Time stepping for numerical models of geophysical fluid dynamics

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What is time stepping?

Consider a system of PDEs :

$$\frac{\partial x}{\partial t} = N(x, \nabla x, \dots)$$

Now discretize in space using whatever method you prefer (finite-difference, finite-element, finite-volume, etc.):

$$\frac{\partial x}{\partial t} = N(x)$$

to get a system of ODEs. This is the **method of lines**. We will ignore coupled space-time approaches such as space-time finite elements here. Thus the problem of time stepping reduces to problem of solving a system of ODEs.

Desirable Characteristics of Time Stepping Schemes

1. Convergence/Accuracy, Consistency: Lax-Richtmyer theorem (consistent $+$ stable $=$ convergent)
2. Stability (A, L, B) and Maximum Stable Time Step (CFL condition): important for stiff problems (very common in geophysical fluids)
3. Strong stability preserving (SSP) or Total variation diminishing (TVD): preserve monotonicity properties of spatial schemes
4. Dispersion properties: minimize phase and amplitude errors
5. No computational modes (ie single step schemes)
6. Cost ($\#$ of rhs evaluations, need for linear or nonlinear solves, memory usage and movement)
7. Preserve linear invariants (ex. mass)
8. Geometric properties: symplectic, preserve phase-space volume and/or invariants (energy, enstrophy, entropy)

General Linear Methods (I)

Many time stepping schemes can be unified using **General Linear Methods**: schemes with r **time levels** and s **stages** (collocation points). Specifically, we have s **stage values** Y_i and **stage derivatives** $N_i = N(Y_i)$ $(i,j = 1,\ldots,s)$, and r **approximations** y_k^n at time step n and y_k^{n+1} at time step $n+1$ $(k,l = 1,\ldots,r)$, which satisfy:

$$
\begin{aligned}
Y_i &= \sum_{j=1}^{s} a_{ij} \Delta t N_j + \sum_{l=1}^{r} u_{il} y_l^n \\
y_k^{n+1} &= \sum_{j=1}^{s} b_{kj} \Delta t N_j + \sum_{l=1}^{r} v_{kl} y_l^n
\end{aligned}
$$

Can be written in matrix form (analogue of a Butcher tableau) as:

$$
\begin{pmatrix} Y \\ y^{n+1} \end{pmatrix} = \begin{pmatrix} A \otimes I & U \otimes I \\ B \otimes I & V \otimes I \end{pmatrix} \begin{pmatrix} N \\ y^n \end{pmatrix}
$$

with $A = a_{ij}$ $(s \times s)$, $B = b_{kj}$ $(r \times s)$, $U = u_{il}$ $(s \times r)$ and $V = v_{kl}$ $(r \times r)$, and I is $(m \times m)$ identity matrix ($m =$ the number of discrete degrees of freedom).

General Linear Methods (II)

Properties of GLM:

- If $r = 1$: **Runge-Kutta method** (single-step)
- If $s = 1$: **Linear Multistep method** (Adams-Bashford, Adams-Moulton, Backwards Differentiation Formulas, many predictor-corrector schemes)
- If A is strictly lower diagonal, scheme is **explicit** (might not require linear solves, does not require nonlinear solves) and usually **conditionally stable** $\rightarrow$ CFL condition (something similar to $\frac{\Delta t c}{\Delta x} < 1$ with characteristic speed c)
- If A is lower diagonal, scheme is **diagonally implicit** (requires linear and/or nonlinear solves, but stage values can be solved in sequence) and usually **unconditionally stable**
- Otherwise, scheme is **implicit** (requires linear and/or nonlinear solves for all stage values at once) and usually **unconditionally stable**

Consider an ODE where

$$\frac{\partial x}{\partial t} = N(X) = S(x) + F(x)$$

where $S(x)$ is "slow" and $F(x)$ is "fast", ie $S(x)$ has characteristic time scale T and $F(x)$ time scale τ such that $\tau \ll T$. Fully explicit time schemes will have very restrictive stable time steps, in terms of T, relative to step size needed for accuracy of $S(x)$, due to CFL condition on $F(x)$.

This is the usual situation in geophysical fluids: sound waves, barotropic mode, gravity waves, etc. So how do we take time steps dictated by accurate resolution of $S(x)$?

Fast/Slow General Linear Methods (II)

Extend general linear method to

$$\begin{pmatrix} Y \\ y^{n+1} \end{pmatrix} = \begin{pmatrix} A_S \otimes I & A_F \otimes I & U \otimes I \\ B_S \otimes I & B_F \otimes I & V \otimes I \end{pmatrix} \begin{pmatrix} S \\ F \\ y^n \end{pmatrix}$$

ie now we have a pair of tableau's A_S/B_S and A_F/B_F (can extend further to even more tableau's, but not discussed here)

- If A_S is strictly lower triangular and A_F is lower triangular or full, we have an **IMEX (implicit-explicit)** scheme. Often A_F is lower triangular and therefore diagonally implicit so stage values can be solved in sequence. **Horizontally-explicit, vertically-implicit (HEVI)** comes from choosing F such that linear or non-linear solves occur column-wise.
- If both A_S and A_F are strictly lower triangular we have a **split-explicit** or **multirate** scheme. Almost always use many more active approximations for $F(x)$ than $S(x)$, ie many small steps for $F(x)$.

Other Approaches

There are also more sophisticated approaches that don't fit this model:

- **Laplace Transform** integrators
- **Continuous-stage Runge-Kutta** integrators
- **Partitioned Runge-Kutta** integrators
- Some **geometric** integrators (**discrete gradients**, **Lie group** integrators, **variational** integrators)
- **Multiderivative** integrators
- **Staggering in time** and/or using **different tableau**'s for different variables (ie no longer $A \otimes I$)
- **Exponential** integrators (but see next talk!)

Atmospheric Models

- **Dynamico (IPSL/LMD)**: Hydrostatic finite-difference model, uses **explicit Runge-Kutta** designed for maximum stable time step (Kinnmark and Gray)
- **HOMME-NH (US DOE)**: Nonhydrostatic spectral element (horizontal)/finite difference (vertical) model, uses **IMEX/HEVI Runge-Kutta** designed for a balance of accuracy and computational cost/maximal time step, currently exploring many differences choices of splittings and IMEX/HEVI schemes
- **Unified Model (UK Met Office)**: Nonhydrostatic semi-Lagrangian model, uses (slightly) **off-centered Crank-Nicholson** scheme with a **simplified Jacobian** ("semi-implicit"), designed for accurate gravity wave propagation with reasonably long time steps and acceptable computational cost

Examples of Time Integrators for Geophysical Fluids (II)

Oceanic Models

- **NEMO**: Hydrostatic Boussinesq Finite-difference model, uses **leapfrog with Robert-Asselin filter** for 3D dynamics and **generalized forward-backwards scheme** for 2D dynamics (free surface/barotropic mode), cheap, time-reversible, symplectic, 2nd order, unstable for diffusion, computational mode
- **CROCO**: Nonhydrostatic Boussinesq Finite-difference model, uses **split-explicit Runge-Kutta** designed for coupling stability, accurate fast waves and ability to handle both dissipative and non-dissipative processes for 3D dynamics with a single time stepper

Major differences compared to atmospheric models: driven by need to accurately simulate fast modes, and different nature of fast modes (2D/3D coupling vs. vertically propagating)

Discrete Gradient Integrators (I)

Consider the following system of ODEs:

$$\frac{\partial x}{\partial t} = S(x)\nabla H(x)$$

where $\nabla H(x)$ is gradient of $H(x)$ and $S(x)$ is a matrix with either

1. $S(x) = -S(x)^T$ (**antisymmetric, Poisson system**)
   OR
2. $S(x)$ is positive or negative semi-definite (**Dissipative system**)

In the first case, the system will **conserve** H. In the second case, H will be **strictly increasing or decreasing**.

How do we construct an integrator that behaves this way?*

*This extends more generally to an n-tensor $S(x)$ with multiple preserved and/or dissipative quantities

Discrete Gradient Integrators (II)

Use a **discrete gradient** integrator:

$$\frac{x^{n+1} - x^n}{\Delta t} = \tilde{S}(x^{n+1}, x^n)\overline{\nabla} H(x^{n+1}, x^n)$$

where $\tilde{S}(x^{n+1}, x^n)$ is any consistent approximation to $S(x)$ that preserves anti-symmetry or positive/negative semi-definiteness and $\overline{\nabla} H(x^{n+1}, x^n)$ is a **discrete gradient**

$$(x^{n+1} - x^n)^T \overline{\nabla} H(x^{n+1}, x^n) = H(x^{n+1}) - H(x^n) \tag{1}$$

$$\overline{\nabla} H(x^n, x^n) = \nabla H(x^n)$$

Proof of conservation for Poisson systems:

$$\begin{aligned}
\overline{\nabla} H^T (x^{n+1} - x^n) &= \Delta t \overline{\nabla} H^T \tilde{S} \overline{\nabla} H \\
H(x^{n+1}) - H(x^n) &= \Delta t \overline{\nabla} H^T \tilde{S} \overline{\nabla} H = -\Delta t \overline{\nabla} H^T \tilde{S} \overline{\nabla} H \\
H(x^{n+1}) - H(x^n) &= 0
\end{aligned}$$

using (1) and anti-symmetry for $\tilde{S}$. Similar calculations show H strictly increasing/decreasing for dissipative systems.

Discrete Gradient Integrators (III)

Average vector field method (second-order* and fully implicit):

$$
\begin{aligned}
\tilde{S}(x^{n+1}, x^n) &= S(\frac{x^{n+1} + x^n}{2}) \\
\overline{\nabla} H(x^{n+1}, x^n) &= \int_0^1 \nabla H(x^n + \tau(x^{n+1} - x^n) d\tau
\end{aligned}
$$

-Evaluate $\overline{\nabla} H$ via **quadrature rule** → exact for polynomial H, can be made practically exact for arbitrary H by increasing order of quadrature; also conserves **linear and quadratic Casimirs**
-Solve nonlinear system with **Newton's method** and **simplified Jacobian** → **semi-implicit** method very similar to existing UK Met Office scheme!
*Higher-order versions exist
-Alternative discrete gradients are the **Gonzalez midpoint** discrete gradient and the **Itoh-Abe coordinate increment** discrete gradient (also known as **discrete variational derivatives**).