Columbia Engineering
The Fu Foundation School of Engineering and Applied Science

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

Numerical Analysis Research Club — September 21, 2017

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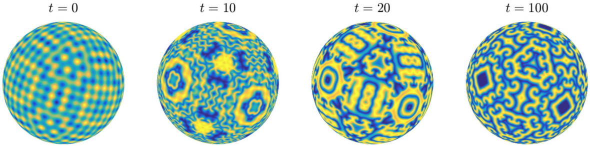
$$u_t = 10^{-4}\Delta u + u - (1+1.5i)u|u|^2$$

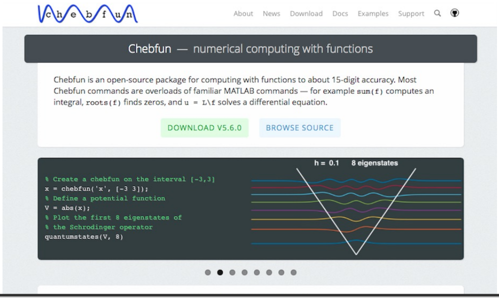


Introduction (1/4)

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);             % initial cond.
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)); % rotated initial cond.
u = spinsphere(S, n, h);                                 % solve
```



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

Introduction (2/4)

Periodicity

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

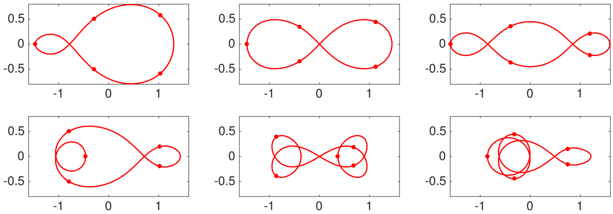


Figure : Choreographies of the n-body problem (Moore, Chenciner, Montgomery, Simó).

- Another type of periodicity is spatial periodicity (e.g., the sphere)
- In both cases, periodicity $\Rightarrow$ fast algorithms

- **Problem:** Computing solutions of stiff 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 and Ginzburg–Landau equations, reaction-diffusion equations, ...

- **Main application:** Pattern formation and dependence on curvature

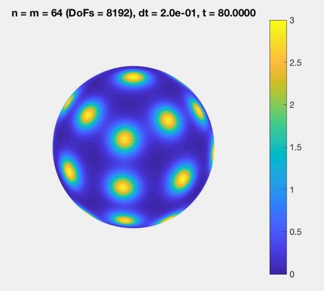


Figure : A spot solution of the Gierer–Meinhardt system in Chebfun.

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

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

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

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

  our contribution: a novel formulation to treat the pole singularity

- **Why implicit-explicit/exponential integrators?** Stiffness

  our contribution: a comparison of implicit-explicit/exponential integrators

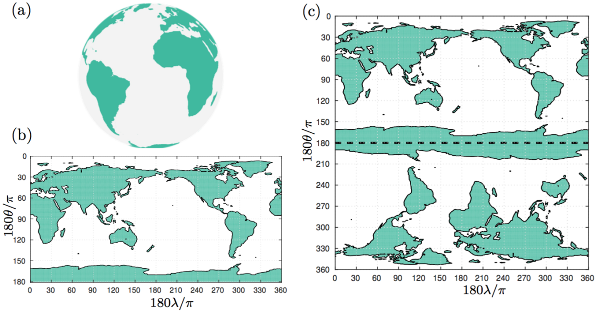
A novel Fourier spectral method (1/3)

Double Fourier Sphere method

- The Double Fourier Sphere method (Meriless, Orszag, Townsend et al.) uses

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

- Functions on the sphere are 2π-periodic in λ but not periodic in θ
- **Key idea:** double up and flip



A novel Fourier spectral method (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

- **Issue:** Division by 0 at the poles
- **Remedy:** Eliminate the singular modes $(1,1,\ldots)^T$ and $(-1,1,-1,1,\ldots)^T$
- Mathematically, truncation as opposed to interpolation
- **Linear Algebra:** Matrix **L** has real and ≤ 0 eigenvalues, can be inverted in $\mathcal{O}(N)$

A novel Fourier spectral method (3/3)

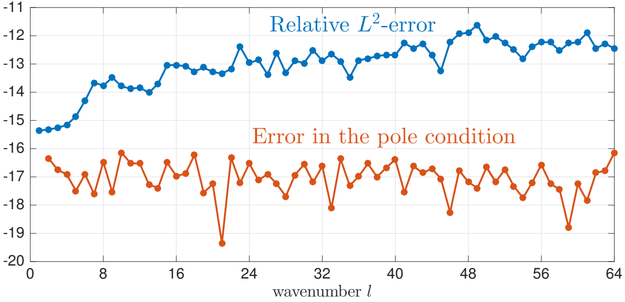
Poisson's equation $\Delta u = f$

Poisson's equation:

$$\Delta u = f_l(\lambda, \theta),$$

on a 128×128 grid with

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



Fourth-order time-stepping (1/3)

Principle

- The PDE $u_t = \alpha\Delta u + \mathcal{N}(u)$ becomes a system of ODEs $\hat{u}'(t) = \mathbf{L}\hat{u} + \mathbf{N}(\hat{u})$

- **Issue:** Stiffness, large eigenvalues of $\mathbf{L}$ forces very small time-steps

- **Remedy:** Exponential integrators and implicit-explicit schemes

- **Exponential integrators (Cox, Matthews, Hochbruck, Ostermann, Kassam):** 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: $\mathcal{O}(N\log N)$ for diffusive, $\mathcal{O}(N^{3/2})$ for dispersive PDEs

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

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

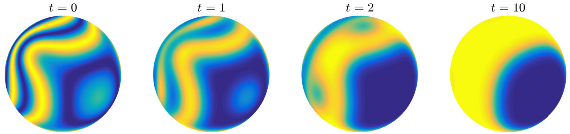
  Dominant cost: $\mathcal{O}(N\log N)$

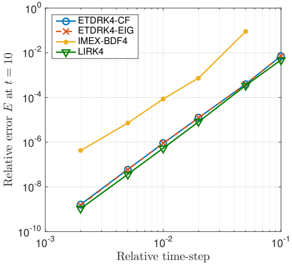
- **Comparisons**: ETDRK4 and two implicit-explicit (IMEX-BDF4 & LIRK4)

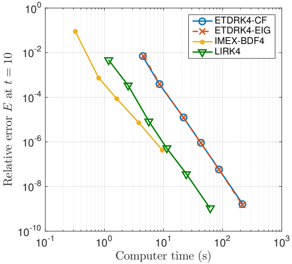
Fourth-order time-stepping (2/3)

Numerical comparisons: diffusive case

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





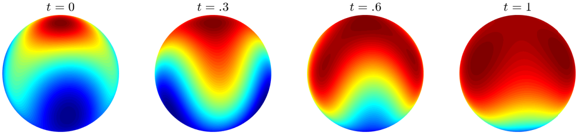


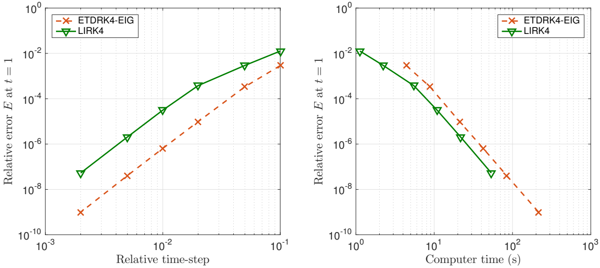
- **Left:** IMEX-BFD4 (yellow) on the left ⇒ the least accurate
- **Right:** IMEX-BFD4 on the left ⇒ the most efficient: implicit-explicit wins

Fourth-order time-stepping (3/3)

Numerical comparisons: dispersive case

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





- **Left:** LIRK4 (green) on the left ⇒ the least accurate
- **Right:** LIRK4 on the left ⇒ the most efficient: implicit-explicit wins again

Conclusions

- 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 wok (1/2)

Barotropic vorticity equation on the sphere

- **Problem:** Solve the barotropic vorticity equation,

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

- **Method:** Double Fourier Sphere with EPIRK schemes (Tokman, Rainwater), e.g.,

$$\hat{u}^{n+1} = \hat{u}^n + \mathbf{J}^{-1}(e^{h\mathbf{J}} - \mathbf{I})\mathbf{N}(\hat{u}^n), \quad \mathbf{J} = \frac{d\mathbf{N}}{d\hat{u}}(\hat{u}),$$

  with Arnoldi iteration for fast $\mathcal{O}(N\log N)$ matrix exponential evaluations

- **Issues:** Solutions might not be smooth and need for local refinement

- **Remedies:** Hyperviscosity and low-rank approximations

Future wok (2/2)

Nonlocal PDEs on the sphere

$$\mathcal{L}_\delta u(\lambda,\theta) = \iint\limits_{\gamma(\sigma,\tau,\lambda,\theta)\leq\delta} \rho_\delta(\gamma)\sin\tau\left[u(\lambda+\sigma,\theta+\tau) - u(\lambda,\theta)\right] d\sigma d\tau$$

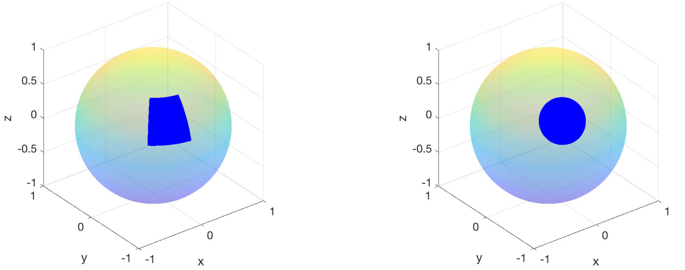


Figure : "Maximum coordinate" (left) and great-circle (right) distances.