Semi-implicit gravity

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Hi Tommaso,

in dreaming up the semi-implicit gravity version in the appendix of your thesis, I think we missed one crucial point. Reconsidering, I came to the conclusion that it is the "explicit part of the implicit step" in the trapezoidal rule that controls vertical velocities, and thus stability, for large time steps. I'll try to highlight this in the following short note.

Best,

Rupert

1 The second step of the implicit trapezoidal rule

Focusing just on the crucial linear terms in the governing equations that are responsible for internal waves, we have – for advection of the background potential temperature and for the vertical momentum,

$$
\begin{aligned}
w_t &= -\frac{\theta}{\Gamma}\left(\pi_z + \Gamma g \chi\right) && (1)\\
\chi_t &= -w\frac{d\overline{\chi}}{dz} && (2)
\end{aligned}
$$

here π is Exner pressure, $\Gamma = (\gamma - 1)/\gamma$ with γ the isentropic exponent, $\chi = 1/\theta$, and the prefactor θ in the first equation is frozen in for the linearization. Suppose that an explicit Euler forward step for these equations over $\Delta t/2$ as well as advection of all quantities have been taken care of in operator splitting-like steps, so that all that is left to do is an implicit, backward Euler step over $\tau = \Delta t/2$.

Suppose that (χ^*, w^*, π^*) denote the state of the relevant solution variables at the start of the implicit substep and $(\delta\chi, \delta w, \delta\pi)$ the respective updates over the implicit step. Then,

$$
\begin{aligned}
w^{n+1} - w^* \equiv \delta w &= -\tau\,\frac{\theta}{\Gamma}\left([\pi^* + \delta\pi]_z + \Gamma g[\chi^* + \delta\chi]\right) && (3)\\
\chi^{n+1} - \chi^* \equiv \delta\chi &= -\tau\left(w^* + \delta w\right)\frac{d\overline{\chi}}{dz}\,. && (4)
\end{aligned}
$$

Now we reorder explicit and implicit contributions, replace $\delta\chi$ in (3) using (4) and solve for δw,

$$
\begin{aligned}
w^{n+1} - w^* = \delta w &= -\tau\,\frac{\theta}{\Gamma}\left(\pi_z^* + \Gamma g \chi^*\right) - \tau\,\frac{\theta}{\Gamma}\left(\delta\pi_z + \Gamma g \delta\chi\right) && (5)\\
&= -\tau\,\frac{\theta}{\Gamma}\left(\pi_z^* + \Gamma g \chi^*\right) - \tau\,\frac{\theta}{\Gamma}\left(\delta\pi_z - \tau\,\Gamma g (w^* + \delta w)\frac{d\overline{\chi}}{dz}\right) && (6)\\
\delta w\left(1 - \tau^2 g\theta\frac{d\overline{\chi}}{dz}\right) &= -\tau\,\frac{\theta}{\Gamma}\left(\pi_z^* + \Gamma g \chi^*\right) + w^*\tau^2 g\theta\frac{d\overline{\chi}}{dz} - \tau\,\frac{\theta}{\Gamma}\delta\pi_z\,. && (7)
\end{aligned}
$$

Letting

$$
N^2 = -g\theta\frac{d\overline{\chi}}{dz} \tag{8}
$$

denote the square of the buoyancy-frequency, we have

$$
\delta w = \frac{1}{1+(\tau N)^2}\left(-\tau\frac{\theta}{\Gamma}\left(\pi_z^* + \Gamma g \chi^*\right) - w^*(\tau N)^2\right) - \tau\frac{\theta/\Gamma}{1+(\tau N)^2}\delta\pi_z \tag{9}
$$

and the update formular for χ subsequently follows from (4).

Consider now the first term on the right in (9), which contains all explicit contributions to the velocity update, and its scaling for large time steps $\tau \to \infty$. The first term in the bracket scales linearly with τ, so that it vanishes in the limit. The second term in the bracket involves $(\tau N)^2$, however, and therefore the limit reads

$$
\delta w\big|_{\tau\to\infty} = -w^*\,. \tag{10}
$$

That is, the first thing the explicit part of the implicit step does is to set the vertical velocity to zero in that limit! This is clearly a stabilizing effect that can capture any large excursion in w^* that may have incurred during the explicit half-time step of the trapezoidal rule.

Tommaso, I think we left this bit out in our earlier attempts. I have implemented a variant of this in my scheme and see the stabilization of vertical velocity very nicely for $N\Delta t$ as large as five. The large scale horizontal domain with a hydrostatic gravity wave still does not quite work yet, but I have two more things to try: (i) locally hydrostatic initialization of pressure - which in my current setup I do not have, and (ii) a preconditioner that addresses the vertical part of the Poisson problem, instead of preconditioning only through division by the diagonal element of the Poisson-matrix. Will keep you posted.

Best,

Rupert

2 Implicit trapezoidal rule – variant 2

2.1 Linear oscillator

To understand the mechanism of stabilization for arbitrary time steps in the implicit trapezoidal rule, we consider

$$\ddot{y} + y = 0 \qquad \text{or rather} \qquad \begin{array}{rcl} \dot{y} & = & v \\ \dot{v} & = & -y \end{array} . \tag{11}$$

The implicit trapezoidal rule for the system version of this problem over one time step reads

$$\begin{array}{rcl} y^{n+1} - y^n & = & \dfrac{\Delta t}{2}\left(v^{n+1} + v^n\right) \\ v^{n+1} - v^n & = & -\dfrac{\Delta t}{2}\left(y^{n+1} + y^n\right) \end{array} . \tag{12}$$

We solve for v^{n+1} first:

$$\begin{array}{rcl} v^{n+1} & = & v^n - \dfrac{\Delta t}{2}\left(y^n + \dfrac{\Delta t}{2}\left(v^{n+1} + v^n\right) + y^n\right) \\ v^{n+1}\left(1 + \dfrac{(\Delta t)^2}{4}\right) & = & v^n\left(1 - \dfrac{(\Delta t)^2}{4}\right) - \Delta t\, y^n \\ v^{n+1} & = & \dfrac{1 - \frac{(\Delta t)^2}{4}}{1 + \frac{(\Delta t)^2}{4}}\, v^n - \dfrac{\Delta t}{1 + \frac{(\Delta t)^2}{4}}\, y^n \end{array} \tag{13}$$

or

$$v^{n+1} - v^n \equiv \delta v = -\, 2v^n\, \frac{\frac{(\Delta t)^2}{4}}{1 + \frac{(\Delta t)^2}{4}} - \frac{\Delta t}{1 + \frac{(\Delta t)^2}{4}}\, y^n \tag{14}$$

Similarly,

$$\begin{array}{rcl} y^{n+1} & = & y^n + \dfrac{\Delta t}{2}\left(v^n - \dfrac{\Delta t}{2}\left(y^{n+1} + y^n\right) + v^n\right) \\ y^{n+1}\left(1 + \dfrac{(\Delta t)^2}{4}\right) & = & y^n\left(1 - \dfrac{(\Delta t)^2}{4}\right) + \Delta t\, v^n \\ y^{n+1} & = & \dfrac{1 - \frac{(\Delta t)^2}{4}}{1 + \frac{(\Delta t)^2}{4}}\, y^n + \dfrac{\Delta t}{1 + \frac{(\Delta t)^2}{4}}\, v^n \end{array} \tag{15}$$

Clearly,

$$\lim_{\Delta t \to \infty} (y^{n+1}, n^{n+1}) = -(y^n, v^n)\,, \tag{16}$$

and this characterizes the energy-preserving, oscillatory nature, and unconditional neutrality of the scheme in the large-time step limit.

Can we understand the implicit trapezoidal rule as a two-step scheme involving a forward Euler predictor and a backward Euler corrector? Let's see.

Forward Euler predictor:

$$\begin{array}{rcl} y^* - y^n & = & \dfrac{\Delta t}{2}\, v^n \\ v^* - v^n & = & -\dfrac{\Delta t}{2}\, y^n \end{array} . \tag{17}$$

Backward Euler corrector:

$$\begin{array}{rcl} y^{n+1} - y^* & = & \dfrac{\Delta t}{2}\, v^{n+1} \\ v^{n+1} - v^* & = & -\dfrac{\Delta t}{2}\, y^{n+1} \end{array} . \tag{18}$$

Obviously, adding the two equation sets we get back the implicit trapezoidal rule from (12). Solving for the new time data, however, given the predicted ones, we obtain

$$\begin{aligned} v^{n+1} &= v^* - \frac{\Delta t}{2}\left(y^* + \frac{\Delta t}{2}\, v^{n+1}\right) \\ v^{n+1}\left(1 + \frac{(\Delta t)^2}{4}\right) &= v^* - \frac{\Delta t}{2}\, y^* \\ v^{n+1} &= \frac{1}{1+\frac{(\Delta t)^2}{4}}\, v^* - \frac{1}{2}\frac{\Delta t}{1+\frac{(\Delta t)^2}{4}}\, y^* \end{aligned} \tag{19}$$

For the increment within the half timestep we have

$$v^{n+1} - v^* \equiv \delta v = -\, v^* \frac{\frac{(\Delta t)^2}{4}}{1+\frac{(\Delta t)^2}{4}} - \frac{1}{2}\frac{\Delta t}{1+\frac{(\Delta t)^2}{4}}\, y^* \tag{20}$$

To get back to the original formula from (13) we re-insert the predictor step to obtain

$$\begin{aligned} v^{n+1} &= \frac{1}{1+\frac{(\Delta t)^2}{4}}\, v^* - \frac{1}{2}\frac{\Delta t}{1+\frac{(\Delta t)^2}{4}}\, y^* \\ &= \frac{1}{1+\frac{(\Delta t)^2}{4}}\left(v^n - \frac{\Delta t}{2} y^n\right) - \frac{1}{2}\frac{\Delta t}{1+\frac{(\Delta t)^2}{4}}\left(y^n + \frac{\Delta t}{2} v^n\right) \\ &= \frac{1-\frac{(\Delta t)^2}{4}}{1+\frac{(\Delta t)^2}{4}}\, v^n - \frac{\Delta t}{1+\frac{(\Delta t)^2}{4}}\, y^n \end{aligned} \tag{21}$$

And analogously for y^{n+1}, i.e.,

$$y^{n+1} = \frac{1-\frac{(\Delta t)^2}{4}}{1+\frac{(\Delta t)^2}{4}}\, y^n + \frac{\Delta t}{1+\frac{(\Delta t)^2}{4}}\, v^n \tag{22}$$

We distinguish the cases of $(y^n, v^n) = \mathcal{O}(1)$ and $y^n = 0$ or $v^n = 0$ and consider the limit $\Delta t \to \infty$:

1. Obviously, when $(y^n, v^n) = \mathcal{O}(1)$, we have

$$y^{n+1}\big|_{\Delta t\to\infty} = -y^n\,. \qquad \text{and} \qquad v^{n+1}\big|_{\Delta t\to\infty} = -v^n \tag{23}$$

2. However, if the respective initial datum is zero, the limiting behavior changes as follows. Suppose $y^n = 0$, but $v^n \neq 0$. Then,

$$y^{n+1} = \frac{\Delta t}{1+\frac{(\Delta t)^2}{4}}\, v^n \qquad \text{and} \qquad v^{n+1} = \frac{1-\frac{(\Delta t)^2}{4}}{1+\frac{(\Delta t)^2}{4}}\, v^n \to -v^n\,. \tag{24}$$

Now, can we also understand the implicit trapezoidal rule as a two-step scheme involving a first the backward and second the forward Euler step? Let's see.

Backward Euler step:

$$\begin{aligned} y^* - y^n &= \frac{\Delta t}{2}\, v^* \\ v^* - v^n &= -\frac{\Delta t}{2}\, y^* \end{aligned}\,. \tag{25}$$

Forward Euler step:

$$\begin{aligned} y^{n+1} - y^* &= \frac{\Delta t}{2}\, v^* \\ v^{n+1} - v^* &= -\frac{\Delta t}{2}\, y^* \end{aligned} . \tag{26}$$

Solving for the intermediate time data first we obtain

$$\begin{aligned} v^* &= v^n - \frac{\Delta t}{2} y^* \\ y^* &= y^n + \frac{\Delta t}{2} v^* = y^n + \frac{\Delta t}{2}\left(v^n - \frac{\Delta t}{2} y^*\right) \\ y^*\left(1 + \frac{(\Delta t)^2}{4}\right) &= y^n + \frac{\Delta t}{2}\, v^n \\ y^* &= \frac{1}{1+\frac{(\Delta t)^2}{4}}\, \left(y^n + \frac{\Delta t}{2}\, v^n\right) \end{aligned} \tag{27}$$

and then,

$$\begin{aligned} v^* &= v^n - \frac{\Delta t}{2} y^* \\ &= v^n - \frac{\frac{\Delta t}{2}}{1+\frac{(\Delta t)^2}{4}} \left(y^n + \frac{\Delta t}{2} v^n\right) \\ &= \frac{1}{1+\frac{(\Delta t)^2}{4}} \left(v^n - \frac{\Delta t}{2} y^n\right) \end{aligned} \tag{28}$$

Next we insert into the forward Euler step in (26) to obtain,

$$\begin{aligned} v^{n+1} &= v^* - \frac{\Delta t}{2} y^* \\ &= \frac{1}{1+\frac{(\Delta t)^2}{4}} \left(v^n - \frac{\Delta t}{2} y^n - \frac{\Delta t}{2}\left(y^n + \frac{\Delta t}{2} v^n\right)\right) \\ &= \frac{1-\frac{(\Delta t)^2}{4}}{1+\frac{(\Delta t)^2}{4}} v^n - \frac{\Delta t}{1+\frac{(\Delta t)^2}{4}} y^n \end{aligned} \tag{29}$$

and that is the same as found in (13).

2.1.1 Summary

Euler forward over Δt:

$$\begin{aligned} y^{\text{new}} &= y^{\text{old}} + \Delta t\, v^{\text{old}} \\ v^{\text{new}} &= v^{\text{old}} - \Delta t\, y^{\text{old}} \end{aligned} . \tag{30}$$

Euler backward over Δt:

$$\begin{aligned} y^{\text{new}} &= \frac{1}{1+(\Delta t)^2}\, \left(y^{\text{old}} + \Delta t\, v^{\text{old}}\right) = y^{\text{old}} - \frac{(\Delta t)^2}{1+(\Delta t)^2} y^{\text{old}} + \frac{\Delta t}{1+(\Delta t)^2} v^{\text{old}} \\ v^{\text{new}} &= \frac{1}{1+(\Delta t)^2}\, \left(v^{\text{old}} - \Delta t\, y^{\text{old}}\right) = v^{\text{old}} - \frac{(\Delta t)^2}{1+(\Delta t)^2} v^{\text{old}} - \frac{\Delta t}{1+(\Delta t)^2} y^{\text{old}} \end{aligned} \tag{31}$$

Implicit trapezoidal rule over Δt:

$$
\begin{aligned}
y^{\mathrm{new}} &= \frac{1-\frac{(\Delta t)^2}{4}}{1+\frac{(\Delta t)^2}{4}} y^{\mathrm{old}} + \frac{\Delta t}{1+\frac{(\Delta t)^2}{4}} v^{\mathrm{old}} &= y^{\mathrm{old}} - \frac{2\frac{(\Delta t)^2}{4}}{1+\frac{(\Delta t)^2}{4}} y^{\mathrm{old}} + \frac{\Delta t}{1+\frac{(\Delta t)^2}{4}} v^{\mathrm{old}} \\
v^{\mathrm{new}} &= \frac{1-\frac{(\Delta t)^2}{4}}{1+\frac{(\Delta t)^2}{4}} v^{\mathrm{old}} - \frac{\Delta t}{1+\frac{(\Delta t)^2}{4}} y^{\mathrm{old}} &= v^{\mathrm{old}} - \frac{2\frac{(\Delta t)^2}{4}}{1+\frac{(\Delta t)^2}{4}} v^{\mathrm{old}} - \frac{\Delta t}{1+\frac{(\Delta t)^2}{4}} y^{\mathrm{old}}
\end{aligned}
\tag{32}
$$

2.2 Implicit gravity

2.2.1 Explicit part of the implicit trapezoidal rule

Focusing just on the crucial linear terms in the governing equations that are responsible for internal waves, we have – for advection of the background potential temperature and for the vertical momentum,

$$
w_t = -\frac{\theta}{\Gamma}\left(\pi_z + \Gamma g \chi\right) \tag{33}
$$

$$
\chi_t = -w \frac{d\overline{\chi}}{dz} \tag{34}
$$

here π is Exner pressure, $\Gamma = (\gamma - 1)/\gamma$ with γ the isentropic exponent, $\chi = 1/\theta$, and the prefactor θ in the first equation is frozen in for the linearization. Suppose we wish to integrate these equations using the implicit trapezoidal rule over a time step Δt. Then,

$$
w^{n+1} - w^n \equiv \delta w = -\Delta t \, \frac{\theta}{\Gamma}\left(\left[\pi^n + \frac{\delta\pi}{2}\right]_z + \Gamma g \left[\chi^n + \frac{\delta\chi}{2}\right]\right) \tag{35}
$$

$$
\chi^{n+1} - \chi^n \equiv \delta\chi = -\Delta t \left(w^n + \frac{\delta w}{2}\right)\frac{d\overline{\chi}}{dz} \, . \tag{36}
$$

Now we reorder explicit and implicit contributions, replace $\delta\chi$ in (35) using (36) and solve for δw,

$$
\begin{aligned}
w^{n+1} - w^n = \delta w &= -\Delta t \, \frac{\theta}{\Gamma}\left(\pi_z^n + \Gamma g \chi^n\right) - \frac{\Delta t}{2}\,\frac{\theta}{\Gamma}\left(\delta\pi_z + \Gamma g \delta\chi\right) && (37)\\
&= -\Delta t \, \frac{\theta}{\Gamma}\left(\pi_z^n + \Gamma g \chi^n\right) - \frac{\Delta t}{2}\,\frac{\theta}{\Gamma}\left(\delta\pi_z - \Delta t \, \Gamma g\left(w^n + \frac{\delta w}{2}\right)\frac{d\overline{\chi}}{dz}\right) && (38)\\
\delta w \left(1 - \frac{(\Delta t)^2}{4} g\theta \frac{d\overline{\chi}}{dz}\right) &= -\Delta t \, \frac{\theta}{\Gamma}\left(\pi_z^n + \Gamma g \chi^n\right) + w^n \frac{(\Delta t)^2}{2} g\theta \frac{d\overline{\chi}}{dz} - \frac{\Delta t}{2}\,\frac{\theta}{\Gamma}\delta\pi_z \, . && (39)
\end{aligned}
$$

Letting

$$
N^2 = -g\theta \frac{d\overline{\chi}}{dz} \tag{40}
$$

denote the square of the buoyancy-frequency, we have

$$
\delta w = \frac{1}{1+\left(\frac{N\Delta t}{2}\right)^2}\left(-\Delta t \frac{\theta}{\Gamma}\left(\pi_z^n + \Gamma g \chi^n\right) - 2\, w^n \left(\frac{N\Delta t}{2}\right)^2\right) - \frac{\Delta t}{2}\,\frac{\theta/\Gamma}{1+\left(\frac{N\Delta t}{2}\right)^2}\delta\pi_z \tag{41}
$$

and the update formula for χ subsequently follows from (36). We summarize these results in the following formulae for the new time level data,

$$
w^{n+1} = \frac{1-\left(\frac{N\Delta t}{2}\right)^2}{1+\left(\frac{N\Delta t}{2}\right)^2} w^n - \frac{\Delta t}{1+\left(\frac{N\Delta t}{2}\right)^2}\left(\frac{\theta}{\Gamma}\left(\pi_z^n + \Gamma g \chi^n\right)\right) - \frac{\Delta t}{2}\,\frac{\theta/\Gamma}{1+\left(\frac{N\Delta t}{2}\right)^2}\delta\pi_z \tag{42}
$$

$$
\chi^{n+1} = \frac{1-\left(\frac{N\Delta t}{2}\right)^2}{1+\left(\frac{N\Delta t}{2}\right)^2}\chi^n - \frac{\Delta t}{1+\left(\frac{N\Delta t}{2}\right)^2}\frac{d\overline{\chi}}{dz} w^n \, . \tag{43}
$$

It is also interesting to note the change in time of the momentum source term for frozen π^n in the following fashion,

$$\left(\chi + \frac{\pi_z}{\Gamma g}\right)^{n+1} = \frac{1 - \left(\frac{N\Delta t}{2}\right)^2}{1 + \left(\frac{N\Delta t}{2}\right)^2} \left(\chi + \frac{\pi_z}{\Gamma g}\right)^{n} - \frac{\Delta t}{1 + \left(\frac{N\Delta t}{2}\right)^2} \frac{d\overline{\chi}}{dz}\, w^n . \tag{44}$$

Consider now the first term on the right in (42), which contains all explicit contributions to the velocity update, and its scaling for large time steps $\Delta t \to \infty$. The first term in the bracket scales linearly with Δt, so that it vanishes in the limit. The second term in the bracket involves $(\Delta t N)^2$, however, and therefore the limit reads

$$\delta^{\text{expl}} w\big|_{\Delta t \to \infty} = -2w^n \qquad \text{or} \qquad w^{n+1} = -w^n . \tag{45}$$

That is, the first thing the explicit part of the implicit step does is to impose a timestep–to–timestep oscillation as expected. This is the energy-preserving property of the implicit trapezoidal rule in the linear case.

2.2.2 Application to advective flux calculations

Here we have to consider the joint evolution of P and $P\chi = \rho$ in the vertical split half time step, i.e.,

$$(P\chi)_t = -(P\overline{\chi}w)_z \tag{46}$$

$$(P)_t = -(Pw)_z \tag{47}$$

and utilize the implicit trapezoidal rule as worked out in (42) to determine the advecting fluxes (Pw). Thus,

$$(P\chi)_j^{n+\frac{1}{2}} - (P\chi)_j^n = -\frac{\Delta t}{2\Delta z}\left((P\overline{\chi}w)_{j+\frac{1}{2}}^{n+\frac{1}{4}} - (P\overline{\chi}w)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right) \tag{48}$$

$$P_j^{n+\frac{1}{2}} - P_j^n = -\frac{\Delta t}{2\Delta z}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}} - (Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right) \tag{49}$$

What I want to show is that the update $\chi_j^{n+\frac{1}{2}} - \chi_j^n$ is as nicely controlled for large Δt as is the nonconservative update from (43).

Rewrite (48) as

$$
\begin{aligned}
P_j^{n+\frac{1}{4}*}\left(\chi_j^{n+\frac{1}{2}}-\chi_j^n\right) &= -\left(P_j^{n+\frac{1}{2}}-P_j^n\right)\chi_j^{n+\frac{1}{4}*}-\frac{\Delta t}{2\Delta z}\left((P\overline{\chi}w)_{j+\frac{1}{2}}^{n+\frac{1}{4}}-(P\overline{\chi}w)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right) &\quad (50)\\
&= -\frac{\Delta t}{2\Delta z}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}}(\overline{\chi}_{j+\frac{1}{2}}-\chi_j^{n+\frac{1}{4}*})-(Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}(\overline{\chi}_{j-\frac{1}{2}}-\chi_j^{n+\frac{1}{4}*})\right) &\quad (51)\\
&= -\frac{\Delta t}{2\Delta z}\,\frac{1}{2}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}}+(Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right)\left(\overline{\chi}_{j+\frac{1}{2}}-\overline{\chi}_{j-\frac{1}{2}}\right) &\quad (52)\\
&\quad -\frac{\Delta t}{2\Delta z}\left(\frac{1}{2}\left(\overline{\chi}_{j+\frac{1}{2}}-2\chi_j^{n+\frac{1}{4}*}+\overline{\chi}_{j-\frac{1}{2}}\right)\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}}-(Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right)\right)\\
&= -\frac{\Delta t}{2\Delta z}\,\frac{1}{2}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}}+(Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right)\left(\overline{\chi}_{j+\frac{1}{2}}-\overline{\chi}_{j-\frac{1}{2}}\right) &\quad (53)\\
&\quad +\frac{\Delta t}{2}(\Delta z)^2\frac{2}{\Delta t}\left(P_j^{n+\frac{1}{2}}-P_j^n\right)\frac{1}{2(\Delta z)^2}\left(\overline{\chi}_{j+\frac{1}{2}}-2\chi_j^{n+\frac{1}{4}*}+\overline{\chi}_{j-\frac{1}{2}}\right)\\
&= -\frac{\Delta t}{2\Delta z}\,\frac{1}{2}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}}+(Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right)\left(\overline{\chi}_{j+\frac{1}{2}}-\overline{\chi}_{j-\frac{1}{2}}\right) &\quad (54)\\
&\quad -\left(P_j^{n+\frac{1}{2}}-P_j^n\right)\left(\chi_j^{n+\frac{1}{4}*}-\overline{\chi}_j^n\right)\\
&\quad +\frac{\Delta t}{16}(\Delta z)^2\frac{2}{\Delta t}\left(P_j^{n+\frac{1}{2}}-P_j^n\right)\frac{4}{(\Delta z)^2}\left(\overline{\chi}_{j+\frac{1}{2}}-2\overline{\chi}_j^n+\overline{\chi}_{j-\frac{1}{2}}\right)\\
&= -\frac{\Delta t}{2\Delta z}\,\frac{1}{2}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}}+(Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right)\left(\overline{\chi}_{j+\frac{1}{2}}-\overline{\chi}_{j-\frac{1}{2}}\right) &\quad (55)\\
&\quad -\left(P_j^{n+\frac{1}{2}}-P_j^n\right)\left(\chi_j^{n+\frac{1}{4}*}-\overline{\chi}_j^n\right)+\frac{\Delta t(\Delta z)^2}{16}\left(\frac{\partial P}{\partial t}\right)_j^{n+\frac{1}{4}}\left(\frac{\partial^2\overline{\chi}}{\partial z^2}\right)_j^n
\end{aligned}
$$

where we have used the abbreviations

$$X^{n+\frac{1}{4}*}=\frac{1}{2}\left(X^{n+\frac{1}{2}}+X^n\right)\,. \tag{56}$$

While the last term in (55) is arguably of higher order and may be neglected unless we want to demonstrate some rigorous bound on χ or the like, the next to last term is not negligible. It is the very kind of contribution that induces us to carry the P-variable along in our scheme even if we solve the pseudo-incompressible equations despite the fact that in that equation set, $\partial_t P \equiv 0$: In each split step of our OpSplit procedure, that derivative will be nonzero and of order unity in general.

We understand that our scheme is better than one may think at this point if instead of considering only the linearized update for $P\chi$ according to (46), we consider the full nonlinear expression

$$\frac{\partial P\chi}{\partial t}=-\frac{\partial(P\chi w)}{\partial z} \tag{57}$$

which turns (54) into

$$
\begin{aligned}
\frac{2}{\Delta t}\left(\chi_j^{n+\frac{1}{2}} - \chi_j^n\right) &= -\frac{1}{2P_j^{n+\frac{1}{4}*}}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}} + (Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right)\frac{\chi_{j+\frac{1}{2}}^{n+\frac{1}{4}} - \chi_{j-\frac{1}{2}}^{n+\frac{1}{4}}}{\Delta z} && (58)\\
&\quad + \frac{(\Delta z)^2}{8}\frac{2}{\Delta t}\left(P_j^{n+\frac{1}{2}} - P_j^n\right)\frac{4}{(\Delta z)^2}\left(\chi_{j+\frac{1}{2}}^{n+\frac{1}{4}} - 2\chi_j^{n+\frac{1}{4}*} + \chi_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right) \\
&= -\frac{1}{2P_j^{n+\frac{1}{4}*}}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}} + (Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right)\frac{\chi_{j+\frac{1}{2}}^{n+\frac{1}{4}} - \chi_{j-\frac{1}{2}}^{n+\frac{1}{4}}}{\Delta z} && (59)\\
&\quad + \frac{(\Delta z)^2}{8}\left(\frac{\partial P}{\partial t}\right)_j^{n+\frac{1}{4}}\left(\frac{\partial^2 \chi}{\partial z^2}\right)_j^{n+\frac{1}{4}} + o\left((\Delta z)^2\right) .
\end{aligned}
$$

For a second-order MUSCL-scheme we can do even better. In that case, reconstruction at $t^{n+\frac{1}{4}}$ is piecewise linear, $\chi_j^{n+\frac{1}{4}*} = \chi_j^{n+\frac{1}{4}} + \mathcal{O}\left((\Delta t)^2\right)$, and the edge values $\chi_{j+\frac{1}{2}}^{n+\frac{1}{4}}$ are determined on an upwind basis.

Suppose, for case 1, that χ is smooth and does not have an extremum, and that $(Pw)_{j\pm\frac{1}{2}}^{n+\frac{1}{4}} > 0$, then

$$
\begin{aligned}
\chi_{j+\frac{1}{2}}^{n+\frac{1}{4}} - 2\chi_j^{n+\frac{1}{4}*} + \chi_{j-\frac{1}{2}}^{n+\frac{1}{4}} &= \chi_{j,+}^{n+\frac{1}{4}} - 2\chi_j^{n+\frac{1}{4}*} + \chi_{j-1,+}^{n+\frac{1}{4}} && (60)\\
&= \chi_{j,+}^{n+\frac{1}{4}} - 2\chi_j^{n+\frac{1}{4}} + \chi_{j,-}^{n+\frac{1}{4}} && (61)\\
&\quad + \left(\chi_{j-1,+}^{n+\frac{1}{4}} - \chi_{j,-}^{n+\frac{1}{4}}\right) - 2\left(\chi_j^{n+\frac{1}{4}*} - \chi_j^{n+\frac{1}{4}}\right) && (62)\\
&= \left(\chi_{j-1,+}^{n+\frac{1}{4}} - \chi_{j,-}^{n+\frac{1}{4}}\right) + \mathcal{O}\left((\Delta t)^2\right) && (63)\\
&= \left(\chi_{j-1}^{n+\frac{1}{4}} + \frac{\Delta z}{2}S_{j-1} - \chi_j^{n+\frac{1}{4}} + \frac{\Delta z}{2}S_j\right) + \mathcal{O}\left((\Delta t)^2\right) && (64)\\
&= \Delta z\left(\frac{1}{2}\left(S_{j-1} + S_j\right) - \frac{\chi_j^{n+\frac{1}{4}} - \chi_{j-1}^{n+\frac{1}{4}}}{\Delta z}\right) + \mathcal{O}\left((\Delta t)^2\right) && (65)\\
&= \mathcal{O}\left((\Delta t)^2 + (\Delta z)^2\right) && (66)
\end{aligned}
$$

Issues to be addressed: This latter result is not "better", as we have already assumed in the previous estimate that this expression is basically $(\Delta z)^2(\partial^2\chi/\partial z^2)$. What we do have to worry about are extrema of χ, where the slope reconstruction deteriorates and we only have a spacial first-order accurate reconstruction, and about the $\mathcal{O}\left((\Delta t)^2\right)$ term.
That term can deteriorate for large Δt, which is the current focus! Checking where it comes from, we have to make sure that both $\chi_{j,\pm}^{n+\frac{1}{4}}$ (from the reconstruction) and $\chi_{j,\pm}^{n+\frac{1}{4}*}$ (from the time update within cell j) are controlled as $\Delta t \to \infty$ as displayed above in working out the explicit part of the semi-implicit time integrator.

Let us, for the moment, not worry about the second derivative term that is an unwanted left-over imprint from the time changes of P, but rather focus on the dominant part of the χ-update in

(59).

$$\frac{2}{\Delta t}\left(\chi_j^{n+\frac{1}{2}} - \chi_j^n\right) \quad = \quad -\frac{1}{2P_j^{n+\frac{1}{4}*}}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}} + (Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right)\frac{\chi_{j+\frac{1}{2}}^{n+\frac{1}{4}} - \chi_{j-\frac{1}{2}}^{n+\frac{1}{4}}}{\Delta z} + \mathcal{O}\left((\Delta z)^2\right) \,. \tag{67}$$

Following the MUSCL strategy translated into the implicit trapezoidal context, we insert a discretization of

$$w_t \quad = \quad -\frac{\theta}{\Gamma}\left(\pi_z^n + \Gamma g \chi\right) \tag{68}$$

$$\chi_t \quad = \quad -w\frac{d\overline{\chi}}{dz} \tag{69}$$

over a half time step and then utilize $w^{n+\frac{1}{4}} = \frac{1}{2}\left(w^{n+\frac{1}{4}} + w^n\right)$ to extract the half of a half time step level vertical velocities. According to the previous considerations in (42), this yields

$$w^{n+\frac{1}{2}} \quad = \quad \frac{1-\left(\frac{N\Delta t}{4}\right)^2}{1+\left(\frac{N\Delta t}{4}\right)^2}\, w^n - \frac{\Delta t/2}{1+\left(\frac{N\Delta t}{4}\right)^2}\left(\frac{\theta}{\Gamma}\left(\pi_z^n + \Gamma g \chi^n\right)\right) \tag{70}$$

$$w^{n+\frac{1}{4}} = \frac{1}{2}\left(w^{n+\frac{1}{2}} + w^n\right) \quad = \quad \frac{1}{1+\left(\frac{N\Delta t}{4}\right)^2}\left(w^n - \frac{\Delta t}{4} g\theta\left(\chi^n + \frac{\pi_z^n}{\Gamma g}\right)\right) \tag{71}$$

$$\equiv \quad \frac{1}{1+\left(\frac{N\Delta t}{4}\right)^2}\left(w^n - \frac{\Delta t}{4} g\theta\, \widetilde{\chi}^n\right) \tag{72}$$

With this we find, neglecting the error term for the moment, and with an obvious abbreviation for the vertical χ derivative,

$$P_j^{n+\frac{1}{4}*}\left(\widetilde{\chi}_j^{n+\frac{1}{2}} - \widetilde{\chi}_j^n\right) \quad = \quad -\frac{\Delta t}{4}\left((Pw)_{j+\frac{1}{2}}^{n+\frac{1}{4}} + (Pw)_{j-\frac{1}{2}}^{n+\frac{1}{4}}\right)\left.\frac{\partial \chi}{\partial z}\right|_j^{n+\frac{1}{4}} \tag{73}$$

$$= \quad -\frac{\Delta t}{4}\left(\frac{P_{j+\frac{1}{2}}^{n+\frac{1}{4}} w_{j+\frac{1}{2}}^n}{1+\left(\frac{N_{j+\frac{1}{2}}\Delta t}{4}\right)^2} + \frac{P_{j-\frac{1}{2}}^{n+\frac{1}{4}} w_{j-\frac{1}{2}}^n}{1+\left(\frac{N_{j-\frac{1}{2}}\Delta t}{4}\right)^2}\right)\left.\frac{\partial \chi}{\partial z}\right|_j^{n+\frac{1}{4}} \tag{74}$$

$$-\left(\frac{N_j^*\Delta t}{4}\right)^2\left(\frac{P_{j+\frac{1}{2}}^{n+\frac{1}{4}} \widetilde{\chi}_{j+\frac{1}{2}}^n}{1+\left(\frac{N_{j+\frac{1}{2}}\Delta t}{4}\right)^2} + \frac{P_{j-\frac{1}{2}}^{n+\frac{1}{4}} \widetilde{\chi}_{j-\frac{1}{2}}^n}{1+\left(\frac{N_{j-\frac{1}{2}}\Delta t}{4}\right)^2}\right) \tag{75}$$

where

$$\left(N_{j*}\right)^2 = -g\theta\left.\frac{\partial \chi}{\partial z}\right|_j^{n+\frac{1}{4}} \tag{76}$$

and where, on the left hand side, we have replace the χ-difference by the $\widetilde{\chi}$-difference by adding a zero.

Thus, what we obtain is

$$\widetilde{\chi}_j^{n+\frac{1}{2}} = \widetilde{\chi}_j^n - \frac{\left(\frac{N_j^* \Delta t}{4}\right)^2}{P_j^{n+\frac{1}{4}*}} \left(\frac{P_{j+\frac{1}{2}}^{n+\frac{1}{4}} \widetilde{\chi}_{j+\frac{1}{2}}^n}{1+\left(\frac{N_{j+\frac{1}{2}}\Delta t}{4}\right)^2} + \frac{P_{j-\frac{1}{2}}^{n+\frac{1}{4}} \widetilde{\chi}_{j-\frac{1}{2}}^n}{1+\left(\frac{N_{j-\frac{1}{2}}\Delta t}{4}\right)^2} \right) \tag{77}$$

$$-\frac{\Delta t}{2} \frac{1}{2P_j^{n+\frac{1}{4}*}} \left(\frac{P_{j+\frac{1}{2}}^{n+\frac{1}{4}} w_{j+\frac{1}{2}}^n}{1+\left(\frac{N_{j+\frac{1}{2}}\Delta t}{4}\right)^2} + \frac{P_{j-\frac{1}{2}}^{n+\frac{1}{4}} w_{j-\frac{1}{2}}^n}{1+\left(\frac{N_{j-\frac{1}{2}}\Delta t}{4}\right)^2} \right) \left.\frac{\partial \chi}{\partial z}\right|_j^{n+\frac{1}{4}} \tag{78}$$

The result does look like a complex variant of the explicit part of the implicit trapezoidal rule, although with weirdly weighted old time level data entering.

Of interest is the limit behavior as $\Delta t \to \infty$ with everything else fixed. What we obtain is

$$\widetilde{\chi}_j^{n+\frac{1}{2}} \to \widetilde{\chi}_j^n - 2\widetilde{\chi}_j^{n*} \tag{79}$$

where

$$\widetilde{\chi}_j^{n*} = \frac{1}{2} \frac{N_{j*}^2}{P_j^{n+\frac{1}{4}*}} \left(\frac{P_{j+\frac{1}{2}}^{n+\frac{1}{4}}}{N_{j+\frac{1}{2}}^2} \widetilde{\chi}_{j+\frac{1}{2}}^n + \frac{P_{j-\frac{1}{2}}^{n+\frac{1}{4}}}{N_{j-\frac{1}{2}}^2} \widetilde{\chi}_{j-\frac{1}{2}}^n \right) . \tag{80}$$

2.2.3 Oscillator with slow forcing over a two-step cycle?

Here we consider

$$y^{n+1} = y^n + \Delta t v^{n+\frac{1}{2}} \tag{81}$$

3 Todos

- advect only perturbations of $1/\theta$
  - modify density flux accordingly by superimposing reconstructed theta-perturbations and background values at cell faces, or
  - by advecting theta-perturbations as a separate scalar and then recomputing full density after the full advection cycle.
  - Tried this, it doesn't improve things, and is also somewhat against our philosophy. So, let's forget about this.

- Apply explicit part of first-order backward Euler of the pressure-gravity combo to P-fluxes, but that of the implicit trapezoidal rule to the cell-centered momenta.
  - try just using the current implicit variant on both forward steps – looks good
  - fluxes – produces controlled updates for very large time steps
  - cell-centered momenta – partial success: vertical velocity gathers oscillatory but controlled updates, yet the buoyancy does not undergo the flip-flop in time that would be expected under the implicit trapezoidal rule for large time steps. Reason: advection of background theta is done with the first-order updated P-fluxes. I have to pull this part out.
  - pull background-θ out of density flux and place it back in a source-term like expression. – This is not appropriate because then I begin to handle the density flux not consistently with the fluxes of other density-weighted variables. That should be avoided.
  - What about going back to separately computing $\tilde{S}$, i.e., fluctuations of $1/\theta$ only for buoyancy computations and resynchronizing after each step?
  - Meanwile tested applying backward Euler half time step for the P-fluxes in the first OpSplit cycle and forward Euler in the second. This formally should yield second order in the end as it would be the equivalent of the implicit midpoint rule, and it does give the most favorable results so far.

- 2016.12.01: I seem to be missing some part of the θ-update in calculating buoyancy for the final momentum update. Options:
  1. Add a final θ-buoyancy contribution when the second projection is done.
     I tried this: It does improve the asymmetries in the advected gravity wave test case, but it introduces unfavorable behavior in the non-advected case. For rather large time steps, checkerboard modes kick in. I think that the asymmetry arising with mean advection has to do with how I link the advection split steps (especially the horizontal ones) to the first projection.
     Yet, I still have a suspicion that we cannot keep the implicit gravity discretization out of the second projection entirely. So, this is where I stand as of August 18, 2017.
  2. Memorize all pressure-gradient / gravity terms over the predictor cycle and recalculate them after the first projection based on the old and new time level θs and on the nodal pressure. This would effectively provide a true trapezoidal rule implementation of these terms albeit with a separate update, done in the predictor and first projection, for θ.

3. We get an interesting variant of this approach when we go back to the nodal-pressure only version of the flux divergence control. KEEP THIS IN MIND!
4. Run scheme as is right now, but flip the x- and y-sweeps in the predictor. Then we get buoyancy evaluated at the beginning and true end of the x-sweep of advection. In the end, this is a switch from a midpoint to a trapezoidal discretization. Why should this make a difference? Unclear. Also, we would have to implement the decomposition of one semi-implicit predictor into two steps, which is somewhat of an arbitrary procedure.

- 2016.12.01: The errors in the current version appear to be too large. Before I try modifications that seem all to be variants of a second-order accurate scheme, should I not first hunt for a bug that destroys second order in the first place?

In (9) we use the abbreviation $\Gamma g \chi^* = -\pi_z^{\mathrm{hy}}$ to obtain

$$\delta w = \frac{1}{1+(\tau N)^2}\left(-\tau\frac{\theta}{\Gamma}\left(\pi_z^* - \pi_z^{\mathrm{hy}}\right) - w^*(\tau N)^2\right) - \tau\frac{\theta/\Gamma}{1+(\tau N)^2}\delta\pi_z \tag{82}$$

$$\delta w = \delta^{\mathrm{expl}} w + \delta^{\pi} w \tag{83}$$

$$\delta\chi = -\tau\left(w^* + \delta^{\mathrm{expl}} w\right)\frac{d\overline{\chi}}{dz} + \frac{1}{\Gamma g}\frac{1}{1+(\tau N)^2}(\tau)^2 g\theta\frac{d\overline{\chi}}{dz}\delta\pi_z \tag{84}$$

$$\delta\chi = -\tau\left(w^* + \delta^{\mathrm{expl}} w\right)\frac{d\overline{\chi}}{dz} + \frac{1}{\Gamma g}\frac{(\tau N)^2}{1+(\tau N)^2}\delta\pi_z \tag{85}$$

It is clear how to implement this in a split fashion outside of the advection routines. It needs to be implemented also, however, in the flux calculations, and it is less clear how that could be achieved.

4 Preconditioning

So far, this is a side issue. It looks as if the code converges very rapidly when all the components fit well together, even with vanilla BiCGStab. We can get back to this when we have the basic scheme running well.

4.1 Introductory thoughts

Let me recall: Given $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$ find $x \in \mathbb{R}^n$ such that

$$Ax = b \tag{86}$$

Preconditioning from the left means multiplying by a matrix $B^{-1} \in \mathbb{R}^{n\times n}$ and considering the problem

$$(B^{-1}A)x = B^{-1}b \tag{87}$$

with the hope that $B^{-1}A$ is better conditioned than A.

Using this strategy, a solver will remain unchanged except for

1. Computation of the rescaled right hand side $b \to B^{-1}b$ and
2. Extending the call to Ax by the composition of calls $B^{-1} \circ A\, x$.

An interesting question besides this more or less trivial operation concerns the computation of the stopping criterion for an iterative scheme. In some sense, lacking the exact solution, one will want to use information on the residual to assess how close one has come to the solution of the problem.

Thus, there are two alternatives,

$$\| b - Ax^n \| < \varepsilon \qquad \text{or} \qquad \| B^{-1}b - (B^{-1}A)x^n \| < \varepsilon\,. \tag{88}$$

What are the implications?

To get an intuition, let's take the standard case in meteorology where we need to compute a solution in a deep atmosphere, across which the density falls off by a factor 10^{-4} or an even more extreme one. In the present implementation that solves the $P \equiv \overline{\rho\theta}$ equation implicitly and uses an Exner type pressure variable, $x \equiv \delta\pi$, the matrix A is dominated by the discrete approximation of

$$\nabla \cdot \left(\frac{P\theta}{\Gamma} \nabla \delta\pi\right) \sim \nabla \cdot \left(\rho\theta^2 \nabla \delta\pi\right) \tag{89}$$

and the right hand side is

$$b = \nabla \cdot (P\boldsymbol{v})^*\,, \tag{90}$$

where the $(\ )^*$ superscript denotes the predicted values before the implicit divergence controlling step. The divergence constraint in the pseudo-incompressible limit reads $\nabla \cdot (P\boldsymbol{v}) = 0$, but the quantity of real interest is the velocity field. Therefore, we would want the factor of P, which has a dynamic range comparable to the density, to be scaled out of the div-control. This means we would want to control

$$\mathrm{diag}(P)^{-1}\,(b - Ax) < \| \,\mathrm{diag}(P)^{-1} \| \ \ \varepsilon\,. \tag{91}$$

Since division by the diagonal (or the main culprit for extreme dynamic range in the diagonal) corresponds simply to diagonal preconditioning, the answer to the question raised above should be: Control the residual of the preconditioned problem,

$$\| B^{-1}(b - A)x^n \| < \| B^{-1} \| \ \ \varepsilon\,, \tag{92}$$

and not the raw residuum.

4.2 Preconditioning w.r.t. vertical columns

4.2.1 Columnwise preconditioning for the first projection

The pressure stencil for the first projection can be read as follows:

$$
\begin{aligned}
\left(\mathcal{L}^{1\text{st}}\pi\right)_{i,j} = {} & \frac{h^x_{i+\frac{1}{2},j}\left(\overline{\pi}^y_{i+1,j} - \overline{\pi}^y_{i,j}\right) - h^x_{i-\frac{1}{2},j}\left(\overline{\pi}^y_{i,j} - \overline{\pi}^y_{i-1,j}\right)}{dx^2} \\
& + \frac{h^y_{i,j+\frac{1}{2}}\left(\overline{\pi}^x_{i,j+1} - \overline{\pi}^x_{i,j}\right) - h^y_{i,j-\frac{1}{2}}\left(\overline{\pi}^x_{i,j} - \overline{\pi}^x_{i,j-1}\right)}{dy^2}
\end{aligned}
\tag{93}
$$

where

$$
\begin{aligned}
\overline{\pi}^x_{i,j} &= \frac{\alpha}{2}\pi_{i-1,j} + (1-\alpha)\,\pi_{i,j} + \frac{\alpha}{2}\pi_{i+1,j} \\
\overline{\pi}^y_{i,j} &= \frac{\alpha}{2}\pi_{i,j-1} + (1-\alpha)\,\pi_{i,j} + \frac{\alpha}{2}\pi_{i,j+1}
\end{aligned}
\tag{94}
$$

The dominant vertical derivative part of the operator thus reads

$$
\left(\mathcal{L}^{1\text{st}}\pi\right)_{j} = \frac{h^y_{i,j+\frac{1}{2}}\overline{\pi}^x_{i,j+1} - \left(h^y_{i,j+\frac{1}{2}} + h^y_{i,j-\frac{1}{2}}\right)\overline{\pi}^x_{i,j} + h^y_{i,j-\frac{1}{2}}\overline{\pi}^x_{i,j-1}}{dy^2}
\tag{95}
$$

where

$$
\overline{\pi}^x_{i,j} = \frac{\alpha}{2}\pi_{i-1,j} + (1-\alpha)\,\pi_{i,j} + \frac{\alpha}{2}\pi_{i+1,j}\,.
\tag{96}
$$

To solve the equation

$$
\left(\mathcal{L}^{1\text{st}}\pi\right)_{j} = r_j
\tag{97}
$$

we can obviously first solve for $\overline{\pi}$ using the Thomas Algorithm for the j-direction, and then for π by inverting the x-averaging – again using the Thomas Algorithm.

5 Hydrostatic initialization

The semi-implicit part of the time integration scheme that we intend to use is either implicit trapezoidal or implicit midpoint. In both cases we have an explicit contribution (Euler forward) followed or preceded by an implicit one (Euler backward). Especially with my implementation up to Jan 2018, the Euler forward is first, and this implies potentially very large deviations from the balanced state in the course of the first few time steps. This is indeed observed. Now, due to the advective nonlinearity, these large deviations can leave a heavy imprint on the later solution, and this must be avoided.

Here I describe a pressure initialization by the hydrostatic model. This is a preliminary exercise also on our way towards constructing a blended hydrostatic/nonhydrostatic solver.

The linearized hydrostatic pseudo-incompressible equations for a vertical slice read

$$
\begin{aligned}
(P\boldsymbol{u})_t + \frac{P\theta}{\Gamma}\pi_x &= 0 &\quad (98a)\\
\frac{\theta}{\Gamma}\pi_z &= -g &\quad (98b)\\
\theta_t &= -w\frac{d\overline{\Theta}}{dz} &\quad (98c)\\
(P\boldsymbol{u})_x + (PW)_z &= 0 &\quad (98d)
\end{aligned}
$$

Integrate (98d) from $z = 0$ to $z = h$ and then from 0 to x, use the rigid lid conditions on w, take the time derivative, let $\pi = \pi_0(t,x) + \widetilde{\pi}(t,x,z)$, where

$$
\widetilde{\pi}(t,x,z) = -\int_0^z \frac{\Gamma g}{\theta(t,x,\zeta)}\,d\zeta \tag{99}
$$

and obtain

$$
\int_0^h (P\boldsymbol{u})_t\,dz = \langle (PU)_t\rangle\,(t) = -\left\langle \frac{P\theta}{\Gamma}\right\rangle \pi_x^0 - \left\langle \frac{P\theta}{\Gamma}\widetilde{\pi}_x\right\rangle . \tag{100}
$$

This yields

$$
\pi_x^0 = -\frac{\langle (PU)_t\rangle}{\langle P\theta/\Gamma\rangle} - \frac{\langle P\theta\widetilde{\pi}_x/\Gamma\rangle}{\langle P\theta/\Gamma\rangle} . \tag{101}
$$

Integration in x yields the bottom pressure π^0 when $\langle (PU)_t\rangle$ is adjusted so as to satisfy the pressure boundary conditions, e.g., periodic ones.

6 Newton iteration for the P-equation

The determination of the advective fluxes $P\boldsymbol{v}$ at the half time level involve a backward Euler discretization of the half time step for

$$
P_t + \nabla\cdot(P\boldsymbol{v}) = 0 . \tag{102}
$$

Starting from an initial explicit guess that already includes the advection terms, the semi-implicit discretization is written for the Exner pressure variable as

$$
\frac{P(\pi^{n+\frac{1}{2}}) - P^n}{\Delta t/2} + \nabla\cdot\left((P\boldsymbol{v})^* - \frac{\Delta t}{2}P\theta\nabla\pi^{n+\frac{1}{2}}\right) = 0 . \tag{103}
$$

The function $P(\pi)$ is nonlinear and we intend to solve (103) by a Newton iteration. Let ν denote the Newton iteration counter and

$$\delta\pi^{\nu} = \pi^{n+\frac{1}{2},\nu+1} - \pi^{n+\frac{1}{2},\nu}\,, \tag{104}$$

then the linearization of the pressure function according to Newton's method yields

$$\frac{\frac{\partial P}{\partial \pi}\delta\pi^{\nu} + P(\pi^{n+\frac{1}{2},\nu}) - P^n}{\Delta t/2} + \nabla\cdot\left((P\boldsymbol{v})^* - \frac{\Delta t}{2}P\theta\nabla\left[\pi^{n+\frac{1}{2},\nu} + \delta\pi^{\nu}\right]\right) = 0\,, \tag{105}$$

where we assume the coefficients $\frac{\partial P}{\partial \pi}$ and $P\theta$ to be constant as assessed after the first explicit half time step. Improvements can be developed later as part of the iteration.

Thus, the Newton iteration requires the solution of

$$-\frac{4}{\Delta t^2}\frac{\partial P}{\partial \pi}\delta\pi^{\nu} + \nabla\cdot\left(P\theta\nabla\delta\pi^{\nu}\right) = \frac{4}{\Delta t^2}\left(P(\pi^{n+\frac{1}{2},\nu}) - P^n\right) + \frac{2}{\Delta t}\nabla\cdot\left((P\boldsymbol{v})^{n+\frac{1}{2},\nu}\right)\,. \tag{106}$$

Considering (105) with ν replaced with $\nu-1$ and recalling that $\pi^{n+\frac{1}{2},\nu-1} + \delta\pi^{\nu-1} = \pi^{n+\frac{1}{2},\nu}$, we have

$$\frac{2}{\Delta t}\nabla\cdot\left((P\boldsymbol{v})^{n+\frac{1}{2},\nu}\right) = -\frac{4}{\Delta t^2}\left(\frac{\partial P}{\partial \pi}\delta\pi^{\nu-1} + P(\pi^{n+\frac{1}{2},\nu-1}) - P^n\right)\,, \tag{107}$$

and re-insertion into (107) yields

$$-\frac{4}{\Delta t^2}\frac{\partial P}{\partial \pi}\delta\pi^{\nu} + \nabla\cdot\left(P\theta\nabla\delta\pi^{\nu}\right) = \frac{4}{\Delta t^2}\left(\left[P(\pi^{n+\frac{1}{2},\nu}) - P(\pi^{n+\frac{1}{2},\nu-1})\right] - \frac{\partial P}{\partial \pi}\delta\pi^{\nu-1}\right)\,. \tag{108}$$

and this constitutes the recursion relation for the right hand side of subsequent Newton steps.

The start of the iteration consists of the original step in which the nonlinear P-π-relation is simply linearized, i.e., we let

$$\pi^{n+\frac{1}{2},0} = \pi^n \qquad \text{and} \qquad P(\pi^{n+\frac{1}{2},0}) - P^n = 0 \tag{109}$$

according to the result of the iteration in the previous time step as a first guess, and then (105) can be cast into the standard form for the semi-implicit, linearized scheme for $\pi^{n+\frac{1}{2},1} = \pi^n + \delta\pi^0$,

$$-\frac{4}{\Delta t^2}\frac{\partial P}{\partial \pi}\pi^{n+\frac{1}{2},1} + \nabla\cdot\left(P\theta\nabla\left[\pi^{n+\frac{1}{2},1}\right]\right) = -\frac{4}{\Delta t^2}\frac{\partial P}{\partial \pi}\pi^n + \frac{2}{\Delta t}\nabla\cdot(P\boldsymbol{v})^*\,, \tag{110}$$

and then the iteration starts with

$$\delta\pi^0 = \pi^{n+\frac{1}{2},1} - \pi^n\,. \tag{111}$$