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

PDEs on the Sphere 2017, ENS Ulm

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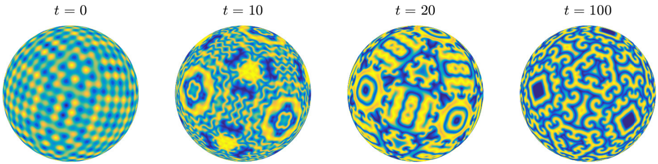
$$u_t = 10^{-4}\Delta u + u - (1 + 1.5i)u|u|^2$$

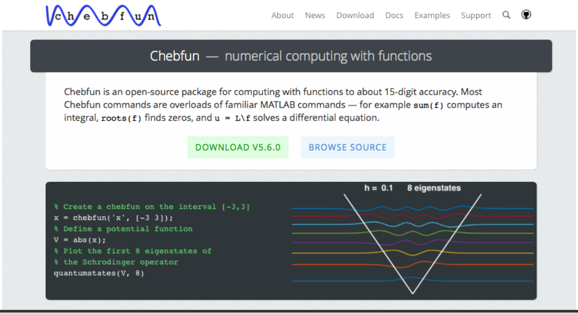


Introduction (1/3)

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
```



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

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

This includes the Allen–Cahn ($\mathcal{L} = \epsilon\Delta$, $\mathcal{N}(u) = u - u^3$) and Schrödinger ($\mathcal{L} = i\Delta$, $\mathcal{N}(u) = iu|u|^2$) equations, reaction-diffusion equations, and the barotropic vorticity equation ($\mathcal{L} = 0$),

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

- **Aim:** Spectral accuracy in space & fourth-order time-stepping
- **Method:** Double Fourier Sphere & implicit-explicit/exp integrators
- **Why Double Fourier Sphere?** $\mathcal{O}(N\log N)$ complexity
  $\rightarrow$ **our contribution:** a novel formulation to treat the pole singularity
- **Why implicit-explicit/exp integrators?** Clustering of points near the poles implies severe CFL restrictions for standard time-stepping schemes
  $\rightarrow$ **our contribution:** a comparison of implicit-explicit/exp integrators ($\mathcal{L} \neq 0$)

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

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

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

$$\hat{u}'(t) = \mathbf{L}\hat{u} + \mathbf{N}(\hat{u}), \quad \hat{u}(0) = \hat{u}_0,$$

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

- **Time discretization:** implicit-explicit schemes and exponential integrators

- **Advantages:**

Novel multiplication matrices in coefficient space: no pole singularity

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

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

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

The Double Fourier Sphere method

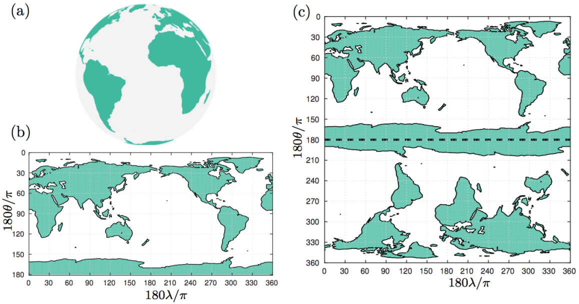
- The Double Fourier Sphere method (1970s—Meriless, Orszag, Boyd, Townsend et al.) uses the longitude-colatitude coordinate transforms,

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

  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 (2/3)

The Laplacian matrix

- The Laplacian operator,

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

  appears in the linear (e.g., Allen–Cahn) or nonlinear part (e.g., barotropic)

- Using Fourier matrices and Kronecker products it can be discretized with

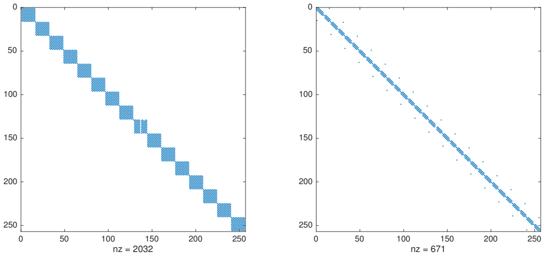
$$\mathbf{L} = \mathbf{I}_n \otimes \left(\mathbf{D}_m^2 + \mathbf{T}_{\sin^2}^{-1}\mathbf{T}_{\cos\sin}\mathbf{D}_m\right) + \mathbf{D}_n^2 \otimes \mathbf{T}_{\sin^2}^{-1}$$

- In value space: $\mathbf{M}^v_{\sin^2}$ is diagonal with zeros at $\theta = 0, \pi \Rightarrow$ singular
- In coefficient space: $\mathbf{M}_{\sin^2} = \mathbf{F}\mathbf{M}^v_{\sin^2}\mathbf{F}^{-1} \Rightarrow$ singular
- New matrix in coefficient space: $\mathbf{T}_{\sin^2} = Q\mathbf{M}_{\sin^2}P \Rightarrow$ nonsingular
- This matrix truncates the extreme wavenumbers to eliminate the modes $(1, 1, \ldots)^T$ and $(-1, 1, -1, 1, \ldots)^T$, which correspond to the nullspace

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

Sparsity pattern of the Laplacian matrix

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



- Each block of $\mathbf{L}$: dense
- Each 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 $\mathcal{O}(N)$ operations since it is equivalent to solving

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

Fourth-order time-stepping on the sphere for $\mathcal{L} \neq 0$ (1/3)
Principle

- We want to solve $u_t = \mathcal{L}u + \mathcal{N}(u) \;\Rightarrow\; \hat{u}'(t) = \mathbf{L}\hat{u} + \mathbf{N}(\hat{u})$
- Large eigenvalues of $\mathbf{L}$: severe restrictions for generic explicit 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): matrix-vector products with $e^{h\mathbf{L}} = \mathcal{O}(N^{3/2})$

  (unless $\mathbf{L}$ has real eigenvalues: reduces to $\mathcal{O}(N\log N)$ using CF method)

- **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 $= \mathcal{O}(N\log N)$

- Key observation: in both cases smoothness at the poles is preserved

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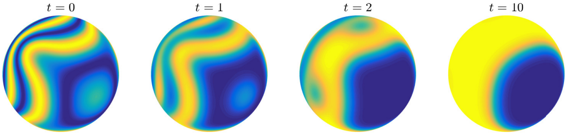
Fourth-order time-stepping on the sphere for $\mathcal{L} \neq 0$ (2/3)

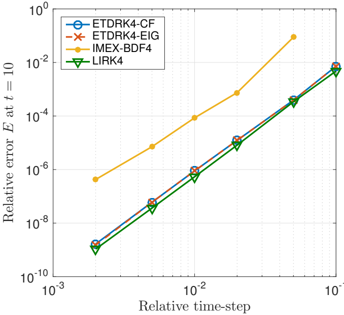
Numerical comparisons: diffusive case

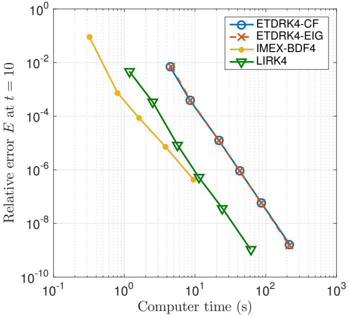
Allen-Cahn:

$$u_t = 10^{-2}\Delta u + u - u^3,$$

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



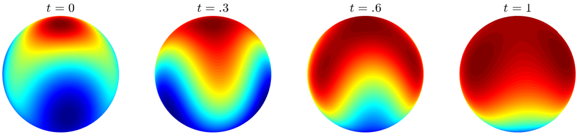


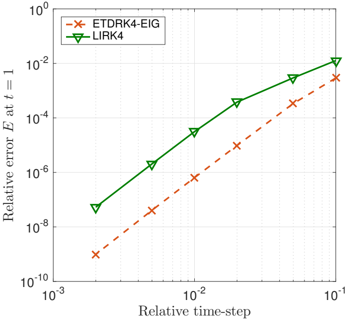


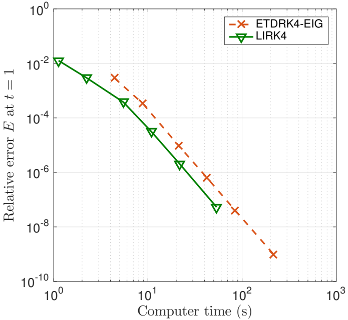
Fourth-order time-stepping on the sphere for $\mathcal{L} \neq 0$ (3/3)

Numerical comparisons: dispersive case

Nonlinear Schrödinger: $$u_t = i\Delta u + iu|u|^2,$$
up to $t = 1$ with $m = n = 256$ and $u(t=0,\lambda,\theta) = 2/(2-\sqrt{2}\cos(\theta)) - 1 + Y_3^3(\lambda,\theta)$







Fourth-order time-stepping on the sphere for $\mathcal{L} = 0$ (1/2)

Principle

- We want to solve $u_t = \mathcal{N}(u) \;\Rightarrow\; \hat{u}'(t) = \mathbf{N}(\hat{u})$
- **Jacobian-based exp integrators (2000s—Tokman):** linearize and apply the exponential on the Jacobian, e.g.,

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

  with closed-form expressions for the Jacobian $\mathbf{J}^n$

- **Dominant cost:** matrix-vector products with $e^{h\mathbf{J}^n} = \mathcal{O}(N \log N)$ with Arnoldi
- Key observation: smoothness at the poles not necessarily preserved
- Remedy: fast $\mathcal{O}(N \log N)$ spherical harmonic-like filter using the FFT

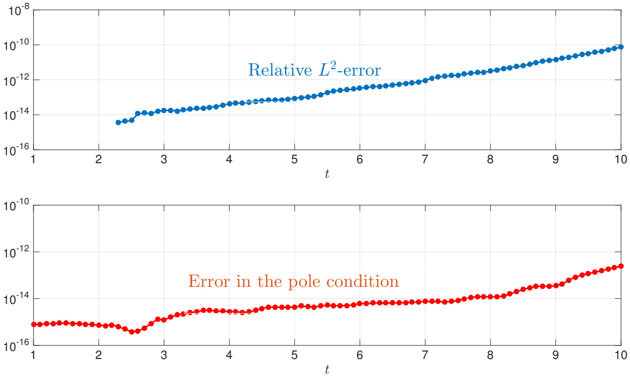
Fourth-order time-stepping on the sphere for $\mathcal{L} = 0$ (2/2)

Numerical example: Rossby–Haurwitz wave

Barotropic vorticity equation:

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

up to $t = 10$ with $m = n = 32$ and $u(t = 0, \lambda, \theta) = \frac{2\pi}{7}\cos\theta + 30\cos\theta\sin^4\theta\cos 4\lambda$



Conclusion

- For $\mathcal{L} \neq 0$: implicit-explicit + Double Fourier Sphere method $= \mathcal{O}(N \log N)$
- Exp integrators are $\mathcal{O}(N^{3/2})$ for dispersive PDEs
- Implicit-explicit schemes outperform exponential integrators in both cases

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

- For $\mathcal{L} = 0$: Jacobian-based exp integrators + FFT harmonic filter $= \mathcal{O}(N \log N)$
- Future work includes generalization to the shallow-water equations with low-rank approximations for local refinement