Fourier Spectral Computing for PDEs on the Sphere

- an FFT-based method with implicit-explicit timestepping
- a simple & efficient approach

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Remote Participation

▷ simple Matlab demos for familiar PDEs can be run in real-time on laptop
  ▷ diffusion & wave equations
  ▷ reaction-diffusion & phase field patterns
  ▷ nonlinear Schrödinger equation

▷ operation count: DFTs on sphere scale as 2D FFTs
  ▷ all latitude calculations done in $O(N)$ operations: scaling reduced by factor of $N \sim 64-256$

▷ matlab demos indicated by footnotes: new demo indicated in red

http://www.irmacs.sfu.ca/events/coast-coast-abs#8253
Applications

- computing PDEs on the sphere driven by geophysics
  - meteorology: atmospheric fluid dynamics
  - climatology: aqua-planet oceanography
  - seismology: Rayleigh surface waves
- Fourier analysis on the sphere
  - tomography, crystallography, computer graphics
- computing on a manifold: constant, positive curvature

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PDEs on the Sphere: Applications & Computation

Computation

- numerical schemes
  - finite-difference, finite-volume, finite-element, spectral element . . .
  - spherical harmonics
- gridding
  - logically-rectangular, cubed sphere, longitude-latitude (long-lat), \textit{yin-yang} overset grid . . .
  - parallelization, mesh refinement & adaptivity

Fourier Spectral Method

- spectrally-fast: uses FFT for Fourier-based spectral transform
- simple implementation: uses long-lat grid & resembles FFT computing on 2D periodic rectangle
PDEs on the Sphere: Applications & Computation

Computation

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  - finite-difference, finite-volume, finite-element, spectral element . . .
  - spherical harmonics

- gridding
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Periodicity of the Sphere

When is a Sphere not a Sphere? . . . When it is a Torus!

- double mapping of a sphere to a periodic rectangle
  - north (NP) & south pole (SP) become lines of constant value
  - longitude $\rightarrow \lambda$-axis ($-\pi \leq \lambda \leq +\pi$)
  - co-latitude $\rightarrow \phi$-axis ($0 \leq \phi \leq 2\pi$)
- spherical symmetry: smooth extension from long-lat sphere to torus
  
  $f(\lambda, \phi) = \begin{cases} f(\lambda, \phi) & \text{for } 0 \leq \phi \leq \pi \\ f(\pi - \lambda, 2\pi - \phi) & \text{for } \pi \leq \phi \leq 2\pi \end{cases}$

- PDE should preserve spherical symmetry

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Fourier Modes with Spherical Symmetry ($m = 0$)

- natural Fourier modes in longitude: $Q_{nm}(\lambda, \phi) = q_{nm}(\phi) e^{im\lambda}$
- trigonometric modes for latitude:
  
  $$q_{nm}(\phi) = \begin{cases} 
  \cos n\phi & \text{for } m = 0 \\
  \sin \phi \sin n\phi & \text{for } m \text{ even} \\
  \sin n\phi & \text{for } m \text{ odd}
  \end{cases}$$

- smoothness at the poles
  - $m$ even modes have even symmetry across poles & are zero at poles for $m \neq 0$
  - $m$ odd modes have odd symmetry across poles & are zero at poles

**demo01:** $n = 3, m = 0$
Fourier Modes with Spherical Symmetry \((m = 0)\)

- natural Fourier modes in longitude: \(Q_{nm}(\lambda, \phi) = q_{nm}(\phi) e^{im\lambda}\)
- trigonometric modes for latitude:
  \[
  q_{nm}(\phi) = \begin{cases} 
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  \]

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Fourier Modes on the Sphere

Fourier Modes with Spherical Symmetry ($m$ even)

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demo01: $n = 4, m = 4$
Fourier Modes on the Sphere

Fourier Modes with Spherical Symmetry ($m$ even)

- natural Fourier modes in longitude: $Q_{nm}(\lambda, \phi) = q_{nm}(\phi) e^{im\lambda}$
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- smoothness at the poles
  
  - $m$ even modes have even symmetry across poles & are zero at poles for $m \neq 0$
  - $m$ odd modes have odd symmetry across poles & are zero at poles

demo01: $n = 4, m = 4$
Fourier Modes on the Sphere

Fourier Modes with Spherical Symmetry ($m$ odd)

- natural Fourier modes in longitude: $Q_{nm}(\lambda, \phi) = q_{nm}(\phi) e^{im\lambda}$
- trigonometric modes for latitude:
  
  $$q_{nm}(\phi) = \begin{cases} 
  \cos n\phi & \text{for } m = 0 \\
  \sin \phi \sin n\phi & \text{for } m \text{ even} \\
  \sin n\phi & \text{for } m \text{ odd}
  \end{cases}$$

- smoothness at the poles
  - $m$ even modes have even symmetry across poles & are zero at poles for $m \neq 0$
  - $m$ odd modes have odd symmetry across poles & are zero at poles

demo01: $n = 5$, $m = 3$
Fourier Modes with Spherical Symmetry ($m$ odd)

- natural Fourier modes in longitude: $Q_{nm}(\lambda, \phi) = q_{nm}(\phi) e^{im\lambda}$
- trigonometric modes for latitude:
  
  \[
  q_{nm}(\phi) = \begin{cases} 
  \cos n\phi & \text{for } m = 0 \\
  \sin \phi \sin n\phi & \text{for } m \text{ even} \\
  \sin n\phi & \text{for } m \text{ odd}
  \end{cases}
  \]

- smoothness at the poles
  
  - $m$ even modes have even symmetry across poles & are zero at poles for $m \neq 0$
  - $m$ odd modes have odd symmetry across poles & are zero at poles

demo01: $n = 5, m = 3$
Double Fourier Series on the Sphere

Fourier Geometry for Spherically-Symmetric Functions

- double sum over $Q_{nm}$ modes

$$f(\lambda, \phi, t) = \sum_{m=-\infty}^{+\infty} \sum_{n=0}^{\infty} \tilde{f}_{nm}(t) \ Q_{nm}(\lambda, \phi) = \sum_{m=-\infty}^{+\infty} e^{im\lambda} \sum_{n=0}^{\infty} \tilde{f}_{nm}(t) \ q_{nm}(\phi)$$

- PDE must respect spherical symmetry

demo02: $n = 4$, $m = 7$, $a = 45^\circ$
Diffusion on the Sphere

Initial Decay and Steady-State Forcing, $N = 64$

- forced diffusion on sphere, $u(\lambda, \phi, t)$
  \[ u_t = \nabla^2 u + f(\lambda, \phi) \]
- initial condition: $u_0(\lambda, \phi, 0) = c_1 \{ Y_{10}^{12}(\lambda, \phi) + \text{conj} \}$
- steady forcing, $f(\lambda, \phi)$ is rotated spherical harmonic: $c_2 \{ Y_3^7(\lambda, \phi) + \text{conj} \}$
- exponential-in-$t$ solutions
  \[ u(\lambda, \phi, t) = e^{-156t} u_0(\lambda, \phi) + (1 - e^{-72t}) f(\lambda, \phi) \]
- FFT-based routines for spherical data: \texttt{fftS.m} \& \texttt{ifftS.m}
- 3\textsuperscript{rd}-order accurate timestepping
Uni-Directional Wavepacket, $N = 64$

- propagation on sphere, $u(\lambda, \phi, t)$ & $v(\lambda, \phi, t)$
  \[
  u_t = v, \quad v_t = \nabla^2 u
  \]

- initial wavepacket: masked spherical harmonic, $u_0(\lambda, \phi) = c_1\{Y_{16}^{16}(\lambda, \phi) + \text{conj}\}$

- propagation follows a great circle

- wavespeeds $\rightarrow 1^+$, in short wave limit

- 2nd-order accurate timestepping scheme for stability
Waves on the Sphere

Forced Waves, \( N = 64 \)

- Radiation on the sphere, \( u(\lambda, \phi, t) \) & \( v(\lambda, \phi, t) \)
  
  \[
  \begin{align*}
  u_t & = v \\
  v_t & = \nabla^2 u + f_1(\lambda, \phi) \sin 24t + f_2(\lambda, \phi) \sin 12t
  \end{align*}
  \]

- Zero initial condition: \( u_0(\lambda, \phi, 0) = 0 \)

- Oscillatory forcings: \( f_j(\lambda, \phi) \) are spatially localized

- 2\(^{nd}\)-order accurate timestepping

- No problems at the pole: geometrical distortions, or time-step restriction from over-resolution
Spectral Computing on the Sphere

Spherical Harmonics (SH)

- characteristics of $Y_l^m(\lambda, \phi)$
  - $l$-index indicates spatial resolution on the sphere
  - SH modes preserve spatial resolution under coordinate rotations
  - SH spectrum is Fourier in $\lambda$-direction; $m$-index gives direction ($-l \leq m \leq +l$)
  - eigenfunctions of the surface Laplacian

- fast SH transform (S2kit), based on Driscoll & Healy (1989)
  - high-complexity algorithm: fast interpolations, fast multipole, WKB approximation . . .

PDE Computing with Spherical Harmonics

- spectral method of choice for geophysical fluid codes
- elliptic solves & timestepping schemes
- Swartztrauber’s 1979 assessment:
  
  “the theoretical gap which exists between the states of the art for discrete spectral approximations on a sphere and on a rectangle.”
Spectral Derivatives on the Sphere

Spectral Differentiation of $Q_{nm}(\lambda, \phi) = q_{nm}(\phi) e^{im\lambda}$

- longitude differentiation
  \[ \frac{\partial}{\partial \lambda} Q_{nm} = im Q_{nm} \]

- latitude differentiation, typically non-constant coefficient
  \[ \sin \phi \frac{\partial}{\partial \phi} Q_{nm} = a_1 Q_{(n-2)m} + a_2 Q_{nm} + a_3 Q_{(n+2)m} \]

- tri-diagonal differentiation matrices: $\sin^2 \phi \nabla^2$, $\sin^2 \phi$

- forward & inverse operations remain $O(N^2)$

Double Fourier Series

- derivative operations on the spectral representation . . .
  \[ u(\lambda, \phi, t) = \sum_m e^{im\lambda} \sum_n \tilde{u}_{nm}(t) q_{nm}(\phi) \]

  . . . act on Fourier coefficients $\tilde{u}_{nm}$ as vectors $(\tilde{u}_n)_m$
Timestepping for Fourier Methods

Diffusion on a Rectangle

- Fourier representation
  \[ u(x, y, t) = \sum_m \sum_n \tilde{u}_{nm}(t) e^{i(mx+ny)} \]

- Forced diffusion on sphere
  \[ u_t - \nabla^2 u = f(\lambda, \phi, t) \]

- Spectral equation
  \[ \frac{d}{dt} \tilde{u}_{nm} + (m^2 + n^2) \tilde{u}_{nm} = \tilde{f}_{nm}(t) \]

Fourier Timestepping Strategies

- Integrating factor treats Laplacian exactly \( \rightarrow \) ODE solve
  \[ \frac{d}{dt} \left\{ e^{(m^2+n^2)t} \tilde{u}_{nm} \right\} = e^{(m^2+n^2)t} \tilde{f}_{nm}(t) \]

- Exponential time-differencing \( \rightarrow \) numerical quadrature
  \[
  \tilde{u}_{nm}(t) = \tilde{u}_{nm}(0) e^{-(m^2+n^2)t} + \int_0^t e^{(m^2+n^2)(s-t)} \tilde{f}_{nm}(s) \, ds
  \]
IMEX Timestepping for Fourier on Sphere

Diffusion on the Sphere

▷ Fourier representation & \((\tilde{u}_n)_m\) as column vector data

\[
\begin{align*} u(x, y, t) &= \sum_m \sum_n (\tilde{u}_n)_m q_{nm}(\phi) e^{im\lambda} \\
\end{align*}
\]

▷ forced diffusion on sphere

\[
\begin{align*} \sin^2 \phi \ u_t - \sin^2 \phi \nabla^2 u &= \sin^2 \phi f(\lambda, \phi, t) \\
\end{align*}
\]

▷ spectral equation

\[
\begin{align*} [\sin^2 \phi] \frac{d}{dt} (\tilde{u}_n)_m - [\sin^2 \phi \nabla^2] (\tilde{u}_n)_m &= [\sin^2 \phi] (\tilde{f}_n)_m \\
\end{align*}
\]

IMEX Scheme [Ascher, Ruuth, Wetton (1995)]

▷ 2\textsuperscript{rd}-order BDF in time

\[
\begin{align*} [\sin^2 \phi] \left\{ \frac{3(\tilde{u}_n)_m^{j+1} - 4(\tilde{u}_n)_m^j + (\tilde{u}_n)_m^{j-1}}{2\Delta t} \right\} \\
- [\sin^2 \phi \nabla^2] (\tilde{u}_n)_m^{j+1} &= [\sin^2 \phi] \left\{ 2(\tilde{f}_n)_m^j - (\tilde{u}_n)_m^{j-1} \right\} \\
\end{align*}
\]
IMEX Timestepping for Fourier on Sphere

Diffusion on the Sphere

- Fourier representation & \((\tilde{u}_n)_m\) as column vector data
  \[
u(x, y, t) = \sum_m \sum_n (\tilde{u}_n)_m q_{nm}(\phi) e^{im\lambda}\]

- forced diffusion on sphere
  \[
sin^2 \phi \, u_t - sin^2 \phi \nabla^2 u = sin^2 \phi \, f(\lambda, \phi, t)\]

- spectral equation
  \[
  [sin^2 \phi] \frac{d}{dt} (\tilde{u}_n)_m - [sin^2 \phi \nabla^2] (\tilde{u}_n)_m = [sin^2 \phi] (\tilde{f}_n)_m
  \]

IMEX Scheme [Ascher, Ruuth, Wetton (1995)]

- 2\textsuperscript{nd}-order BDF in time
  \[
  \left\{ \begin{array}{l}
  \frac{3}{2\Delta t} [sin^2 \phi] - [sin^2 \phi \nabla^2] \\
  [sin^2 \phi]
  \end{array} \right\} (\tilde{u}_n)^{j+1}_m = \]
  \[
  \frac{4(\tilde{u}_n)^{j}_m - (\tilde{u}_n)^{j-1}_m}{2\Delta t} + 2(\tilde{f}_n)^{j}_m - (\tilde{u}_n)^{j-1}_m
  \]
Application: Fitz-Hugh Nagumo Equations

Pattern Formation & Front Dynamics, \( N = 256 \)

- bi-stable \((0, 1)\) activator, \(u(\lambda, \phi, t)\) & long-range inhibitor, \(v(\lambda, \phi, t)\)

\[
\begin{align*}
    u_t &= \frac{\epsilon^2}{r^2} \nabla^2 u + u(u-a)(u-1) + \rho (v-u) \\
    0 &= \frac{1}{r^2} \nabla^2 v + (v-u)
\end{align*}
\]

- labyrinth forming region in parameter space [Goldstein, DJM, Petrich, 1992]

- \(0 < \epsilon \ll 1 \ll r\) → sharp fronts in \(u\) & large spherical domain
- \(0 < a - 1/2 \ll 1\) → \(u = 0, 1\) bistability with weak bias to red
- \(0 < \rho \ll 1\) → weak inhibition producing blue
Application: Fitz-Hugh Nagumo Equations

Pattern Formation & Front Dynamics, \( N = 256 \)

- bi-stable \((0, 1)\) activator, \(u(\lambda, \phi, t)\) & long-range inhibitor, \(v(\lambda, \phi, t)\)

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \frac{\epsilon^2}{r^2} \nabla^2 u + u(u - a)(u - 1) + \rho(v - u) \\
0 &= \frac{1}{r^2} \nabla^2 v + (v - u)
\end{align*}
\]

- labyrinth forming region in parameter space [Goldstein, DJM, Petrich, 1992]

\(\nabla^2\) \(0 < \epsilon \ll 1 \ll r\) \(\rightarrow\) sharp fronts in \(u\) & large spherical domain

\(\nabla^2\) \(0 < a - 1/2 \ll 1\) \(\rightarrow\) \(u = 0, 1\) bistability with weak bias to red

\(\nabla^2\) \(0 < \rho \ll 1\) \(\rightarrow\) weak inhibition producing blue
Application: Phase-Field Model

Diffusion Fronts & Triple Point Dynamics

- complex-valued FFTs: `fftSc.m` & `ifftSc.m`
- complex-valued gradient flow, $\psi(\lambda, \phi, t) \rightarrow$ diffusion & tri-stability
  \[
  \psi_t = \frac{\delta \mathcal{F}}{\delta \psi^*} ; \quad \mathcal{F}[\psi, \psi^*] = \int_S \left\{ \epsilon |\nabla \psi|^2 + \frac{1}{\epsilon} |\psi - z_1|^2 |\psi - z_2|^2 |\psi - z_3|^2 \right\} dS
  \]
- $z_j^3 = 1 \quad \rightarrow$ phases defined by 3 cube roots of unity
- $0 < \epsilon \ll 1 \quad \rightarrow$ sharp fronts separating phases
- slow drift of phase fronts $\rightarrow$ conformity
- on the plane, steady boundary-supported $120^\circ$ triple junctions [Bronsard/Reitich, 1993]
Application: Phase-Field Model

Diffusion Fronts & Triple Point Dynamics

- complex-valued FFTs: `fftSc.m` & `ifftSc.m`
- complex-valued gradient flow, $\psi(\lambda, \phi, t) \rightarrow$ diffusion & tri-stability

$$
\psi_t = \frac{\delta F}{\delta \psi^*} \quad ; \quad F[\psi, \psi^*] = \int_S \left\{ \epsilon |\nabla \psi|^2 + \frac{1}{\epsilon} |\psi - z_1|^2 |\psi - z_2|^2 |\psi - z_3|^2 \right\} \, dS
$$

- $z_j^3 = 1 \quad \rightarrow$ phases defined by 3 cube roots of unity
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Waves with Dispersion & Nonlinearity

▶ complex-valued, $\psi(\lambda, \phi, t)$

$$i\psi_t = \nabla^2 \psi \mp |\psi|^2 \psi$$

▶ $\mp$ defocussing; $+$ focussing

▶ near spherical harmonic initial condition

▶ on the plane: singularity possible in focussing case
Simple & Spectrally-Fast PDE Computing

- Fourier-based spectral transform
- implicit-explicit timestepping schemes
- suite of matlab routines
- follows paradigm for Fourier spectral method
- stability issues for fluid flows
- advection of rotating shallow water potential vorticity, DJM & Blazenko