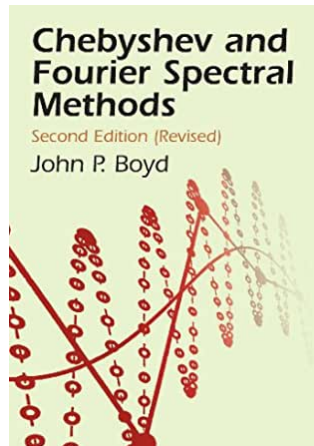
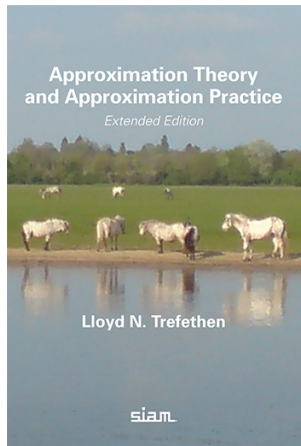
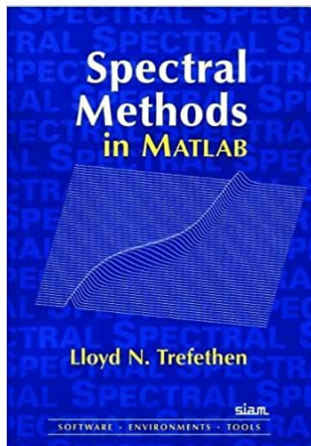


# *modern* ^ Spectral methods

Dan Fortunato  
CCM

# Based on...

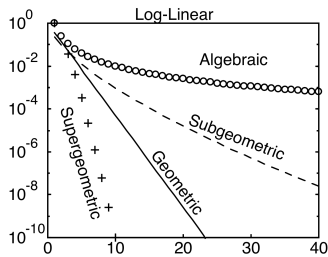
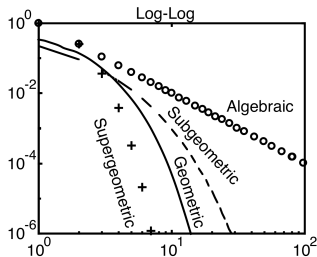


# What is a spectral method?

## 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” / “ $m$ th order”  $\rightarrow O(N^{-m})$
  - $\infty$ -differentiable? “superalgebraic” / “subgeometric”  $\rightarrow O(N^{-m})$  for every  $m \geq 0$
  - analytic? “geometric” / “exponential”  $\rightarrow O(c^{-N})$  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?

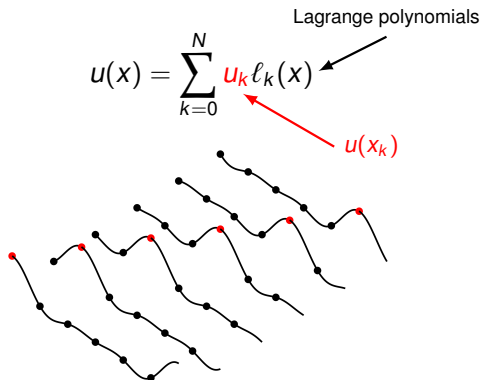


# Representing functions on a computer

## Values or coefficients?

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### Values at grid points



“nodal”, “pseudospectral”, “collocation”

# Representing functions on a computer

## Values or coefficients?

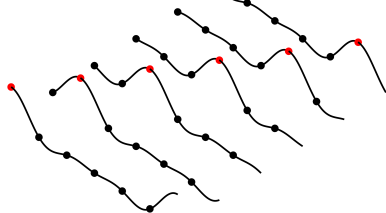
Suppose we are approximating a function  $u(x)$  defined on  $[-1, 1]$ . How should we discretize  $u$  so that we may compute with it to spectral accuracy?

### Values at grid points

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

Lagrange polynomials

$u(x_k)$



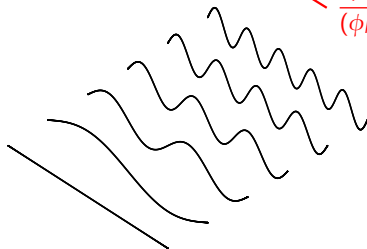
“nodal”, “pseudospectral”, “collocation”

### Coefficients of basis functions

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

orthogonal polynomials

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



“modal”, “spectral”, “frequency domain”

fast transforms

# 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)

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

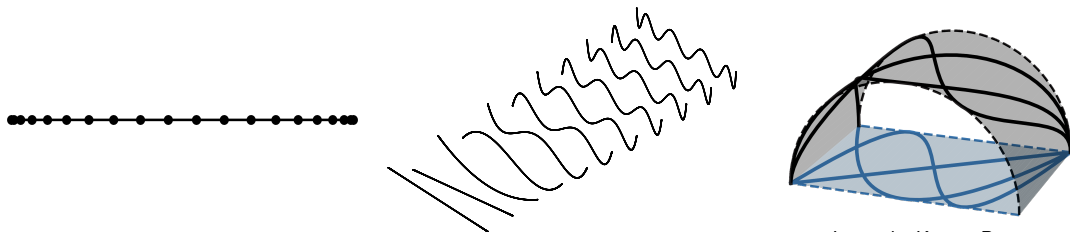


Image by Keaton Burns

# 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.

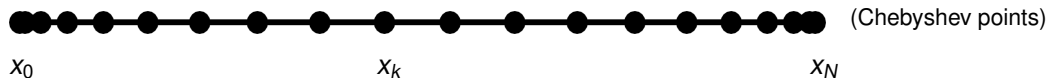
# Value-based spectral methods

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

# Value-based spectral methods

## Differentiation

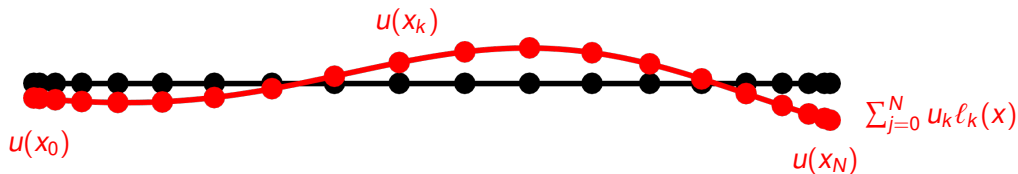
Given values on a grid, what are the values of the derivative on that same grid?



# Value-based spectral methods

## Differentiation

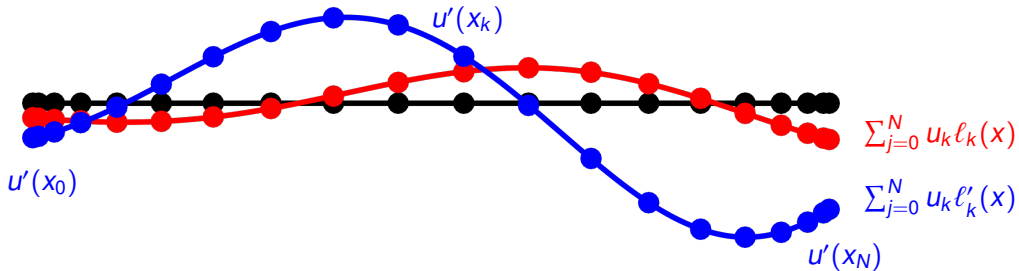
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# Value-based spectral methods

## Differentiation

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



Differentiation  $\{x_k\} \rightarrow \{x_k\}$  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**.

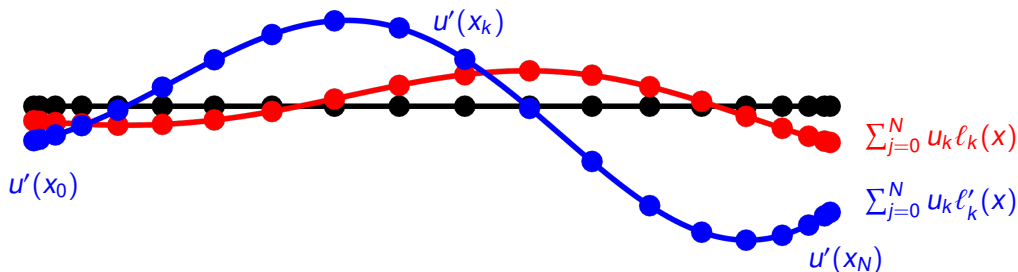
[Fornberg, 1998], [Trefethen, 2000]



# Value-based spectral methods

## Differentiation

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

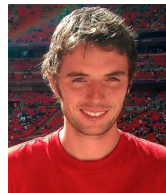
## Rectangular differentiation

Modern take: [Driscoll & Hale, 2015]

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



Toby Driscoll



Nick Hale

# Value-based spectral methods

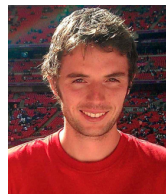
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# Value-based spectral methods

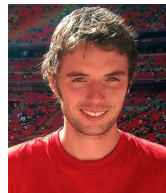
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- That is,  $D_N$  should be rectangular:  $\tilde{D}_N \in \mathbb{R}^{N \times (N+1)}$ .



Toby Driscoll



Nick Hale

# Value-based spectral methods

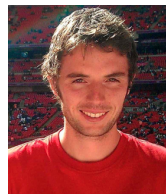
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- That is,  $D_N$  should be rectangular:  $\tilde{D}_N \in \mathbb{R}^{N \times (N+1)}$ .
- If  $P_{N-1,N}$  is a resampling matrix from the  $(N + 1)$ -point grid to the  $N$ -point grid, then  $\tilde{D}_N = P_{N-1,N} D_N$ .



Toby Driscoll



Nick Hale

# Value-based spectral methods

## Rectangular differentiation

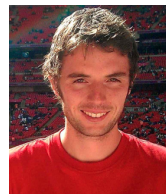
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Why is this useful? Boundary conditions.



Toby Driscoll



Nick Hale

# Value-based spectral methods

Rectangular collocation [Driscoll & Hale, 2015]

Consider the ODE

$$\begin{aligned}u'(x) + a(x)u(x) &= f(x), & x \in [-1, 1] \\ u(-1) &= c\end{aligned}$$

# Value-based spectral methods

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

Traditional spectral collocation:

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

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

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

System is rectangular — one too many rows.



# Value-based spectral methods

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Delete a row. But which one...

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

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# Value-based spectral methods

Rectangular collocation [Driscoll & Hale, 2015]

Consider the ODE

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

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

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

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

# Value-based spectral methods

Rectangular collocation [Driscoll & Hale, 2015]

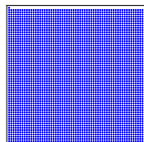
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$$\mathbf{u} = \begin{bmatrix} c \\ P_{N-1,N}\mathbf{f} \end{bmatrix}$$

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

# Value-based spectral methods

Rectangular collocation [Driscoll & Hale, 2015]

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



**DIFFERENTIATION  
IS  
SQUARE**



**DIFFERENTIATION  
IS  
RECTANGULAR**

# Coefficient-based spectral methods

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

# Coefficient-based spectral methods

## Fourier differentiation

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  $\phi_k(x) = e^{i\pi kx}$ :

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



# Coefficient-based spectral methods

## Fourier differentiation

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

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

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

Differentiation  $\{e^{i\pi kx}\} \rightarrow \{e^{i\pi kx}\}$  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  $u$ .

# Coefficient-based spectral methods

## Fourier differentiation

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

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

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

# Coefficient-based spectral methods

## Chebyshev differentiation

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

---

# Coefficient-based spectral methods

## Chebyshev 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  $\phi_k(x) = T_k(x)$ :

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

# 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  $\{T_k(x)\} \rightarrow \{T_k(x)\}$  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?

---

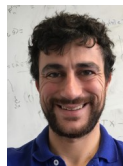
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$$u(x) = \sum_{k=0}^N \hat{u}_k T_k(x)$$

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

$$T'_k(x) = kC_{k-1}^{(1)}(x), \quad T''_k(x) = 2kC_{k-2}^{(2)}(x), \quad T'''_k(x) = 8kC_{k-3}^{(3)}(x), \quad \dots$$

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



Sheehan Olver Alex Townsend

# Coefficient-based spectral methods

Ultraspherical spectral method [Olver & Townsend, 2012]

Differentiation:

$$T'_k(x) = kC_{k-1}^{(1)}(x), \quad \hat{D}_N = \begin{pmatrix} 0 & 1 & & & \\ & & 2 & & \\ & & & 3 & \\ & & & & \ddots \\ & & & & & \ddots \end{pmatrix}$$

Conversion:

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

Multiplication:

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

# Coefficient-based spectral methods

Ultraspherical spectral method [Olver & Townsend, 2012]

Consider the ODE

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



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Ultraspherical spectral method [Olver & Townsend, 2012]

Consider the ODE

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

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

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Ultraspherical spectral method [Olver & Townsend, 2012]

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

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Last row is all zeros. Delete it.

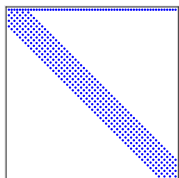
# Coefficient-based spectral methods

Ultraspherical spectral method [Olver & Townsend, 2012]

Consider the ODE

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

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



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

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

# Coefficient-based spectral methods

Ultraspherical spectral method [Olver & Townsend, 2012]

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



**CHEBYSHEV'**



**CHEBYSHEV**



**CHEBYSHEV'**



**ULTRASPHERICAL**

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Multiplication can be global ✗ in coefficient space.

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However, if the degree of variable coefficients is high this sparsity can be lost ✗.

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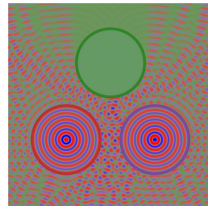
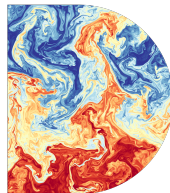
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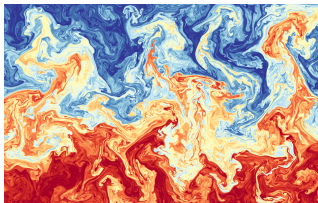
# Software for spectral methods

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

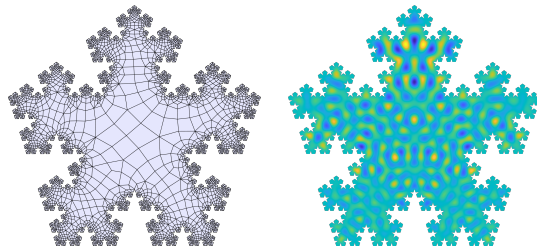
chebfun



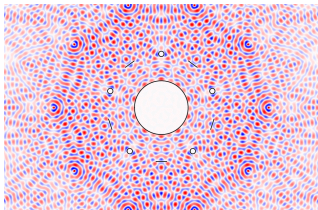
# Applications



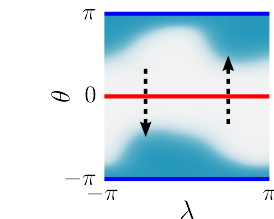
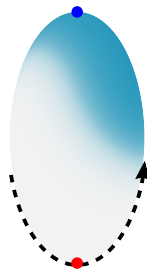
High Reynolds number flows  
[Dedalus Project, 2019]



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.*