RocMLMs: Predicting Rock Properties through Machine Learning Models

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Introduction

- *Phase transformations strongly impact mantle convection*
- *Lookup Tables and GFEM programs like Perple_X are effective at implementing phase changes, but too slow for high-resolution geodynamic simulations*
- *We developed RocMLMs to emulate dynamic phase changes instead of using Lookup Tables or GFEM programs*
- ***We hypothesized that RocMLMs will be faster than Lookup Tables and GFEM programs, while maintaining accuracy***

Methods

- *RocMLM training data were designed to be relevant for convection in the dry upper mantle (1–28 GPa, 773–2273 K, lherzolite to harzburgite)*
- *3111 natural peridotite samples were used to define a mixing array between hypothetical mantle endmember compositions DSUM & PSUM*
- *128 synthetic bulk compositions were sampled from the hypothetical mixing array for the RocMLM training dataset*
- ***Different ML algorithms (DT, KN, NN1, NN2, NN3) were trained on 2^{21} (~2.1M) phase equilibria calculations to predict density, Vp, and Vs at upper mantle PTX conditions***

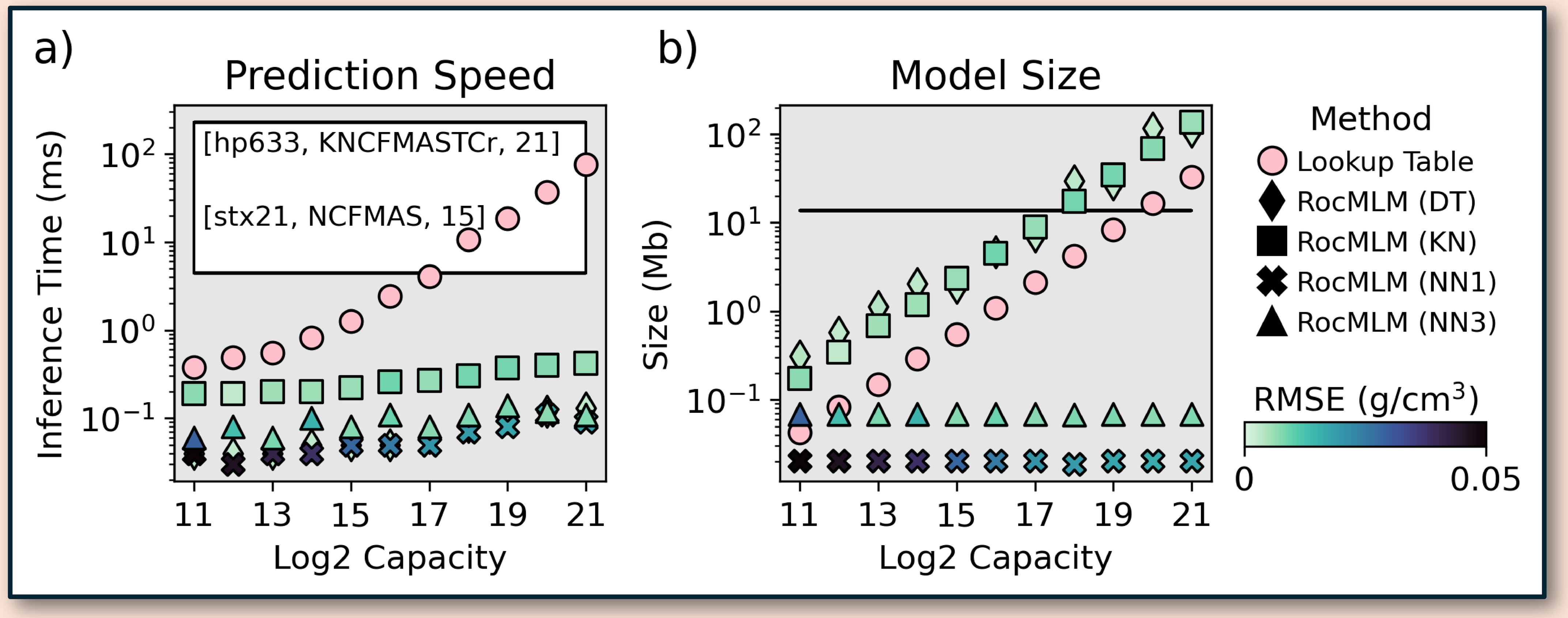
Results

- ***RocMLMs are 10^1–10^3 times faster than Lookup Tables and Perple_X***
- *RocMLM training data show good agreement with PREM and STW105 for an average mantle geotherm*

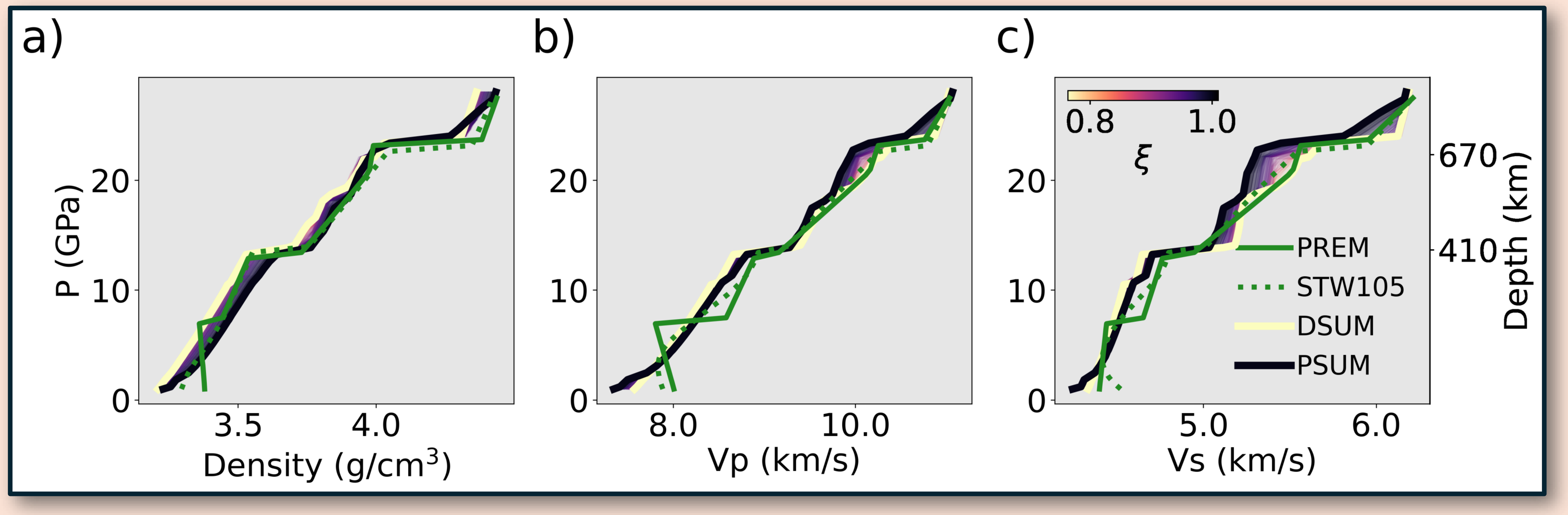
Conclusions

- ***RocMLM prediction speed makes thermodynamically self-consistent mantle convection within high-resolution numerical geodynamic models practical for the first time***
- *RocMLMs trained with moderately deep (3 hidden layers) NNs are more robust and efficient compared other ML algorithms, and are therefore the most practical models for coupling with numerical geodynamic codes*

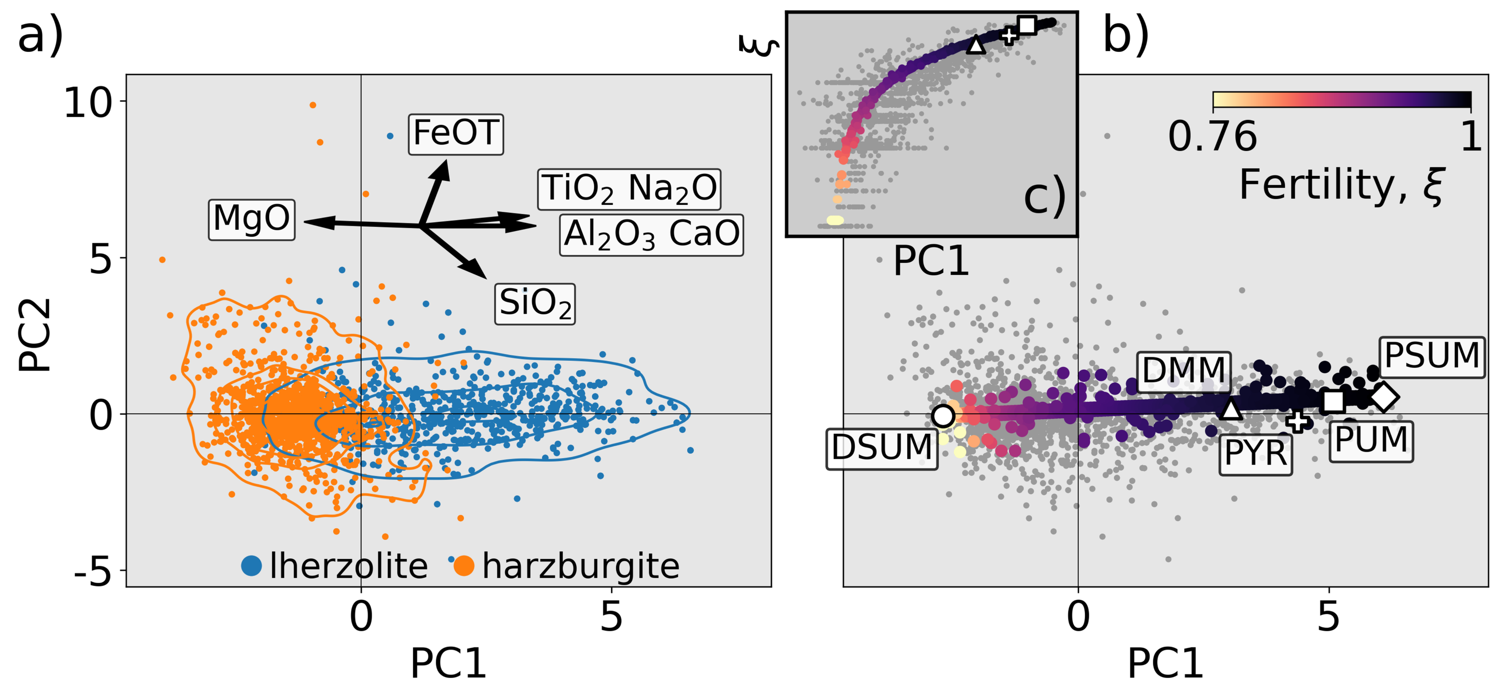
RocMLMs predict density and elastic properties of dry mantle rocks with high accuracy and are up to 10^1–10^3 faster than commonly used methods: Lookup Tables and Perple_X



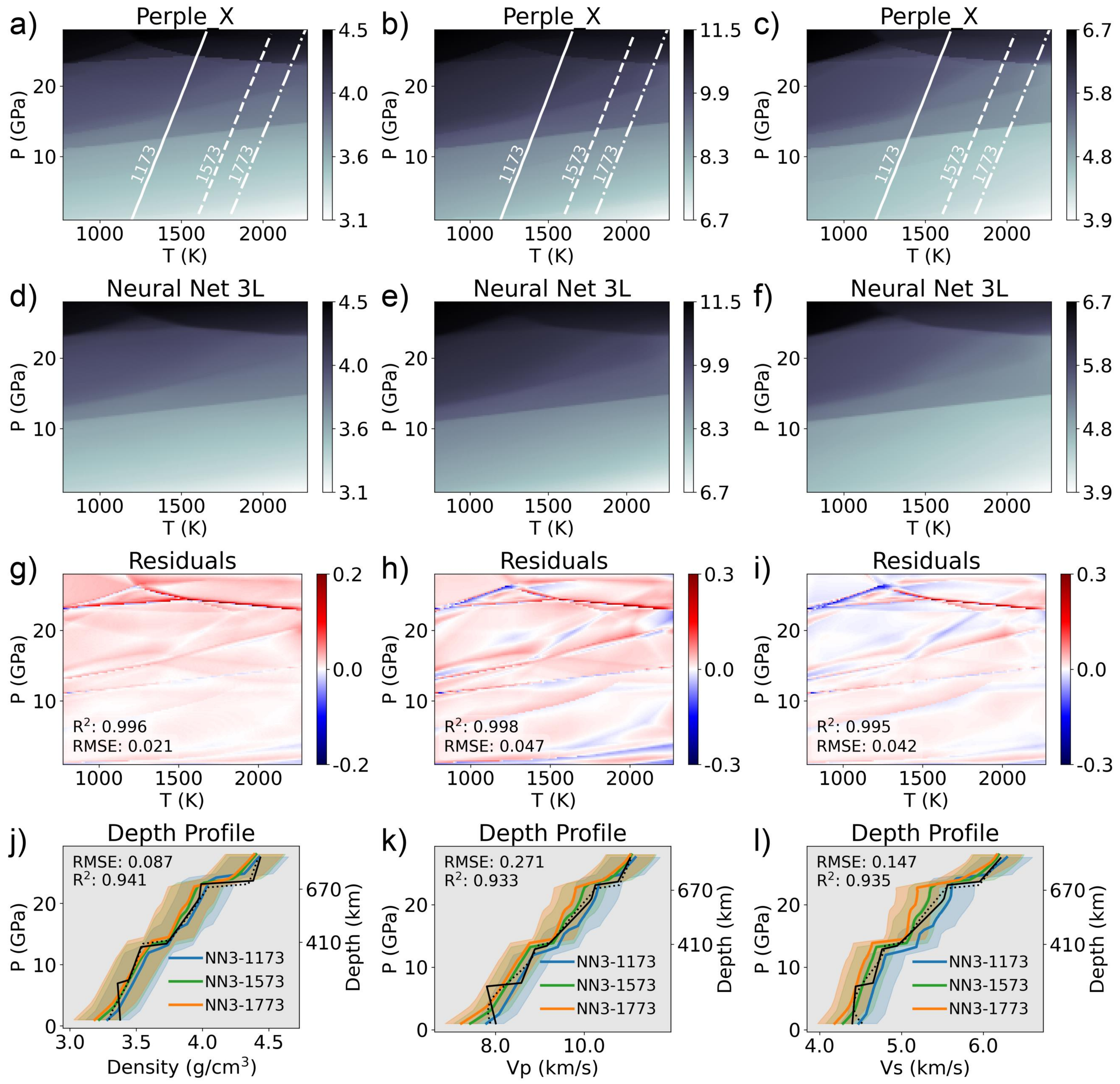
Computational efficiency of various approaches in terms of prediction speed (a) and model size (b). "Capacity" (x-axis) is a proxy for the petrological "knowledge", or predictive capabilities, of Lookup Tables and RocMLMs. The white region in (a) indicates GFEM prediction speed for different Perple_X configurations (thermodynamic dataset, chemical system, and number of solution phases are indicated in square brackets). GFEM model size is constant (bold black line). stx21: Stixrude and Lithgow-Bertelloni (2022), hp633: Holland and Powell (2011) updated in Holland et al. (2018). Perple_X was run without multilevel grid refinement. RMSE is measured using kfold cross-validation with k=5.



Depth profiles of RocMLM training data along a 1573 K mantle adiabat showing the sensitivities of thermodynamic estimates of density (a), Vp (b), and Vs (c) to changes in bulk mantle composition (as represented by the Fertility Index, ξ). Geophysical profiles PREM and STW105 (green lines) and the profiles of synthetic mantle end-member compositions PSUM and DSUM (thick colored lines) are shown for reference. Thin colored lines show profiles for the entire range of RocMLM training data.



PC1-PC2 diagrams showing the standardized geochemical dataset of natural peridotite samples (a) and a mixing array between hypothetical end-member mantle compositions Primitive Synthetic Upper Mantle (PSUM) and Depleted Synthetic Upper Mantle (DSUM, b). Black arrows in (a) indicate PCA loading vectors. Colored data points in (b) are the synthetic mantle compositions used to train RocMLMs, which were sampled independently from the natural peridotite samples (gray data points). The inset (c) shows how the Fertility Index (ξ) changes nonlinearly with PC1. DMM, PUM, and PYR are Workman and Hart (2005), Sun and McDonough (1989), and Green (1979), respectively.



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Open Research

All data, code, and relevant information for reproducing this work are published at github.com/buchanankerswell/kerswell_et_al_rocmlm and archived on the Open Science Framework data repository doi.org/10.17605/OSF.IO/K23TB. All code is MIT Licensed and free for use and distribution (see license details). Reference models PREM and STW105 are freely available from the Incorporated Research Institutions for Seismology Earth Model Collaboration (Trabant et al., 2012). All computations were made using CPUs of a Macbook Pro (2022; M2 chip) with macOS 14.5 and using Python 3.12.3.

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