UNIVERSITY OF OXFORD

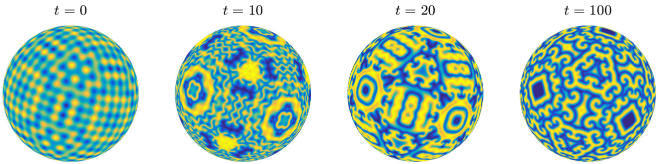
Fourth-order time-stepping for stiff PDEs on the sphere

Oxford Student SIAM Chapter 2017

Hadrien Montanelli and Yuji Nakatsukasa

May 17, 2017

$$u_t = 10^{-4}\Delta u + u - (1+1.5i)u|u|^2$$



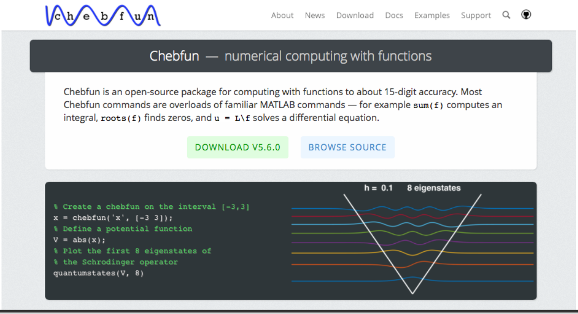
UNIVERSITY OF OXFORD

Introduction (1/3)

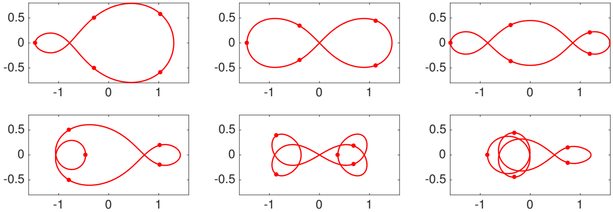
The code that produced those pictures

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

```
n = 1024;                                            % number of grid pts
h = 1e-1; tspan = [0 100];                           % time-step/time interval
S = spinopsphere(tspan);                             % initialize operator
S.lin = @(u) 1e-4*lap(u);                            % linear part
S.nonlin = @(u) u-(1+1.5i)*u.*abs(u).^2;             % nonlinear part
u0 = @(x,y,z) cos(40*x)+cos(40*y)+cos(40*z);
th = pi/8; c = cos(th); s = sin(th);
S.init = 1/3*spherefun(@(x,y,z) u0(c*x-s*z,y,s*x+c*z)); % initial condition
u = spinsphere(S, n, h);                             % solve
```



- A large number of phenomena in natural and social sciences exhibit periodicity
- These phenomena vary in time but recur at intervals: temporal periodicity



- Another type of periodicity is spatial periodicity: e.g., the sphere
- In both cases, periodicity is a feature that we can take advantage of for developing fast $\mathcal{O}(N \log N)$ algorithms

- **Problem:** Computing solutions of PDEs of the form

$$u_t = \alpha\Delta u + \mathcal{N}(u), \quad u(t=0,\lambda,\theta) = u_0(\lambda,\theta),$$

  e.g., Allen–Cahn, Ginzburg–Landau and Schrödinger equations, reaction-diffusion equations, ...

- **Method:** Double Fourier Sphere & implicit-explicit/exponential integrators

- **Why Double Fourier Sphere?** Spectral accuracy & $\mathcal{O}(N \log N)$ complexity

  $\rightarrow$ **our contribution:** a novel formulation to treat the pole singularity

- **Why implicit-explicit/exponential integrators?** Standard time-stepping schemes require very small time-steps

  $\rightarrow$ **our contribution:** a comparison of implicit-explicit/exponential integrators

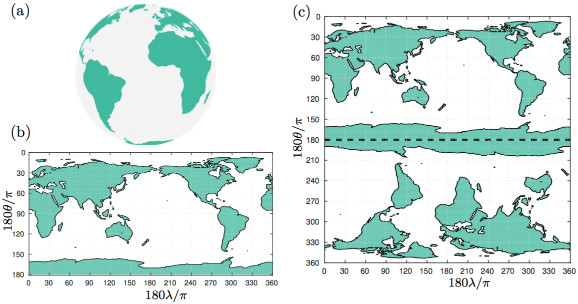
A Fourier spectral method in coefficient space (1/3)

Double Fourier Sphere method

- The Double Fourier Sphere method (1970s—Meriless, Orszag) uses longitude-colatitude coordinates,

$$x = \cos\lambda \sin\theta, \; y = \sin\lambda \sin\theta, \; z = \cos\theta, \quad (\lambda, \theta) \in [-\pi, \pi] \times [0, \pi]$$

- Functions $u(\lambda, \theta)$ on the sphere are 2π-periodic in λ but not periodic in θ
- Key idea: double up $u(\lambda, \theta)$ and flip it to make it periodic in both directions, and then use approximations with Fourier series



A Fourier spectral method in coefficient space (2/3)

The Laplacian matrix for $u_t = \alpha\Delta u + \mathcal{N}(u)$

- Functions are approximated by Fourier series,

$$u(t,\lambda,\theta) \approx \sum_{j=-m/2}^{m/2}{}' \sum_{k=-n/2}^{n/2}{}' \hat{u}_{jk}(t) e^{ij\theta} e^{ik\lambda}$$

- Laplace operator,

$$\Delta u = u_{\theta\theta} + \frac{\cos\theta\sin\theta}{\sin^2\theta} u_\theta + \frac{1}{\sin^2\theta} u_{\lambda\lambda},$$

  discretized with a matrix **L** that acts on Fourier coefficients

- **Problem**: Division by 0 at the poles
- **Remedy**: New matrix **L** that eliminates the modes $(1,1,\ldots)^T$ and $(-1,1,-1,1,\ldots)^T$, which correspond to the delta functions at 0 and π
- **Linear Algebra**: The matrix **L** can be inverted in $\mathcal{O}(N)$ operations

A Fourier spectral method in coefficient space (3/3)

Poisson's equation $\Delta u = f$

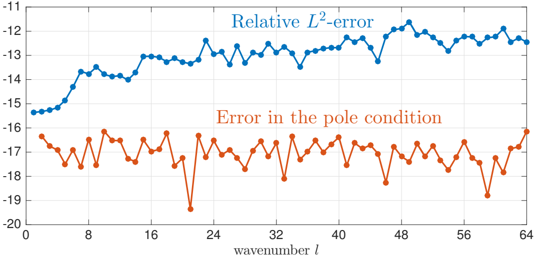
Poisson's equation:

$$\Delta u = f(\lambda,\theta), \quad (\lambda,\theta) \in [-\pi,\pi] \times [0,\pi],$$

$$\int_0^{\pi}\int_{-\pi}^{\pi} u(\lambda,\theta)\sin\theta d\lambda d\theta = 0,$$

on a 128×128 grid with right-hand sides

$$f_l(\lambda,\theta) = l(l+1)\sin^l\theta\cos(l\lambda) + (l+1)(l+2)\cos\theta\sin^l\theta\cos(l\lambda), \quad 1 \le l \le 64$$



Fourth-order time-stepping on the sphere (1/3)

Principle

- We want to solve $u_t = \alpha\Delta u + \mathcal{N}(u) \;\Rightarrow\; \hat{u}'(t) = \mathbf{L}\hat{u} + \mathbf{N}(\hat{u}),\; \mathbf{N}(\hat{u}) = \mathbf{F}\mathcal{N}(\mathbf{F}^{-1}\hat{u})$
- Large eigenvalues of $\mathbf{L}$: very small time-steps for standard time-stepping schemes
- **Exponential integrators (2000s—Cox, Matthews, Hochbruck, Ostermann, Kassam, Trefethen):** integrate $\mathbf{L}$ exactly with matrix exponential, numerical scheme for $\mathbf{N}$, e.g.,

$$\hat{u}^{n+1} = e^{h\mathbf{L}}\hat{u}^n + \mathbf{L}^{-1}(e^{h\mathbf{L}} - \mathbf{I})\mathbf{N}(\hat{u}^n)$$

  Dominant cost (per time-step): FFT $= \mathcal{O}(N\log N)$ for diffusive PDEs, matrix-vector products $= \mathcal{O}(N^{3/2})$ for dispersive PDEs

- **Implicit-explicit:** implicit formula for $\mathbf{L}$, explicit formula for $\mathbf{N}$, e.g.,

$$(3\mathbf{I} - 2h\mathbf{L})\hat{u}^{n+1} = 4\hat{u}^n - \hat{u}^{n-1} + 4h\mathbf{N}(\hat{u}^n) - 2h\mathbf{N}(\hat{u}^{n-1})$$

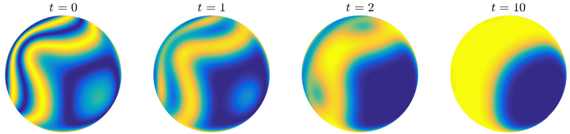
  Dominant cost (per time-step): FFT $= \mathcal{O}(N\log N)$

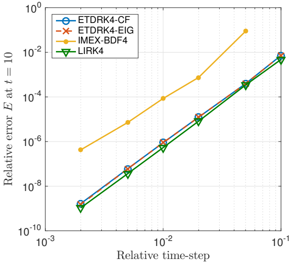
- **Comparisons**: two exponential integrators (ETDRK4-CF & ETDRK4-EIG) and two IMEX-schemes (IMEX-BDF4 & LIRK4)

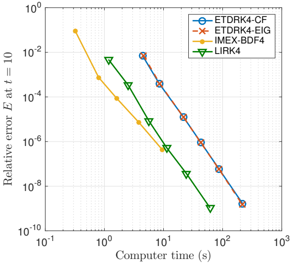
Fourth-order time-stepping on the sphere (2/3)

Numerical comparisons: diffusive case

Allen-Cahn: $$u_t = 10^{-2}\Delta u + u - u^3$$





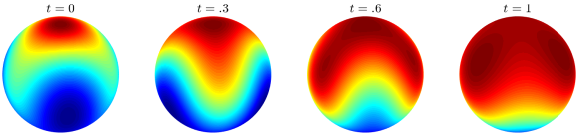


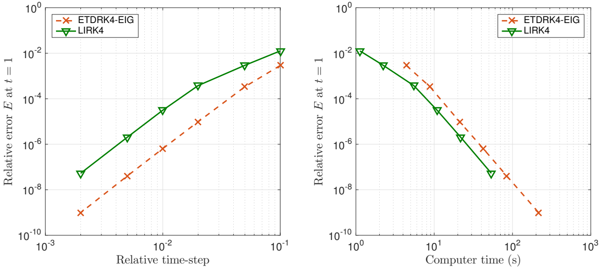
- **Left:** IMEX-BFD4 (yellow) on the left, i.e., the least accurate
- **Right:** IMEX-BFD4/LIRK4 on the left, i.e., the most efficient $\Rightarrow$ IMEX wins

Fourth-order time-stepping on the sphere (3/3)

Numerical comparisons: dispersive case

Nonlinear Schrödinger: $u_t = i\Delta u + iu|u|^2$





- **Left:** LIRK4 (green) on the left, i.e., the least accurate
- **Right:** LIRK4 on the left, i.e., the most efficient $\Rightarrow$ IMEX wins again

Conclusion

- Implicit-explicit + Double Fourier Sphere = $\mathcal{O}(N \log N)$
- Exponential integrators + Double Fourier Sphere = $\mathcal{O}(N \log N)$ or $\mathcal{O}(N^{3/2})$
- Implicit-explicit schemes outperform exponential integrators in both cases

	diffusive PDEs	**dispersive PDEs**
diagonal problems	$\mathcal{O}(N \log N)$	$\mathcal{O}(N \log N)$
	Exponential	Exponential
non-diagonal problems	$\mathcal{O}(N \log N)$	$\mathcal{O}(N \log N)$
fast sparse direct solver	Implicit-explicit	Implicit-explicit
non-diagonal problems	$\mathcal{O}(N^2)$	$\mathcal{O}(N^2)$
dense solver	TBD	TBD

- Future work includes hyperbolic equations, e.g., shallow-water equations