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Two Dimensional Continuum Model of Ice

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Two-Dimensional Quasi-Liquid Mediated Continuum Model of Ice

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Figure 1. Visual Introduction

Why does roughening occur?

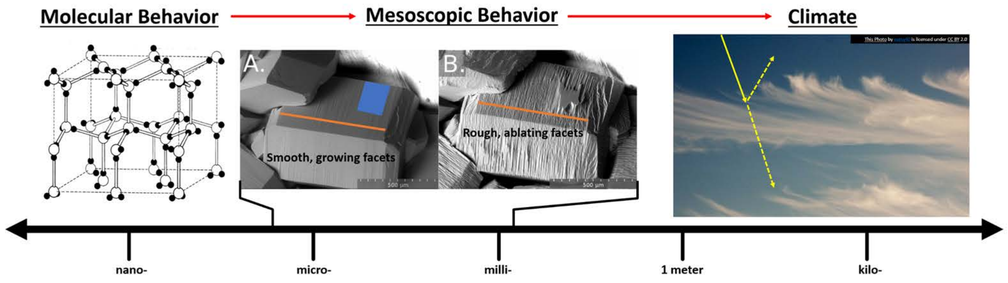


Figure 2. Molecular Dynamics of Ice[1]

- Quasi-liquid layer on ice varies in thickness cyclically as ice layers form
- Model parameters informed by these simulations

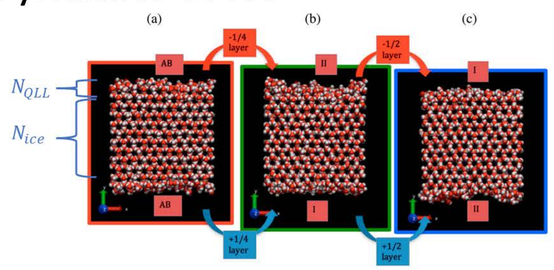
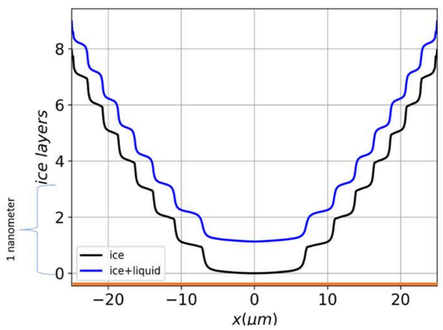


Figure 3. Quasi-Liquid Mediated Continuum Model (2016)[1]

Smooth growing facet from 1D continuum model



Model of water vapor saturation surrounding an ice facet

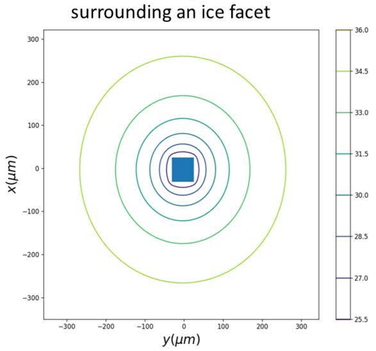


Figure 4. Partial Differential Equations Describing the Model

$$\frac{\partial N_{\mathrm{QLL}}}{\partial t} = D\nabla^2 N_{\mathrm{QLL}} + \sigma_m v_{\mathrm{kin}} N'_{\mathrm{QLL}},$$

$$\frac{\partial N_{\mathrm{ice}}}{\partial t} = \sigma_m v_{\mathrm{kin}} \left(1 - N'_{\mathrm{QLL}}\right),$$

What the continuum model has explained[1]:

- How does faceted growth occur in one dimension?
  - "Diffusive slowdown" leads to steady-state faceted growth
  - Increased step density counteracts increased vapor at corner

What we are exploring:

A. How does faceted *ablation* occur in one dimension?
B. How does faceted growth occur in *two dimensions*?
C. How does faceted ablation occur in two dimensions?
D. How does meso-scale roughness arise from molecular steps of ice?

B. Faceted growth in 2D.
Smooth, faceted growth shown by the 2d continuum model.

- Adaptation of ∇^2 and σ_m to two dimensions
- Optimization of algorithm (500x speedup)
- Changing integration method (LSODA to RK45)

C. Faceted ablation in 2D.
Smooth, faceted ablation also shown by the 2d continuum model.

- Everything in model remains the same except for supersaturation (lowered)
- Model consistent with observed behavior

D. How stable is faceted growth?
Both the 1d and 2d model show the behavior of a stable limit cycle, with high spatial frequency noise being dissipated over time in the growth and ablation cases.

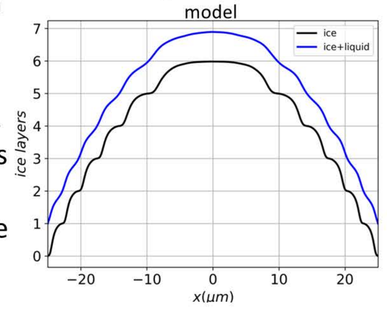
Materials and Methods

- Python 3.9 with NumPy, SciPy, Matplotlib, and Numba
- Model from 2016 sped up using Numba Python-to-C runtime compilation and CPU parallelization
- Explicit Runge-Kutta method of order 5(4) used for integration of partial differential equations

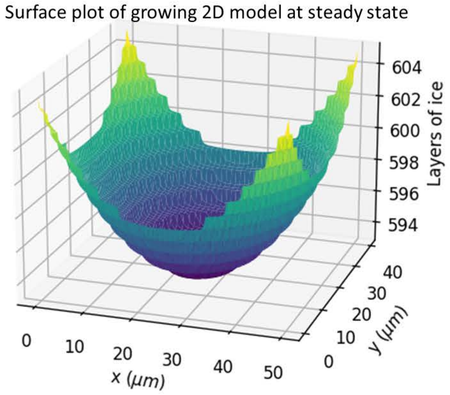
Results

A. Faceted ablation in 1D. Smooth, faceted ablation demonstrated by 1D continuum model. Width of steps decreases toward facet corners, reaching steady state like in growth.

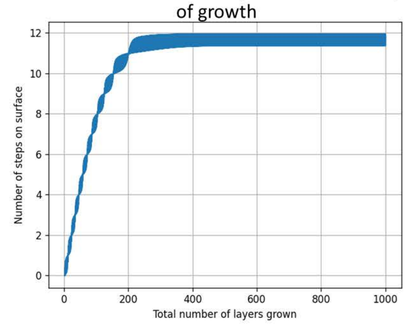
Smooth ablating facet from 1D continuum model



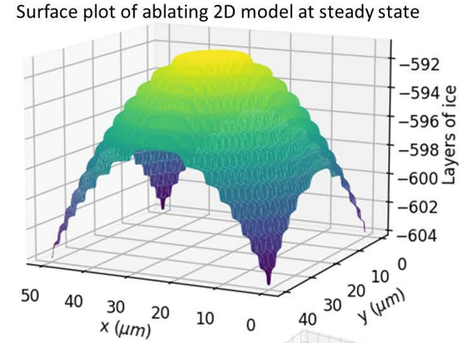
Surface plot of growing 2D model at steady state



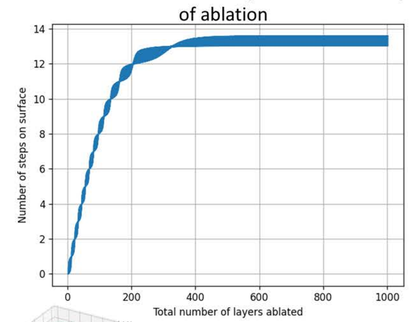
Surface of ice reaches steady state after 400 layers of growth

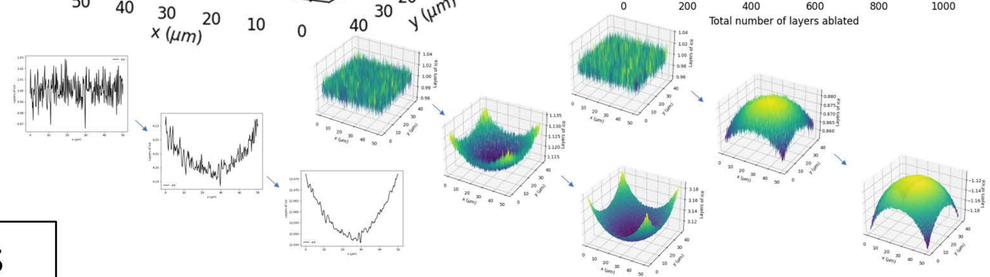


Surface plot of ablating 2D model at steady state



Surface of ice reaches steady state after 400 layers of ablation





Future Directions

- 1D and 2D model exhibit faceted growth and ablation, but not meso-scale roughness yet
  - Prof. Jake Price is investigating this with Fourier analysis
  - Low spatial frequency perturbations may induce roughness
  - Growth and ablation cycles may lead to accumulated roughness
- Implement and test behavior of model with a spiral dislocation

Acknowledgements

- Jake Price for Fourier analysis of the model
- University of Puget Sound Summer Research Grant

1. Neshyba, S.; Adams, J.; Reed, K.; Rowe, P. M.; Gladich, I. A Quasi-Liquid Mediated Continuum Model of Faceted Ice Dynamics. *Journal of Geophysical Research: Atmospheres* **2016**, *121* (23), 14,035-14,055. https://doi.org/10.1002/2016JD025458