L17

Spectral methods for PDEs

Suppose we wish to numerically solve

$$q_t - S(q) = 0 \qquad a < x < b \qquad (*)$$

where $S(q)$ is an operator involving spatial derivs., e.g. $S(q) = -\bar{u} q_x$ for 1D scalar advection by a constant velocity $\bar{u}$. Spectral methods seek an approximate soln in the form (a form of function space methods)

$$Q(x,t) = \sum_{n=1}^{N} \hat{q}_n(t)\, \varphi_n(x) \qquad (1)$$

where the $\{\varphi_n(x)\}$ are a set of orthogonal basis functions wrt some positive weight fn $w(x)$ (e.g. $w(x) \equiv 1$, the commonest choice):

$$\langle \varphi_m, \varphi_n \rangle \equiv \int_a^b w(x)\varphi_m^*(x)\varphi_n(x)\,dx = 0 \qquad m \neq n.$$

In the simplest case, if $q(x,t)$ satisfies homogeneous BCs at $x = a, b$, we also insist the $\{\varphi_n(x)\}$ satisfy the same BCs, so (1) will also automatically satisfy the BCs.

To obtain expressions for the expansion coeffs $\hat{q}_n(t)$ we form a residual

$$R[Q](x,t) = Q_t - S(Q)$$

and attempt to minimize some measure of R at each time wrt the $\hat{q}_n(t)$. As in Amath 585, we recall that three strategies are:

(1) Minimize $\|R\|_2^2 = \langle R, R \rangle$

(2) [Galerkin method] Require R to be orthogonal to the φ_n's:

$$\langle \varphi_n, R \rangle = 0 \qquad, n = 1, \ldots, N$$

(3) [Collocation method] Require R be zero at gridpoints x_j, $j = 1, \ldots, N$

$$R[Q](x_j, t) = 0 \qquad, j = 1, \ldots, N.$$

For problems of form $(*)$, strategies (1) and (2) are equivalent. Letting $\dot{\hat{q}}_n = d\hat{q}_n/dt$, (1) $\Rightarrow$

$$0 = \frac{\partial}{\partial \dot{\hat{q}}_n}\langle R, R\rangle = \frac{\partial}{\partial \dot{\hat{q}}_n}\int_a^b w(x)\left\{\sum_n \dot{\hat{q}}_n\varphi_n - S\left(\sum_n \hat{q}_n\varphi_n\right)\right\}^* \left\{\sum_n \dot{\hat{q}}_n\varphi_n - S\left[\sum_n \hat{q}_n\varphi_n\right]\right\}dx$$

$$= \int_a^b w(x)\varphi_n^*\left[\sum_n \dot{\hat{q}}_n\varphi_n - S\sum_n \hat{q}_n\varphi_n\right]dx$$

$$= \langle \varphi_n, R\rangle$$

which is strategy (2).

Fourier spectral methods on a periodic domain $0<x<L$

If the differential operator $S(q)$ includes x-derivs through order p, $q(x,t)$ obeys periodic BCs if q and its first $p-1$ x-derivs are equal at $x=0$ and $x=L$, e.g., for

$$q_t + 6qq_x + q_{xxx} = 0 \qquad 0<x<1 \qquad (*')$$

periodic BCs would be:

$$q(0,t) = q(1,t)$$
$$q_x(0,t) = q_x(1,t)$$
$$q_{xx}(0,t) = q_{xx}(1,t)$$

In this case $q(x,t)$ may be ~~regarded~~ extended into a 1-periodic fn, satisfying $(*')$ on $-\infty<x<\infty$ and a natural spectral representation for approximating q is a finite Fourier series approximation

$$Q(x,t) = \sum_{n=1}^{N} \hat{q}_n(t)\varphi_n(x) \qquad (F)$$

where (notation chosen with 20/20 foresight)

$$\varphi_n(x) = N^{-1} e^{iK_n x} \qquad \left(\langle \varphi_m, \varphi_n\rangle = \int_0^L \varphi_m^*(x)\varphi_n(x)\,dx = \frac{L}{N^2}\delta_{mn}\right)$$

With a complex Fourier series we must include both positive and negative wavenos, a la Amath 585:

$$K_n = \begin{cases} \frac{2\pi}{L}(n-1) & 1 \le n \le \frac{N}{2} \\ \frac{2\pi}{L}(n-1-N) & \frac{N}{2} < n \le N \end{cases}$$

Note ambiguity: $K_{\frac{N}{2}+1} = \frac{2\pi}{L}\left(\frac{N}{2}\right)$ or $\frac{2\pi}{L}\left(-\frac{N}{2}\right)$? (as chosen here)

The p-th derivative of Q is just

$$\frac{\partial^p Q}{\partial x^p}(x,t) = \mathrm{Re}\left[\sum_{n=1}^{N} (iK_n)^p \hat{q}_n(t)\varphi_n(x)\right]$$

Re[ ] will automatically take care of above ambiguity.

Relation to Discrete Fourier Transform (DFT)

For any N-vector $\vec{y} = \{y_j\}$, its DFT $\hat{\vec{y}} = \{\hat{y}_n\}$ is

$$\hat{y}_n = \sum_{j=1}^{N} y_j e^{\frac{-2\pi i(j-1)(n-1)}{N}}, \quad n=1,\dots,N$$

with inverse DFT

$$y_j = N^{-1}\sum_{n=1}^{N} \hat{y}_n e^{\frac{2\pi i(j-1)(n-1)}{N}}, \quad j=1,\dots,N$$