Evolution equations with spectral methods: the case of the wave equation

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Plan

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Time discretization

It seems that, in general, there is no efficient spectral decomposition for the time coordinate...

$\Rightarrow$use of finite-differences schemes ! t is discretized (usually) on an equally-spaced grid, with a times-step δt : $U^J = U(J \times \delta t)$.

$$\frac{dU}{dt} = F(U) = L(U) + Q(U)$$

Study, for different integration schemes of :

- stability : $\forall n \|U^n\| \leq C e^{Kt} |U^0\|$, for some $\delta t < \delta_{\text{lim}}$,
- region of absolute stability : when considering

  $$\frac{dU}{dt} = \lambda U,$$

  the region in the complex plane for $\lambda \delta t$ for which $\|U^n\|$is bounded for all n,
- unconditional stability : if δ is independent from N (level of spectral truncation).

One-dimensional study

To use the knowledge of the region of absolute stability, it is necessary to diagonalize the matrix L and study its eigen-values λ_i.
In one dimension :

First-order Fourier

For $L = d/dx$, one finds $\max |\lambda_i| = O\left(N\right)$

First-order Chebyshev

For $L = d/dx$, one finds $\max |\lambda_i| = O\left(N^2\right)$

Second-order Fourier

For $L = d/dx^2$, one finds $\max |\lambda_i| = O\left(N^2\right)$

Second-order Chebyshev

For $L = d^2/dx^2$, one finds $\max |\lambda_i| = O\left(N^4\right)$

Time integration schemes

Most popular...

Explicit

- first-order Adams-Bashford scheme (a.k.a forward Euler) :

$$U^{n+1} = U^n + \delta t F\left(U^n\right),$$

- second-order Adams-Bashford scheme :

$$U^{n+1} = U^n + \delta t \left[\frac{23}{12} F\left(U^n\right) - \frac{16}{12} F\left(U^{n-1}\right) + \frac{5}{12} F\left(U^{n-2}\right)\right],$$

- Runge-Kutta schemes...

All these exhibit a bounded region of absolute stability
$\Rightarrow \exists K > 0, \quad \delta t \leq K / \max |\lambda_i|$ (Courant condition ...).

Time integration schemes
Most popular...

Implicit

Adams-Moulton :

- first-order (a.k.a backward Euler scheme)

$$U^{n+1} = U^n + \delta t F\left(U^{n+1}\right),$$

- second-order (a.k.a. Crank-Nicholson scheme)

$$U^{n+1} = U^n + \frac{1}{2}\delta t\left[F\left(U^{n+1}\right) + F\left(U^n\right)\right].$$

Both have an unbounded region of absolute stability in the left complex half-plane ⇒unconditionally stable schemes.
Higher-order AM schemes have only a bounded region of absolute stability.

Schemes can be mixed and various source terms can be treated in different ways (*e.g.* linear ⇒implicit / non-linear ⇒explicit).

Wave equation

The three-dimensional wave equation in spherical coordinates :

$$\Box\phi = -\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} + \frac{\partial^2\phi}{\partial r^2} + \frac{2}{r}\frac{\partial\phi}{\partial r} + \frac{1}{r^2}\Delta_{\theta\varphi}\phi = \sigma;$$

with

$$\Delta_{\theta\varphi} \equiv \frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

In 1D, it admits two characteristics : $\pm c$: $f(ct - x)$ and $f(ct + x)$.
To be well-posed, the initial-boundary value problem needs :

- $\phi(t = 0)$ and $\partial\phi/\partial t(t = 0)$,
- a boundary condition at every domain boundary (Dirichlet, von Neumann, mixed).

An explicit scheme for the wave equation

Using a second-order scheme to evaluate the second time derivative

$$\left.\frac{\partial^2 \phi}{\partial t^2}\right|_{t=t^J} = \frac{\phi^{J+1} - 2\phi^J + \phi^{J-1}}{\delta t^2} + O\left(\delta t^4\right),$$

one recovers the forward Euler scheme

$$\phi^{J+1} = 2\phi^J - \phi^{J-1} + \delta t^2 \left(\Delta \phi^J + \sigma\right) + O(\delta t^4).$$

Solution of the initial-boundary value problem inside a sphere or $r \leq R$:

- initial profiles at $t = t^0$ and $t = t^1$,
- $\forall t > t^1$, a value for $\phi(r = R)$.

With spectral methods using Chebyshev polynomials in r, time-step limitation is coming from the second radial derivative :

$$\delta t^2 \leq K/N^4.$$

Complete 3D problem $\Rightarrow$regularity conditions at the origin too, for $\ell > 1$.

Implicit scheme

With the same formula for the second time derivative and the Crank-Nicholson scheme :

$$\left[1 - \frac{\delta t^2}{2}\Delta\right]\phi^{J+1} = 2\phi^J - \phi^{J-1} + \delta t^2\left(\frac{1}{2}\Delta\phi^{J-1} + \sigma^J\right).$$

One must invert the operator $1 - 1/2\delta t^2\Delta$; one way is :

- consider the spectral representation of ϕ in terms of spherical harmonics ($\Delta_{\theta\varphi}Y_\ell^m = -\ell(\ell+1)Y_\ell^m$) ;
- solve the ordinary differential equation in r as a simple linear system, using *e.g.* the tau method.

⇒one can add boundary and regularity conditions depending on the multipolar momentum ℓ.
⇒beware of the condition number of the operator matrix !
⇒sometimes regularity is better imposed (stable) using a Galerkin base.

Domain boundaries

Contrary to the Laplace operator Δ, the d'Alembert one $\Box$ is not invariant under inversion / sphere.

- one cannot *a priori* use a change of variable $u = 1/r$!
- the distance between two neighboring grid points becomes larger than the wavelength...

$\Rightarrow$domain of integration bounded (*e.g.* within a sphere of radius R).

Two types of BCs :

- reflecting BC : $\phi(r = R) = 0$,
- absorbing BC...

An absorbing BC can be seen in 1D : at $x = 1$ one imposes no incoming characteristic ⇒only $f(ct - x)$ mode.
In spherical 3D geometry : asymptotically, the solution must match

$$\phi \sim_{r\to\infty} \frac{1}{r} f(ct - r),$$

equivalently,

$$\lim_{r\to\infty} \frac{\partial(r\phi)}{\partial t} + c\frac{\partial(r\phi)}{\partial t} = 0.$$

At finite distance R :

$$\left.\left(\frac{1}{c}\frac{\partial\phi}{\partial t} + \frac{\partial\phi}{\partial r} + \frac{\phi}{r}\right)\right|_{r=R} = 0;$$

which is exact in spherical symmetry.

General form of the solution

The homogeneous wave equation $\Box\phi = 0$ admits as asymptotic development of its solution

$$\phi(t, r, \theta, \varphi) = \sum_{k=1}^{\infty} \frac{f_k(t - r, \theta, \varphi)}{r^k}.$$

One can show that the contribution from a mode ℓ exists only for $k \leq \ell + 1$. Moreover, the operators :

$$B_1 f = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial r} + \frac{f}{r}, \qquad B_{n+1} f = \left(\frac{\partial}{\partial t} + \frac{\partial}{\partial r} + \frac{2n+1}{r} \right) B_n f$$

are such that the condition $B_n\phi = 0$ matches the first n terms ($B_n\phi = O\left(1/r^{2n+1}\right)$). It follows that

$$B_n\phi = 0$$

- is a n^{th}-order BC,
- is exact for all modes $\ell \leq n - 1$,
- is asymptotically exact with an error decreasing like $1/R^{n+1}$,
- is the generalization of the Sommerfeld BC at finite distance ($n = 1$).

Absorbing BC for $l \leq 2$

The condition $B_3\phi = 0$ at $r = R$ writes

$$\forall (t, \theta, \varphi), \quad B_1\phi|_{r=R} = \left(\frac{\partial}{\partial t} + \frac{\partial}{\partial r} + \frac{1}{r} \right) \phi(t, r, \theta, \varphi) \Big|_{r=R} = \xi(t, \theta, \varphi),$$

with $\xi(t, \theta, \varphi)$ verifying a wave-like equation on the sphere $r = R$

$$\frac{\partial^2 \xi}{\partial t^2} - \frac{3}{4R^2}\Delta_{\theta\varphi}\xi + \frac{3}{R}\frac{\partial \xi}{\partial t} + \frac{3\xi}{2R^2} = \frac{1}{2R^2}\Delta_{\theta\varphi}\left(\frac{\phi}{R} - \frac{\partial \phi}{\partial r}\Big|_{r=R} \right).$$

- easy to solve if ξ is decomposed on the spectral base of spherical harmonics !
- looks like a perturbation of the Sommerfeld BC...
- exact for $\ell \leq 2$ and the error decreases as $1/R^4$ for other modes.