

# Introduction to the Mars Subsurface Ice Model (MSIM) Program Collection

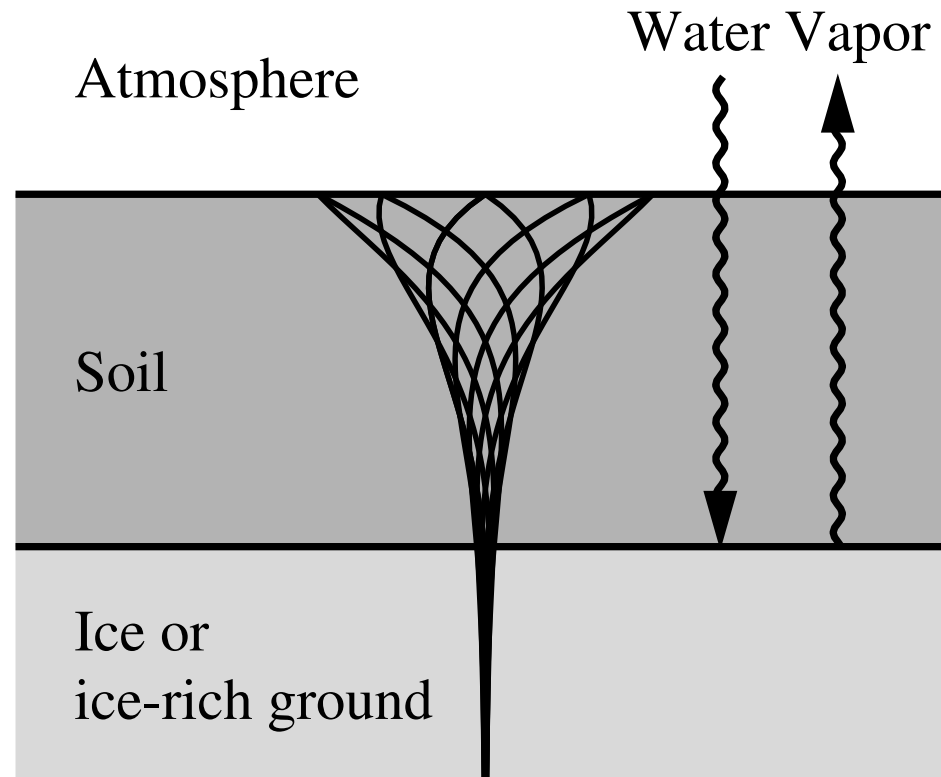
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November 2024

<https://github.com/nschorgh/MSIM/>

# Ground Ice in Diffusive Contact with Atmospheric Water Vapor



Vapor diffusion in the presence of temperature variations

# Mars Subsurface Ice Model (MSIM)

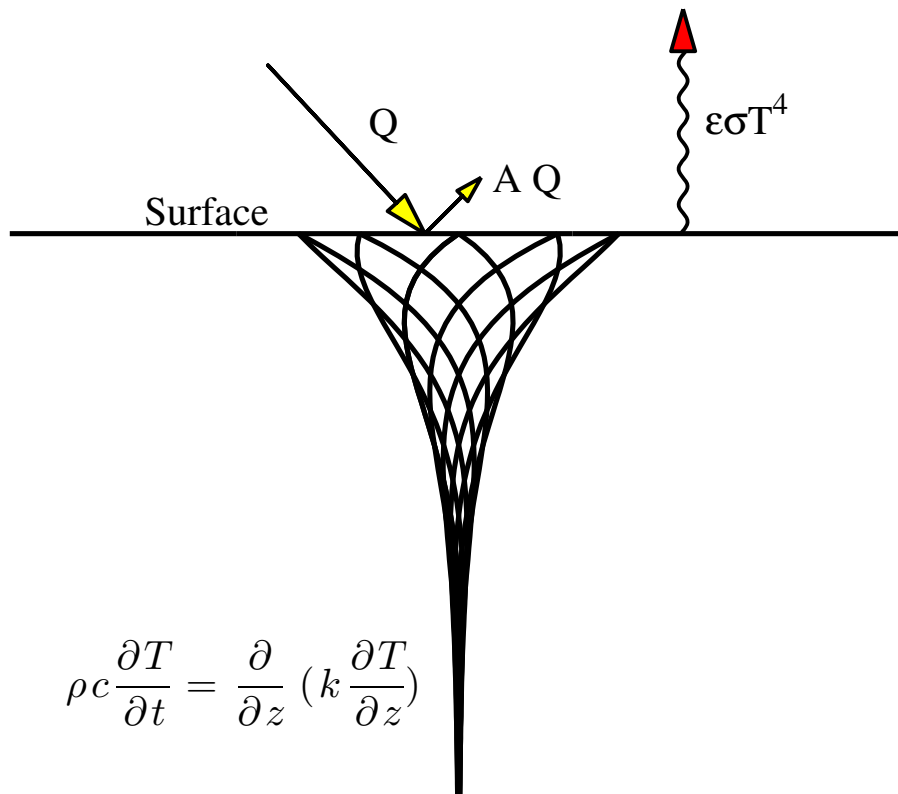
<https://github.com/nschorgh/MSIM/>

Component			Typical time step
Thermal model	semi-implicit + nonlinear b.c.		15 mins
Microphysical model	diffusion, adsorption, sublimation		seconds
Equilibrium ice table	vapor equilibrium		—
Non-equilibrium ice	net vapor flux & ice content		100 yr

<https://github.com/nschorgh/Planetary-Code-Collection/>

3D surface energy balance	slopes & shadows	Megapixels
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# Subsurface Heat Storage (1D)



Heat equation with non-linear boundary condition

1) Flux-conservative discretization (heat conservation) on irregular grid

2) Time-marching scheme that is *not* subject to

$$\Delta t < \Delta z^2 / (2\kappa).$$

Semi-implicit solver,

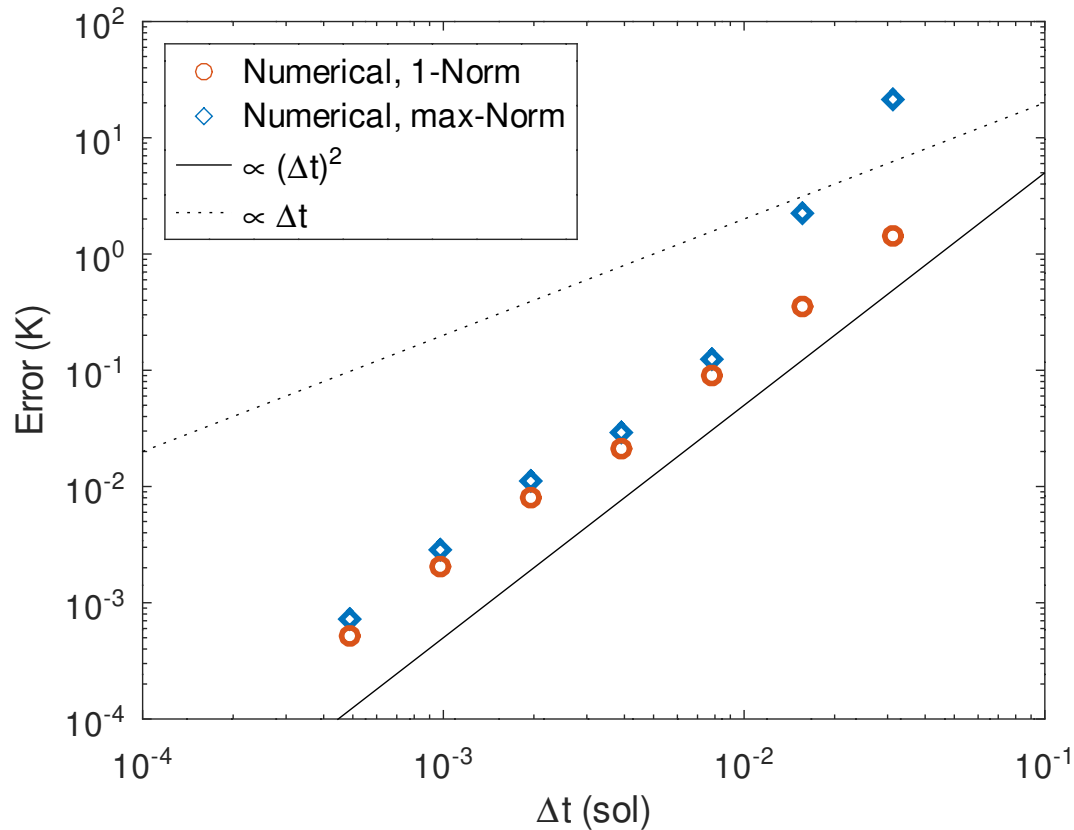
$$\Delta t \lesssim (\text{Solar Day}) / 100$$

# Numerical Solver for Heat Equation

Semi-implicit finite-difference method (Crank-Nicolson)

2nd order

unconditionally stable (for linear b.c.)



Convergence with time step  $\Delta t$  for the Crank-Nicolson method with nonlinear boundary condition.

(Many common Mars thermal models use explicit time steps, which lack both of these advantages.)

# Surface Energy Balance

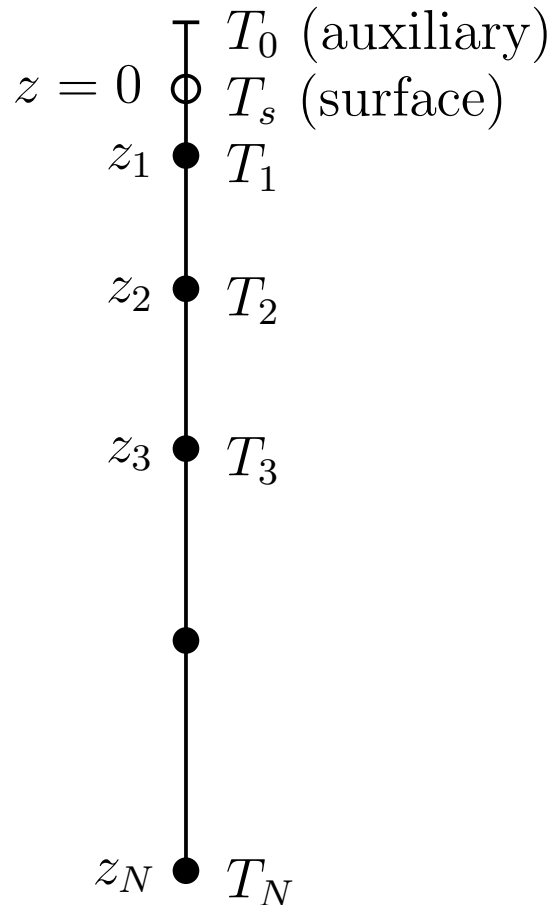
Surface energy balance:

$$k \frac{\partial T}{\partial z} = \epsilon \sigma T^4 - Q(t)$$

nonlinear boundary condition, because dependence on  $T$  itself  
(superposition fails)

- In MSIM, Stefan-Boltzmann term is linearized, so it can be incorporated into implicit method (*Schorghofer & Khattiwala 2004*)
- Nonlinear implies fully-implicit and semi-implicit schemes are no longer unconditionally stable (*Williams & Curry 1977*)  
For Mars and flat ground, stability is not an issue;  
For airless bodies and slopes, this can be a common issue at sunrise

# Grid Spacing



- Flux is defined in between grid points, so surface boundary condition should be imposed there too.  
 $\Rightarrow (z_1 - 0) = \frac{1}{2}(z_2 - z_1)$
- Otherwise grid-spacing is arbitrary

# Thermal Model Performance

Full surface energy balance:

$$\underbrace{(1 - A)Q_0 \sin \theta}_{\text{direct insolation}} + Q_{\text{sky}} + \underbrace{k \frac{\partial T}{\partial z}}_{\substack{\text{subsurf.} \\ \text{heat}}} = \underbrace{\epsilon \sigma T^4}_{\substack{\text{Stefan-} \\ \text{Boltzmann}}} - \underbrace{L \frac{dm_{\text{CO}_2}}{dt}}_{\substack{\text{latent heat of} \\ \text{seasonal CO}_2}}$$

Benchmark (3.6 GHz Intel Xeon E5-1650, gfortran 11.4.0):

10 Mars years (6686 sols), 100 steps/sol (15 mins), 80 grid points: **only 1.1 seconds** (with 2nd order accuracy)

For example, 1 million thermal model runs over 10 Mars years on a 10-core (20 threads) CPU take 15 hours, hence feasible on a simple workstation.



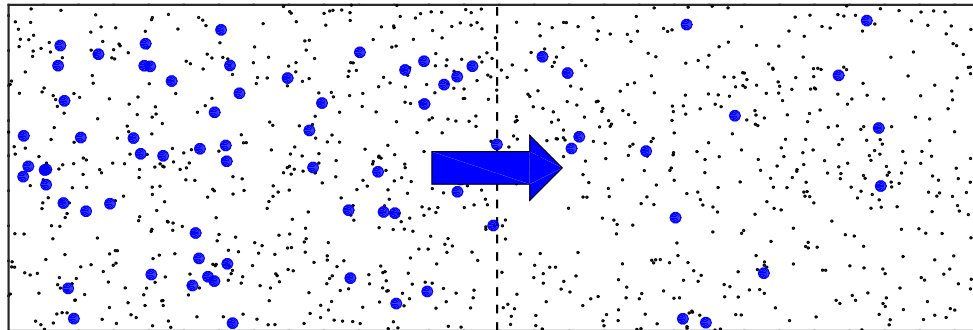
# Vapor Transport in Non-Isothermal Sublimation Environments

Phases of H<sub>2</sub>O incorporated: *vapor, adsorbed H<sub>2</sub>O, and ice*

Vapor flux in non-isothermal environment (*Landau & Lifshitz*):

$$\vec{J} = -D\rho_{\text{atm}} \vec{\nabla} \left( \frac{\rho_v}{\rho_{\text{atm}}} \right) + (\text{exotic terms}) + (\text{advection}) \approx -D \vec{\nabla} \rho_v$$

$\vec{J}$ ...vapor flux;  $D$ ...diffusion coefficient;  $\rho_v$ ...H<sub>2</sub>O vapor density



Vapor diffuses along gradient of **absolute humidity** (kg/m<sup>3</sup>), not necessarily along gradients of relative humidity.

E.g., diffusion from warm unsaturated to cold saturated region

# Microphysical Model Equations

Diffusion of water vapor in porous medium with phase transitions (adsorption and sublimation) on 1-dimensional irregular grid

*Governing Equations*

**Conservation of mass:** 
$$\frac{\partial}{\partial t}(\bar{\rho}_v + \bar{\rho}_f + \bar{\rho}_a) + \frac{\partial \bar{J}}{\partial z} = 0$$

**Vapor transport:** 
$$J = -D \frac{\partial \rho_v}{\partial z}$$

**Adsorption:**  $\bar{\rho}_a = \bar{\rho}_a(p, T)$  reversible and not kinetically-limited

**Sublimation:**  $p \leq p_{sv}(T)$  excess vapor converted to ice

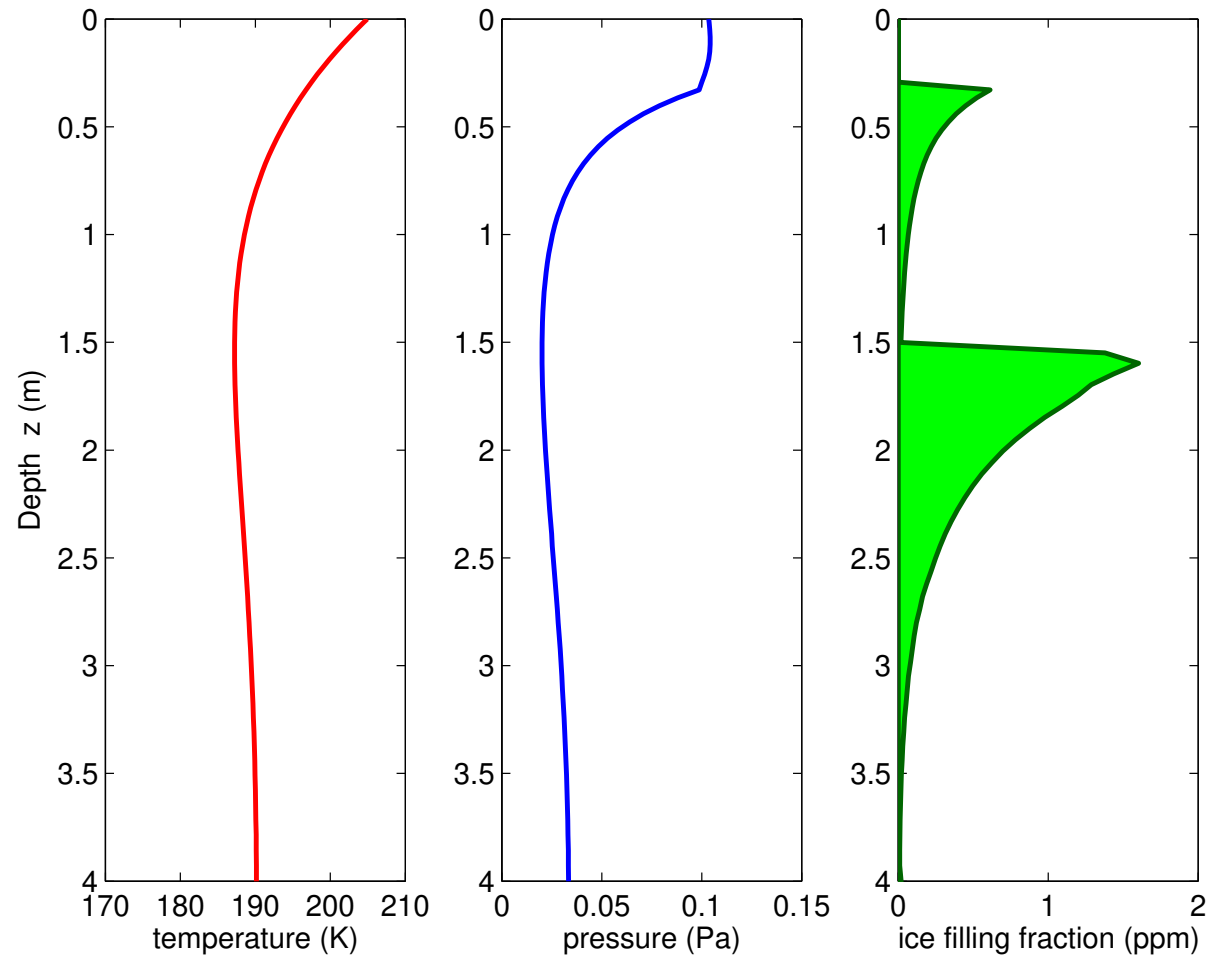
Indices:  $v$  ... vapor,  $f$  ... ice,  $a$  ... adsorbed water

$\bar{\rho}$  ... mass per total volume,  $\bar{J}$  ... vapor flux per total area

# Microphysical Model Numerics

- Flux-conservative discretization on irregular 1d grid (there are several options)
- Threshold for phase transition implies problem is non-linear  
⇒ forward-time discretization (explicit time step)

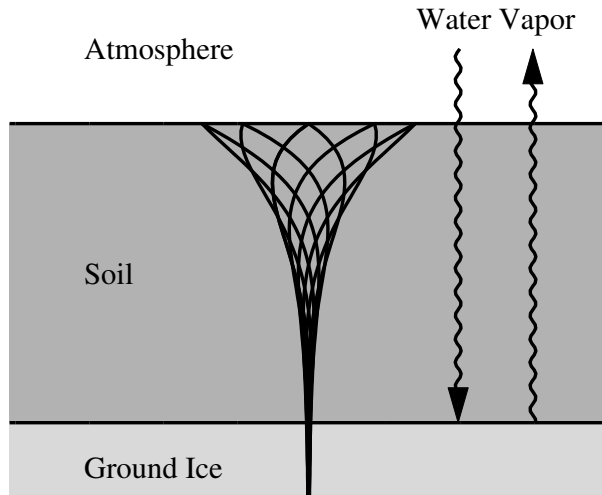
# Accumulation of Subsurface Ice



Snapshot of temperature cycles that pump atmospheric humidity into the ground; movie is on [GitHub](#)

# Time-Averaging of Transport Equations

Microphysics is complicated, but time averages can help us.



$$J = -D \frac{\partial \rho_v}{\partial z}$$

$J$  ... vapor flux;  $D$  ... diffusion coefficient

$\rho_v$  ... H<sub>2</sub>O vapor density;  $z$  ... vertical coordinate

Time average over period  $P$  :

$$\langle X \rangle = \frac{1}{P} \int_0^P X dt$$

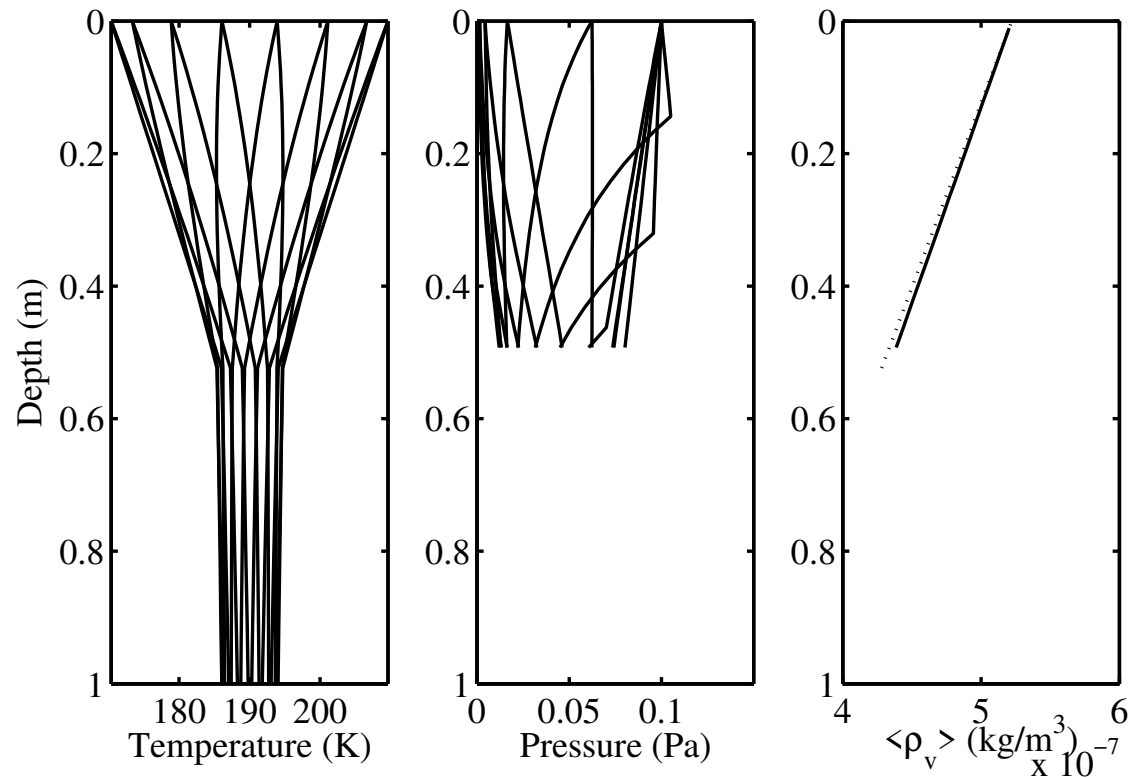
$$\langle J \rangle = - \left\langle D \frac{\partial \rho_v}{\partial z} \right\rangle \approx - \langle D \rangle \left\langle \frac{\partial \rho_v}{\partial z} \right\rangle = - \langle D \rangle \frac{\partial \langle \rho_v \rangle}{\partial z}$$

The **time-averaged flux** is given by the gradient of the **time-averaged vapor density**.  $\Rightarrow$  Net vapor flux can be calculated without microphysical processes.  $\Rightarrow$  “Fast” computational methods for subsurface ice evolution.

## Boundary-Value Formulation

If averaging period is one solar year, time-average of  $\rho_v$  is determined by the boundary values at the surface and the ice table.

$$\text{(mass conservation)} \quad \frac{\partial(\rho_v + \rho_{ads} + \rho_{ice})}{\partial t} + \frac{\partial J}{\partial z} = 0 \quad \Rightarrow \quad \left\langle \frac{\partial J}{\partial z} \right\rangle = 0$$

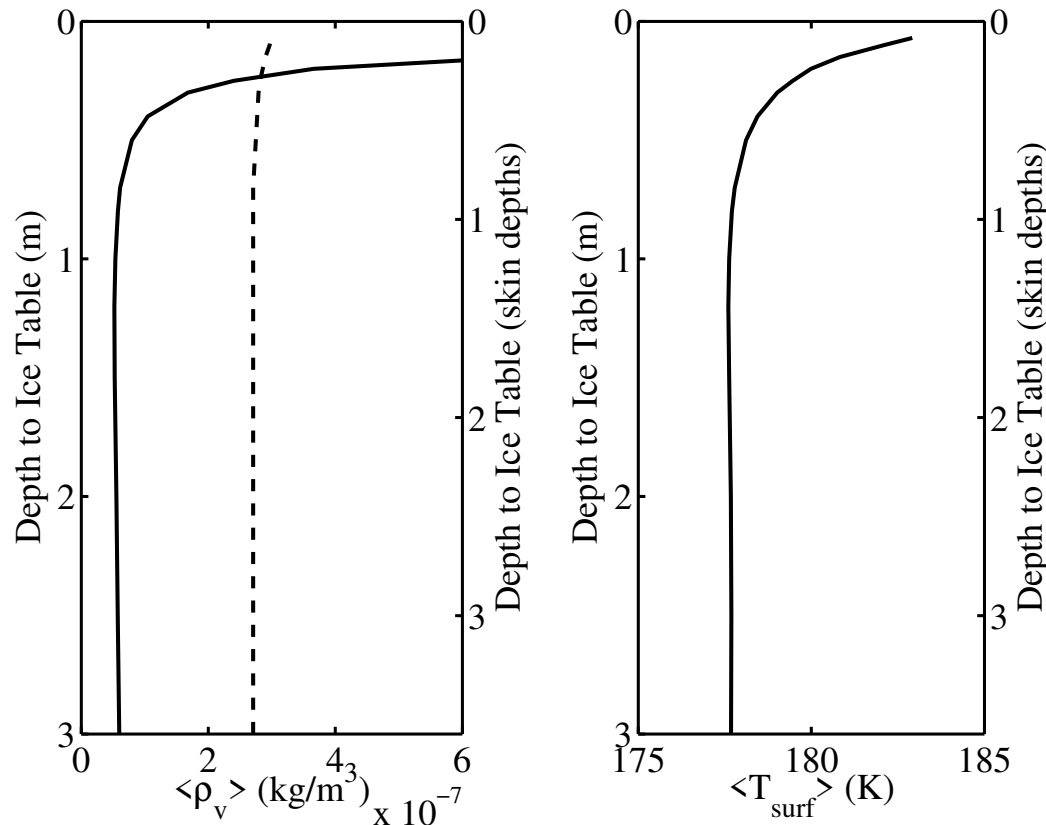


$\langle J \rangle$  is constant with depth;  $\langle \rho_v \rangle$  is linear with depth; solid lines are microphysics simulation; dotted line connects boundary values

# Equilibrium Ice Table $\langle J \rangle = 0$

Depth of equilibrium ice table:

$$\langle \rho_v(\text{surface}) \rangle = \langle \rho_v(\text{ice table}) \rangle$$

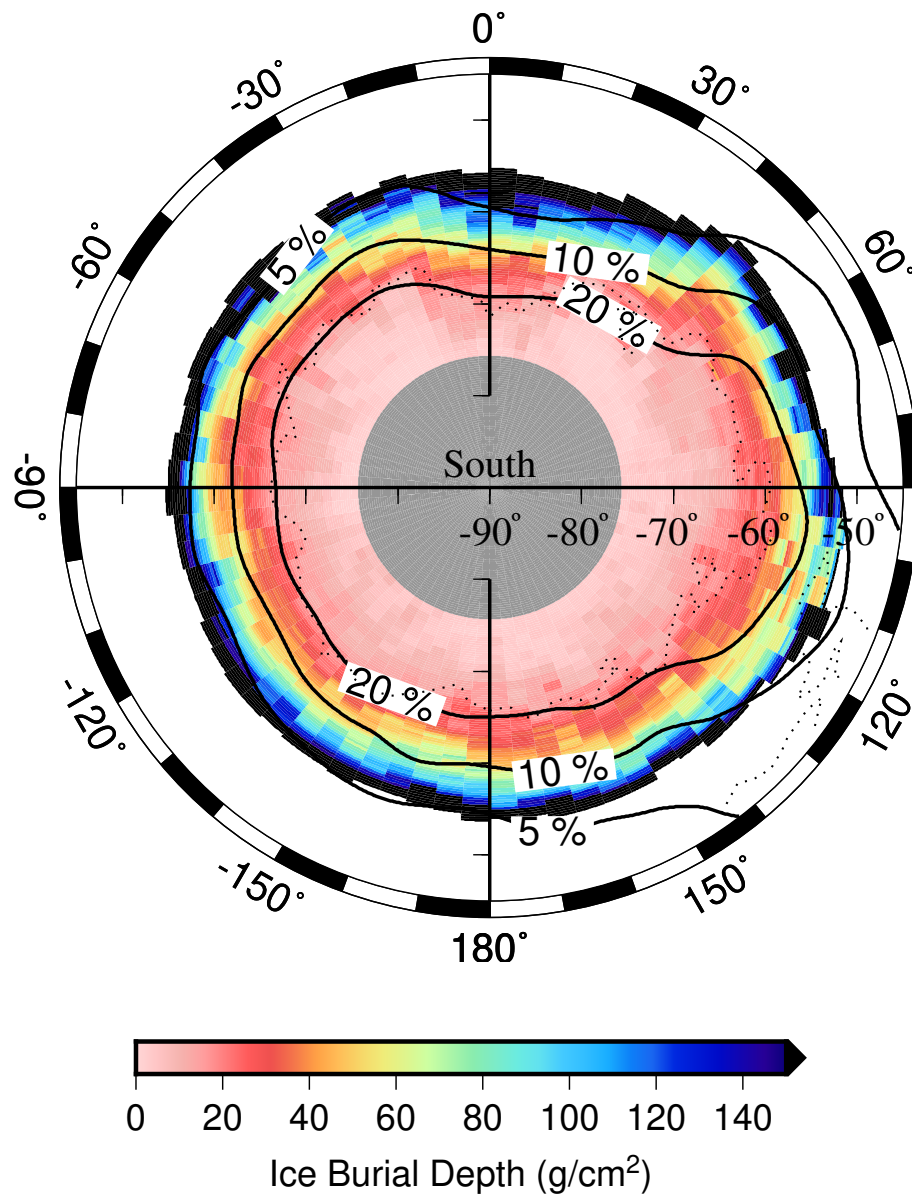


For each depth to ice table, thermal model was equilibrated and  $\langle \rho_v \rangle$  was calculated for the last Mars year.

Depth to equilibrium ice table: **Nonlinear root-finding**

I usually use bisection method, and turn off geothermal heat to avoid missing a root.

## Example Result



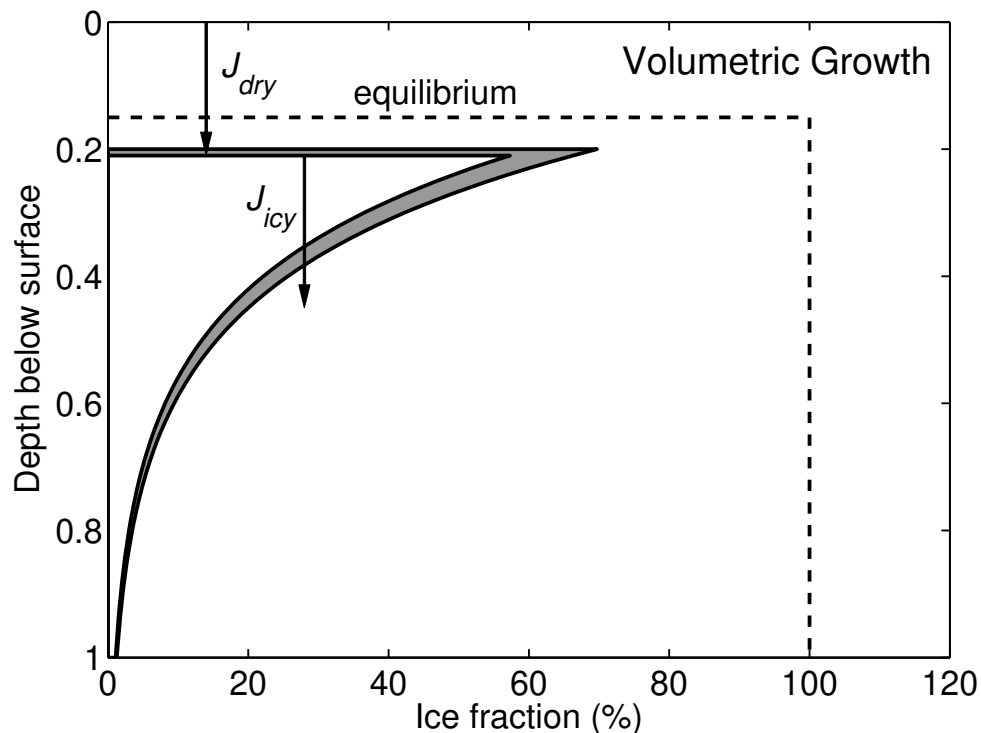
Depth to equilibrium ice table (colors) in the south polar region of Mars compared to results from nuclear spectroscopy (solid contours).

*Schorghofer & Aharonson (2005)*



# Beyond Equilibrium:

## Recharge of Subsurface Ice



- Subsurface ice can be sequestered from atmospheric vapor (*Melton & Jakosky 1993*)
- Interface is below equilibrium depth
- Interface is sharp
- Interface is moving (i.e., between grid points)

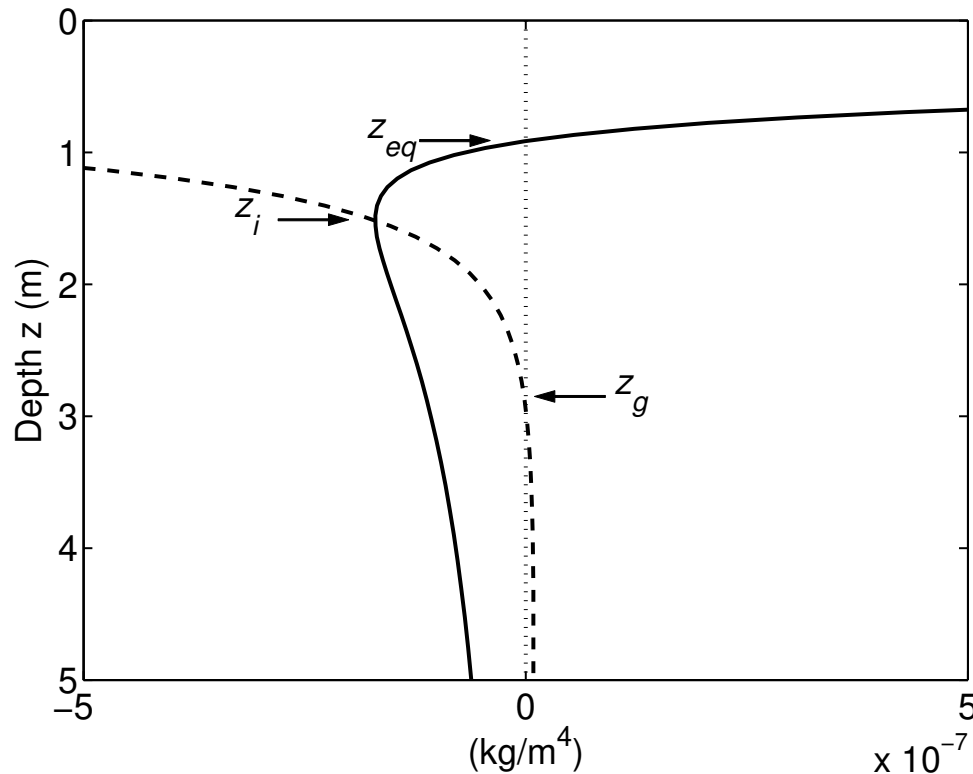
Gray area shows incremental ice growth. Ice fraction is relative to pore volume.

## Location of $z_{eq}$ , $z_i$ , and $z_g$

$z_{eq}$  ... equilibrium depth

$z_i$  ... interface depth

$z_g$  ... geothermal limit



solid line ...  $\frac{\langle \rho_{sv} \rangle(z) - \langle \rho(0) \rangle}{z}$

dash line ...  $\partial \langle \rho_{sv} \rangle / \partial z$

All three of these depths migrate with changing ice content.

for realistic Mars subsurface temperatures at  $60^\circ\text{N}$ .

# Numerics of Interface Retreat

Depth of uppermost ice  $z_p$ , might or might not cross grid-point during advance

Mass conservation:

$$\frac{dz_p}{dt} f(z_p) \Phi_0 \rho_{\text{ice}} = -\langle J \rangle = \eta D \frac{\Delta \langle \rho_v \rangle}{z_p}$$

$z_p$  ... shallowest depth with pore ice;  $f$  ... fraction of pore filled with ice;

$\Phi_0$  ... ice-free porosity;  $0 \leq \eta \leq 1$  ... constriction of diffusion

Integrate over one time step  $\Delta t_B$ :

$$\int_{z_p(0)}^{z_p(\Delta t_B)} f(z) z dz = \int_0^{\Delta t_B} \frac{1}{\Phi_0 \rho_{\text{ice}}} \eta D \Delta \langle \rho_v \rangle dt$$

$$\sum_{j=0}^{z_p} f(z_j) z_j \Delta z_j = \frac{1}{\Phi_0 \rho_{\text{ice}}} \eta D \Delta \langle \rho_v \rangle \Delta t_B$$

To find  $z_p(\Delta t_B)$ , sum until this equality is exceeded.

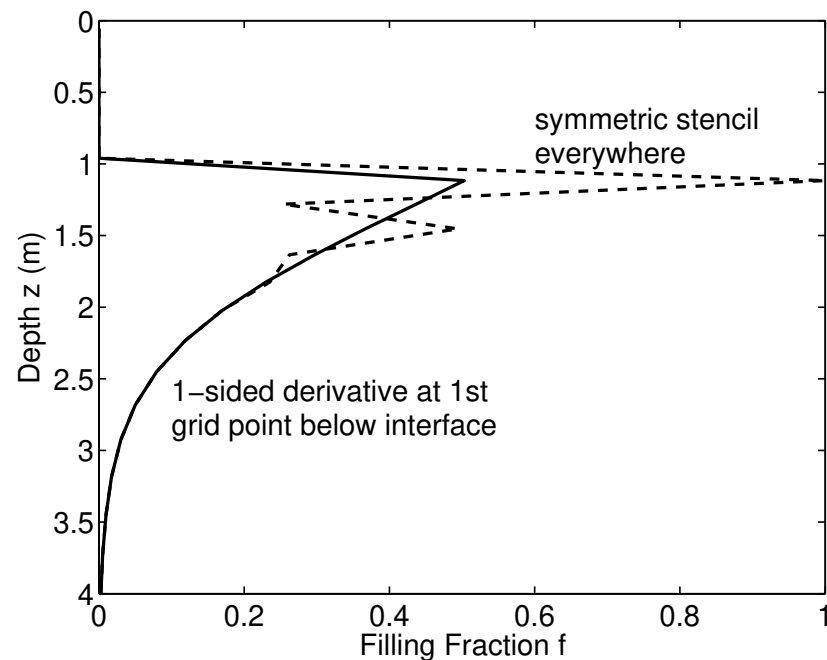
# Numerics with Partial Pore Filling

We have to deal with  $\sigma(z, t)$ , not just depth-to-ice-table  $z_T(t)$ .  
 $\sigma$  ... ice density; Mass change for interstitial ice:

$$\frac{\partial \sigma}{\partial t} = \frac{\partial}{\partial z} \left( \eta D_{\text{icefree}} \frac{\partial \langle \rho_{sv} \rangle}{\partial z} \right)$$

$\eta$  ... constriction of diffusion (discontinuous at interface)

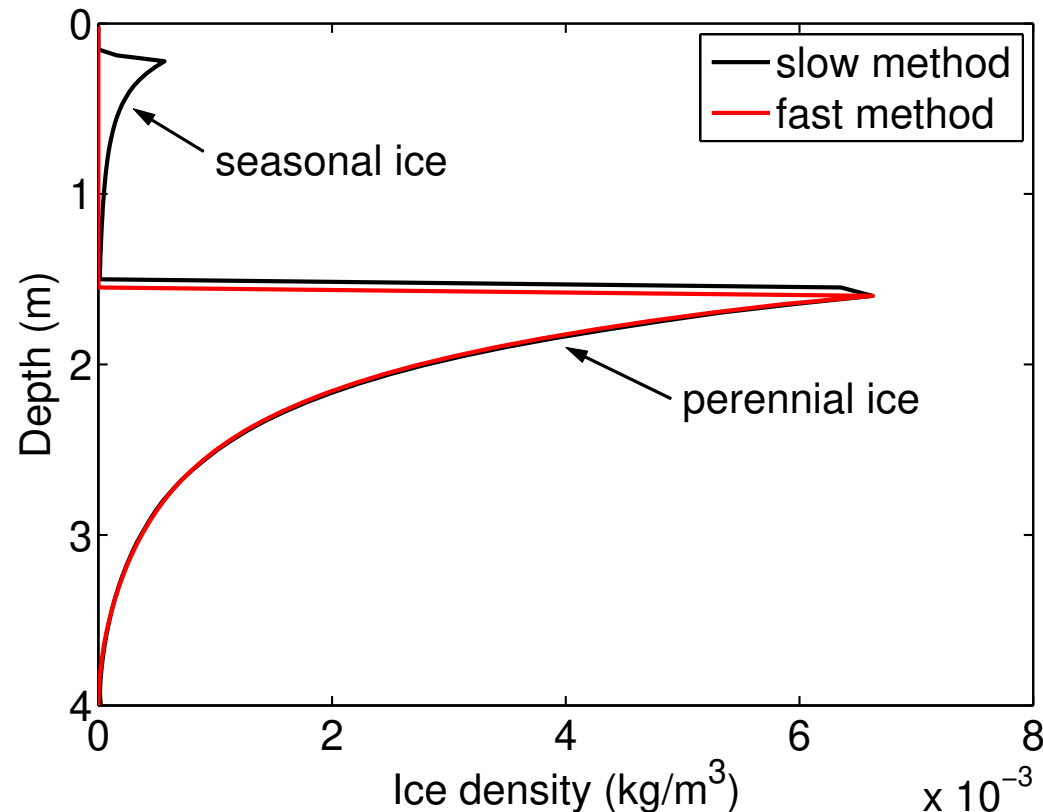
This involves 2nd spatial derivative of  $\rho_{sv}$  (difficult near interface  
 $\Rightarrow$  one-sided finite-differences from below)



# Comparison between Fast and Slow Method

*slow* ... microphysical model

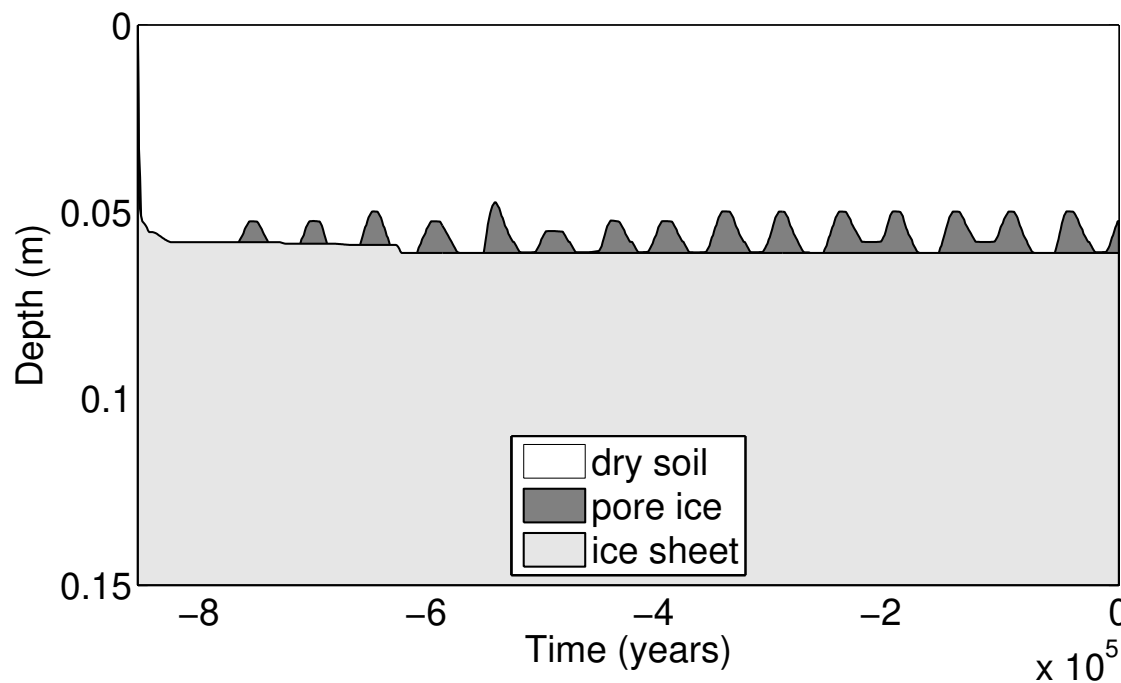
*fast* ... time-averaged transport equations



Speedup is  $\sim 10^4$ -fold! About same speed as a thermal model.  
Fast method does not resolve diurnal and seasonal cycle.

# Example: Phoenix Landing Site

massive ice sheet formed 863 ka ago (local obliquity maximum)



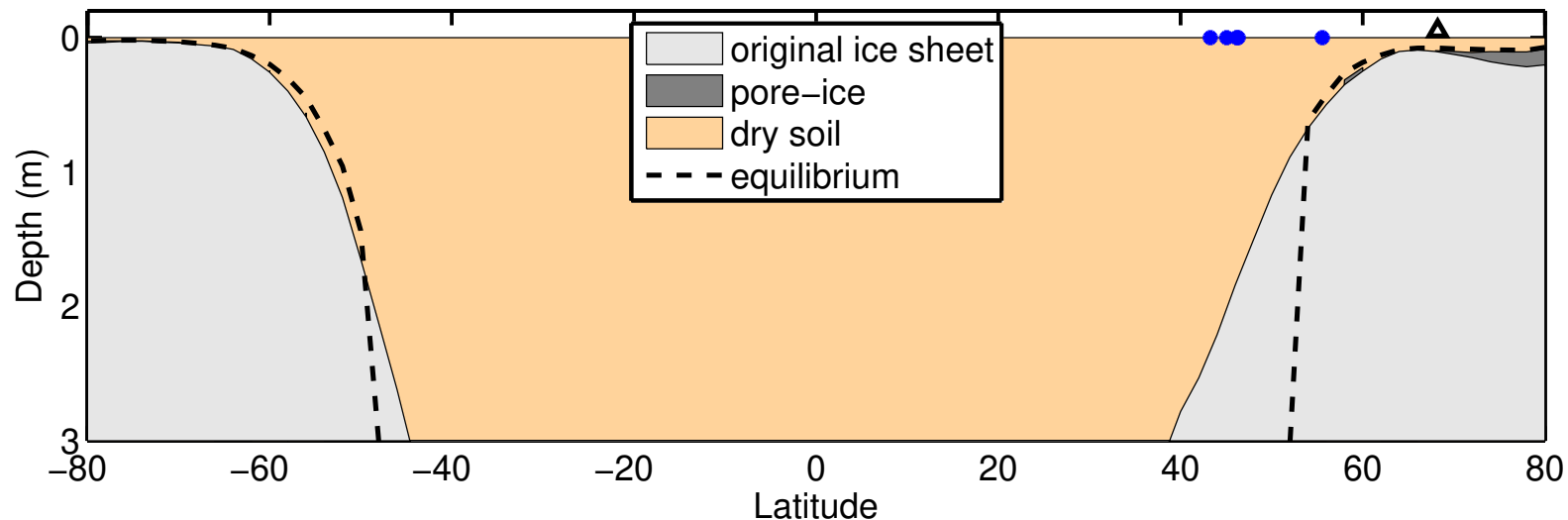
Filling fraction is always 100% (vertical growth mode).

Present-day thickness of pore ice layer is only 9 mm. Phoenix observed mostly pore-ice, while neutron spectroscopy reveals massive ice.

*(Schorghofer & Forget 2012)*

# Example: Present-day Ice Distribution

Scenario: Massive ice sheet formed 1 Ma ago



consistent with: MONS geographic boundary, MONS burial depths, MONS ice content, pore ice at Phoenix Landing Site, mid-latitude icy impact sites (*Schorghofer & Forget 2012*)

# Summary

1. MSIM includes a powerful subsurface thermal model (semi-implicit, 2<sup>nd</sup> order accurate, stabilized)
2. MSIM also includes microphysical model for vapor transport and adsorption, but it is computationally slow.
3. Method for fast subsurface ice modeling: **Solve time-averaged transport equations**
4. Non-equilibrium model with partial pore filling is fast but complex (whereas retreat or growth with full pores is easy)
5. MSIM is publicly available (but it includes a few third-party routines) <https://github.com/nschorgh/MSIM/>



# References

**MSIM** is publicly available at <https://github.com/nschorgh/MSIM/> (but not open-source yet, because of third-party routines)

## Methods:

1. [https://github.com/nschorgh/MSIM/blob/main/MSIM\\_Methods.pdf](https://github.com/nschorgh/MSIM/blob/main/MSIM_Methods.pdf)
2. Thermal model: *Schörghofer & Khatiwala, PSJ (2024)*  
(most of it was written 2001–2003)
3. Fast non-equilibrium model: *Schörghofer, Icarus (2010)*

## Science Applications:

1. Vapor diffusion: *Schorghofer & Aharonson, JGR (2005)*
2. Equilibrium ice table: *Schorghofer & Aharonson, JGR (2005)*,  
*Aharonson & Schorghofer, JGR (2006)*
3. Non-equilibrium ice evolution: *Schorghofer, Nature (2007)*,  
*Schorghofer & Forget, Icarus (2012)*, *Vos et al., JGR (2022, 2023)*