Pattern formation on the sphere

Courant Institute Numerical Analysis and Scientific Computing Seminar

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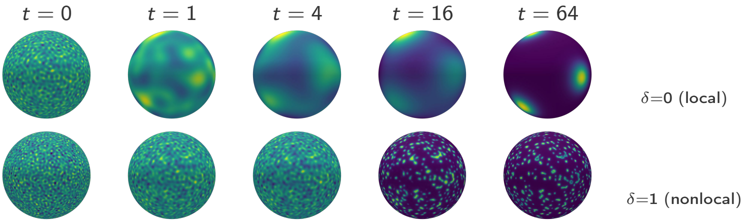
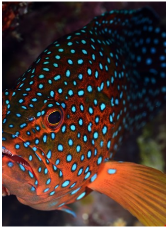
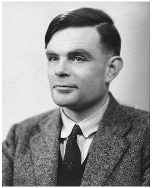


- Nature exhibits a seemingly endless array of patterns



- Alan Turing: those patterns are somehow similar
- He came up with a simple model[1] that could give rise to all manner of patterns: reaction-diffusion equations



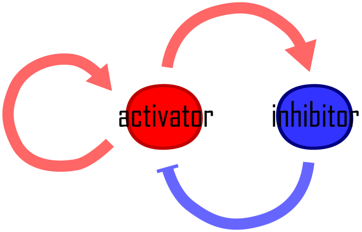
[1] Turing, *The chemical basis of morphogenesis* (1952)

- Pray-predator system

  Inside each organism there are two substances: activator & inhibitor

  Activator: stimulates production

  Inhibitor: slows production down



- Notion of spreading rate

- Mathematically: reaction-diffusion equations

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

- Spherical geometry relevant to : development of embryos, growth of tumors, convective patterns

Introduction (3/3)

My contributions

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

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

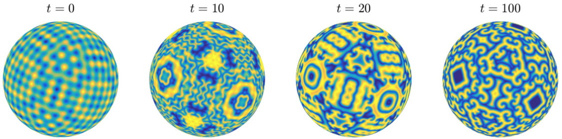
- **Method:** expand u in a spectral basis & time-stepping on expansion coefficients

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

  My contribution: a new spectral method

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

  My contribution: nonlocal reaction-diffusion equations & a spectral method



δ=0 (local)

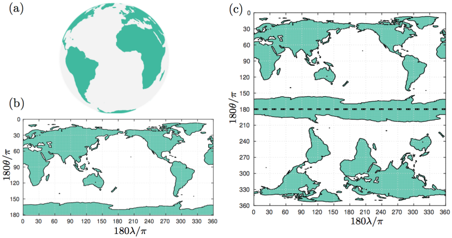
Local PDEs: Algorithms (1/3)

Discretizing space with 2D Fourier series

- 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:

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

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

Local PDEs: Algorithms (2/3)

The local Laplace–Beltrami matrix

- 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 to filter out the sawtooth mode

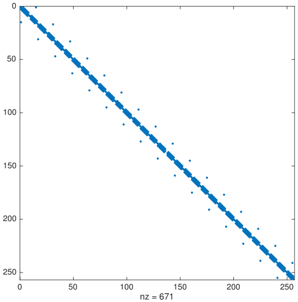
- $\mathbf{L}$ has good numerical properties:

  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)

Local PDEs: Algorithms (3/3)

Time-stepping with implicit-explicit schemes

- 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: $\hat{u}^k = \hat{u}(k\Delta t)$
- Implicit-explicit (Ascher et al.[4]): implicit formula for $\mathbf{L}$, explicit for $\mathbf{N}$

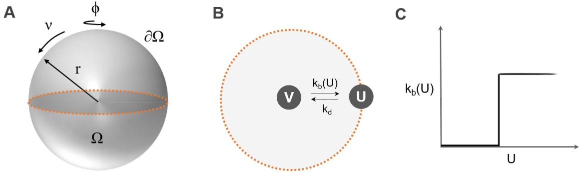
$$(3\mathbf{I} - 2\Delta t \epsilon^2 \mathbf{L})\hat{u}^{k+1} = 4\hat{u}^k - \hat{u}^{k-1} + 4\Delta t \mathbf{N}(\hat{u}^k) - 2\Delta t \mathbf{N}(\hat{u}^{k-1})$$

Nonlinear term in physical space: $\mathbf{N}(\hat{u}^k) = \mathbf{F}\mathcal{N}(\mathbf{F}^{-1}\hat{u}^k)$ *with FFT matrix* $\mathbf{F}$

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:

$$\begin{cases} U_t = \frac{\epsilon_U^2}{r^2}\Delta U + k_b H(U-\Theta)V - k_d(U-U_0) \text{ on } \partial\Omega, \\ V_t = \epsilon_V^2 \Delta V \text{ in } \Omega, \\ \epsilon_V^2(\nabla V \cdot n) = -k_b H(U-\Theta)V + k_d U \end{cases}$$

Nondimensionalization:

$$u = k_d U / k_b V_{max}, \quad \tau = k_d t,$$
$$\epsilon^2 = \epsilon_u^2 / k_d r^2, \quad \alpha = 3k_b/2k_d r,$$
$$\theta = k_d \Theta / k_b V_{max}$$

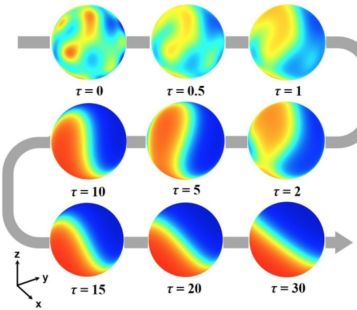
$$u_\tau = \epsilon^2 \Delta u + \left(1 - \frac{\alpha}{2\pi}\bar{u}\right) H(u-\theta) - u + \beta$$

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

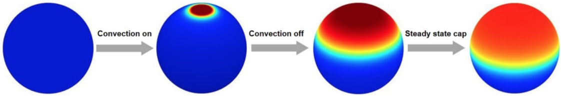
Local PDEs: Applications (2/6)

Spherical caps in embryogenesis

- Random initial conditions relax to a single cap



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



Local PDEs: Applications (3/6)

Symmetric spirals

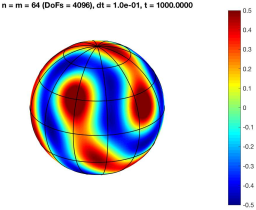
- Swift–Hohenberg free energy functional:

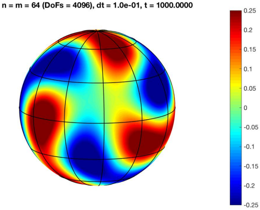
$$F(u) = \int_{\mathbb{S}^2} \left(\frac{1}{2}(\Delta u)^2 - |\nabla u|^2 - \frac{\mu - 1}{2} u^2 + \frac{1}{4} u^4 \right) d\Omega$$

- Swift–Hohenberg equation:

$$u_t = -\frac{\delta F}{\delta u} = -\Delta^2 u - 2\Delta u + (\mu - 1)u - u^3$$

- For $\mu = 0.2$ (left) and $\mu = 0.1$ (right):





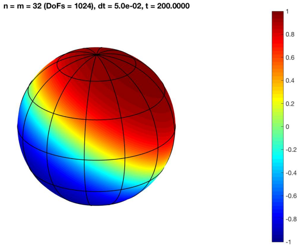
- Consider the free energy functional:

$$F(u, v) = \int_{\mathbb{S}^2} \left(\frac{\epsilon_u^2}{2} |\nabla u|^2 + \frac{1}{4}(1 - u^2)^2 + \frac{\epsilon_v^2}{2} |\nabla v|^2 + \frac{b}{4}(1 - |v|^2)^2 + cu|v|^2 \right) d\Omega$$

- The dynamics is then given by:

$$\begin{aligned} u_t &= M\Delta \frac{\delta F}{\delta u} = -M\epsilon_u^2 \Delta^2 u + M\Delta \left(u^3 - u + c|v|^2 \right), \\ v_t &= -\frac{\delta F}{\delta v} = \epsilon_v \Delta v + b(1 - |v|^2)v - 2cuv \end{aligned}$$

- For $c = 0$:



Local PDEs: Applications (5/6)

Numerical optimization of energy functional

- Find steady-states of $u_t = -\delta F/\delta u$ for some energy functional $F(u)$, e.g.:

$$F(u) = \int_{\mathbb{S}^2} \left(\frac{1}{2}(\Delta u)^2 - |\nabla u|^2 - \frac{\mu - 1}{2} u^2 + \frac{1}{4} u^4 \right) d\Omega$$

- Expand u in 2D Fourier series:

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

- Write $F(u)$ as a function of Fourier coefficients and optimize[6]

- 1D example, Allen–Cahn equation $u_t = \epsilon^2 u_{xx} + u - u^3$:

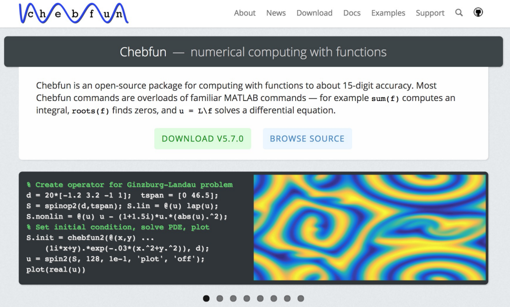
$$F(u) = \int_{-\pi}^{\pi} \frac{\epsilon^2}{2} |u_x|^2 + \frac{1}{4}(u^2 - 1)^2 dx$$

[6] M. & Gushterov, *Computing planar and spherical choreographies* (2016)

Local PDEs: Applications (6/6)

Software

- Chebfun: MATLAB package for computing to $\approx$ 15 digits of accuracy



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

Nonlocal PDEs: Algorithms (1/3)

Discretizing space with spherical harmonics

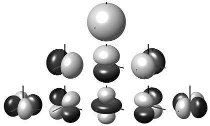
- Nonlocal PDEs:

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

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

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

$$Y_\ell^m(\theta,\varphi) = e^{im\varphi} P_\ell^m(\cos\theta)$$



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

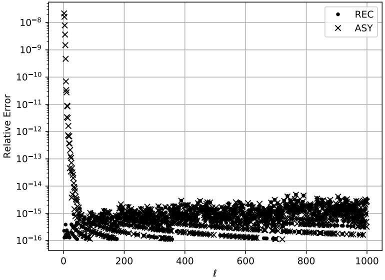
$$\lambda_\delta(\ell) = 2\pi \int_{-1}^{1} (P_\ell(t) - 1)\rho_\delta\left(\sqrt{2(1-t)}\right) dt$$

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

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

  mod. Clenshaw–Curtis quadrature[8]

  recurrence $\mathcal{O}(\ell^2)$ & asymptotic $\mathcal{O}(\ell \log \ell)$ formulas



[7] Slevinsky, M. & Du, *A spectral method for nonlocal diffusion operators on the sphere* (2018)
[8] Trefethen, *Is Gauss quadrature better than Clenshaw–Curtis?* (2008)

- 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: $\tilde{u}^k = \tilde{u}(k\Delta t)$
- Exponential integrators (Cox & Matthews, Hochbruck & Ostermann[9]): integrate $\mathbf{L}_\delta$ exactly with matrix exponential, numerical scheme for $\mathbf{N}$

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

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: $\mathcal{O}(N \log^2 N)$

[9] Hochbruck & Ostermann, *Exponential integrators* (2010)

Nonlocal PDEs: Applications (1/3)

Brusselator model

- Brusselator model:[10]

$$A \to U$$
$$2U + V \to 3U$$
$$B + U \to V + C$$
$$U \to D$$

Equations:

$$\begin{cases} U_T = \epsilon_u^2 \mathcal{L}_\delta U + A - (B+1)U + U^2 V, \\ V_T = \epsilon_v^2 \mathcal{L}_\delta V + BU - U^2 V \end{cases}$$

Scaling:

$$u = \epsilon_u U / \sqrt{(B+1)\epsilon_v^2}, \; f = B/(B+1)$$
$$v = \sqrt{(B+1)\epsilon_v^2} V / B\epsilon_u, \; t = (B+1)T$$
$$\epsilon = \epsilon_u / \sqrt{B+1}, \; \tau = (B+1)/\epsilon_v^2$$

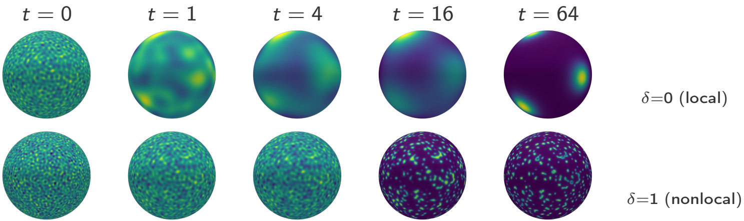
$$u_t = \epsilon^2 \mathcal{L}_\delta u + \epsilon^2 E - u + f u^2 v, \quad \tau v_t = \mathcal{L}_\delta v + \epsilon^{-2}(u - u^2 v)$$

[10] Prigogine & Lefever, *Symmetry breaking instabilities in dissipative systems* (1968)

Nonlocal PDEs: Applications (2/3)

Brusselator model

- Local case: perturbations from the steady state relax to spot patterns[11]
- Nonlocal case: speckled solution
- Nonlocal diffusion operators introduce new qualitative behaviors



[11] Trinh & Ward, *The dynamics of spot patterns for reaction-diffusion systems on the sphere* (2016)

Nonlocal PDEs: Applications (3/3)

Software

- Julia: `FastTransforms.jl` and `SpectralTimeStepping.jl` packages

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Julia is a high-level, high-performance dynamic programming language for numerical computing. It provides a sophisticated compiler, distributed parallel execution, numerical accuracy, and an extensive mathematical function library. Julia's Base library, largely written in Julia itself, also integrates mature, best-of-breed open source C and Fortran libraries for linear algebra, random number generation, signal processing, and string processing. In addition, the Julia developer community is contributing a number of external packages through Julia's built-in package manager at a rapid pace. IJulia, a collaboration between the Jupyter and Julia communities, provides a powerful browser-based graphical notebook interface to Julia.

Julia programs are organized around multiple dispatch; by defining functions and overloading them for different combinations of argument types, which can also be user-defined. For a more in-depth discussion of the rationale and advantages of Julia over other systems, see the following highlights or read the introduction in the online manual.

- Also available in MATLAB, `mex-ing` from Julia

Discussion

- Fast algorithms for solving both local and nonlocal PDEs on the sphere
- Applications in biology and physics
- Algorithms available online (Chebfun website & hadrien-montanelli.github.io)
- Possible extensions:

  Numerical optimization of energy functional

  Local and nonlocal phase-field crystal models on the sphere

  Local and nonlocal advection equations on the sphere

  PDEs on spheroids