

# FWAM Session B: Function Approximation and Differential Equations

**Alex Barnett<sup>1</sup> and Keaton Burns<sup>2</sup>**

Wednesday afternoon, 10/30/19

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# LECTURE 1

interpolation, integration, differentiation, spectral methods

## Goals and plan

Overall: graph of  $f(x)$  needs  $\infty$  number of points to describe, so how handle  $f$  to user-specified accuracy in computer w/ least cost? (bytes/flops)

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task: given exact  $f(x_j)$  at some  $x_j$ , model  $f(x)$  at other points  $x$ ?

App: cheap but accurate “look-up table” for possibly expensive func.

Contrast: fit noisy data = learning (pdf for) params in model, via likelihood/prior

- Numerical integration:

App: computing expectation values, given a pdf or quantum wavefunc.

App: integral equation methods for PDEs (Jun Wang's talk)

- Numerical differentiation:

App: build a matrix (linear system) to approximate an ODE/PDE (Lecture II)

App: get gradient  $\nabla f$ , eg for optimization (cf adjoint methods)

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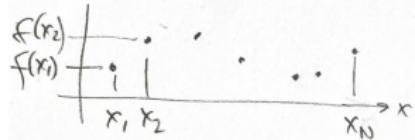
Plus: good 1D tools, pointers to codes, higher dim methods, opinions!

# Interpolation in 1D ( $d = 1$ )

Say  $y_j = f(x_j)$  known at nodes  $\{x_j\}$      $N$ -pt "grid"

note: exact data, not noisy

want interpolant  $\tilde{f}(x)$ , s.t.  $\tilde{f}(x_j) = y_j$

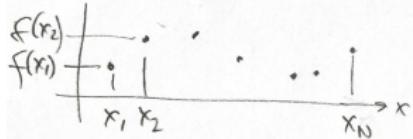


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hopeless w/o assumptions on  $f$ , eg smoothness, otherwise...

- extra info helps, eg  $f$  periodic, or  $f(x) = \text{smooth} \cdot |x|^{-1/2}$

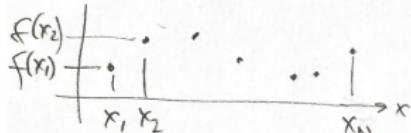


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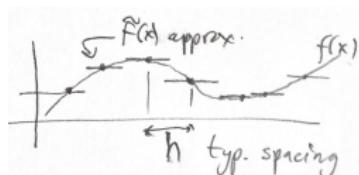
Simplest: use value at  $x_j$  nearest to  $x$

"snap to grid"

Error  $\max_x |\tilde{f}(x) - f(x)| = \mathcal{O}(h)$  as  $h \rightarrow 0$

holds if  $f'$  bounded; ie  $f$  can be nonsmooth but not crazy

Recap notation " $\mathcal{O}(h)$ ": exists  $C, h_0$  s.t. error  $\leq Ch$  for all  $0 < h < h_0$

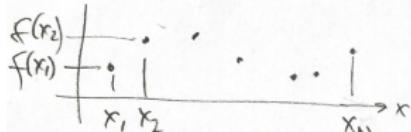


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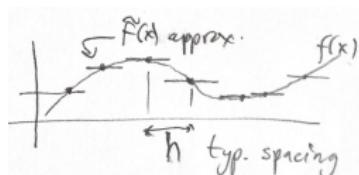
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Piecewise linear:

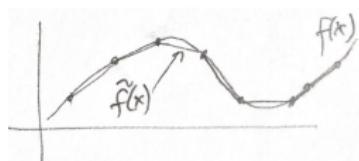
"connect the dots"

max error =  $\mathcal{O}(h^2)$  as  $h \rightarrow 0$

needs  $f''$  bounded, ie smoother than before



Message: a higher order method is *only* higher order if  $f$  smooth enough



## Interlude: convergence rates

Should know or measure convergence rate of any method you use

- “effort” parameter  $N$       eg # grid-points =  $1/h^d$  where  $h$  = grid spacing,  $d$  = dim
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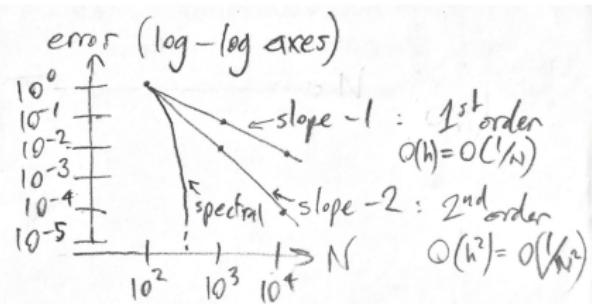
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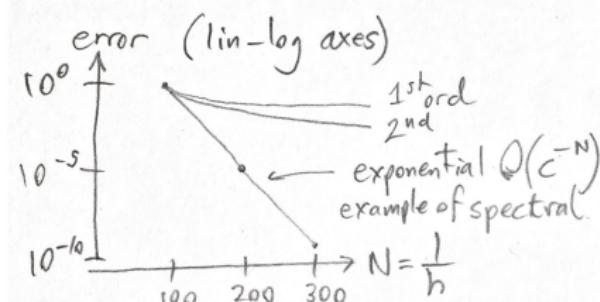
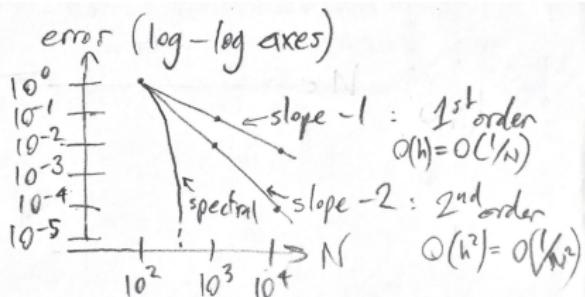
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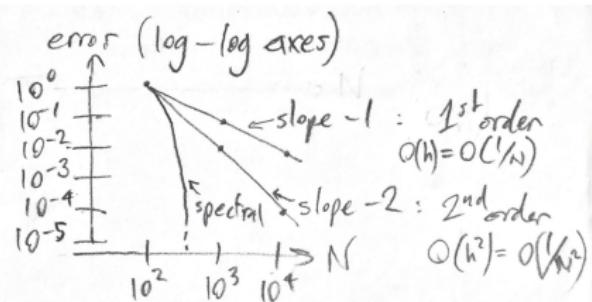
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Note how spectral gets many digits for small  $N$

crucial for eg 3D prob.

“spectral” = “superalgebraic”, beats  $\mathcal{O}(N^{-p})$  for any  $p$

- how many digits to you want? for 1-digit (10% error), low order ok, easier to code

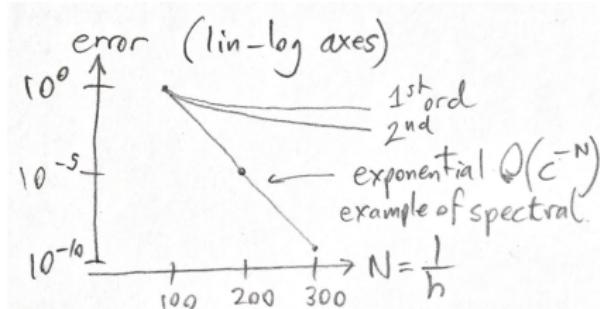
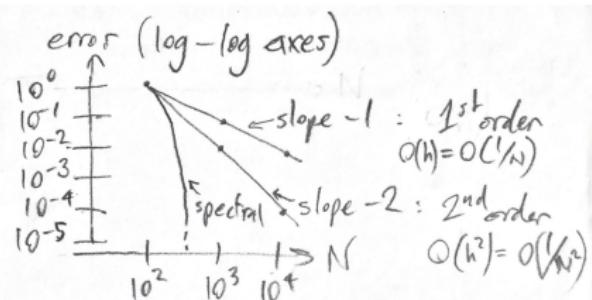
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<rant> test your code w/ known exact soln to check error conv. <\rant>

How big is prefactor  $C$  in error  $\leq Ch^p$ ? Has asympt. rate even kicked in yet? :)

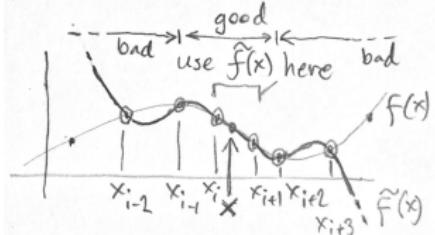
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Pick a  $p$ , eg 6. For any target  $x$ , use only the nearest  $p$  nodes:

Exists unique degree- $(p-1)$  poly,  $\sum_{k=0}^{p-1} c_k x^k$   
which matches local data  $(x_j, y_j)_{j=1}^p$

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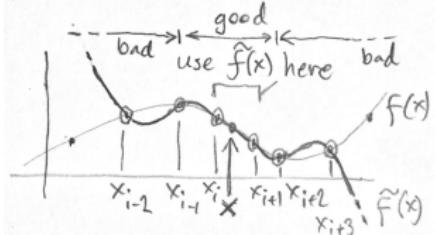
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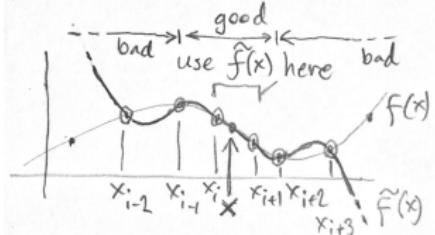
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ie,  $V\mathbf{c} = \mathbf{y}$        $V$ ="Vandermonde" matrix, is ill-cond. but works

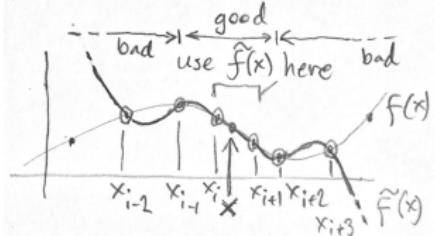
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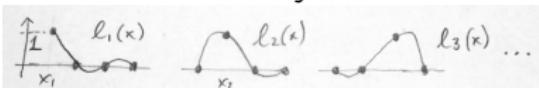
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2) traditional: barycentric formula  $\tilde{f}(x) = \frac{\sum_{j=1}^p \frac{y_j}{x-x_j} w_j}{\sum_{j=1}^p \frac{1}{x-x_j} w_j} \quad w_j = \frac{1}{\prod_{i \neq j} (x_j - x_i)}$  [Tre13, Ch. 5]

Either way,  $\tilde{f}(x) = \sum_{j=1}^p y_j \ell_j(x)$  where  $\ell_j(x)$  is  $j$ th Lagrange basis func:

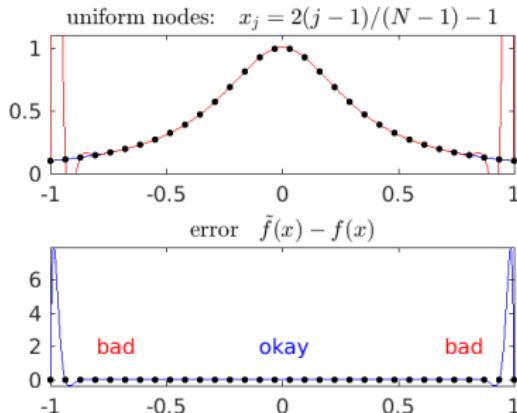


## Global polynomial (Lagrange) interpolation?

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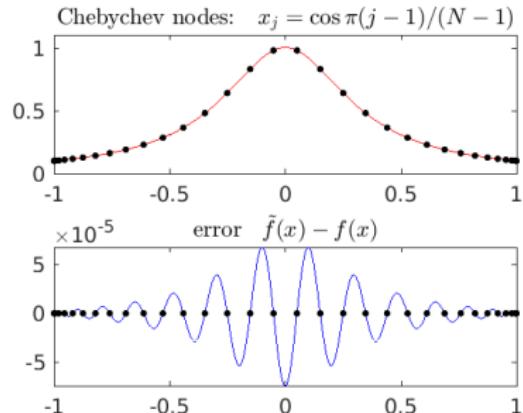
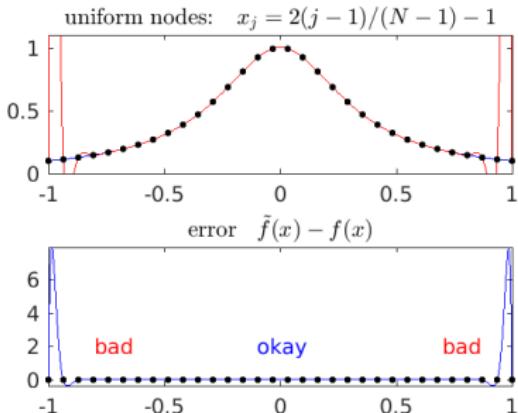
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 $p = N = 32$ , smooth (analytic)  $f(x) = \frac{1}{1+9x^2}$  on  $[-1, 1]$  :    (Runge 1901)



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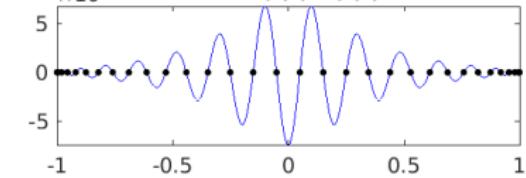
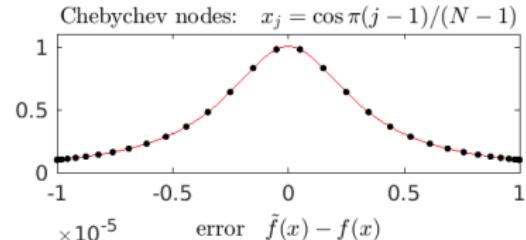
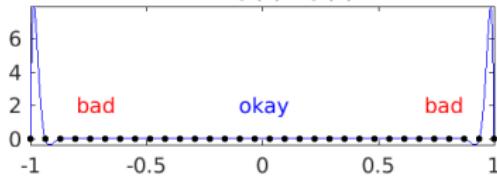
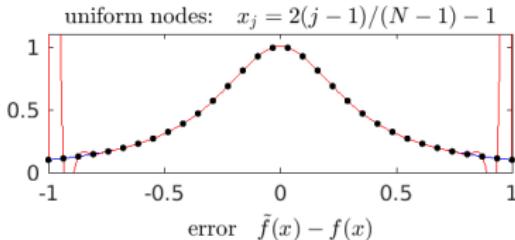
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But exists good choice of nodes...

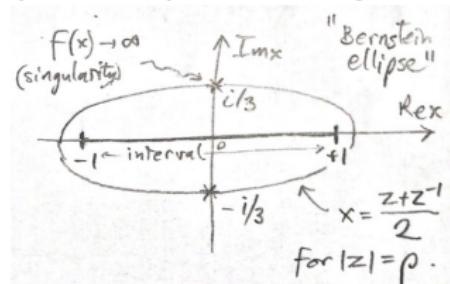
"Chebychev": means non-unif. grid density  $\sim \frac{1}{\sqrt{1-x^2}}$

- our first spectral method

$$\max \text{err} = \mathcal{O}(\rho^{-N})$$

exponential conv!

$\rho > 1$  "radius" of largest ellipse in which  $f$  analytic



## Node choice and adaptivity

Recap: poly approx.  $f(x)$  on  $[a, b]$ : exist good & bad node sets  $\{x_j\}_{j=1}^N$

**Question:** Do you get to choose the set of nodes at which  $f$  known?

- data fitting applications: No (or noisy variants: kriging, Gaussian processes, etc)  
use local poly (central region only!), or something stable (eg splines) [GC12]
- almost all else, interp., quadrature, PDE solvers: Yes so pick good nodes!

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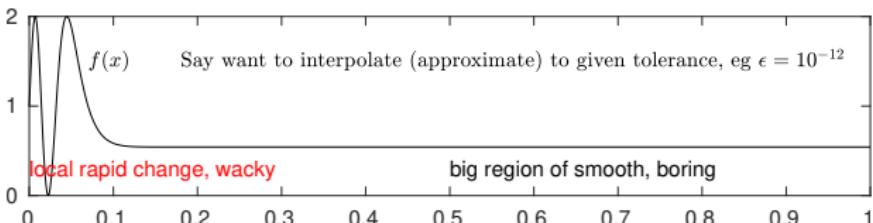
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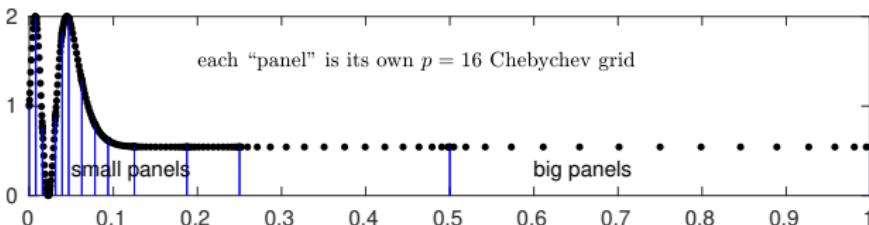
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automatically split  
(recursively) panels  
until max err  $\leq \epsilon$

via test for local error

1D adaptive interpolator codes to try:

- [github:dbstein/function\\_generator](#) py+numba, fast (Stein '19)
- [chebfun for MATLAB](#) big- $N$  Cheb. grids done via FFTs! (Trefethen et al.)

App.: replace nasty expensive  $f(x)$  by cheap one!

optimal “look-up table”

# Global interpolation of periodic functions I

Just did  $f$  on intervals  $[a, b]$ . global interp. (& integr., etc.) of smooth *periodic*  $f$  differs!

Periodic:  $f(x + 2\pi) = f(x)$  for all  $x$ ,  $f(x) = \sum_{n \in \mathbb{Z}} \hat{f}_k e^{ikx}$  Fourier series

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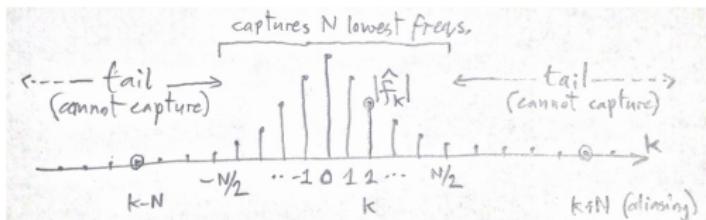
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What's best you can do?

get  $N$  coeffs right  $c_k = \hat{f}_k$

error  $\sim$  size of tail  $\{\hat{f}_k\}_{|k| \geq N/2}$



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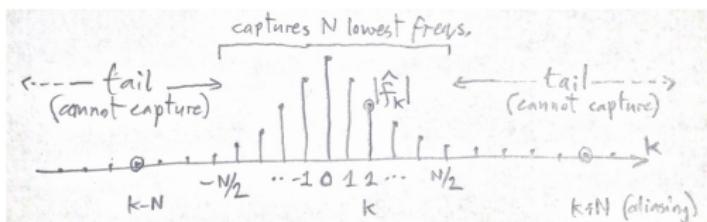
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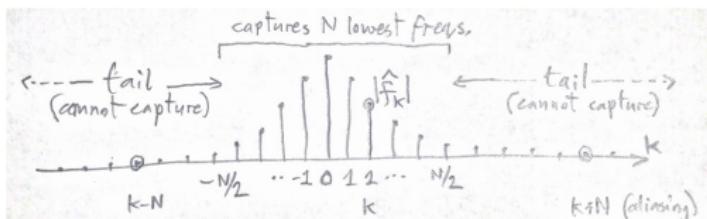
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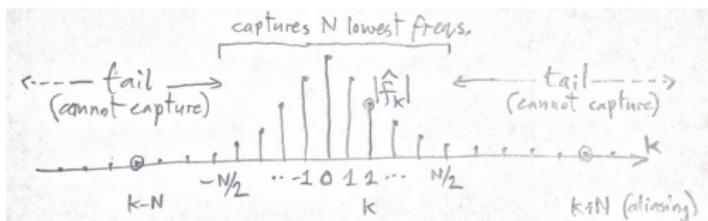
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Summary: given  $N$  samples  $f(x_j)$ , interp. error = truncation + aliasing

a crude bound is  $\max_{x \in [0, 2\pi)} |\tilde{f}(x) - f(x)| \leq 2 \sum_{|k| \geq N/2} |\hat{f}_k|$

ie error controlled by sum of tail

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That's theory. In real life you always measure your conv. order/rate!

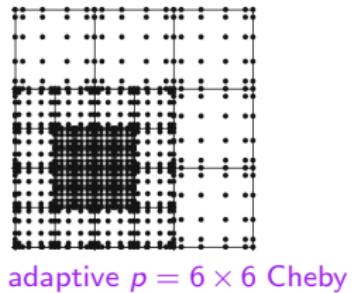
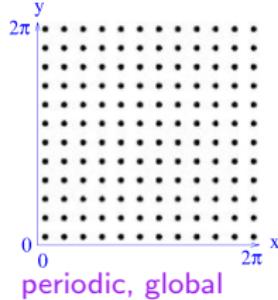
Messages:

- $f$  smooth, periodic, global interpolation w/ uniform grid: spectral acc.
- key to spectral methods. FFT cost  $\mathcal{O}(N \log N)$  swaps from  $f(x_j)$  grid to  $\hat{f}_k$

## Flavor of interpolation in higher dims $d > 1$

If you *can* choose the nodes:

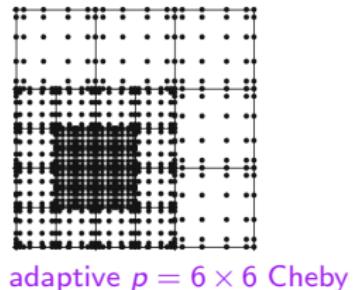
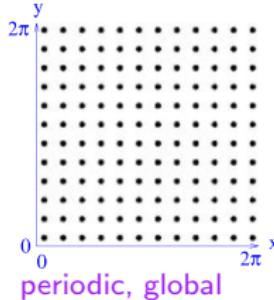
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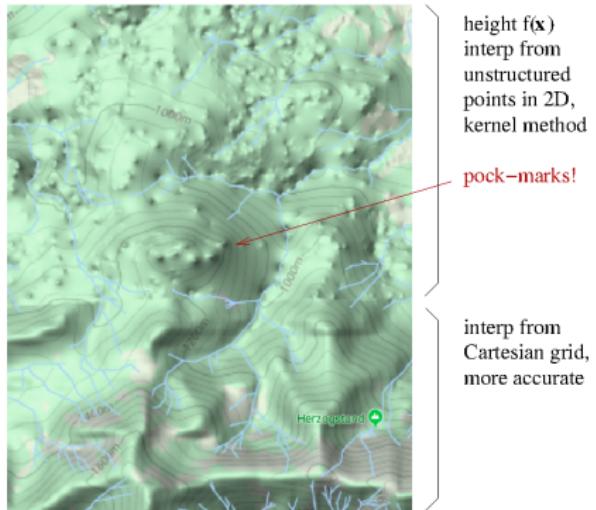
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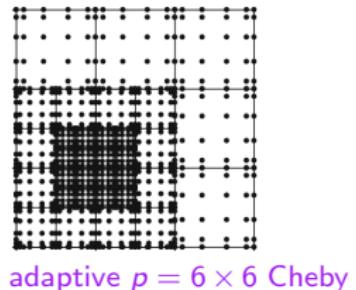
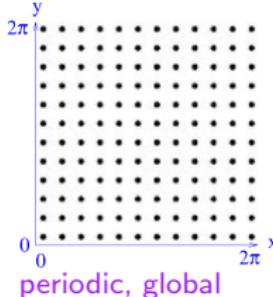
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But if know  $f$  smooth:

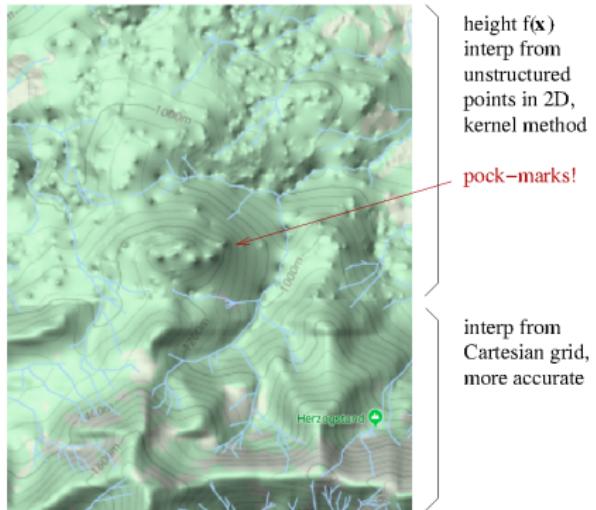
locally fit multivariate polynomials

If also data noisy, many methods:

kriging (Gauss. proc.), NUFFT, RBF...

If also high dim  $d \gg 1$ :

tensor train, neural networks...



## Numerical integration (back to $d = 1$ )

Task: eval.  $\int_a^b f(x)dx$  accurately w/ least number of func. evals,  $N$

“quadrature”: nodes  $\{x_j\}$ , weights  $\{w_j\}$ , s.t.  $\int_a^b f(x)dx \approx \sum_{j=1}^N w_j f(x_j)$

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demo:  $N=14$ ;  $\text{sum}(\exp(\cos(2*\pi*(1:N)/N)))/N - \text{besseli}(0,1)$   
ans = 1.3e-15

# Advanced integration

- custom quadr. for singularity eg  $f(x) = \text{smooth} \cdot |x|^{-1/2}$  (Rokhlin school)  
or for arb. set of funcs. "generalized Gaussian quad." (CCM: Manas Rachh)
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code: `integral2`, etc, `quadpy`

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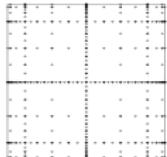
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Much higher  $d \gg 1$

tensor prod: exp. # f evals.  $N = n^d$  kills you :( "curse of dim."

- "sparse grids" scale better as  $N \sim n(\log n)^d$  (Smolyak '63)
- (quasi-)Monte Carlo:  $\sum_{j=1}^N f(\mathbf{x}_j)$ , for random  $\mathbf{x}_j$  err  $\mathcal{O}(N^{-1/2})$ , slow conv!  
importance sampling (Thurs am session), custom transformations...



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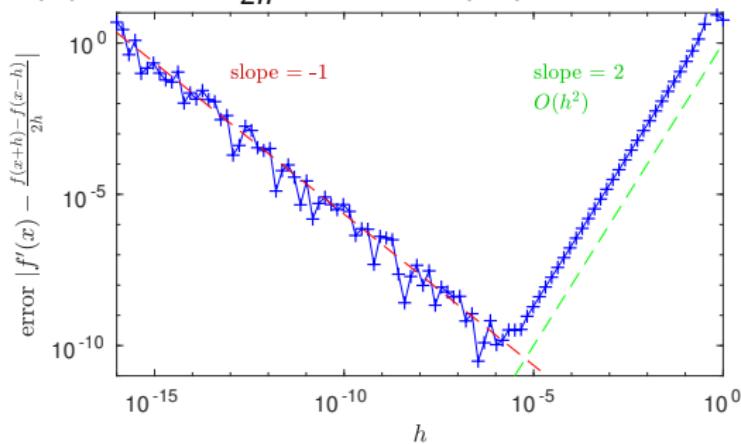
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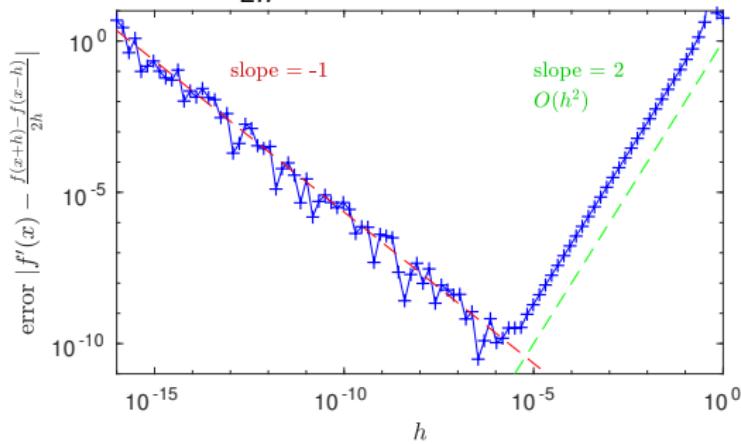
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- CPU arithmetic done only to relative "rounding error"  $\epsilon_{\text{mach}} \sim 10^{-16}$
- subtracting v. close  $f(x+h)$  and  $f(x-h)$ : "catastrophic cancellation"
- balance two error types:  $h_{\text{best}} \sim \epsilon_{\text{mach}}^{1/3} \sim 10^{-5}$

Essential reading: floating point, backward stability [GC12, Ch. 5–6] [TBI97, Ch. 12–15]

## High-order (better!) differentiation, $d = 1$

As w/ integration: get interpolant  $\rightarrow$  differentiate it exactly [Tre00, Ch. 6]

Get  $N \times N$  matrix  $D$  acting on func. values  $\{f(x_j)\}$  to give  $\{f'(x_j)\}$ . Has simple formula

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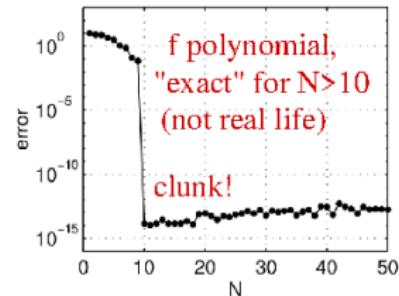
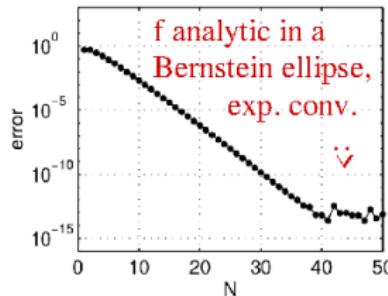
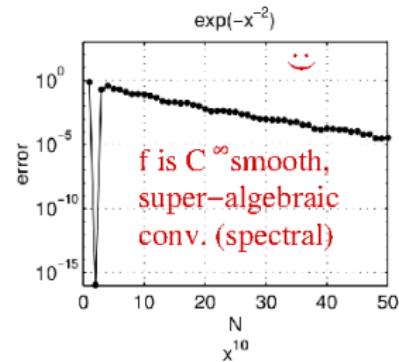
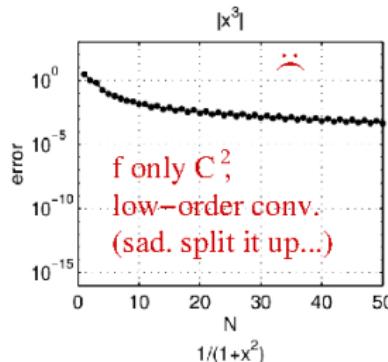
As w/ integration: get interpolant  $\rightarrow$  differentiate it exactly [Tre00, Ch. 6]

Get  $N \times N$  matrix  $D$  acting on func. values  $\{f(x_j)\}$  to give  $\{f'(x_j)\}$ . Has simple formula

Examples:

$N$  Chebychev nodes  
in  $[-1, 1]$

shown: max error in  $f'$



- for  $N$  large, the dense  $D$  is never formed, merely applied via FFT

spectral solvers for ODE/PDEs. codes: chebfun, PseudoPack, dedalus... Lecture II

## Summary: we scratched the surface

Can integrate & differentiate smooth funcs given only point values  $f(x_j)$

Both follow from building a good (fast-converging) interpolant

For  $f$  smooth in 1D, can & should easily get many (10+) digits accuracy

### Concepts:

convergence order/rate      how much effort will you have to spend to get more digits?

smoothness      smooth  $\Leftrightarrow$  fast convergence; nonsmooth needs custom methods

global      (one interpolation formula/basis for the whole domain)

vs local      (distinct formulae for  $x$  in different regions)

spectral method      global, converge v. fast, even non-per. can exploit FFT

adaptivity      auto split boxes to put nodes only where they need to be

rounding error & catastrophic cancellation      how not shoot self in the foot

tensor products for 2D, 3D      for higher dims: randomized/NN/TN (Th/Fr sessions)

See recommended books at end, and come discuss stuff!

# LECTURE II: numerical differential equations

## Motivation

Produce numerical approximations to the solutions of ODEs/PDEs.

## Goals for today

Basic overview of how different methods work. Understand error properties and suitability for different equations.

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- Boundary Integral Methods Linear problems w/ boundary data

## Reminder of types and applications of diff. eq.

- ODEs: eg pendulum  $u''(t) + \sin(u(t)) = 0$   
Task: solve  $u(t)$  given initial conditions    e.g.  $u(0) = 1, u'(0) = 0$

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Task: solve  $u(x)$  given forcing, boundary conditions  
Steady state of heat/diffusion, Gauss's law for conservative forces  
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 $\Delta u$  means Laplacian  $\partial^2 u / \partial x^2 + \partial^2 u / \partial y^2 + \dots =$  curvature of  $u$   
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[Mike will overview the three flavors of PDE in next talk]

BCs: simple (eg periodic cube) vs complicated ( $u = 0$  on a nasty surface)

# Typical solution strategies

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ODEs:

- Treat spatial problems as time-indep. PDEs “boundary value problems”
- Evolve temporal problems with finite differences “initial value problems”

# Finite difference methods

Basic viewpoint:

- Discretize variables on a discrete grid
- Construct Taylor-series approximations to values at neighboring points
- For  $N$  points, expand to  $N$  terms (error  $\mathcal{O}(h^N)$ )
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E.g. Centered differences on 3 points:  $x - h, x, x + h$

$$u(x + h) = u(x) + u'(x)h + u''(x)h^2/2 + \mathcal{O}(h^3) \quad (1)$$

$$u(x - h) = u(x) - u'(x)h + u''(x)h^2/2 + \mathcal{O}(h^3) \quad (2)$$

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Extra order here due to symmetry

# Finite difference methods

Alternate viewpoint:

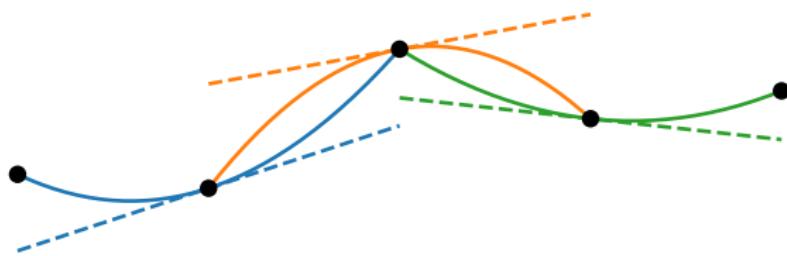
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- Differentiate the local interpolant to approximate derivatives.

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E.g. Centered differences using 3 points:



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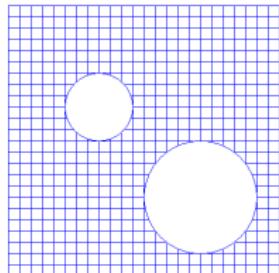
$$u'(t) = -\lambda u(t) \quad \lambda > 0 \quad (8)$$

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$$u_{n+1} = (1 + k\lambda)^{-1}u_n \quad (10)$$

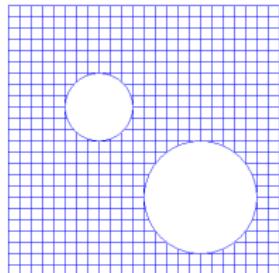
# Finite difference methods

- Extends to multiple dimensions with regular grids
- Simple to adjust order of accuracy
- Some more advanced techniques:
  - Conservative schemes
  - Select stencils term by term “upwinding”
  - Adaptive stencil selection for jumps “WENO”
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Resources: LeVeque “Finite Difference Methods for ODE/PDE”

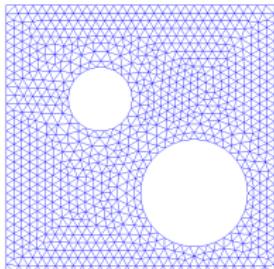
Codes: e.g. Pencil code (magnetohydrodynamics)

# Finite element methods

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$$u(\mathbf{x}) = \sum_{n=1}^N u_n \phi_n(\mathbf{x}) \quad (11)$$

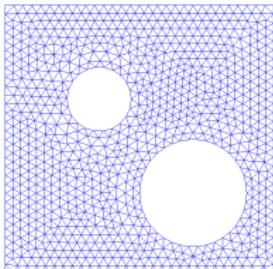
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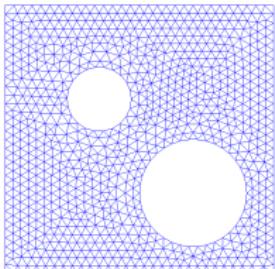
$$\int \psi_m(\mathbf{x}) [\partial_t u(\mathbf{x}) + L u(\mathbf{x}) - f(\mathbf{x})] \, d\mathbf{x} = 0 \quad (13)$$

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- Solve resulting algebraic system:

$$M \cdot \partial_t \mathbf{u} + S \cdot \mathbf{u} = M \cdot \mathbf{f} \quad (14)$$

“Mass matrix”  $M$ , “stiffness matrix”  $S$

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Codes: Arepo, Athena, OpenFOAM

Many local experts in CCA!

# Finite element methods

## Traditional FEM

- Use piecewise linear “tent” functions. Continuous
- “Weak form” from integrating by parts:

$$\int \psi_m \nabla^2 u \, d\mathbf{x} = - \int \nabla \psi_m \cdot \nabla u \, d\mathbf{x} \quad (16)$$

Lowers order of derivatives, allows piecewise linear representation

- Not conservative and  $M \neq I$ , need implicit schemes or to invert  $M$
- Easy to adjust order of accuracy. Use higher degree polynomials, “p adaptivity”

## Modern research: high-order FEM

- Discontinuous Galerkin (FVM + FEM): high order inside elements, but allow discontinuities. Need Riemann solvers again
- Spectral elements: very high order internal representations

Codes: FEniCS, deal.II

# Spectral methods

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- Solve Galerkin projection of equations. *But don't integrate by parts*
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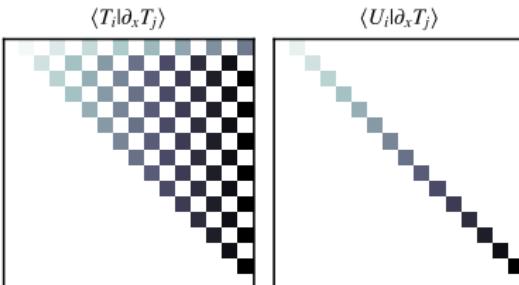
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Non-periodic intervals: Chebyshev polynomials  $T_n(x)$ . Fast w/ DCT

Traditional: "collocation" using values at Chebyshev nodes. Dense matrices.

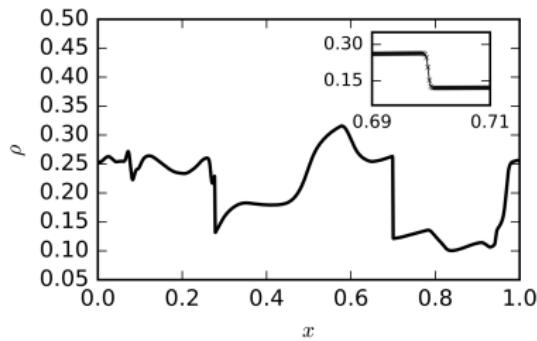
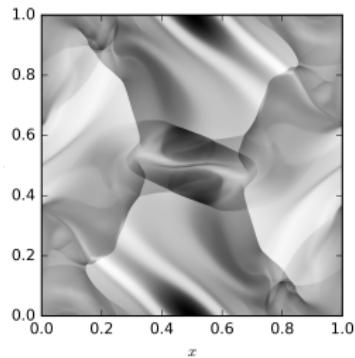
Modern:  $M$  and  $S$  banded with right choice of test functions.



Other geometries: other polynomials, spherical harmonics, ...

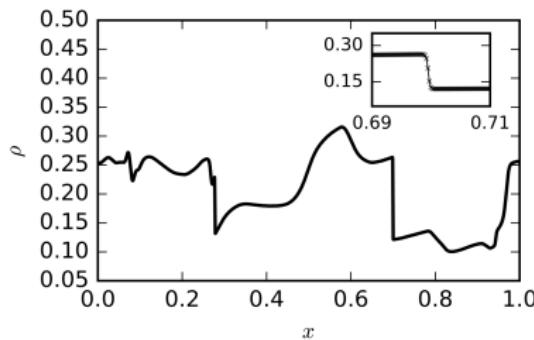
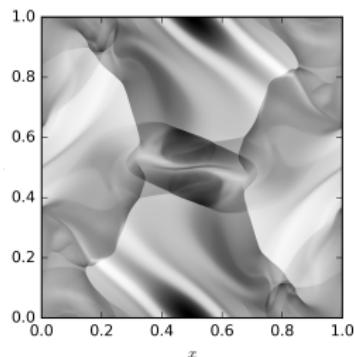
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- **Exponential** accuracy for smooth solutions. Need to regularize discontinuities



# Spectral methods

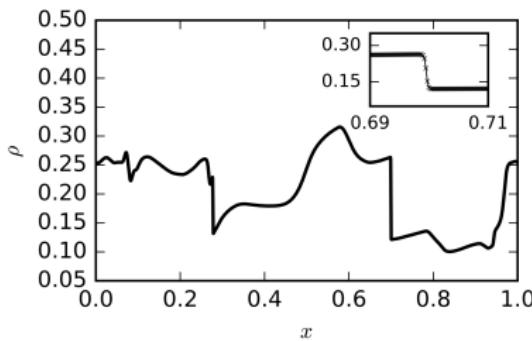
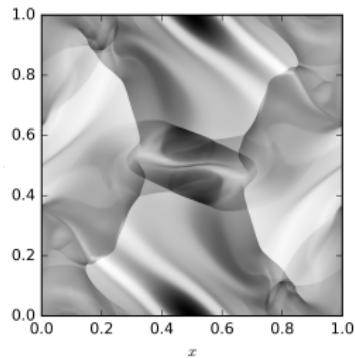
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- Very flexible in terms of equations.
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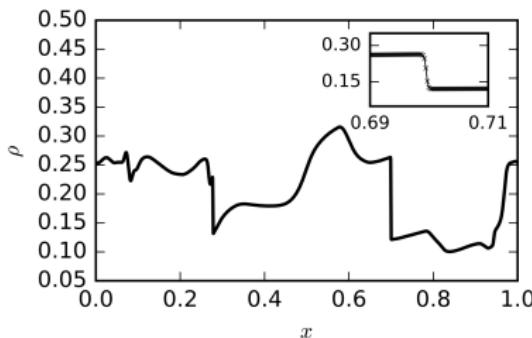
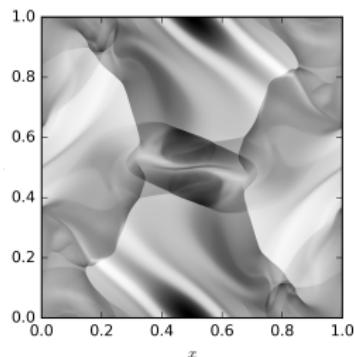


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Resources: Boyd “Chebyshev and Fourier Spectral Methods”

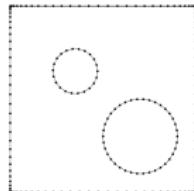
Codes: Chebfun (MATLAB), ApproxFun (julia), Dedalus (Python)

# Boundary integral methods

Use knowledge of PDEs in constructing numerical solutions:

A Green's func  $G$  (fundamental soln) needed

eg  $\Delta G = \delta$



For linear PDEs dominated by boundary rather than bulk terms, compute solution by forming integral equation of the fundamental solution/Green's function. Reduced dimensionality. Improved conditioning. Low-rank interactions and fast methods. Reconstruct solution in the bulk.

Examples: Stokes flow, Helmholtz, Maxwell, typically with homogeneous media

heavily uses high-order integration methods

- see Jun Wang's talk later today!

# Summary

## Recommended accessible reading

- [GC12] A Greenbaum and T P Chartier, *Numerical methods*, Princeton University Press, 2012.
- [TBI97] L. N. Trefethen and D. Bau III, *Numerical linear algebra*, SIAM, 1997.
- [Tre00] Lloyd N. Trefethen, *Spectral methods in MATLAB*, Software, Environments, and Tools, vol. 10, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2000.
- [Tre13] L. N. Trefethen, *Approximation theory and approximation practice*, SIAM, 2013,  
<http://www.maths.ox.ac.uk/chebfun/ATAP>.

This document: <https://github.com/ahbarnett/fwam-numpde>

See code directory for MATLAB code used to generate figures