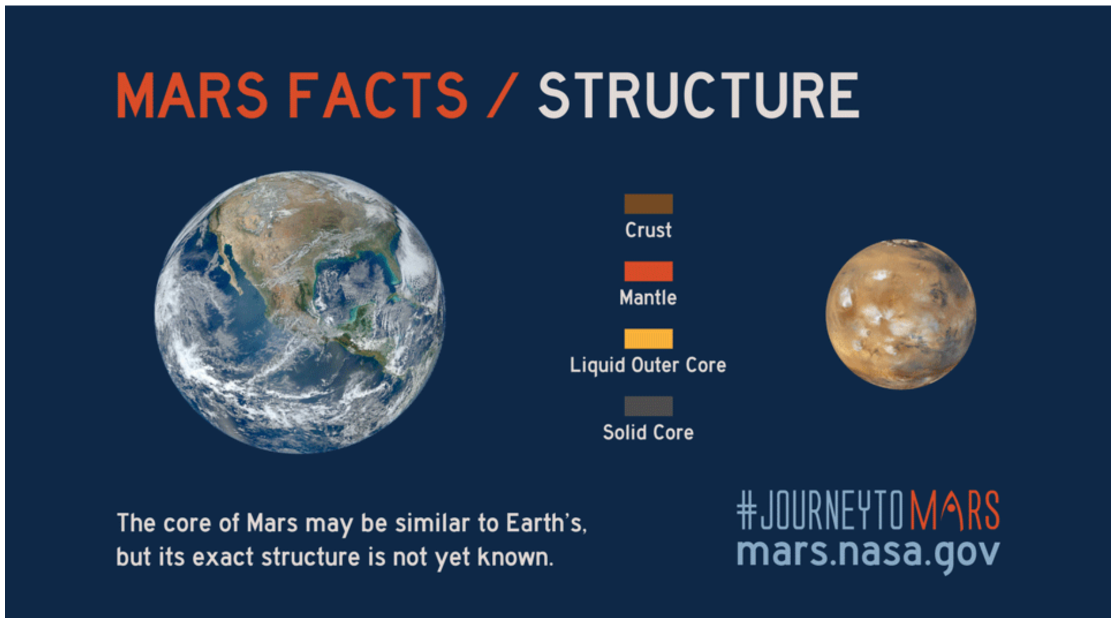
Introduction

Mantle convection is an important driver of thermal evolution of terrestrial planets



[NASA]

Introduction

Inputs

Viscosity

Initial temperature

Uranium

⋮

GAIA [Hüttig, Stemmer 2008]

$$\nabla . (\rho\vec{u}) = 0$$

$$0 = -\nabla P + \nabla . \tau + \rho\vec{g}$$

$$\rho c_p \frac{DT}{Dt} - \alpha T \frac{DP}{Dt} = \nabla . (k\nabla T) + \rho H + \phi$$

Outputs

Surface heat flux

Radial contraction

Crustal thickness

⋮

- Mantle convection is governed by poorly constrained parameters and initial conditions

Introduction

Inputs

Viscosity

Initial temperature

Uranium

⋮

Outputs

Surface heat flux

Radial contraction

Crustal thickness

⋮

- Mantle convection is governed by poorly constrained parameters and initial conditions
- In planetary science, the outputs are observable (…sometimes)

Introduction

Inputs

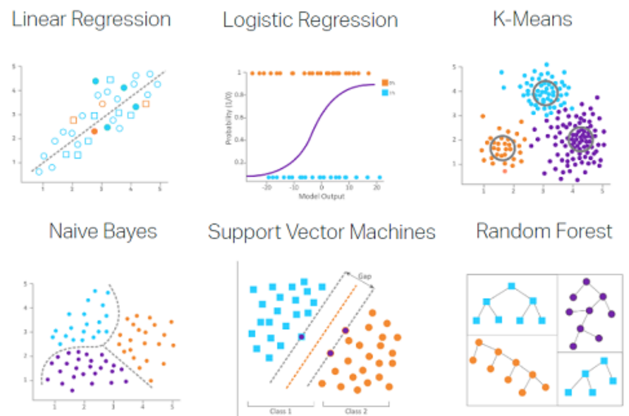
Viscosity

Initial temperature

Uranium

⋮

Machine Learn?



[Datanami]

Outputs

Surface heat flux

Radial contraction

Crustal thickness

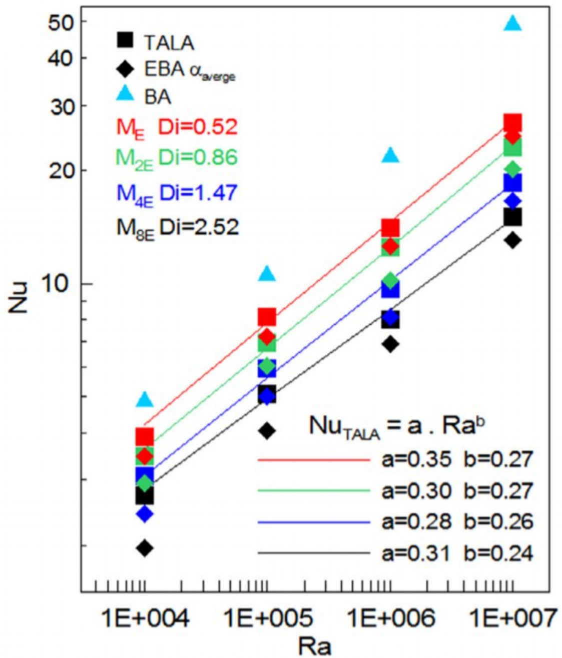
⋮

- Mantle convection is governed by poorly constrained parameters and initial conditions
- In planetary science, the outputs are observable (…sometimes)
- Can we find a mapping using ML to rapidly scan the parameter space?

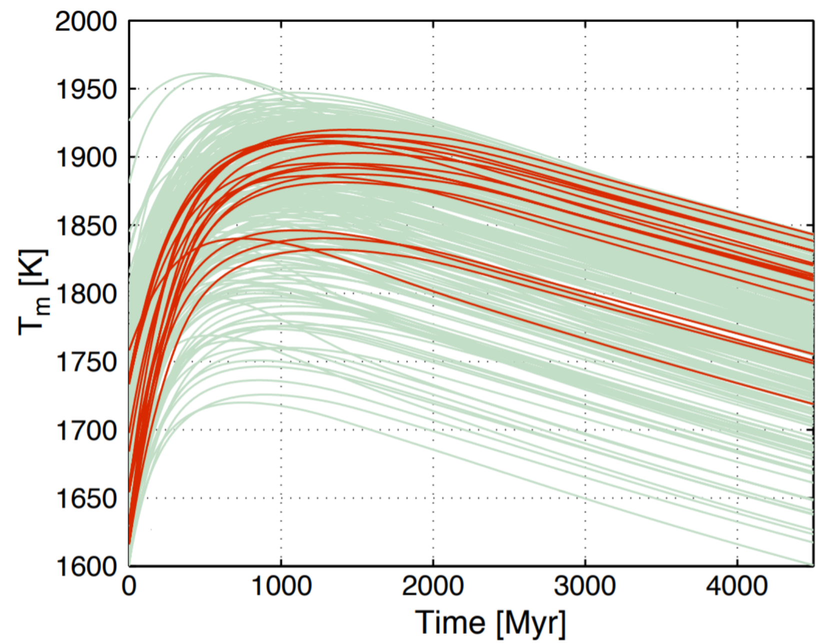
Data and Results I

Steady-State Simulations

Traditional 0D surrogate models are limited to simple flows



[Čížková et al. 2017]



[Grott et al. 2011]

Steady-State Simulations

Traditional 0D surrogate models are limited to simple flows

We can leverage ML to find higher-dimensional mappings for more complex flows

Parameters

Ra ∈ [1e+4, 1e+9] *(vigor of convection)*

RaQ/Ra ∈ [0, 10] *(vigor of convection from internal heating)*

Di ∈ [0, 2] *(compressibility)*

$\boldsymbol{\eta_T}$ ∈ [1e+0, 1e+10] *(Temperature dependence of viscosity)*

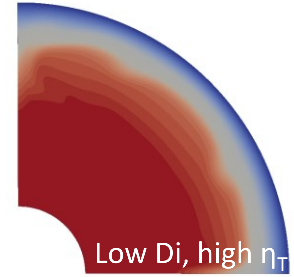
$\boldsymbol{\eta_V}$ ∈ [1e+0, 1e+4] *(Pressure dependence of viscosity)*

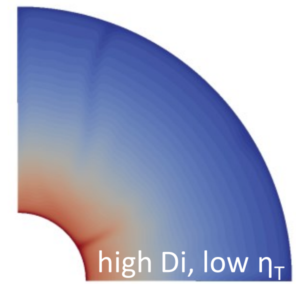
→ 1-D Temperature profile

Steady-State Simulations

~40000, 2-D, quarter-cylinder, **steady-state** simulations

~9TB of data generated using ~1 million CPU hours





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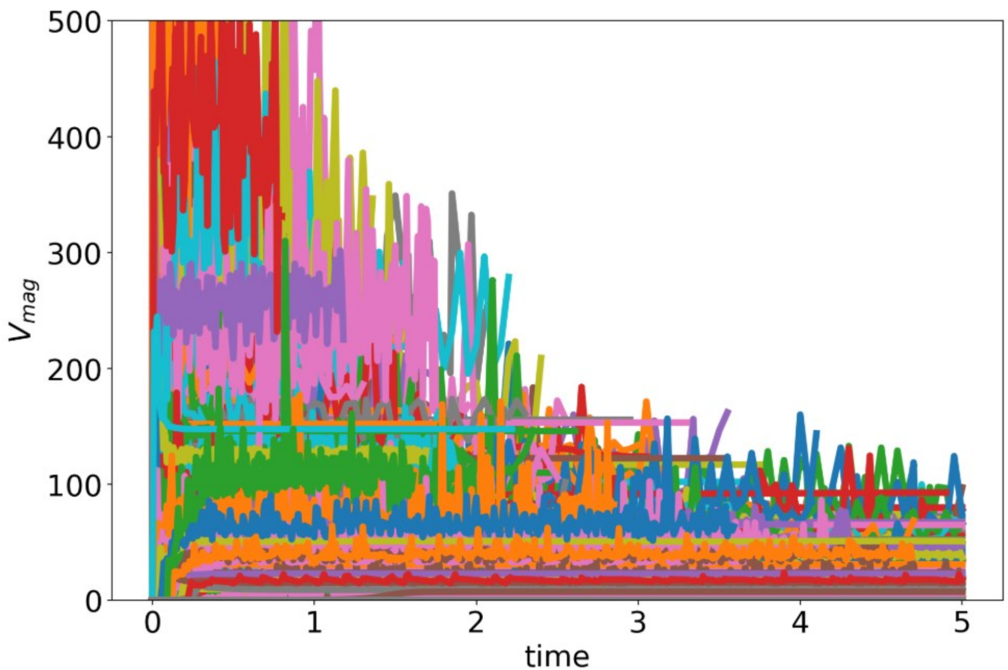
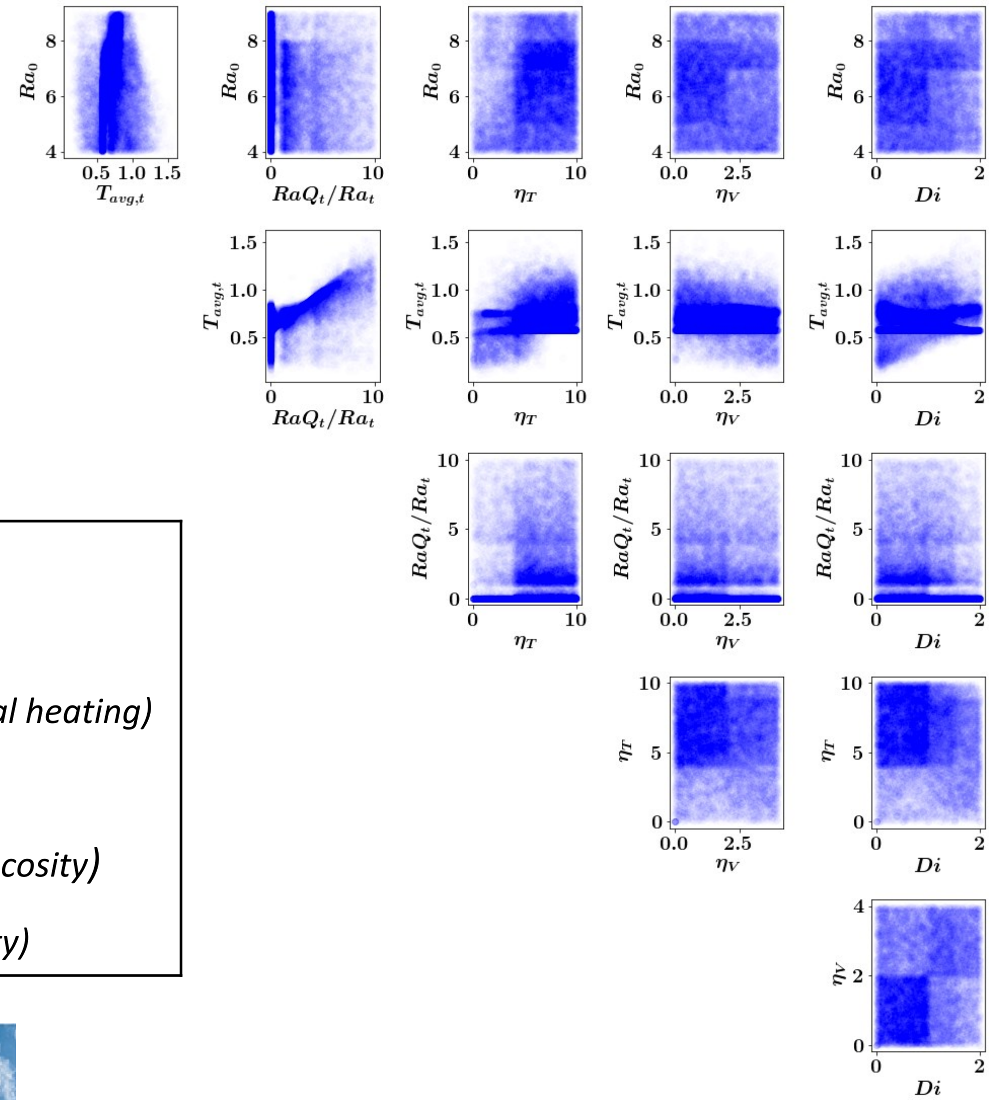
→ 1-D Temperature profile

Steady-State Simulations

~27000 simulations reached statistical steady-state



Steady-State Simulations



Parameters

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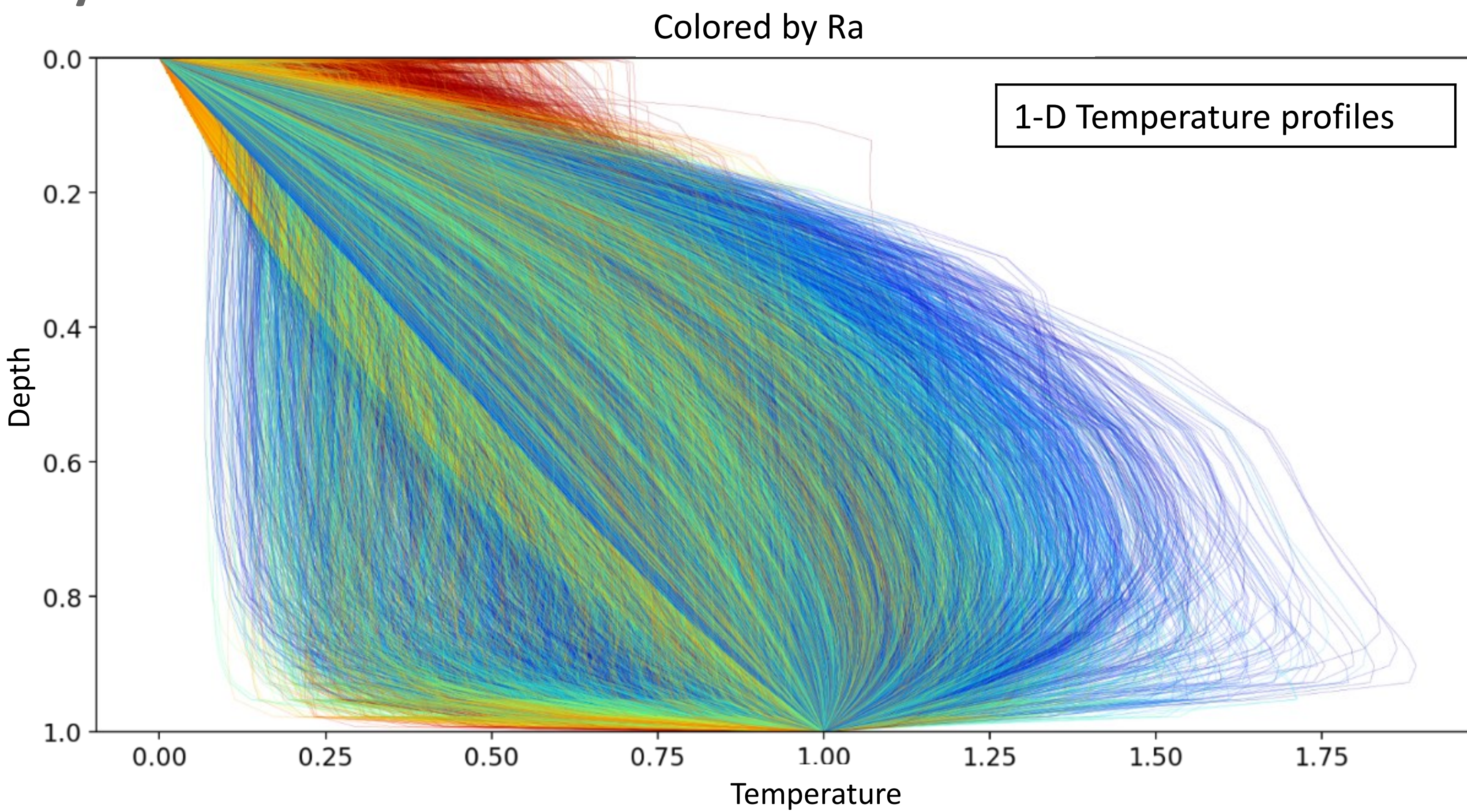
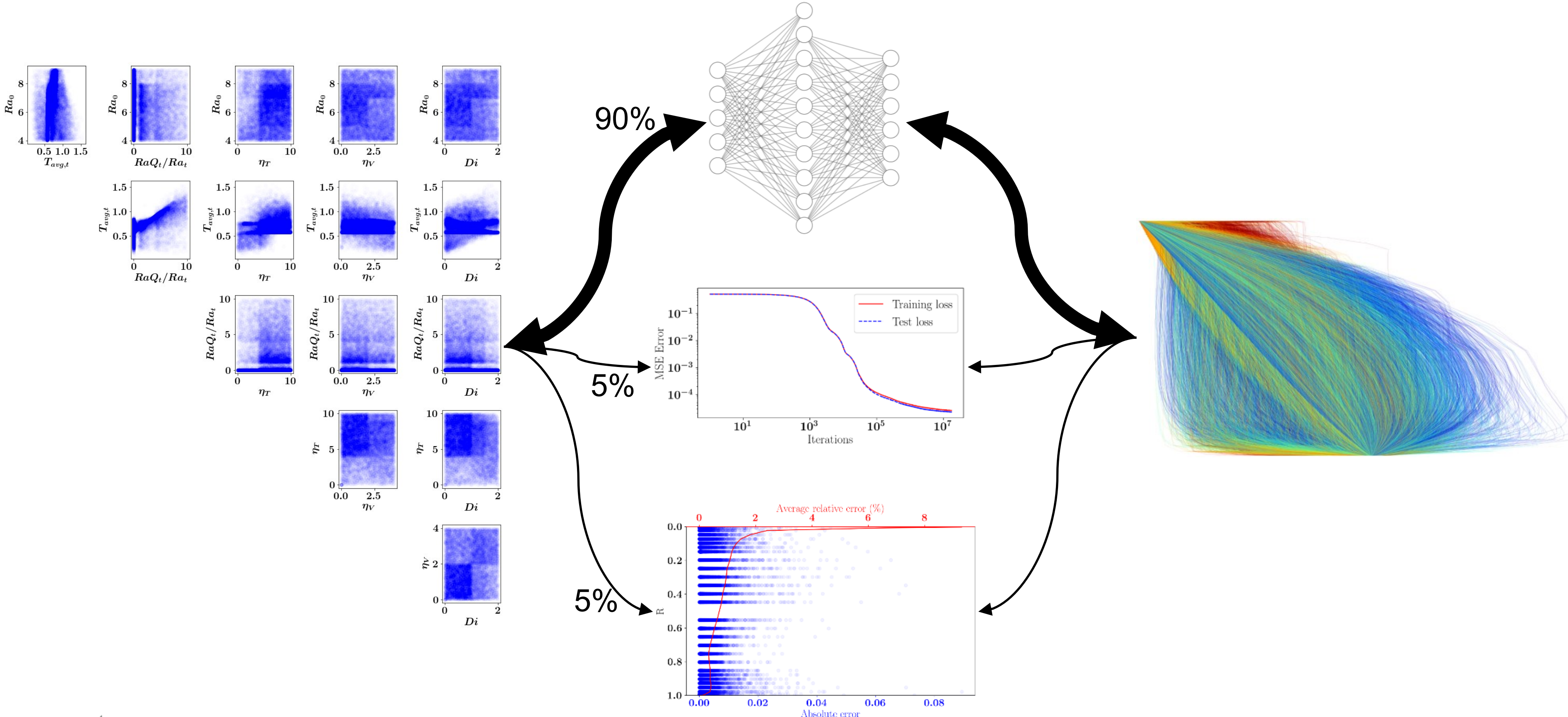
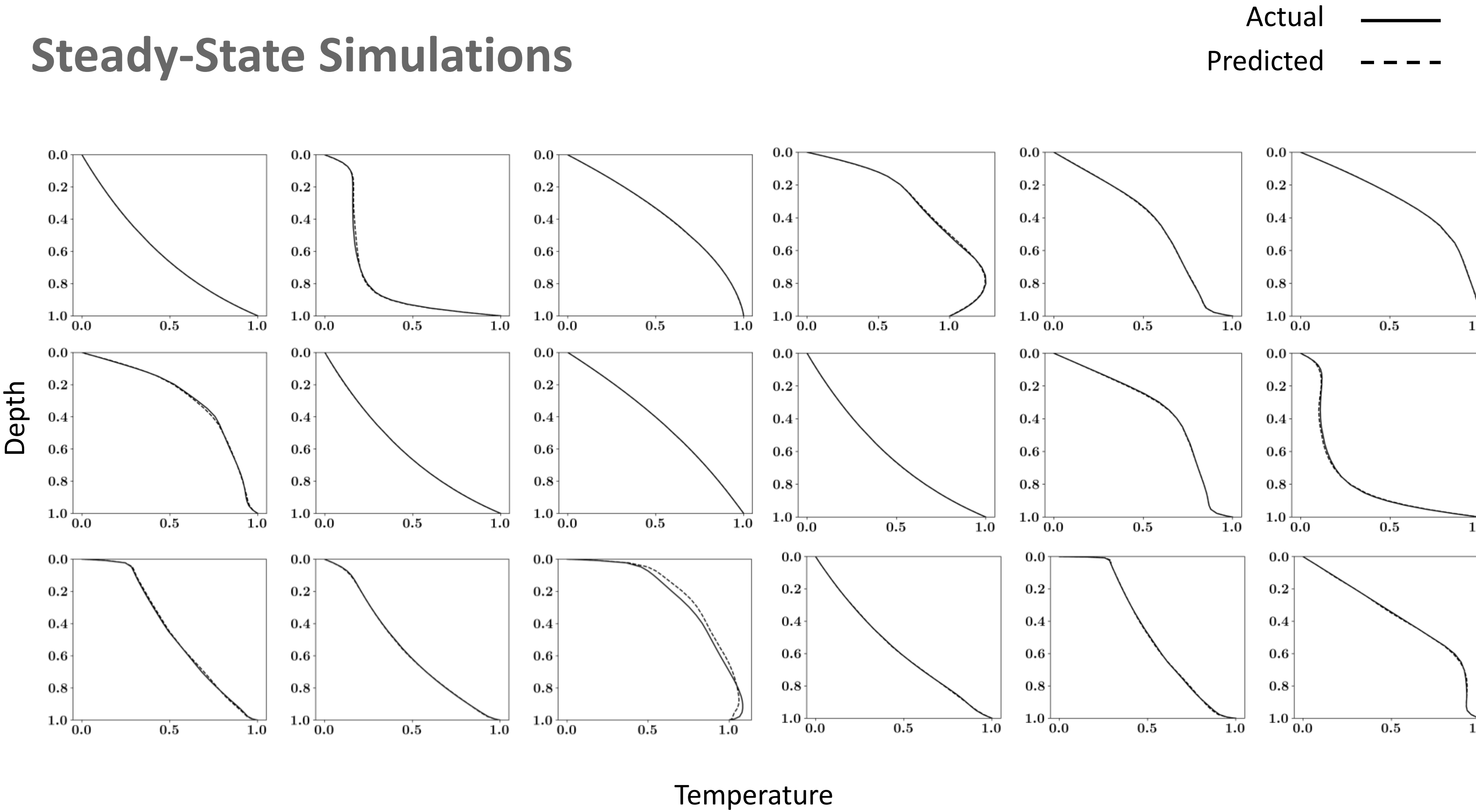
Steady-State Simulations



Steady-State Simulations



Steady-State Simulations



Steady-State Simulations

Average train error: 1.23%

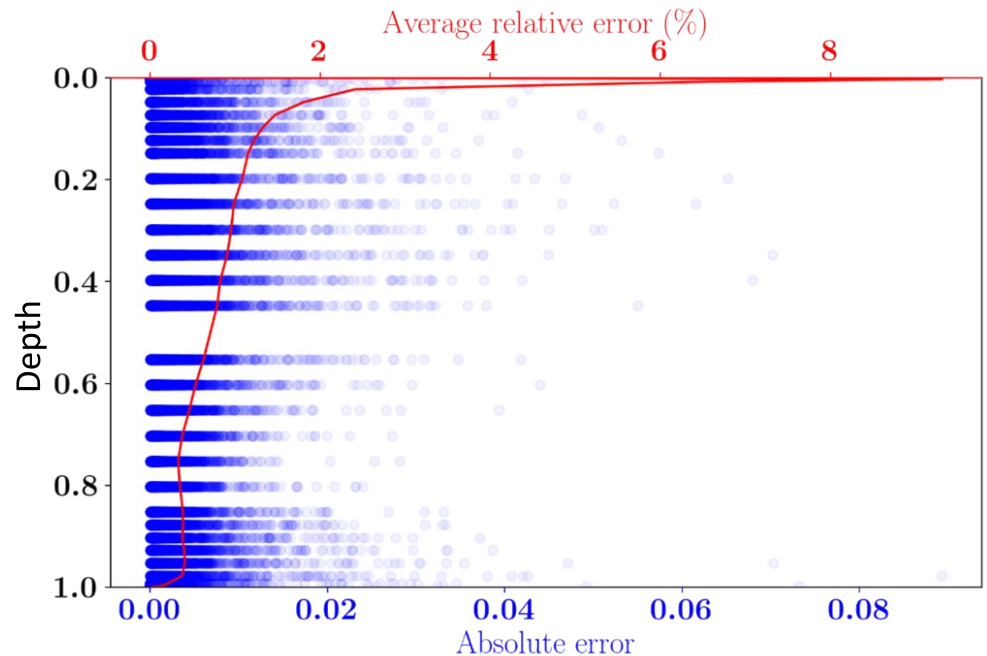
Average test error: 1.25%

Average train error surface heat flux: 6.65%

Average test error surface heat flux: 6.42%

Average train error core heat flux: 22.73%

Average test error core heat flux: 23.54%



Steady-State Simulations

We can now run evolution models

$q_{c,t-1}$

$q_{s,t-1}$

$$\rho_m c_p \frac{d}{dt}\int_{R_c}^{R_p} r^2 T(r,t)\,dr = R_c^2 q_{c,t-1} - R_p^2 q_{s,t-1} + \rho_m \frac{R_p^3 - R_c^3}{3} H_{t-1}$$

Ra'_t

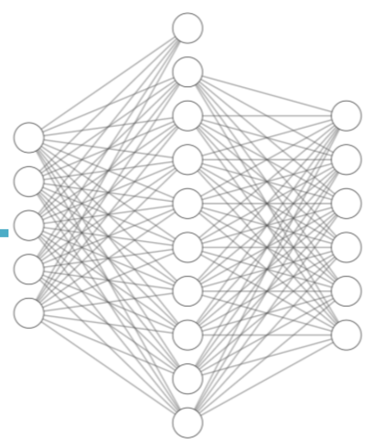
$(RaQ_t / Ra_t)'$

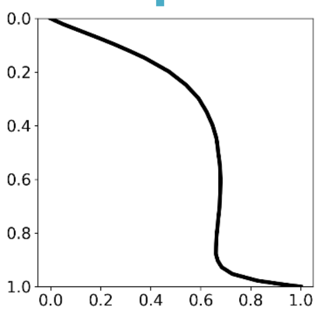
$\Delta\eta'_T$

$\Delta\eta'_V$

Di'

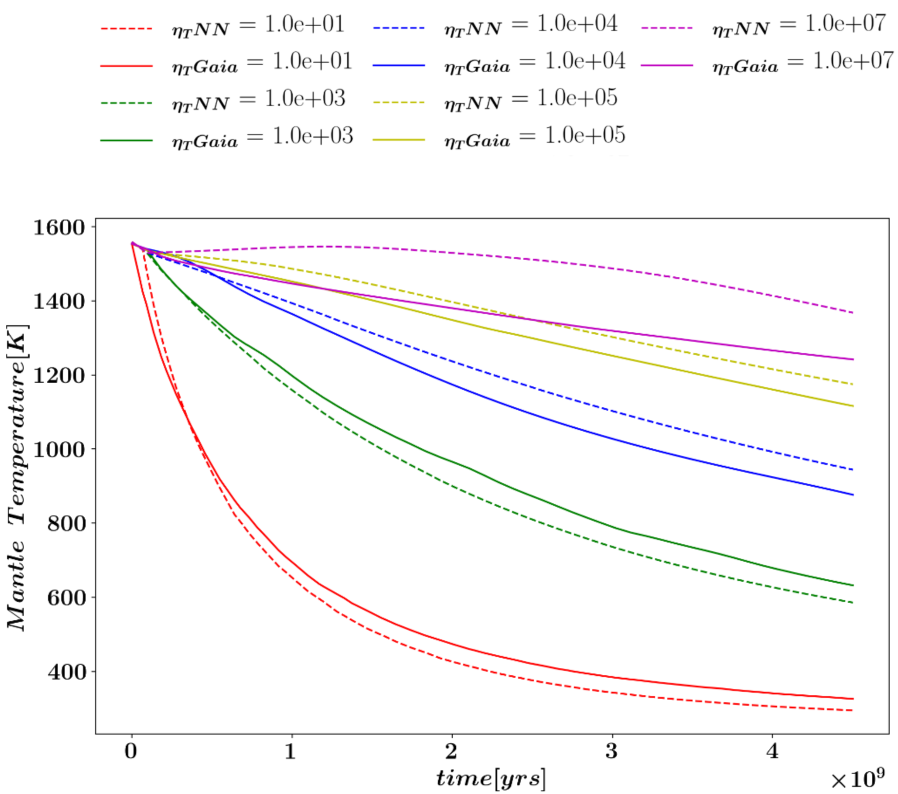
$T'_{avg,t}$

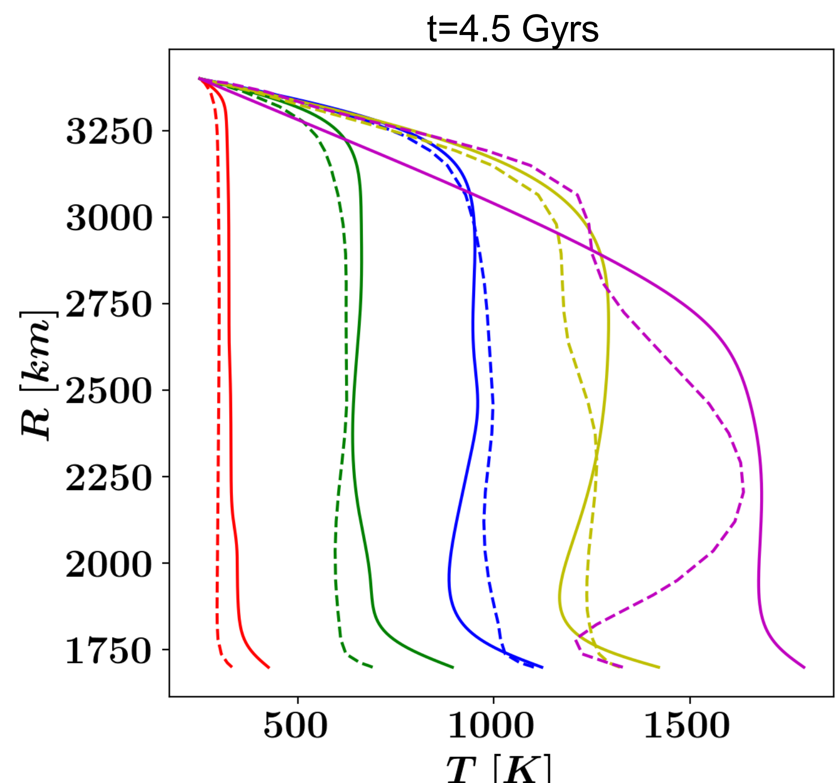




$T'_{profile,\,t}$

Steady-State Simulations

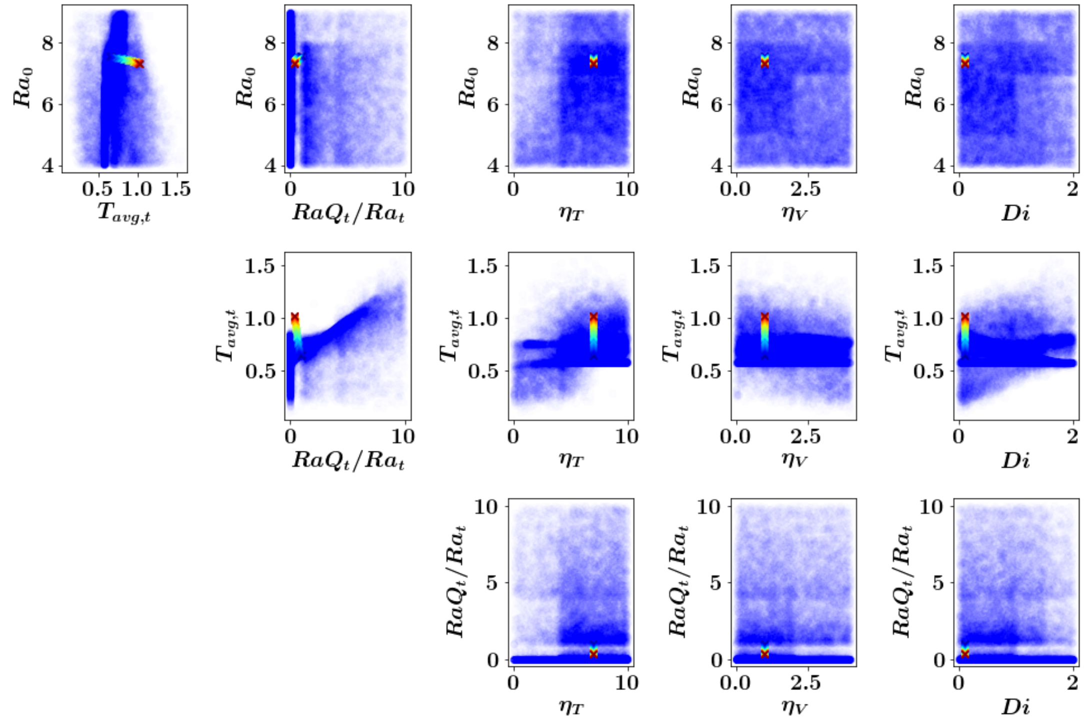




Steady-State Simulations

Possible sources of error:

- Movement of parameters out of the data manifold during evolution



Steady-State Simulations

Possible sources of error:

- Movement of parameters out of the data manifold during evolution

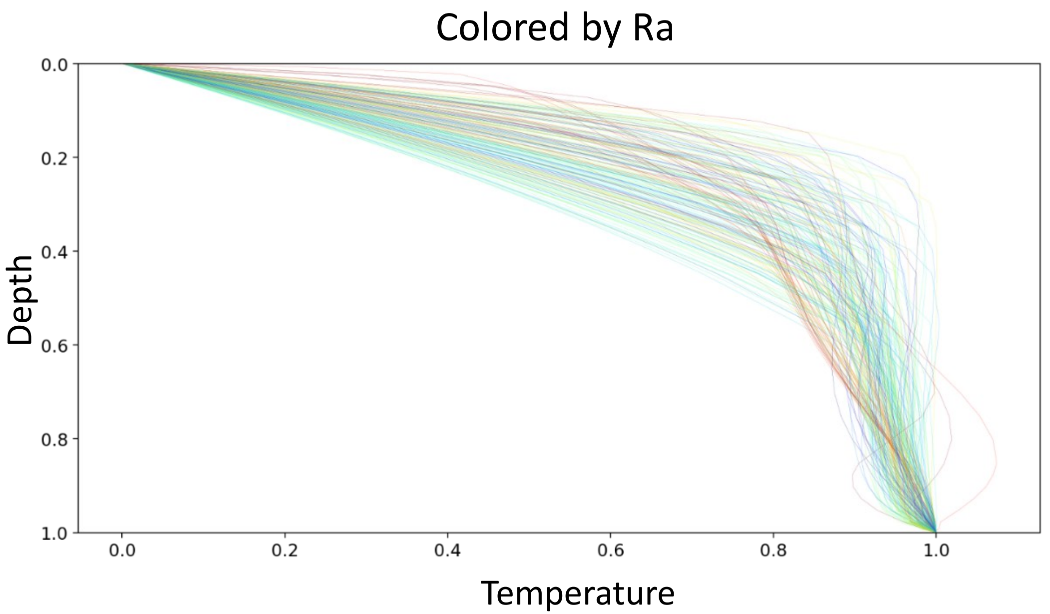
- Use of the 0D energy equation

$$\boxed{\rho_m c_p \frac{d}{dt}\int_{R_c}^{R_p} r^2 T(r,t)dr = R_c^2 q_c - R_p^2 q_s + \rho_m \frac{R_p^3 - R_c^3}{3} H_t}$$

Steady-State Simulations

Possible sources of error:

- Movement of parameters out of the data manifold during evolution
- Use of the 0D energy equation
- Only 1% of the profiles 'stagnant lid'



Data and Results II

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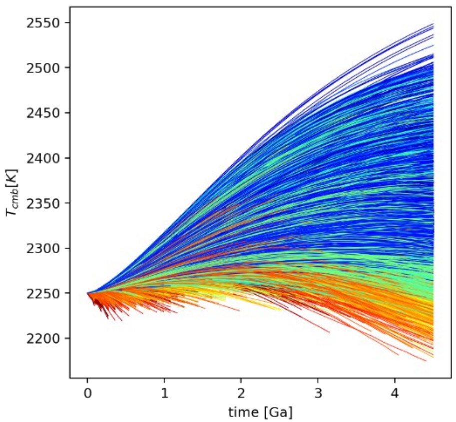
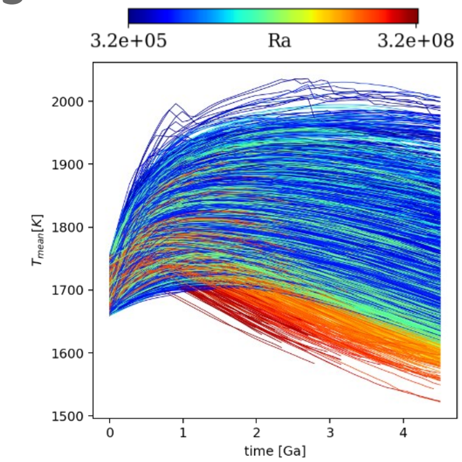
Evolution Simulations





Parameters

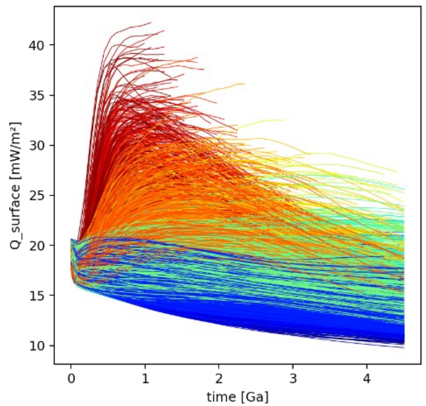
Ra (η_{ref} ϵ *[1e+19, 1e+22 Pa s]*)

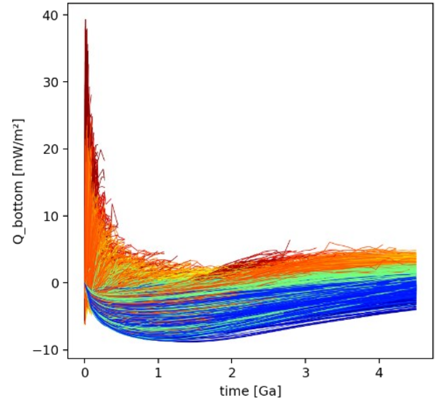
RaQ (*Λ ϵ [1, 50], η_{ref}*)

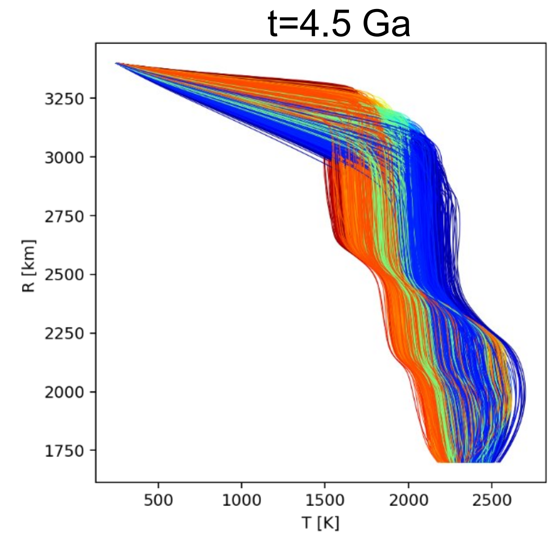
$\mathbf{T_{initial}}$ ϵ [1600, 1800 K]

E ϵ [1e+5, 5e+5 J mol^{-1}]

V ϵ [4e-6, 10e-6 m^3 mol^{-1}]



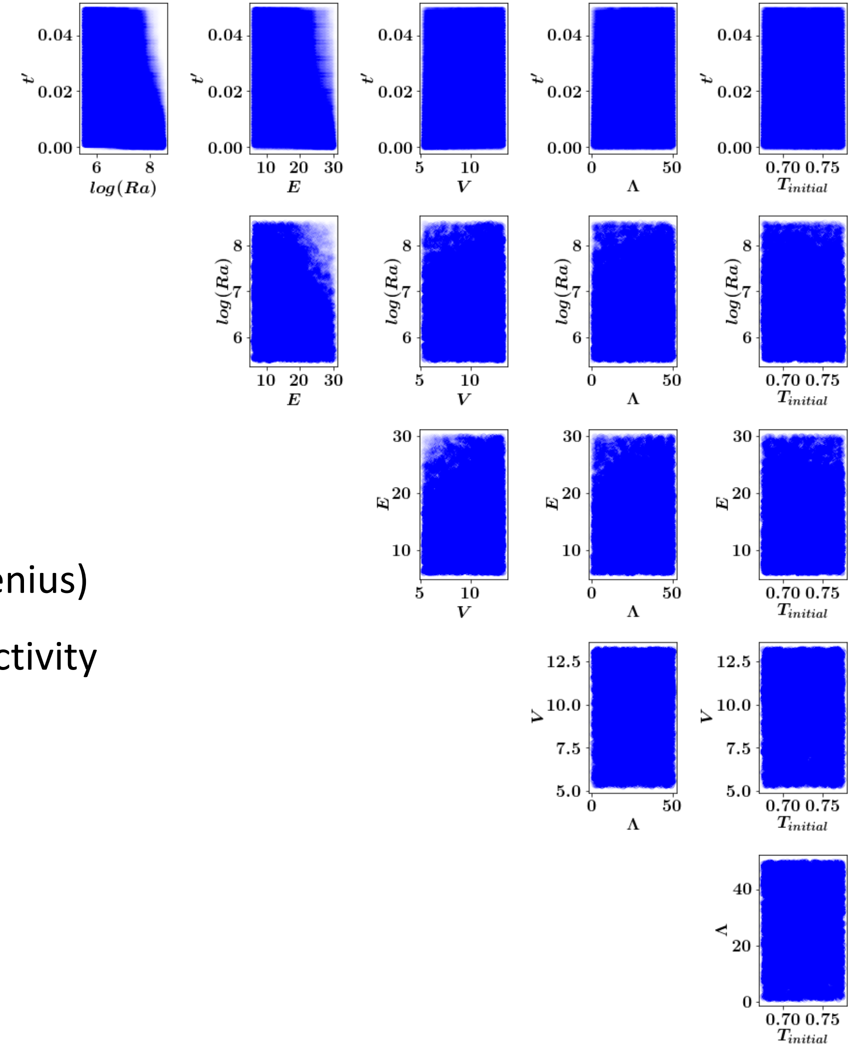




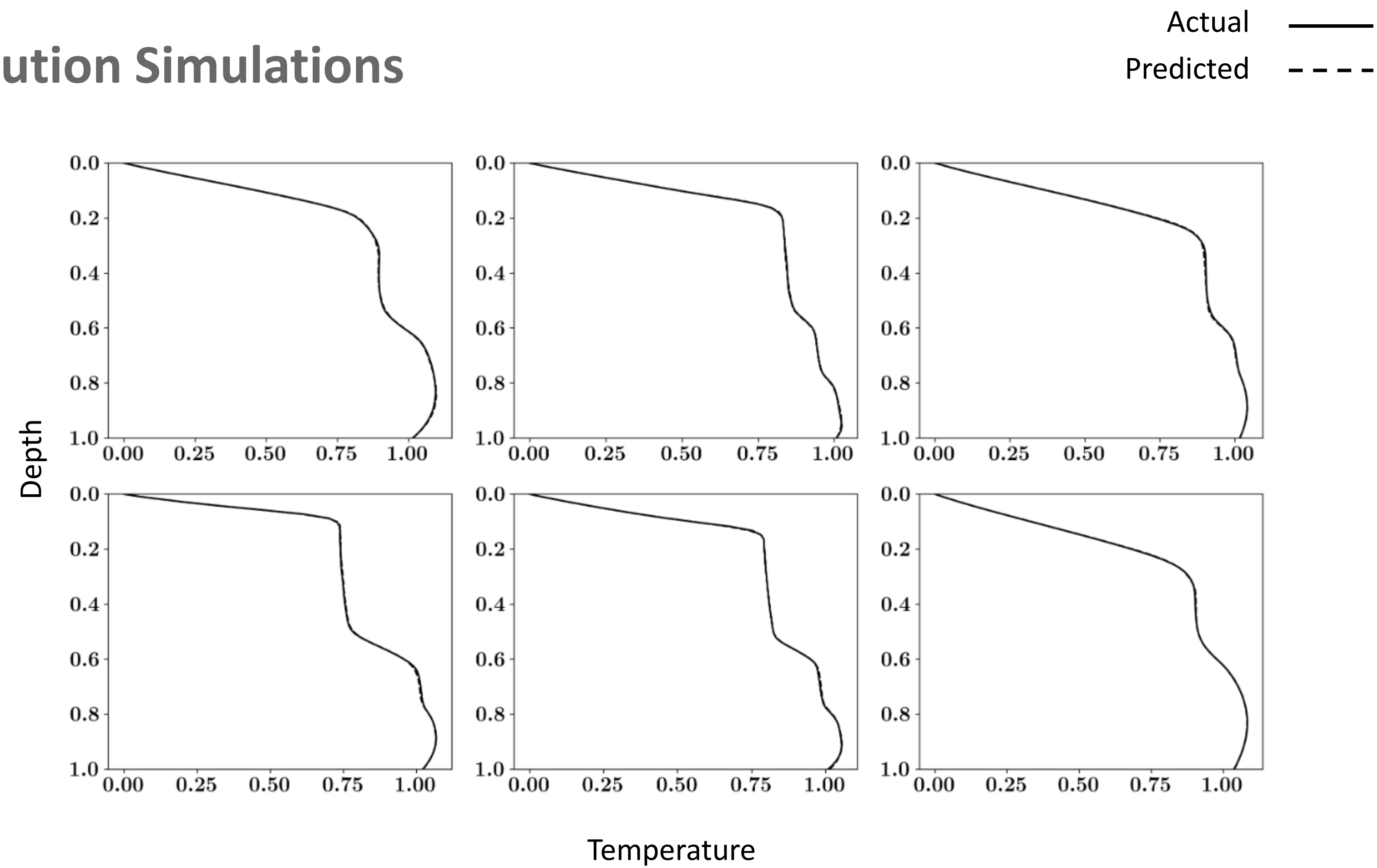
Evolution Simulations

Generated ~10000 **evolution** simulations for Mars with:

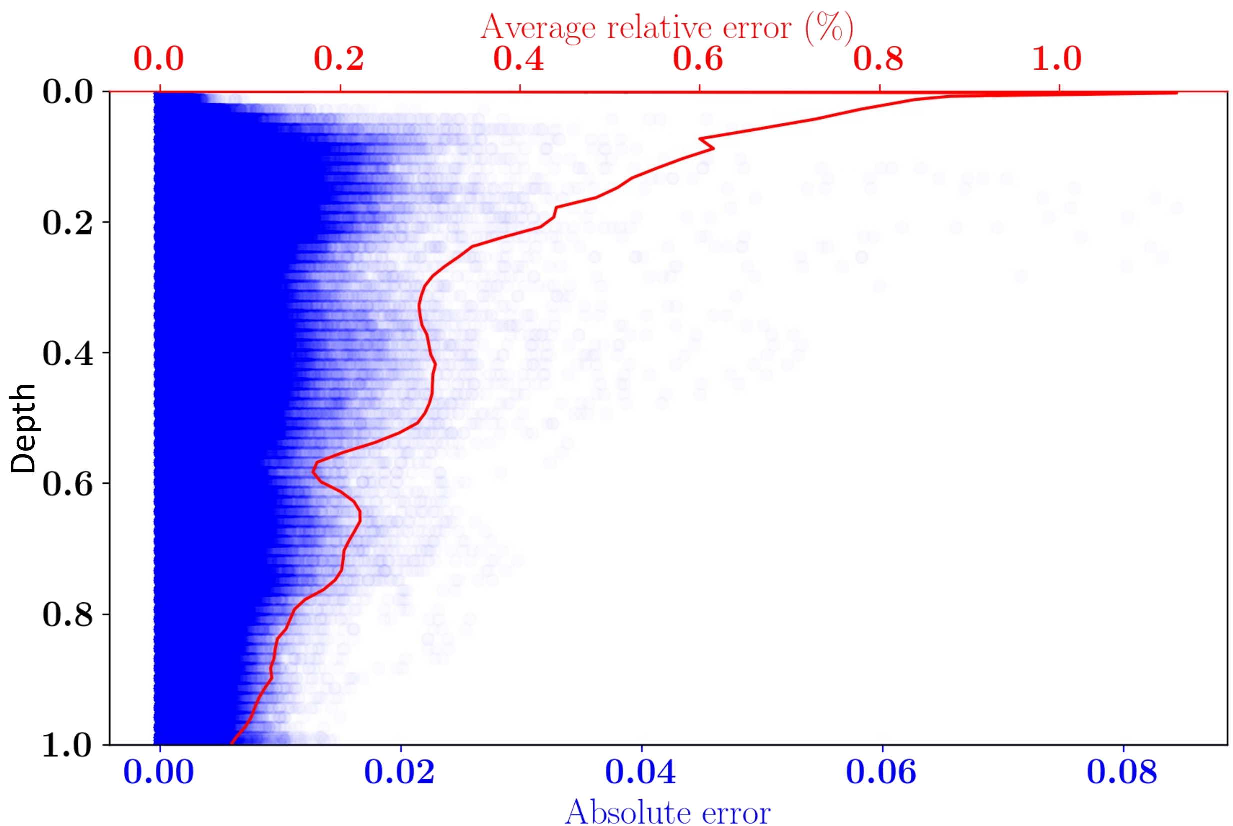
- Compressible convection (EBA)
- Heat production from core and radiogenic elements
- Temperature and pressure dependent viscosity (Arrhenius)
- Temperature and pressure dependent thermal conductivity and thermal expansion
- Solid phase transitions



Evolution Simulations

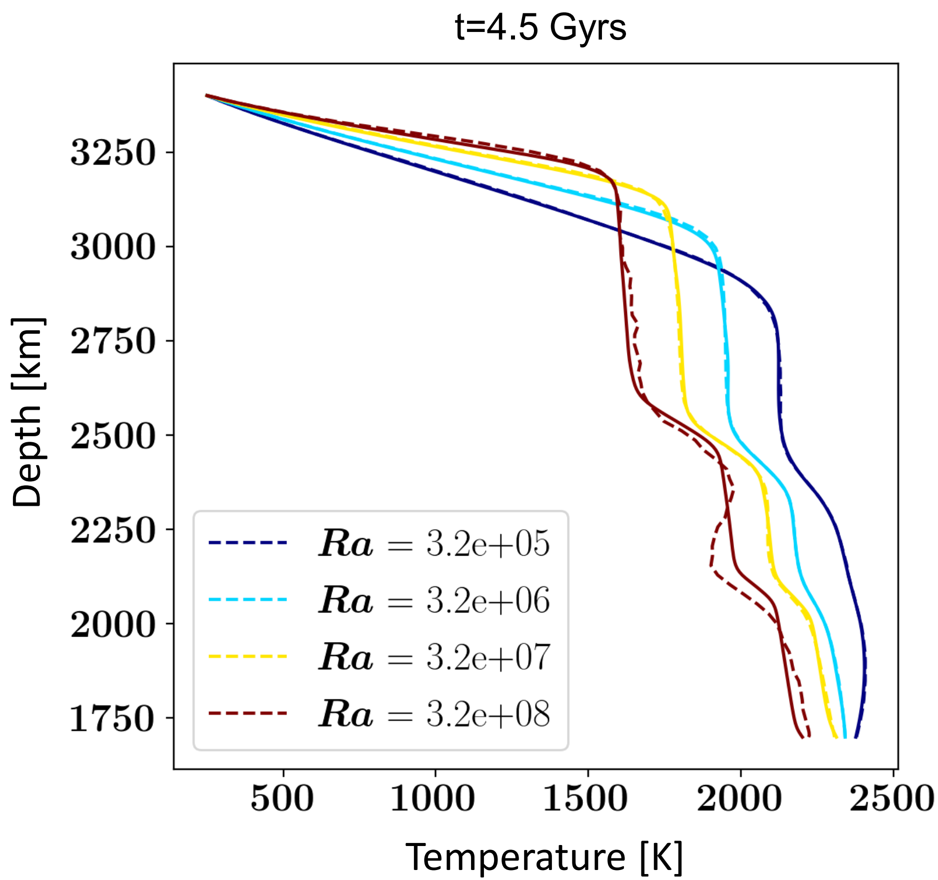


Evolution Simulations



Evolution Simulations

Actual ———
Predicted - - - -



Conclusion

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Conclusion

- Algorithms like NNs allow for regression in higher-dimensions in space and time
- Data for training on *steady-state* simulations is hard to generate
- Evolution models built from *steady-state* simulations offer reasonable accuracy in certain sub-spaces of the parameter manifold
- Data for training on *evolution* simulations is easier to generate and offers *t* times more data
- Evolution models learned directly from *evolution* simulations offer better accuracy

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Backup Slides

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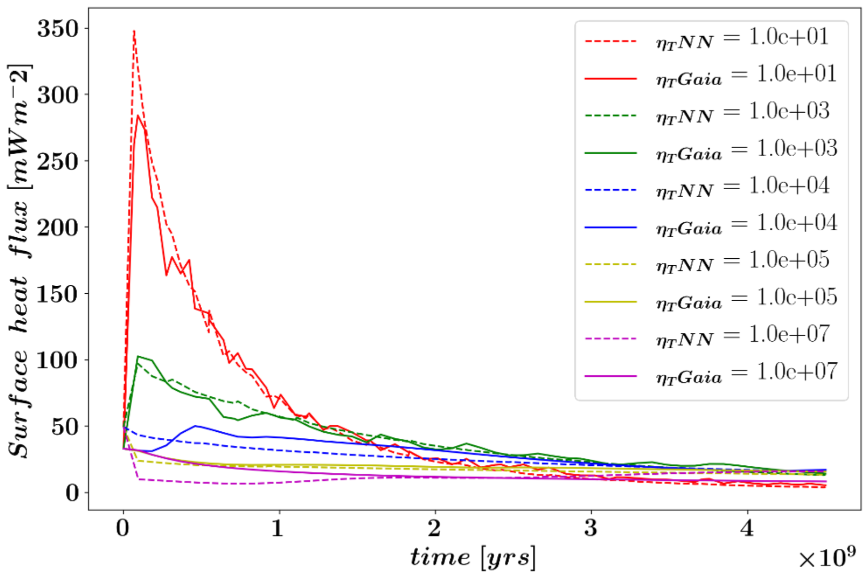
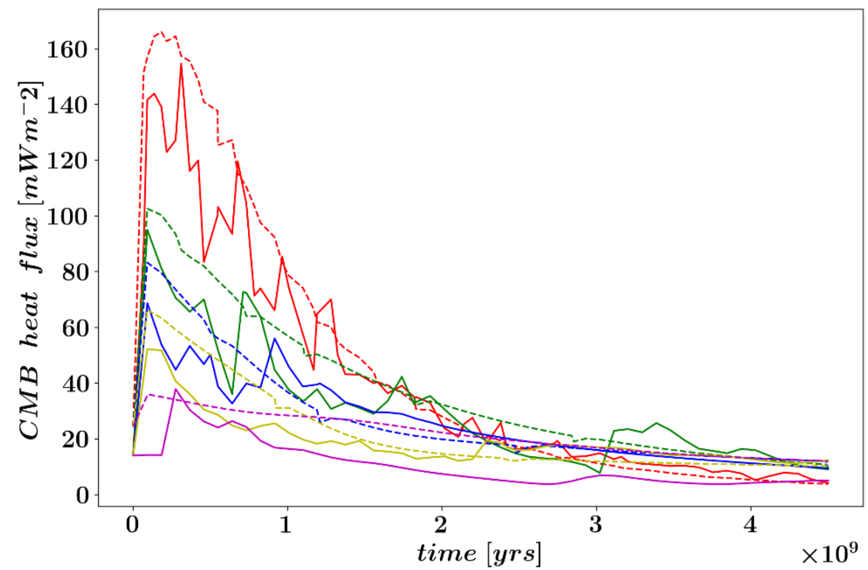
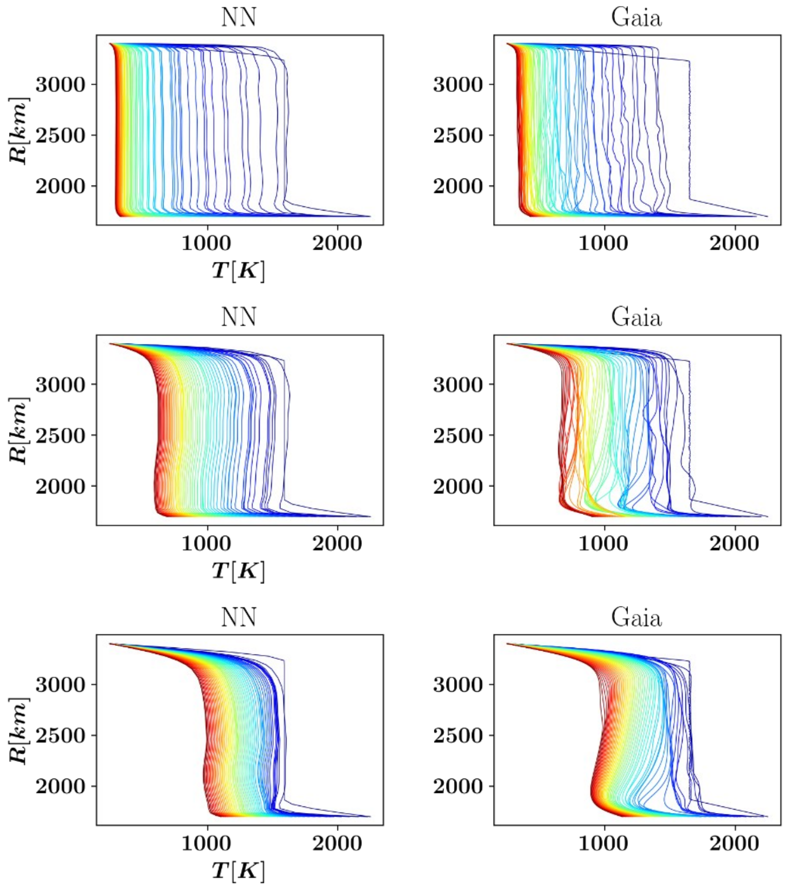
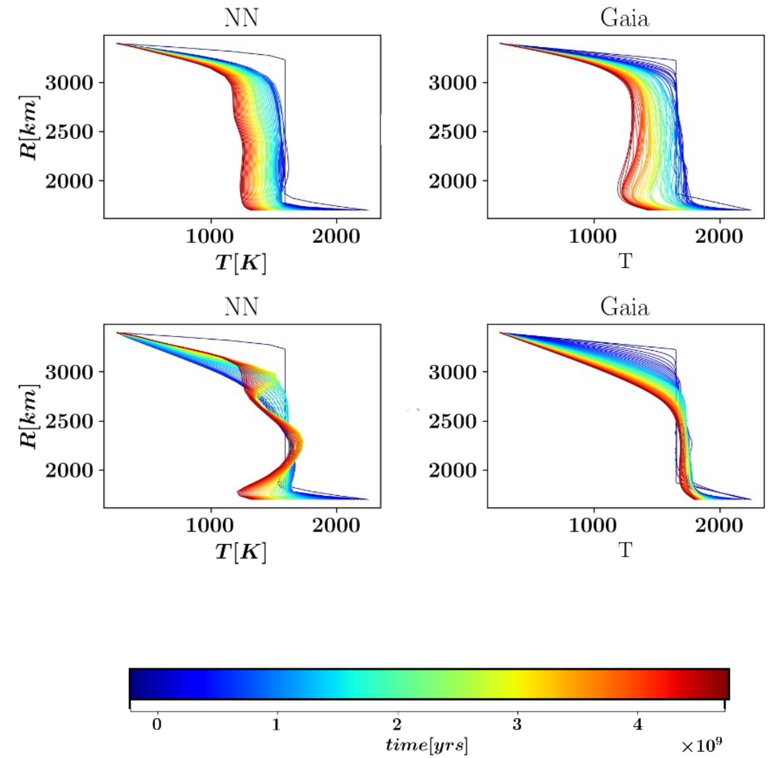
Steady-State Simulations



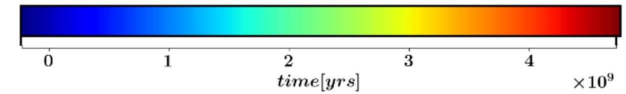


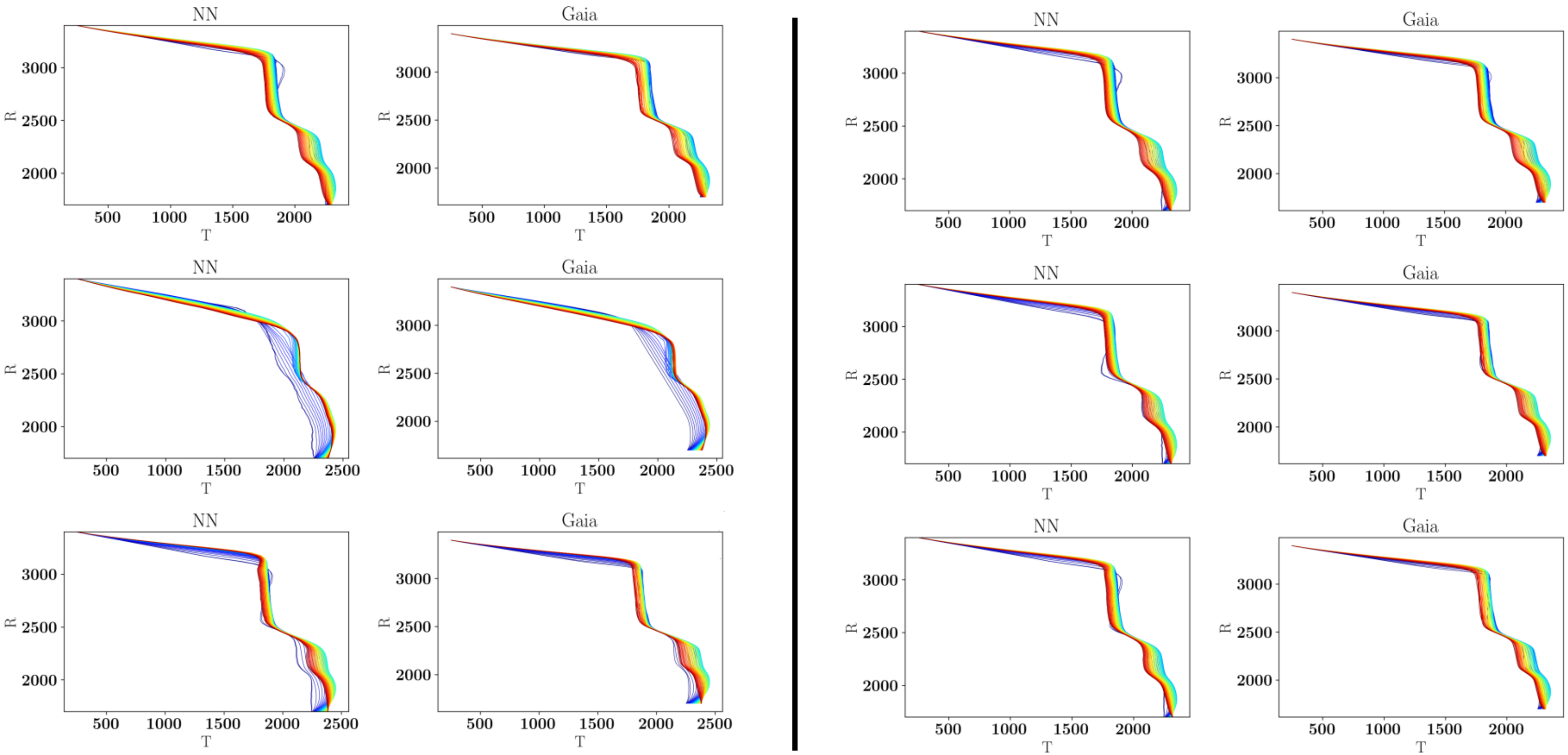
Steady-State Simulations





Evolution Simulations





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