UNIVERSITY OF OXFORD

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

Seminar of Numerical Analysis, MATHICSE, EPFL

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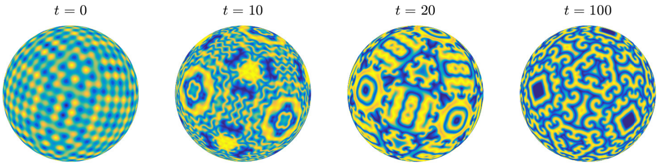
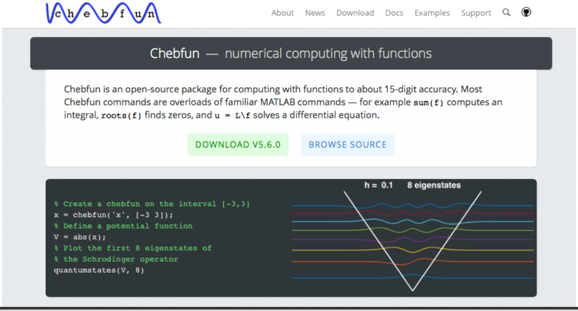
$$u_t = 10^{-4}\Delta u + u - (1 + 1.5i)u|u|^2$$



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
```



Introduction (2/4)

The Numerical Analysis group at Oxford

Numerical Analysis Group (Prof.): Nick Trefethen, Endre Süli, Andrew Wathen, Jared Tanner, Coralia Cartis, Patrick Farrell, Raphael Hauser, Gunnar Martinsson

- **Problem:** Computing smooth solutions of stiff PDEs on the unit sphere of the form

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

- **Aim:** Spectral accuracy in space and fourth-order time-stepping
- **Method:** Double Fourier Sphere method and implicit-explicit schemes
- **Why Double Fourier Sphere?** Spherical harmonics is $O(N^{3/2})$, RBFs is $O(N^2)$ while Double Fourier Sphere is $O(N\log N)$ $\rightarrow$ **our contribution:** a novel formulation in coefficient space to treat the pole singularity
- **Why Implicit-explicit?** We approached this assuming exponential integrators was the way to go—something surprising turned up $\rightarrow$ **our contribution:** a practical comparison of implicit-explicit schemes and exponential integrators
- **Applications:** Allen–Cahn, nonlinear Schrödinger and Ginzburg–Landau equations, reaction-diffusion equations and pattern formation on the sphere

- **Problem:** Computing smooth solutions of stiff PDEs on the unit sphere of the form

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

- **Space discretization:** A variant of the Double Fourier Sphere method in coefficient space

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

Leads to a system of $N = nm$ ODEs for $\hat{u}(t) = \{\hat{u}_{jk}(t)\}$

$$\hat{u}'(t) = \alpha\mathbf{L}\hat{u} + \mathbf{N}(\hat{u}), \quad \hat{u}(0) = \hat{u}(0)$$

- **Time discretization:** Exponential integrators and implicit-explicit schemes
- **Advantages:**

Novel multiplication matrices in coefficient space: no pole singularity

Implicit-explicit/exponential integrators: no severe restrictions on the time-steps

Special structure of the discrete Laplacian: $O(N\log N)$ complexity

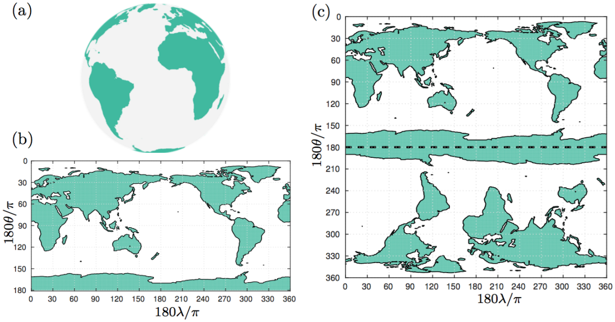
A Fourier spectral method in coefficient space (1/5)

The Double Fourier Sphere method

- The Double Fourier Sphere method (1970s—Meriless, Orszag, Boyd, Townsend et al.) uses the longitude-latitude coordinate transforms,

$$x = \cos\lambda\sin\theta,\ y = \sin\lambda\sin\theta,\ z = \cos\theta,$$

  with $(\lambda, \theta) \in [-\pi, \pi] \times [0, \pi]$
- 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



A Fourier spectral method in coefficient space (2/5)

The Laplacian matrix

- We want to solve $u_t = \alpha\Delta u + \mathcal{N}(u)$ with

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

- The DFS method leads to a system of nm ODEs for $\hat{u}(t) = \{\hat{u}_{jk}(t)\}$,

$$\hat{u}'(t) = \alpha\mathbf{L}\hat{u} + \mathbf{N}(\hat{u}), \quad \mathbf{L} = \mathbf{I}_n \otimes (\mathbf{D}_m^2 + \mathbf{T}_{\sin^2}^{-1}\mathbf{T}_{\cos\sin}\mathbf{D}_m) + \mathbf{D}_n^2 \otimes (\mathbf{T}_{\sin^2}^{-1}),$$

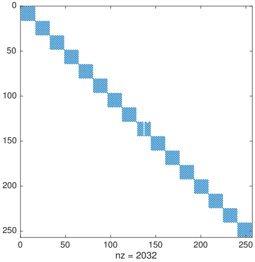
$$\mathbf{N}(\hat{u}) = \mathbf{F}\mathcal{N}(\mathbf{F}^{-1}\hat{u})$$

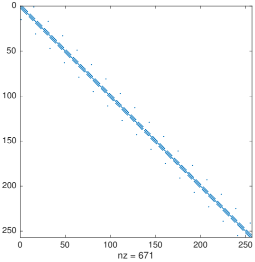
- In value space: $\mathbf{M}_{\sin^2}^{v}$ is diagonal zeros at $\theta = 0, \pi \Rightarrow$ singular
- In coefficient space: $\mathbf{M}_{\sin^2} = \mathbf{F}\mathbf{M}_{\sin^2}^{v}\mathbf{F}^{-1} \Rightarrow$ singular
- New matrix in coefficient space: $\mathbf{T}_{\sin^2} = Q\mathbf{M}_{\sin^2}P \Rightarrow$ nonsingular

A Fourier spectral method in coefficient space (3/5)

Sparsity pattern of the Laplacian matrix

- Sparsity patterns of $\mathbf{L}$ (left) and $\mathbf{T}_{\sin^2}\mathbf{L}$ (right) with $m = n = 16$:





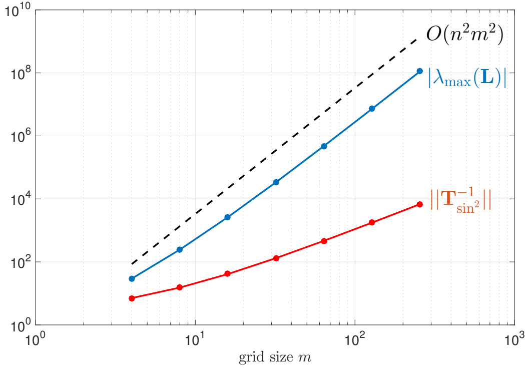
- Each $m \times m$ block of $\mathbf{L}$: dense
- Each $m \times m$ block of $\mathbf{T}_{\sin^2}\mathbf{L}$: pentadiagonal with two (near-)corner elements
- Consequence:

$$(z\mathbf{I} + h\mathbf{L})x = b$$

can be solved in $O(nm)$ operations since it is equivalent to solving

$$(z\mathbf{T}_{\sin^2} + h\mathbf{T}_{\sin^2}\mathbf{L})x = \mathbf{T}_{\sin^2} b$$

- Eigenvalues of the Laplacian operator: $-l(l+1)$ with integer $l \geq 0$
- Eigenvalues of the Laplacian matrix: real and nonpositive (Yuji Nakatsukasa)
- Largest in magnitude grows as $O(n^2 m^2)$



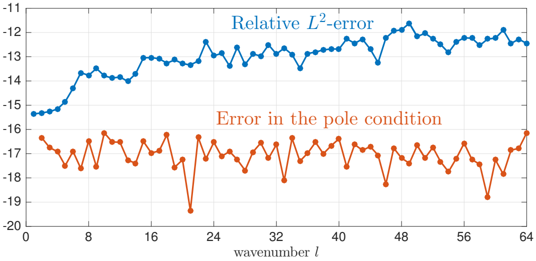
Poisson's equation

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

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

on a 128×128 grid with right-hand sides

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



Fourth-order time-stepping on the sphere (1/4)

Solving stiff systems of ODEs

- We want to use a fourth-order time-stepping algorithm for solving

$$\hat{u}'(t) = \mathbf{L}\hat{u} + \mathbf{N}(\hat{u}), \quad \hat{u}(0) = u_0 \qquad (\mathbf{L} = \alpha\mathbf{L})$$

- Large eigenvalues of **L**: severe restrictions for generic explicit schemes
- Remedy: Exponential integrators and implicit-explicit schemes
- Exponential integrators: integrate **L** exactly with matrix exp., numerical scheme for **N**, e.g.,

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

- Implicit-explicit: implicit formula for **L**, explicit formula for **N**, e.g.,

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

- Exponential integrators: 2000s—Hochbruck, Ostremann, Cox, Matthews, Tokman, Minchev, Trefethen, Kassam
- Survey paper under review (with Niall Bootland), compares 30 exp. integrators: hard to do much better than the ETDRK4 scheme of Cox and Matthews (2002)

ETDRK4 (Cox and Matthews, 2002)

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

$$\hat{b}^n = e^{h\mathbf{L}/2}\hat{u}^n + \mathbf{L}^{-1}(e^{h\mathbf{L}/2} - \mathbf{I})\mathbf{N}(\hat{a}^n)$$

$$\hat{c}^n = e^{h\mathbf{L}/2}\hat{a}^n + \mathbf{L}^{-1}(e^{h\mathbf{L}/2} - \mathbf{I})\left[2\mathbf{N}(\hat{b}^n) - \mathbf{N}(\hat{u}^n)\right]$$

$$\hat{u}^{n+1} = e^{h\mathbf{L}}\hat{u}^n + hf_1(h\mathbf{L})\mathbf{N}(\hat{u}^n) + hf_2(h\mathbf{L})\left[\mathbf{N}(\hat{a}^n) + \mathbf{N}(\hat{b}^n)\right] + hf_3(h\mathbf{L})\mathbf{N}(\hat{c}^n)$$

- In general: $O(nm^3)$ precomputation of $e^{h\mathbf{L}}$ ($\mathbf{L} = \mathbf{V}\Lambda\mathbf{V}^{-1}$ with $\mathrm{cond}(\mathbf{V}) < 100$), $O(nm^2)$ per time-step $\rightarrow$ **ETDRK4-EIG**
- Real eigenvalues ($\alpha \in \mathbb{R}$): no precomputation, matrix-vector products computed with Carathéodory–Fejér method, $O(nm \log nm)$ per time-step $\rightarrow$ **ETDRK4-CF**

Fourth-order time-stepping on the sphere (3/4)

Implicit-explicit schemes

- Implicit-explicit schemes: 1990s—Ascher, Ruuth, Wetton; 2000s—Pareshi, Russo, Calvo, de Frutos, Novo; 2010s—Cardone, Constatinescu, Sandu
- Four steps, stable for diffusive ($\alpha \in \mathbb{R}$) PDEs only:

$$\textbf{IMEX} - \textbf{BDF4} \qquad \begin{aligned}(25\mathbf{I} - 12h\mathbf{L})\hat{u}^{n+1} &= 48\hat{u}^{n} - 36\hat{u}^{n-1} + 16\hat{u}^{n-2} - 3\hat{u}^{n-3}\\ &+ 48h\mathbf{N}(\hat{u}^{n}) - 72h\mathbf{N}(\hat{u}^{n-1})\\ &+ 48h\mathbf{N}(\hat{u}^{n-2}) - 12h\mathbf{N}(\hat{u}^{n-3})\end{aligned}$$

- One step and six stages, stable for both diffusive and dispersive ($\alpha \in i\mathbb{R}$) PDEs:

LIRK4 (Calvo, de Frutos and Novo, 2001)

$$\begin{aligned}\hat{v}_1 &= \hat{u}^{n}\\ (\mathbf{I} - \tfrac{1}{4}h\mathbf{L})\hat{v}^{2} &= \hat{u}^{n} + \tfrac{1}{4}h\mathbf{N}(\hat{v}^{1})\\ (\mathbf{I} - \tfrac{1}{4}h\mathbf{L})\hat{v}^{3} &= \hat{u}^{n} + \tfrac{1}{2}h\mathbf{L}\hat{v}^{2} - \tfrac{1}{4}h\mathbf{N}(\hat{v}^{1}) + h\mathbf{N}(\hat{v}^{2})\\ &\vdots\\ \hat{u}^{n+1} &= \hat{u}^{n} + h\sum_{i=1}^{6} b_i\mathbf{L}\hat{v}^{i} + h\sum_{i=1}^{6} \tilde{b}_i\mathbf{N}(\hat{v}^{i})\end{aligned}$$

- For both: $O(nm \log nm)$ cost per time-step

Fourth-order time-stepping on the sphere (4/4)

Computational costs

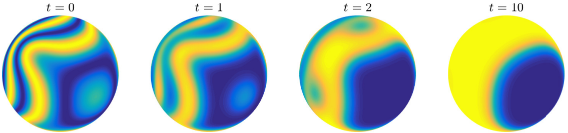
	Exponential integrators		Implicit-explicit	
	ETDRK4-CF	ETDRK4-EIG	IMEX-BDF4	LIRK4
# $O(nm \log nm)$ FFTs	8	8	2	12
# $O(nm)$ linear solves	$9p = 108$	0	1	5
# $O(nm^2)$ matrix-vector prod.	0	9	0	0
diffusive PDEs	✓	✓	✓	✓
dispersive PDEs	×	✓	×	✓

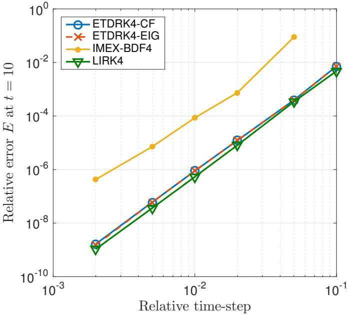
Numerical comparisons (1/2)

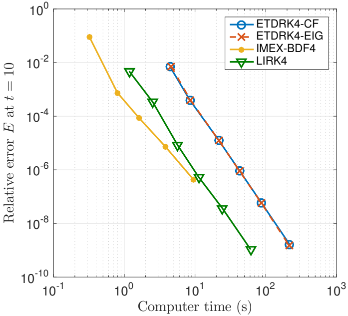
Diffusive case

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

up to $t = 10$ with $m = n = 256$ and $u(t=0,x,y,z) = \cos(\cosh(5xz) - 10y)$





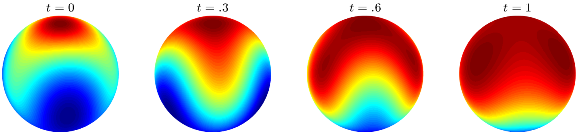


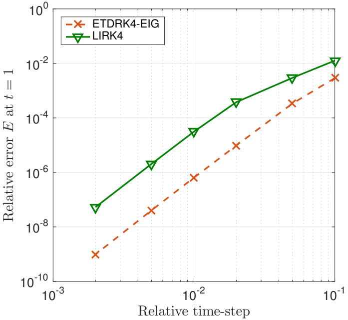
Numerical comparisons (2/2)

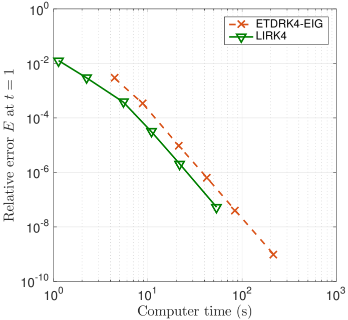
Dispersive case

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

up to $t = 1$ with $m = n = 256$ and $u(t = 0, \lambda, \theta) = 2/(2 - \sqrt{2}\cos(\theta)) - 1 + Y_3^3(\lambda, \theta)$







Conclusion

- Exponential integrators/implicit-explicit with Double Fourier Sphere method: $O(N \log N)$ for diffusive PDEs
- Exponential integrators are $O(N^{3/2})$ for dispersive PDEs
- Implicit-explicit schemes outperform exponential integrators in both cases

	diffusive PDEs	dispersive PDEs
diagonal problems	$O(N \log N)$ ETDRK4	$O(N \log N)$ ETDRK4
non-diagonal problems fast sparse direct solver	$O(N \log N)$ IMEX-BDF4	$O(N \log N)$ LIRK4
non-diagonal problems dense solver	$O(N^2)$ TBD	$O(N^2)$ TBD

- Future work includes hyperbolic PDEs, e.g., barotropic vorticity equation

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

with Double Fourier Sphere plus Jacobian-based exponential integrators, e.g.,

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