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

Norbert Schörghofer (norbert@hawaii.edu)

These notes were originally written around 2003
and last updated on June 27, 2014

Part 1

Conduction of Heat

originally developed by Samar Khatiwala in 2001 (including upper radiation boundary condition)
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

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

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

1.2 Semi-Implicit Scheme on Irregular Grid

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

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

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

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

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

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

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.

Upper boundary condition:

a) Radiation

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

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

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

$T = T_r + T'$ $\qquad$ 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 $\Delta z = z_2 - z_1 = 2 z_1$, define $\beta = \frac{\Delta t}{(\rho c)_1} \frac{1}{2 \Delta z^2}$, then $\alpha_1 = \beta k_{3/2}$ and $\gamma_1 = \beta k_{1/2}$

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

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

b) prescribed T

standard formula 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`

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

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

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.)

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

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

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

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

$c_{\text{obs}} \approx 800$ J/(kg K), $c_{\text{ice}} \approx 2000$ J/(kg K), $\rho_{\text{ice}} \approx 926$ kg/m^3, $k_{\text{ice}} \approx 2.4$ W/(m K)
$\Rightarrow \quad I_{\text{ice}} = \sqrt{k_{\text{ice}}\rho_{\text{ice}}c_{\text{ice}}} \approx 2100$, in SI units
at around 200 Kelvin: $c_{\text{ice}} = 1540$ J/(kg K), $\rho_{\text{ice}} = 927$ kg/m^3, $k_{\text{ice}} = 3.2$ 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 $c = \rho_v/\rho_0$
ρ_{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)
$\epsilon(1 - \rho_f/\rho_{\mathrm{ice}})$ ... fraction of space available to gas
$\bar{\rho}_v = \rho_v \epsilon(1 - \rho_f/\rho_{\mathrm{ice}})$ ρ_v ... vapor density in void space
$\bar{\rho}_f = \rho_f \epsilon$ ρ_f ... ice density in volume not occupied by regolith

$\bar{J} = J\epsilon(1 - \rho_f/\rho_{\text{ice}})$ 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

Possible discretizations of spatial derivatives:

Note: The spatial discretizations are probably not 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)

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

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)

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

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)

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

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

Discretization of time derivative:

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

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

derivatives of the isotherm are not expanded to keep it linear

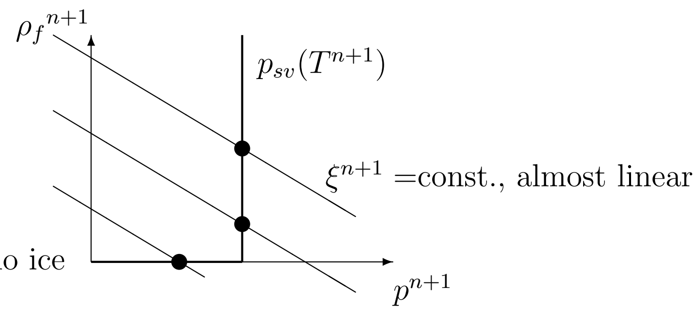
Complete scheme:

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

Upper boundary condition:

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

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

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

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

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)

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

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

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

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

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

$$\frac{\varphi^{n+1}}{\varphi^n} \approx 1 + \frac{\rho_v^{n+1}-\rho_v^n}{\rho_{\rm ice}} - i\frac{\Delta t D}{\Delta z}\frac{\rho_v'}{\rho_{\rm ice}}\sin(k\Delta z) \quad \text{where} \quad \rho_v' = \partial_z\rho_v$$
$$\left|\frac{\varphi^{n+1}}{\varphi^n}\right|^2 \approx 1 + 2\frac{\dot\rho_v\Delta t}{\rho_{\rm ice}}$$

growth $O(\rho_v/\rho_{\rm ice})$ 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

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

$\Delta t \le \dfrac{\Delta z^2}{2D}$

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

(see mathematica notebook discretization3.nb)

$$\partial_z(a\partial_z b) = \frac{ab'}{\Delta z}\left((1-2c)(-1+\cos(hk)) + i\sin(hk)\right)$$
$$\frac{\varphi^{n+1}}{\varphi^n} = 1 - \frac{\Delta t D}{\Delta z}\frac{\partial_z\rho_v}{\rho_{\rm ice}}\left((1-2c)(-1+\cos(hk)) + i\sin(hk)\right)$$

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

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

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

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