Math 6620: Analysis of Numerical Methods, II
Fourier spectral methods, II

See Hesthaven, S. Gottlieb, and D. Gottlieb 2007, Chapter 3

Akil Narayan[1]

[1] **Department of Mathematics, and Scientific Computing and Imaging (SCI) Institute**
University of Utah

Time-dependent problems

We will now (briefly) discuss time-dependent problems:

$$\frac{\partial u}{\partial t} = \mathcal{L}(u),$$

with periodic boundary conditions in the one-dimensional spatial variable x.

We will frequently take $\mathcal{L}$ as a linear operator (but this need not be the case).

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In contrast to establishing rigorous convergence for such problems, we'll focus on stability, and on practical implementation considerations.

In particular we'll consider "strong form" Galerkin and collocation methods.

As with other time-dependent problems, we'll construct semi-discrete schemes, and not wade into the time-stepping details.

A simple example

We seek to develop a Fourier-Galerkin scheme for the PDE,

$$\frac{\partial u}{\partial t} = c\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2},$$

with constants $c \in \mathbb{R}$ and $\nu > 0.$ We will assume the initial condition is smooth.

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The exact solution satisfies an energy stability property:

$$\int_0^{2\pi} u\frac{\partial u}{\partial t} = c\int_0^{2\pi} u\frac{\partial u}{\partial x}\mathrm{d}x + \nu\int_0^{2\pi} u\frac{\partial^2 u}{\partial x^2}\mathrm{d}x$$

Using $uu_t = \frac{1}{2}(u^2)_t$, $uu_x = \frac{1}{2}(u^2)_x$ and periodic boundary conditions:

$$\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{L^2} = 0 - \nu\|u_x\|^2_{L^2} \leqslant 0,$$

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The Fourier-Galerkin method will seek a solution u_N given by,

$$u_N(x,t) = \sum_{|k|\leqslant N} \widehat{u}_k(t)\phi_k(x), \qquad \phi_k(x) = \frac{1}{\sqrt{2\pi}}e^{ikx},$$

i.e., $u_N(\cdot,t) \in V_N = \mathrm{span}_{|k|\leqslant N}e^{ikx}$ for every t.

A simple Fourier Galerkin scheme

The Fourier-Galerkin scheme for this problem is given by:

$$\left\langle \frac{\partial u_N}{\partial t}, v \right\rangle = c \left\langle \frac{\partial u_N}{\partial x}, v \right\rangle + \nu \left\langle \frac{\partial^2 u_N}{\partial x^2}, v \right\rangle, \qquad \forall \;\; v \in V_N$$

Choosing $v = \phi_k$ for every $|k| \leqslant N$, this yields a size-$(2N+1)$ ODE system given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{u}} = c\widehat{\boldsymbol{D}}_1 \hat{\boldsymbol{u}} + \nu \widehat{\boldsymbol{D}}_2 \hat{\boldsymbol{u}},$$

$\frac{d\hat{u}}{dt} = \underline{\underline{A}}\,\underline{\hat{u}}$, $\underline{\underline{A}}$: diagonal

where $\widehat{D}_1$ and $\widehat{D}_2$ are spectral differentiation matrices, which are diagonal:

$$\widehat{\boldsymbol{D}}_1 = \mathrm{diag}\left(-iN, -i(N-1), \cdots, iN\right), \qquad \widehat{\boldsymbol{D}}_2 = \mathrm{diag}\left(-N^2, -(N-1)^2, \cdots, -N^2\right).$$

Thus, these ODEs are actually uncoupled, and we can compute an exact solution:

$$\widehat{u}_k(t) = \widehat{u}_k(0) e^{(-\nu k^2 + ick)t}, \qquad |k| \leq N$$

which has non-increasing magnitude in time, just as we expect from the (exact) stability condition.

$$u_N(x,t) = \sum_{|k| \leq N} \hat{u}_k(0)\, \phi_k(x)\, e^{-(\nu k^2 + ick)t}$$

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In addition, these (uncoupled) ODE's are actually the evolution of the *exact* projection coefficients, i.e., with $\widehat{u}_k(t)$ the exact solution to the ODE above, then

$$\widehat{u}_k(t) = \left\langle u, \phi_k \right\rangle,$$

where u is the exact solution.

A second example, I

To understand why the Fourier-Galerkin method can be difficult to implement, consider

$$\frac{\partial u}{\partial t} = \sin x \, \frac{\partial u}{\partial x},$$

again with periodic boundary conditions over $x \in [0, 2\pi]$. Taking $u_N \in V_N$ as before, the scheme is given by,

$$\left\langle \frac{\partial u_N}{\partial t}, v \right\rangle = \left\langle \sin x \, \frac{\partial u_N}{\partial x}, v \right\rangle, \qquad \forall \;\; v \in V_N$$

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We use the property,

$$\phi_k(x)\phi_\ell(x) = \frac{1}{\sqrt{2\pi}} \phi_{k+\ell}(x), \qquad k, \ell \in \mathbb{Z},$$

which implies,

$\frac{1}{2i}\left(e^{ix} - e^{-ix}\right)$

$$\sin x \, \phi_k'(x) = -i\sqrt{\frac{\pi}{2}} \left(\phi_1(x) - \phi_{-1}(x)\right)(ik)\phi_k(x) = \frac{k}{2}\left(\phi_{k+1}(x) - \phi_{k-1}(x)\right).$$

A second example, II

Hence, the Fourier-Galerkin scheme can again be written as an ODE system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\boldsymbol{u}} = \boldsymbol{A}\widehat{\boldsymbol{u}},$$

where

$$\boldsymbol{A} = \begin{pmatrix} 0 & \frac{-N}{2} & & & \\ \frac{(N-1)}{2} & 0 & \frac{-(N-1)}{2} & & \\ & \ddots & & \ddots & \\ & & & & \\ & & & \frac{-N}{2} & 0 \end{pmatrix}$$

A third example, I

The previous example was not too bad, but things can get out of hand quickly. Consider,

$$\frac{\partial u}{\partial t} = u \, \frac{\partial u}{\partial x},$$

Then the Fourier-Galerkin scheme is,

$$\left\langle \frac{\partial u_N}{\partial t}, v \right\rangle = \left\langle u_N \, \frac{\partial u_N}{\partial x}, v \right\rangle, \qquad\qquad \forall \;\; v \in V_N.$$

Setting $v \leftarrow \phi_r$ for some $|r| \leqslant N$, we need to compute the inner product:

$$\left\langle \left(\sum_{|k| \leqslant N} \widehat{u}_k(t) \phi_k \right) \left(\sum_{|\ell| \leqslant N} i\ell \widehat{u}_\ell(t) \phi_\ell \right), \phi_r \right\rangle$$

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We use the fact that

$$\sum_{|k|,|\ell| \leqslant N} i\ell \widehat{u}_k(t) \widehat{u}_\ell(t) \phi_k \phi_\ell = \sum_{|k|,|\ell| \leqslant N} \frac{i\ell}{\sqrt{2\pi}} \widehat{u}_k(t) \widehat{u}_\ell(t) \phi_{k+\ell} = \sum_{|s| \leqslant 2N} a_s \phi_s,$$

where

$a \vee b = \max\{a, b\}$

$a \wedge b = \min\{a, b\}$

$$a_s = \sum_{\ell=(-N)\vee(s-N)}^{N \wedge (s+N)} \frac{i\ell}{\sqrt{2\pi}} \widehat{u}_{s-\ell}(t) \widehat{u}_\ell(t)$$

A third example, II

So the scheme is,

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\boldsymbol{u}} = \boldsymbol{a}(\widehat{\boldsymbol{u}}),$$

where

$$a_k = \sum_{\ell=(-N)\vee(k-N)}^{N\wedge(k+N)} \frac{i\ell}{\sqrt{2\pi}}\widehat{u}_{k-\ell}(t)\widehat{u}_\ell(t).$$

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Our PDE was nonlinear, so it's no surprise that our semi-discrete form is nonlinear.

In particular, it involves a (discrete) convolution.

From an implementation standpoint, this is pretty expensive: The operation

$$\widehat{\boldsymbol{u}} \mapsto \boldsymbol{a}\left(\widehat{\boldsymbol{u}}\right),$$

is an $\mathcal{O}(N^2)$ operation.

A fourth example

Things can get even worse:

$$\frac{\partial u}{\partial t} = \sin u \, \frac{\partial u}{\partial x},$$

In this case, it is entirely unclear how to compute,

$$\left\langle \sin u_N(x,t) \frac{\partial}{\partial u_N}, \phi_k \right\rangle,$$

since the $\sin u_N$ term cannot be easily expanded in terms of the basis ϕ_ℓ.

Thus, in some cases one cannot even form the true Galerkin system.

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As we briefly discussed before, one can employ a pseudospectral approach, which would use collocation values $\boldsymbol{u}$ in intermediate computations:

$$\widehat{\boldsymbol{u}} \xrightarrow{DFT} \boldsymbol{u} \rightarrow \sin \boldsymbol{u} \xrightarrow{DFT} \widehat{\sin \boldsymbol{u}},$$

which corresponds to the approximation:

$$\sin u_N \approx I_N \sin u_N.$$

(Or one could interpolate the entire $\sin u_N \; \frac{\partial}{\partial x} u_N$ term).

Collocation

Collocation methods are, of course, much easier, but they come with a price.

Consider our first example,

$$\frac{\partial u}{\partial t} = c\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2}.$$

The collocation (Petrov-Galerkin) formulation of this problem corresponds to the trial function,

$$u_N(x,t) = \sum_{k=1}^{M} u_k(t)\ell_k(x), \qquad M = 2N+1,$$

where ℓ_k is the cardinal Lagrange function at x_k for the space V_N.

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With collocation values $\boldsymbol{u}(t) = (u_k(t))_{k\in[M]}$, as our degrees of freedom, and δ_{x_k} for $k \in [M]$ our test functions, then our scheme reads,

$$\left\langle \frac{\partial u_N}{\partial t}, v \right\rangle = \left\langle c\frac{\partial u_N}{\partial x} + \nu\frac{\partial^2 u_N}{\partial x^2}, v \right\rangle, \qquad v \in \mathrm{span}_{k\in[M]}\delta_{x_k}$$

which just means we enforce zero residual at the points x_k:

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u} = c\widetilde{\boldsymbol{D}}_1\boldsymbol{u} + \nu\widetilde{\boldsymbol{D}}_2\boldsymbol{u},$$

where $\widetilde{\boldsymbol{D}}_1$ and $\widetilde{\boldsymbol{D}}_2$ are the collocation differentiation matrices (dense) for the first and second derivatives, respectively.

A second collocation example

Collocation makes a lot of things much easier. E.g., for

$$\frac{\partial u}{\partial t} = \sin u \, \frac{\partial u}{\partial x},$$

the collocation scheme is just,

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u} = (\sin \boldsymbol{u}) \odot \left(\widetilde{\boldsymbol{D}}_1 \boldsymbol{u}\right),$$

where $\odot$ is the elementwise product between vectors and $\sin \boldsymbol{u}$ is interpreted elementwise.

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Therefore, many of the analytical challenges with Galerkin methods (even if using pseudospectral approaches) are mitigated by using collocation schemes.

The main difference between Galerkin and collocation methods in this context is

$$\frac{\mathrm{d}}{\mathrm{d}t} u_N = P_N \mathcal{L}(u_N) \qquad \text{vs.} \qquad \frac{\mathrm{d}}{\mathrm{d}t} u_N = I_N \mathcal{L}(u_N),$$

and hence the aliasing error for $\mathcal{L}(u_N)$ is what sets these two methods apart.

Naturally, there is no free lunch: although collocation is easier to formulate/implement, it's generally easier to prove things (e.g., stability) for Galerkin approaches.

Recall: semi-bounded operators

Stability for time-dependent Fourier spectral methods begins with similar considerations at the continuous level.

Consider again our prototypical example,

$$u_t = \mathcal{L}(u),$$

with periodic boundary conditions on $[0, 2\pi]$ with $\mathcal{L}$ a linear operator.

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The adjoint $\mathcal{L}^*$ of the operator $\mathcal{L}$ is defined by the condition,

$$\langle \mathcal{L}^* u, v \rangle = \langle u, \mathcal{L} v \rangle,$$

for every periodic $u, v \in L^2$.

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We call $\mathcal{L}$ semi-bounded if,

$$\mathcal{L} + \mathcal{L}^* \leqslant CI,$$

for some $C \in \mathbb{R}$. This means that,

$$\left\langle \left(\mathcal{L} + \mathcal{L}^*\right) u, u \right\rangle \leqslant \langle Cu, u \rangle = C\|u\|_{L^2}^2$$

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Note the following result: If $\mathcal{L}$ is semi-bounded, then $u_t = \mathcal{L}u$ is a well-posed PDE, and the solution satisfies the stability condition,

$$\|u(t)\|_{L^2} \leqslant e^{(C/2)t}\|u(0)\|_{L^2}.$$

$\mathcal{L} + \mathcal{L}^* \leq C I$

$u_t = \mathcal{L}(u) = \mathcal{L}u$

$\langle u_t, u \rangle = \langle \mathcal{L}u, u \rangle \qquad \langle u, u_t \rangle = \langle u, \mathcal{L}u \rangle$

$\shortparallel \qquad\qquad\qquad\qquad \shortparallel$

$\frac{1}{2} \frac{d}{dt} \|u\|_{L^2}^2 \qquad\qquad \frac{1}{2} \frac{d}{dt} \|u\|_{L^2}^2$

$$\frac{d}{dt} \|u\|_{L^2}^2 = \langle (\mathcal{L} + \mathcal{L}^* u), u \rangle \leq C \|u\|_{L^2}^2$$

$\Rightarrow$ Gronwall's ineq. $\Rightarrow$ $\|u\|_{L^2}^2 \leq \|u_0\|_{L^2}^2 \cdot \exp(Ct)$

$$\|u\|_{L^2} \leq \|u_0\|_{L^2} \cdot \exp\left(\frac{C}{2} t\right)$$

Some examples, I

We will use the notion of semi-bounded operators, so it is useful to consider some examples.

Example

Consider

$$u_t = \mathcal{L}(u) := c(x) u_x.$$

This is a variable wavespeed advection equation. We assume c is real-valued and periodic.

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$$u_t = \mathcal{L}(u) := c(x) u_x.$$

This is a variable wavespeed advection equation. We assume c is real-valued and periodic. We compute $\mathcal{L}^*$ through integration by parts:

$$\begin{aligned} \langle \mathcal{L}u, v \rangle = \langle c(x) u_x, v \rangle &= \int_0^{2\pi} c(x) u_x \overline{v} \mathrm{d}x \\ &\stackrel{\text{IbP}}{=} u \overline{v} c(x) \Big|_0^{2\pi} - \int_0^{2\pi} u \left(c(x) \overline{v} \right)_x \mathrm{d}x. \end{aligned}$$

If we also assume that c is differentiable:

$$\begin{aligned} \langle \mathcal{L}u, v \rangle &= -\int_0^{2\pi} u \left(c'(x) \overline{v} + c(x) \overline{v}_x \right) \mathrm{d}x \\ &= \left\langle u, -c'(x) v - c(x) v_x \right\rangle = \left\langle u, \mathcal{L}^* v \right\rangle. \end{aligned}$$

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$$\mathcal{L}^* = -c(x) \frac{\partial}{\partial x} - c'(x) I$$

Therefore,

$$\mathcal{L} + \mathcal{L}^* = c(x) \frac{\partial}{\partial x} - c(x) \frac{\partial}{\partial x} - c'(x) I = -c'(x) I.$$

Finally: if $c(x)$ is periodic, differentiable, and has bounded derivative, then $\mathcal{L}$ is semi-bounded with $\mathcal{L} + \mathcal{L}^* \leqslant CI$, with $C = \max |c'(x)|$.

Example

Consider

$$u_t = \mathcal{L}(u) := \frac{\partial}{\partial x}\kappa(x)\frac{\partial}{\partial x}u,$$

where κ is a real, non-negative, periodic and differentiable function.

Again with integration by parts:

$$\begin{aligned}\langle \mathcal{L}u, v\rangle &= \int_0^{2\pi} \frac{\partial}{\partial x}\kappa(x)\frac{\partial}{\partial x}u, \overline{v}\mathrm{d}x \\ &= -\int_0^{2\pi} \kappa(x)u_x\overline{v}_x\mathrm{d}x \\ &= \int_0^{2\pi} u\frac{\partial}{\partial x}\kappa(x)\frac{\partial}{\partial x}\overline{v}\mathrm{d}x = \left\langle u, \left(\frac{\partial}{\partial x}\kappa(x)\frac{\partial}{\partial x}\right) v\right\rangle.\end{aligned}$$

IbP

Therefore,

$$\mathcal{L} + \mathcal{L}^* = 2\frac{\partial}{\partial x}\kappa(x)\frac{\partial}{\partial x}.$$

Example

Consider

$$u_t = \mathcal{L}(u) := \frac{\partial}{\partial x}\kappa(x)\frac{\partial}{\partial x}u,$$

where κ is a real, non-negative, periodic and differentiable function.

To show that this is semi-bounded, note that,

$$\left\langle(\mathcal{L}+\mathcal{L}^*)u, u\right\rangle = 2\left\langle \frac{\partial}{\partial x}\kappa(x)u_x, u\right\rangle = -2\left\langle\kappa(x)u_x, u_x\right\rangle \leqslant 0\|u\|^2_{L^2}.$$

Fourier-Galerkin stability

A particularly attractive property of the Fourier-Galerkin method: if $\mathcal{L}$ is semi-bounded, not only is the original PDE well-posed with a stability condition, but the Fourier-Galerkin solution obeys the same stability condition.

Theorem

Assume $\mathcal{L}$ is semi-bounded with $\mathcal{L} + \mathcal{L}^* \leqslant CI$, and consider the PDE $u_t = \mathcal{L}(u)$. Then the Fourier-Galerkin solution is stable and obeys the bound,

$$\|u_N(t)\|_{L^2} \leqslant e^{(C/2)t} \|u_N(0)\|_{L^2}$$

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The first step is to show that $P_N = P_N^*$:

$$\begin{aligned}\langle P_N u, v\rangle = \langle P_N u, P_N v\rangle + \langle P_N u, (I - P_N)v\rangle \\ &= \langle P_N u, P_N v\rangle \\ &= \langle P_N u, P_N v\rangle + \langle (I - P_N)u, P_N v\rangle \\ &= \langle u, P_N v\rangle .\end{aligned}$$

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$$\|u_N(t)\|_{L^2} \leqslant e^{(C/2)t} \|u_N(0)\|_{L^2}$$

The second step uses $u_N = P_N u_N$ to formulate a PDE that u_N satisfies:

$$\frac{\partial}{\partial t} u_N = P_N \mathcal{L} u_N \quad \Longrightarrow \quad \frac{\partial}{\partial t} u_N = P_N \mathcal{L} P_N u_N =: \mathcal{L}_N u_N.$$

Then,

$$\begin{aligned} \mathcal{L}_N + \mathcal{L}_N^* &= P_N \mathcal{L} P_N + (P_N \mathcal{L} P_N)^* \\ &= P_N \mathcal{L} P_N + P_N \mathcal{L}^* P_N \\ &= P_N \left(\mathcal{L} + \mathcal{L}^*\right) P_N \leqslant C P_N. \end{aligned}$$

Therefore,

$$\frac{d}{dt}\|u_N\|_{L^2}^2 = \left\langle (\mathcal{L}_N + \mathcal{L}_N^*) u_N, u_N \right\rangle \leqslant C \left\langle P_N u_N, u_N \right\rangle = C \|u_N\|_{L^2}^2,$$

which implies the result.

Collocation stability

Collocation stability is more delicate and technical.

For example, for the rather simple problem

$$u_t = c(x) u_x,$$

then the Fourier collocation method is stable only if c is bounded away from 0.
(Recall for Fourier Galerkin, and in the general continuous problem, $c(x)$ changing sign is no problem.)

Collocation stability is more delicate and technical.

For example, for the rather simple problem

$$u_t = c(x)u_x,$$

then the Fourier collocation method is stable only if c is bounded away from 0.
(Recall for Fourier Galerkin, and in the general continuous problem, $c(x)$ changing sign is no problem.)

The instability is "weak" and often does not surface in practice; nevertheless it is there.

One must resort to some somewhat clever alternatives to fix the problem. In particular, consider the rewritten problem,

$$u_t = \frac{1}{2}c(x)u_x + \frac{1}{2}\frac{\partial}{\partial x}\left(c(x)u\right) - \frac{1}{2}c'(x)u,$$

which is called the *skew-symmetric form*. Note that if a is differentiable, this is equivalent to the original PDE.

The Fourier collocation method applied to the skew-symmetric form is stable.

The difference between the two schemes is that the scheme for the skew-symmetric form effectively adds a term that compensates for aliasing error.

Hesthaven, Jan S., Sigal Gottlieb, and David Gottlieb (2007). *Spectral Methods for Time-Dependent Problems*. Cambridge University Press. ISBN: 0-521-79211-8.