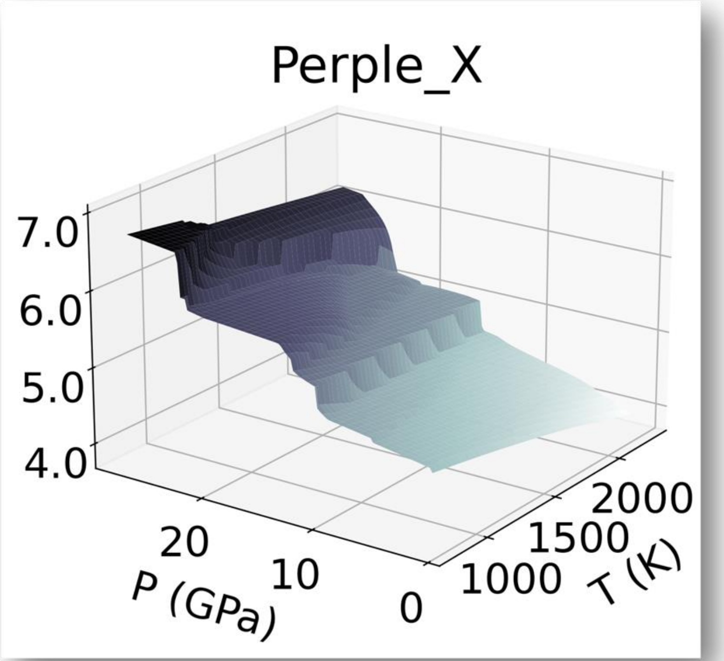
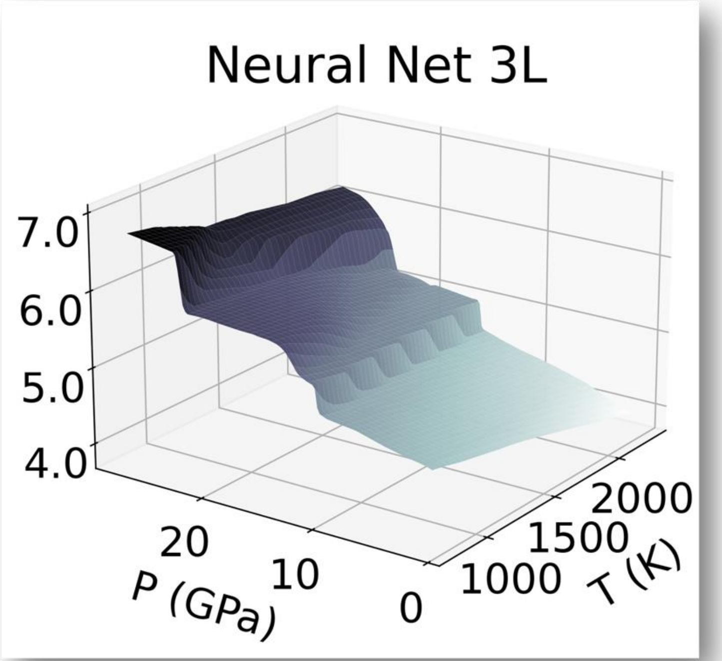
# RocMLMs

## *Predicting Rock Properties through Machine Learning Models*

<u>*Training Dataset*</u>




<u>*RocMLM Predictions*</u>





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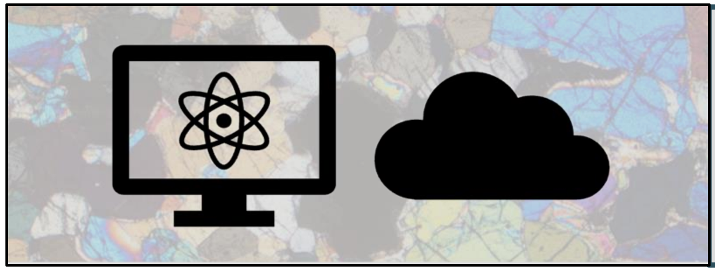
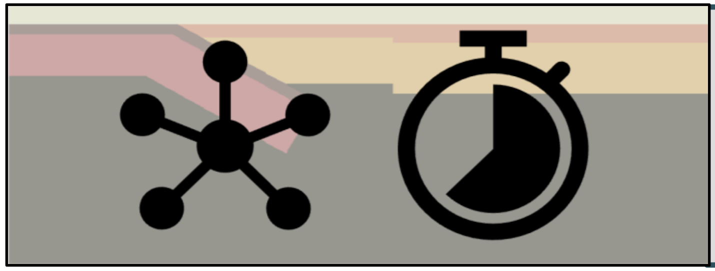
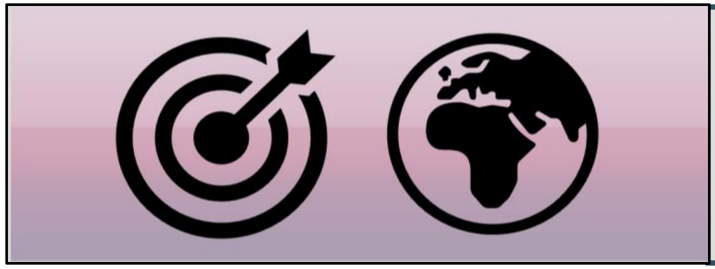
# *We developed RocMLMs to emulate dynamic phase changes in numerical simulations of mantle convection*



*Training Dataset*



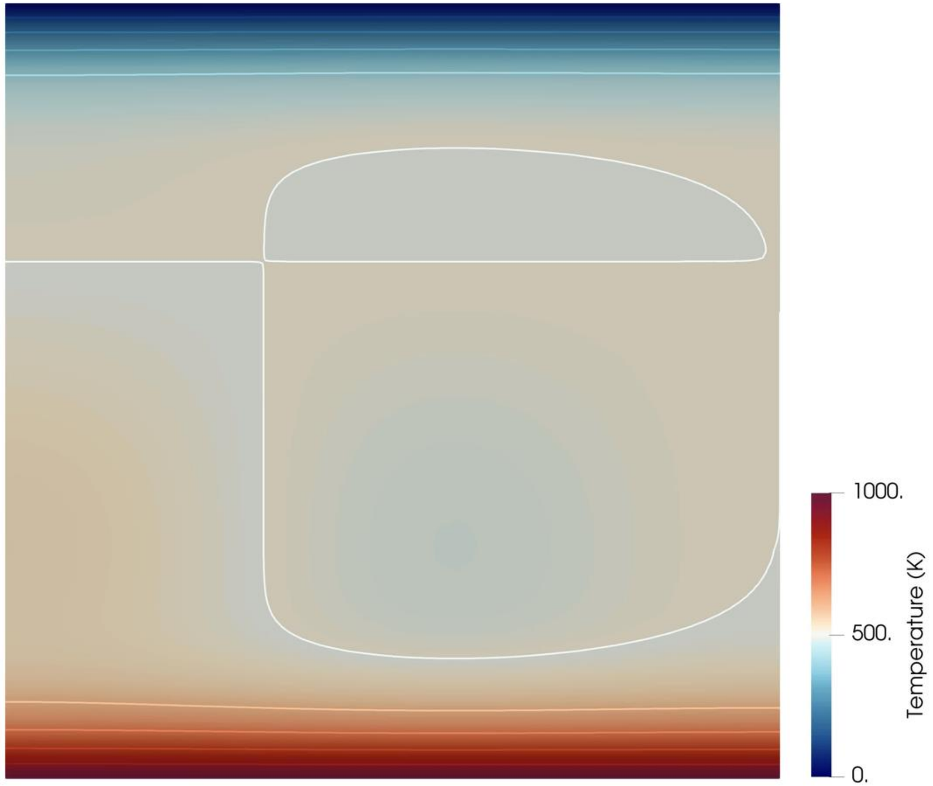
*Performance*



*Accuracy*

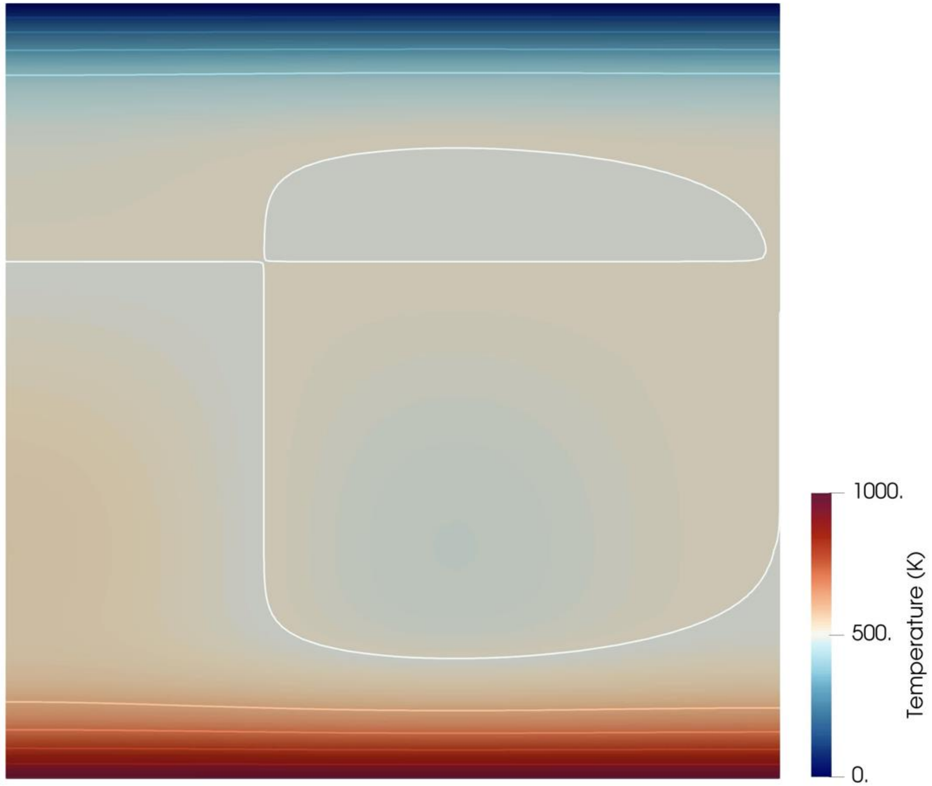
# Phase transformations strongly impact mantle convection

*No phase change*




Blankenbach et al. (1989; *GJI*)

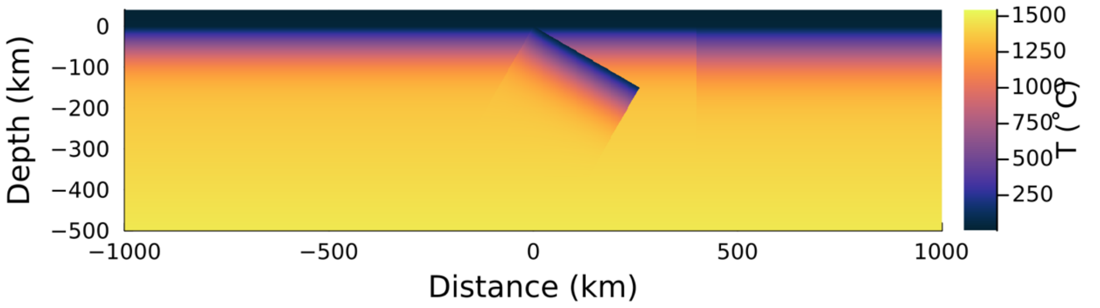
*Phase change with:* $\rho_1 > \rho_2$



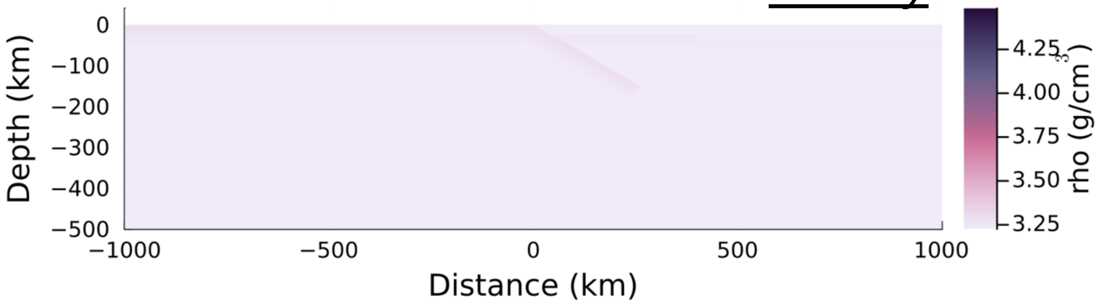

Christensen & Yuen (1985; *JGR:SE*)

# Lookup Tables are effective at implementing phase changes

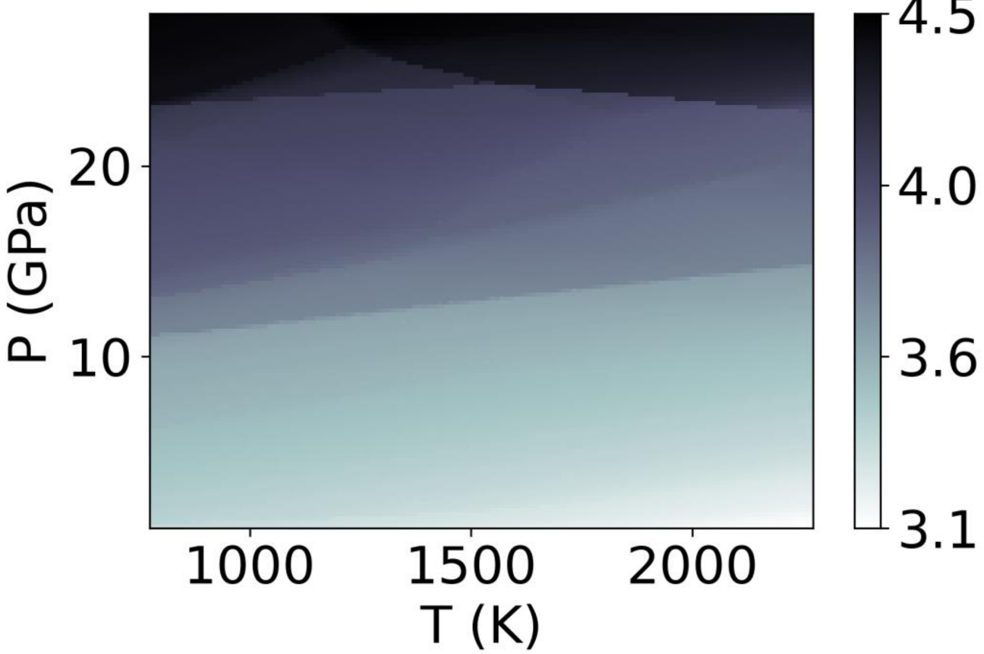
*Temperature*



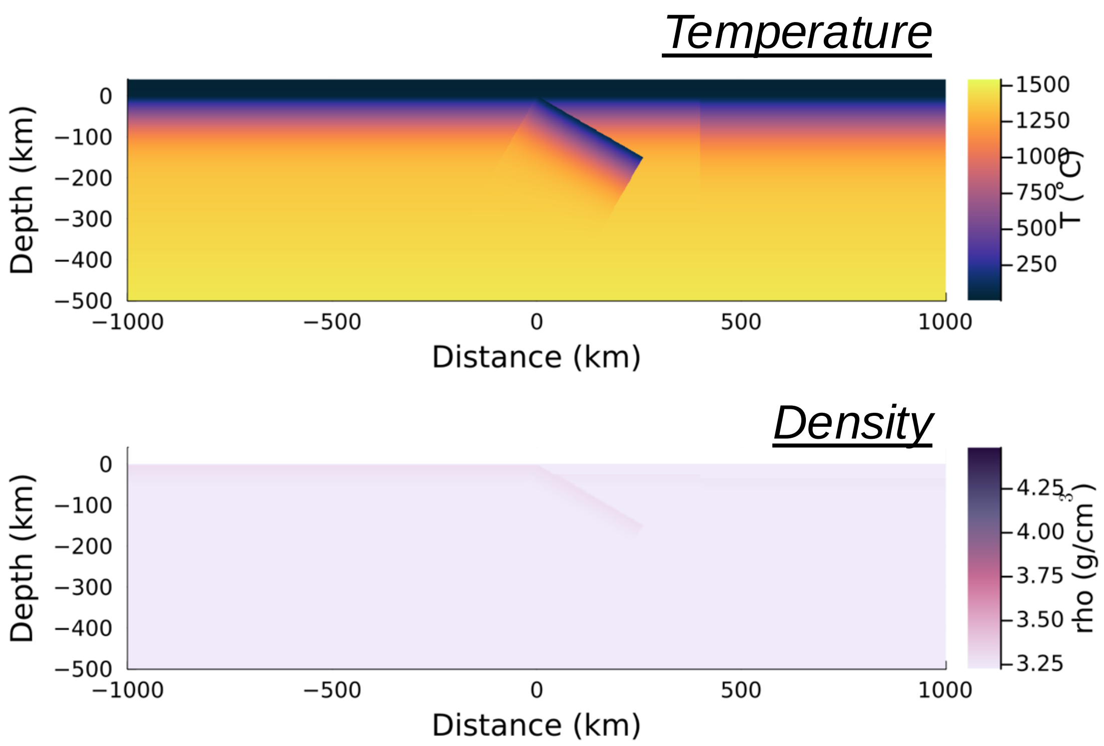

*Density*

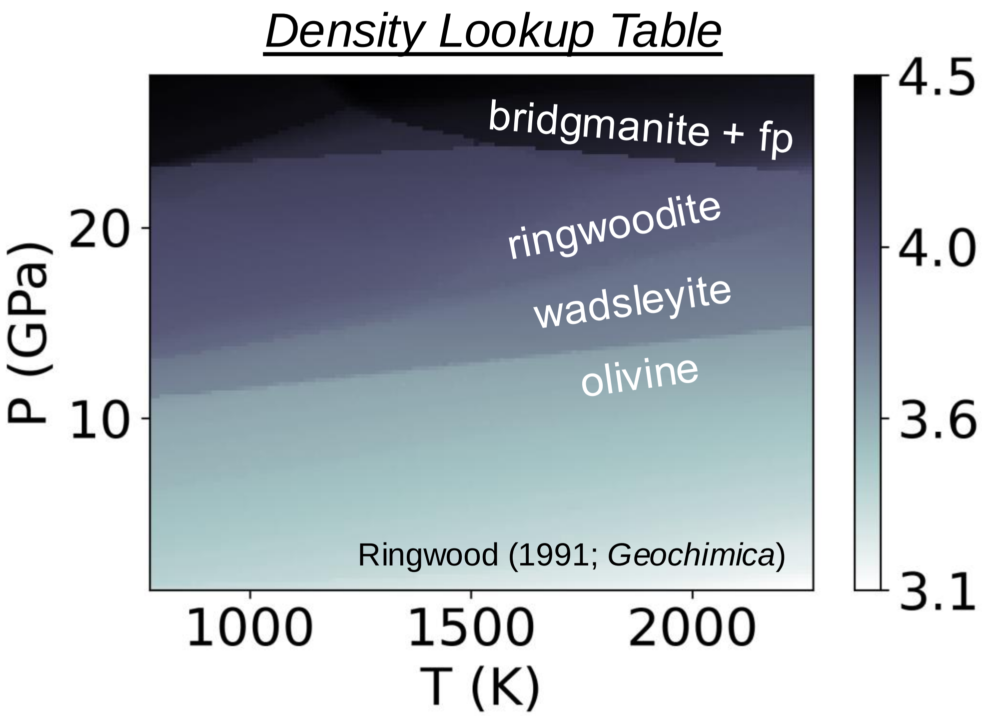



*Density Lookup Table*

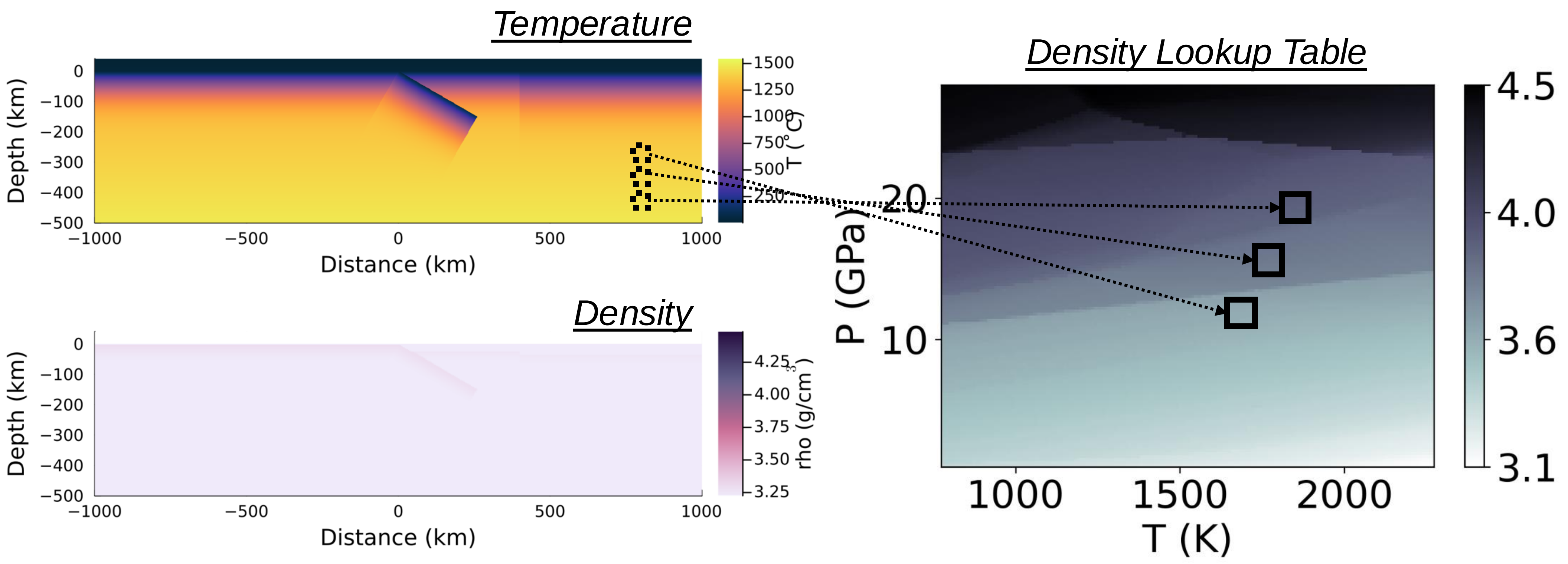


# Lookup Tables are effective at implementing phase changes

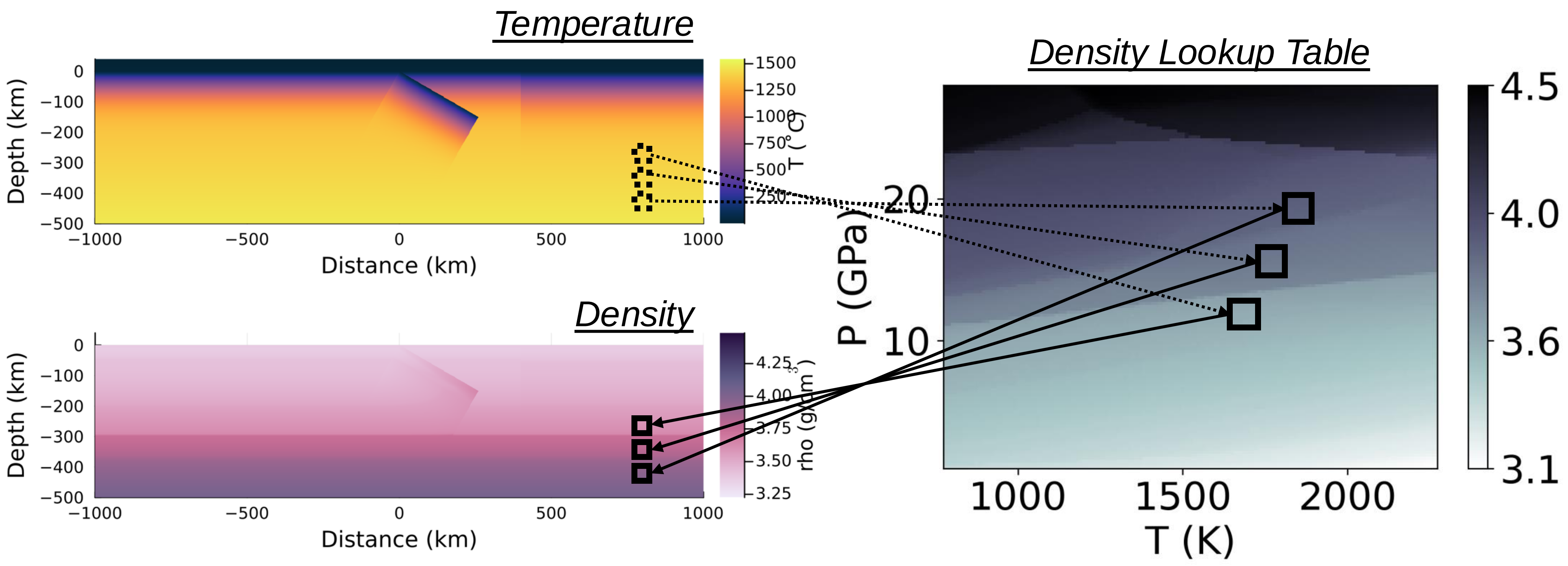


# Lookup Tables are effective at implementing phase changes



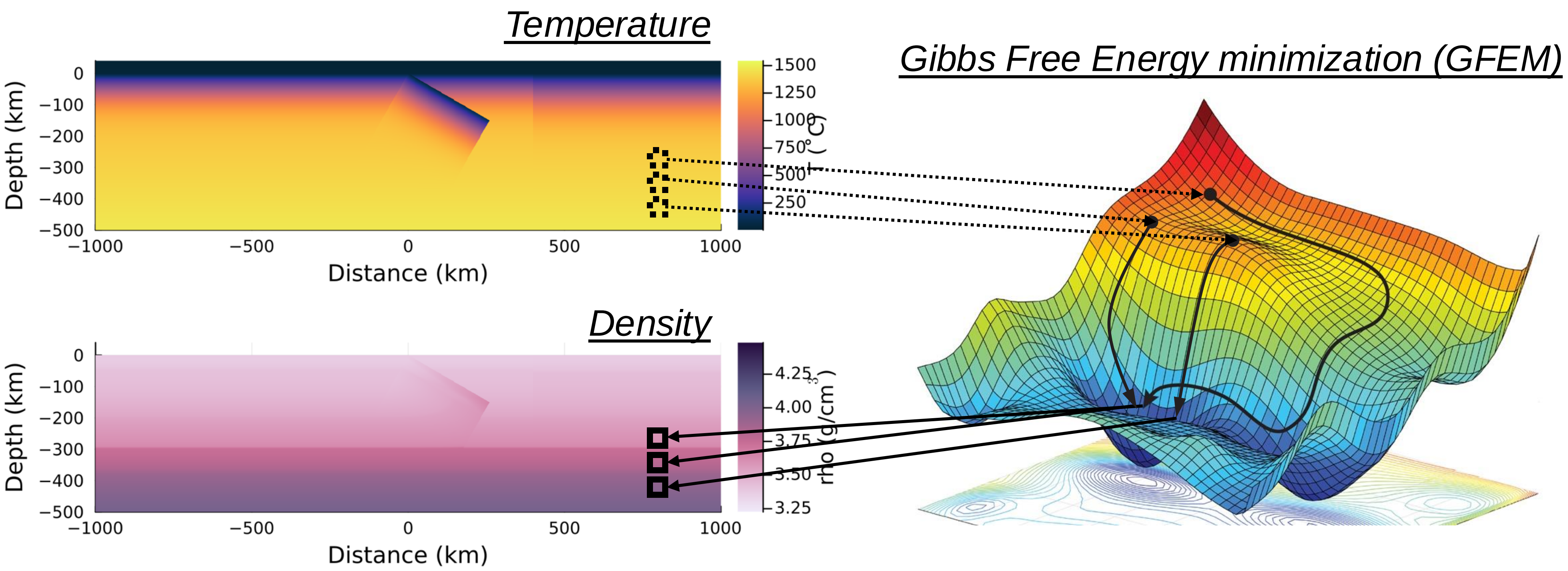
# Lookup Tables are effective at implementing phase changes




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

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

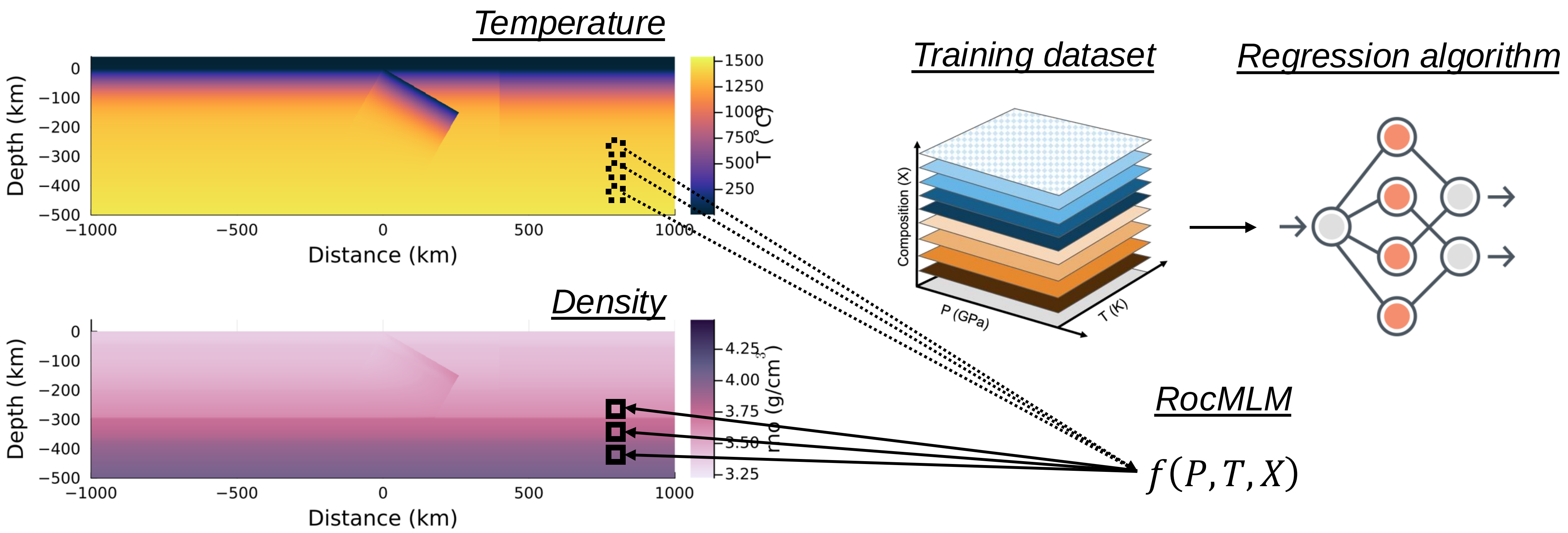
# *Phase equilibria modeling is more effective, but slow*




**+ :** *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

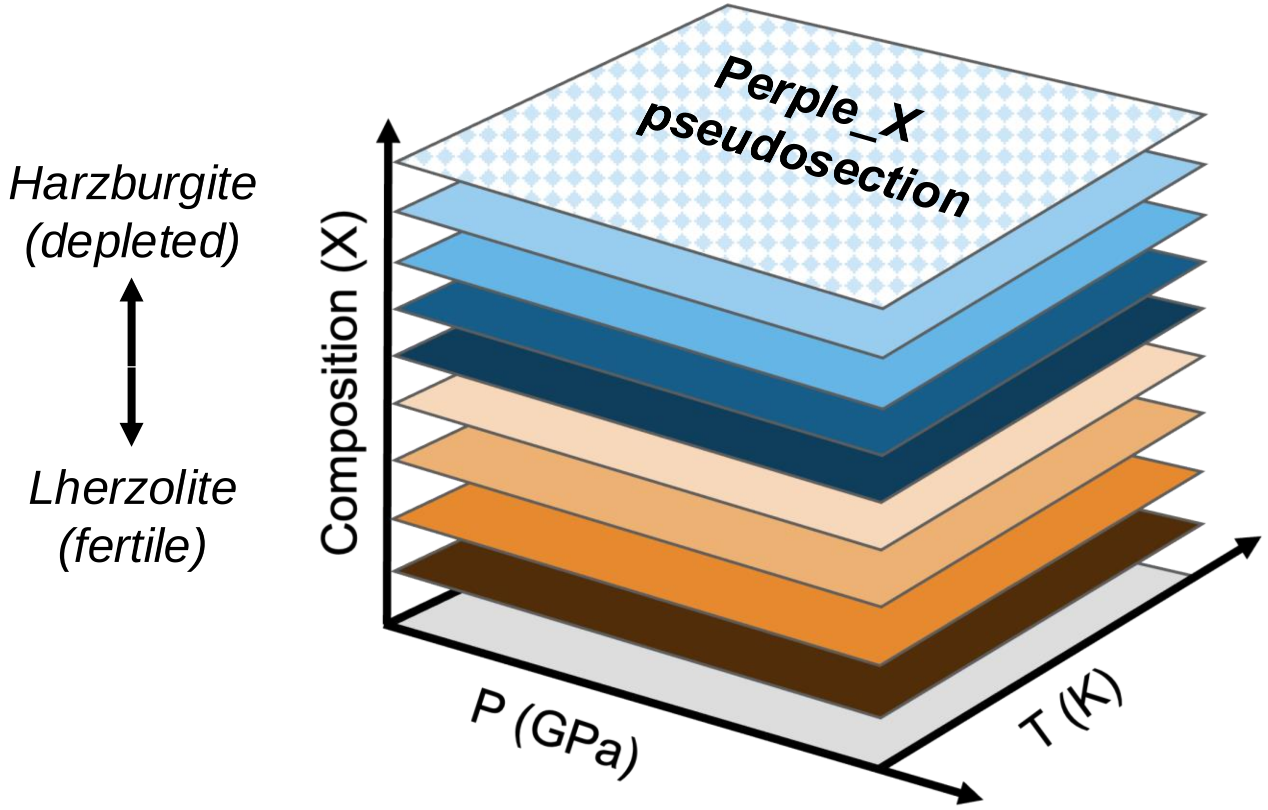



**+ :** *potentially much faster than Lookup Tables and GFEM*

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

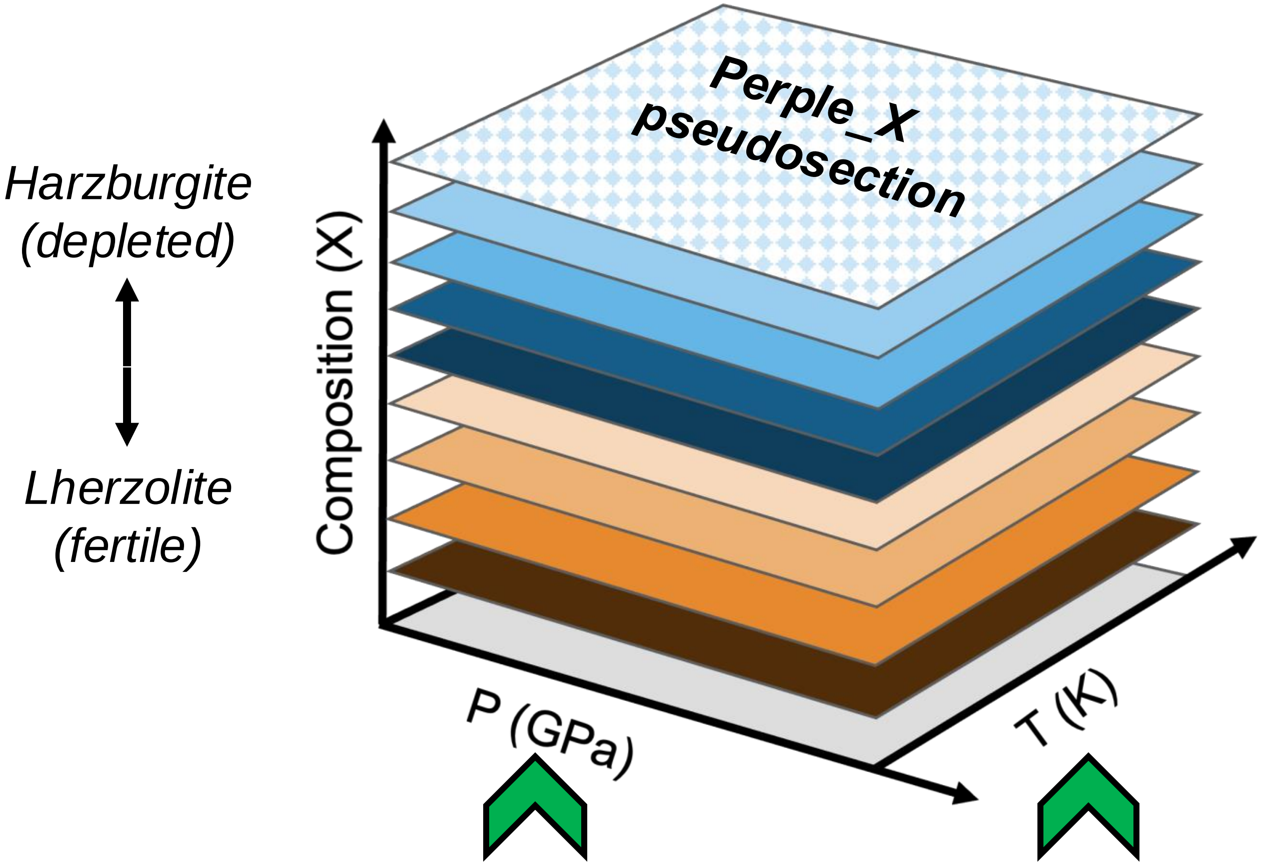
Kerswell et al. (2024; in review JGR:MLC)

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




Kerswell et al. (2024; in review JGR:MLC)

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

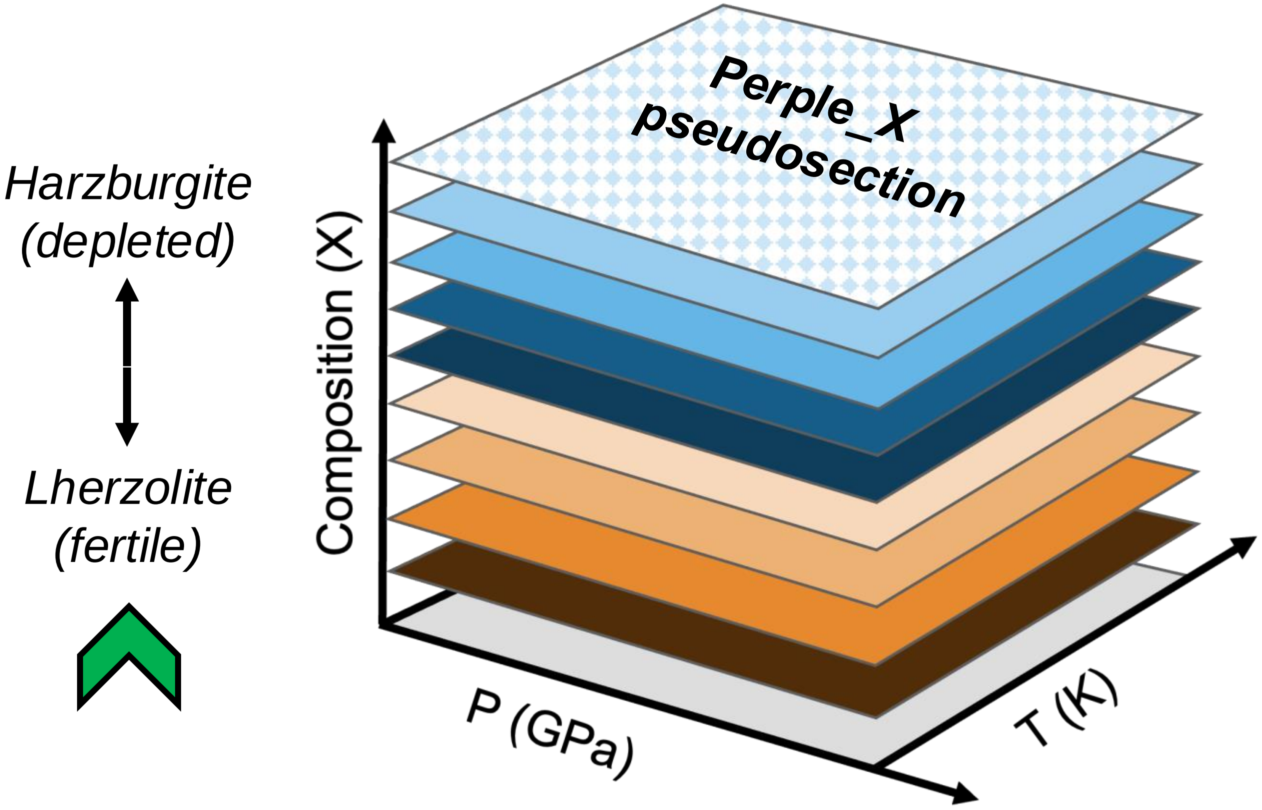



**P :** *1–28 GPa*

**T :** *773–2273 K*

Kerswell et al. (2024; in review JGR:MLC)

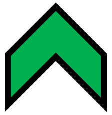
# *RocMLM training data were designed to be relevant for convection in the upper mantle*




***P :*** *1–28 GPa*

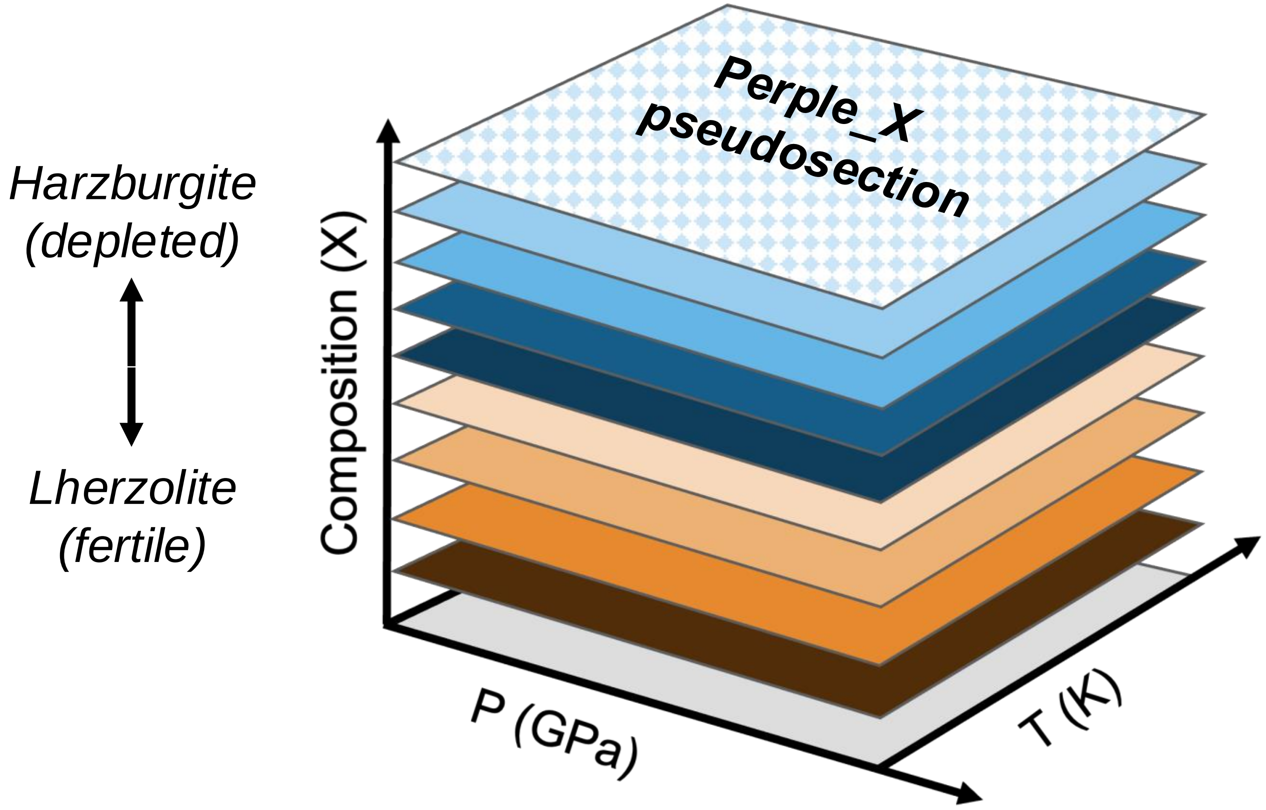
***T :*** *773–2273 K*

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



Kerswell et al. (2024; in review JGR:MLC)

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




***P :*** *1–28 GPa*

***T :*** *773–2273 K*

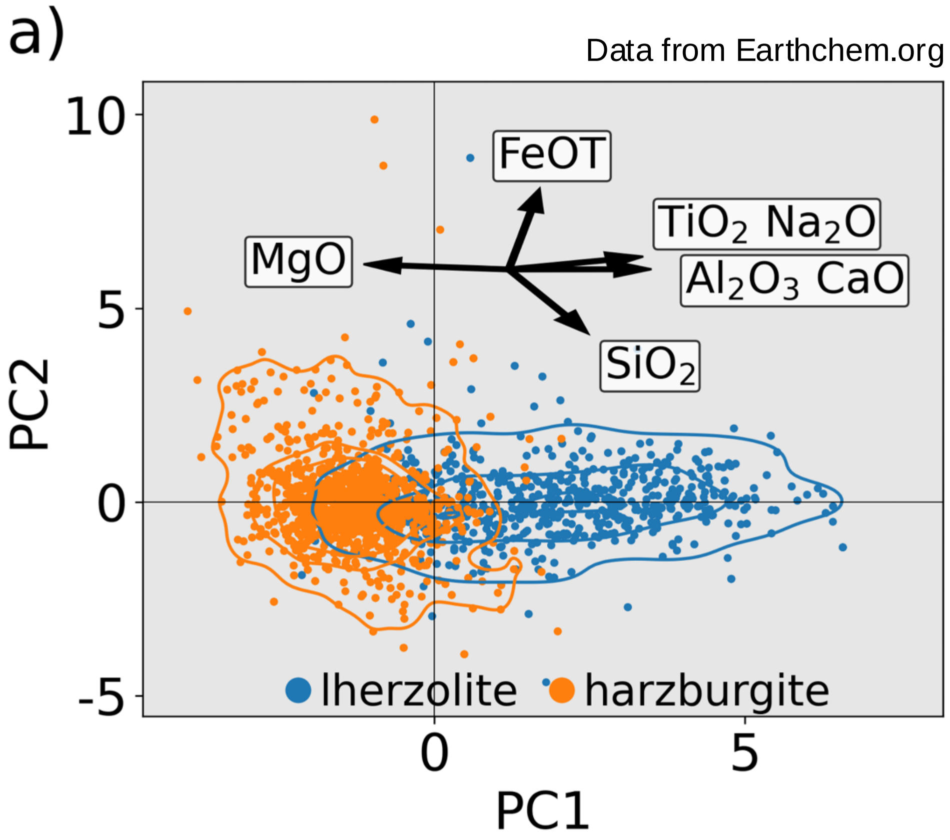
***X :*** *[ $Na_2O$-CaO-FeO-MgO-$Al_2O_3$-$SiO_2$ ]*

***Dimensions*** **:** *2 + 6 = 8*

***Need to reduce this !***

Kerswell et al. (2024; in review JGR:MLC)

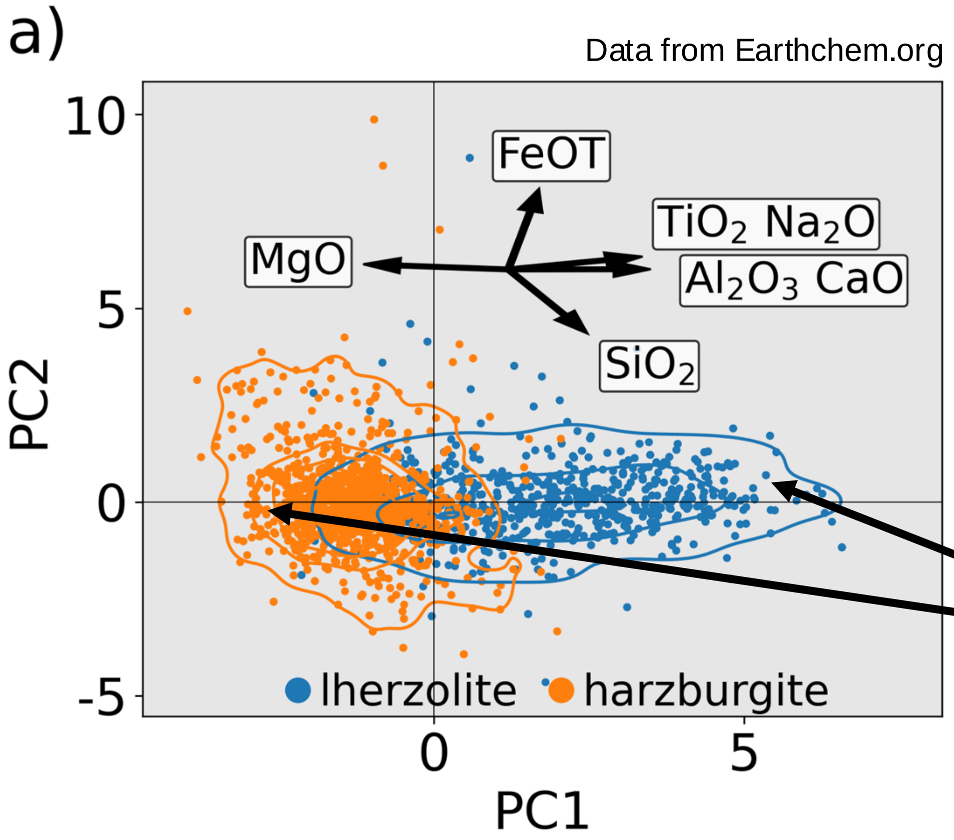
# *3111 natural peridotite samples were reduced by PCA to 2 "chemical" components: PC1 & PC2*




*PC loading vectors*

Kerswell et al. (2024; in review JGR:MLC)

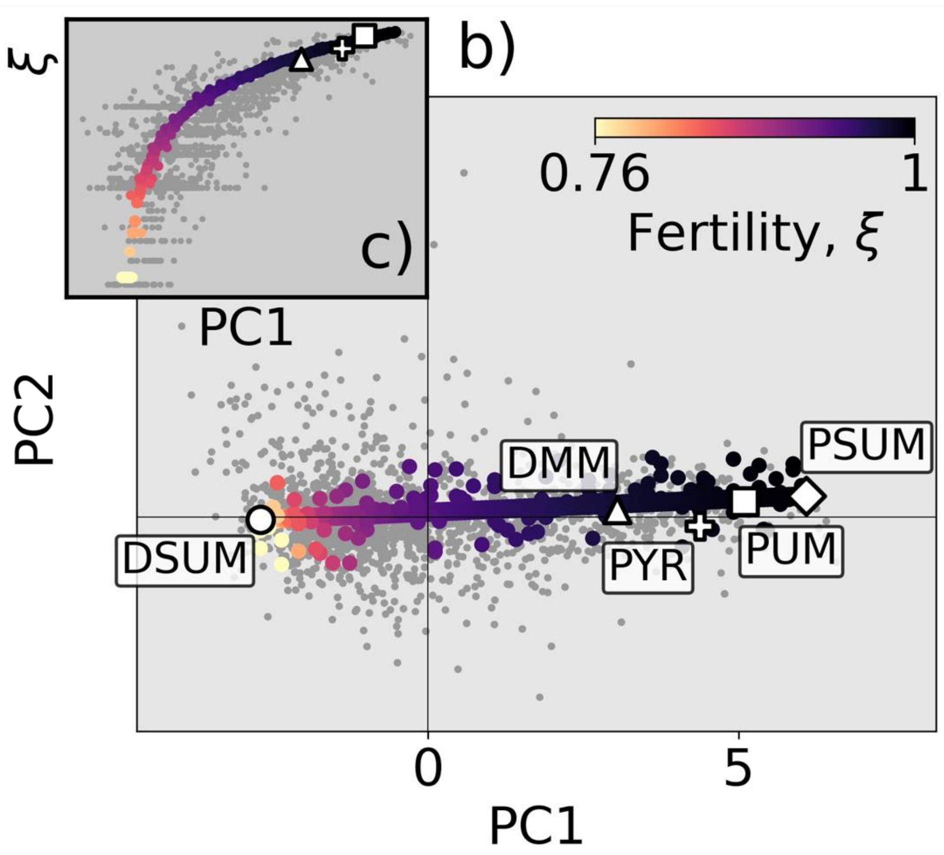
# *3111 natural peridotite samples were reduced by PCA to 2 "chemical" components: PC1 & PC2*




***<u>Hypothetical mantle endmembers</u>***

Kerswell et al. (2024; in review JGR:MLC)

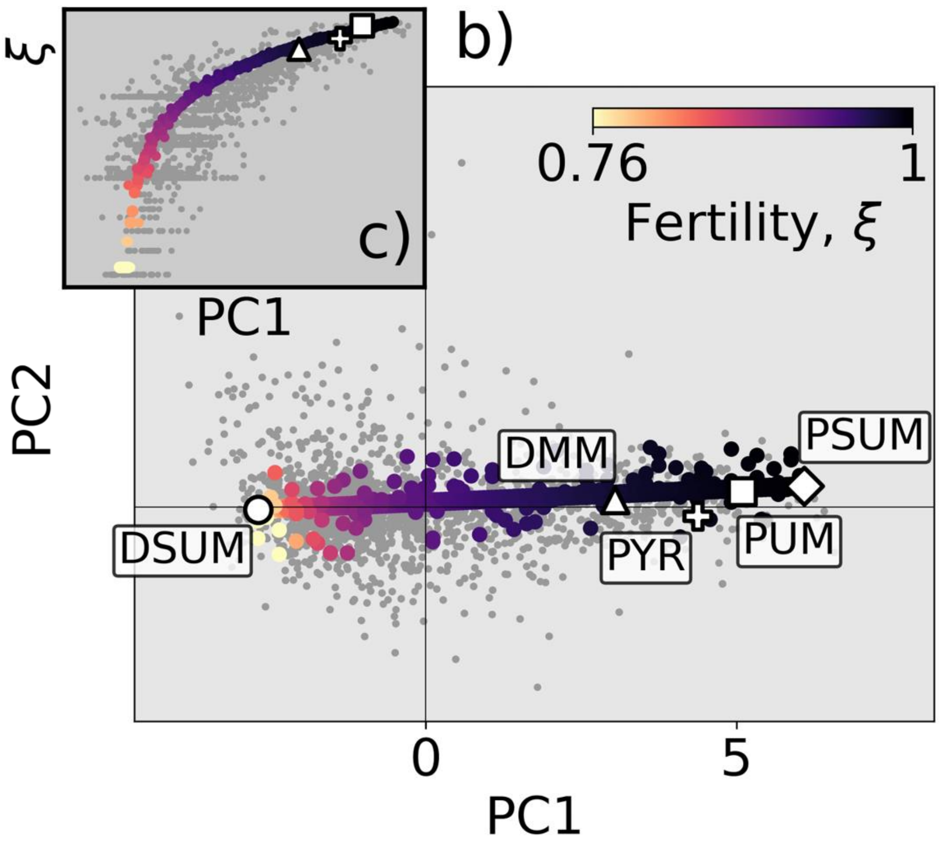
# *A hypothetical mixing array was used to sample synthetic bulk compositions for RocMLM training*




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

Kerswell et al. (2024; in review JGR:MLC)

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




*ξ Fertility Index parameter represents composition*

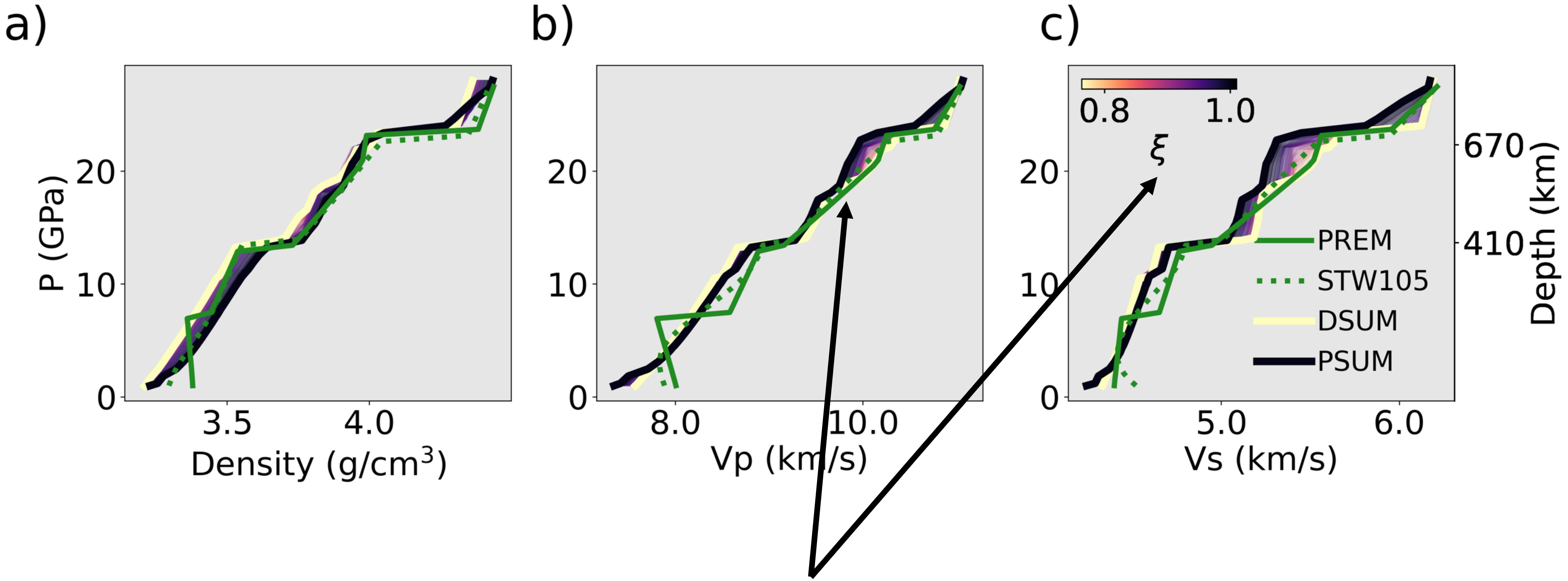
$\xi$ : [ $Na_2O$-$CaO$-$FeO$-$MgO$-$Al_2O_3$-$SiO_2$ ]

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

Shaw (1970; *Geochimica*)

Kerswell et al. (2024; in review JGR:MLC)

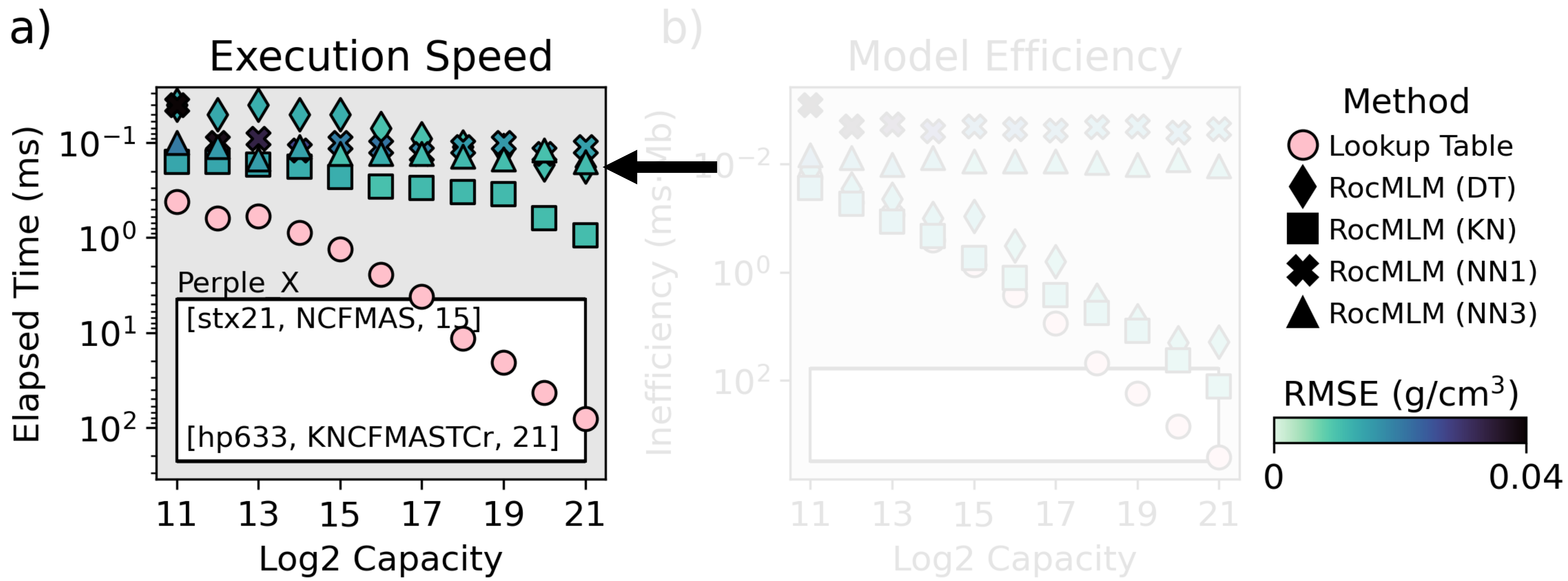
# *RocMLM training dataset contains $2^{21}$ (~2.1M) phase equilibria across an array of 128 mantle comp's from fertile → depleted*




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

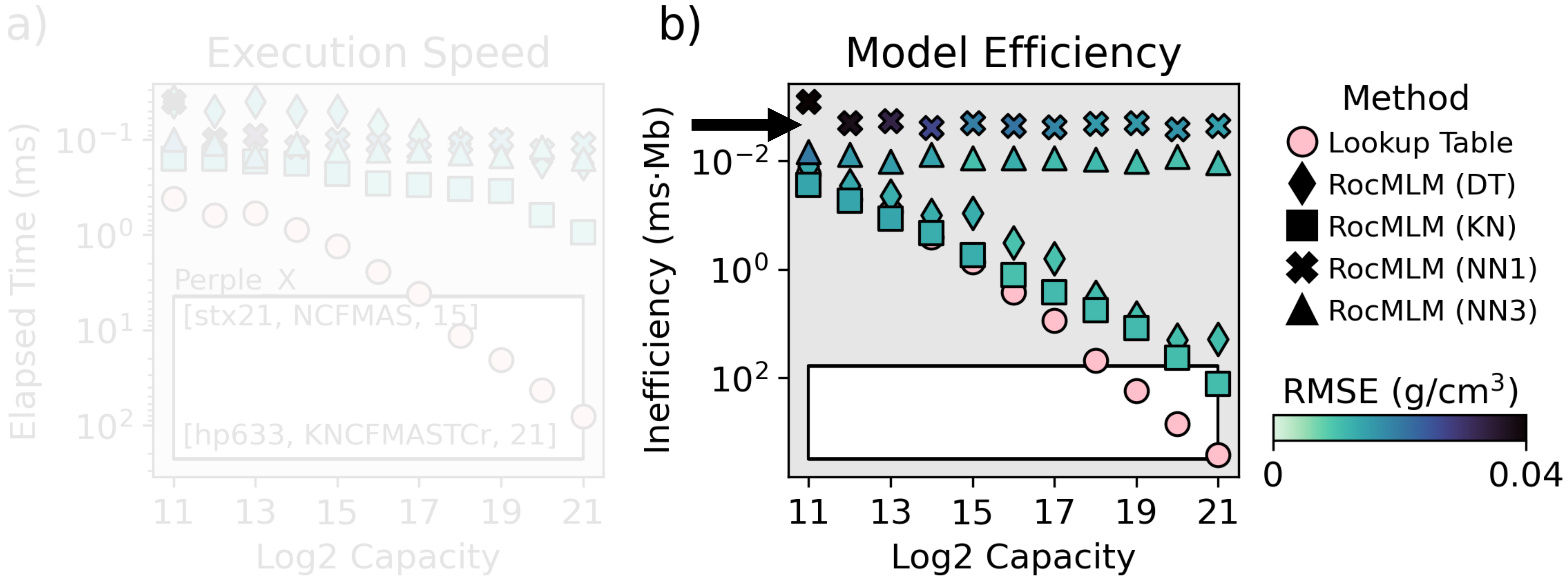
Kerswell et al. (2024; in review JGR:MLC)

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




Kerswell et al. (2024; in review JGR:MLC)

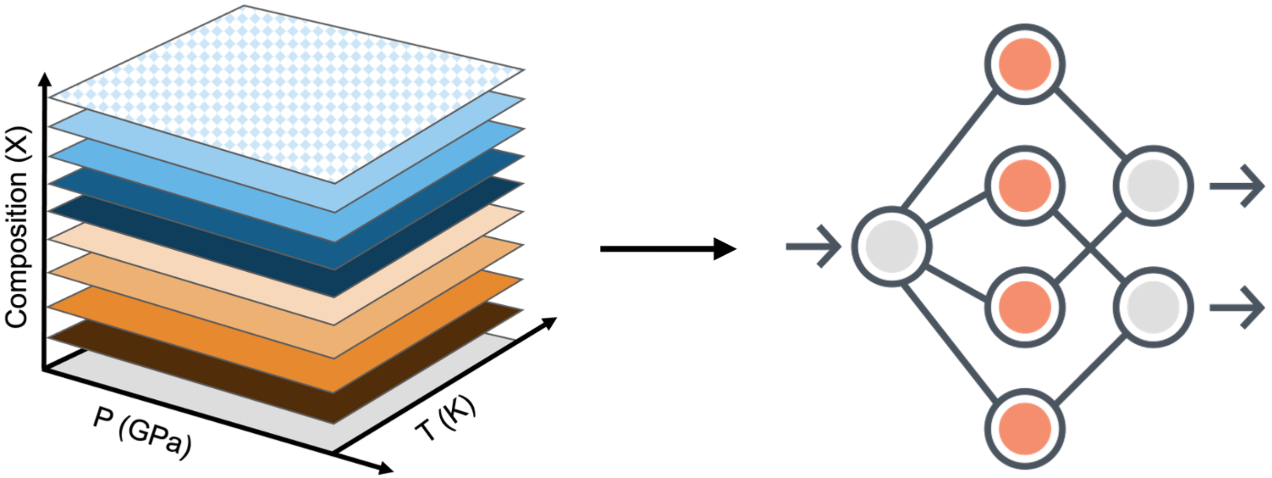
# *Neural Networks are more scalable than other algorithms*




Kerswell et al. (2024; in review JGR:MLC)

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

***Training dataset*** ***Regression algorithm***



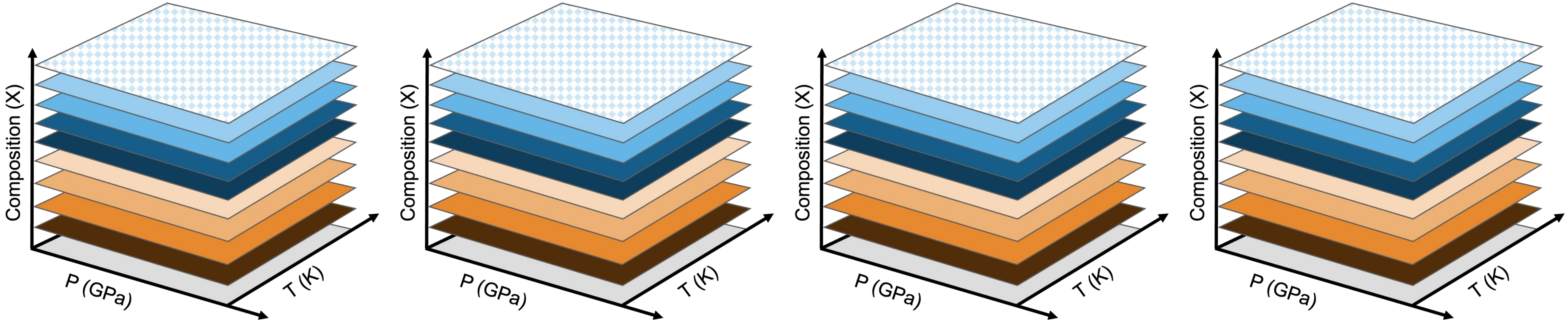

RocMLMs are $10^1$–$10^3$ times faster than GFEM programs and Lookup Tables

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?**

# RocMLM2: extending training dataset to include H2O



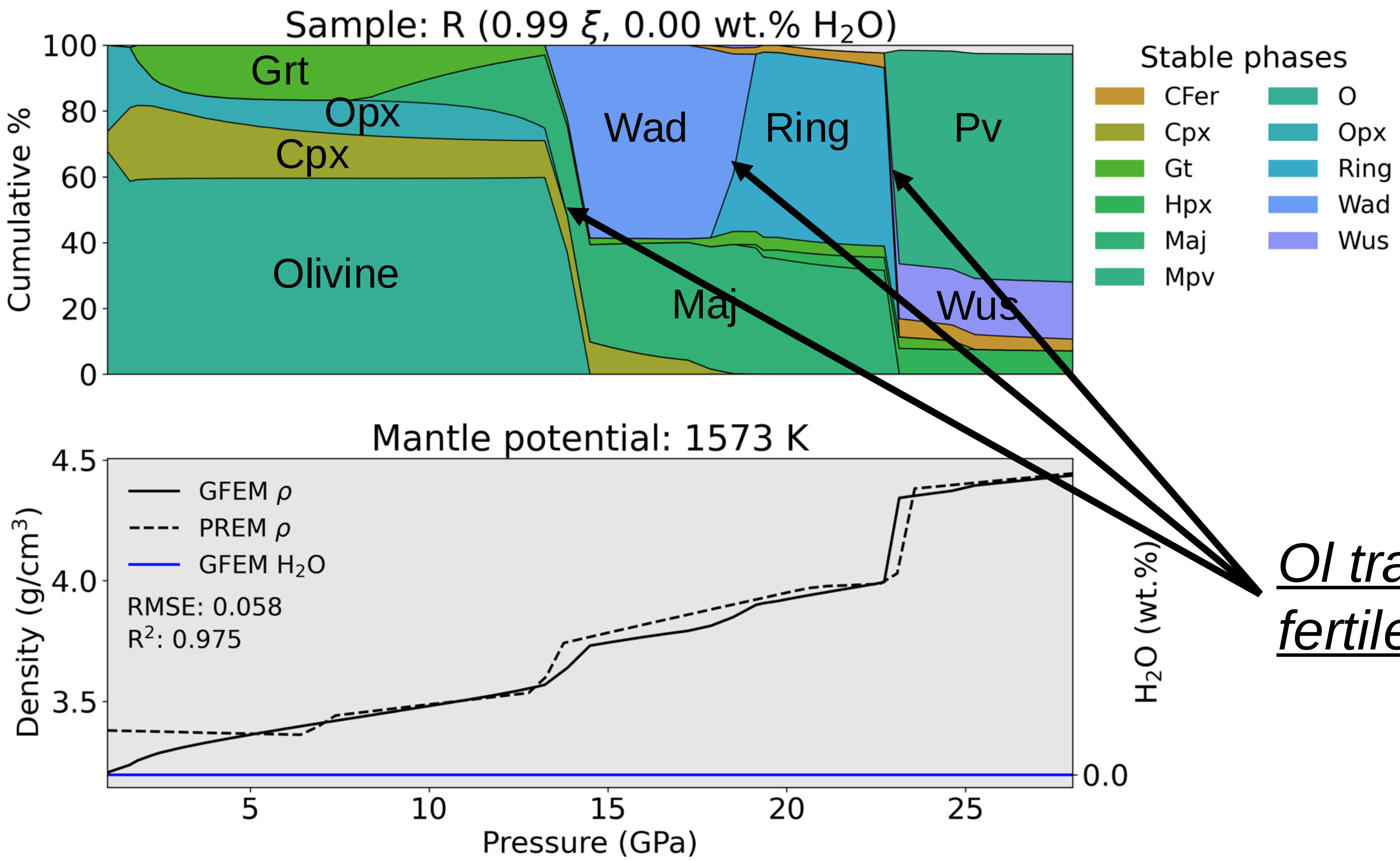

***0.1 %H2O*** … ***0.2 %H2O*** … ***1 %H2O*** … ***5 %H2O***

***P :*** *1–28 GPa* ***X :*** *[$Na_2O$-CaO-FeO-MgO-$Al_2O_3$-$SiO_2$-**$H_2O$**] → [ξ, H2O ]*

***T :*** *773–2273 K* **Dimensions :** 2 + 2 = 4 **Size :** *5,292,032*

Kerswell et al. (2024; in prep)

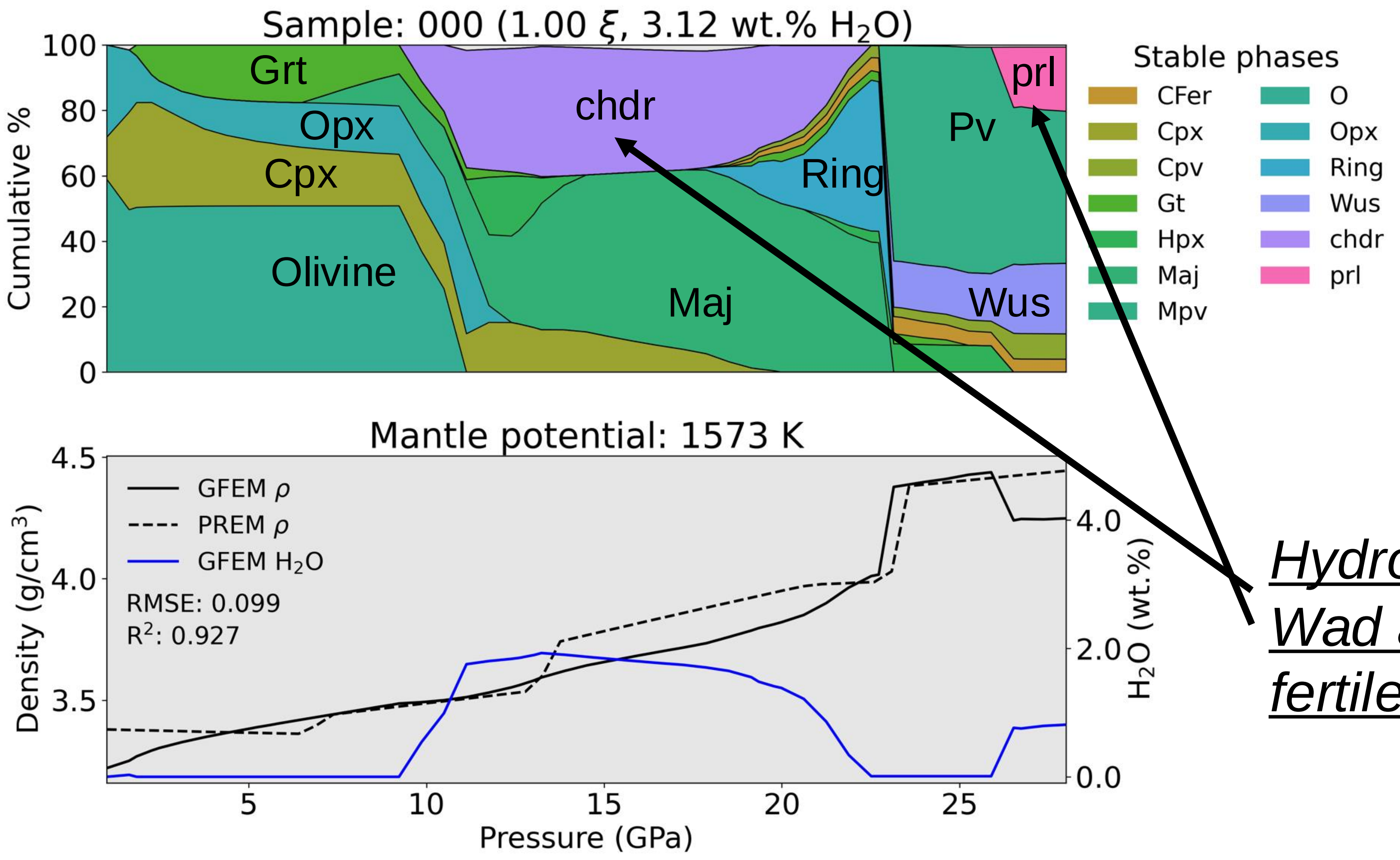
# Dry mantle compositions show sharp density discontinuities where Ol transforms into denser Mg-Fe-rich phases




***Ol transitions in a dry fertile mantle***

Kerswell et al. (2024; in prep)

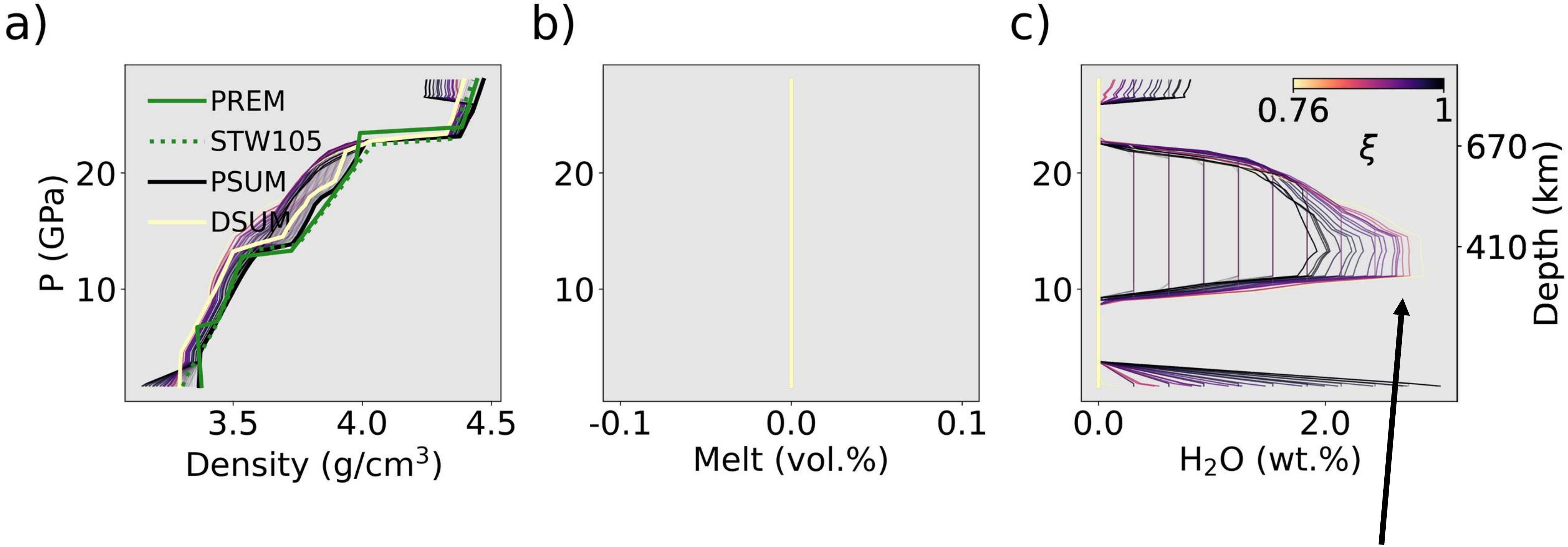
# Adding water hydrates the MTZ by stabilizing high-density Mg silicate minerals




***Hydrous phases replace Wad and Pv in a wet fertile mantle***

Kerswell et al. (2024; in prep)

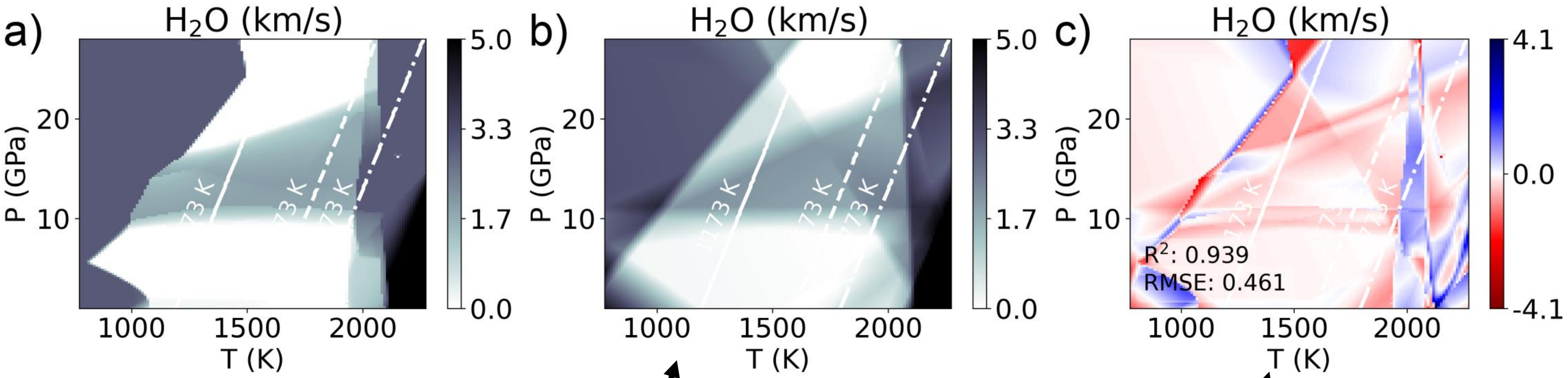
# Adding water smooths out sharp density discontinuities within the MTZ but does not produce melting




*<u>More depleted mantle compositions can potentially store more water</u>*

Kerswell et al. (2024; in prep)

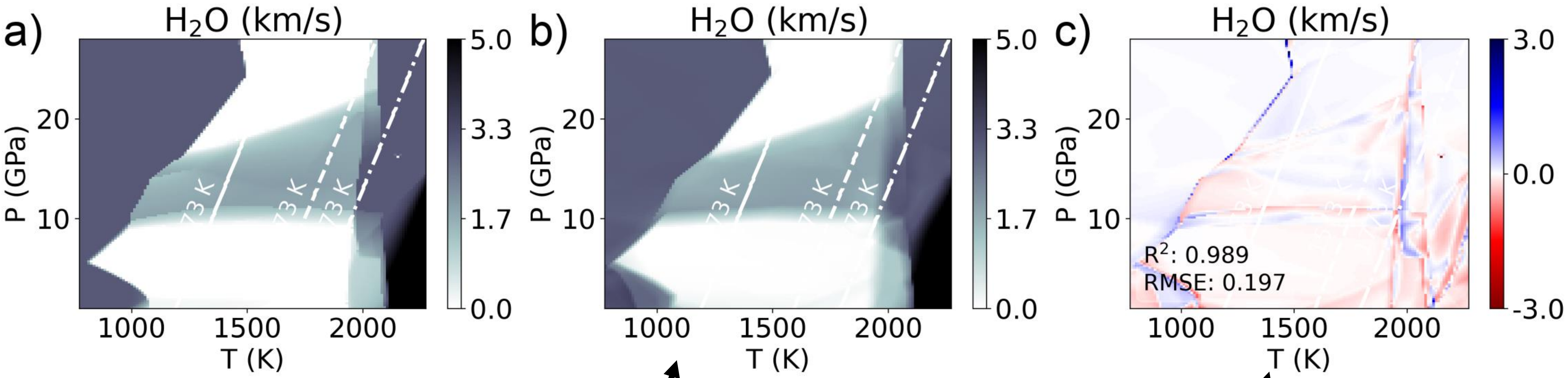
# Some ML algorithms (small NN) show bias due to strongly irregular training data distributions




*<u>Artefacts induced from density distribution = large residuals</u>*

Kerswell et al. (2024; in prep)

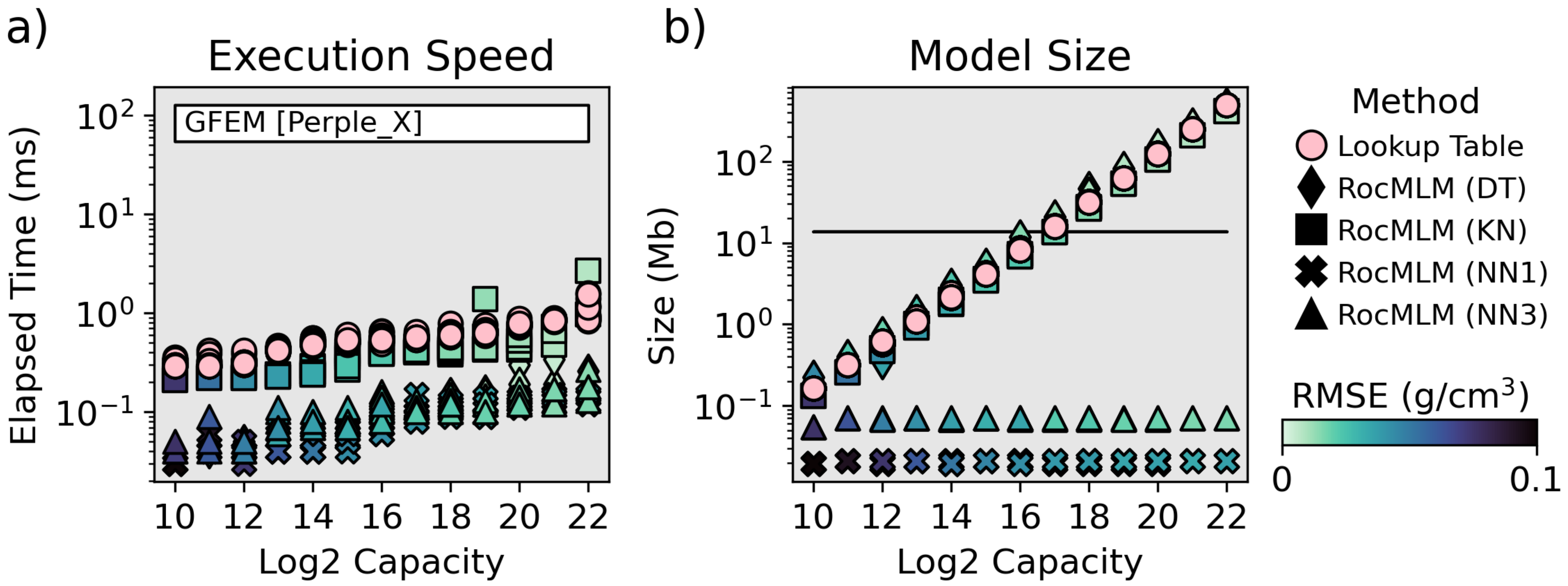
# Larger NN (and other ML algorithms) show better predictions and higher internal accuracies




*Artefacts from density distribution disappear = small residuals*

Kerswell et al. (2024; in prep)

# RocMLM performance continues to exceed GFEM and Lookup Table approaches




Kerswell et al. (2024; in prep)