The physics-dynamics coupling mechanism in weather and climate models

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Canonical problem

Consider the following *canonical problem* for a generic (vectorial) variable $\psi = \psi(\boldsymbol{x}, t)$:

$$\frac{\partial \psi}{\partial t} - \mathscr{D}\psi = \sum_{m=1}^{M} \mathscr{P}_m \psi + R(\boldsymbol{x}, t) = \mathscr{P}\psi + R(\boldsymbol{x}, t) \,, \tag{1}$$

where

- $\mathscr{D}$ is the spatial operator modeling the dynamics (it includes, e.g., advection by the mean flow and the pressure gradient forcing);
- the operator $\mathscr{P}_m$ models the $m-$th physical process (e.g., radiative transfer), with $\mathscr{P} = \sum_{m=1}^{M} \mathscr{P}_m$; and
- R represents a forcing term indendent of ψ (e.g., the orographic forcing).

Canonical problem: analytical solution

If $\mathscr{D}$ and $\mathscr{P}$ do not depend on time, and $R \equiv 0$, the exact solution to (1) is

$$\psi(t) = \psi(0) \exp\left[t\left(\mathscr{D} + \mathscr{P}\right)\right],$$

where

$$\exp\left[t\left(\mathscr{D} + \mathscr{P}\right)\right] = I + t\left(\mathscr{D} + \mathscr{P}\right) + \frac{t^2}{2}\left(\mathscr{D} + \mathscr{P}\right)^2 + \frac{t^3}{6}\left(\mathscr{D} + \mathscr{P}\right)^3 + \dots,$$

with I the identity operator. Therefore,

$$\begin{aligned}\psi(t + \Delta t) &= \exp\left[\Delta t\left(\mathscr{D} + \mathscr{P}\right)\right] \psi(t) \\ &= \left[I + \Delta t\left(\mathscr{D} + \mathscr{P}\right) + \frac{\Delta t^2}{2}\left(\mathscr{D} + \mathscr{P}\right)^2 + \frac{\Delta t^3}{6}\left(\mathscr{D} + \mathscr{P}\right)^3 + \dots\right] \psi(t).\end{aligned}$$

Canonical problem in the literature

Specific choices for $\mathscr{D}$, $\mathscr{P}$ and R proposed in the literature to study stability and accuracy properties of coupling strategies in a simplified setting:

- In [2, 8]:

$$\mathscr{D} \equiv 0\,, \quad \mathscr{P}\psi = -\sigma\psi\,, \quad R(\boldsymbol{x}, t) \equiv G\,,$$

  with σ a complex constant and G a real constant.

- In [3, 4, 9]:

$$\mathscr{D}\psi = -U\frac{\partial \psi}{\partial x} + i\alpha\psi\,, \quad \mathscr{P}\psi = -\beta\psi\,, \quad R(x, t) = R_k \exp\left[i\left(kx + \Omega_k t\right)\right]\,,$$

  with U, α, $\beta \geq 0$, k and Ω_k real constants, and R_k a complex constant.

Canonical problem: semi-discretized version

Let $\mathbb{D}$ and $\mathbb{P}_m$ be numerical approximations to $\mathscr{D}$ and $\mathscr{P}_m$, respectively. A semi-discretized form of (1) then reads

$$\frac{d\psi_j}{dt} - \mathbb{D}\psi_j = \mathbb{P}\psi_j + R_j(t), \tag{2}$$

with $\psi_j = \psi_j(t) \approx \psi(\boldsymbol{x}_j, t)$ and $R_j(t) = R(\boldsymbol{x}_j, t)$.

Note. In what follows, the subscript denoting the spatial location is omitted for ease of notation.

Dynamical core

For the sake of tractability, we limit ourselves to two-time-level multi-step time integration schemes. The inviscid and adiabatic dynamical core can then be cast in the form

$$\psi^{n+1} = \mathbf{L}(\Delta t,\ \mathbb{D})\psi^n, \tag{3}$$

where

- Δt denotes the timestep size;
- $\psi^n \approx \psi(n\Delta t)$;
- $\mathbf{L} = \mathbf{L}(\Delta t,\ \mathbb{D})$ is the (nonlinear) numerical update operator.

Example. Any one-step update operators can be written as

$$\mathbf{L}\psi^n = \psi^n + (1-\xi)\,\Delta t\,\mathbb{D}\psi^n + \xi\,\Delta t\,\mathbb{D}\psi^{n+1}, \qquad 0 \le \xi \le 1.$$

$\xi = 0$ gives the forward (explicit) Euler method, $\xi = 1$ gives the backward (implicit) Euler method, and $\xi = 1/2$ gives the Crank-Nicholson method. The latter is the only one-step two-time-level scheme being second-order accurate.

Coupling strategies

Four coupling mechanisms will be presented in the following:

- concurrent method (CM),
- parallel splitting (PS),
- sequential-update splitting (SUS), and
- symmetric sequential-update splitting (SSUS).

Concurrent method (CM) (1)

$$\psi^{n+1} = \mathbf{L}(\Delta t,\ \mathbb{D} + \mathbb{P} + R)\psi^n$$

Example. Using a one-step time integrator:

$$\begin{aligned}\frac{\psi^{n+1} - \psi^n}{\Delta t} = {} & \xi_D \mathbb{D}\psi^{n+1} + (1 - \xi_D)\mathbb{D}\psi^n \\ & + \sum_{m=1}^{M} \left[\xi_m \mathbb{P}_m \psi^{n+1} + (1 - \xi_m)\mathbb{P}_m \psi^n \right] \\ & + \xi_R R^{n+1} + (1 - \xi_R) R^n ,\end{aligned}$$

with $0 \leq \xi_D \leq 1$, $0 \leq \xi_m \leq 1$, for $m = 1, \dots, M$, and $0 \leq \xi_R \leq 1$.

Concurrent method (CM) (2)

Advantages:

– Perfect representation of the steady-state solution [2].

Disadvantages:

– Not a clear separation between physical parameterizations and dynamical core.
– This hinders a modular code design.

Notes:

– Semi-implicit and fully implicit methods difficult to implement in presence of nonlinear terms.

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Example. Using only one-step integrators:

(i) $$\frac{\psi^{n+1,D} - \psi^n}{\Delta t} = \xi_D \mathbb{D}\psi^{n+1,D} + (1 - \xi_D)\mathbb{D}\psi^n$$

(ii) $$\frac{\psi^{n+1,m} - \psi^n}{\Delta t} = \xi_m \mathbb{P}_m \psi^{n+1,m} + (1 - \xi_m)\mathbb{P}_m \psi^n, \quad m = 1,\dots,M$$

(iii) $$\frac{\psi^{n+1,R} - \psi^n}{\Delta t} = \xi_R R^{n+1} + (1 - \xi_R) R^n$$

Parallel splitting (PS) (2)

Advantages:

- Parameterizations are treated in isolation, and independently of the dynamical core.
- This allows for a modular code design, and enables a high level of parallelism.
- Physics ordering does not matter.
- Different processes may be integrated using different schemes.

Disadvantages:

- Not suitable to model interactions between physical processes as all parameterizations "see" the same state.
- $\mathcal{O}(\Delta t)$ accurate, independently of the accuracy of single integrators.
- To get some useful insight on this last assertion, let us consider a convenient case.

Parallel splitting (PS) (3)

Let $M = 1$ and $R \equiv 0$, so that the exact solution to problem (2) is

$$\psi(t) = \exp\left[t\left(\mathbb{D} + \mathbb{P}_1\right)\right]\psi(0) = \exp\left[t\left(\mathbb{D} + \mathbb{P}\right)\right]\psi(0)\,.$$

Then, assuming that only one-step time schemes are used:

(i) $\quad \psi^{n+1,D} = \left(I - \Delta t\xi_D\mathbb{D}\right)^{-1}\left(I + \Delta t(1-\xi_D)\mathbb{D}\right)\psi^n\,,$

(ii) $\quad \psi^{n+1,1} = \left(I - \Delta t\xi_1\mathbb{P}\right)^{-1}\left(I + \Delta t(1-\xi_1)\mathbb{P}\right)\psi^n\,.$

If $\mathbb{D}$ and $\mathbb{P}$ are both *linear*, Taylor expansion yields

(iv) $\quad \psi^{n+1} = \left[I + \Delta t\left(\mathbb{D} + \mathbb{P}\right) + \Delta t^2\left(\xi_D\mathbb{D}^2 + \xi_1\mathbb{P}^2\right) + \mathcal{O}(\Delta t^3)\right]\psi^n\,.$

A direct comparison of the preceding with the exact update operator,

$$\exp\left[\Delta t\left(\mathbb{D} + \mathbb{P}\right)\right] = I + \Delta t\left(\mathbb{D} + \mathbb{P}\right) + \frac{\Delta t^2}{2}\left(\mathbb{D} + \mathbb{P}\right)^2 + \mathcal{O}(\Delta t^3)\,,$$

unravels the poor accuracy of PS, which is $\mathcal{O}(\Delta t)$ accurate independently of ξ_D and ξ_1, viz, even if both dynamics and physics are integrated using a second-order scheme. Actually, $\mathcal{O}(\Delta t^2)$ accuracy is retrieved when

$$\xi_D = \xi_1 = 1/2 \qquad \text{and} \qquad \mathbb{D}\mathbb{P} = -\mathbb{P}\mathbb{D}\,.$$

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Example. Using only one-step integrators:

(i) $$\frac{\psi^{n+1,0} - \psi^n}{\Delta t} = \xi_D \mathbb{D}\psi^{n+1,D} + (1 - \xi_D)\mathbb{D}\psi^n$$

(ii) $$\frac{\psi^{n+1,m} - \psi^{n+1,m-1}}{\Delta t} = \xi_m \mathbb{P}_m \psi^{n+1,m} + (1 - \xi_m)\mathbb{P}_m \psi^{n+1,m-1}, \quad m = 1, \dots, M$$

(iii) $$\frac{\psi^{n+1} - \psi^{n+1,M}}{\Delta t} = \xi_R R^{n+1} + (1 - \xi_R) R^n$$

Sequential-update splitting (SUS) (2)

Advantages:

- Parameterizations are treated in isolation $\Rightarrow$ Modular code design.
- Any parameterization feels the effect of all preceding parameterizations.

Disadvantages:

- Physics ordering matters!
- Dependencies among parameterizations erodes room for parallelization.
- Only first-order accurate, unless all operators commute [5].

Consider again one-step integrators, with $M = 1$ and $R \equiv 0$. Under the assumption of linearity:

(i) $\psi^{n+1,0} = (I - \Delta t \xi_D \mathbb{D})^{-1} (I + \Delta t (1 - \xi_D) \mathbb{D}) \psi^n$,

(ii)
$$\begin{aligned}
\psi^{n+1} &= (I - \Delta t \xi_1 \mathbb{P})^{-1} (I + \Delta t (1 - \xi_1) \mathbb{P}) \psi^{n+1,0} \\
&= (I - \Delta t \xi_1 \mathbb{P})^{-1} (I + \Delta t (1 - \xi_1) \mathbb{P}) (I - \Delta t \xi_D \mathbb{D})^{-1} (I + \Delta t (1 - \xi_D) \mathbb{D}) \psi^n \\
&= \left[I + \Delta t (\mathbb{D} + \mathbb{P}) + \Delta t^2 \left(\xi_D \mathbb{D}^2 + \mathbb{P}\mathbb{D} + \xi_1 \mathbb{P}^2 \right) + \mathcal{O}(\Delta t^3) \right] \psi^n .
\end{aligned}$$

Therefore, the numerical composite update operator is second-order only if

$$\xi_D = \xi_1 = 1/2 \quad \text{and} \quad \mathbb{D}\mathbb{P} = \mathbb{P}\mathbb{D} .$$

Note that the second condition is independent of the temporal discretization used, and it is hardly met in reality.

Symmetrized sequential-update splitting (SSUS) (1)

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(iii) $$\psi^{n+1,M+1} = \mathbf{L}_D(\Delta t,\ \mathbb{D})\widetilde{\psi}^M$$

(iv) $$\psi^{n+1,m} = \mathbf{L}_m((1-\eta)\Delta t,\ \mathbb{P}_m)\psi^{n+1,m+1}, \quad m = M, \dots, 1$$

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Symmetrized sequential-update splitting (SSUS) (2)

Example. Using only one-step integrators:

(i) $$\frac{\widetilde{\psi}^0 - \psi^n}{\eta \Delta t} = \xi_R R^{n+\eta} + (1 - \xi_R) R^n$$

(ii) $$\frac{\widetilde{\psi}^m - \widetilde{\psi}^{m-1}}{\eta \Delta t} = \xi_m \mathbb{P}_m \widetilde{\psi}^m + (1 - \xi_m) \mathbb{P}_m \widetilde{\psi}^{m-1}, \quad m = 1, \dots, M$$

(iii) $$\frac{\psi^{n+1,M+1} - \widetilde{\psi}^M}{\Delta t} = \xi_D \mathbb{D} \psi^{n+1,M+1} + (1 - \xi_D) \mathbb{D} \widetilde{\psi}^M$$

(iv) $$\frac{\psi^{n+1,m} - \psi^{n+1,m+1}}{(1-\eta)\Delta t} = \xi_m \mathbb{P}_m \psi^{n+1,m} + (1 - \xi_m) \mathbb{P}_m \psi^{n+1,m+1}, \quad m = M, \dots, 1$$

(iv) $$\frac{\psi^{n+1} - \psi^{n+1,1}}{(1-\eta)\Delta t} = \xi_R R^{n+1} + (1 - \xi_R) R^{n+\eta}$$

Symmetrized sequential-update splitting (SSUS) (3)

First, all parameterizations are scanned in a given order, and each is moved $\eta\Delta t$ forward in time. After that a full dynamical step is carried out, all parameterizations are scanned in the reverse order, and stepped by the remaining fraction of the time step, i.e., $(1-\eta)\Delta t$.

The resulting procedure is close in spirit to SUS. Yet, in contrast to SUS, SSUS is symmetric around the dynamics, with η controlling the degree of off-centering. Actually, SUS is recovered in the limit $\eta \to 0$.

In the linear case, with $M = 1$ and $R \equiv 0$, simple calculations yield

$$\begin{aligned}\psi^{n+1} = \big[& I + \Delta t\,(\mathbb{D} + \mathbb{P}) \\ & + \Delta t^2 \left(\xi_D \mathbb{D}^2 + \eta \mathbb{D}\mathbb{P} + (1-\eta)\mathbb{P}\mathbb{D} + (2\eta^2 \xi_1 - 2\eta\xi_1 + \eta - \eta^2 + \xi_1)\mathbb{P}^2 \right) \\ & + \mathcal{O}(\Delta t^3) \big] \psi^n .\end{aligned}$$

Necessary and sufficient conditions for the preceding to be $\mathcal{O}(\Delta t^2)$ accurate:

$$\xi_D = \xi_1 = \eta = \frac{1}{2} .$$

Note. SSUS with $\eta = 1/2$ is known as *Strang splitting* [10].

A real-life example

The COSMO model features a three-stages Runge-Kutta dynamical core, and pursues a fully explicit parallel splitting strategy:

$$\psi^* = \psi^n + \frac{\Delta t}{3}\mathbb{D}\psi^n + \frac{\Delta t}{3}\mathbb{P}\psi^n, \tag{4a}$$

$$\psi^{**} = \psi^n + \frac{\Delta t}{2}\mathbb{D}\psi^* + \frac{\Delta t}{2}\mathbb{P}\psi^n, \tag{4b}$$

$$\psi^{n+1} = \psi^n + \Delta t\mathbb{D}\psi^{**} + \Delta t\mathbb{P}\psi^n. \tag{4c}$$

Note. Explicity parallel splitting is equivalent to the concurrent method.

Remark. Physical tendencies are held constant throughout the whole time step. If $\mathbb{D}$ and $\mathbb{P}$ are linear, a more compact form of (4),

$$\psi^{n+1} = \left[I + \Delta t\,(\mathbb{D} + \mathbb{P}) + \frac{\Delta t^2}{2}\left(\mathbb{D}^2 + \mathbb{D}\mathbb{P}\right) + \frac{\Delta t^3}{6}\left(\mathbb{D}^3 + \mathbb{D}^2\mathbb{P}\right) \right] \psi^n,$$

reveals the crucial drawback of degrading accuracy from $\mathcal{O}(\Delta t^3)$ to $\mathcal{O}(\Delta t)$.

Isentropic model (1)

For a non-adiabatic atmosphere (i.e., $\dot{\theta} \neq 0$), the flux form of the continuity equation, the momentum equation, and the conservation law for a passive, non-precipitating tracer ϕ in isentropic coordinates read:

$$\frac{\partial \sigma}{\partial t} + \nabla \cdot (\sigma \boldsymbol{v}) = -\frac{\partial \sigma \dot{\theta}}{\partial \theta}, \tag{5a}$$

$$\frac{\partial \sigma \boldsymbol{v}}{\partial t} + \nabla \cdot (\sigma \boldsymbol{v} \otimes \boldsymbol{v}) + \sigma \nabla M = -\frac{\partial \sigma \boldsymbol{v} \dot{\theta}}{\partial \theta}, \tag{5b}$$

$$\frac{\partial \sigma \phi}{\partial t} + \nabla \cdot \left(\sigma \boldsymbol{v} \phi \right) = -\frac{\partial \sigma \phi \dot{\theta}}{\partial \theta} + \sigma S_{\phi}. \tag{5c}$$

Here, $\nabla = \left[\partial / \partial x, \partial / \partial y \right]^T$ is the horizontal nabla operator, σ is the *isentropic mass density*, $\boldsymbol{v} = [u, v]^T$ is the horizontal velocity vector, $M = M(\sigma)$ is the Montgomery potential, and S_{ϕ} models physical source-sink rates for ϕ.

Isentropic model (2)

The differential system (5) can be cast into the canonical form (1):

$$\psi = \begin{bmatrix} \sigma \\ \boldsymbol{u} \\ \phi \end{bmatrix}, \quad \mathscr{D} = \begin{bmatrix} -\nabla \cdot (\sigma \boldsymbol{v}) \\ -\nabla \cdot (\sigma \boldsymbol{v} \otimes \boldsymbol{v}) - \sigma \nabla M(\sigma) \\ -\nabla \cdot \big(\sigma \boldsymbol{v} \phi\big) \end{bmatrix},$$

$$\mathscr{P}_1 = \begin{bmatrix} -\dfrac{\partial \sigma \dot{\theta}}{\partial \theta} \\ -\dfrac{\partial \sigma \boldsymbol{v} \dot{\theta}}{\partial \theta} \\ -\dfrac{\partial \sigma \phi \dot{\theta}}{\partial \theta} \end{bmatrix}, \quad \mathscr{P}_2 = \begin{bmatrix} 0 \\ 0 \\ \sigma S_\phi \end{bmatrix}, \quad \mathscr{R} \equiv 0 .$$

Question. How to handle the saturation adjustment? Is it likely to degrade accuracy to first order?

Use case

- Two proposals:
  - *dry* thermally forced low Froud number flow past an isolated Gaussian-shaped mountain [6];
  - slowly-varying tropical cyclone [1].
- To prevent the formation of zero-mass-thick layers:
  - MacCormack coupled with some sort of flux-limiting mechanism (see, e.g., [11]);
  - second-order MPDATA [7].
- Within this framework, distinguishing between parameterizations performed *before* or *after* the dynamics is not relevant (except from the saturation adjustment?).
- Rather, we distinguish coupling performed *before* the dynamics, from coupling carried out *after* the dynamics.

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