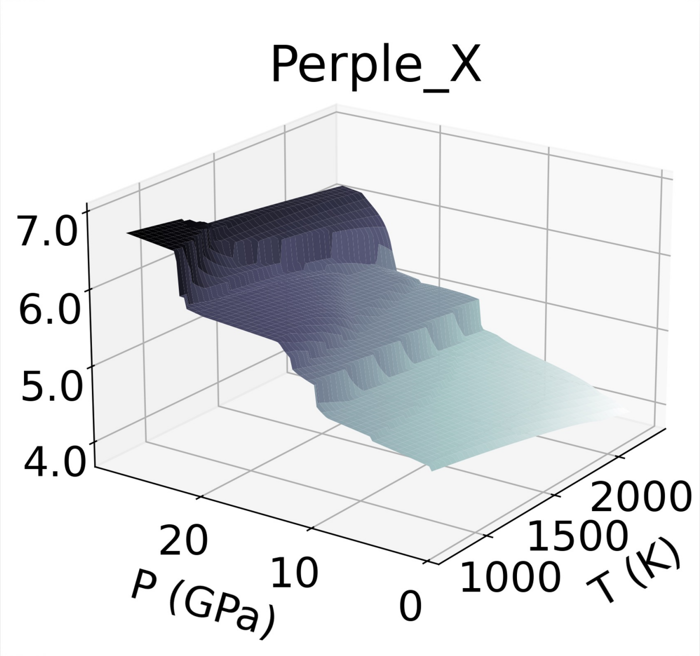
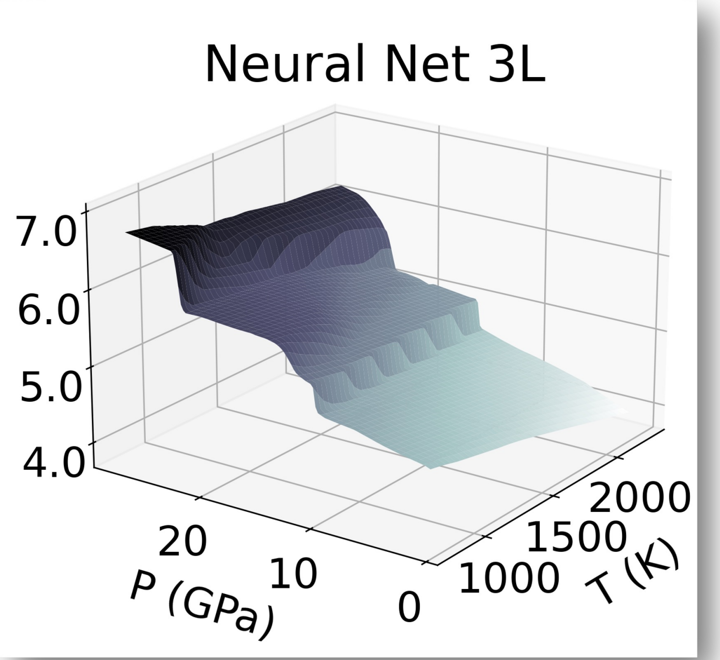
RocMLMs

Predicting Rock Properties through Machine Learning Models

Training Dataset



RocMLM Predictions



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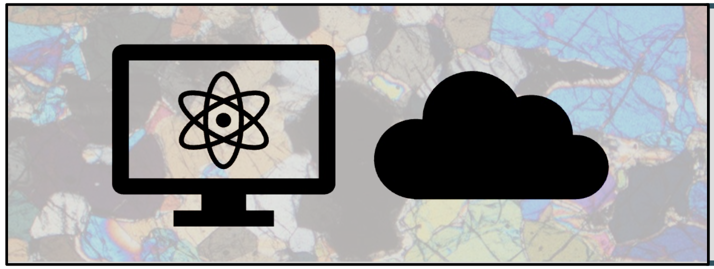
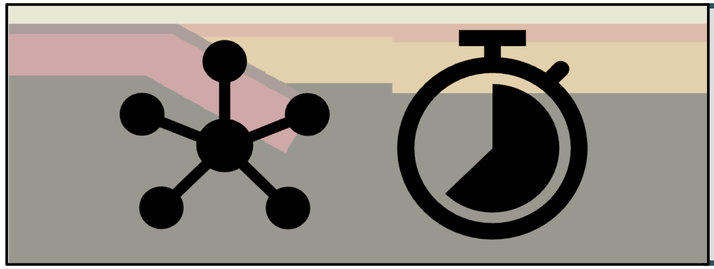
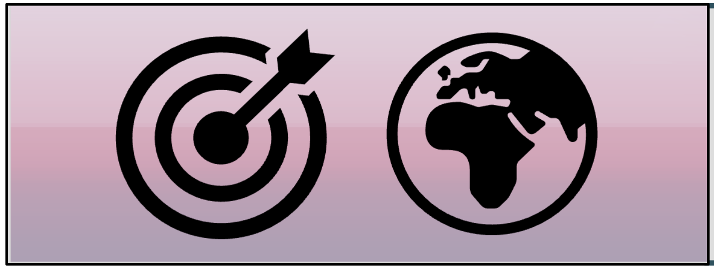
We developed RocMLMs to emulate dynamic phase changes in numerical simulations of mantle convection



Training Dataset



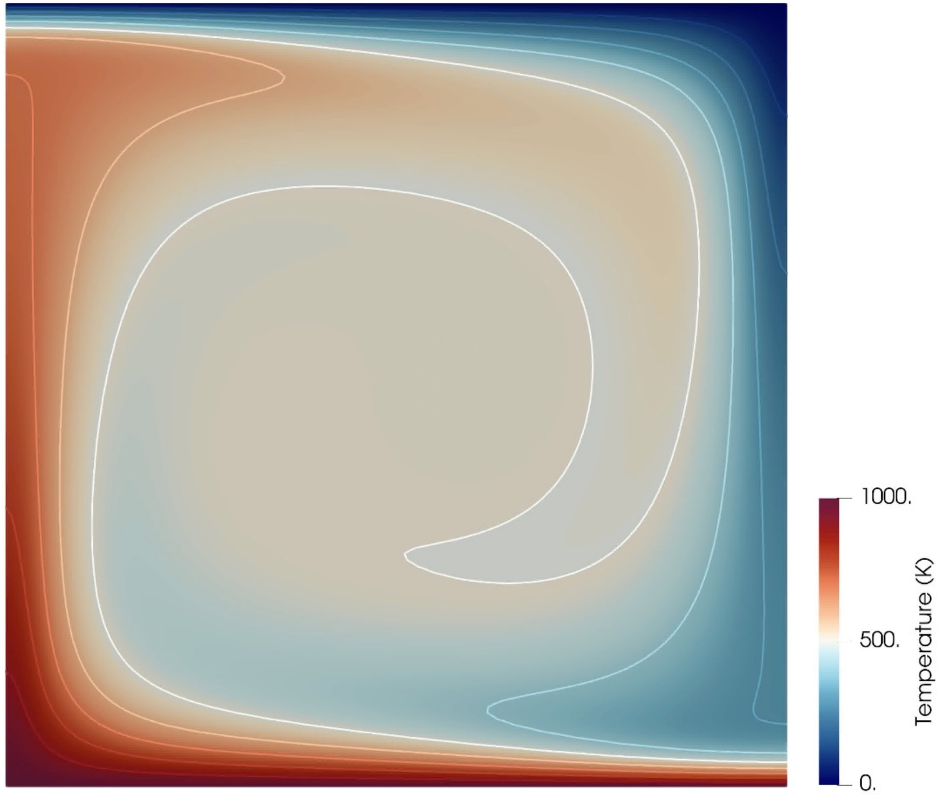
Performance



Accuracy

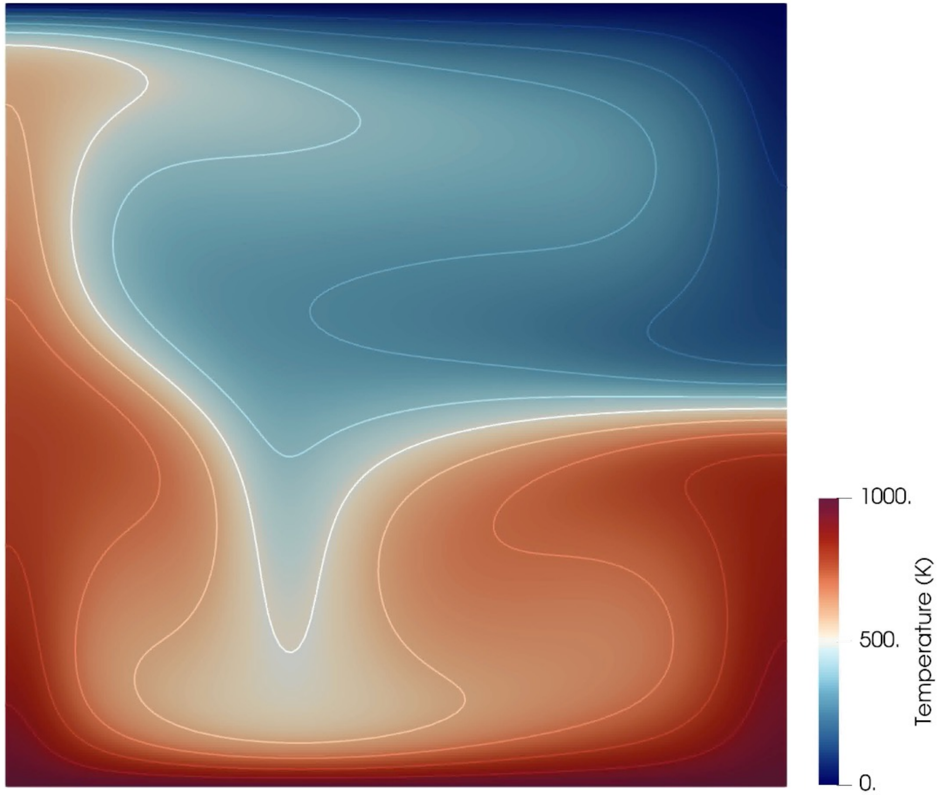
Phase transformations strongly impact mantle convection

No phase change



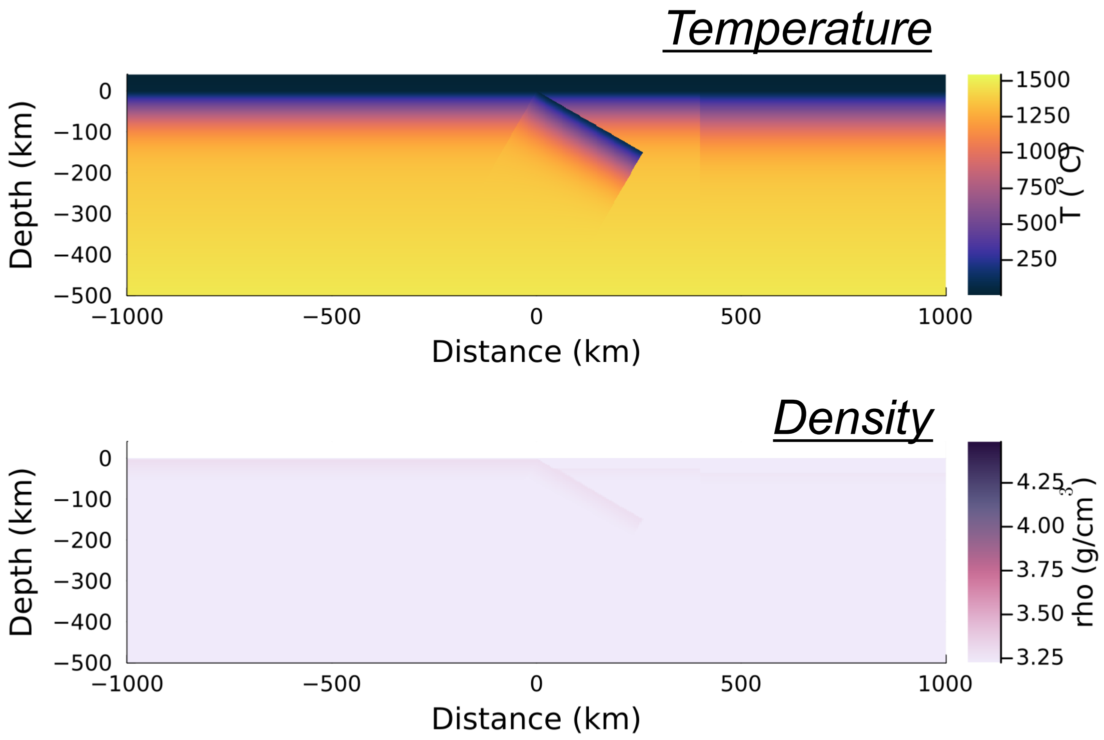
Blankenbach et al. (1989; *GJI*)

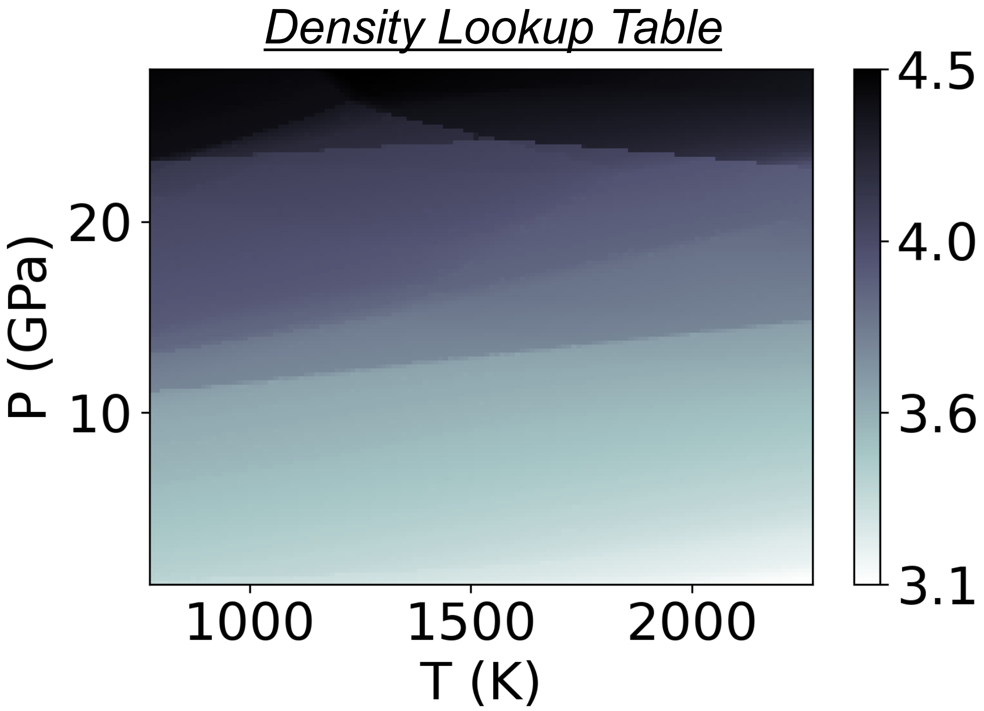
Phase change with: $\rho_1 > \rho_2$



Christensen & Yuen (1985; *JGR:SE*)

Lookup Tables are effective at implementing phase changes





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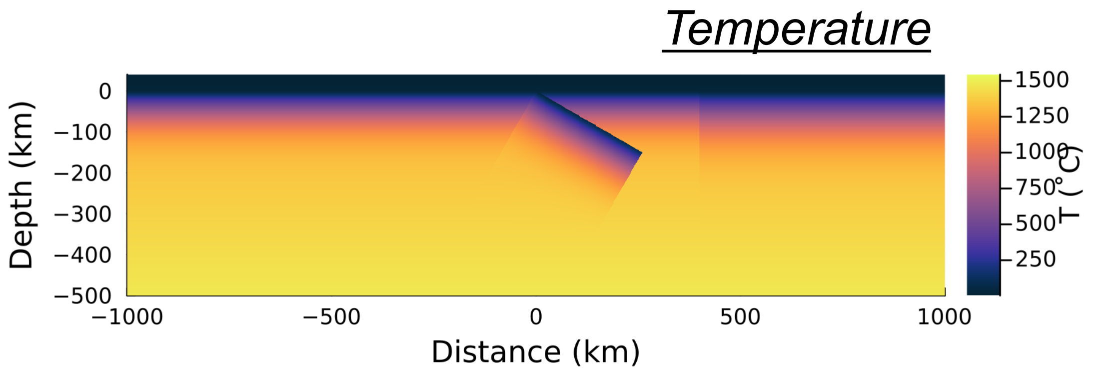

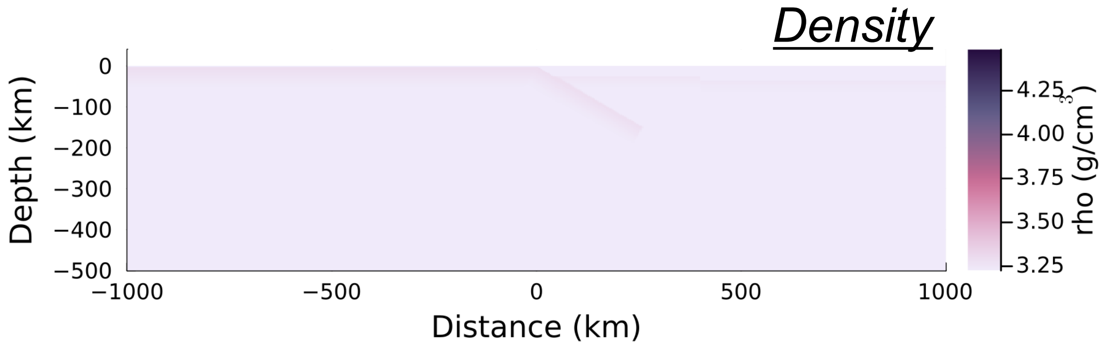

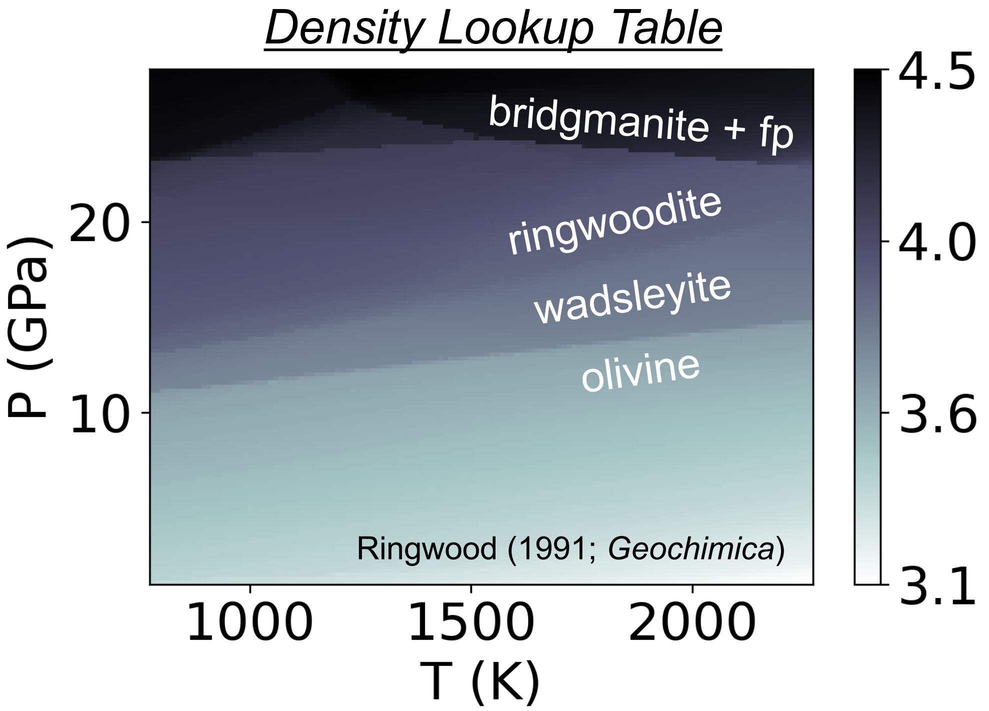

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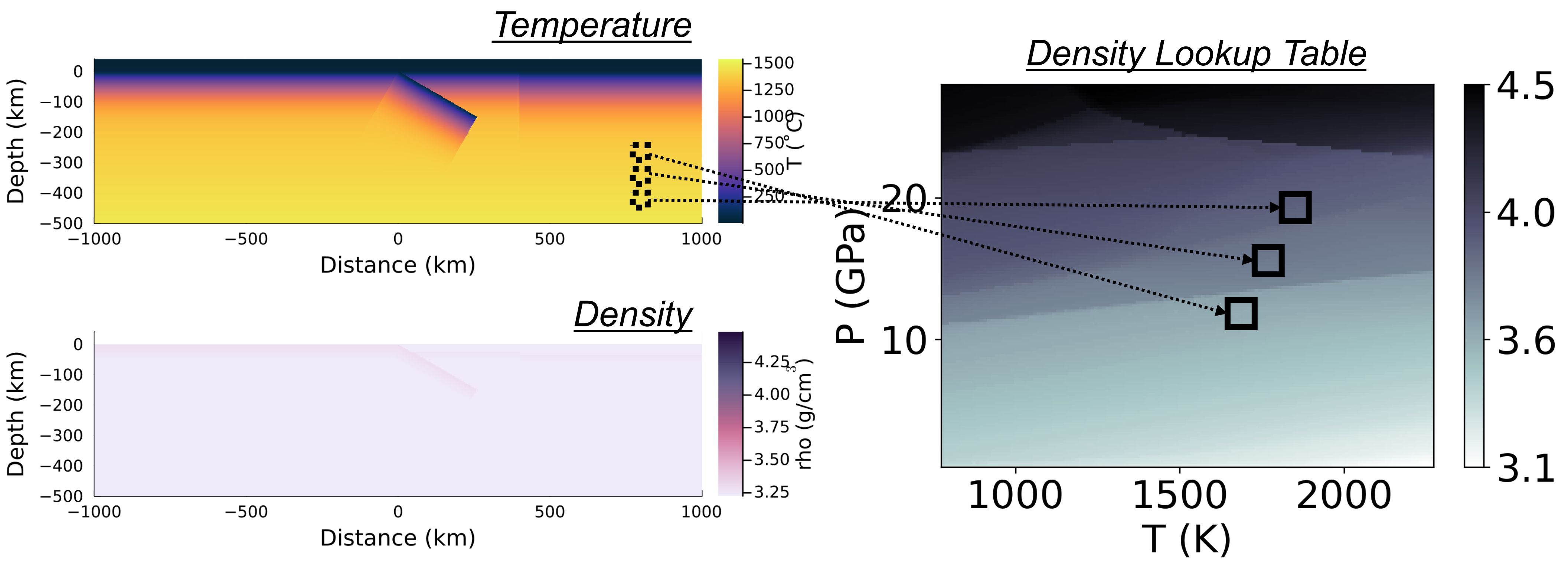
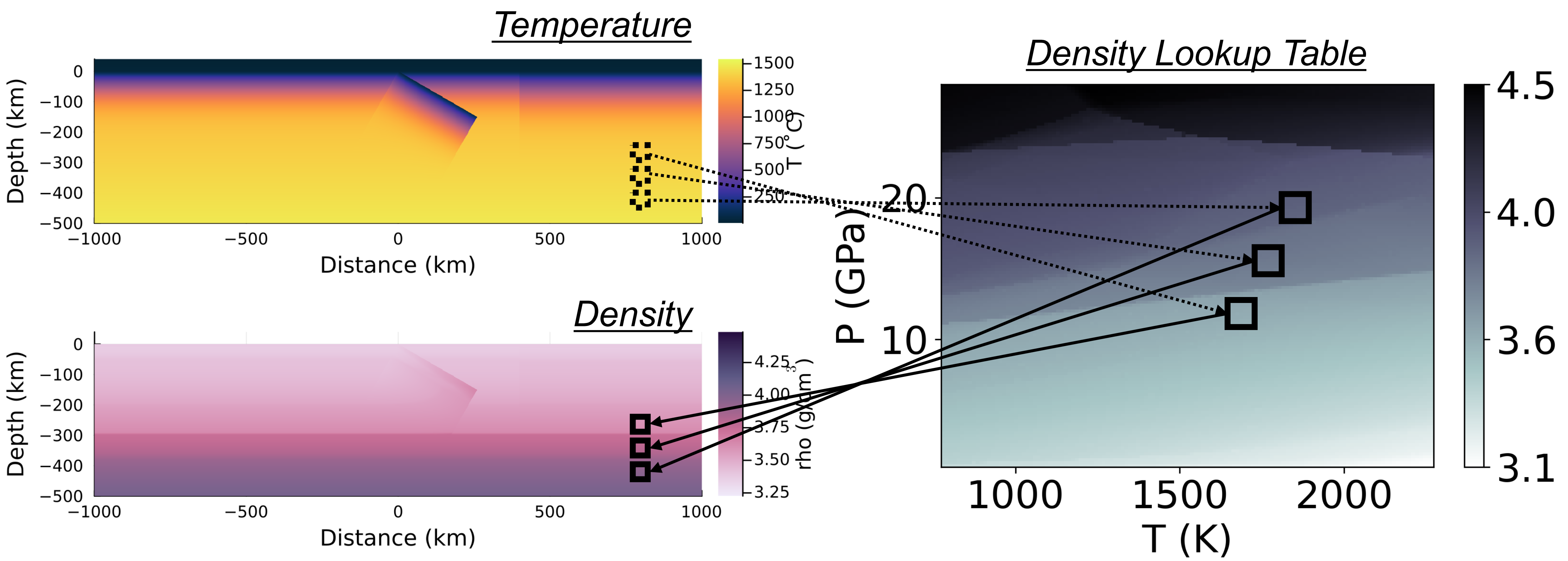


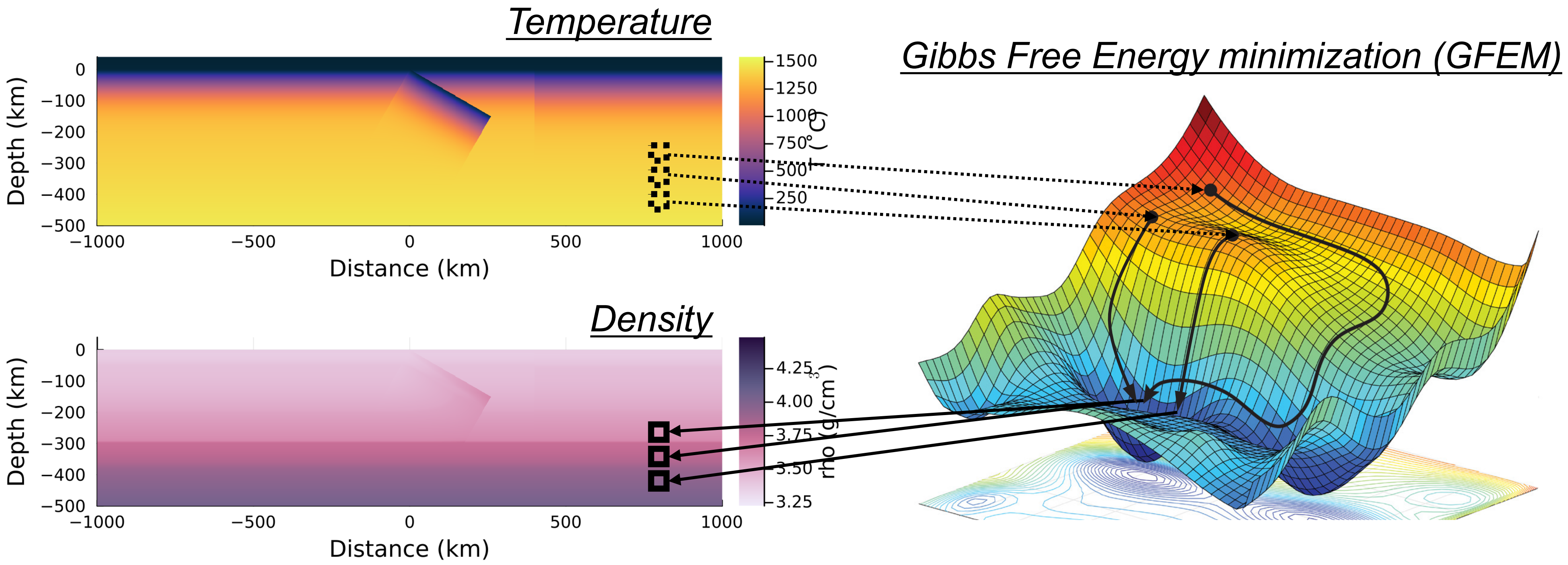
Lookup Tables are effective at implementing phase changes



+ : *adds a degree of thermodynamic self-consistency*

– : *need Lookup Tables for each rock composition and rock property*

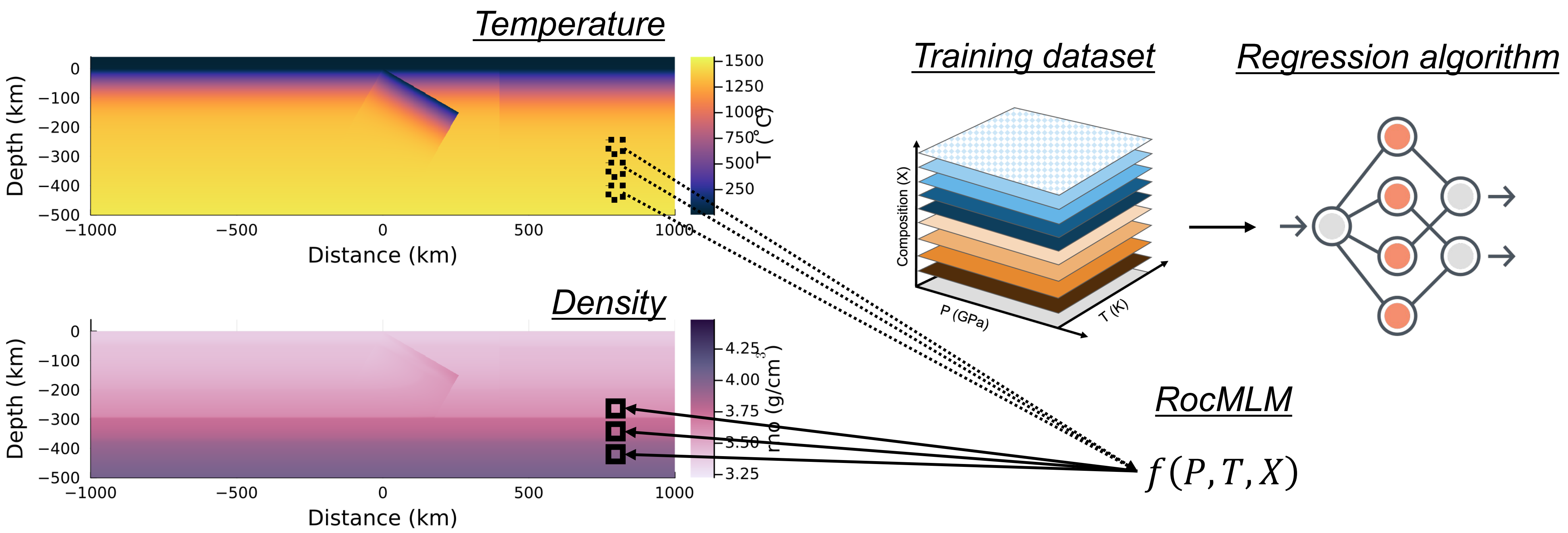
Phase equilibria modeling is more effective, but slow



+ : *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

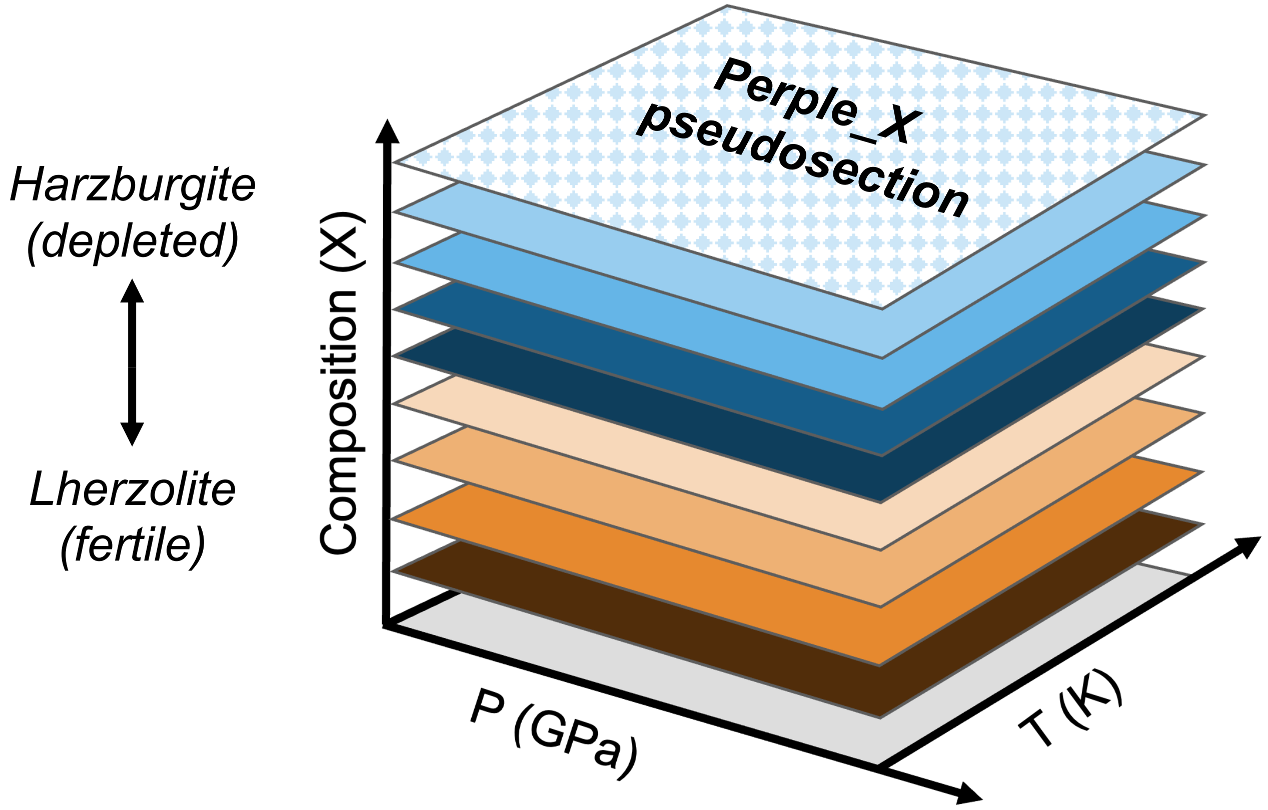


+ : *potentially much faster than Lookup Tables and GFEM*

– : *requires building and training on a large dataset*

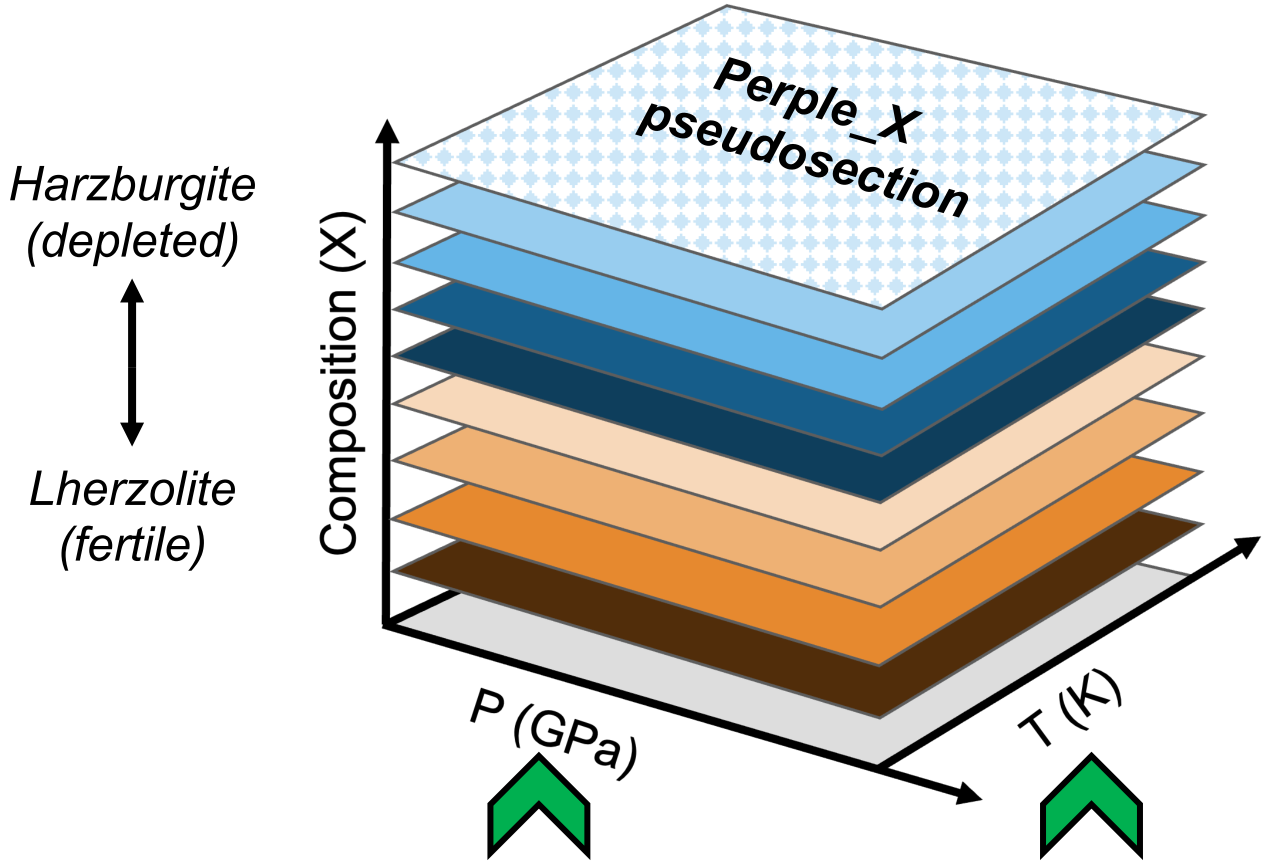
Kerswell et al. (2024; submitted G3)

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



Kerswell et al. (2024; submitted G3)

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



P : *1–28 GPa*

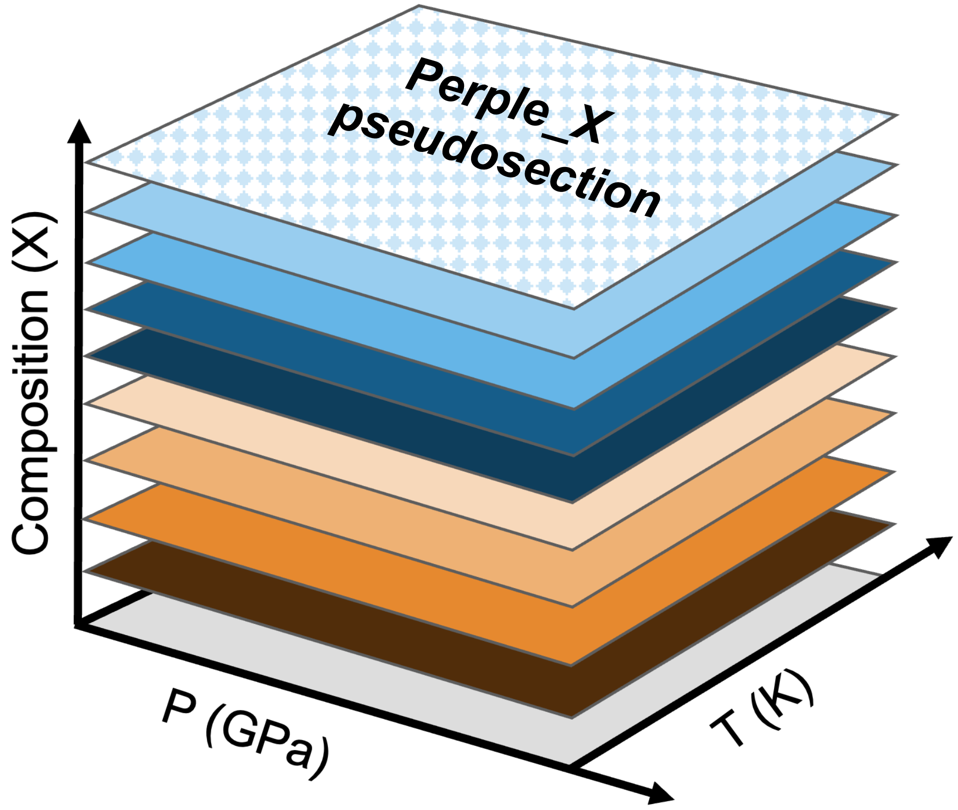
T : *773–2273 K*

Kerswell et al. (2024; submitted G3)

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

Harzburgite (depleted)

Lherzolite (fertile)



P : *1–28 GPa*

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X : *[Na_2O-CaO-FeO-MgO-Al_2O_3-SiO_2]*

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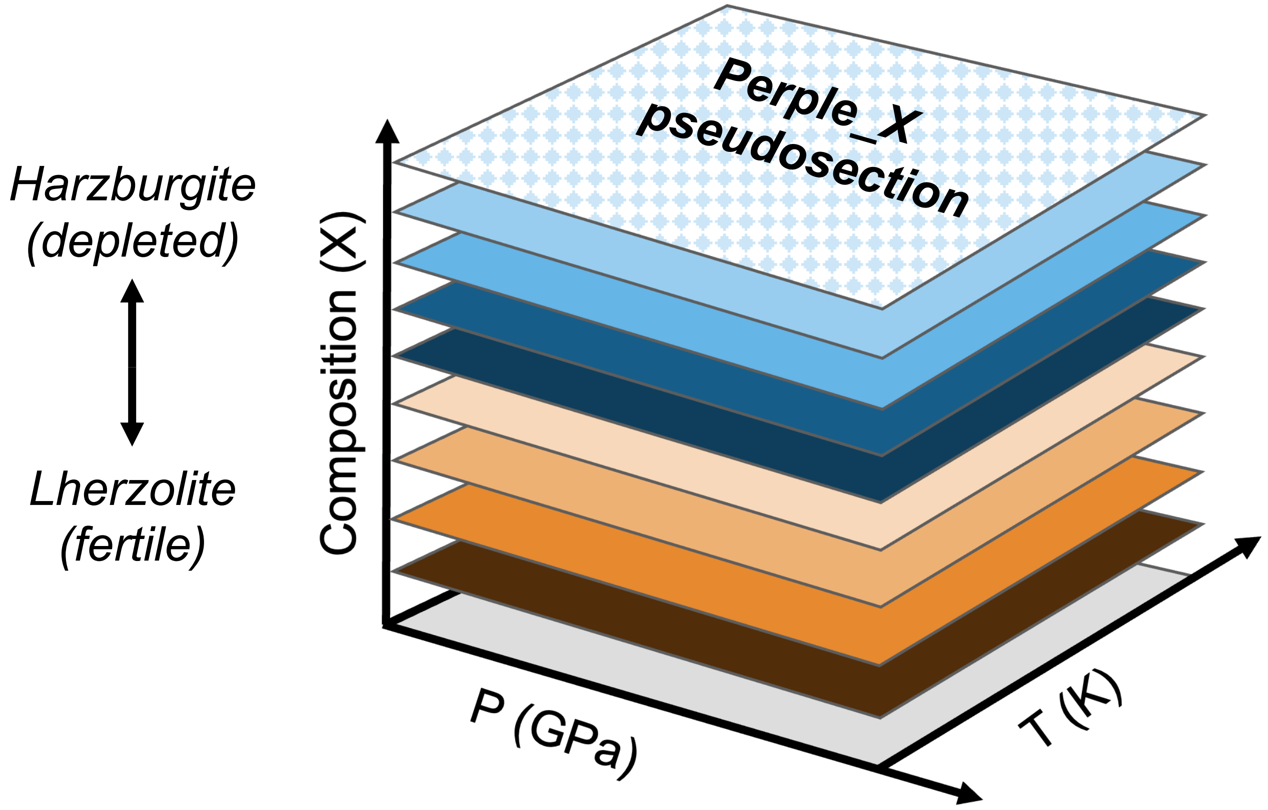
RocMLM training data were designed to be relevant for convection in the upper mantle



P : *1–28 GPa*

T : *773–2273 K*

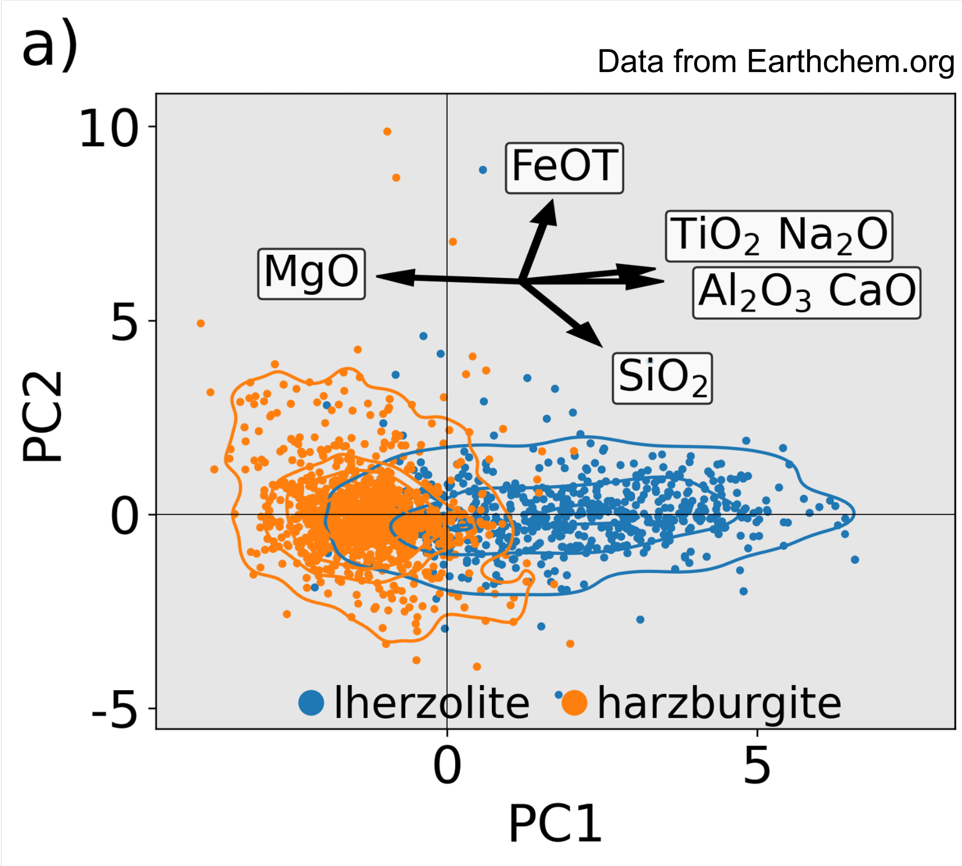
X : *[Na_2O-CaO-FeO-MgO-Al_2O_3-SiO_2]*

<u>Dimensions</u> : *2 + 6 = 8*

Need to reduce this !

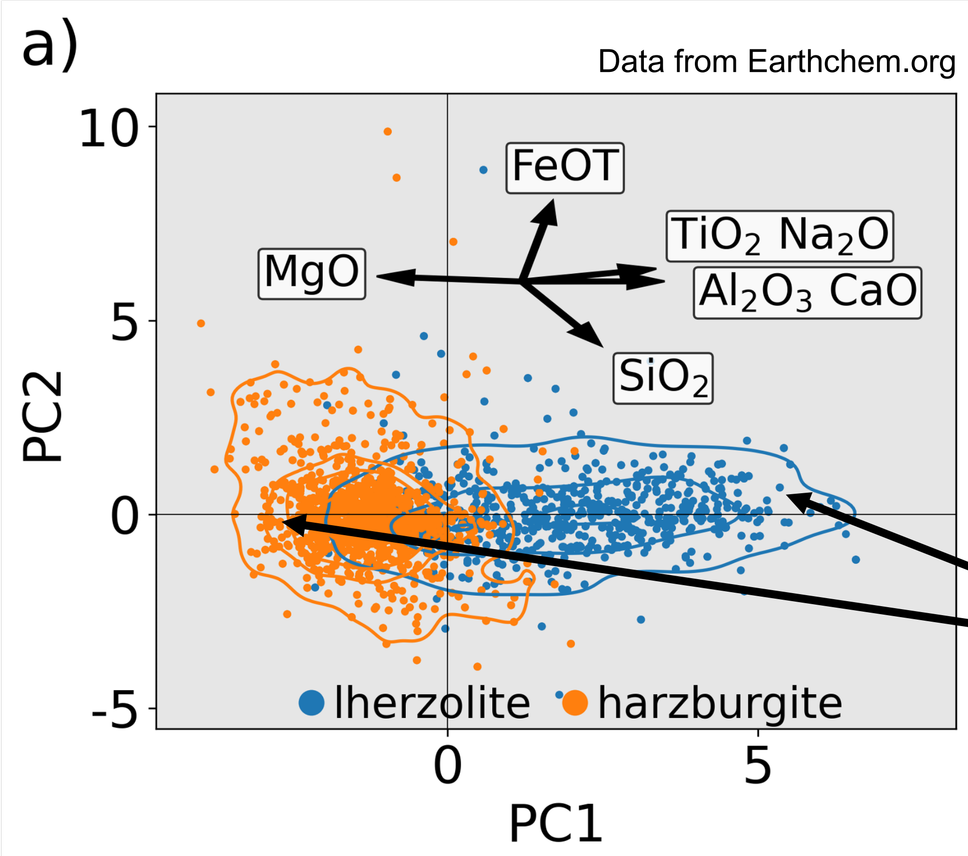
Kerswell et al. (2024; submitted G3)

3111 natural peridotite samples were reduced by PCA to 2 "chemical" components: PC1 & PC2



PC loading vectors

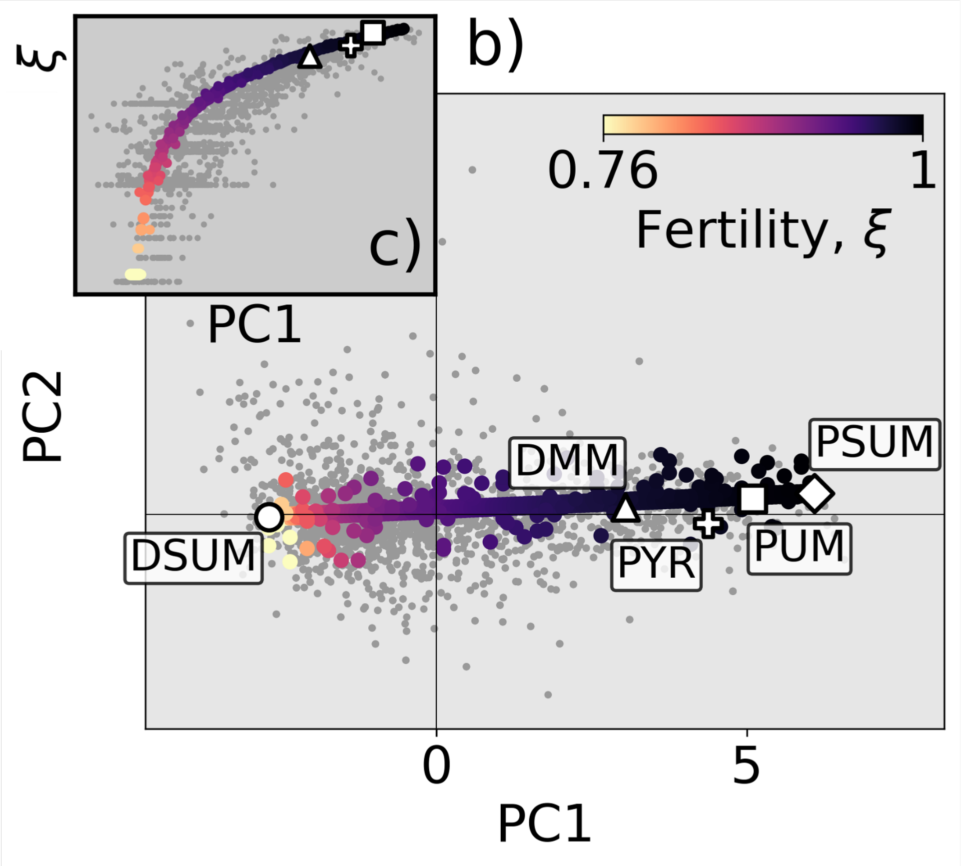
3111 natural peridotite samples were reduced by PCA to 2 "chemical" components: PC1 & PC2



Hypothetical mantle endmembers

Kerswell et al. (2024; submitted G3)

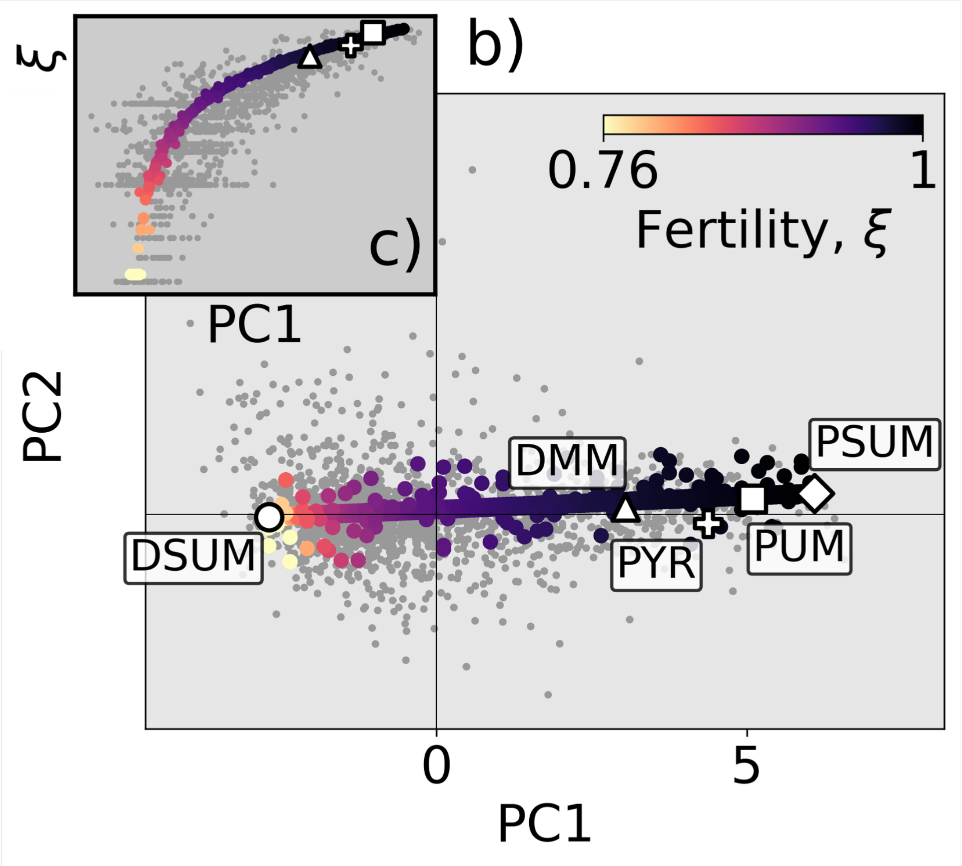
A hypothetical mixing array was used to sample synthetic bulk compositions for RocMLM training



← *<u>Synthetic samples used for RocMLM training</u>*

Kerswell et al. (2024; submitted G3)

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



<u>ξ Fertility Index parameter represents composition</u>

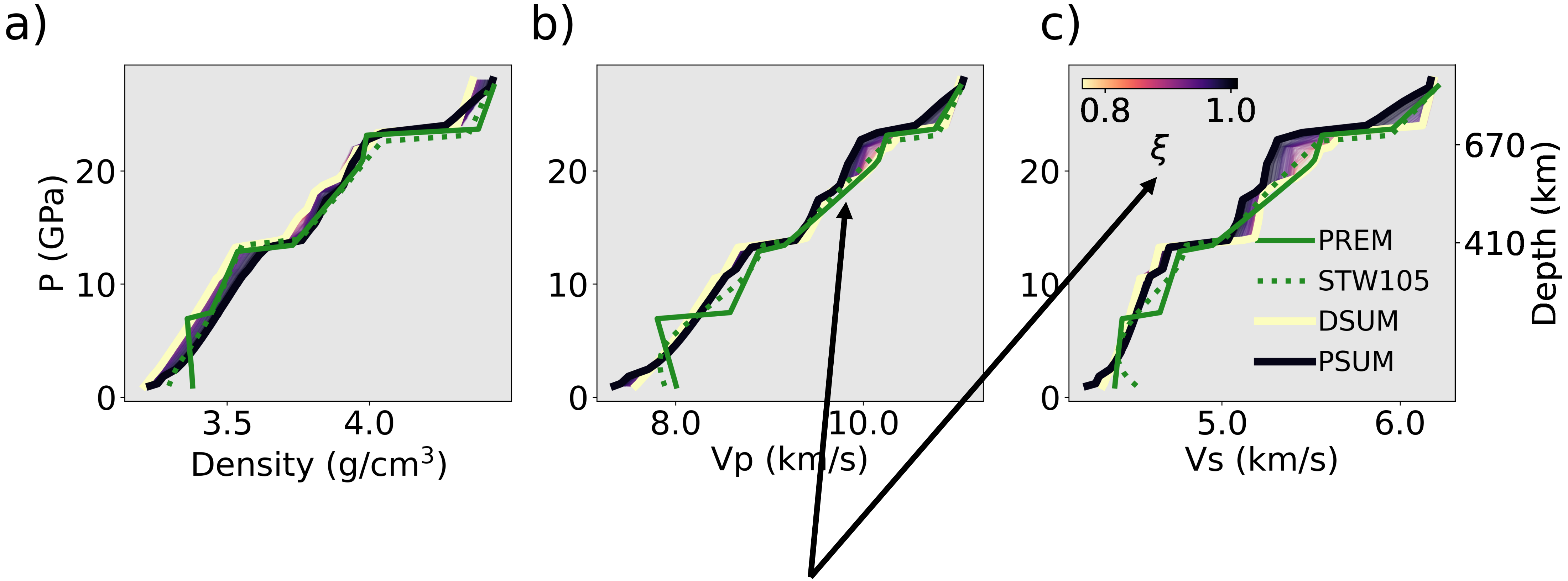
ξ : [Na_2O-CaO-FeO-MgO-Al_2O_3-SiO_2]

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

Shaw (1970; *Geochimica*)

Kerswell et al. (2024; submitted G3)

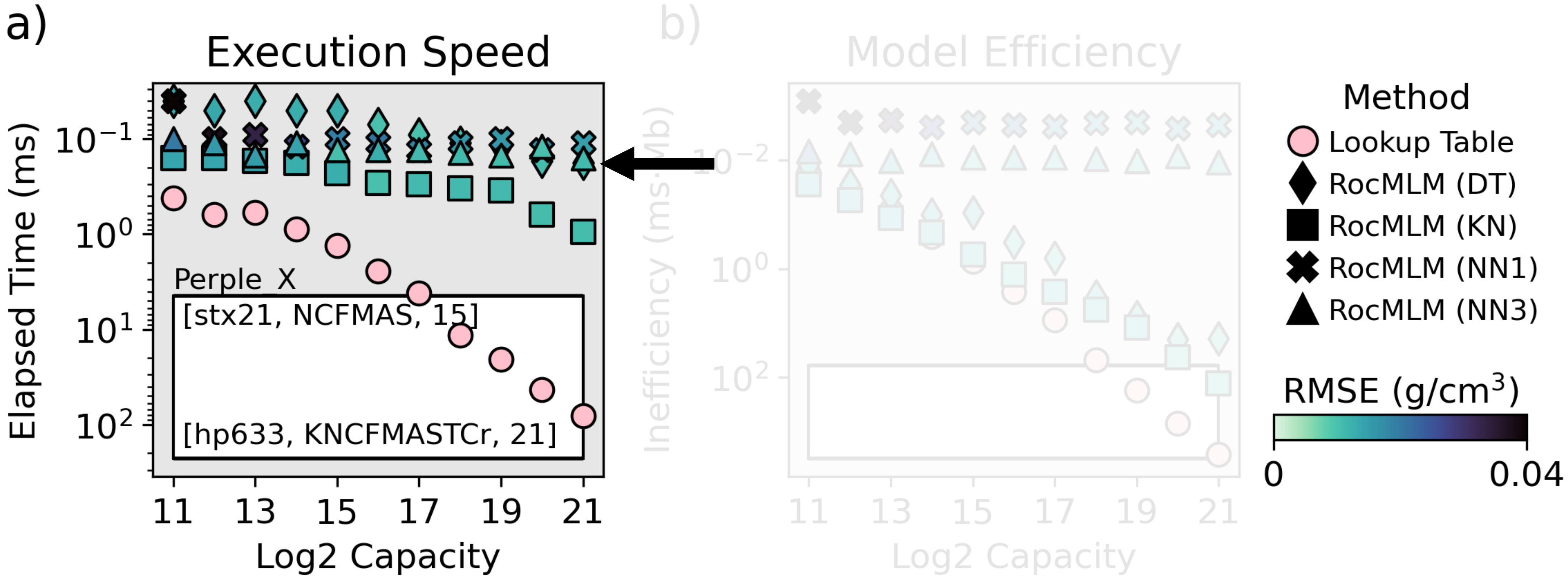
RocMLM training dataset contains 2^{21} (~2.1M) phase equilibria across an array of 128 mantle comp's from fertile → depleted



<u>Training data are sensitive to mantle composition</u>

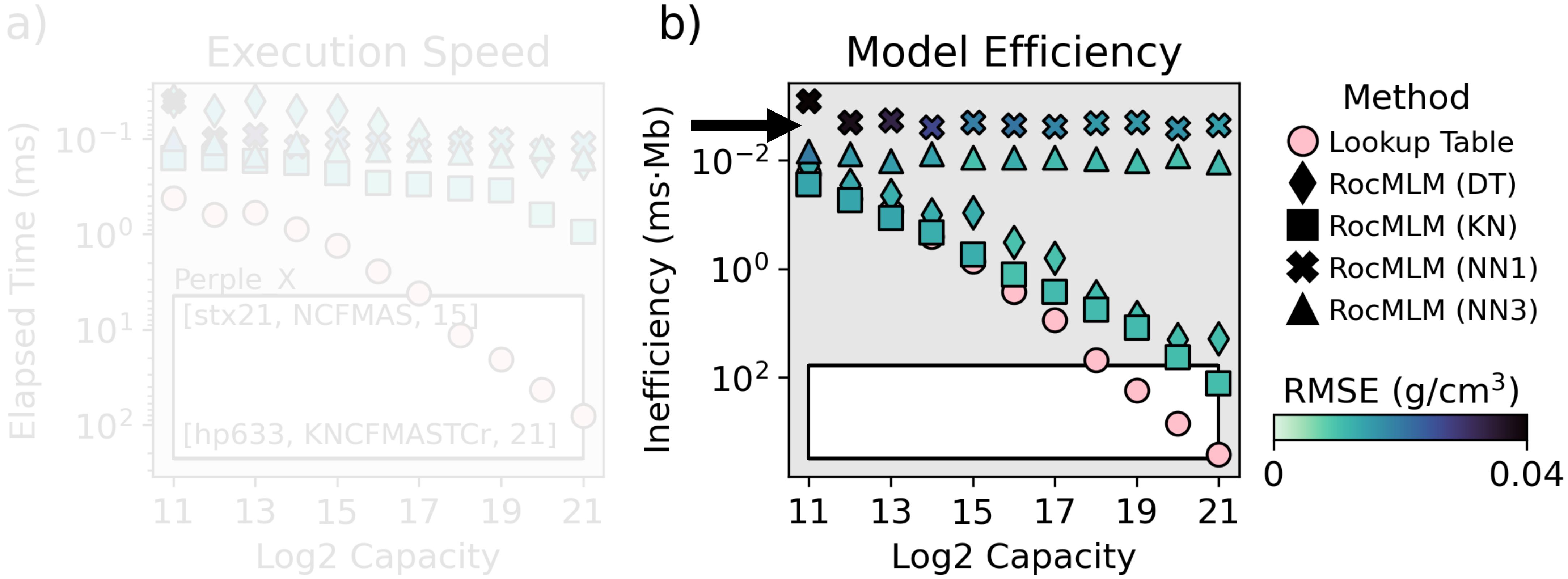
Kerswell et al. (2024; submitted G3)

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



Kerswell et al. (2024; submitted G3)

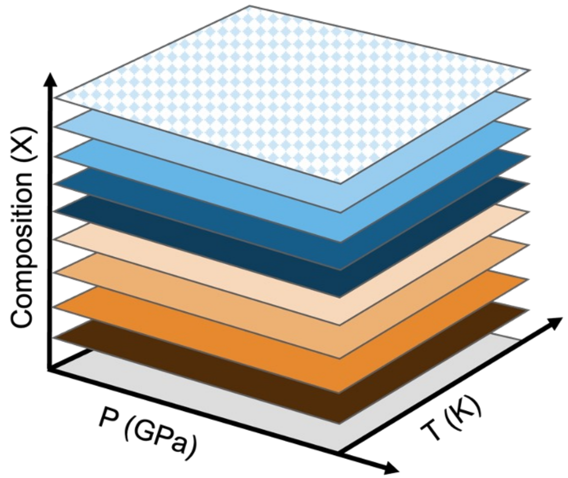
Neural Networks are more scalable than other algorithms



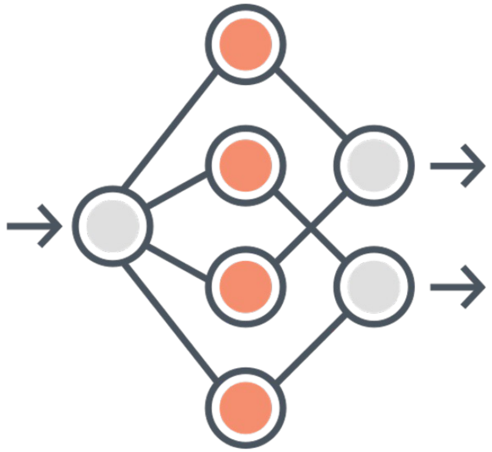
Kerswell et al. (2024; submitted G3)

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?