Exascale algorithms for numerical weather and climate prediction

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The linear diffusion equation

The linear diffusion equation is

$$\frac{\partial \phi}{\partial t} = K \frac{\partial^2 \phi}{\partial x^2}$$

with K a constant. Assume the domain is periodic in x. If the initial condition is wavelike

$$\phi(x, 0) = e^{ikx} \quad \text{(real part understood)}$$

then the exact solution can be found. Let

$$\phi(x, t) = \Phi(t) e^{ikx}.$$

Then

$$\frac{d\Phi}{dt} = -k^2 K \Phi,$$

so

$$\Phi = \Phi(0) e^{-k^2 K t}; \quad \Phi(0) = 1$$

$$\phi(x, t) = e^{-k^2 K t} e^{ikx}.$$

The solution is a stationary wave decreasing in amplitude.

Stability of some example schemes—von Neumann stability analysis

Divide the periodic space domain into N equal intervals of size Δx so that $x_j = j\Delta x$, $j = 0,\ 1,\ 2, \ldots,\ N$. Choose a time step Δt and let $t^{(n)} = n\Delta t$, $n = 0,\ 1,\ 2,\ \ldots$. Write ϕ_j^n for the numerical approximation to $\phi(x_j, t^{(n)})$.
Consider first a centred difference scheme:

$$\frac{\phi_j^{(n+1)} - \phi_j^{(n-1)}}{2\Delta t} = K\left(\frac{\phi_{j+1}^{(n)} - 2\phi_j^{(n)} + \phi_{j-1}^{(n)}}{\Delta x^2}\right).$$

This scheme is second order in space and second order in time, meaning that if we substitute the true solution into the finite difference scheme then the dominant terms in the residual are a term proportional to Δx^2 and a term proportional to Δt^2.

Von Neumann stability analysis

On a *periodic domain* any function can be decomposed into Fourier components. If the evolution of the function is governed by a *linear equation* with *constant coefficients* then its behaviour can be determined by looking at the behaviour of each Fourier component.

Look for numerical solutions of the form

$$\phi_j^{(n)} = A^n e^{ikj\Delta x}$$

where A is a (possibly complex) constant—the *amplification factor*. If we find $|A| > 1$ then the numerical solution is growing with time.

Von Neumann stability analysis

Substitute into the numerical scheme and cancelling powers of A and $e^{ikj\Delta x}$ leaves a quadratic equation for A:

$$A^2 + \frac{2K\Delta t}{\Delta x^2}\left(2 - 2\cos k\Delta x\right)A - 1 = 0.$$

There are two roots for A, corresponding to the physical mode and the computational mode.

$$A = -\frac{2K\Delta t}{\Delta x^2}\left(1 - \cos k\Delta x\right) \pm \left[\left(\frac{2K\Delta t}{\Delta x^2}\right)^2\left(1 - \cos k\Delta x\right)^2 + 1\right]^{1/2}.$$

Both roots A^+ and A^- are real and their product is $A^+A^- = -1$. A^+ lies between 0 and 1 and this corresponds to the physical mode ($A^+ \to 1$ as $\Delta x,\ \Delta t/\Delta x \to 0$). On the other hand, $A^- < -1$ and this corresponds to the computational mode. The computational mode is unconditionally unstable. Therefore, this centred difference scheme is a poor choice for the diffusion equation.

An alternative scheme uses a forward Euler rather than a centred time step:

$$\frac{\phi_j^{(n+1)} - \phi_j^{(n)}}{\Delta t} = K \left(\frac{\phi_{j+1}^{(n)} - 2\phi_j^{(n)} + \phi_{j-1}^{(n)}}{\Delta x^2} \right).$$

This is first-order accurate in time and second-order accurate in space.
Von Neumann analysis leads to the following expression for the amplification factor:

$$A = 1 - \frac{2K\Delta t}{\Delta x^2} \left(1 - \cos k\Delta x\right).$$

Now $0 \leq (1 - \cos k\Delta x) \leq 2$, so $|A| \leq 1$ if $2K\Delta t/\Delta x^2 \leq 1$. This scheme is conditionally stable. Note that, because of the quadratic dependence on Δx, a moderate increase in resolution might require a much smaller time step.

Another alternative scheme uses a backward Euler time step:

$$\frac{\phi_j^{(n+1)} - \phi_j^{(n)}}{\Delta t} = K \left(\frac{\phi_{j+1}^{(n+1)} - 2\phi_j^{(n+1)} + \phi_{j-1}^{(n+1)}}{\Delta x^2} \right).$$

Again, this is first-order accurate in time and second-order accurate in space.
Von Neumann analysis leads to

$$A = \left(1 + \frac{2K\Delta t}{\Delta x^2} (1 - \cos k\Delta x) \right)^{-1}.$$

For this scheme $|A| \leq 1$ for any value of Δt, so it is unconditionally stable. However, the unknown $\phi^{(n+1)}$ appears on both sides of the equation defining the scheme, so it is non-trivial to solve for $\phi^{(n+1)}$. In this linear one-dimensional example $\phi^{(n+1)}$ can be found by solving a tridiagonal system of simultaneous equations, which can be done efficiently using Gaussian elimination.

The linear advection equation

Consider the equation

$$\frac{D\phi}{Dt} = \frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = 0 \tag{1}$$

where u is a constant velocity, the domain is $0 \leq x \leq 1$ with periodic boundary conditions $\phi(0, t) = \phi(1, t)$, and the initial condition is given as $\phi(x, 0) = F(x)$.
The solution of this problem is

$$\phi(x, t) = F(x - ut),$$

(where $x - ut$ is understood to be taken modulo 1 to account for the periodicity). The initial function is advected with speed u, and its shape is preserved.

The upstream scheme

Divide the periodic space domain into N equal intervals of size Δx so that $x_j = j\Delta x,\ j = 0,\ 1,\ 2,\ \ldots,\ N$. Choose a time step Δt and let $t^{(n)} = n\Delta t,\ n = 0,\ 1,\ 2,\ \ldots$. Let $\phi_j^{(n)}$ be the numerical approximation to $\phi(x_j, t^{(n)})$.
Consider a forward in time, backward in space (FTBS) approximation:

$$\frac{\phi_j^{(n+1)} - \phi_j^{(n)}}{\Delta t} + u\frac{\phi_j^{(n)} - \phi_{j-1}^{(n)}}{\Delta x} = 0$$

Von Neumann stability analysis gives an equation for the amplification factor. Let $\phi_j^{(n)} = A^n e^{ikj\Delta x}$. Then

$$A^{n+1} e^{ikj\Delta x} - A^n e^{ikj\Delta x} + \frac{u\Delta t}{\Delta x}\left(A^n e^{ikj\Delta x} - A^n e^{ik(j-1)\Delta x}\right) = 0.$$

Define $c = u\Delta t/\Delta x$; c is called the *Courant number*. Cancel powers of A and $e^{ikj\Delta x}$ to obtain

$$A - 1 + c\left(1 - e^{-ik\Delta x}\right) = 0.$$

The amplification factor is complex, as it must be for a propagating solution. The numerical solution will be stable if $|A| \le 1$. $|A|^2$ is given by A times its complex conjugate. After some algebra

$$|A|^2 = 1 - 2c(1-c)(1 - \cos k\Delta x).$$

Now $(1 - \cos k\Delta x)$ is always greater than or equal to zero, so $|A|^2$ will be less than or equal to 1 provided $c(1-c) \ge 0$, i.e. provided $0 \le c \le 1$.

Note that the FTBS scheme is unstable for $u < 0$. But in that case we could switch to using a forward in time forward in space (FTFS) scheme. In the general case, for which u could take either sign, we must use FTBS when $u > 0$ and FTFS when $u < 0$, so that we always use information from the upstream side of the point whose new value we are trying to calculate. This combined FTBS/FTFS scheme is called the *upstream scheme*.

When the time step is small enough so that the upstream scheme is stable, $|A| \leq 1$. For the numerical scheme to reproduce the true solution we would need $|A| = 1$. In general the numerical solution is damped. Damping error, or excessive numerical diffusion, is the dominant truncation error in the first-order upstream scheme.

The Courant-Friedrichs-Lewy criterion

The FTBS scheme is conditionally stable. In fact the criterion just derived from von Neumann stability analysis happens to coincide exactly with the Courant-Friedrichs-Lewy (CFL) criterion. *The CFL criterion states that, for a hyperbolic system, a necessary condition for stability is that the domain of dependence of the numerical solution should include the domain of dependence of the original partial differential equation.*
In the numerical solution information can propagate only from left to right, and can do so no faster than one grid length per time step. It is clear that the numerical domain of dependence will contain the physical domain of dependence provided that $1/u \geq \Delta t/\Delta x$, i.e. $0 \leq u\Delta t/\Delta x \leq 1$.

The CTCS scheme

As an alternative to the upstream scheme, consider the centred in time centred in space (CTCS) scheme

$$\frac{\phi_j^{(n+1)} - \phi_j^{(n-1)}}{2\Delta t} + u\,\frac{\phi_{j+1}^{(n)} - \phi_{j-1}^{(n)}}{2\Delta x} = 0.$$

This scheme is second-order accurate in space and time. It is a three-time-level formula since it involves values of ϕ at times $t^{(n-1)}$, $t^{(n)}$, and $t^{(n+1)}$. To start the integration values of ϕ are needed at times $t^{(0)}$ and $t^{(1)}$, but only $\phi_j^{(0)}$ is given as initial data, so another formula such as FTCS must be used to obtain $\phi_j^{(1)}$.

The CTCS scheme

Von Neumann stability analysis leads to the following quadratic equation for the amplification factor:

$$A^2 + (2ic \sin k\Delta x)A - 1 = 0,$$

with roots

$$A = -ic \sin k\Delta x \pm \left[1 - (c \sin k\Delta x)^2\right]^{1/2}.$$

There are two cases to consider...

The CTCS scheme

- (i) $|c| < 1$
  Then $(c \sin k\Delta x)^2 < 1$, and

  $$|A|^2 = 1$$

  The solution is stable and, moreover, there is no damping error.
- (ii) $|c| > 1$
  Then, for some $k\Delta x$, $(c \sin k\Delta x)^2 > 1$, and

  $$|A|^2 = \left\{ c \sin k\Delta x \pm \left[(c \sin k\Delta x)^2 - 1 \right]^{1/2} \right\}^2$$

  One of the roots has $|A| > 1$, so the numerical solution is unstable.

Computational mode in the CTCS scheme

Because the CTCS scheme gives two roots for the amplification factor

$$A^{\pm} = -ic \sin k\Delta x \pm \left[1 - (c \sin k\Delta x)^2\right]^{1/2},$$

say, the general form of the numerical solution with wavenumber k is

$$\phi_j^{(n)} = \left[C_1 \left(A^{+}\right)^n + C_2 \left(A^{-}\right)^n\right] e^{ikj\Delta x}.$$

Assuming $|c| < 1$ so that $|A| = 1$, it is convenient to write

$$A^{+} = e^{-i\alpha}, \qquad A^{-} = -e^{i\alpha},$$

where $\sin\alpha = c \sin k\Delta x$, $\cos\alpha = \left[1 - (c \sin k\Delta x)^2\right]^{1/2}$. In the limit $\Delta x \to 0$, $\Delta t \to 0$ we find $\alpha \to uk\Delta t$, so that

$$\begin{aligned} \phi_j^{(n)} &= C_1 e^{ik(j\Delta x - un\Delta t)} + (-1)^n C_2 e^{ik(j\Delta x + un\Delta t)} \\ &= C_1 e^{ik(x-ut)} + (-1)^n C_2 e^{ik(x+ut)}. \end{aligned} \tag{2}$$

In this limit the first term becomes proportional to the exact solution $e^{ik(x-ut)}$ and is therefore called the *physical mode*. The second term does not correspond to any solution of the original equation; it is an artefact of the numerical method and is called the *computational mode*. Two characteristics of the computational mode for this scheme are (i) it oscillates in time from one step to the next (because of the $(-1)^n$ factor) and (ii) it propagates in the opposite direction to the physical solution (because of the $+un\Delta t$ in the exponential instead of $-un\Delta t$).

The CTCS scheme

The solution $\phi_j^{(n+1)}$ depends on $\phi_{j\pm1}^{(n)}$ and $\phi_j^{(n-1)}$, but not on $\phi_j^{(n)}$. Except at the initial time, the solution is found on two sets of points that are not coupled: those with $n+j$ even, and those with $n+j$ odd. At any point x_j the solution oscillates between the two uncoupled solutions. To keep the amplitude of the computational mode small. it is necessary to couple the solutions on the two sets of alternating grid points. A common way to do this is to apply a time filter that strongly damps oscillations of period $2\Delta t$, e.g. the *Robert-Asselin filter*.

For a centred in time scheme

$$\phi^{(n+1)} = \phi^{(n-1)} + 2\Delta t(\text{other terms})$$

we replace $\phi^{(n-1)}$ by a filtered value

$$\overline{\phi}^{(n-1)} = \phi^{(n-1)} + \varepsilon \left(\phi^{(n)} - 2\phi^{(n-1)} + \overline{\phi}^{(n-2)} \right),$$

i.e., at each step compute

$$\phi^{(n+1)} = \overline{\phi}^{(n-1)} + 2\Delta t(\text{other terms})$$

then compute

$$\overline{\phi}^{(n)} = \phi^{(n)} + \varepsilon \left(\phi^{(n+1)} - 2\phi^{(n)} + \overline{\phi}^{(n-1)} \right),$$

for use in the next time step. This filter introduces some artificial damping of the physical mode, so ε should be kept small, e.g. $\varepsilon = 0.1$.