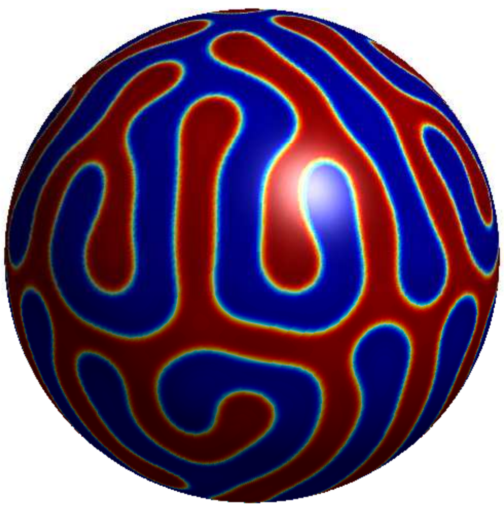
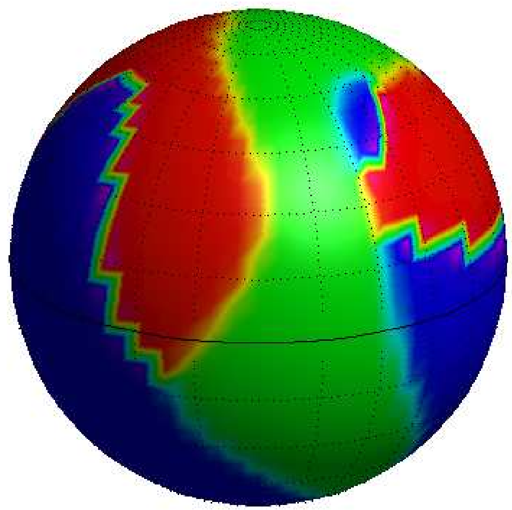
Fourier Spectral Computing for PDEs on the Sphere

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

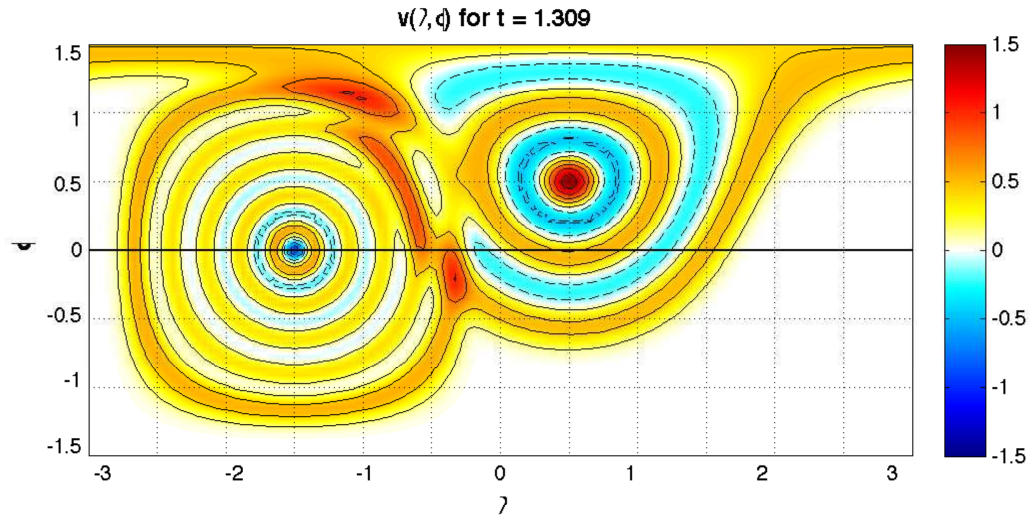


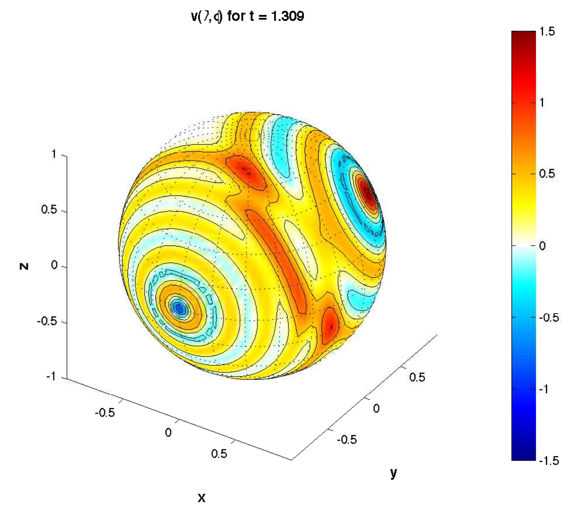


▷ Dave Muraki, Andrea Blazenko & Kevin Mitchell

Mathematics, Simon Fraser University

Matlab Demos Online



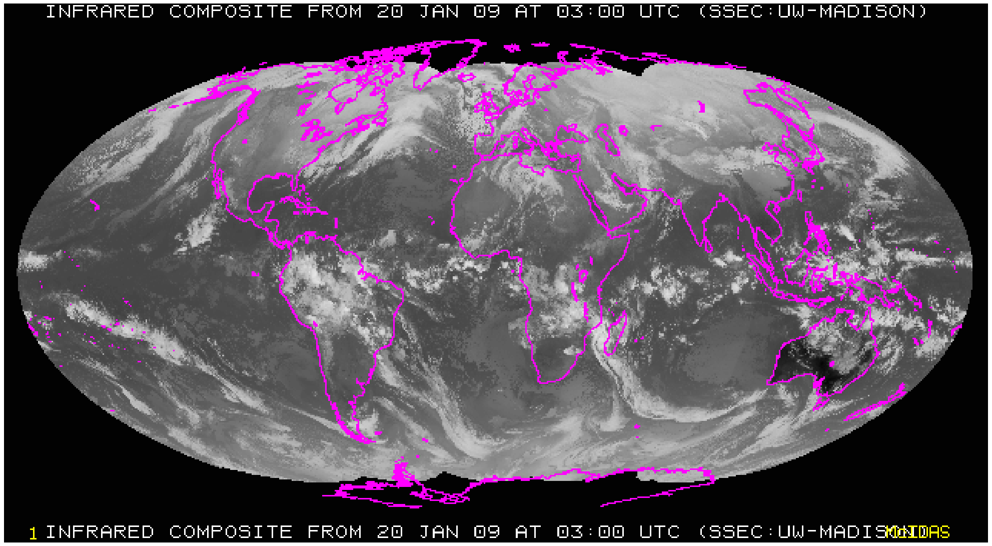


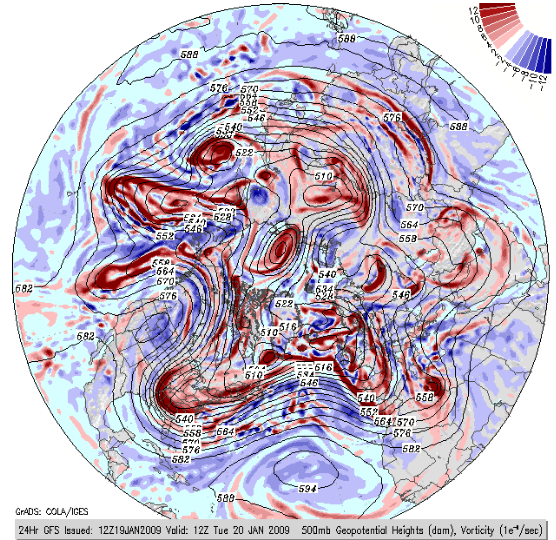
Remote Participation

- 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

PDEs on the Sphere: Applications & Computation

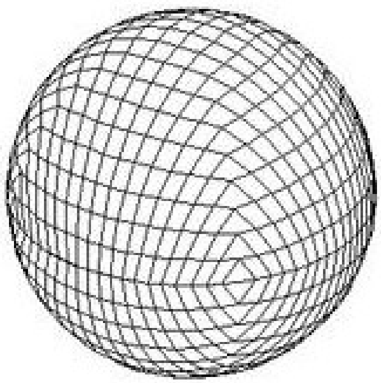


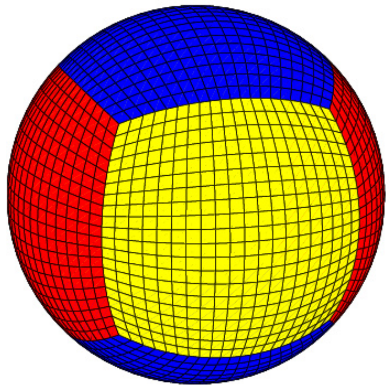


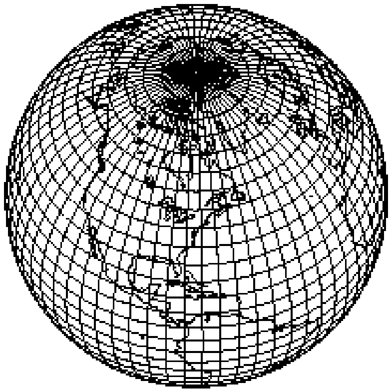
Applications

- ▷ 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

PDEs on the Sphere: Applications & Computation







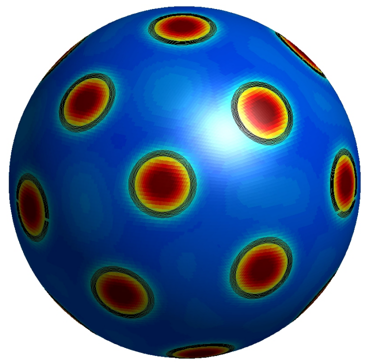
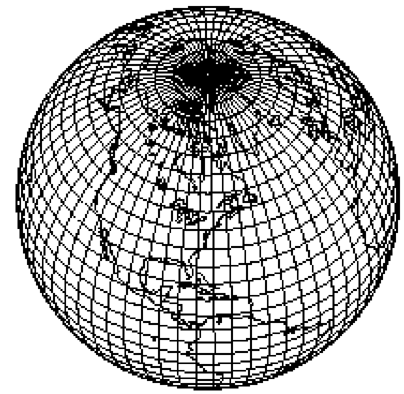
Computation

- ▷ numerical schemes
  - ▷ finite-difference, finite-volume, finite-element, spectral element . . .
  - ▷ spherical harmonics
- ▷ gridding
  - ▷ logically-rectangular, cubed sphere, longitude-latitude (long-lat), *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

- ▷ numerical schemes [Calhoun, Helzel & LeVeque, 2008]
  - ▷ finite-difference, finite-volume, finite-element, spectral element . . .
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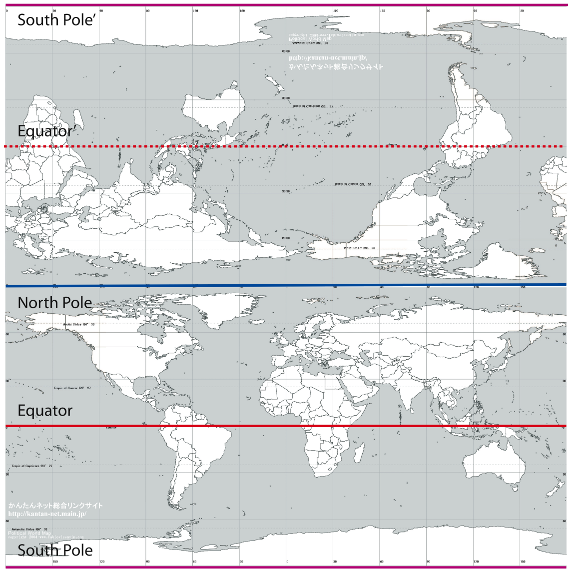
Periodicity of the Sphere

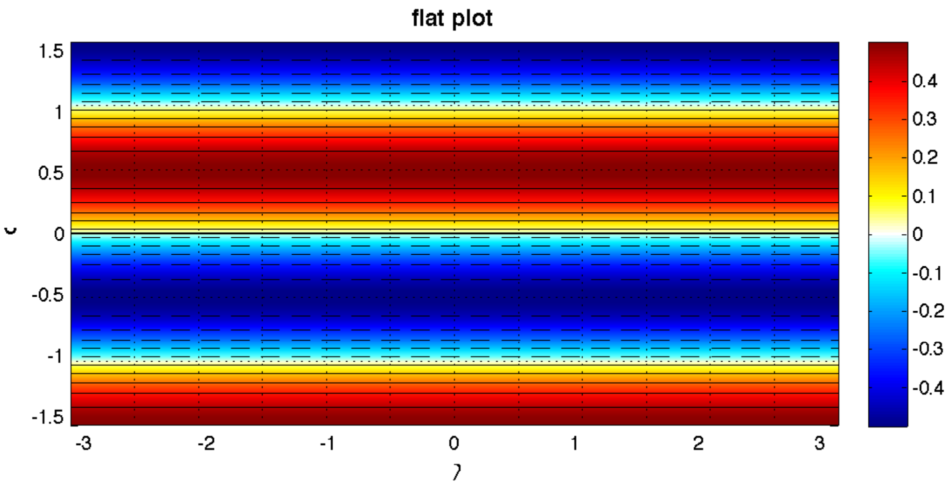


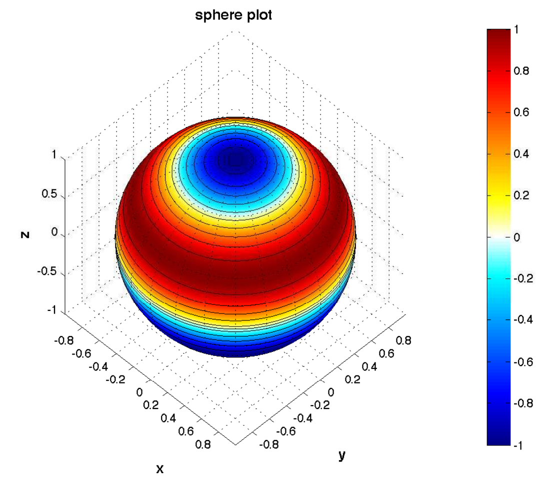
When is a Sphere is not a Sphere? . . . When it is a Torus!

- double mapping of a sphere to a periodic rectangle
  - north (NP) & south pole (SP) become lines of constant value
  - longitude $\longrightarrow$ λ-axis ($-\pi \leq \lambda \leq +\pi$)
  - co-latitude $\longrightarrow$ ϕ-axis ($0 \leq \phi \leq 2\pi$)
- spherical symmetry: smooth extension from long-lat sphere to torus

$$f(\lambda,\phi) = \begin{cases} f(\lambda,\phi) & \text{for} \quad 0 \leq \phi \leq \pi \\ f(\pi-\lambda, 2\pi-\phi) & \text{for} \quad \pi \leq \phi \leq 2\pi \end{cases} .$$

- PDE should preserve spherical symmetry





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

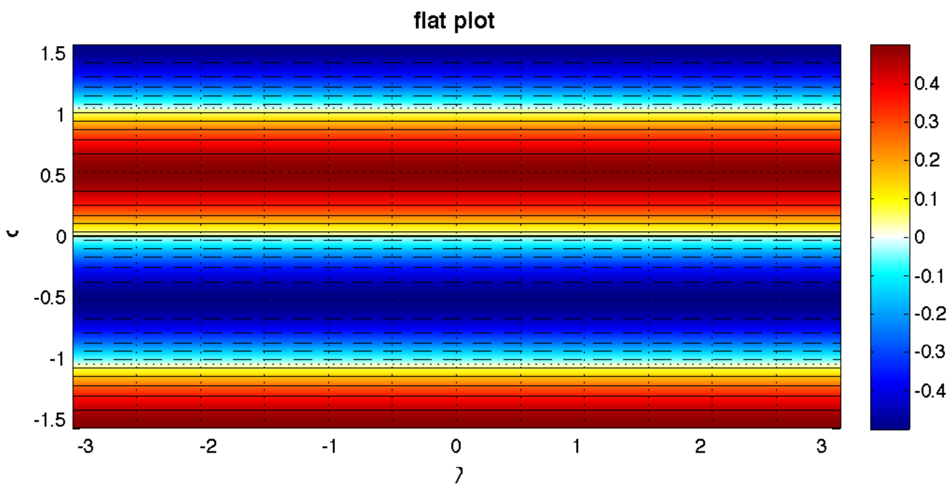
- natural Fourier modes in longitude: $Q_{nm}(\lambda, \phi) = q_{nm}(\phi)\ e^{im\lambda}$
- trigonometric modes for latitude:

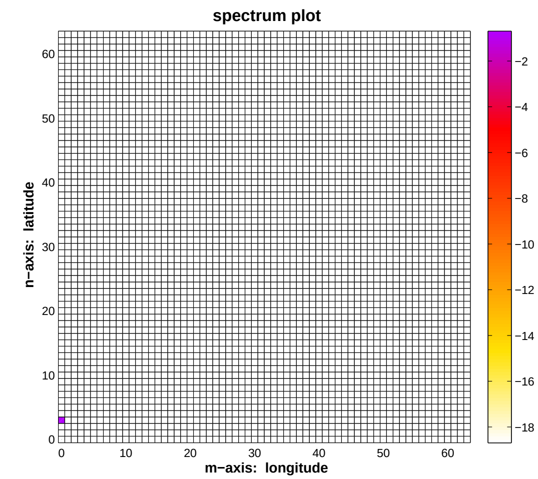
$$q_{nm}(\phi) = \begin{cases} \cos n\phi & \text{for} \quad m = 0 \\ \sin\phi\ \sin n\phi & \text{for} \quad m \text{ even} \\ \sin n\phi & \text{for} \quad m \text{ odd} \end{cases}$$

- 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 on the Sphere





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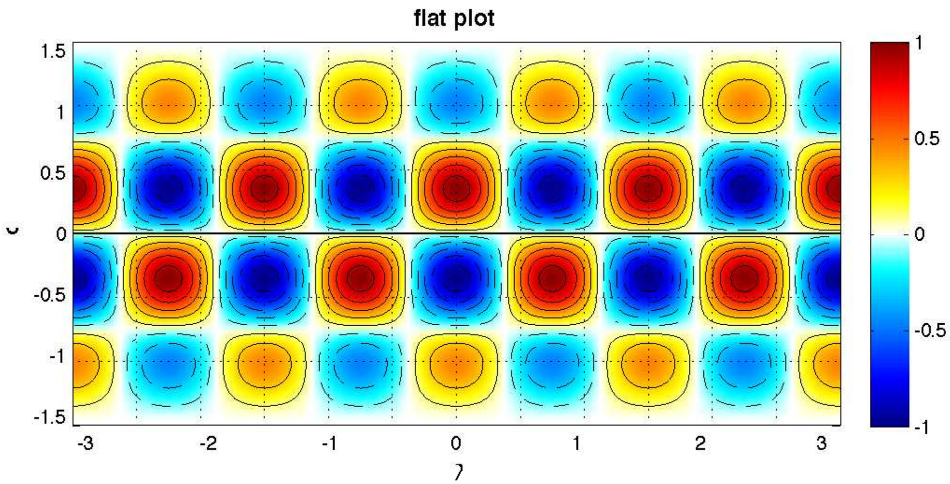

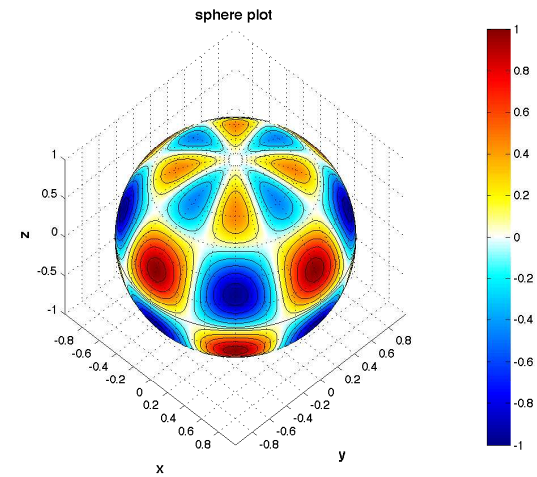

Fourier Modes with Spherical Symmetry (m even)

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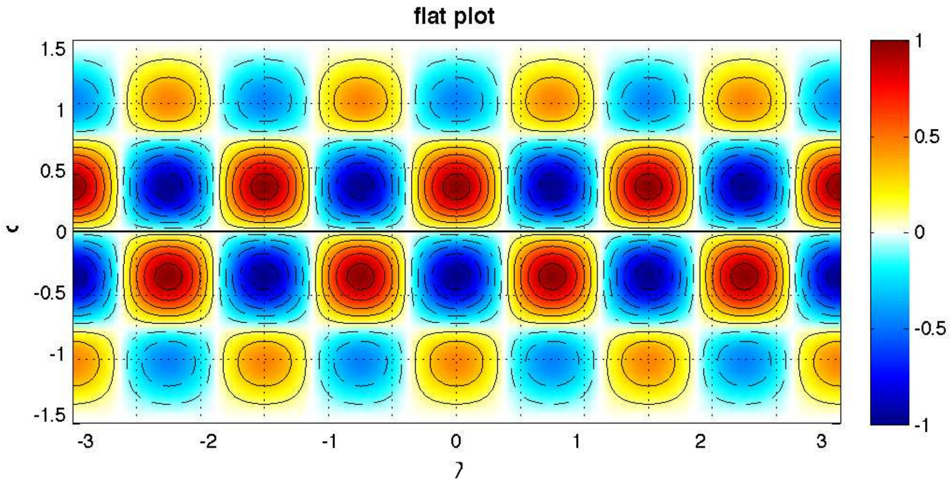
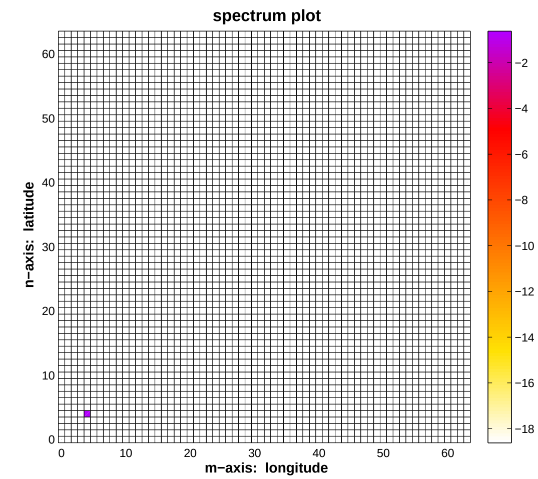
demo01: $n = 4$, $m = 4$





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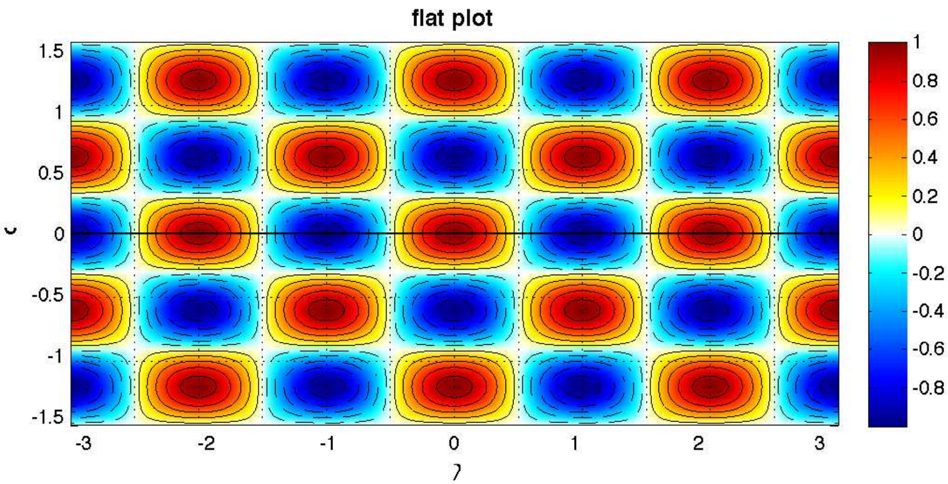
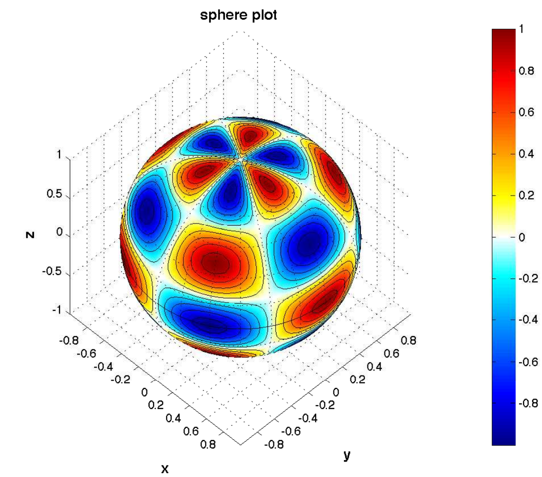
Fourier Modes on the Sphere





Fourier Modes with Spherical Symmetry (m odd)

- natural Fourier modes in longitude: $Q_{nm}(\lambda, \phi) = q_{nm}(\phi)\ e^{im\lambda}$
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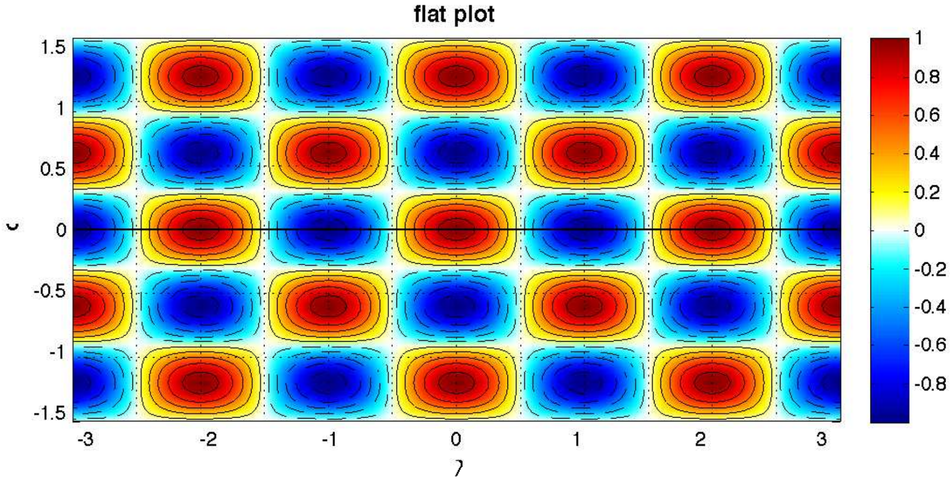
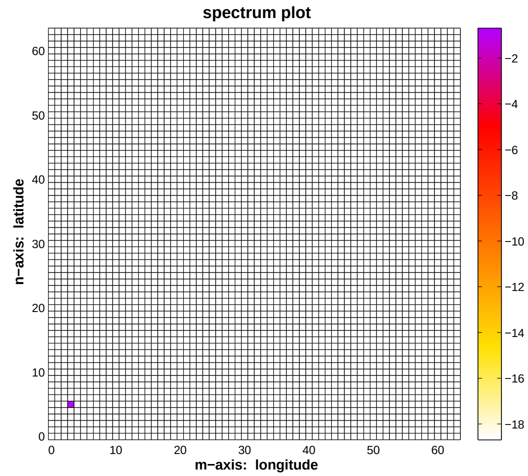
demo01: $n = 5$, $m = 3$

Fourier Modes on the Sphere





Fourier Modes with Spherical Symmetry (m odd)

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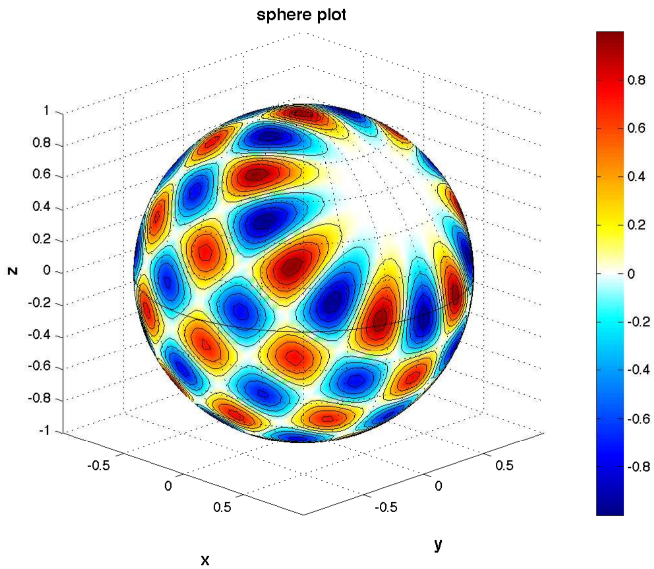
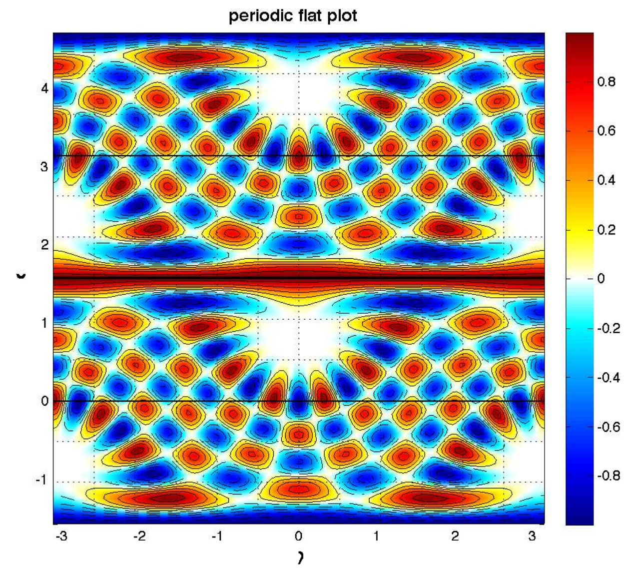




Fourier Geometry for Spherically-Symmetric Functions

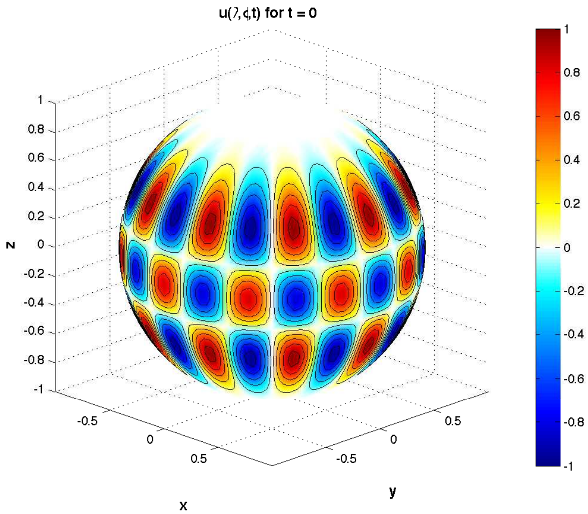
- double sum over Q_{nm} modes

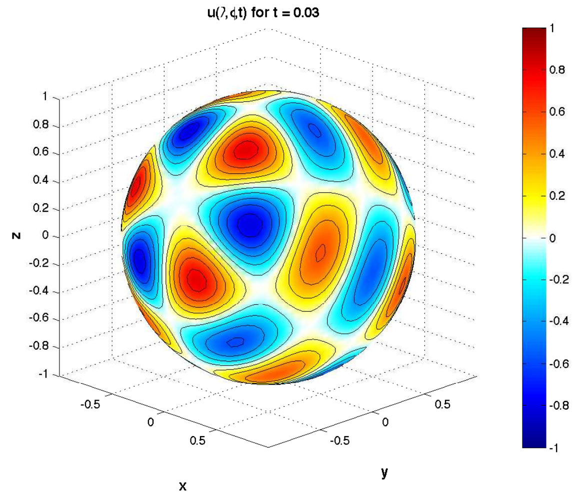
$$f(\lambda,\phi,t) = \sum_{m=-\infty}^{+\infty} \sum_{n=0}^{\infty} \tilde{f}_{nm}(t)\ Q_{nm}(\lambda,\phi) = \sum_{m=-\infty}^{+\infty} e^{im\lambda} \sum_{n=0}^{\infty} \tilde{f}_{nm}(t)\ q_{nm}(\phi)$$

- early works: Merilees, (1973), Orszag (1973), Boer/Steinberg (1974), Boyd (1978)
- elliptic solves: Yee (1981), Moorthi/Higgins (1992)
- fluid flow: Fornberg (1997), Spotz, et.al. (1998), Cheong et.al. (2000-2006), Layton/Spotz (2003)

- PDE must respect spherical symmetry

demo02: $n = 4$, $m = 7$, $a = 45^{\circ}$





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

- forced diffusion on sphere, $u(\lambda, \phi, t)$

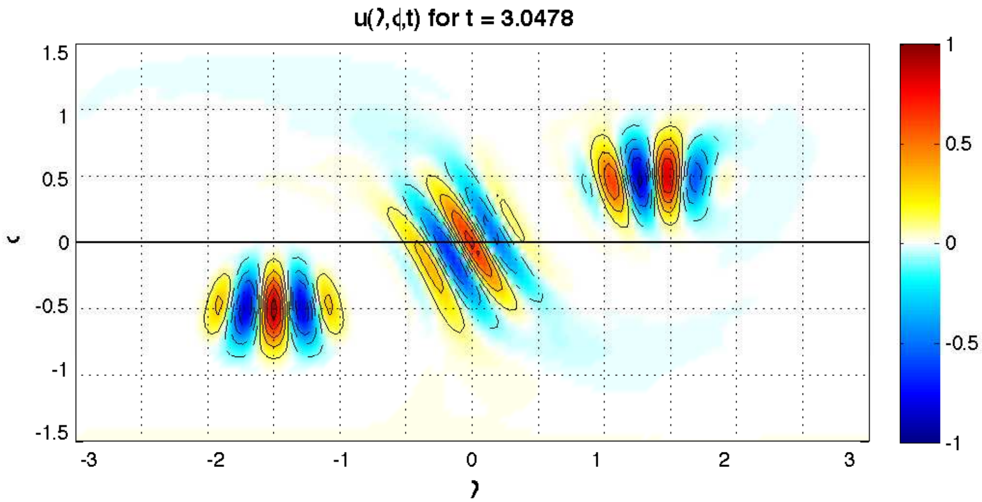
$$u_t = \nabla^2 u + f(\lambda, \phi)$$

  - initial condition: $u_0(\lambda, \phi, 0) = c_1 \{Y_{12}^{10}(\lambda, \phi) + \mathrm{conj}\}$
  - steady forcing, $f(\lambda, \phi)$ is rotated spherical harmonic: $c_2 \{Y_7^3(\lambda, \phi) + \mathrm{conj}\}$

- 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: *fftS.m* & *ifftS.m*
- 3$^{\mathrm{rd}}$-order accurate timestepping



Uni-Directional Wavepacket, $N = 64$

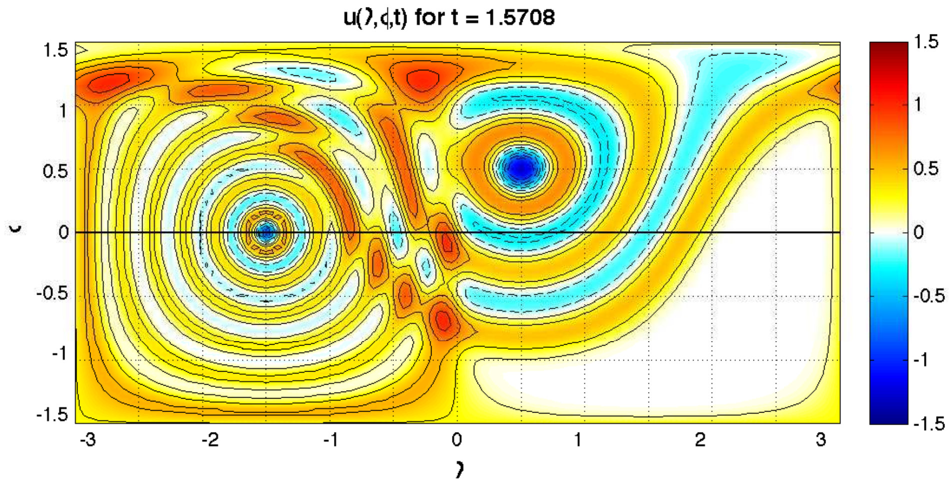
- propagation on sphere, $u(\lambda, \phi, t)$ & $v(\lambda, \phi, t)$

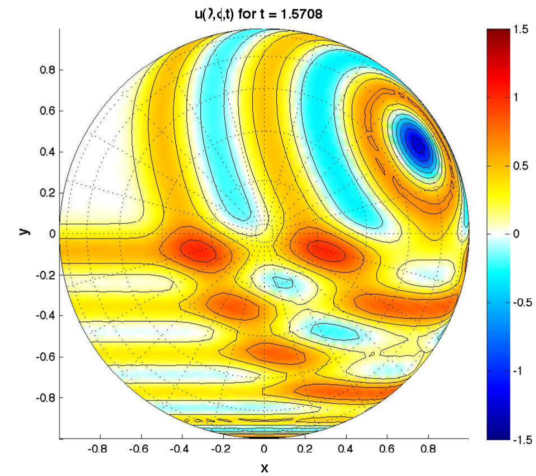
$$\begin{aligned} u_t &= v \\ v_t &= \nabla^2 u \end{aligned}$$

  - initial wavepacket: masked spherical harmonic, $u_0(\lambda, \phi) = c_1\{Y_{16}^{16}(\lambda, \phi) + \text{conj}\}$
  - propagation follows a great circle
  - wavespeeds $\longrightarrow 1^+$, in short wave limit

- 2^{nd}-order accurate timestepping scheme for stability

demo04





Forced Waves, $N = 64$

- radiation on the sphere, $u(\lambda, \phi, t)$ & $v(\lambda, \phi, t)$

$$\begin{aligned} u_t &= v \\ v_t &= \nabla^2 u + f_1(\lambda, \phi) \sin 24t + f_2(\lambda, \phi) \sin 12t \end{aligned}$$

  - 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 λ-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 . . .
  - Orszag (1986), Jakob-Chien/Alpert (1997), Suda/Takami (2001)

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."

Spatial 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

$$u_t \quad - \quad \nabla^2 u \quad = \quad f(\lambda, \phi, t)$$

- spectral equation

$$\frac{d}{dt}\tilde{u}_{nm} + (m^2 + n^2)\,\tilde{u}_{nm} \quad = \quad \tilde{f}_{nm}(t)$$

Fourier Timestepping Strategies

- integrating factor treats Laplacian exactly $\longrightarrow$ 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 $\longrightarrow$ 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

$$u(x,y,t) = \sum_m \sum_n (\tilde{u}_n)_m \, q_{nm}(\phi) \; e^{im\lambda}$$

- forced diffusion on sphere

$$\sin^2\phi \; u_t \quad - \quad \sin^2\phi \; \nabla^2 u \quad = \; \sin^2\phi \; f(\lambda,\phi,t)$$

- 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^{rd}-order BDF in time

$$[\sin^2\phi] \left\{ \frac{3(\tilde{u}_n)_m^{j+1} - 4(\tilde{u}_n)_m^{j} + (\tilde{u}_n)_m^{j-1}}{2\triangle t} \right\}$$

$$- \, [\sin^2\phi \; \nabla^2] \, (\tilde{u}_n)_m^{j+1} \quad = \quad [\sin^2\phi] \left\{ 2(\tilde{f}_n)_m^{j} - (\tilde{u}_n)_m^{j-1} \right\}$$

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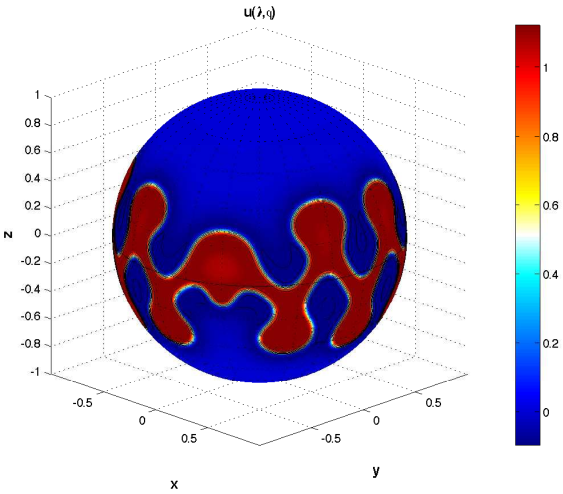
IMEX Scheme [Ascher, Ruuth, Wetton (1995)]

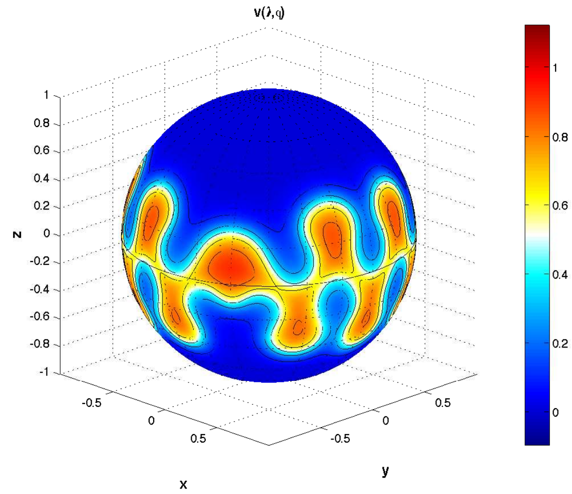
- 2^{rd}-order BDF in time

$$\left\{ \frac{3}{2\triangle t} [\sin^2\phi] - [\sin^2\phi \, \nabla^2] \right\} (\tilde{u}_n)_m^{j+1} \quad =$$

$$[\sin^2\phi] \left\{ \frac{4(\tilde{u}_n)_m^j - (\tilde{u}_n)_m^{j-1}}{2\triangle t} + 2(\tilde{f}_n)_m^j - (\tilde{u}_n)_m^{j-1} \right\}$$

Application: Fitz-Hugh Nagumo Equations





Pattern Formation & Front Dynamics, $N = 256$

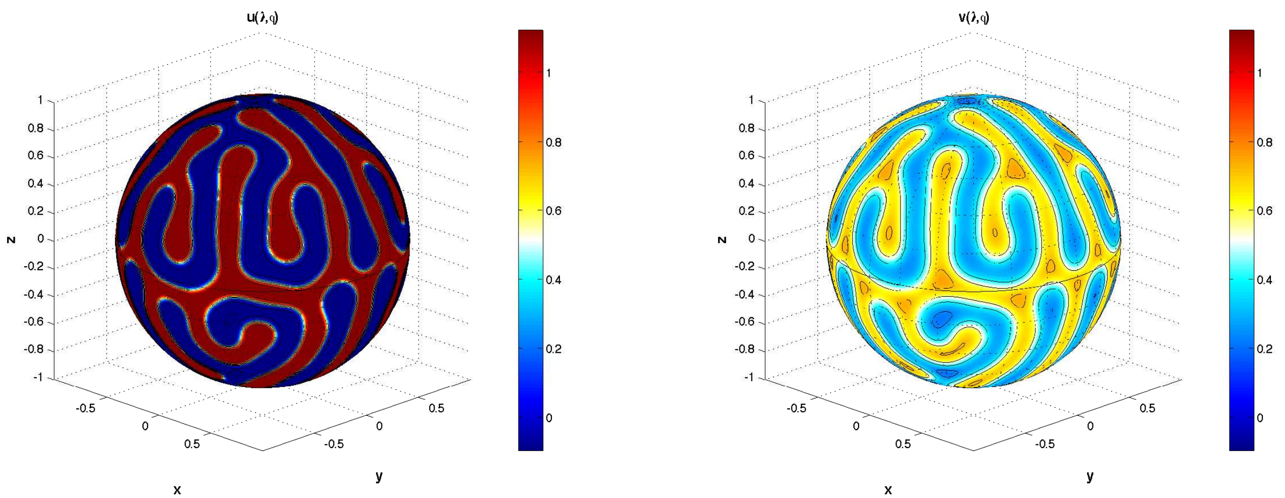
- ▷ bi-stable (0, 1) activator, $u(\lambda, \phi, t)$ & long-range inhibitor, $v(\lambda, \phi, t)$

$$u_t = \frac{\epsilon^2}{r^2} \nabla^2 u + u(u - a)(u - 1) + \rho\,(v - u)$$

$$0 = \frac{1}{r^2} \nabla^2 v + (v - u)$$

- ▷ labyrinth forming region in parameter space [Goldstein, DJM, Petrich, 1992]
  - ▷ $0 < \epsilon \ll 1 \ll$ r $\longrightarrow$ sharp fronts in u & large spherical domain
  - ▷ $0 < a - 1/2 \ll 1$ $\longrightarrow$ $u = 0, 1$ bistability with weak bias to red
  - ▷ $0 < \rho \ll 1$ $\longrightarrow$ weak inhibition producing blue

Application: Fitz-Hugh Nagumo Equations



Pattern Formation & Front Dynamics, $N = 256$

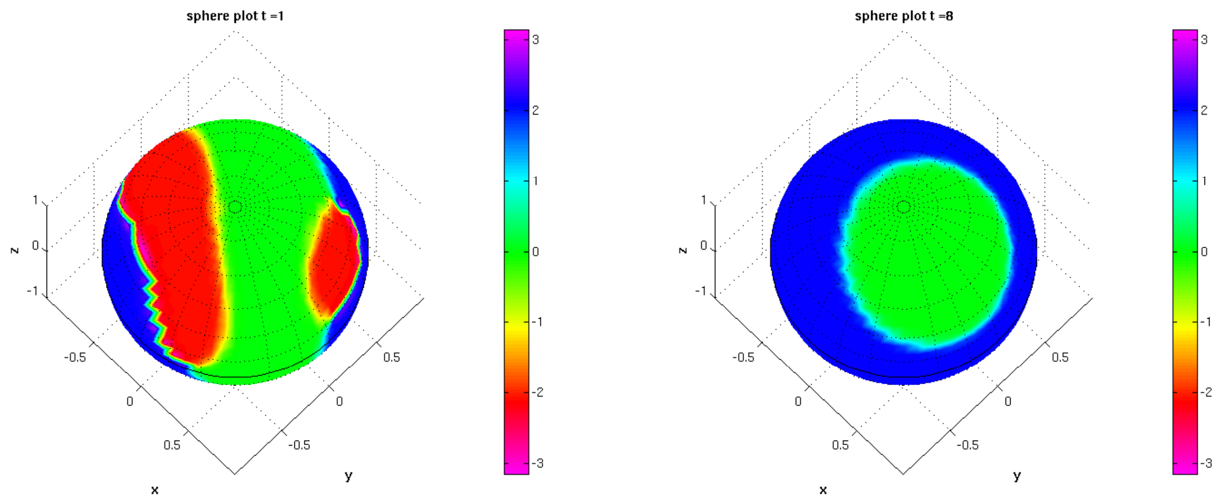
- bi-stable (0, 1) activator, $u(\lambda, \phi, t)$ & long-range inhibitor, $v(\lambda, \phi, t)$

$$u_t = \frac{\epsilon^2}{r^2} \nabla^2 u + u(u - a)(u - 1) + \rho\,(v - u)$$

$$0 = \frac{1}{r^2} \nabla^2 v + (v - u)$$

- labyrinth forming region in parameter space [Goldstein, DJM, Petrich, 1992]
  - $0 < \epsilon \ll 1 \ll$ r $\longrightarrow$ sharp fronts in u & large spherical domain
  - $0 < a - 1/2 \ll 1$ $\longrightarrow$ $u = 0, 1$ bistability with weak bias to red
  - $0 < \rho \ll 1$ $\longrightarrow$ weak inhibition producing blue

Application: Phase-Field Model



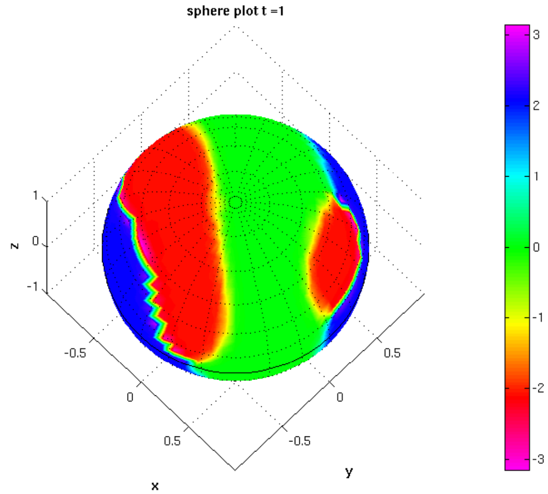
Diffusion Fronts & Triple Point Dynamics

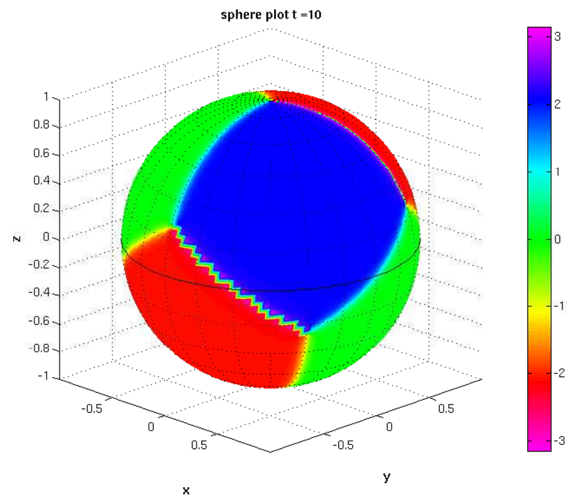
- complex-valued FFTs: $fftSc.m$ & $ifftSc.m$
- complex-valued gradient flow, $\psi(\lambda, \phi, t) \longrightarrow$ diffusion & tri-stability

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

  - ${z_j}^3 = 1 \quad \longrightarrow$ phases defined by 3 cube roots of unity
  - $0 < \epsilon \ll 1 \quad \longrightarrow$ sharp fronts separating phases
- slow drift of phase fronts $\longrightarrow$ conformity
- on the plane, steady boundary-supported 120° triple junctions [Bronsard/Reitich, 1993]

Application: Phase-Field Model





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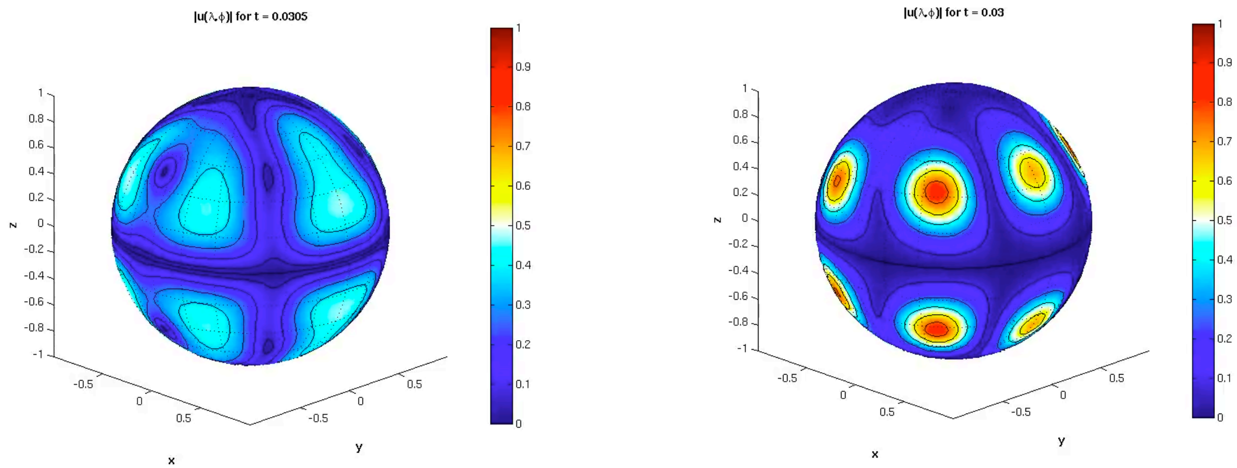
Application: Nonlinear Schrödinger Equation



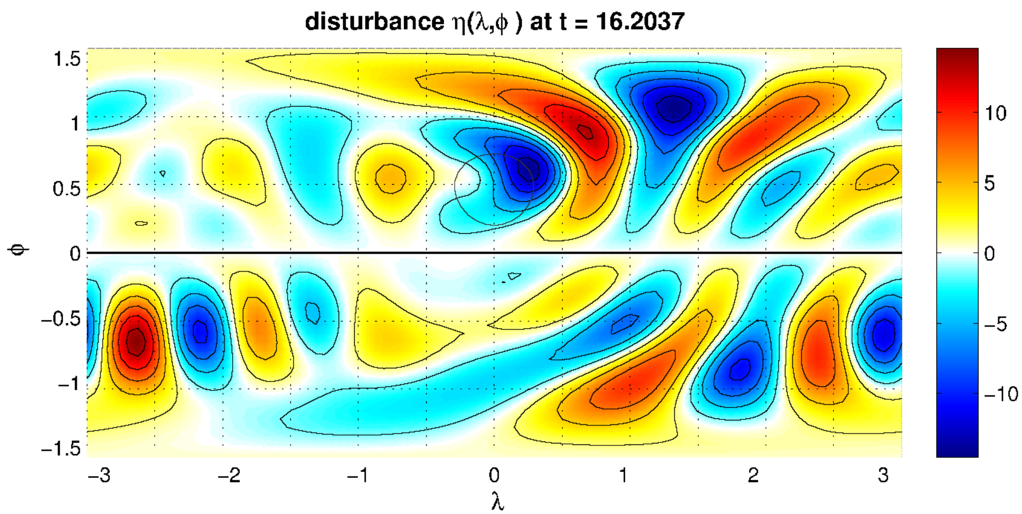
Waves with Dispersion & Nonlinearity

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

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

  - $-$ $\longrightarrow$ defocussing; $+$ $\longrightarrow$ focussing
- near spherical harmonic initial condition
- on the plane: singularity possible in focussing case

In Closing



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