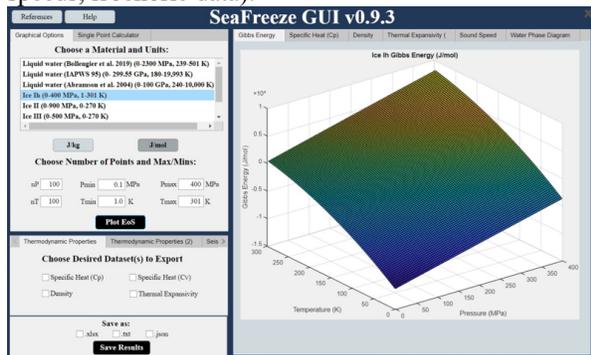


**SeaFreeze: a code to obtain the accurate thermodynamics of water ice polymorphs, “salted ices” and solutions at any conditions found in icy worlds of the solar system.** B. Journaux<sup>1</sup>, J. M. Brown<sup>1</sup>, S. Vance<sup>2</sup>, O. Bollengier<sup>3</sup>, <sup>1</sup>University of Washington, Seattle, WA, USA (correspondence: bjournau@uw.edu), <sup>2</sup>NASA Jet Propulsion Laboratory, Pasadena, CA, USA, <sup>3</sup>Université de Nantes, France.

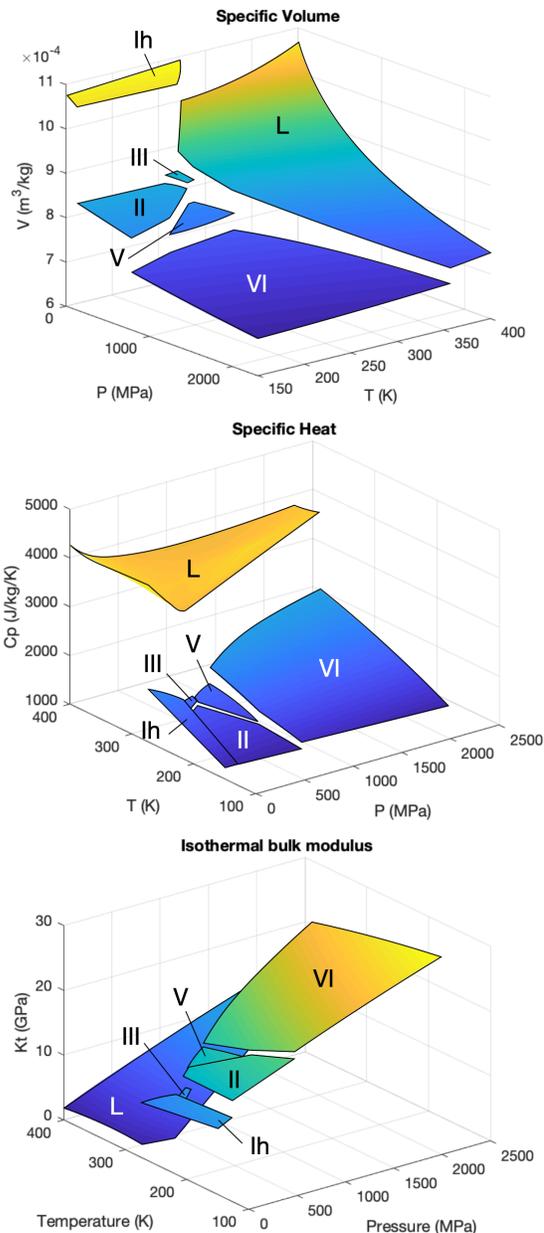
**Introduction:** The water-rich layers of icy moons contains several forms of ices and solids depending on pressure, temperature and chemistry [1]. Many of the geological processes on these moons, like cryovolcanisms, tectonics, oceanic evolution, involves processes of partial melting and fractional crystallization that are controlled by the stability of ices and “salted ices” (hydrates) and the coordinates of their eutectic [2]. As the conditions inside these moons far exceed the one found in Earth oceans, pressure is expected to have a major and under investigated role on the properties and stability of water-rich phases inside icy worlds.

**SeaFreeze:** and SeaFreeze GUI codes released in 2020 [3] (Fig. 1) allows to compute from fundamental potentials (Gibbs energy) derived from experimental data the most accurate thermodynamic properties (e.g. density, bulk modulus, heat capacity) and elastic properties ( $V_p$ ,  $V_s$ ) for ice polymorphs and liquid water as a function of pressure and temperature (Fig. 2). Since, we have been working on implementing the effect of chemistry (on solids) in the  $H_2O$ -( $Na^+$ ,  $Cl^+$ ,  $Mg^{2+}$ ,  $SO_4^{2-}$ ,  $NH_3$ ) systems from new experimental measurements (X-Ray diffraction, ultrasonic sound speeds, isochoric data).



**Figure 1:** SeaFreeze GUI available on GitHub

We will present how to use Seafreeze and how it can be easily and quickly implemented in existing frameworks and routines (Pyhton, matlab, GUI) and how new data can be implemented into SeaFreeze. We will also present new results on salted ice phases (hydrates) that demonstrate an unexpected diversity of structure at high pressure. Finally, we will discuss the implication for chemical physics/mineralogy as well as for the upcoming exploration of icy worlds of our solar system by NASA and ESA robotic space missions



**Figure 2:** Example of the evolution of thermodynamic properties computed with SeaFreeze for ices and liquid water up to 2300 MPa and between 100 and 400K.

**References:** [1] Journaux et al. *Space Sci. Rev.*, 216, 7. [2] Vance et al. (2020), *JGR-Planets*, 126, e2020JE006736. [3] Journaux B. et al. (2020) *JGR-Planets*, 125, e2019JE006176.