Fourth-order time-stepping for PDEs on the sphere—and more

École Polytechnique & INRIA – DEFI Internal Seminar

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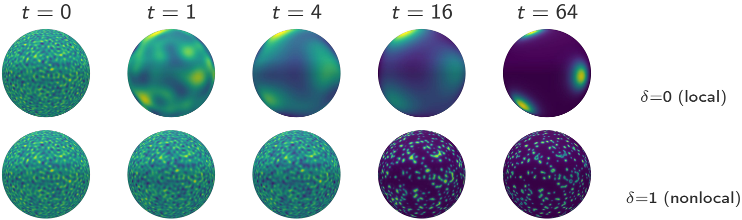
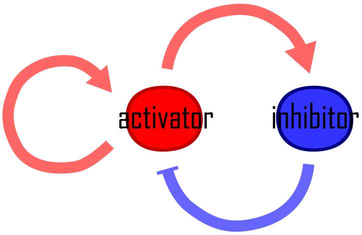


- Reaction-diffusion equations[1]

$$\begin{cases} u_t = \epsilon_u^2 \Delta u + F(u,v), \\ v_t = \epsilon_v^2 \Delta v + G(u,v) \end{cases}$$



- Pray-predator system (time)

  activator versus inhibitor

  activator—stimulates production

  inhibitor—slows production down

- Notion of spreading rate (space)

- Spherical geometry: embryogenesis, growth of tumors, convective patterns

[1] Turing, *The chemical basis of morphogenesis* (1952)

- **Problem:** Computing solutions of local and nonlocal PDEs of the form

$$u_t(t,\theta,\varphi) = \epsilon^2 \mathcal{L}_\delta u + \mathcal{N}(u), \quad (\theta,\varphi) \in \times[0,\pi] \times [-\pi,\pi)$$

- **Method:** expand u in a spectral basis & time-stepping on expansion coefficients

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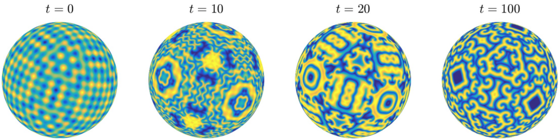
- **Local PDEs:** 2D Fourier series & implicit-explicit schemes

  My contribution: a spectral method

- **Nonlocal PDEs:** spherical harmonics & exponential integrators

  My contributions: def. nonlocal diffusion operator & a spectral method

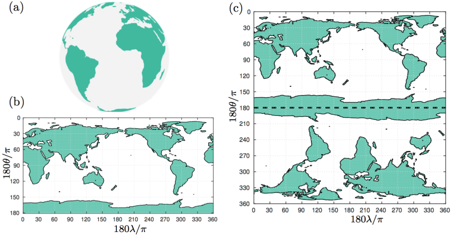


δ=0 (local)

- Local PDEs:

$$u_t = \epsilon^2 \Delta u + \mathcal{N}(u), \quad \Delta u = u_{\theta\theta} + \frac{\cos\theta}{\sin\theta} u_\theta + \frac{1}{\sin^2\theta} u_{\varphi\varphi}$$

- Double Fourier Sphere method (Meriless, Orszag, Townsend et al.[2])



- Approximations by 2D Fourier series with $N = n^2$ coeffs:

$$u(t,\theta,\varphi) \approx \sum_{\ell=-n/2}^{n/2-1} \sum_{m=-n/2}^{n/2-1} \hat{u}_{\ell m}(t) e^{i(\ell\theta + m\varphi)}, \quad \hat{u}_{\ell,m} = \hat{u}_{-\ell,m}(-1)^m$$

[2] Townsend, Wilber & Wright, *Computing with functions in spherical and polar geometries* (2016)

- Operator Δ discretized with a $N \times N$ matrix $\mathbf{L}$ acting on Fourier coefficients $\hat{u}$
- PDE $u_t = \epsilon^2 \Delta u + \mathcal{N}(u) \longrightarrow$ system of ODEs $\hat{u}'(t) = \epsilon^2 \mathbf{L}\hat{u} + \mathbf{N}(\hat{u})$

- Method for constructing $\mathbf{L}$:[3]

  standard Fourier matrices

  projection matrices

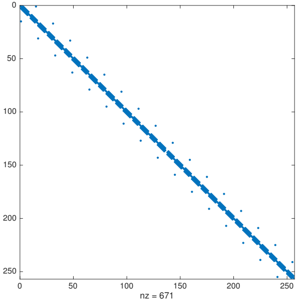
- $\mathbf{L}$ has good numerical properties:

  preserves doubled-up symmetry

  preserves smoothness at the poles

  has real and negative eigenvalues

  can be inverted in $\mathcal{O}(N)$ operations



[3] M. & Nakatsukasa, *Fourth-order time-stepping for PDEs on the sphere* (2018)

- PDE $u_t = \epsilon^2 \Delta u + \mathcal{N}(u)$ $\longrightarrow$ system of ODEs $\hat{u}'(t) = \epsilon^2 \mathbf{L}\hat{u} + \mathbf{N}(\hat{u})$

- Discretization with time-step Δt: $\hat{u}^k = \hat{u}(k\Delta t)$, $k = 0, 1, \ldots$
- Large $\mathcal{O}(N^2)$ eigenvalues: stiffness, standard explicit time-stepping impractical

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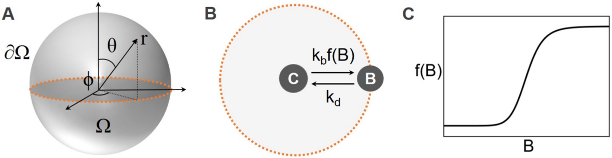
- Implicit-explicit (Ascher et al.[4]): implicit formula for **L**, explicit for **N**

$$(3\mathbf{I} - 2\Delta t\epsilon^2\mathbf{L})\hat{u}^{k+1} = 4\hat{u}^k - \hat{u}^{k-1} + 4\Delta t\mathbf{N}(\hat{u}^k) - 2\Delta t\mathbf{N}(\hat{u}^{k-1}) \quad \text{(second order)}$$

- In practice, fourth-order schemes such as IMEX-BDF4 or LIRK4
- Nonlinear term in physical space: $\mathbf{N}(\hat{u}^k) = \mathbf{F}\mathcal{N}(\mathbf{F}^{-1}\hat{u}^k)$ with FFT matrix **F**
- Cost per time-step: $\mathcal{O}(N \log N)$

[4] Ascher, Ruuth & Wetton, *Implicit-explicit methods for time-dependent PDEs* (1995)

- Embryogenesis model:[5]



Equations:

$$\begin{cases} U_t = \epsilon_U^2 \Delta U + k_b f(U) V - k_d U \text{ on } \partial\Omega, \\ V_t = \epsilon_V^2 \Delta V \text{ in } \Omega, \\ \epsilon_V^2 (\nabla V \cdot n) = -k_b f(U) V + k_d U \end{cases}$$

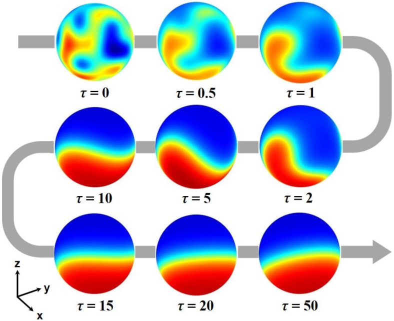
Nondimensionalization:

$$u = k_d U / k_b V_0,$$
$$\tau = k_d t,$$
$$\epsilon^2 = \epsilon_U^2 / k_d$$

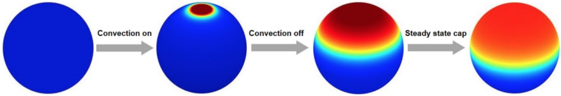
$$u_\tau = \epsilon^2 \Delta u + \mathcal{N}(u)$$

[5] Diegmiller, M., Muratov & Shvartsman, *Spherical caps in cell polarization* (2018)

- Random initial conditions relax to a single cap



- Constant initial conditions with transient convection also relax to a single cap



Local PDEs: Applications (3/3)

Software

- Chebfun: MATLAB package for computing to ≈ 15 digits of accuracy
- Function approximation and PDE solvers in 1D/2D/3D, on the sphere, etc.
- Led by Nick Trefethen at the University of Oxford

Aurentz, Austin, Driscoll, Filip, Güttel, Hale, Hashemi, Nakatsukasa, Platte, Townsend, Trefethen, Wright

- Standard differential operators are local:

$$Df(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- It is possible to define nonlocal analogues: [6]

$$D_\delta f(x) = \int_0^\delta \frac{f(x+h) - f(x)}{h} dh$$

- Examples include fractional differential operators and integral operators
- When are they useful?
  - The phenomenon we are interested in is intrinsically nonlocal, *e.g.*, peridynamics
  - The phenomenon is local but hard to discretize—approximating the local phenomenon with a nonlocal model, and then discretizing the latter may be easier
  - We do not know—the parameter δ gives more flexibility in the modeling process

[6] Du, *Nonlocal modeling, analysis, and computation* (2019)

- Nonlocal PDEs:

$$u_t = \epsilon^2 \mathcal{L}_\delta u + \mathcal{N}(u), \quad \mathcal{L}_\delta u(\boldsymbol{x}) = \int_{\mathbb{S}^2} \rho_\delta(|\boldsymbol{x} - \boldsymbol{y}|)\, [u(\boldsymbol{y}) - u(\boldsymbol{x})]\, d\Omega(\boldsymbol{y})$$

- Operator $\mathcal{L}_\delta$ decouples the spherical harmonic modes ($\ell \geq 0$, $-\ell \leq m \leq \ell$):

$$\mathcal{L}_\delta Y_\ell^m(\theta,\varphi) = \underbrace{\left(2\pi \int_{-1}^{1} (P_\ell(t) - 1)\rho_\delta(\sqrt{2(1-t)})\, dt\right)}_{\lambda_\delta(\ell)} Y_\ell^m(\theta,\varphi),$$

$$\mathcal{L}_0 Y_\ell^m(\theta,\varphi) = \Delta Y_\ell^m(\theta,\varphi) = -\ell(\ell+1) Y_\ell^m(\theta,\varphi)$$

- Approximations by spherical harmonic series with $N = (n+1)(2n+1)$ coeffs:

$$u(t,\theta,\varphi) \approx \sum_{\ell=0}^{n} \sum_{m=-\ell}^{+\ell} \tilde{u}_{\ell m}(t) Y_\ell^m(\theta,\varphi)$$

- $\mathcal{L}_\delta$ discretized[7] with a matrix $\mathbf{L}_\delta$ acting on spherical harmonics coefficients $\tilde{u}$
- PDE $u_t = \epsilon^2 \mathcal{L}_\delta u + \mathcal{N}(u) \longrightarrow$ system of ODEs $\tilde{u}'(t) = \epsilon^2 \mathbf{L}_\delta \tilde{u} + \mathbf{N}(\tilde{u})$

- $\mathbf{L}_\delta$ is diagonal with entries $\lambda_\delta(\ell)$:

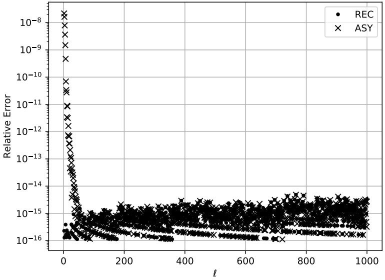
$$\lambda_\delta(\ell) = 2\pi \int_{-1}^{1} (P_\ell(t) - 1)\, \rho_\delta\left(\sqrt{2(1-t)}\right) dt$$

$$\rho_\delta\left(\sqrt{2(1-t)}\right) \propto \frac{1}{(1-t)^{1-\alpha}} \chi_{[0,\delta]}$$

- Computation of $\lambda_\delta(\ell)$:

  modified Clenshaw–Curtis quadrature

  recurrence & asymptotic formulas



[7] Slevinsky, M. & Du, *A spectral method for nonlocal diffusion operators on the sphere* (2018)

- PDE $u_t = \epsilon^2 \mathcal{L}_\delta u + \mathcal{N}(u) \;\longrightarrow\;$ system of ODEs $\tilde{u}'(t) = \epsilon^2 \mathbf{L}_\delta \tilde{u} + \mathbf{N}(\tilde{u})$

- Discretization with time-step Δt: $\tilde{u}^k = \tilde{u}(k\Delta t),\ k = 0, 1, \dots$
- Larges $\mathcal{O}(N)$ eigenvalues: stiffness, standard explicit time-stepping impractical

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- Exponential integrators (Hochbruck & Ostermann[8]): exact $\mathbf{L}_\delta$, numerical $\mathbf{N}$

$$\tilde{u}^{k+1} = e^{\Delta t \epsilon^2 \mathbf{L}_\delta}\,\tilde{u}^k + (\epsilon^2 \mathbf{L}_\delta)^{-1}(e^{\Delta t \epsilon^2 \mathbf{L}_\delta} - \mathbf{I})\mathbf{N}(\tilde{u}^k) \quad \text{(first order)}$$

- In practice, fourth-order schemes such as ETDRK4 (best for diagonal problems[9])
- Nonlinear term in physical space: $\mathbf{N}(\tilde{u}^k) = \mathbf{G}\mathcal{N}(\mathbf{G}^{-1}\tilde{u}^k)$ with FST matrix $\mathbf{G}$
- Cost per time-step: $\mathcal{O}(N \log^2 N)$

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[8] Hochbruck & Ostermann, *Exponential integrators* (2010)
[9] M. & Bootland, *Solving periodic stiff PDEs in 1D, 2D and 3D with exponential integrators* (2020)

Background

- Nonlinear advection equations on the sphere such as the barotropic vorticity equation are of significant importance in atmospheric numerical modeling

$$u_t + \frac{(\Delta^{-1}u)_\theta}{\sin\theta}u_\lambda - \frac{(\Delta^{-1}u)_\lambda}{\sin\theta}(u_\theta - 2\Omega\sin\theta) = 0$$

- A first step towards solving the shallow water & Navier–Stokes equations
- Spectral accuracy in space: spherical harmonics, RBFs, DFS method
- DFS is the only one that has $\mathcal{O}(N\log N)$ cost per time-step for N grid points

Goal

- Extend my DFS-based algorithm to solve nonlinear advection equations

Challenges

- Pole conditions—for reaction-diffusion equations, numerically satisfied; for advection equations, have to be enforced while maintaining spectral accuracy

$$\sum_{j=-m/2}^{m/2-1}\hat{u}_{j,k} = \sum_{j=-m/2}^{m/2-1}(-1)^j\hat{u}_{j,k} = 0, \quad |k| \geq 1$$

- Aliasing instabilities—for reaction-diffusion equations, Laplacian had a stabilizing effect; for advection equations, stabilization needed with, *e.g.*, vanishing viscosity

Background

- Nonlocal models are ubiquitous in applied fields including materials science, fluid dynamics, fracture mechanics, and image analysis
- Already introduced nonlocal diffusion operators on the sphere

$$\mathcal{L}_\delta u(\boldsymbol{x}) = \int_{\mathbb{S}^2} \rho_\delta(|\boldsymbol{x} - \boldsymbol{y}|)\,[u(\boldsymbol{y}) - u(\boldsymbol{x})]\,d\Omega(\boldsymbol{y})$$

Goal

- Develop a nonlocal vector calculus on the sphere, including nonlocal surface divergence, gradient, and curl operators together with their adjoints

$$\boldsymbol{\mathcal{G}}_\delta u(\boldsymbol{x}) = \int_{\mathbb{S}^2} [u(\boldsymbol{x}, \boldsymbol{y}) + u(\boldsymbol{y}, \boldsymbol{x})]\,\boldsymbol{\alpha}_\delta(\boldsymbol{x}, \boldsymbol{y})d\Omega(\boldsymbol{y})$$

Challenges

- Requires the use of vector spherical harmonics—expansions in vector spherical harmonics may be easily obtained from the Helmholtz–Hodge decomposition
- Nonlocal operators and their adjoints act on one- or two-point functions

$$\boldsymbol{\mathcal{G}}_\delta^* \boldsymbol{V}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\alpha}_\delta(\boldsymbol{x}, \boldsymbol{y}) + \boldsymbol{V}(\boldsymbol{y}) \cdot \boldsymbol{\alpha}_\delta(\boldsymbol{y}, \boldsymbol{x})$$

- Vector fields on manifolds are tricky to handle

Background

- Consider the following 3D Helmholtz equation,

$$-\left(\Delta + k^2\right) u(\boldsymbol{x}) = 0, \qquad \boldsymbol{x} \in \mathbb{R}^3 \setminus \overline{\Omega},$$
$$u(\boldsymbol{x}) = f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma$$

- This is a Dirichlet exterior problem whose solution is given by $u = \mathcal{S}\left[\frac{\partial u}{\partial n}\right]$ with

$$\int_\Gamma G(\boldsymbol{x}, \boldsymbol{y}) \left[\frac{\partial u}{\partial n}\right](\boldsymbol{y}) d\Gamma(\boldsymbol{y}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma$$

Goals

- Design a fast hierarchical solver for high-order boundary elements on curved surfaces

Challenges

- Curved surfaces (*e.g.*, unit sphere)—high-order polynomials need to be combined with high-order meshes (*i.e.*, curved elements)
- Singular integrals—regularization or/and semi-analytic methods
- Dense matrices—hierarchical matrices for faster matrix-vector products

Background

- Why and when do deep networks break the curse of dimensionality?
- For a real-valued function u in $\mathbb{R}^d$ with smoothness m and for some prescribed $\epsilon > 0$,

$$\|u - u_W\| \leq \epsilon \quad \text{with} \quad W = \mathcal{O}(\epsilon^{-\frac{d}{m}})$$

- Above result: curse of dimensionality, *i.e.*, W grows geometrically with d
- Bandlimited functions u of the form[10]

$$u(\boldsymbol{x}) = \int_{\mathbb{R}^d} G(\boldsymbol{x} \cdot \boldsymbol{y}) f(\boldsymbol{y}) d\boldsymbol{y}, \quad G \text{ is analytic}, \quad \operatorname{supp} f \subset [-1, 1]^d,$$

  can be approximated with error ϵ by networks of size $W = \mathcal{O}\left(\epsilon^{-2} \log^2 \epsilon^{-1}\right)$
- It resembles the solution to Helmholtz equation $-\left(\Delta + k^2\right) u = f$ in $\mathbb{R}^d$

Goal

- Study the curse of dimensionality in the solutions of high-dimensional PDEs

Challenge

- Approximation of G—for Helmholtz equation, it is in general singular

[10] M., Yang & Du, *Deep ReLU networks for bandlimited functions* (2020)