Uranus as a Water World: Utilizing Machine Learning to Predict Conditions of Ice Phases in Extreme Environments

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Research Objective

With this study, we look to enhance the current understanding of the phase conditions of ice and the melting curve. Therefore, we can apply this knowledge to the systems of Uranus and other icy celestial bodies.

Introduction

What We Do (And Don't) Know About Uranus

- Uranus is the second outermost planetary body in our solar system.
- Unique characteristics include its tilted axis, offset magnetic field, and unknown interior.
- The only visit to Uranus was in 1986 with Voyager 2.
- NASA's upcoming mission, the Uranus Orbiter and Probe (UOP), is scheduled for launch around 2032.

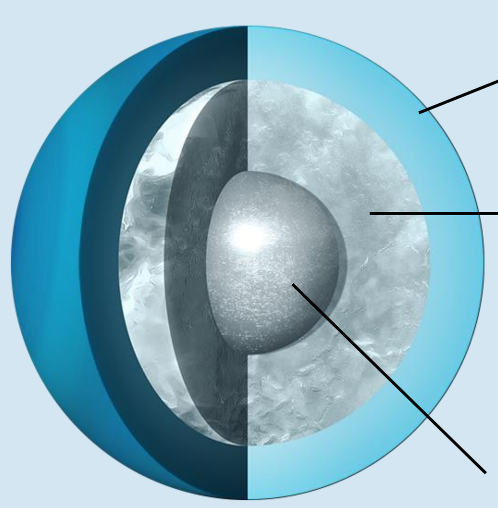

Fig 1. Current model of Uranus[1].

Crystalline Ice Phases

The most common phase of ice is Ice-Ih. However, when higher pressures are introduced, such as those within a planet, the water molecules can be arranged differently.

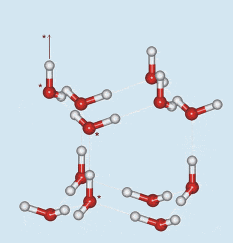

Fig 2. Structure of Ice-Ih[2].

Results

Melting Curve of Ice Phases

- The result of training the machine learning code with collected experimental data (Fig 3).
- Different ice phases can be observed at different pressure and temperature parameters.

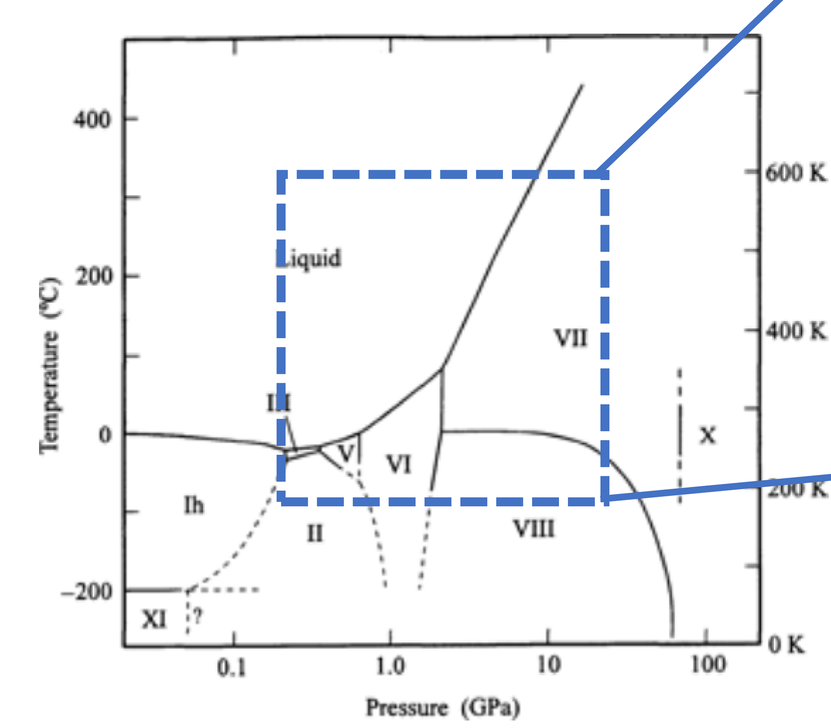

Fig 4. Phase diagram showing the stable phases of the ice-water system drawn from past beliefs about phase boundaries[3]. The dotted area is the region focused on in our project.

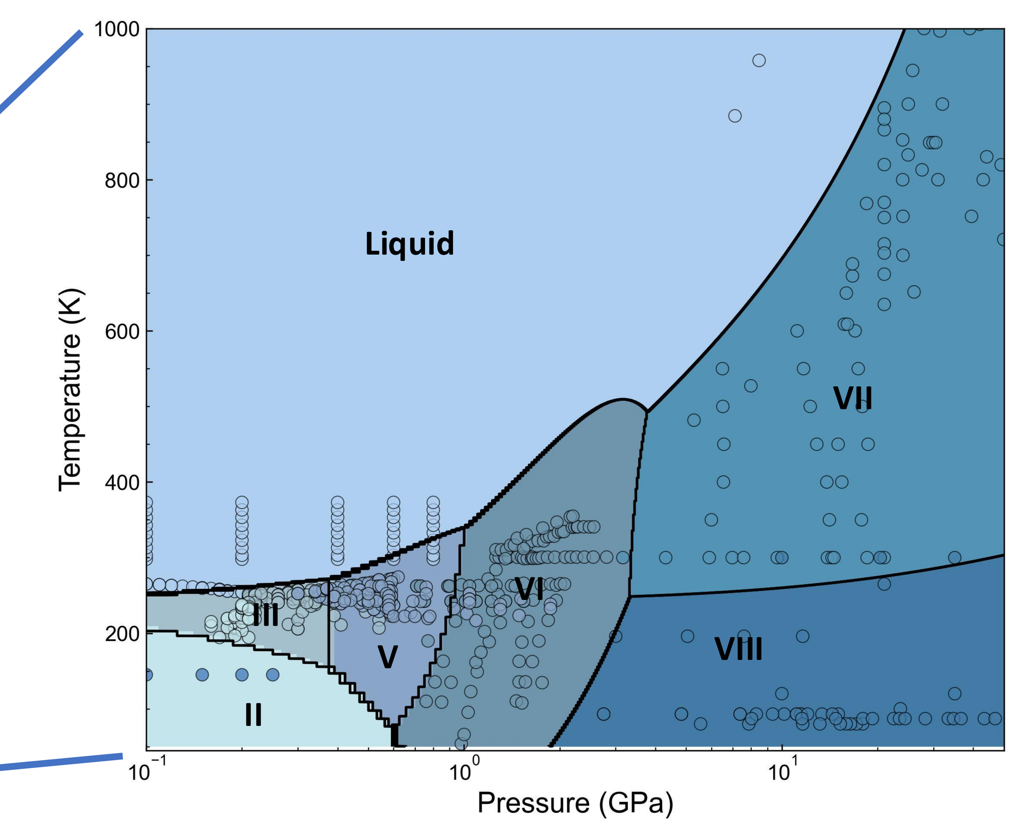

Fig 3. Machine learning prediction of melting curve phase diagram showing the stable phases of the ice-water system on a logarithmic scale of pressure.

Phase Structures Seen in Resulting Phase Diagram

- On the molecular level, differences between ices phases are visual and physical.

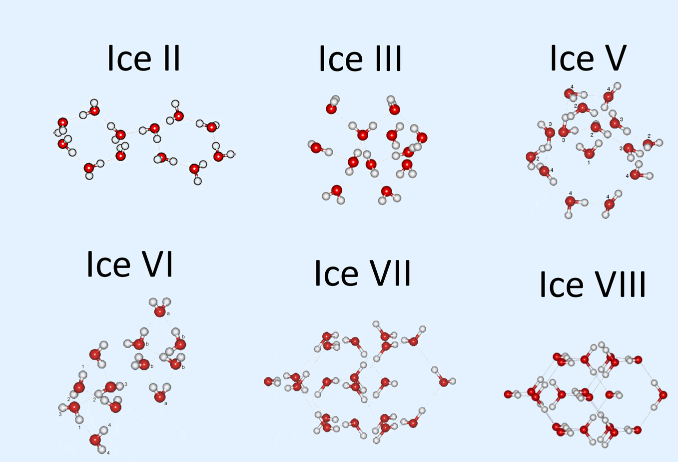

Fig 5. Structures of other ice phases[2].

Methodology

Finding Melting Curve Using Machine Learning

Experimental data was reviewed and compiled from literature covering various ice phases. Then, supervised machine learning techniques were utilized to define the phase equilibrium.

Multi-Class Logistic Regression

This approach trains separate binary classifiers for each phase, selecting the one with the highest predicted probability for classification.

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

Sigmoid function for logistic regression algorithms.

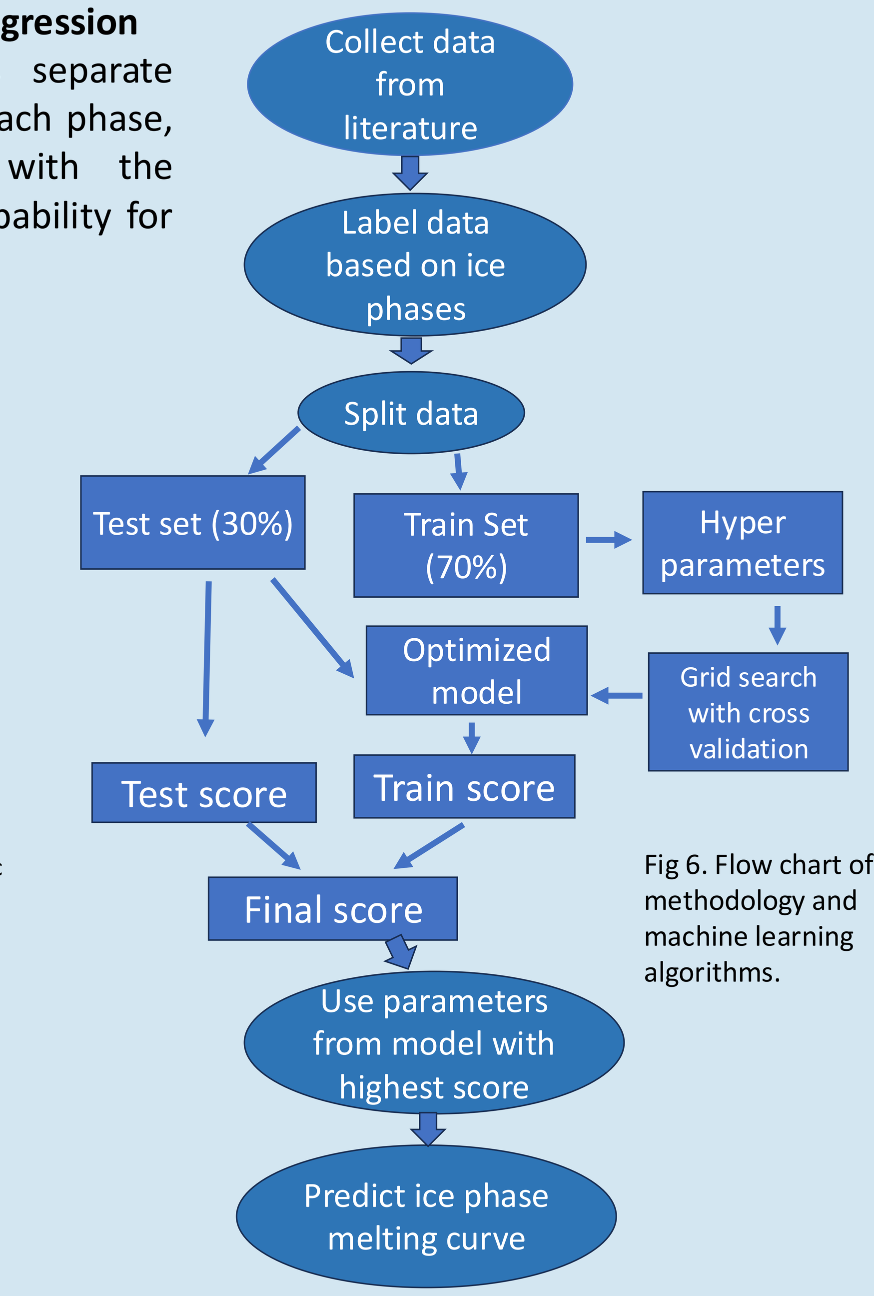

Fig 6. Flow chart of methodology and machine learning algorithms.

Cross-Validation

Cross-validation, specifically k-fold cross-validation, was used to evaluate model performance. Our dataset was split into k subsets to train and test the model. The model with the best fit was selected to construct the final phase diagram.

Best Parameters

The algorithm attempts to find the best machine learning parameters for predicting the melting curve. For logistic regression, these parameters were tested and values for the model with the best fit are as follows:

Polynomial Degree = 2
Regularization strength = 1000
Class Weight = None
Multi-Class = One vs. Rest
Penalty = L1 (Lasso Regularization)
Solver = Liblinear

With these parameters, an F1-Score is calculated, which is used for selecting the best model. The current model uses the parameters above.

Discussion

Uranus

- Most of the middle layer of Uranus is water in liquid form, with Ice VII forming deeper within the planet.
- Can expect an ocean sitting on top of ice.
  - Ice VII is 1.5 times denser than Ice-Ih.
- Ice VII is observed in shock wave experiments.

Going Further

- Many exoplanets are rich in water.
- Lower pressure (1-10 GPa) ice phases are especially relevant in Icy Moons.
  - Lower dielectric constants and lower solubility.
  - These ices explain features such as subsurface oceans and cryovolcanoes.

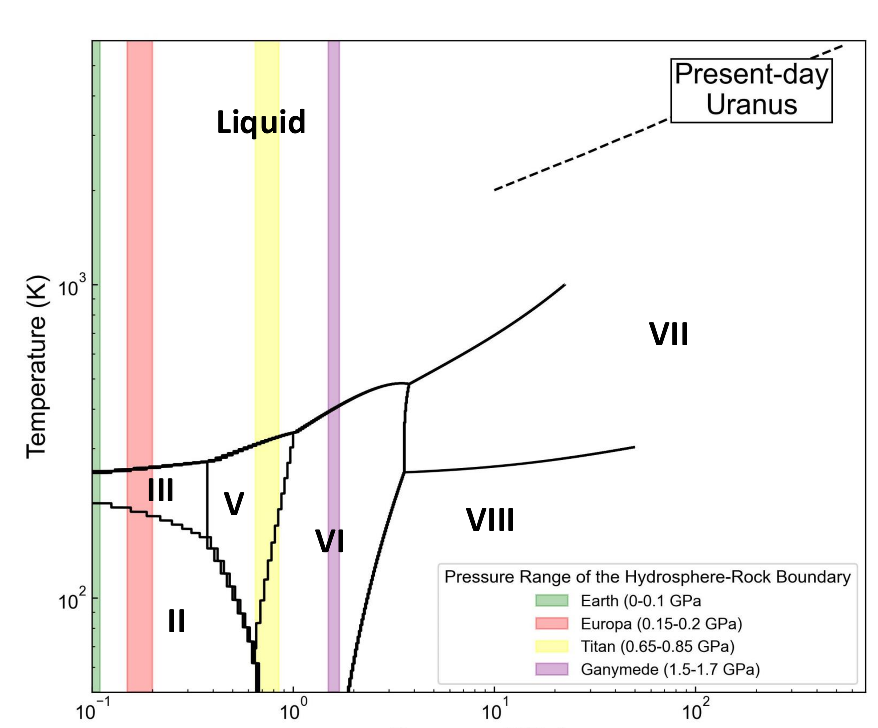

Figure 7. Machine learning prediction of phase diagram. The highlighted regions detail the pressure ranges of the hydrosphere rock boundaries of different celestial bodies[4]. The dotted line depicts the estimated P-T conditions of Uranus[5].

Fig 8. Uranus

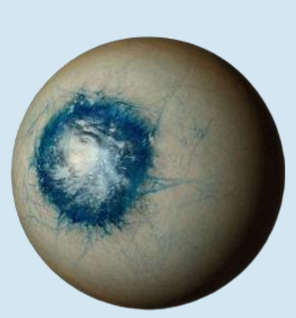

Fig 9. LHS 1140 b, exoplanet

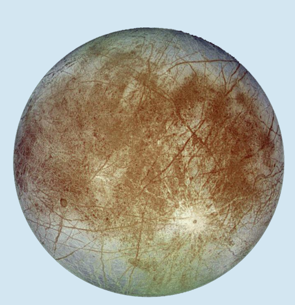

Fig 10. Europa, moon of Jupiter

Fig 11. Ganymede, moon of Jupiter

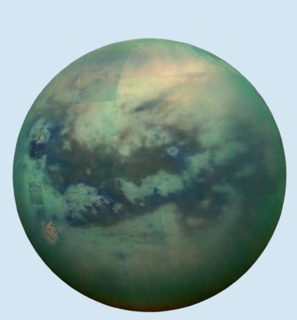

Fig 12. Titan, moon of Saturn

Acknowledgements

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References: [1] Nettelmann, N. *Icarus* **2016**, 275. [2] Martin Chaplin: "Ice Phases." The Ice Phases of Water. [3] Petrenko, V. F. *Clarendon Press* **2006**. [4] Journaux, B. *Space Science Reviews* **2020**, 216. [5] Hofstadter, M. D. *Keck Institute for Space Studies*, **2024**. [6] Bridgman, P. W. *Proceedings of the American Academy of Arts and Sciences* **1912**, *47*. [7] Bridgman, P. W. *The Journal of Chemical Physics* **1937**, *5*. [8] Fortes, A. D. *J Appl Cryst* **2012**, *45*. [9] Huang C. *Monthly Notices of the Royal Astronomical Society* **2021**, *503*. [10] Journaux, B. *Journal of Geophysical Research: Planets* **2020**, *125*. [11] Wagner, W. *Journal of Physical and Chemical Reference Data* **2011**, *40*. [12] Bezacier, L. *The Journal of Chemical Physics* **2014**, *141*. [13] Herrig, S. *Journal of Physical and Chemical Reference Data* **2018**, *47*. [14] Komatsu, K. *Proceedings of the National Academy of Sciences of the United States of America* **2020**, *117*. [15] Klotz, S. *Phys. Rev. B* **2017**, *95*. [17] Strässle, T. *J. Phys.: Condens. Matter* **2005**, *17*. [18] Feistel, R. *J Mar Res* **2005**, *63*. [19] Yoshimura, Y. *J. Chem. Phys.* **2006**, *124*. [20] Choukroun, M. *The Journal of Chemical Physics* **2007**, *127*. [21] León, G. C. *Journal of Physics and Chemistry of Solids* **2002**, *63*. [22] Besson, J. M. *Phys. Rev. B* **1994**, *49*.