NOTES
1-Dimensional Numerical Model of Thermal Conduction and Vapor Diffusion in the Planetary Subsurface

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Part 1

Conduction of Heat

originally developed by Samar Khatiwala in 2001 (including upper radiation boundary condition for semi-implicit scheme)
extended to variable thermal properties and irregular grid by Norbert Schörghofer 2002–2003

1.1 Governing Equation

T ... temperture, t ... time, z ... depth, ρc ... volumetric heat capacity, k ... thermal conductivity

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z} \right) \tag{1.1}$$

$F = k\dfrac{\partial T}{\partial z}$ ... heat flux

1.2 Semi-Implicit Scheme on Irregular Grid

$$\frac{\partial}{\partial z} F_j = \frac{F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}}{(z_{j+1} - z_{j-1})/2} = 2 \frac{k_{j+\frac{1}{2}} \frac{T_{j+1}-T_j}{z_{j+1}-z_j} - k_{j-\frac{1}{2}} \frac{T_j - T_{j-1}}{z_j - z_{j-1}}}{z_{j+1} - z_{j-1}}$$

$$\begin{aligned}(\rho c)_j \frac{\partial T_j}{\partial t} &= \frac{2k_{j+\frac{1}{2}}}{(z_{j+1}-z_j)(z_{j+1}-z_{j-1})} T_{j+1} - \frac{2}{z_{j+1}-z_{j-1}} \left(\frac{k_{j+\frac{1}{2}}}{z_{j+1}-z_j} + \frac{k_{j-\frac{1}{2}}}{z_j - z_{j-1}} \right) T_j + \\ &\quad + \frac{2k_{j-\frac{1}{2}}}{(z_j - z_{j-1})(z_{j+1}-z_{j-1})} T_{j-1}\end{aligned}$$

$$\text{introduce} \quad \alpha_j = \frac{\Delta t}{(\rho c)_j} \frac{k_{j+\frac{1}{2}}}{(z_{j+1}-z_j)(z_{j+1}-z_{j-1})} \quad \text{and} \quad \gamma_j = \frac{\Delta t}{(\rho c)_j} \frac{k_{j-\frac{1}{2}}}{(z_j - z_{j-1})(z_{j+1}-z_{j-1})}$$

$$\Delta t \frac{\partial T_j}{\partial t} = 2\alpha_j T_{j+1} - 2(\alpha_j + \gamma_j) T_j + 2\gamma_j T_{j-1}$$

$$T_j^{n+1} - T_j^n = \alpha_j T_{j+1}^{n+1} - (\alpha_j + \gamma_j) T_j^{n+1} + \gamma_j T_{j-1}^{n+1} + \alpha_j T_{j+1}^n - (\alpha_j + \gamma_j) T_j^n + \gamma_j T_{j-1}^n$$

$$\boxed{-\alpha_j T_{j+1}^{n+1} + (1+\alpha_j+\gamma_j)T_j^{n+1} - \gamma_j T_{j-1}^{n+1} = \alpha_j T_{j+1}^n + (1-\alpha_j-\gamma_j)T_j^n + \gamma_j T_{j-1}^n} \quad 1<j<N$$

Superscript n refers to time step. Index j refers to position z_j. The conductivity k is defined on half-points. In the program, $2(\rho c)_j = (\rho c)_{j+\frac{1}{2}} + (\rho c)_{j-\frac{1}{2}}$. In this way, the parameters k and ρc do not need to be defined at an interface of two layers with different thermal properties. Since indices in the program must be integers, we choose $k(j) = k_{j-\frac{1}{2}}$ and the same for ρc.

1.2.1 Upper boundary condition:

a) Radiation

$$Q + k\left.\frac{\partial T}{\partial z}\right|_{z=0} = \epsilon\sigma T^4\big|_{z=0} \tag{1.2}$$

Q is the incoming solar flux including the atmospheric contribution.
introduce auxiliary quantity T_0, such that surface temperature $T_s = (T_0+T_1)/2$

$$\left.\frac{\partial T}{\partial z}\right|_{z=0} = \frac{T_1-T_0}{\Delta z} \quad \text{and} \quad T^4\big|_{z=0} = \left(\frac{T_0+T_1}{2}\right)^4 \quad \text{with} \quad \Delta z = 2z_1$$

$T = T_r + T'$ $\qquad$ T_r is a reference temperature around which we linearize

$$\begin{aligned} Q + k_{1/2}\frac{T_1-T_0}{\Delta z} &= \epsilon\sigma\left(\frac{2T_r + T_0' + T_1'}{2}\right)^4 \\ &\approx \epsilon\sigma T_r^4 + 2\epsilon\sigma T_r^3(T_0'+T_1') \\ &= -3\epsilon\sigma T_r^4 + 2\epsilon\sigma T_r^3(T_0+T_1) \end{aligned}$$

$T_0\left(\frac{k_{1/2}}{\Delta z} + B(T_r)\right) = Q + 3\epsilon\sigma T_r^4 + T_1\left(\frac{k_{1/2}}{\Delta z} - B(T_r)\right)$ where $B(T_r) = 2\epsilon\sigma T_r^3$
introduce $a = (Q + 3\epsilon\sigma T_r^4)/(\frac{k}{\Delta z} + B)$ and $b = (\frac{k_{1/2}}{\Delta z} - B)/(\frac{k_{1/2}}{\Delta z} + B)$

$$-\alpha_1 T_2^{n+1} + (1+\alpha_1+\gamma_1-\gamma_1 b^n)T_1^{n+1} = \alpha_1 T_2^n + (1-\alpha_1-\gamma_1+\gamma_1 b^n)T_1^n + \gamma_1\frac{Q^n + Q^{n+1} + 6\epsilon\sigma T_r^4}{\frac{k_{1/2}}{\Delta z} + B^n}$$

choose $\Delta z = z_2 - z_1 = 2z_1$, define $\beta = \frac{\Delta t}{(\rho c)_1}\frac{1}{2\Delta z^2}$, then $\alpha_1 = \beta k_{3/2}$ and $\gamma_1 = \beta k_{1/2}$

$$\text{surface temperature} \quad T_s = \frac{1}{2}(T_1+T_0) = \frac{1}{2}\left(\frac{Q+3\epsilon\sigma T_r^4}{k_{1/2}/\Delta z + B} + T_1 + bT_1\right) = \frac{Q + 3\epsilon\sigma T_r^4 + \frac{2k}{\Delta z}T_1}{2(k_{1/2}/\Delta z + B)}$$

choose $T_r^n = T_s^{n-1}$
implemented in `conductionQ.f`

b) prescribed T

standard formulas (**??**,**??**) with $T_0 = T_s$ and $z_0 = 0$

$$\alpha_1 = \frac{\Delta t}{(\rho c)_1} \frac{k_{3/2}}{(z_2 - z_1) z_2}, \qquad \gamma_1 = \frac{\Delta t}{(\rho c)_1} \frac{k_{1/2}}{z_1 z_2}$$

$$-\alpha_1 T_2^{n+1} + (1 + \alpha_1 + \gamma_1) T_1^{n+1} = \alpha_1 T_2^n + (1 - \alpha_1 - \gamma_1) T_1^n + \gamma_1 (T_s^n + T_s^{n+1})$$

implemented in `conductionT.f`

1.2.2 Lower boundary condition:

(assume $z_{N+1} - z_N = z_N - z_{N-1}$)
say, no heat flux: $F_{N+\frac{1}{2}} = 0 \quad \Rightarrow \quad k_{N+\frac{1}{2}}(T_{N+1} - T_N) = 0 \quad \Rightarrow \quad T_{N+1} = T_N$

$$(1 + \gamma_N) T_N^{n+1} - \gamma_N T_{N-1}^{n+1} = (1 - \gamma_N) T_N^n + \gamma_N T_{N-1}^n$$

$$\gamma_N = \frac{\Delta t}{(\rho c)_N} \frac{k_{N-\frac{1}{2}}}{2(z_N - z_{N-1})^2}$$

Or geothermal heating: $F_{N+\frac{1}{2}} = F_{\text{geothermal}} \quad \Rightarrow \quad k_{N+\frac{1}{2}}(T_{N+1} - T_N) = \Delta z F_{\text{geothermal}}$

$$(1 + \gamma_N) T_N^{n+1} - \gamma_N T_{N-1}^{n+1} = (1 - \gamma_N) T_N^n + \gamma_N T_{N-1}^n + \frac{\Delta t}{(\rho c)_N} \frac{F_{\text{geothermal}}}{\Delta z}$$

1.3 With Frost Cover

Add latent heat of CO_2 sublimation

$$Q + k \left. \frac{\partial T}{\partial z} \right|_{z=0} = \epsilon \sigma T^4 \big|_{z=0} + L \frac{d m_{CO_2}}{dt} \tag{1.3}$$

call `conductionQ` if T_s is above CO_2 frost point or if $m_{CO_2} = 0$; call `conductionT` if T_s is below CO_2 frost point or if $m_{CO_2} > 0$; calculate energy difference and add CO_2 mass; adjust surface albedo; repeat this at every call

1.4 Influence of Ice on Thermal Conductivity

(This is only one possible parametrization. In retrospective, it agrees well with the laboratory measurements by Siegler et al., J. Geophs. Res. (2012).)

$$\begin{aligned} \rho c &= (1 - \epsilon) \rho_{\text{regolith}} c_{\text{regolith}} + \epsilon f \rho_{\text{ice}} c_{\text{ice}} \\ k &= (1 - \epsilon) k_{\text{regolith}} + \epsilon f k_{\text{ice}} + (1 - f) \epsilon k_{\text{air}} \end{aligned}$$

ρ ... density; c ... heat capacity; k ... thermal conductivity
ϵ ... porosity (void space / total volume)
f ... ice filling fraction ($f = \rho_f / \rho_{\text{ice}}$, ρ_f =density of free ice)

$$
\begin{aligned}
\rho_{\rm obs} c_{\rm obs} &= (1-\epsilon)\rho_{\rm regolith} c_{\rm regolith} \\
k_{\rm obs} &= (1-\epsilon) k_{\rm regolith} \quad \text{if} \quad k_{\rm air} = 0
\end{aligned}
$$

$$
\rho c = \epsilon f \rho_{\rm ice} c_{\rm ice} + \rho_{\rm obs} c_{\rm obs} \qquad\qquad I = \sqrt{\rho c \left(\epsilon f k_{\rm ice} + I_{\rm obs}^2/(\rho_{\rm obs} c_{\rm obs})\right)}
$$

$c_{\rm obs} \approx 800$ J/(kg K), $c_{\rm ice} \approx 2000$ J/(kg K), $\rho_{\rm ice} \approx 926$ kg/m^3, $k_{\rm ice} \approx 2.4$ W/(m K)
$\Rightarrow \quad I_{\rm ice} = \sqrt{k_{\rm ice} \rho_{\rm ice} c_{\rm ice}} \approx 2100$, in SI units
at around 200 Kelvin: $c_{\rm ice} = 1540$ J/(kg K), $\rho_{\rm ice} = 927$ kg/m^3, $k_{\rm ice} = 3.2$ W/(m K)
See Winter & Saari (1969) for heat capacity of silicates as a function of temperature.
See Handbook of Chemistry and Physics for temperature dependences for ice

In the program, k and ρc are defined on half-points, while ρ_f and T are defined on grid points.

Part 2

Diffusion of Water Vapor with Phase Transitions

developed by Norbert Schörghofer, 2003–2004

3 phases: vapor, free ice, adsorbate
diffusion of water vapor; variable diffusivity; irregular grid
implemented in `vapordiffusioni.f`

2.1 Governing Equations

indices: v ... gas (vapor), f ... free ice (solid), a ... adsorbed water
$\bar{\rho}$ ... mass per total volume, $\bar{J}$ ... vapor flux per total area

conservation of mass:

$$\frac{\partial}{\partial t}(\bar{\rho}_v + \bar{\rho}_f + \bar{\rho}_a) + \nabla \cdot \bar{J} = 0 \tag{2.1}$$

vapor transport: (Landau & Lifshitz, Vol. VI, §57, §58)

$$J = -D\rho_0 \nabla c \tag{2.2}$$

c ... concentration $c = \rho_v/\rho_0$
$\rho_{\rm air}$ ... total density of air, including humidity
ρ_v ... density of vapor

$$p_v = nkT = \rho_v \frac{k}{m_v} T \tag{2.3}$$

m ... mass of molecule; k ... Boltzmann constant

adsorption: $\bar{\rho}_a = A(p,T)$
The amount adsorbed also changes when ice is present.

ϵ ... porosity (= void space / total volume)
$\epsilon(1-\rho_f/\rho_{\rm ice})$ ... fraction of space available to gas
$\bar{\rho}_v = \rho_v \epsilon (1-\rho_f/\rho_{\rm ice})$ ρ_v ... vapor density in void space
$\bar{\rho}_f = \rho_f \epsilon$ ρ_f ... ice density in volume not occupied by regolith

$\bar{J} = J\epsilon(1-\rho_f/\rho_{\text{ice}})$ $\quad$ J ... vapor flux through void area
$\rho_{\text{ice}} \approx 926$ kg/m^3 ... density of ice when it's really cold

Conservation of mass becomes

$$\frac{\partial}{\partial t}\left(\rho_v\left(1-\frac{\rho_f}{\rho_{\text{ice}}}\right)+\rho_f+\frac{1}{\epsilon}\bar{\rho}_a\right)+\partial_z\left(1-\frac{\rho_f}{\rho_{\text{ice}}}\right)J=0$$

$$\frac{\partial}{\partial t}\left[\rho_v\left(1-\frac{\rho_f}{\rho_{\text{ice}}}\right)+\rho_f+\frac{1}{\epsilon}\bar{\rho}_a\right]=\partial_z\left[\left(1-\frac{\rho_f}{\rho_{\text{ice}}}\right)D\partial_z\rho_v\right]$$

introduce $\varphi = 1-\dfrac{\rho_f}{\rho_{\text{ice}}}$ and $\gamma=\dfrac{k}{m}\dfrac{1}{\epsilon}$

$$\partial_t\left(\frac{p}{T}\varphi+\frac{k}{m_v}\rho_f\right)+\gamma\left(\frac{\partial\bar{\rho}_a}{\partial p}\partial_t p+\frac{\partial\bar{\rho}_a}{\partial T}\partial_t T\right)=\partial_z\left[D\varphi\left(\partial_z\frac{p}{T}\right)\right] \tag{2.4}$$

This is an equation for p and ρ_f.

If there is no ice, then

$$\left(\frac{1}{T}+\gamma\frac{\partial\bar{\rho}_a}{\partial p}\right)\partial_t p+\left(-\frac{p}{T^2}+\gamma\frac{\partial\bar{\rho}_a}{\partial T}\right)\partial_t T=\partial_z\left(D\partial_z\frac{p}{T}\right)$$

2.2 Discretizations

2.2.1 Possible discretizations of spatial derivatives:

Note: These spatial discretizations are not necessarily the best possible.

$$\partial_z(a\partial_z b)\big|_j=\frac{1}{\Delta z^2}\left(a_{j+1/2}(b_{j+1}-b_j)-a_{j-1/2}(b_j-b_{j-1})\right)+O(\Delta z^2) \tag{2.5}$$

or

$$\partial_z(a\partial_z b)\big|_j=\frac{1}{2\Delta z^2}\left((a_{j+1}+a_j)(b_{j+1}-b_j)-(a_j+a_{j-1})(b_j-b_{j-1})\right)+O(\Delta z^2) \tag{2.6}$$

or

$$\begin{aligned}\partial_z(a\partial_z b)\big|_j &= a\partial_{zz}b+(\partial_z a)\partial_z b\\ &= \frac{1}{\Delta z^2}\left(a_j(b_{j+1}-2b_j+b_{j-1})+\frac{1}{4}(a_{j+1}-a_{j-1})(b_{j+1}-b_{j-1})\right)+O(\Delta z^2)\end{aligned} \tag{2.7}$$

The most general discretization which is accurate to $O(\Delta z^2)$, rather than just $O(\Delta z)$, is of the following form (see mathematica notebook discretization2.nb)

$$\begin{aligned}\partial_z(a\partial_z b)\big|_j &= \frac{1}{\Delta z^2}(ca_jb_j+(-1-\frac{c}{2})a_{j-1}b_j+(-1-\frac{c}{2})a_{j+1}b_j\\ &\quad -\frac{c}{2}a_jb_{j-1}+\frac{3+c}{4}a_{j-1}b_{j-1}+\frac{1+c}{4}a_{j+1}b_{j-1}\\ &\quad -\frac{c}{2}a_jb_{j+1}+\frac{1+c}{4}a_{j-1}b_{j+1}+\frac{3+c}{4}a_{j+1}b_{j+1})+O(\Delta z^2)\end{aligned} \tag{2.8}$$

Choices (2.6) and (2.7) above correspond to $c = -1$ and $c = -2$, respectively.

Another set of schemes are the ones that do not involve the corner points $a_{j+1}b_{j-1}$ and $a_{j-1}b_{j+1}$. They are of the following form (see mathematica notebook discretization3.nb)

$$\begin{aligned}\partial_z(a\partial_z b)\big|_j &= \frac{1}{\Delta z^2}(-a_jb_j - ca_{j-1}b_j + (-1+c)a_{j+1}b_j + \\ &\quad (1-c)a_jb_{j-1} + ca_{j-1}b_{j-1} + ca_jb_{j+1} + (1-c)a_{j+1}b_{j+1}) + \\ &\quad \left(c - \frac{1}{2}\right)O(\Delta z) + O(\Delta z^2) \qquad (2.9)\\ &= \frac{1}{\Delta z^2}\left[(1-c)a_{j+1}(b_{j+1}-b_j) + ca_{j-1}(b_{j-1}-b_j) + a_j(cb_{j+1} - b_j + (1-c)b_{j-1})\right] + O(\Delta z)\end{aligned}$$

For $c = 1/2$ this reduces to scheme (2.6) above
If starting with complete pore filling, $c > 0$ is required for downward motion of ice table.
On irregular grid: General scheme without corner points (see mathematica notebook discretization6.nb)

$$\begin{aligned}\partial_z(a\partial_z b)\big|_j &= -\frac{2c + (1-2c)h_+/h_-}{h_-h_+}a_jb_j + \frac{-1 + (1-2c)h_+/h_-}{h_-(h_- + h_+)}a_{j-1}b_j + \frac{2c-2}{h_+(h_- + h_+)}a_{j+1}b_j + \\ &\quad + \frac{1 + (1-2c)h_+/h_-}{h_-(h_- + h_+)}a_jb_{j-1} + \frac{1 + (2c-1)h_+/h_-}{h_-(h_- + h_+)}a_{j-1}b_{j-1} + \frac{2c}{h_+(h_- + h_+)}a_jb_{j+1} \\ &\quad + \frac{2-2c}{h_+(h_- + h_+)}a_{j+1}b_{j+1} + O(h_+ + h_-) \qquad (2.10)\end{aligned}$$

where $h_+ = z_{j+1} - z_j$ and $h_- = z_j - z_{j-1}$. For $h_+ = h_- = h$ this reduces to (2.9)

2.2.2 Discretization of time derivative:

use eq. (2.4), $A \equiv f$

$$\begin{aligned}\frac{p_j^{n+1}}{T_j^{n+1}}\varphi_j^{n+1} - \frac{p_j^n}{T_j^n}\varphi_j^n + \frac{k}{\mu}\left({\rho_f}_j^{n+1} - {\rho_f}_j^n\right) + \gamma\left.\frac{\partial f}{\partial p}\right|_j^n (p_j^{n+1} - p_j^n) + \\ +\gamma\left.\frac{\partial f}{\partial T}\right|_j^n (T_j^{n+1} - T_j^n) = \Delta t\left(\partial_z D\varphi\partial_z\frac{p}{T}\right)_j^n \qquad (2.11)\end{aligned}$$

derivatives of the isotherm are not expanded to keep it linear

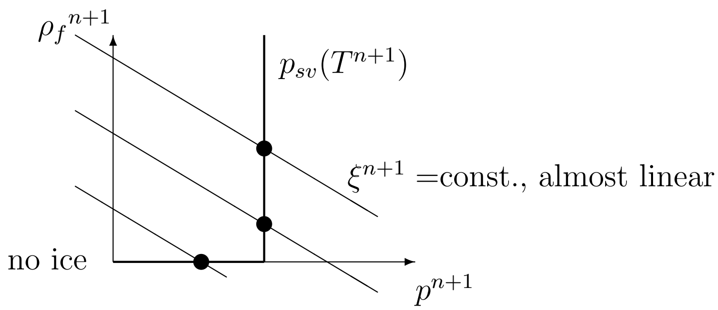
2.2.3 Complete scheme:

using (2.11) and (2.10)

$$\begin{aligned}\xi_j^{n+1} &= \frac{p_j^n}{T_j^n}\varphi_j^n + \frac{k}{\mu}{\rho_f}_j^n + \gamma\left.\frac{\partial f}{\partial p}\right|_j^n p_j^n - \gamma\left.\frac{\partial f}{\partial T}\right|_j^n (T_j^{n+1} - T_j^n) + \\ &\quad \frac{\Delta t}{\Delta z^2}\left[D_j\varphi_j^n\left(\frac{p_{j+1}^n}{T_{j+1}^n} - 2\frac{p_j^n}{T_j^n} + \frac{p_{j-1}^n}{T_{j-1}^n}\right) + \frac{1}{4}(D_{j+1}\varphi_{j+1}^n - D_{j-1}\varphi_{j-1}^n)\left(\frac{p_{j+1}^n}{T_{j+1}^n} - \frac{p_{j-1}^n}{T_{j-1}^n}\right)\right]\end{aligned}$$

where $\xi^{n+1} = \frac{p^{n+1}}{T^{n+1}}\left(1 - \frac{\rho_f^{n+1}}{\rho_{\text{ice}}}\right) + \frac{k}{\mu}{\rho_f}^{n+1} + \gamma \left.\frac{\partial f}{\partial p}\right|^n p^{n+1}$

$p \leq p_{sv}(T)$ and $0 \leq \rho_f \leq \rho_{\text{ice}}$



p_{sv} ... saturation vapor pressure

Try $\rho_f^{n+1} = 0 \quad \Rightarrow \quad p^{n+1} = \frac{T^{n+1} \cdot \xi^{n+1}}{1 + T^{n+1}\gamma \left.\frac{\partial f}{\partial p}\right|^n}$ and $\rho_f^{n+1} = 0$

If $p^{n+1} > p_{sv}(T^{n+1})$ then $p^{n+1} = p_{sv}(T^{n+1})$ and

$$\rho_f^{n+1} = \frac{\xi^{n+1} - \frac{p_{sv}(T^{n+1})}{T^{n+1}} - \gamma \left.\frac{\partial f}{\partial p}\right|^n p_{sv}(T^{n+1})}{\frac{k}{\mu} - \frac{p_{sv}(T^{n+1})}{T^{n+1}\rho_{\text{ice}}}}$$

introduce $p_{\text{frost}}^{n+1} = p_{sv}(T^{n+1})$

2.2.4 Upper boundary condition:

1) $p(z = 0, t) = p_{\text{atm.}}(t)$
2) $D(z = 0) = D_0$
3) $\varphi_0 = 1$

$$\partial_z \left(D\varphi\partial_z \frac{p}{T}\right)\Big|_{j=0} = \frac{1}{\Delta z^2}\left[D_1\varphi_1\left(\frac{p_2}{T_2} - 2\frac{p_1}{T_1} + \frac{p_{\text{atm}}}{T_{\text{surf}}}\right) + \frac{1}{4}(D_2\varphi_2 - D_0\varphi_0)\left(\frac{p_2}{T_2} - \frac{p_{\text{atm}}}{T_{\text{surf}}}\right)\right] \quad (2.12)$$

for half-shifted grid ($z_2 = 3z_1$):

$$a\partial_{zz}b + (\partial_z a)\partial_z b = \frac{1}{\Delta z^2}\left[a_1\left(\frac{8}{3}b_s - 4b_1 + \frac{4}{3}b_2\right) + \left(-\frac{4}{3}a_s + a_1 + \frac{1}{3}a_2\right)\left(-\frac{4}{3}b_s + b_1 + \frac{1}{3}b_2\right)\right] \quad (2.13)$$

2.2.5 Lower boundary condition:

no vapor flux (impermeable) $J = 0 \quad \Rightarrow \quad \partial_z \rho_v = 0 \quad \Rightarrow \quad \partial_z \frac{p}{T} = 0 \quad \Rightarrow \quad \frac{p_{N+1}}{T_{N+1}} = \frac{p_{N-1}}{T_{N-1}}$

$$\partial_z \left(D\varphi\partial_z \frac{p}{T} \right)\Big|_{j=N} = \frac{1}{\Delta z^2} 2D_N\varphi_N \left(\frac{p_{N-1}}{T_{N-1}} - \frac{p_N}{T_N} \right) \tag{2.14}$$

2.3 Numerical Stability

Stability analysis for p (vapor), 2nd order schemes:

consider $b_{j\pm1} = b_j e^{\pm ik\Delta z}$ and $a_{j\pm1} = a_j \pm a'_j\Delta z$ in (2.8)

$$\begin{aligned}
\partial_z(a\partial_z b)\big|_j &= \frac{a_jb_j}{\Delta z^2}(c + (-1-\frac{c}{2})(1-\frac{a'_j\Delta z}{a_j}) + (-1-\frac{c}{2})(1+\frac{a'_j\Delta z}{a_j}) \\
&\quad -\frac{c}{2}e^{-ik\Delta z} + \frac{3+c}{4}(1-\frac{a'_j\Delta z}{a_j})e^{-ik\Delta z} + \frac{1+c}{4}(1+\frac{a'_j\Delta z}{a_j})e^{-ik\Delta z} \\
&\quad -\frac{c}{2}e^{+ik\Delta z} + \frac{1+c}{4}(1-\frac{a'_j\Delta z}{a_j})e^{+ik\Delta z} + \frac{3+c}{4}(1+\frac{a'_j\Delta z}{a_j})e^{+ik\Delta z}) + O(\Delta z^2) \\
&= \frac{a_jb_j}{\Delta z^2}\left(-2 + 2\cos(k\Delta z) - i\frac{a'_j\Delta z}{a_j}\sin(k\Delta z)\right), \quad \text{independent of } c
\end{aligned}$$

introduce $\rho = p/T$, then

$$\rho^{n+1} = \rho^n + \frac{\Delta t D\rho^n}{\Delta z^2}\left(-2 + 2\cos(k\Delta z) - i\frac{D'\Delta z}{D}\sin(k\Delta z)\right)$$

$$\frac{\rho^{n+1}}{\rho^n} = 1 + \frac{2D\Delta t}{\Delta z^2}\left(-1+\cos(k\Delta z)\right) - i\frac{\Delta t}{\Delta z}D'\sin(k\Delta z)$$

$$\left|\frac{\rho^{n+1}}{\rho^n}\right|^2 = \left(1 + \frac{2D\Delta t}{\Delta z^2}(-1+\cos(k\Delta z))\right)^2 + \left(\frac{\Delta t}{\Delta z}D'\right)^2\sin(k\Delta z)$$

extremum must be at $\cos(k\Delta z) = +1, -1, \text{or } \frac{1-\frac{\Delta z^2}{2D\Delta t}}{1-\left(\frac{D'\Delta z}{D}\right)^2}$. The corresponding amplification factors are

$$1, \quad 1 - \frac{4D\Delta t}{\Delta z^2}, \quad D'\sqrt{\frac{-4D\Delta t + (D'\Delta t)^2 + \Delta z^2}{-4D^2 + (D'\Delta z)^2}}$$

Leading to the stability criterion

$$\Delta t \le \min\left(\frac{\Delta z^2}{2D}, \frac{2D}{D'^2}\right) \quad \text{where} \quad D' = \max(|\partial_z D|)$$

Stability analysis for φ (ice), 2nd order schemes:

consider $a_{j\pm1} = a_j e^{\pm ik\Delta z}$ and $b_{j\pm1} = b_j \pm b'_j\Delta z$ in (2.8), then

$$\partial_z(a\partial_z b)\big|_j = i\frac{a_jb'_j}{\Delta z}\sin(k\Delta z)\text{independent of } c$$

$$r^{n+1}\varphi^{n+1} + \frac{k}{\mu}\rho_{\text{ice}}(1-\varphi^{n+1}) = r^n\varphi^n + \frac{k}{\mu}\rho_{\text{ice}}(1-\varphi^n) + i\frac{\Delta t D\varphi^n}{\Delta z}r'\sin(k\Delta z)$$

$$\varphi^{n+1}(r^{n+1} - \frac{k}{\mu}\rho_{\text{ice}}) = \varphi^n\left(r^n - \frac{k}{\mu}\rho_{\text{ice}} + i\frac{\Delta t D}{\Delta z}r'\sin(k\Delta z)\right)$$

$\rho_v \ll \rho_{\text{ice}}$

$$\frac{\varphi^{n+1}}{\varphi^n} \approx 1 + \frac{\rho_v^{n+1}-\rho_v^n}{\rho_{\text{ice}}} - i\frac{\Delta t D}{\Delta z}\frac{\rho_v'}{\rho_{\text{ice}}}\sin(k\Delta z) \quad \text{where} \quad \rho_v' = \partial_z\rho_v$$

$$\left|\frac{\varphi^{n+1}}{\varphi^n}\right|^2 \approx 1 + 2\frac{\dot{\rho}_v\Delta t}{\rho_{\text{ice}}}$$

growth $O(\rho_v/\rho_{\text{ice}})$ corresponds to physical growth. marginally stable

Stability analysis for p (vapor), corner-free schemes:

(see mathematica notebook discretization3.nb)

$$\frac{\rho^{n+1}}{\rho^n} = 1 + \frac{\Delta t}{\Delta z^2}\left((2D + (1-2c)\Delta z D')(-1+\cos(hk)) + i\Delta z D'\sin(hk)\right)$$

for $D' = 0$ it becomes independent of c

$$\left|\frac{\rho^{n+1}}{\rho^n}\right| = 1 + \frac{2\Delta t D}{\Delta z^2}(-1+\cos(hk))$$

$$\Delta t \leq \frac{\Delta z^2}{2D}$$

Stability analysis for φ (ice), corner-free schemes:

(see mathematica notebook discretization3.nb)

$$\partial_z(a\partial_z b) = \frac{ab'}{\Delta z}\left((1-2c)(-1+\cos(hk)) + i\sin(hk)\right)$$

$$\frac{\varphi^{n+1}}{\varphi^n} = 1 - \frac{\Delta t D}{\Delta z}\frac{\partial_z\rho_v}{\rho_{\text{ice}}}\left((1-2c)(-1+\cos(hk)) + i\sin(hk)\right)$$

$$\begin{aligned} |A|^2 &= [-1 + g(1-2c) + (2c-1)g\cos(hk)]^2 + g^2\sin^2(hk) \quad \text{where} \quad g = \frac{\Delta t D}{\Delta z}\frac{\partial_z\rho_v}{\rho_{\text{ice}}} \ll 1 \\ &\approx 1 - 2g(1-2c)(1-\cos(hk)) \leq 1 - 4g(1-2c) \end{aligned}$$

Thus, $c \leq 1/2$ is necessary for stability
from $1 \geq 2g(1-2c) \geq 0$ and $|\partial_z\rho_v| \leq \rho_v/h$ we get

$$\frac{\Delta t D}{\Delta z^2}\frac{\rho_v}{\rho_{\text{ice}}} \leq \frac{1}{2(1-2c)}$$

For $c < 1/2$, the amplification $|A| < 1$ and therefore the scheme is really stable, not just marginally.