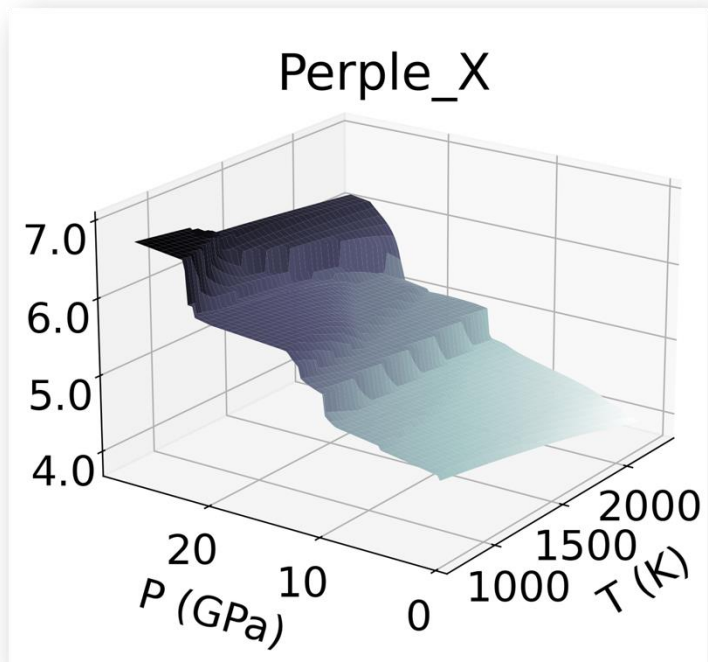


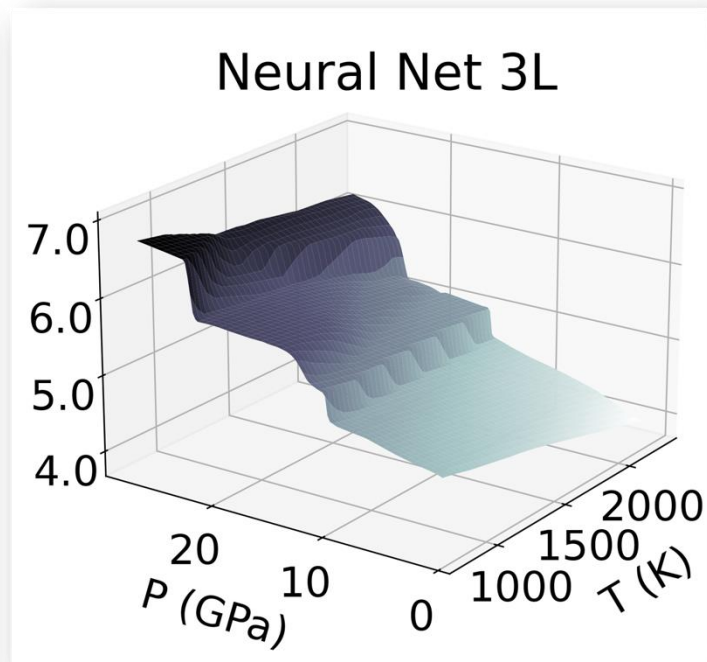
RocMLMs

Predicting Rock Properties through Machine Learning Models

Training Dataset



RocMLM Predictions



¹*Buchanan Kerswell*

¹*Nestor Cerpa**

¹*Andréa Tommasi**

¹*Marguerite Godard*

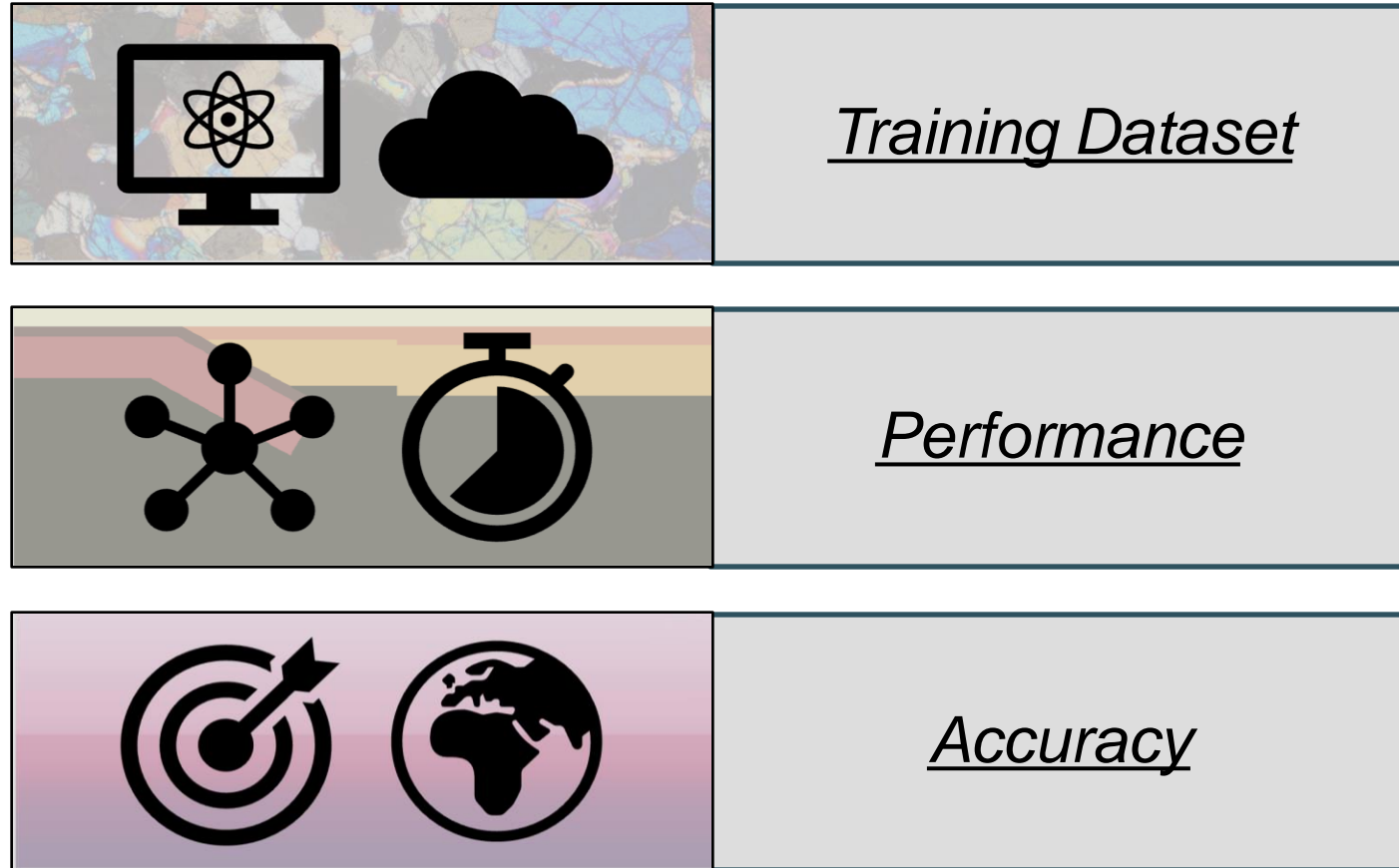
²*José Alberto Padrón-Navarta*

¹*CNRS, Géosciences Montpellier*

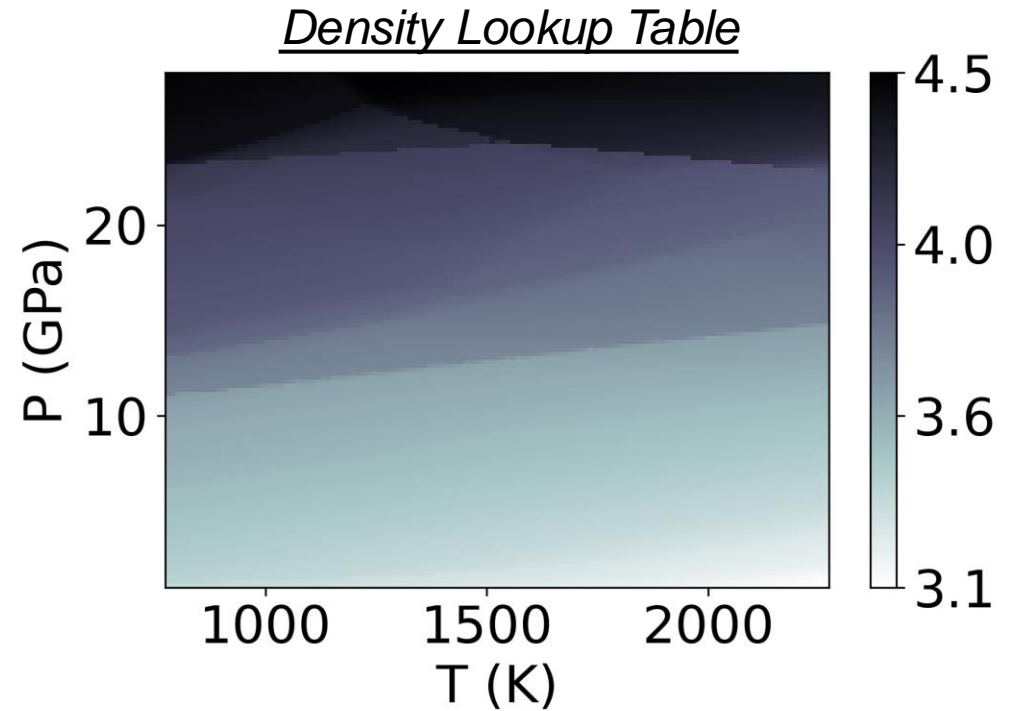
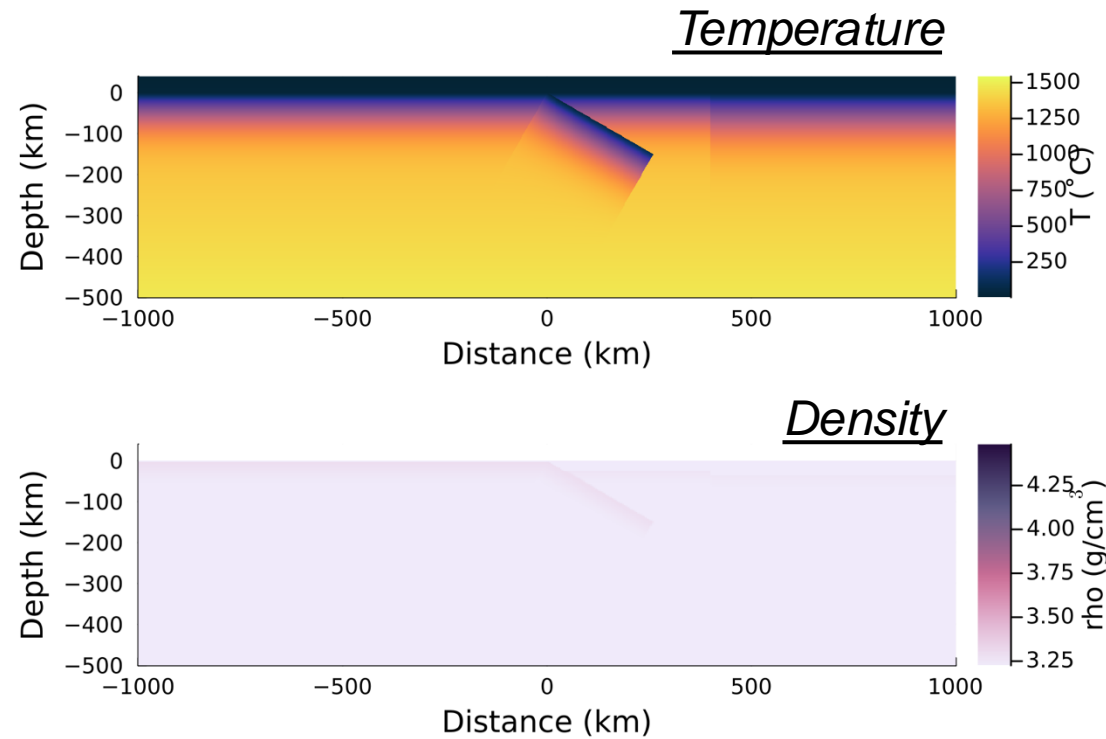
²*Andalusian Earth Science Institute*

April 15, 2024

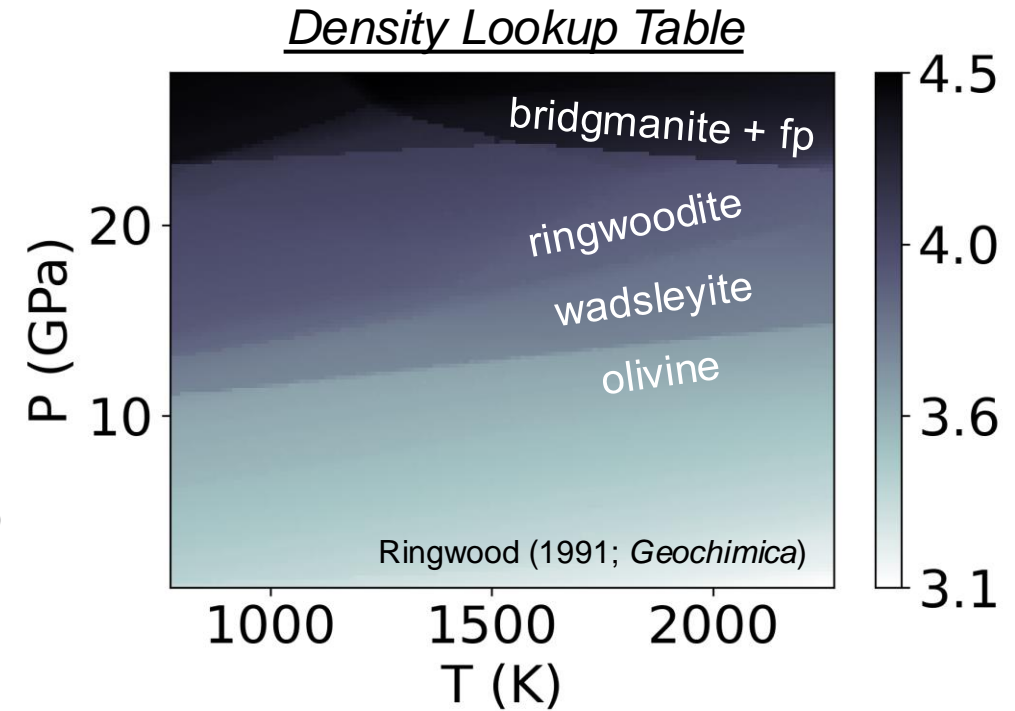
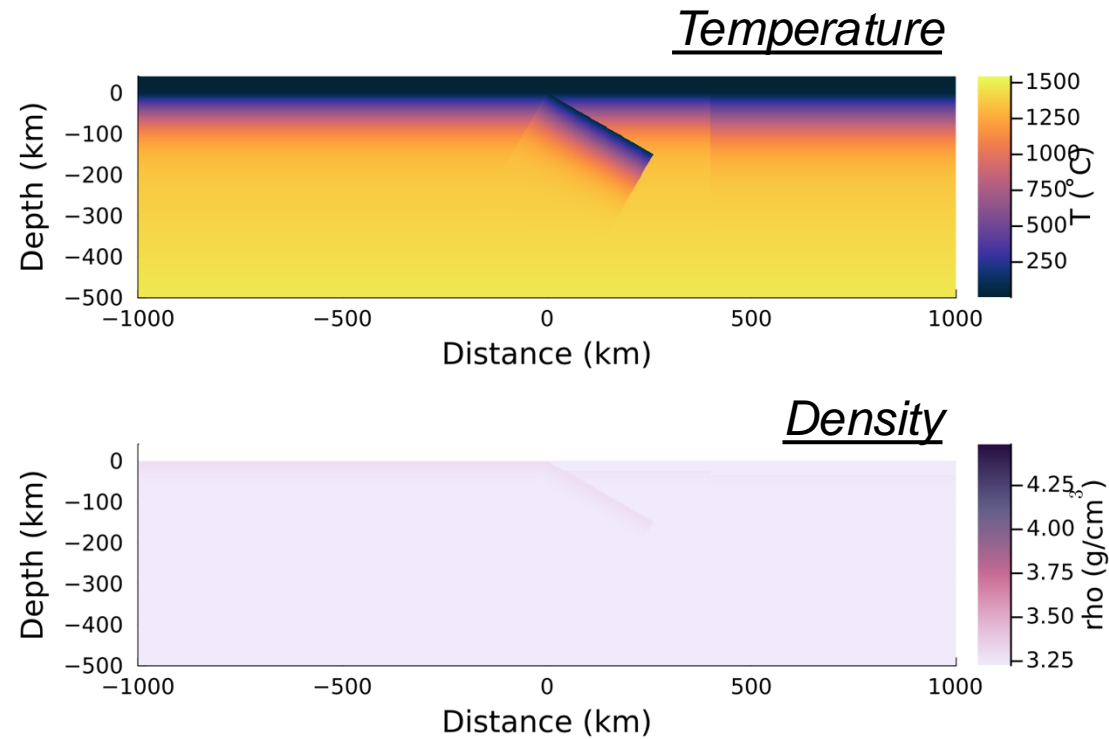
We developed RocMLMs to emulate dynamic phase changes in numerical simulations of mantle convection



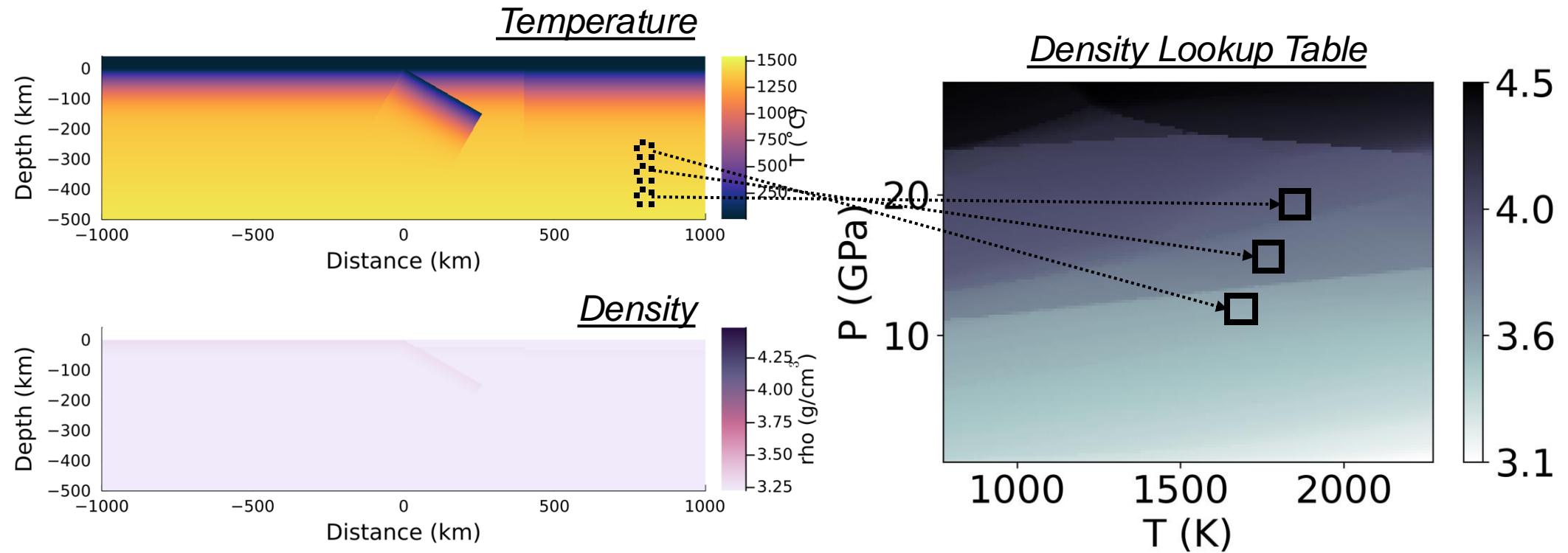
Lookup Tables are effective at implementing phase changes



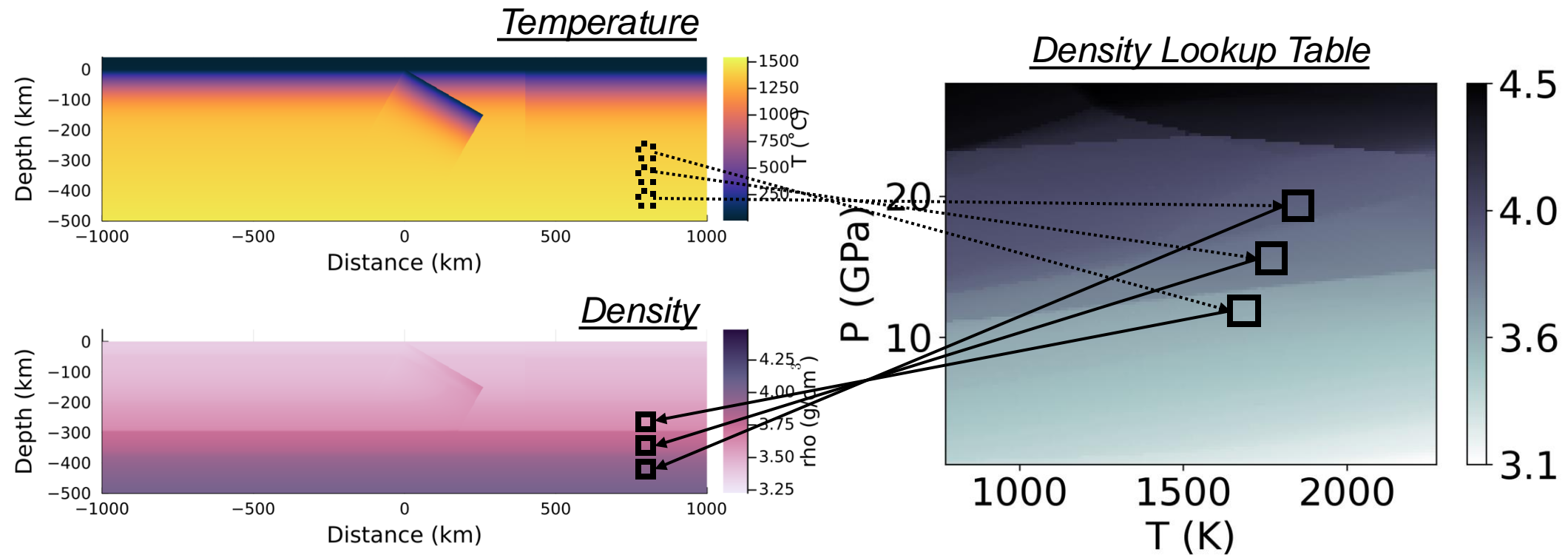
Lookup Tables are effective at implementing phase changes



Lookup Tables are effective at implementing phase changes



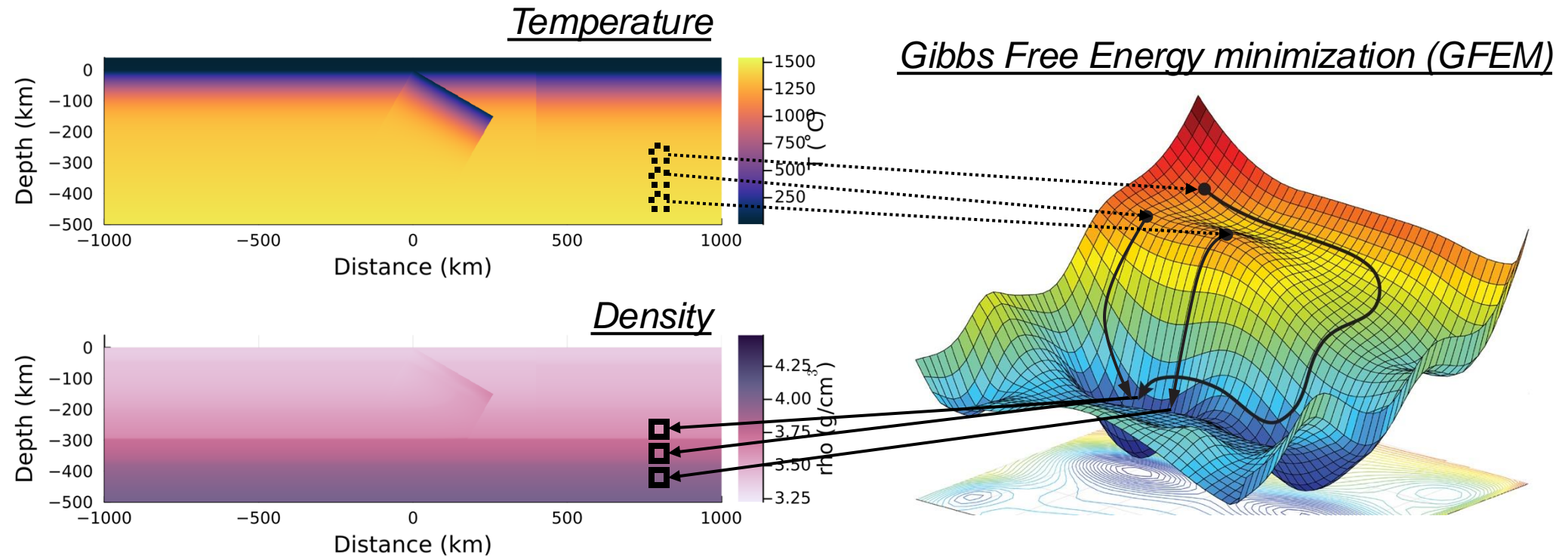
Lookup Tables are effective at implementing phase changes



+ : adds a degree of thermodynamic self-consistency

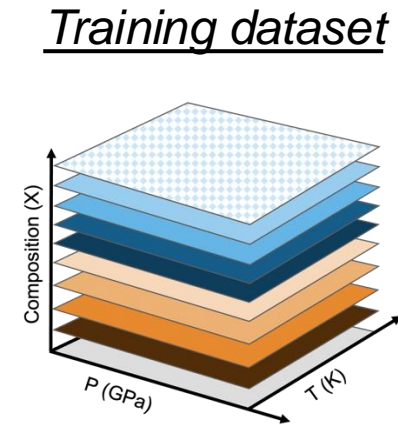
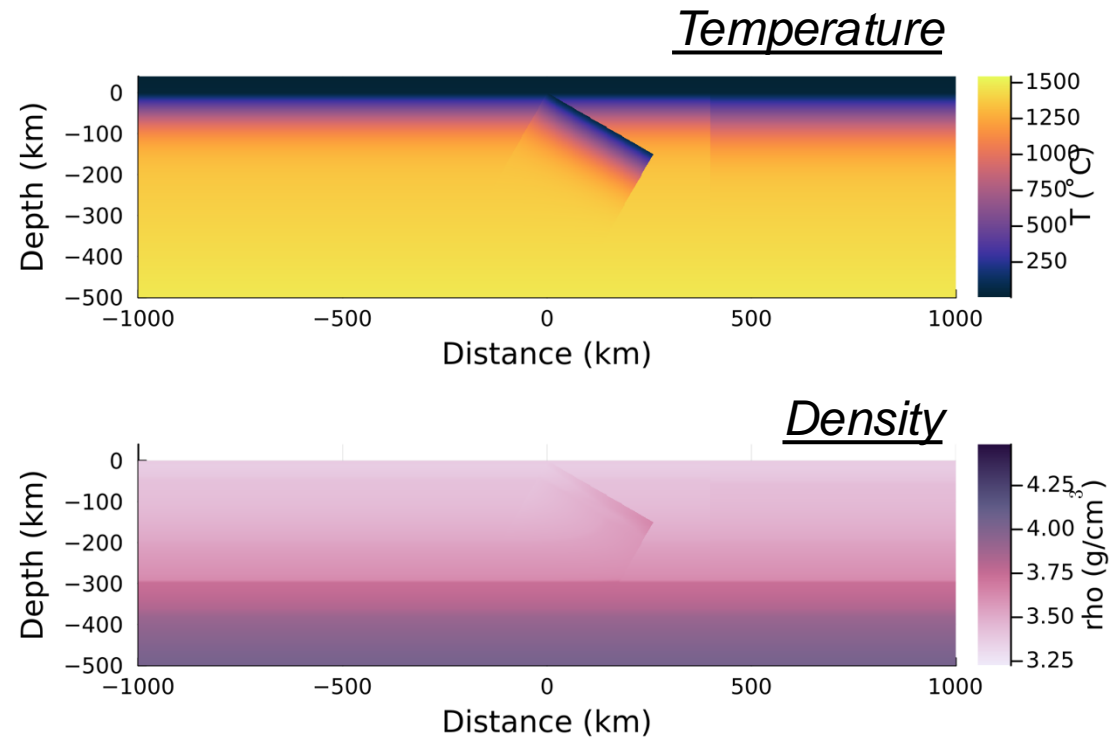
- : need Lookup Tables for each rock composition and rock property

Phase equilibria modeling is more effective, but slow

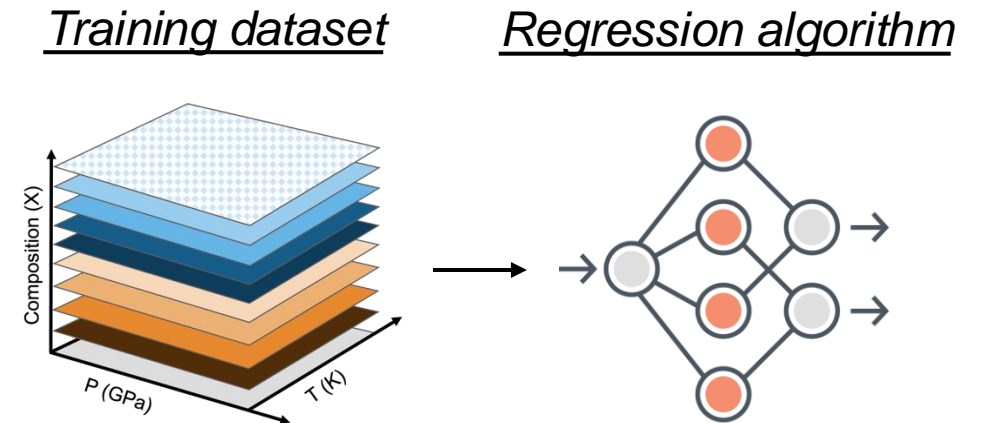
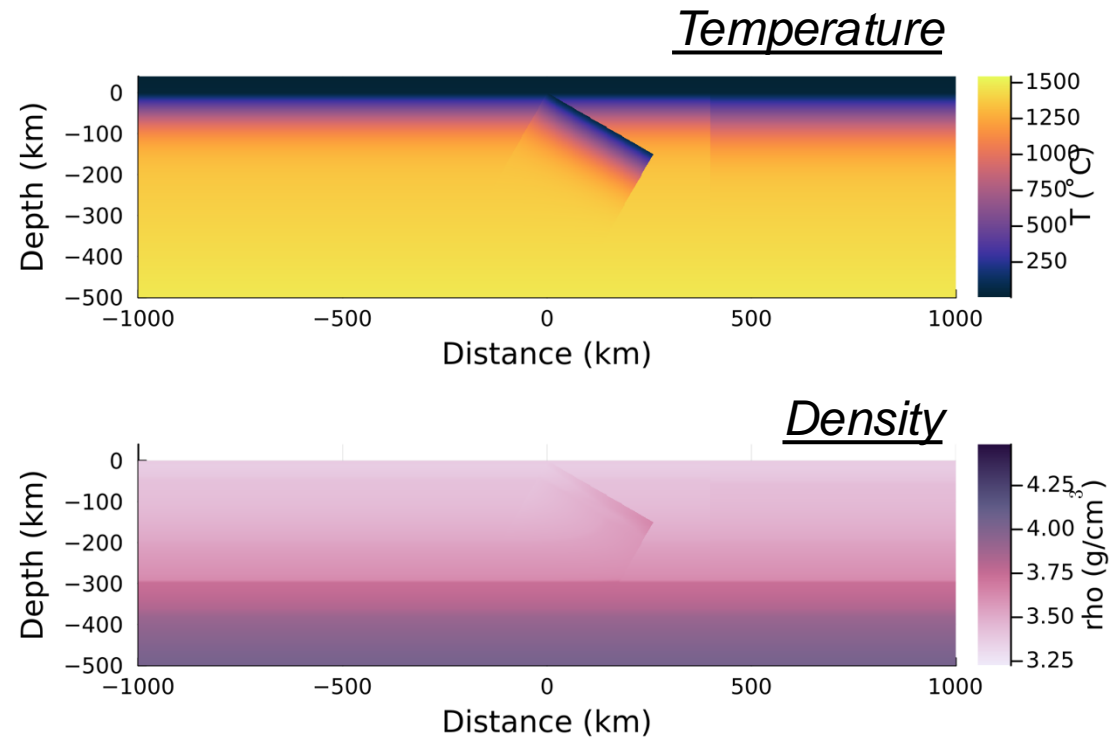


- + : thermodynamically self-consistent, can handle changing compositions***
- : computationally expensive to run (too slow for high-res simulations)***

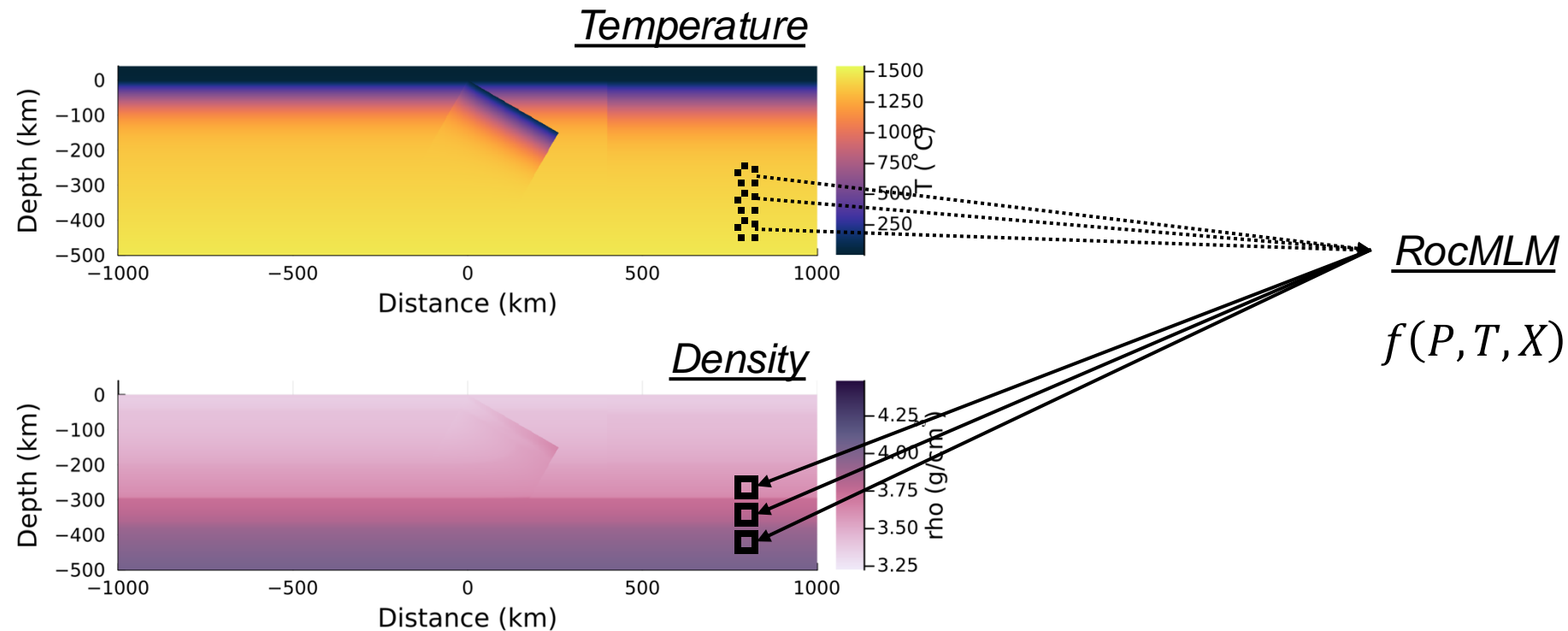
Machine learning models (RocMLM) are effective and fast



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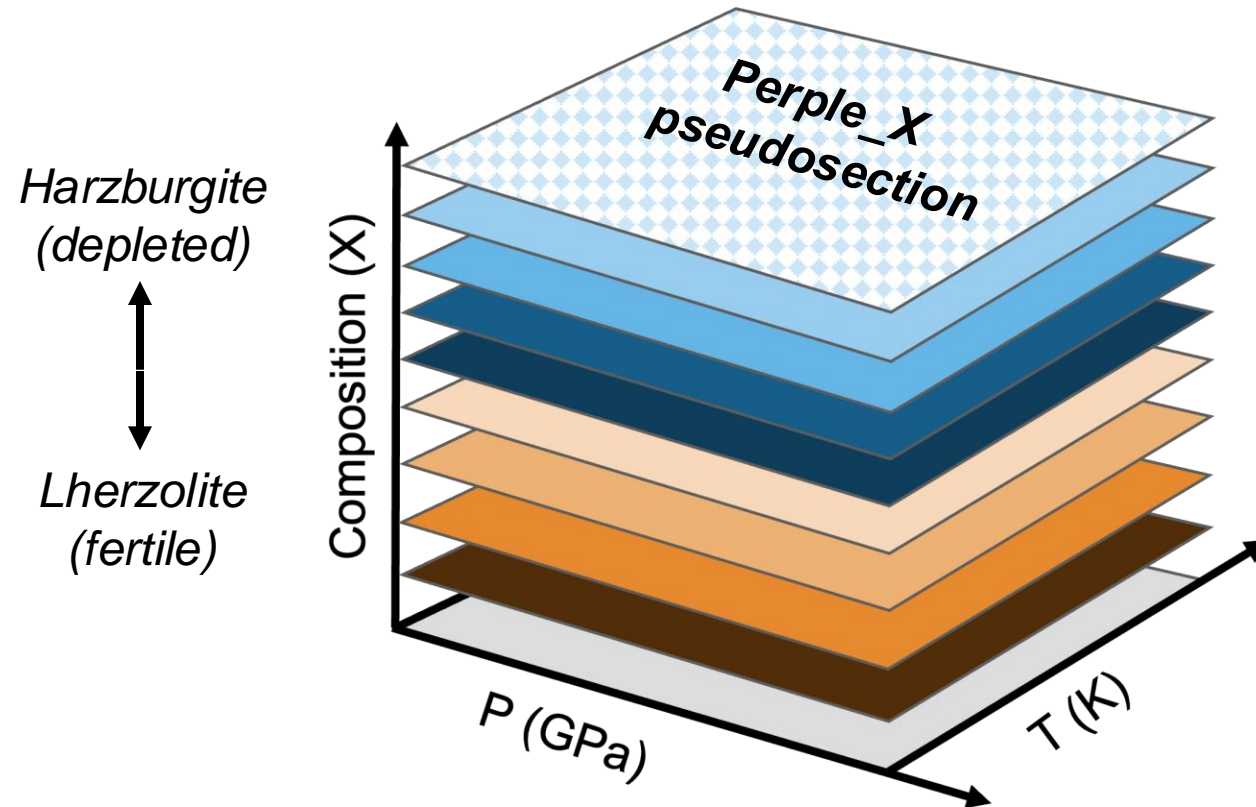


Machine learning models (*RocMLM*) are effective and fast

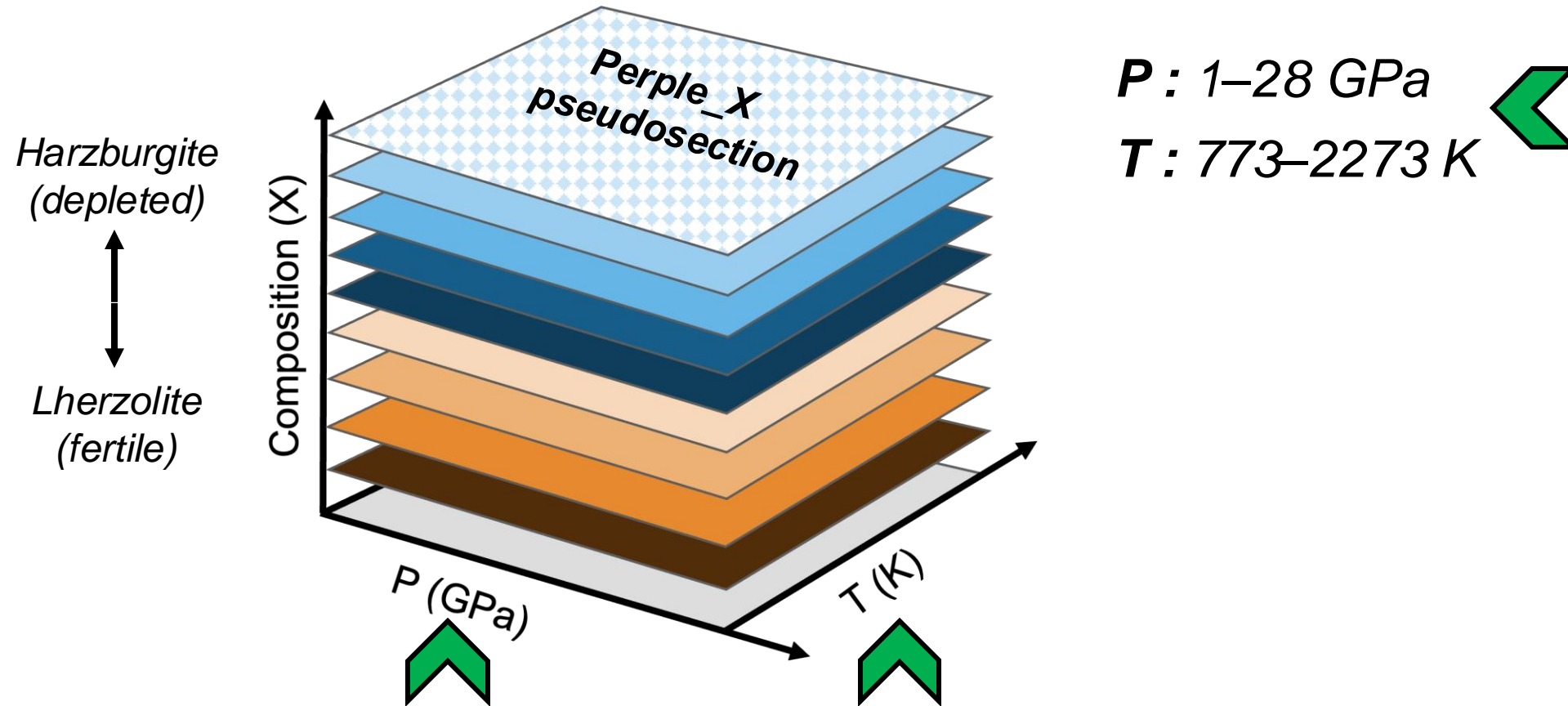


- + : *potentially much faster than Lookup Tables and GFEM*
- : *requires building and training on a large dataset*

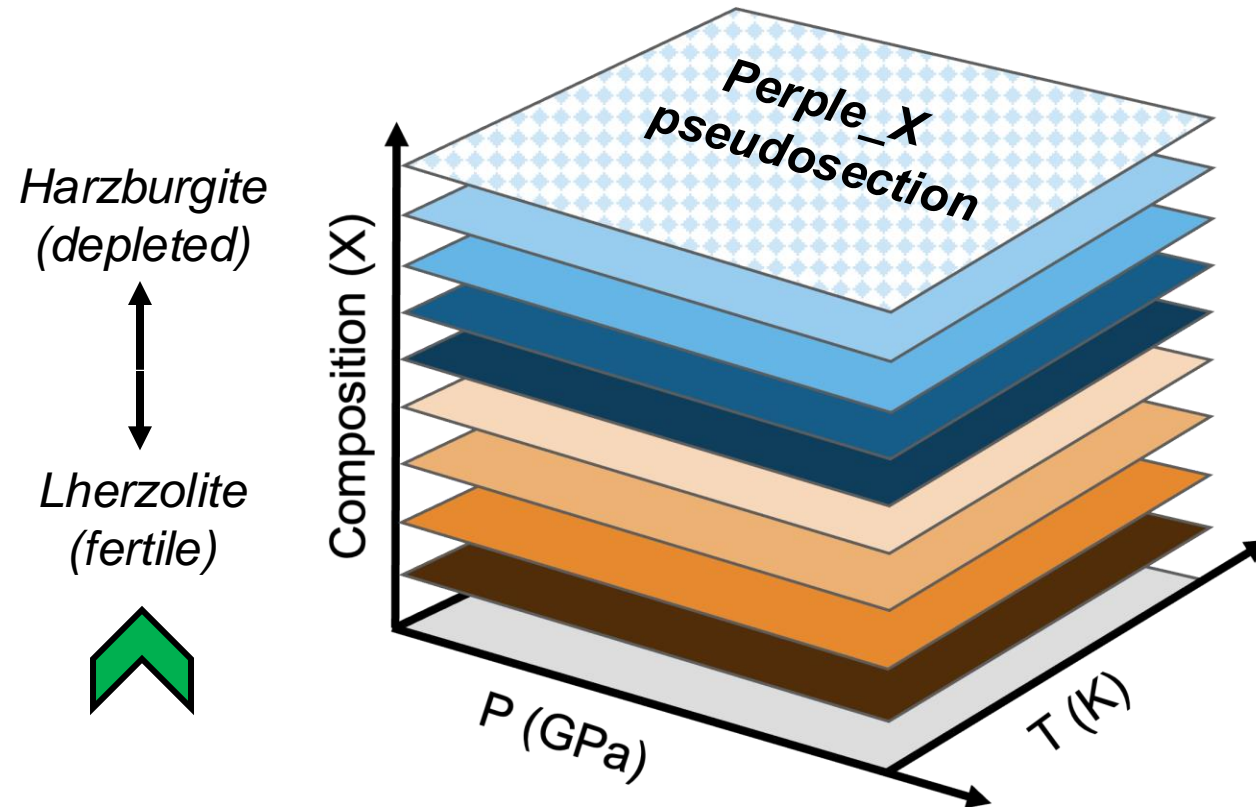
RocMLM training data were designed to be relevant for convection in the upper mantle



RocMLM training data were designed to be relevant for convection in the upper mantle



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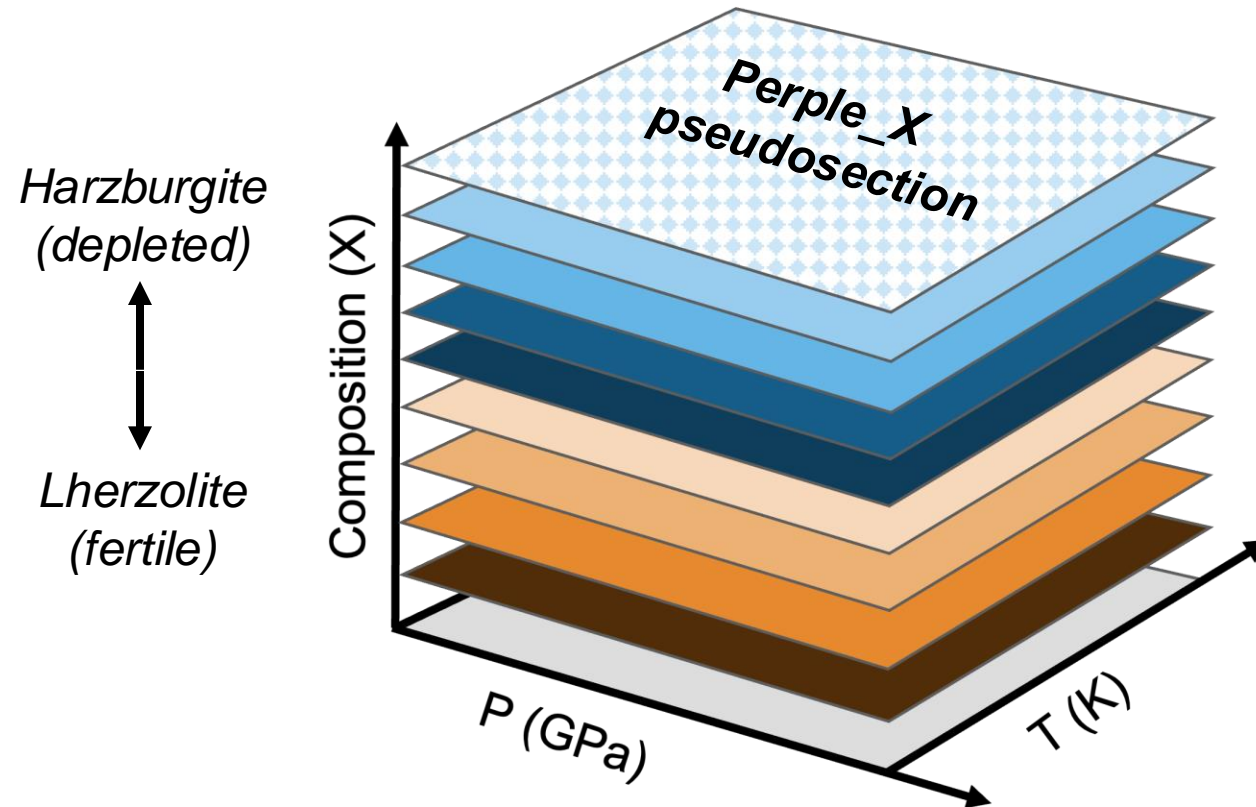
$P : 1\text{--}28 \text{ GPa}$

$T : 773\text{--}2273 \text{ K}$

$X : [\text{Na}_2\text{O-CaO-FeO-MgO-Al}_2\text{O}_3\text{-SiO}_2]$



RocMLM training data were designed to be relevant for convection in the upper mantle



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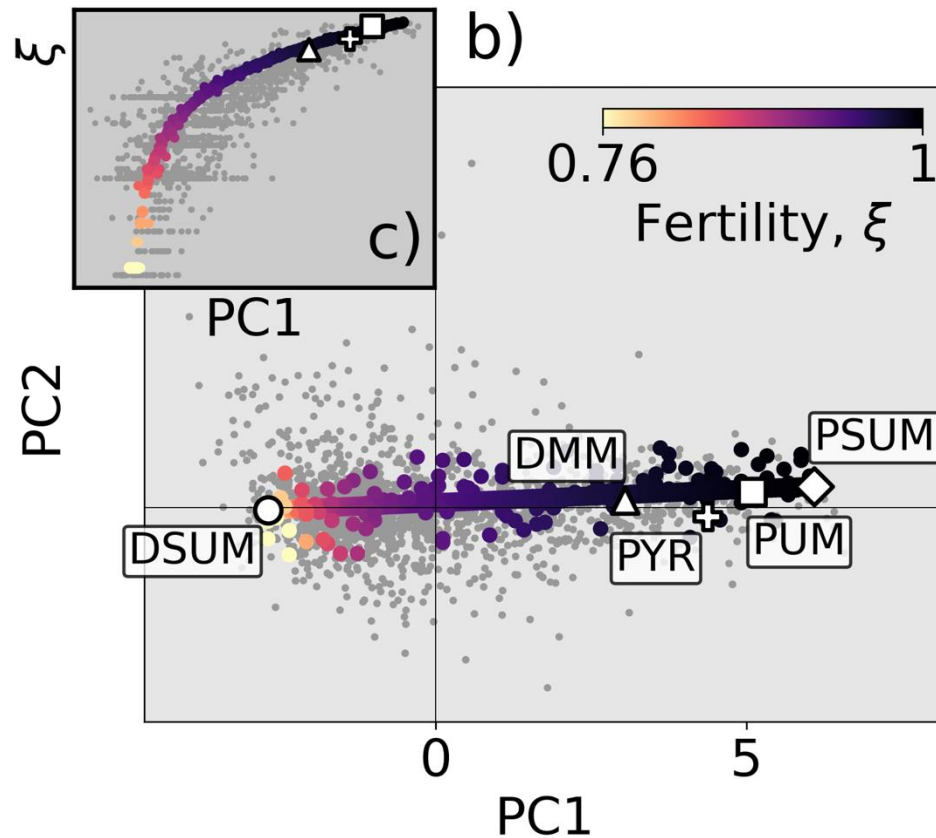
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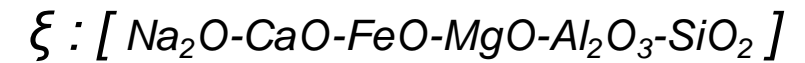
Dimensions : 2 + 6 = 8

Need to reduce this !

A hypothetical mixing array was used to sample synthetic bulk compositions for RocMLM training



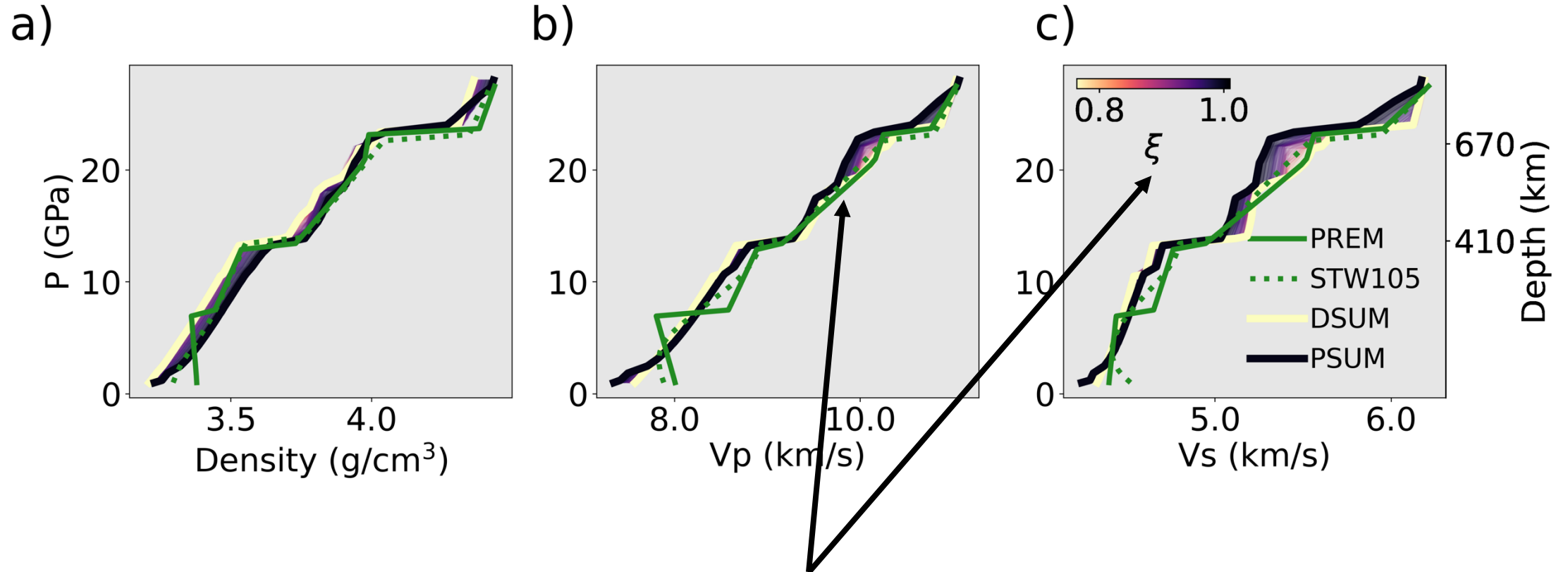
ξ Fertility Index parameter
represents composition



$$\xi = 1 - F = R^{\frac{1}{\left(\frac{1}{D_0}\right)^{-1}}}$$

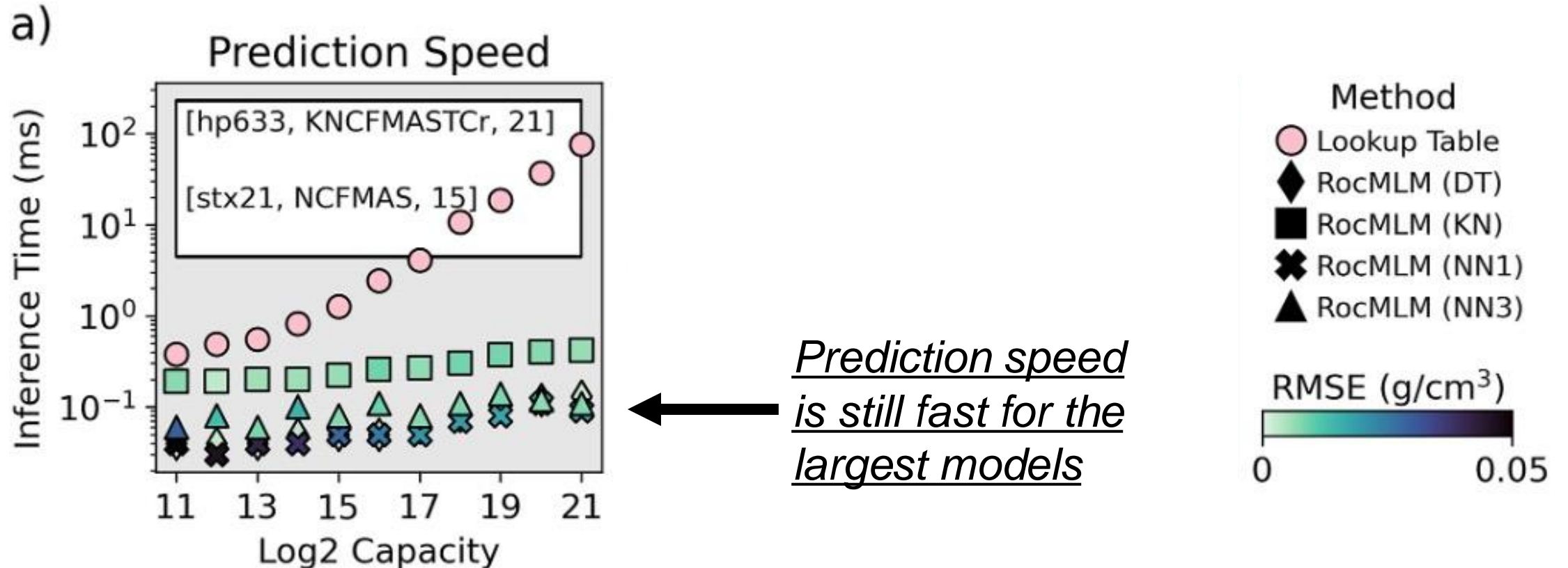
Shaw (1970; *Geochimica*)

RocMLM training dataset contains 2^{21} (~2.1M) phase equilibria across an array of 128 mantle comp's from fertile → depleted



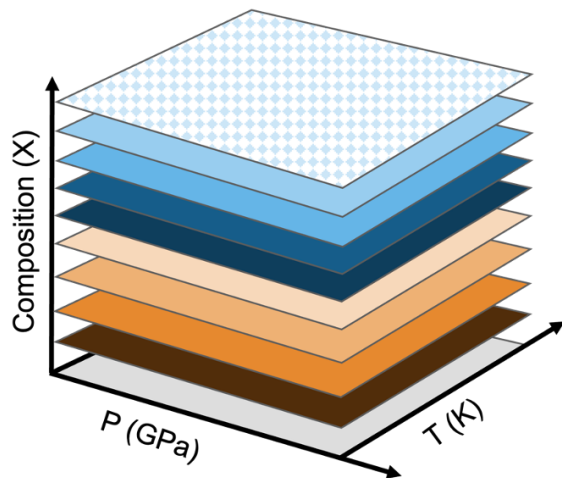
Training data are sensitive to mantle composition

RocMLMs are 10^1 – 10^3 times faster than common methods

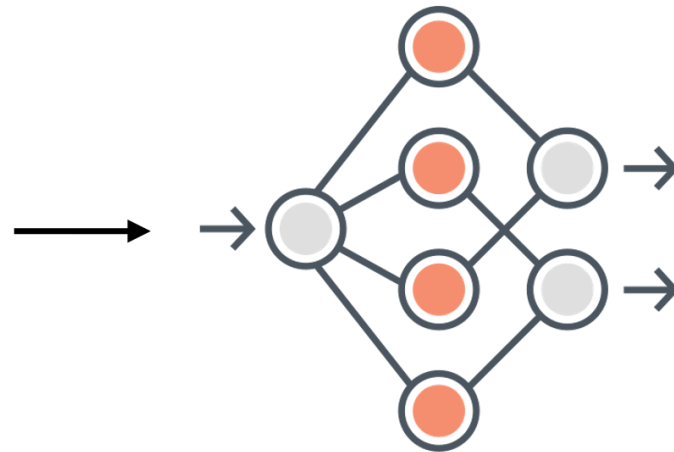


In summary, RocMLMs overcome practical limitations for emulating dynamic phase changes in numerical simulations of mantle convection

Training dataset



Regression algorithm



RocMLMs are 10^1 – 10^3 times faster than GFEM programs and Lookup Tables

RocMLMs trained with Neural Networks are more efficient compared to other regression algorithms

RocMLM training data show good agreement with PREM and STW105 for an average mantle geotherm

Questions?