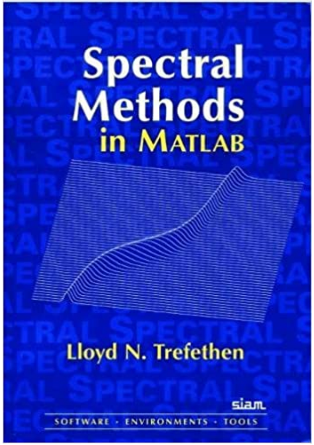
modern Spectral methods

Dan Fortunato
CCM

Based on...


Spectral Methods in MATLAB
Lloyd N. Trefethen
siam
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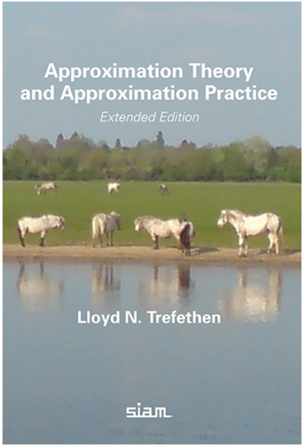
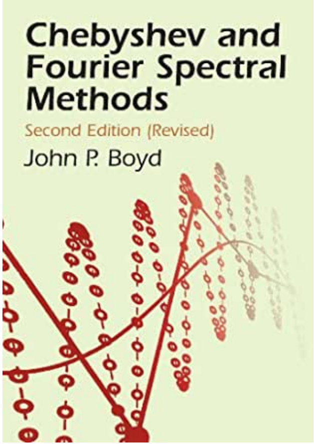

Approximation Theory and Approximation Practice
Extended Edition
Lloyd N. Trefethen
siam

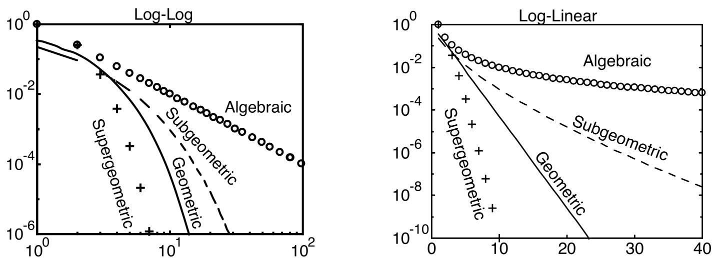

Chebyshev and Fourier Spectral Methods
Second Edition (Revised)
John P. Boyd

What is a spectral method?
Approximation theory

Definition: A numerical method is called a **spectral method** if its convergence rate is as fast as the smoothness of the answer allows.

Smoother

- m-differentiable? "*algebraic*" / "mth order" $\rightarrow \mathcal{O}(N^{-m})$
- ∞-differentiable? "*superalgebraic*" / "subgeometric" $\rightarrow \mathcal{O}(N^{-m})$ for every $m \geq 0$
- analytic? "*geometric*" / "exponential" $\rightarrow \mathcal{O}(c^{-N})$ for some $c > 1$



Such accuracy is called **spectral accuracy**.

Representing functions on a computer
Values or coefficients?

Suppose we are approximating a function $u(x)$ defined on $[-1, 1]$. How should we discretize u so that we may compute with it to spectral accuracy?

Representing functions on a computer

Values or coefficients?

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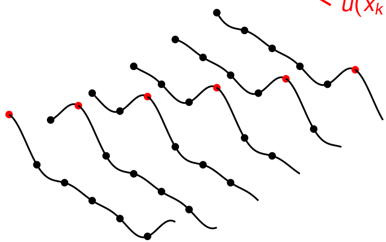
Values at grid points

Lagrange polynomials

$$u(x) = \sum_{k=0}^{N} u_k \ell_k(x)$$

$u(x_k)$



“nodal”, “pseudospectral”, “collocation”

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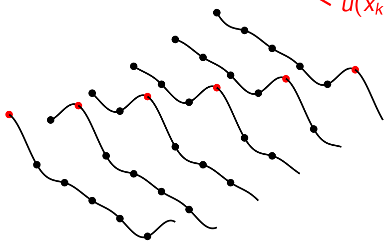


"nodal", "pseudospectral", "collocation"

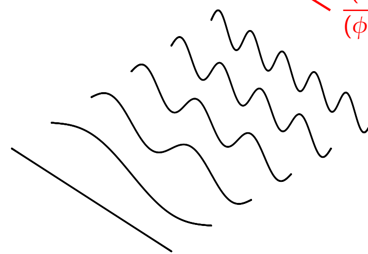
fast transforms

Coefficients of basis functions

orthogonal polynomials

$$u(x) = \sum_{k=0}^{N} \hat{u}_k \phi_k(x)$$

$$\frac{(u, \phi_k)_\phi}{(\phi_k, \phi_k)_\phi}$$



"modal", "spectral", "frequency domain"

Representing functions on a computer
Values or coefficients?

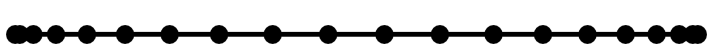
What grid points $\{x_k\}$ or basis functions $\{\phi_k\}$ should we use on $[-1, 1]$?

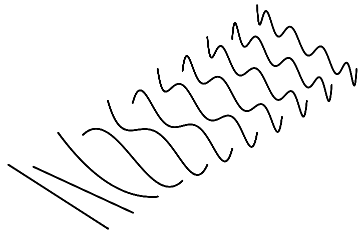
- Periodic? Equispaced nodes / Fourier series

$$x_k = -1 + \frac{2k}{N}, \quad \phi_k(x) = e^{i\pi kx}$$

- Non-periodic? Chebyshev nodes / Chebyshev series (or others – just need to avoid Runge phenomenon)

$$x_k = \cos\left(\frac{k\pi}{N}\right), \quad \phi_k(x) = T_k(x) = \cos(k \cos^{-1} x)$$





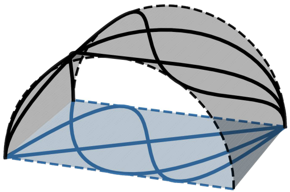


Image by Keaton Burns

Numerical computing with functions

Differentiation, integration, evaluation, convolution, ...

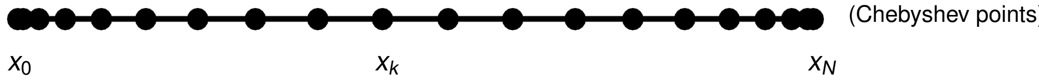
$$u(x) = \sum_{k=0}^{N} u_k \ell_k(x) = \sum_{k=0}^{N} \hat{u}_k \phi_k(x)$$

- Once we have this representation, many operations are easy — just apply the operation to each term in the sum.
- To get a flavor of each representation, let's focus on differentiation using both values and coefficients.
- We'll look at a traditional take and a modern take on each.

Value-based spectral methods

$$u(x) = \sum_{k=0}^{N} u_k \ell_k(x)$$

Given values on a grid, what are the values of the derivative on that same grid?



Value-based spectral methods
Differentiation

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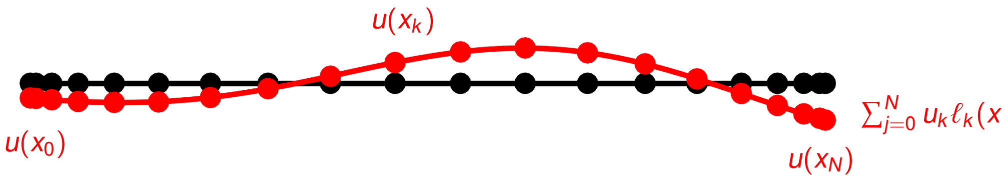

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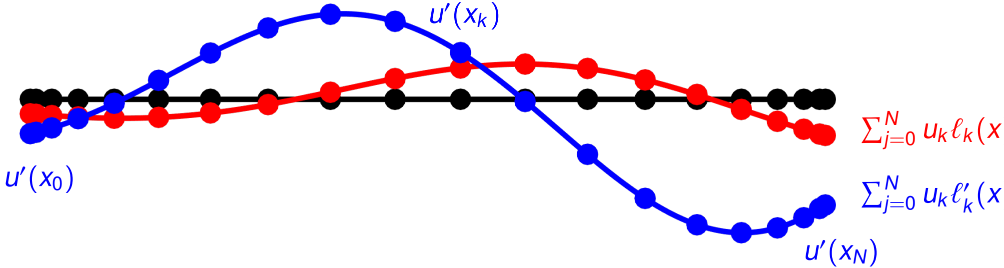


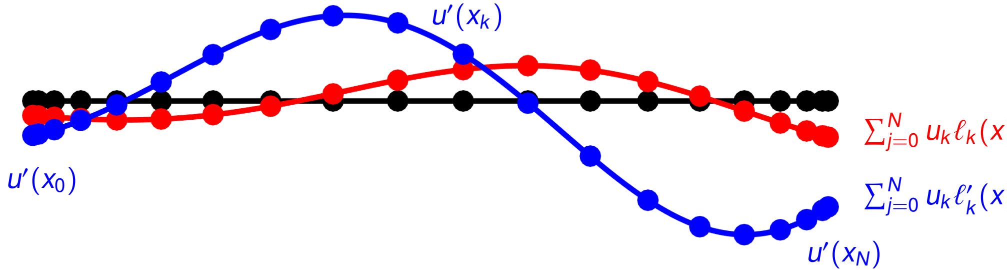
Differentiation $\{x_k\} \to \{x_k\}$ is **dense**:

$$u'(x_j) = \sum_{k=0}^{N} u_k \ell'_k(x_j) = \sum_{k=0}^{N} u'_k \ell_k(x_j)$$

The derivative at the k-th point depends on the values of u **at all points**.

[Fornberg, 1998], [Trefethen, 2000]

Given values on a grid, what are the values of the derivative on that same grid?



We can write down the dense matrix $D_N \in \mathbb{R}^{(N+1)\times(N+1)}$ such that

$$D_N \begin{pmatrix} u_0 \\ \vdots \\ u_N \end{pmatrix} = \begin{pmatrix} u_0' \\ \vdots \\ u_N' \end{pmatrix}$$

Such a matrix is called a **differentiation matrix**.

Value-based spectral methods
Rectangular differentiation

Modern take: [Driscoll & Hale, 2015]

- Differentiating a degree-N polynomial yields a degree-$(N-1)$ polynomial.


Toby Driscoll


Nick Hale

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- Therefore, D_N should map values on an $(N+1)$-point grid to values on an N-point grid.

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- That is, D_N should be rectangular: $\tilde{D}_N \in \mathbb{R}^{N\times(N+1)}$.


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- If $P_{N-1,N}$ is a resampling matrix from the $(N+1)$-point grid to the N-point grid, then $\tilde{D}_N = P_{N-1,N}D_N$.


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Why is this useful? Boundary conditions.

Toby Driscoll

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Value-based spectral methods

Rectangular collocation [Driscoll & Hale, 2015]

Consider the ODE

$$
\begin{aligned}
u'(x) + a(x)u(x) &= f(x), \quad x \in [-1, 1] \\
u(-1) &= c
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Value-based spectral methods

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Consider the ODE

$$u'(x) + a(x)u(x) = f(x), \quad x \in [-1, 1]$$
$$u(-1) = c$$

<u>Traditional spectral collocation</u>:

$$L\boldsymbol{u} = \left(D_N + \begin{bmatrix} a(x_0) & & \\ & \ddots & \\ & & a(x_N) \end{bmatrix} \right) \begin{bmatrix} u(x_0) \\ \vdots \\ u(x_N) \end{bmatrix} = \begin{bmatrix} f(x_0) \\ \vdots \\ f(x_N) \end{bmatrix} = \boldsymbol{f}$$

$$B\boldsymbol{u} = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} u(x_0) \\ \vdots \\ u(x_N) \end{bmatrix} = c$$

$$\begin{bmatrix} B \\ L \end{bmatrix} \boldsymbol{u} = \begin{bmatrix} c \\ \boldsymbol{f} \end{bmatrix}$$

System is rectangular — one too many rows.

Value-based spectral methods
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Value-based spectral methods

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$$\begin{bmatrix} B \\ L(1:N,:) \end{bmatrix} \boldsymbol{u} = \begin{bmatrix} c \\ \boldsymbol{f}(1:N) \end{bmatrix}$$

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$$B\boldsymbol{u} = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} u(x_0) \\ \vdots \\ u(x_N) \end{bmatrix} = c$$

$$\begin{bmatrix} B \\ P_{N-1,N}L \end{bmatrix} \boldsymbol{u} = \begin{bmatrix} c \\ P_{N-1,N}\boldsymbol{f} \end{bmatrix}$$

System is square.
We have precisely the space we need for B.

Value-based spectral methods

Rectangular collocation [Driscoll & Hale, 2015]

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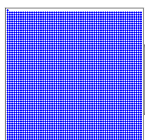

$$\boldsymbol{u} = \begin{bmatrix} c \\ P_{N-1,N}\boldsymbol{f} \end{bmatrix}$$

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Value-based spectral methods
Rectangular collocation [Driscoll & Hale, 2015]

Drake's summary of [Driscoll & Hale, 2015]:

Coefficient-based spectral methods

$$u(x) = \sum_{k=0}^{N} \hat{u}_k \phi_k(x)$$

Given coefficients in a basis, what are the coefficients of the derivative in that same basis?

Coefficient-based spectral methods

Fourier differentiation

Given coefficients in a basis, what are the coefficients of the derivative in that same basis?

Suppose $u(x)$ is periodic on $[-1, 1]$. Let's represent u using a Fourier series, so $\phi_k(x) = e^{i\pi kx}$:

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Differentiation $\left\{e^{i\pi kx}\right\} \to \left\{e^{i\pi kx}\right\}$ is **sparse**:

$$u'(x) = \sum_{k=-N/2}^{N/2} \hat{u}_k \phi_k'(x) = \sum_{k=-N/2}^{N/2} \hat{u}_k i\pi k e^{i\pi kx} = \sum_{k=-N/2}^{N/2} \hat{u}_k' e^{i\pi kx}$$

The k-th coefficient of the derivative depends **only** on the k-th coefficient of u.

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Fourier differentiation

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We can write down the diagonal matrix $\hat{D}_N \in \mathbb{R}^{(N+1)\times(N+1)}$ such that

$$\hat{D}_N \begin{pmatrix} \hat{u}_{-N/2} \\ \vdots \\ \hat{u}_{N/2} \end{pmatrix} = \begin{pmatrix} \hat{u}'_{-N/2} \\ \vdots \\ \hat{u}'_{N/2} \end{pmatrix}$$

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Suppose $u(x)$ is non-periodic on $[-1, 1]$. Let's represent u using a Chebyshev series, so $\phi_k(x) = T_k(x)$:

$$u(x) = \sum_{k=0}^{N} \hat{u}_k T_k(x)$$

Coefficient-based spectral methods
Chebyshev differentiation

Given coefficients in a basis, what are the coefficients of the derivative in that same basis?

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$$u(x) = \sum_{k=0}^{N} \hat{u}_k T_k(x)$$

Differentiation $\{T_k(x)\} \to \{T_k(x)\}$ is **dense**:

$$T_k'(x) = \begin{cases} 2k \sum_{j \text{ odd}}^{k-1} T_j(x), & k \text{ even}, \\ 2k \sum_{j \text{ even}}^{k-1} T_j(x) - 1, & k \text{ odd}. \end{cases}$$

The k-th coefficient of the derivative depends on **many** coefficients of u.

Coefficient-based spectral methods

Ultraspherical differentiation

Given coefficients in a basis, what are the coefficients of the derivative in that same basis?

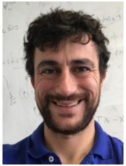
Suppose $u(x)$ is non-periodic on $[-1, 1]$. Let's represent u using a Chebyshev series, so $\phi_k(x) = T_k(x)$:

$$u(x) = \sum_{k=0}^{N} \hat{u}_k T_k(x)$$

Modern take: Let differentiation change the basis. [Olver & Townsend, 2012]

$$T_k'(x) = kC_{k-1}^{(1)}(x), \qquad T_k''(x) = 2kC_{k-2}^{(2)}(x), \qquad T_k'''(x) = 8kC_{k-3}^{(3)}(x), \quad \ldots$$

Then differentiation $\{T_k(x)\} \to \{C_k^{(\lambda)}(x)\}$ is **sparse**.



Sheehan Olver

Alex Townsend

Coefficient-based spectral methods

Ultraspherical spectral method [Olver & Townsend, 2012]

Differentiation:

$$T_k'(x) = kC_{k-1}^{(1)}(x), \qquad \hat{D}_N = \begin{pmatrix} 0 & 1 & & & \\ & & 2 & & \\ & & & 3 & \\ & & & & \ddots \end{pmatrix}$$

Conversion:

$$T_k(x) = \tfrac{1}{2}\left(C_k^{(1)} - C_{k-2}^{(1)}\right), \qquad \hat{S}_N = \begin{pmatrix} 1 & 0 & -\frac{1}{2} & & \\ & \frac{1}{2} & 0 & -\frac{1}{2} & \\ & & \frac{1}{2} & 0 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}$$

Multiplication:

$$a(x) \approx \sum_{k=0}^{m-1} \hat{a}_k T_k(x), \quad T_j(x)T_k(x) = \tfrac{1}{2}\left(T_{|j-k|} + T_{j+k}\right), \quad m\text{-banded operation}$$

Consider the ODE

$$
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Coefficient-based spectral methods

Ultraspherical spectral method [Olver & Townsend, 2012]

Consider the ODE

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$$L\hat{\boldsymbol{u}} = \left(\hat{D}_N + \hat{S}_N \hat{M}_N[a]\right) \begin{bmatrix} \hat{u}_0 \\ \vdots \\ \hat{u}_N \end{bmatrix} = \hat{S}_N \begin{bmatrix} \hat{f}_0 \\ \vdots \\ \hat{f}_N \end{bmatrix} = \hat{S}_N \hat{\boldsymbol{f}}, \qquad B\hat{\boldsymbol{u}} = \begin{bmatrix} T_0(-1) & \cdots & T_N(-1) \end{bmatrix} \begin{bmatrix} \hat{u}_0 \\ \vdots \\ \hat{u}_N \end{bmatrix} = c$$

$$\begin{bmatrix} B \\ L \end{bmatrix} \hat{\boldsymbol{u}} = \begin{bmatrix} c \\ \hat{S}_N \boldsymbol{f} \end{bmatrix}$$

Coefficient-based spectral methods

Ultraspherical spectral method [Olver & Townsend, 2012]

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$$\begin{bmatrix} B \\ L \end{bmatrix} \hat{\boldsymbol{u}} = \begin{bmatrix} c \\ \hat{S}_N \boldsymbol{f} \end{bmatrix}$$

System is rectangular — one too many rows.
Last row is all zeros. Delete it.

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$$\begin{bmatrix}B\\ L(0{:}N-1,:)\end{bmatrix}\hat{\boldsymbol{u}} = \begin{bmatrix}c\\ \hat{S}_{N-1}\hat{\boldsymbol{f}}(0{:}N-1)\end{bmatrix}$$

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Coefficient-based spectral methods

Ultraspherical spectral method [Olver & Townsend, 2012]

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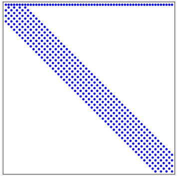

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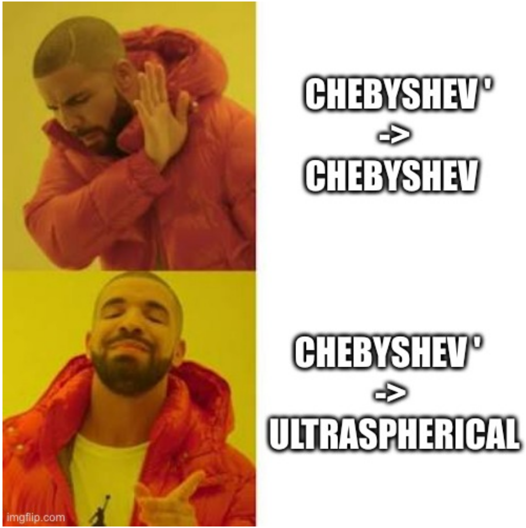
System is rectangular — one too many rows. Last row is all zeros. Delete it.

Drake's summary of [Olver & Townsend, 2012]:



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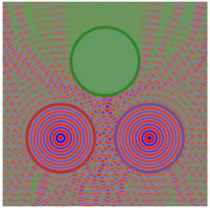
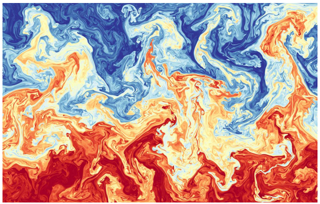
Software for spectral methods

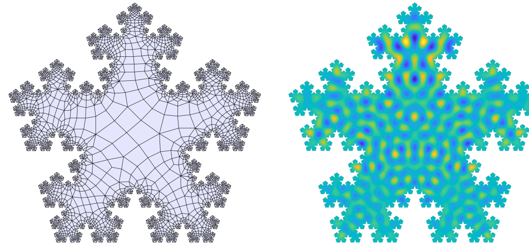
- MATLAB? Chebfun. (chebfun.org)
  - Trefethen, Hale, Driscoll, Austin, Aurentz, Townsend, ...
- Python? Dedalus. (dedalus-project.org)
  - Burns, Vasil, Oishi, Lecoanet, ...
- Julia? ApproxFun. (github.com/JuliaApproximation/ApproxFun.jl)
  - Olver, Slevinsky, Townsend, ...



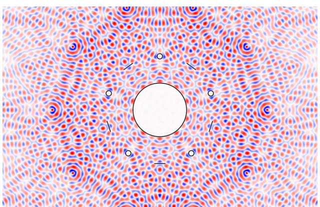
Applications



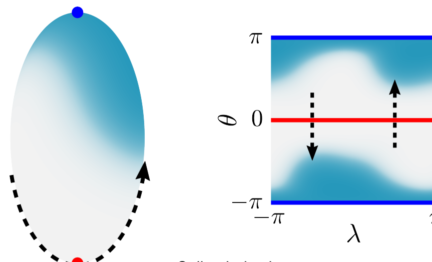
High Reynolds number flows
[Dedalus Project, 2019]



Very high order element methods
[F., Hale, & Townsend, 2020]



High frequency scattering
[Slevinsky & Olver, 2017]



Cell polarization
[F., Miller, Greengard, Shvartsman, in prep.]

I didn’t mention

- **Simple 2D and 3D geometries**
  - Use tensor products of 1D spectral ideas or special basis functions (spherical harmonics, Zernike polynomials, Bessel functions, double Fourier, etc.).
  - Orszag, Trefethen, Driscoll, Townsend, Olver, Slevinsky, Hale, Hashemi, Burns, Vasil, ...
- **Meshes and element methods**
  - Use piecewise high-order patches each of which are each spectral.
  - Sherwin, Fisher, Patera, Hesthaven, Warburton, Persson, Kolev, Ham, Mitchell, Martinsson, Gillman, ...
- **Integral equations**
  - Same ideas apply. Use global spectral or piecewise spectral on boundaries.
  - Greengard, Rokhlin, Barnett, Martinsson, Gillman, Rachh, Malhotra, Kaye, Jiang, Veerapaneni, Vico, O’Neil, Epstein, ...

Lots of spectral folks here at Flatiron!
Talk to us if your problem might be suitable for a spectral method.