High-Pressure Phase Diagrams of H$_2$O, CH$_4$, and NH$_3$ for Ice Giant Interiors: A Machine-Learning Global Inversion from Experimental and Theoretical Data. Junjie Dong$^{1,2}$ and Rebecca A. Fischer$^1$, 1Department of Earth and Planetary Sciences, Harvard University, 2Department of the History of Science, Harvard University. Correspondence to: Junjie Dong (junjiedong@g.harvard.edu).

Ice giants in our Solar System, Uranus and Neptune, are thought to have interiors composed of a mixture of rock and ice, with the ice layer composed primarily of water (H$_2$O), methane (CH$_4$), and ammonia (NH$_3$) [1]. A complete characterization of the structure and evolution of the two ice giants requires accurate high-pressure phase diagrams for H$_2$O, CH$_4$, and NH$_3$ that describe their solid–solid phase transitions, reactions, and melting.

To date, the phase equilibria of all these ice components have been studied up to multi-megabar conditions using high-pressure experiments and first-principles simulations [e.g., 2–4]. However, the exact stability field and melting temperature of each ice phase remains controversial. This is partly due to the fact that traditional approaches to determining high-pressure phase diagrams, which involve free-hand drawing from a subset of experimental or theoretical data, are subject to significant biases and do not quantitatively account for uncertainties across data sets [5].

In this study, we applied a novel inversion strategy to construct pressure–temperature ($P$–$T$) phase diagrams of H$_2$O, CH$_4$, and NH$_3$ up to 1000 GPa. Our approach employs a machine-learning global inversion method based on multi-class logistic regression and supervised learning algorithms [5], which provides comprehensive statistical evaluation across experimental and numerical datasets, resulting in more accurate phase diagrams.

Here, we demonstrate the effectiveness of our inversion strategy through a case study on the $P$–$T$ phase diagram of H$_2$O (Fig. 1a), which is critical for understanding the structure and evolution of ice giants. For example, the H$_2$O melting curve likely determines the location of the fluid–crystalline boundary (FCB) in the ice layer of ice giants and indicates the radius of a growing frozen core as the planet cools (Fig. 1b–c). A thermal boundary layer would develop at the FCB [6], and the size of the frozen core affects the heat trapped in the interior and may contribute to Uranus’ low luminosity. In addition, the size of the frozen core affects the orbits of Uranus’ moons. The H$_2$O melting curve provided here controls the size of the frozen core and thus plays an important role in the thermal and tidal evolution of the ice giants.


Figure 1: $P$–$T$ phase diagram of H$_2$O. (a) Global inversion of a multi-fidelity data collection (experimental and theoretical data combined). The different colored regions correspond to different high-pressure phases of H$_2$O. This pilot test successfully identified the superionic transitions and melting curve of H$_2$O, and their $P$–$T$ conditions were statistically optimized. (b–c) The fluid–crystalline boundary (FCB) in the interior of Uranus occurs where the H$_2$O melting curve intersects the temperature profile of the planet. Early Uranus had a higher average temperature. As the planet cooled, the FCB shifted to lower pressures and temperatures, causing the frozen icy core to grow over time.