The Pseudospectral Fourier Method

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Motivation of the Pseudospectral Method

- Better operators for the spatial derivatives were required. PS is exact up to machine precision in space.
- FD is very memory consuming and PS overcomes this problem by using less spatial grid points.
- First method to be exact at grid points $\rightarrow$ basis for later methods.

History

- The development started in the early 1980s.
- As a method with global communication, it was well suited for serial processing, which was common in HPC at this time.
- Advance from acoustic wave equation to elastic wave equation and complex 3D structures.
- Boundary conditions could be implemented with Chebychev polynomials.
- Grid stretching for better incorporation of topography and internal curves.
- Optimization for parallel computing by mixing FD and PS in different spatial directions.

Problem: Solving the acoustic wave equation

$$\underbrace{\frac{p(x,t+\mathrm{d}t)-2p(x,t)+p(x,t-\mathrm{d}t)}{\mathrm{d}t^2}}_{\text{Finite differences for temporal derivatives}} = c(x)^2 \quad \underbrace{\partial_x^2 p(x,t)}_{\substack{\text{Pseudospectral}\\ \text{method for}\\ \text{spatial derivative}}} \quad + s(x,t)$$

Fourier Series

- Approximate function by a sum over N weighted orthogonal basis functions

$$f(x) \approx g_N(x) = \sum_{i=1}^{N} a_i \Phi_i(x)$$

- Chose trigonometric basis functions in the interval $[-\pi, \pi]$

$$\begin{aligned} \cos(nx) \qquad n &= 0, 1, \ldots, \infty \\ \sin(nx) \qquad n &= 0, 1, \ldots, \infty \end{aligned}$$

- Approximation of 2π-periodic function on $[-\pi, \pi]$

$$\rightarrow f(x) \approx g_n(x) = \frac{1}{2} a_0 + \sum_{k=1}^{n} a_k \cos(kx) + b_k \sin(kx)$$

- Apply least squares problem to find coefficients a_k, b_k

$$\|f(x) - g_N(x)\|_{L2} = \left[\int_a^b \{f(x) - g_N(x)\}^2 \,\mathrm{d}x\right]^{\frac{1}{2}} = \text{Min}$$

$$\rightarrow a_k = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(kx)\mathrm{d}x \qquad k = 0, 1, \ldots, n$$

$$\rightarrow b_k = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin(kx)\mathrm{d}x \qquad k = 0, 1, \ldots, n$$

- For discrete set of points $x_i = \frac{2\pi}{N} i, \qquad i = 0, ..., N$

$$a_k^* = \frac{2}{N} \sum_{j=1}^{N} f(x_j) \cos(kx_j) \qquad k = 0, 1, \ldots, n$$

$$b_k^* = \frac{2}{N} \sum_{j=1}^{N} f(x_j) \sin(kx_j) \qquad k = 0, 1, \ldots, n$$

$$\rightarrow g_n^* := \frac{1}{2} a_0^* + \sum_{k=1}^{n-1} \{ a_k^* \cos(kx) - b_k^* \sin(kx) \} + \frac{1}{2} a_n^* cos(nx)$$

- Exact interpolation at collocation points

$$g_n^*(x_i) = f(x_i)$$

Fourier Transform

- Continuous

$$F(k) = \mathscr{F}[f(x)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{ikx} dx$$

$$f(x) = \mathscr{F}^{-1}[F(k)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{-ikx} dk$$

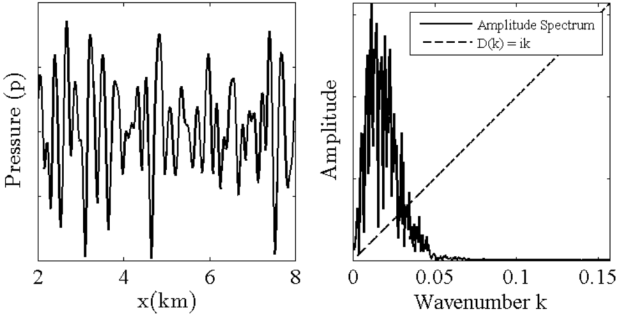
- Discrete

$$F_k = \sum_{j=0}^{N-1} f_j \, e^{i2\pi jk/N}, \;\; k = 0, ..., N$$

$$f_j = \frac{1}{N} \sum_{k=0}^{N-1} F_k \, e^{-i2\pi jk/N}, \;\; j = 0, ..., N$$

- Exploited property for Pseudospectral Method

$$F^{(n)}(k) = (ik)^n F(k)$$
$$\rightarrow f^{(n)}(x) = \mathscr{F}^{-1}[(ik)^n F(k)]$$
$$\rightarrow \partial_x^n f_j = \mathscr{F}^{-1}[(ik)^n F_k]$$



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Comparison PS - FD

Pros

- Exact spatial derivative (up to machine precision)
- Only two grid points per wavelength required
- No grid staggering required
- Memory efficient

Cons

- Computational more expensive (more FLOPS per spatial derivative required)
- Global communication required $\rightarrow$ does not allow parallel computing
- Assumes periodicity of function $\rightarrow$ boundary conditions difficult to implement