

256 Summary

1 High order FD

- *Finite-order finite differences:*

$$\begin{aligned} \mathcal{D}_n f(x_j) &= \frac{f_{j+n} - f_{j-n}}{2n\Delta x} \\ \frac{df}{dx} \Big|_{x_j} &= \sum_{n=1}^m \alpha_n^m \mathcal{D}_n f_j \\ \alpha_n^m &= -2(-1)^n \frac{(m!)^2}{(m-n)!(m+n)!}. \end{aligned}$$

- *Points per Wavelength:*

$$\text{PPW} = \frac{2\pi}{k\Delta x} \geq 2$$

- *Number of passes:*

$$\nu = \frac{kc t}{2\pi}$$

- *Phase error:* Leading term of the relative error. Often

$$\text{PE}(p, \nu) \sim C\nu \left(\frac{2\pi}{\text{PPW}} \right)^{\text{order}}.$$

- *Work per wavelength:*

$$W_m = 2m \times \text{PPW} \times \frac{t}{\Delta t},$$

where $m = \text{order}$.

- *Infinite-order finite differences:* As above with $m \rightarrow \infty$. Demand exactness for trig. polynomial e^{ix} . Find coefficients by comparing with Fourier series for $x \mapsto x$. Rearranging the sum gives

$$\frac{du}{dx} \Big|_{x_j} = \sum_{i=0}^N \underbrace{\frac{1}{2}(-1)^{j+i} \left[\sin\left(\frac{\pi}{N+1}(j-i) \right) \right]^{-1}}_{D_{i,j}} u_i.$$

2 Trigonometric Polynomial Approximation

Assume $u: [0, 2\pi] \rightarrow \mathbb{R}$ periodic.

- N even.
- *Spaces:*

$$\begin{aligned} \hat{B}_N &:= \text{span}\{e^{inx} : |n| \leq N/2\} \quad N+1\text{-dim.} \\ \tilde{B}_N &:= \hat{B}_N \setminus \left\{ \sin\left(\frac{N}{2}x\right) \right\} \quad N\text{-dim.} \end{aligned}$$

2.1 Continuous Expansion

- *Fourier series:*

$$\begin{aligned} \mathcal{P}_N u(x) &= \sum_{n=-\infty}^{\infty} \hat{u}_n e^{inx}, \\ \hat{u}_n &= \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-inx} dx. \end{aligned}$$

- Special cases:
 - u real $\Rightarrow \hat{u}_{-n} = \hat{u}_n^*$,
 - u even \Rightarrow only cosines,
 - u odd \Rightarrow only sines.
- *Approximation:*
 - $\sum_{n=-\infty}^{\infty} |\hat{u}_n|^2 < \infty \Rightarrow \|u - \mathcal{P}_N u\|_{L^2} \rightarrow 0$.
 - $\sum_{n=-\infty}^{\infty} |\hat{u}_n| < \infty \Rightarrow \|u - \mathcal{P}_N u\|_{L^\infty} \rightarrow 0$.
- $u^{(0\dots m-1)}$ (viewed periodically) is continuous, $u^{(m)} \in L^2 \Rightarrow |\hat{u}_n| \sim (1/n)^m$.
- *Spectral convergence:* $u \in C^\infty \Rightarrow \hat{u}_n$ decays faster than any power of n .
- $\mathcal{P}\mathcal{D} = \mathcal{D}\mathcal{P}$. Projection and differentiation commute. (start with expansion above, carry out both.)
- *Truncation error:* $\mathcal{P}_N \mathcal{L}(\text{Id} - \mathcal{P}_N) = 0$.

2.1.1 Approximation Theory for the Continuous Expansion

- *Sobolev norm:*

$$\|u\|_q^2 = \sum_{m=0}^q \|D^m u\|_{L^2}^2 \sim \sum_{n=-\infty}^{\infty} |\hat{u}_n|^2 (1+|n|)^{2q}.$$

- Parseval's Identity:

$$\sum_n |\hat{u}_n|^2 = \frac{1}{2\pi} \int_0^{2\pi} |u|^2.$$

- $h = 1/N$.
- $u \in H^r$:

$$\|u - \mathcal{P}_{2N} u\|_{L^2} \leq C h^q \left\| u^{(q)} \right\|_{L^2}.$$

Proof: Parseval, consider tail, smuggle in an $n^{2q} \cdot \frac{1}{n^{2q}}$.

- u analytic:

$$\|u - \mathcal{P}_{2N} u\|_{L^2} \leq C e^{-cN} \|u\|_{L^2}$$

Proof: $\left\| u^{(q)} \right\|_{L^2} \leq C q! \|u\|_{L^2}$, Stirling's Formula: $q! \sim q^q e^{-q}$, $q \sim N$.

- $u \in H^r$:

$$\|u - \mathcal{P}_{2N} u\|_{H^q} \leq C h^{r-q} \|u\|_{H^r}.$$

Proof: Parseval, $(1+|n|)^{2q} \sim \frac{(1+|n|^{2r})}{N^{2(r-q)}}$.

- $u \in C^q$, $q > 1/2$:

$$\|u - \mathcal{P}_{2N} u\|_{L^\infty} \leq h^{q-1/2} \left\| u^{(q)} \right\|_{L^2}.$$

Proof: $|u - \mathcal{P}_{2N} u|$, smuggle in n^q , CSU.

- \mathcal{L} a constant coefficient differential operator:

$$\mathcal{L}u = \sum_{j=1}^s a_j \frac{d^j u}{dx^j}.$$

$$\|\mathcal{L}u - \mathcal{L}\mathcal{P}_{2N} u\|_{H^q} \leq h^{r-q-s} \|u\|_{H^r}.$$

2.2 Discrete Expansion

2.2.1 Discrete Even Expansion

- $x_j = 2\pi j/N$, $j = 0 \dots N-1$. (N points)

- *Exactness*: Periodic case: Trapezoidal rule is Gauß quadrature.

$$u \in \hat{B}_{2N-2}: \quad \frac{1}{2\pi} \int_0^{2\pi} u(x) dx = \frac{1}{N} \sum_{j=0}^{N-1} u(x_j)$$

Proof: Evaluate geometric series.

- *Coefficients*:

$$\tilde{u}_n = \frac{1}{N\tilde{c}_n} \sum_{j=0}^{N-1} e^{-inx_j} u(x_j),$$

where $c_n = 1 + \mathbf{1}_{n=N/2}$ to compensate for $\tilde{u}_{N/2} = \tilde{u}_{-N/2}$. $\rightarrow N$ coefficients, N quadrature points.

- *Interpolant*:

$$\begin{aligned} \mathcal{I}_N u(x) &= \sum_{|n| \leq N/2} \tilde{u}_n e^{inx} \\ &= \sum_{j=0}^{N-1} g_j(x) u(x_j) \end{aligned}$$

with

$$g_j(x) = \frac{1}{N} \sin\left(N \frac{x - x_j}{2}\right) \cot\left(\frac{x - x_j}{2}\right).$$

- $\mathcal{I}_N: L^2 \rightarrow \tilde{B}_N$.
- $\mathcal{I}_N u(x_j) = u(x_j)$. (rewrite sums, geometric series)
- Two different ways to differentiate: go through mode space—or don't.
- Differentiation matrix is *circulant*.
- $\sin N/2$ consequences:
 - $\mathcal{I}_N \frac{d}{dx} \neq D \mathcal{I}_N$ ($d/dx: \tilde{B}_N \rightarrow \tilde{B}_N$)
 - $D^2 \neq D^{(2)}$.
- Spatial discretization does not cause phase error deterioration.

2.2.2 Discrete Odd Expansion

- $x_j = 2\pi j / (N + 1)$ $j = 0 \dots N$. ($N + 1$ points)
- *Exactness*: Periodic case: Trapezoidal rule is Gauß quadrature.

$$u \in \hat{B}_{2N}: \quad \frac{1}{2\pi} \int_0^{2\pi} u(x) dx = \frac{1}{N+1} \sum_{j=0}^N u(x_j).$$

- *Coefficients*:

$$\tilde{u}_n = \frac{1}{N+1} \sum_{j=0}^N u(x_j) e^{-inx_j}.$$

- *Interpolant*:

$$\begin{aligned} \mathcal{J}_N u(x) &= \sum_{|n| \leq N/2} \tilde{u}_n e^{inx} \\ &= \sum_{l=0}^N u(x_l) h_l(x) \end{aligned}$$

with

$$h_l(x) = \frac{1}{N+1} \frac{\sin\left(\frac{N+1}{2}(x - x_l)\right)}{\sin\left(\frac{1}{2}(x - x_l)\right)} = \sum_{k=-N/2}^{N/2} e^{ik(x-x_l)}.$$

- $\mathcal{J}_N: L^2 \rightarrow \hat{B}_N$.

- $\mathcal{I}_N u(x_j) = u(x_j)$.
- May also be viewed as *Lagrange trigonometric interpolant*:
- Same differentiation matrix as ∞ -order FD.
- $\mathcal{I}_N \frac{d}{dx} = \mathcal{D}\mathcal{I}_N$.

2.2.3 Approximation Theory for Discrete Expansions

- $u \in H^q$, $q > 1/2$:

$$\tilde{c}_n \tilde{u}_n = \hat{u}_n + \sum_{|m| \leq \infty, m \neq 0} \hat{u}_{n+2Nm}$$

Proof: Substitute continuous into discrete, exchange sums because of absolute convergence, smuggle+CSU.

- *Aliasing error*:

$$\mathcal{A}_N u := \tilde{c}_n \tilde{u}_n - \hat{u}_n.$$

- $u \in H^r$, $r > 1/2$:

$$\|\mathcal{A}_N u\|_{L^2} \leq h^r \|u^{(r)}\|_{L^2}.$$

Proof: smuggle, CSU.

- $u \in H^r$, $r > 1/2$:

$$\|u - \mathcal{I}_{2N} u\|_{L^2} \leq h^r \|u^{(r)}\|_{L^2}.$$

Proof: Error = aliasing+truncation.

- $u \in H^r$, $r > 1/2$:

$$\|\mathcal{A}_N u\|_{H^q} \leq h^{r-q} \|u\|_{H^r}.$$

- $u \in H^r$, $r > 1/2$:

$$\begin{aligned} \|u - \mathcal{I}_{2N} u\|_{H^q} &\leq h^{r-q} \|u\|_{H^r}, \\ \|\mathcal{L}u - \mathcal{L}\mathcal{I}_{2N} u\|_{H^q} &\leq h^{r-q-s} \|u\|_{H^r}. \end{aligned}$$

3 Fourier Spectral Methods

Consider $u_t = \mathcal{L}u$.

3.1 Fourier Galerkin

- *Defining assumption*:

$$R_N = \partial_t u_N - \mathcal{L}u_N \perp \hat{B}_N.$$

- *Build method*: Calculate residual, project onto \hat{B}_N , set to zero.
 - Multiplication (for nonlinear problems) becomes convolution. (e.g. Burgers)
 - More complicated nonlinearities: no way.
 - Very efficient for linear, constant-coefficient problems with periodic BCs.

3.1.1 Stability

- \mathcal{L} semi-bounded:

$$\mathcal{L} + \mathcal{L}^* \leq 2\alpha \text{Id}$$

\Rightarrow stability.

- *Proving semi-boundedness*: Integrate by parts.

Examples:

- $\mathcal{L} = a(x)\partial_x$
- $\mathcal{L} = \partial_x b(x)\partial_x$
- \mathcal{L} semi-bounded \Rightarrow Fourier-Galerkin stable.

Proof: show $\mathcal{P}_N = \mathcal{P}_N^*$ by $(\mathcal{P}_N u, v) = (\mathcal{P}_N u, \mathcal{P}_N v)$. Then $\mathcal{L}_N = \mathcal{P}_N \mathcal{L} \mathcal{P}_N$ semi-bounded.

3.2 Fourier Collocation

- *Defining assumption*:

$$R_N|_{y_j} = 0$$

- *Optionally*: Collocation points $\{y_j\} \neq$ Quadrature points $\{x_j\}$. (we won't do that)
- *Build method*: Expand u with Lagrange interpolation polynomial. Obtain residual. Set to zero at collocation points \rightarrow simply replace derivatives by application of the differentiation matrix.

3.2.1 Stability

- $\mathcal{I}_N \neq \mathcal{I}_N^*$, so Fourier Galerkin proof breaks.
- *Discrete inner product*:

$$(u, v)_N = \frac{1}{N+1} \sum_{j=0}^N f(x_j) \overline{g(x_j)}$$

$\|u_N\|_N = \|u_N\|_{L^2}$ for odd expansion.

$\|u_N\|_N \sim \|u_N\|_{L^2}$ for even expansion.

- $\mathcal{L} = a(x)u(x)$, $0 < 1/k \leq |a(x)| \leq k$:
 - $\|u_N(t)\|_N \leq k \|u_N(0)\|$.
Proof: Multiply by u_N/a , obtain $(1/a)d/dt(\sum u^2)$. Use exactness of quad. formula, periodicity to get $d/dt = 0$. Exploit boundedness of a .
 - $\dot{\mathbf{u}} = A D \mathbf{u}$: Use $A^{1/2}$ as a change of variables, then bound $\mathbf{u} = e^{-ADt} \mathbf{u}_0$ by saying $A^{1/2} D A^{-1/2}$ is skew-symmetric.
Proof remains valid for $\dot{\mathbf{u}} = D A \mathbf{u}$, $\mathcal{L} = -a(x)$, ...
- $\mathcal{L} = a(x)u(x)$ with $a(x)$ changing sign, but $|a_x|/2 \leq \alpha$ uniformly
 - *treat skew-symmetric form*

$$\mathcal{L}u = \frac{1}{2}a u_x + \frac{1}{2}(a u)_x - \frac{1}{2}a_x u$$

to get $\|u_N\|_N \leq e^{\alpha t} \|u_0\|_N$:

Proof: Multiply by u_N , get $d/dt \sum u_N^2$. Integrate (exact) by parts in the second term, only third term left over, yields bound.

- skew-symmetric equation can be written

$$\begin{aligned} \frac{\partial u_N}{\partial t} + \frac{1}{2} \mathcal{J}_N a \partial_x u_N + \frac{1}{2} \partial_x \mathcal{J}_N [a u_N] - \frac{1}{2} \mathcal{J}_N (a_x u_N) &= 0, \\ \frac{\partial u_N}{\partial t} + \frac{1}{2} \mathcal{J}_N a \partial_x u_N + \frac{1}{2} \partial_x \mathcal{J}_N [a u_N] - \frac{1}{2} (\mathcal{J}_N \partial_x (a u_N) - \mathcal{J}_N a \partial_x u_N) &= 0, \\ \frac{\partial u_N}{\partial t} + \mathcal{J}_N a \partial_x u_N + \underbrace{\frac{1}{2} \partial_x \mathcal{J}_N [a u_N] - \frac{1}{2} \mathcal{J}_N \partial_x (a u_N)}_{A_N :=} &= 0 \end{aligned}$$

$$\|A_N\|_{L^2} \leq h^{2s-1} \left\| u_N^{(2s)} \right\|_{L^2}$$

(it's $2s - 1$ because A_N contains derivatives). This motivates the...

- ...superviscosity method

$$\tilde{\mathcal{L}}u = \mathcal{L}u + (-1)^s \frac{\varepsilon}{N^{2s-1}} \partial_x^{2s} u_N.$$

Stable if $\varepsilon >$ some constant C .

Proof: Add A_N on both sides, integrate $(u_N, A_N)_N$ by parts, $\leq \|u_N^{(s)}\|_{L^2}$. Bound superviscosity term by same norm, bound for $(u, \partial_t u)_N$ involving $|a_x|$ shows up.

- Using Fourier Galerkin, see that superviscosity = filtering.
- $\mathcal{L} = b(x)\partial_x^2 u$, $b > 0$:
 - matrix method: Define $D^{(2)} = D^2$, note $D^2 \mathbf{u} \in \hat{B}_{N-1}$, $D_{\text{real}}^{(2)} \mathbf{u} \in \tilde{B}_N$, use skew-hermiticity.
 - integral method: $\partial_x^2 := \mathcal{I}_N \partial_x \mathcal{I}_N \partial_x \mathcal{I}_N$, then rewrite as integral.
- $\mathcal{L} = f(U)_x$:

- Spectral viscosity method

$$\partial_t u_N + \partial_x \mathcal{P}_N f(u_N) = \varepsilon_N (-1)^{s+1} \partial_x^s [Q_m * \partial_x^s u_N]$$

where Q_m is a filter

- Superspectral viscosity method

$$\partial_t u_N + \partial_x \mathcal{P}_N f(u_N) = \varepsilon_N (-1)^{s+1} \partial_x^{2s} u_N.$$

4 Orthogonal Polynomials

- $B_N := \text{span}\{x^n: 0 \leq n \leq N\}$.
- Fourier methods achieve exponential accuracy only if u is periodic.
- *Sturm-Liouville operator*:

$$\mathcal{L}\varphi = \partial_x(p\partial_x\varphi) + q\varphi = \lambda w\varphi$$

$p > 0$, $0 \leq q < M$, w the weight function.

- *Parseval identity*:

$$(u, u)_{L_w^2} = \sum \gamma_n \hat{u}_n^2, \quad \gamma_n = (\varphi_n, \varphi_n), \quad \hat{u}_n = \frac{1}{\gamma_n} (u, \varphi_n)_{L_w^2}.$$

- Estimate decay of \hat{u}_n by plugging in eigenvalue problem, using selfadjointness of operator.
- *Singular Sturm-Liouville problem*: p vanishes at boundary.

$$\rightarrow |\hat{u}_n| \sim C \frac{1}{\lambda_n^m} \left\| \left(\frac{\mathcal{L}}{w} \right)^m u \right\|_{L_w^2}.$$

\rightarrow spectral decay for C^∞ functions with zero BCs. (Regular problem: only for periodic problems, otherwise boundary causes error.)

- *Jacobi polynomials*: $P_n^{(\alpha, \beta)}$, $\alpha, \beta > -1$

$$p(x) = (1-x)^{\alpha+1}(1+x)^{\beta+1}, \quad w(x) = (1-x)^\alpha(1+x)^\beta, \quad q(x) = c w.$$

- *Rodrigues' formula*:

$$(1-x)^\alpha(1+x)^\beta P_n^{\alpha, \beta}(x) = \frac{1}{2^n n!} \partial_x^n (1-x)^{\alpha+n}(1+x)^{\beta+n}.$$

- *Derivative*:

$$\frac{d}{dx} P_n^{\alpha, \beta} = \frac{n + \alpha + \beta + 1}{2} P_{n-1}^{(\alpha+1, \beta+1)}(x).$$

- *Odd/Even:*

$$P_n^{(\alpha, \beta)} = (-1)^n P_n^{(\alpha, \beta)}(-x).$$

- *There are various three-term recurrence for these polynomials, $P_0^{(\alpha, \beta)} = 1$, $P_1^{(\alpha, \beta)} = \frac{1}{2}(\alpha + \beta + 2)x + (\alpha - \beta)/2$.*
- *Legendre polynomials: $\alpha = \beta = 0$, $w \equiv 1$, called P_n*
- *Chebyshev polynomials: $p = \sqrt{1 - x^2}$, $q = 0$, $w = p$. $T_n = \cos(n \arccos(x))$.*

$$x T_n = \frac{1}{2} T_{n-1} + T_{n+1}.$$

Chebyshev is best approximation to x^{n+1} among polynomials of degree n .

- *Ultraspherical/Gegenbauer polynomials: $\alpha = \beta$.*
- *PPW for polynomials: ~ 4 . (Gegenbauer expansion, decay of the Bessel function)*

5 Polynomial Expansions

- Can somewhat easily differentiate and integrate, requires three-term stuff and its inverse.
- *Gauß-Lobatto quadrature:* both endpoints part of the quadrature. Exact for B_{2N-1} .
- *Gauß-Radau quadrature:* one endpoint part of the quadrature. Exact for B_{2N} .
- *Pure Gauß quadrature:* no endpoints part of the quadrature. Exact for B_{2N+1} .
- Each different kind of polynomial has a different set of quadrature points and weights because each has a different weight function.
- Chebyshev Quadrature:

$$\begin{array}{ccc} \text{GL} & \text{GR} & G \\ x_j = -\cos\left(\frac{j}{N}\pi\right) & w_j = -\cos\left(\frac{2j}{2N+1}\pi\right) & z_j = -\cos\left(\frac{2j+1}{2N+2}\pi\right) \quad j=0, \dots, N \\ w_j = \frac{\pi}{c_j N} & v_j = \frac{\pi}{c_j} \cdot \frac{1}{2N+1} & u_j = \frac{\pi}{N+1} \end{array}$$

with

$$c_j = 1 + \mathbf{1}_N + \mathbf{1}_0.$$

- $[\cdot, \cdot]_w$ denotes discrete inner product, $\|\cdot\|_{N,w}$ discrete norm.
- *Discrete Gauß-Lobatto norm:* not exact for $n = N$, but equivalent.
- *Discrete Expansion:*

$$\mathcal{I}_N u(x) = \sum_{n=0}^N P_n^{(\alpha)}(x) \tilde{u}_n, \quad \tilde{u}_n = \frac{1}{\tilde{\gamma}_n} \sum_{j=0}^N u(x_j) P_n^{(\alpha)}(x_j) w_j$$

- *Quadrature points are interpolation points.*

Proof: Plug coefficient terms into expansion, exchange sums to find

$$l_j(x) = w_j \sum_{n=0}^N \frac{1}{\tilde{\gamma}_n} P_n^{(\alpha)}(x) P_n^{(\alpha)}(x_j)$$

is the Lagrange interpolation polynomial.

- Differentiation matrices are nilpotent. (Decrease in order)
- GL Differentiation matrix is centro-antisymmetric.
- $D^{(q)} = D^q$.

- *Runge phenomenon*: Wild behavior of polynomials near interval boundaries.
- $u \in C^0[-1, 1]$, $\{x_j\}$ interpolation nodes. Then

$$\|u - \mathcal{I}_N u\|_\infty \leq |1 + \Lambda_N| \|u - p^*\|_\infty,$$

where p^* is the best-approximating polynomial and

$$\Lambda_n = \max_{[-1, 1]} \lambda_n, \quad \lambda_n = \sum_{j=0}^N l_j(x).$$

- $\Lambda_N \geq C \log(N + 1) + C'$.
- *Cauchy interpolation remainder*:

$$u(x) - \mathcal{I}_N u(x) = \frac{u^{(N+1)}(\xi)}{(N+1)!} \prod_{j=0}^n (x - x_j).$$

- Grid points should cluster quadratically near the boundary.

6 Polynomial Spectral Methods & Stability

6.1 Galerkin

- *Defining assumption*: Residual orthogonal to B_N .
- *Stiffness matrix*:

$$S_{k,n} = \frac{1}{\gamma_k} \int \varphi_k \mathcal{L} \varphi_n w dx.$$

Mass matrix:

$$M_{k,n} = \frac{1}{\gamma_k} \int \varphi_k \varphi_n w dx,$$

positive definite because L^2 -norm is a norm.

- Formulation:

$$\dot{\mathbf{a}} = M^{-1} S \mathbf{a}.$$

- Basis constructed as a linear combination of $P_n^{(\alpha)}$ to ensure BCs are kept.
- $u_t = \mathcal{L}u$. If \mathcal{L} is semi-bounded ($\mathcal{L} + \mathcal{L}^* \leq 2\gamma \text{Id}$), then the Galerkin method is stable.
- Linear hyperbolic equation well-posed in Jacobi norm for $\alpha \geq 0$, $\beta \leq 0$, but not for Chebyshev. (Consider $1 - |x|/\varepsilon$. Norm blows up, because Cheb weights blow up.)

6.2 Tau

- *Defining assumption*: Residual orthogonal to B_{N-k} , where k is the number of BCs, demand that it is zero.
- BC coefficients can be obtained once PDE-discretizing coefficients are computed.
- Mass matrix remains diagonal.
- Usable for elliptic problems, allows efficient preconditioners.
- Burgers: Product once again becomes convolution-like term.

6.3 Collocation

- *Defining assumption*: Residual zero at interpolation/quadrature nodes.

- Stability: Usual go-to-integral stuff.

6.4 Penalty Method for Boundary Conditions

- *Example:*

$$Q^-(x) = \frac{(1-x)P'_N(x)}{2P_N(-1)} = \begin{cases} 1 & x = -1, \\ 0 & x = x_j \neq -1. \end{cases}$$

$$\frac{\partial u_N}{\partial t} + a \frac{\partial u_N}{\partial x} = -\tau a Q^-(x)(u_N(-1) - \text{BC})$$

- Consistent because exact solution satisfies scheme exactly.
- Stable: go back to integral, gives boundary values, tweak τ to be bigger than corresponding weight.