1: Introduction to spectral methods & Dedalus

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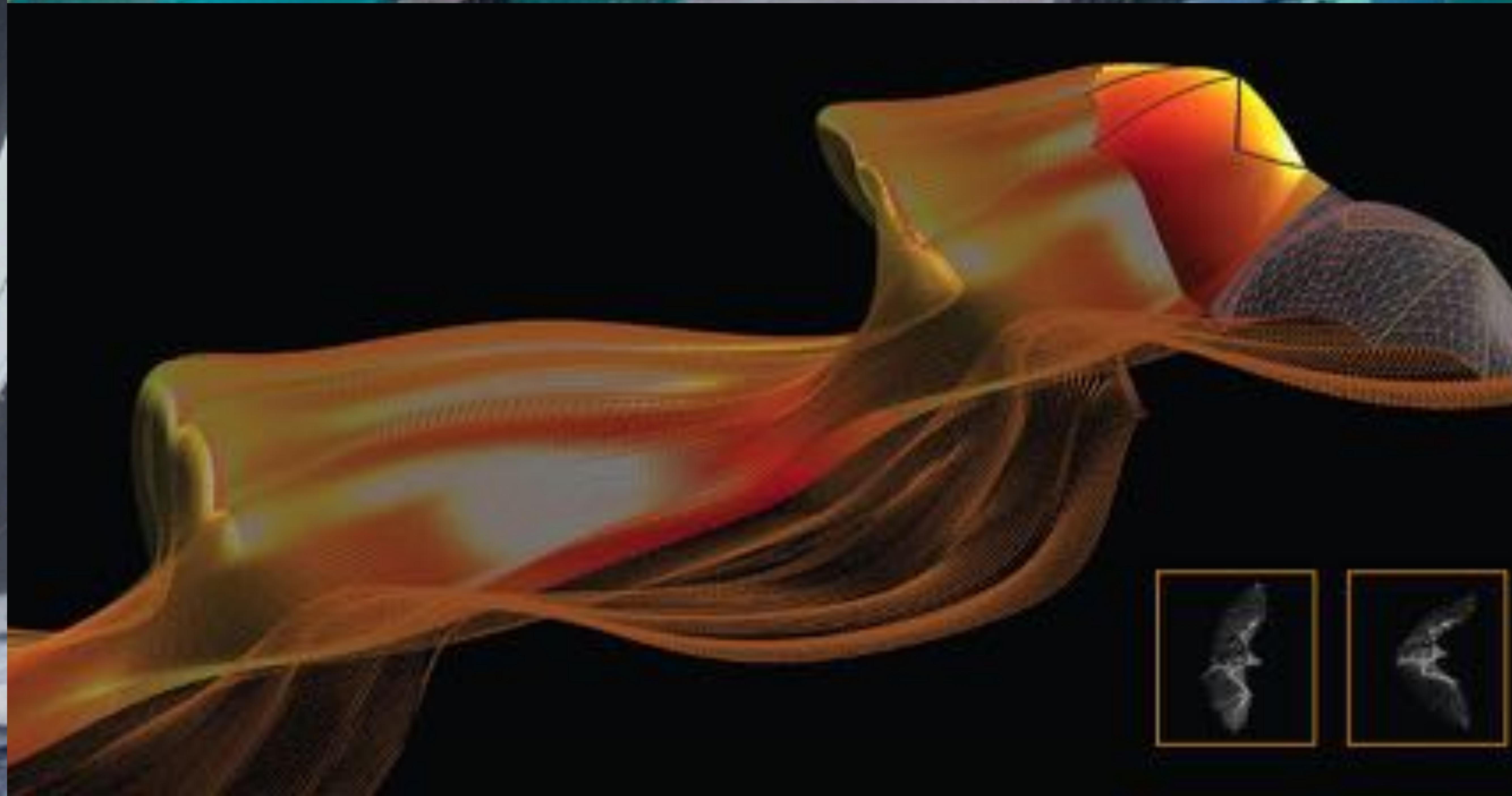
CISM Udine 2023

PDEs across science & engineering

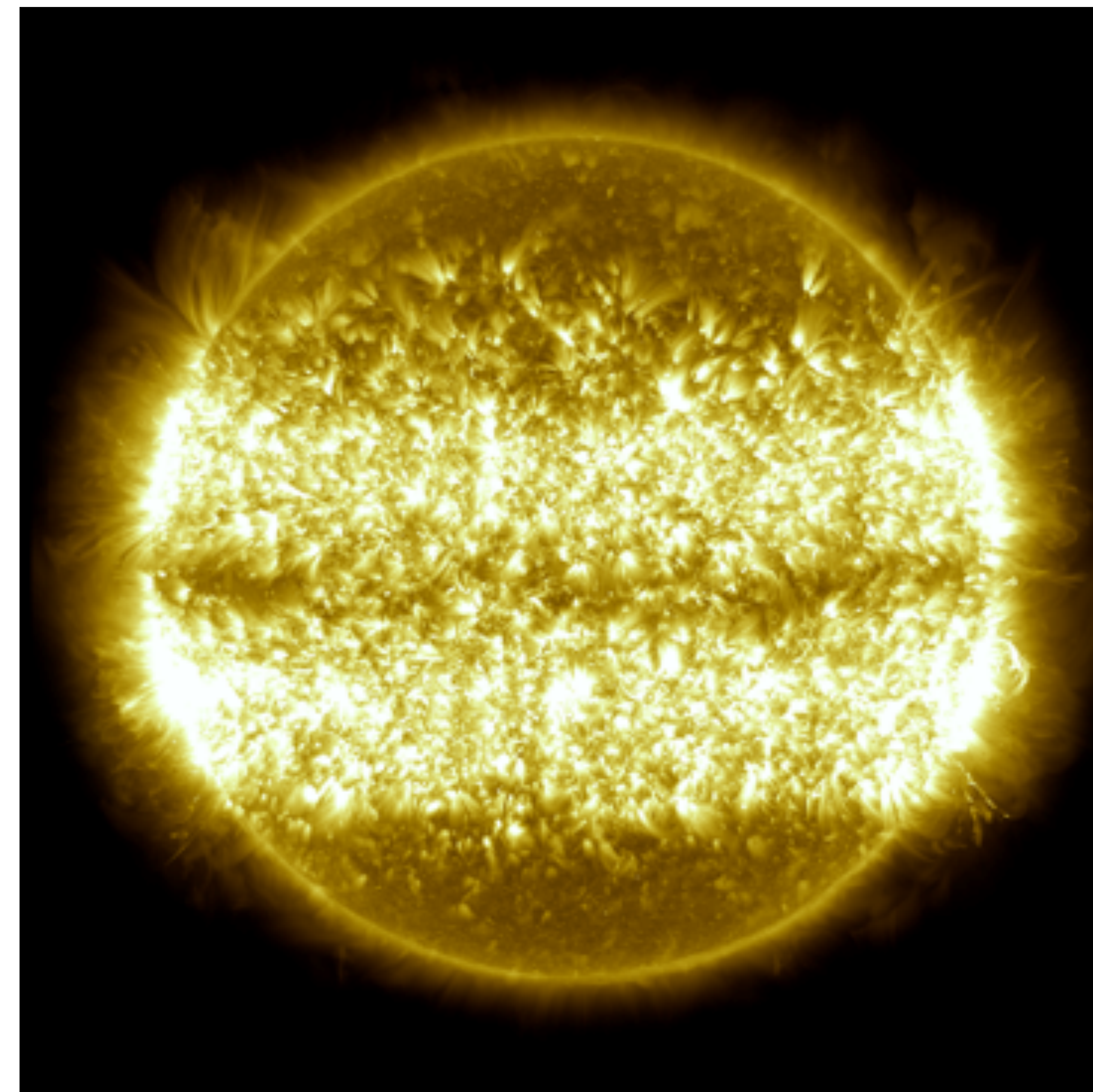


PDEs across science & engineering

Belousov–Zhabotinsky reaction

(Stephen Morris)

Solar convection



(NASA/SDO)

Scientific solvers: fast but narrowly focused

Design goals:

- Realistic parameters
- Maximum performance

Common limitations:

- Low-order methods
- Hard-coded models
- Difficult to modify

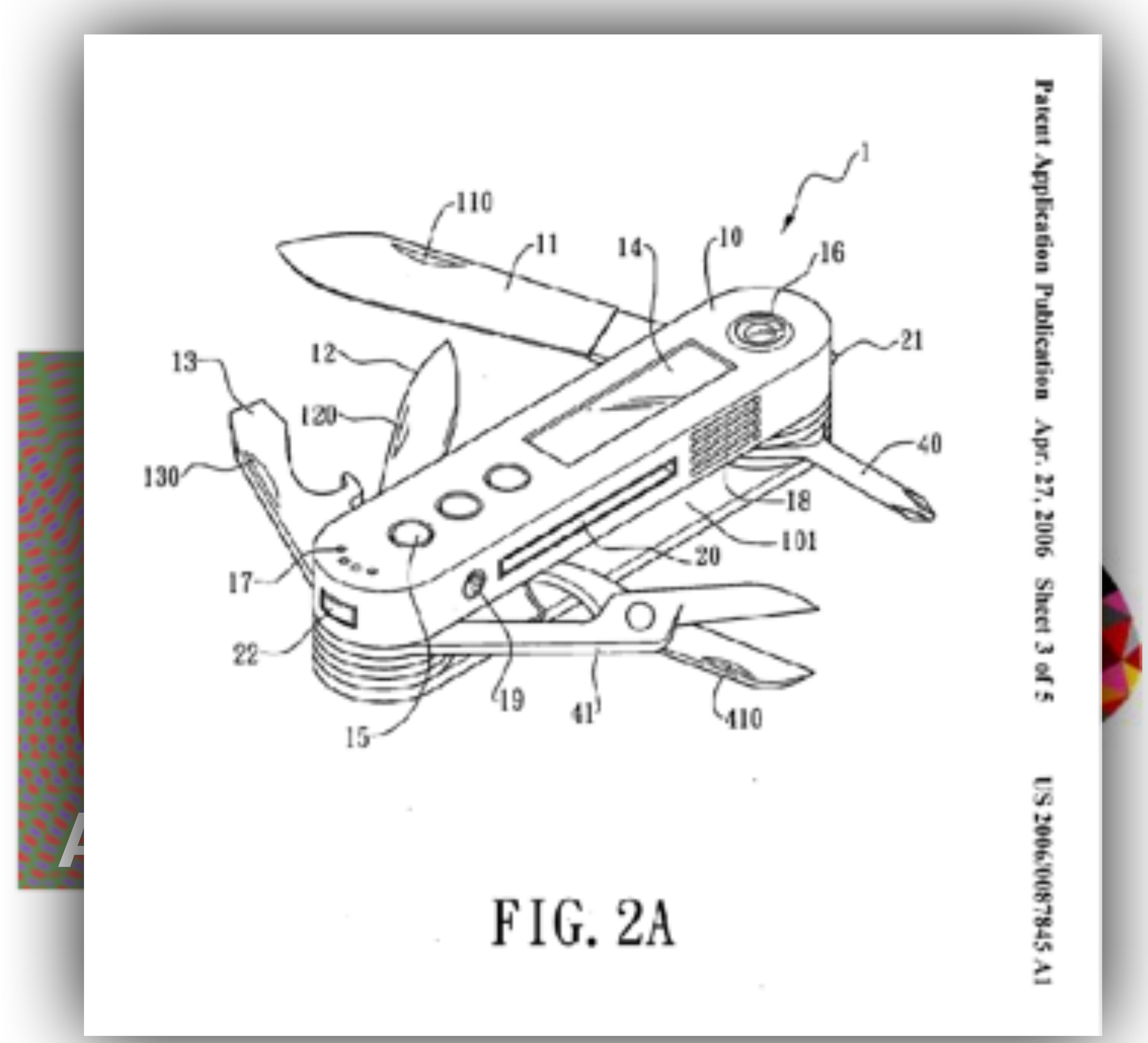
Mathematical solvers: flexible but slow

Design goals:

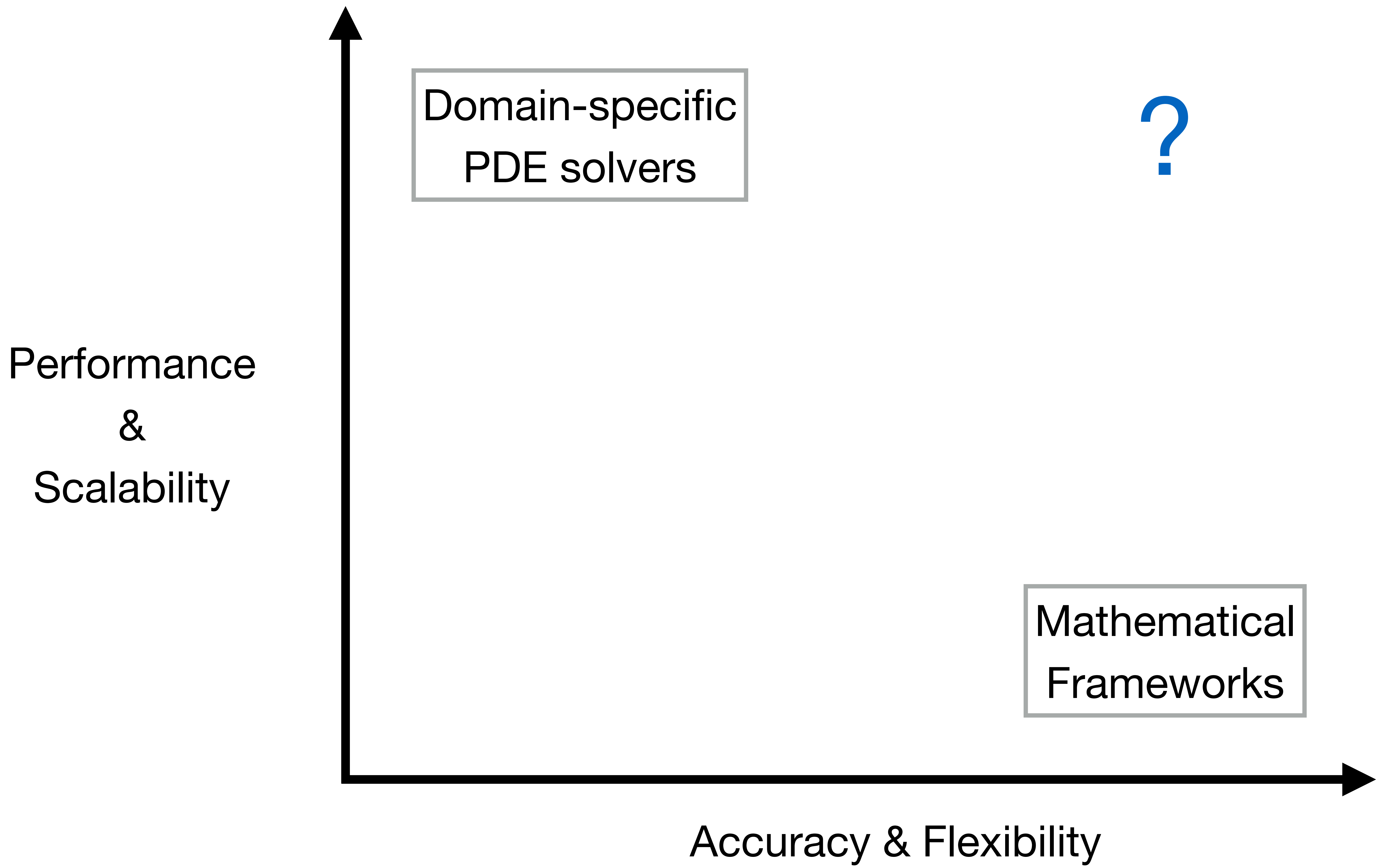
- Newest methods
- High accuracy

Common limitations:

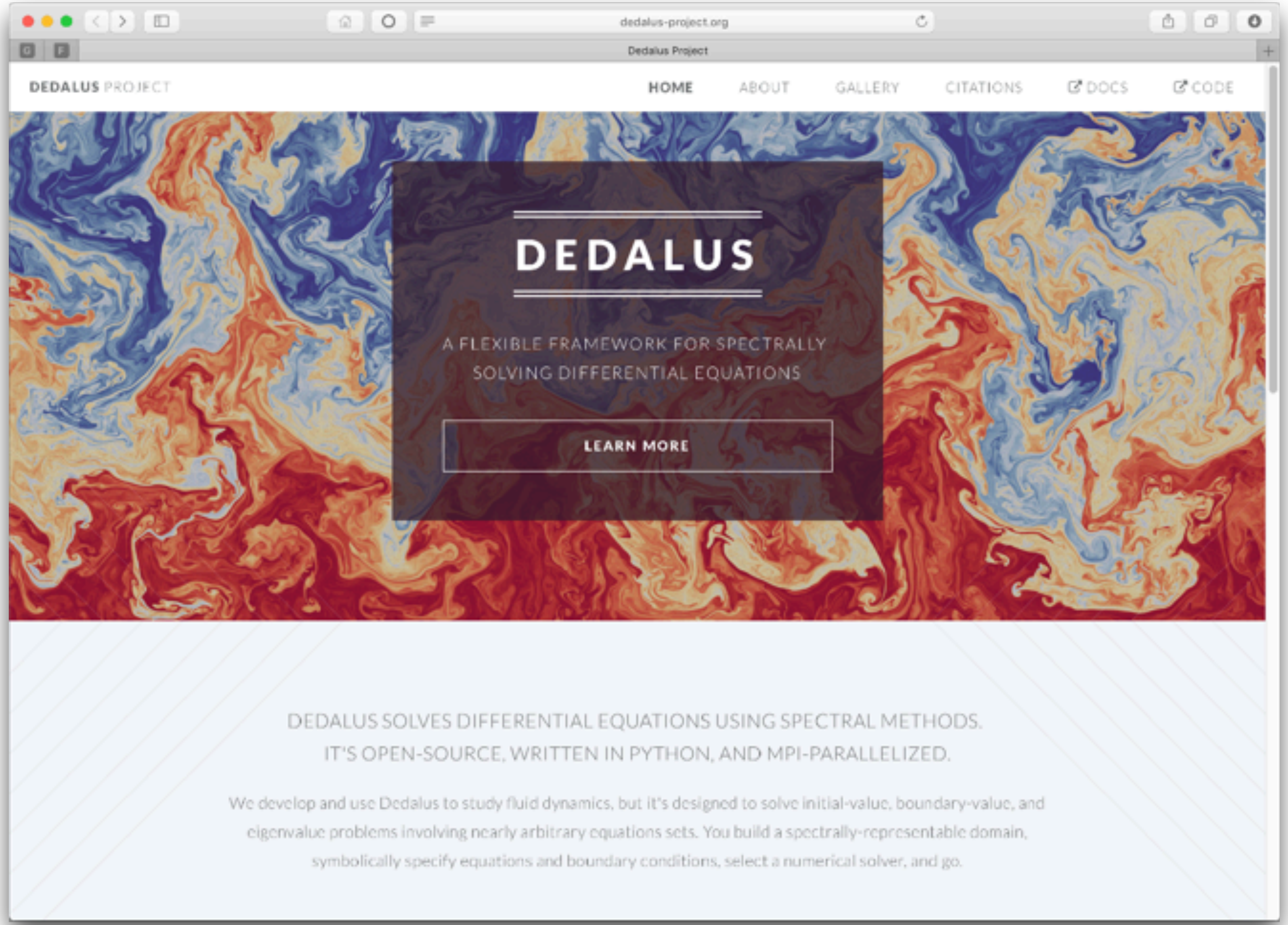
- Nonlinearly unstable
- Only scalar-valued fields
- Don't parallelize / scale



Challenge: high-order & flexible methods at scale



Dedalus Project

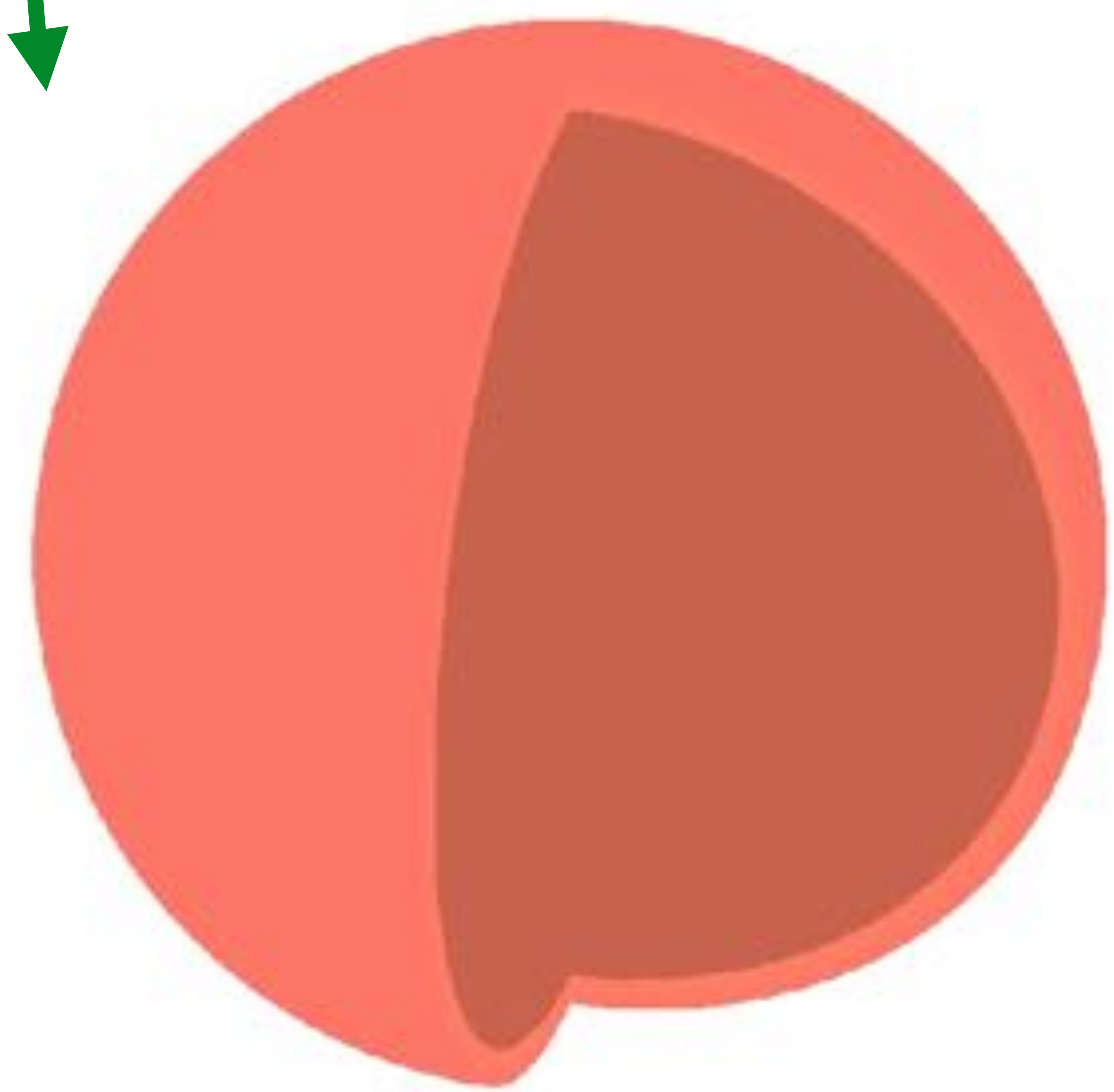


Dedalus Project

```
problem.add_equation("div(u) = 0")
problem.add_equation("dt(u) - ν*Lap(u) + grad(p) + b*g = - u@grad(u)")
problem.add_equation("dt(b) - κ*Lap(b) = - u@grad(b)")
```

Rapid solver development

Spiral-defect chaos

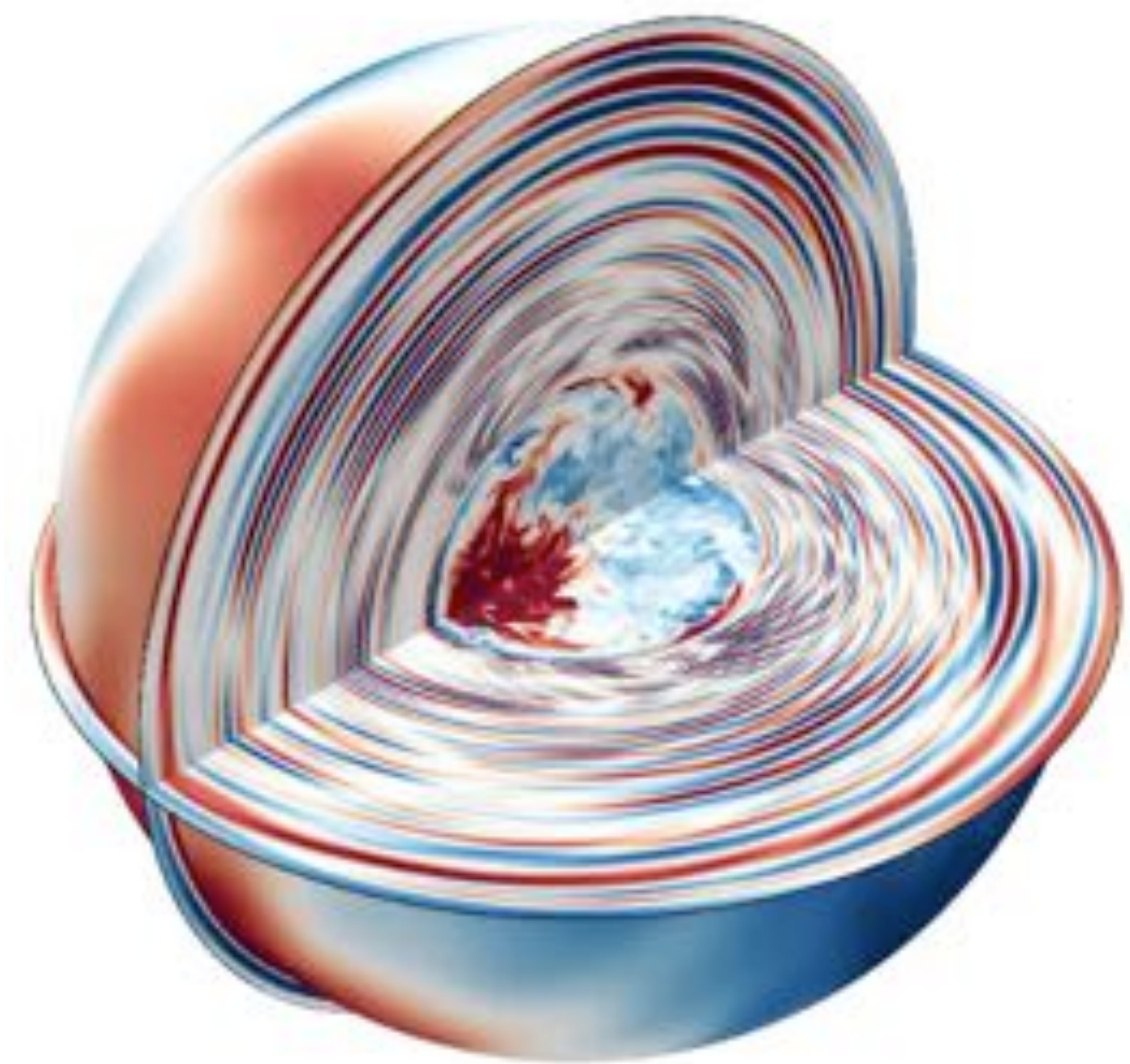


Flexible equations

NLS quantum graphs

High performance

Turbulent wave excitation



Global Spectral Methods

Global spectral discretizations

Expand over **"trial"** functions:

$$u(x) = \sum_{n=0}^{N} u_n \phi_n(x)$$

Project equations against **"test"** functions:

$$\mathscr{L} u(x) = f(x)$$

$$\langle \psi_i | \mathscr{L} u \rangle = \langle \psi_i | f \rangle$$

$$\sum_j \langle \psi_i | \mathscr{L} \phi_j \rangle u_j = \langle \psi_i | f \rangle$$

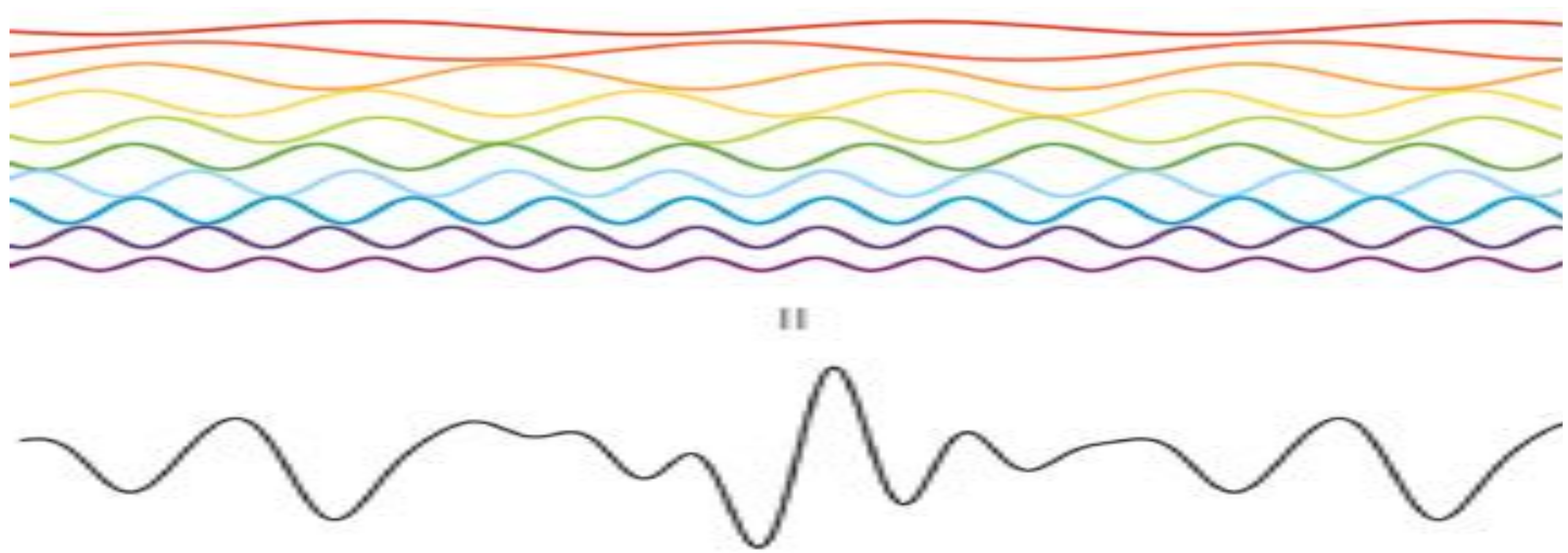
- Easy to adapt to different equations
- **Exponential convergence** for smooth functions
- Only possible in **simple geometries**
- **Fast** if discretized operators are **sparse**
- RHS terms require **spectral transforms**

Fourier spectral methods

Fourier series $\phi_n(x) = e^{inx}$

- **Exponential convergence** for smooth **periodic** functions
- **Fast transforms** for computing coefficients
- **Diagonal** derivative matrix:

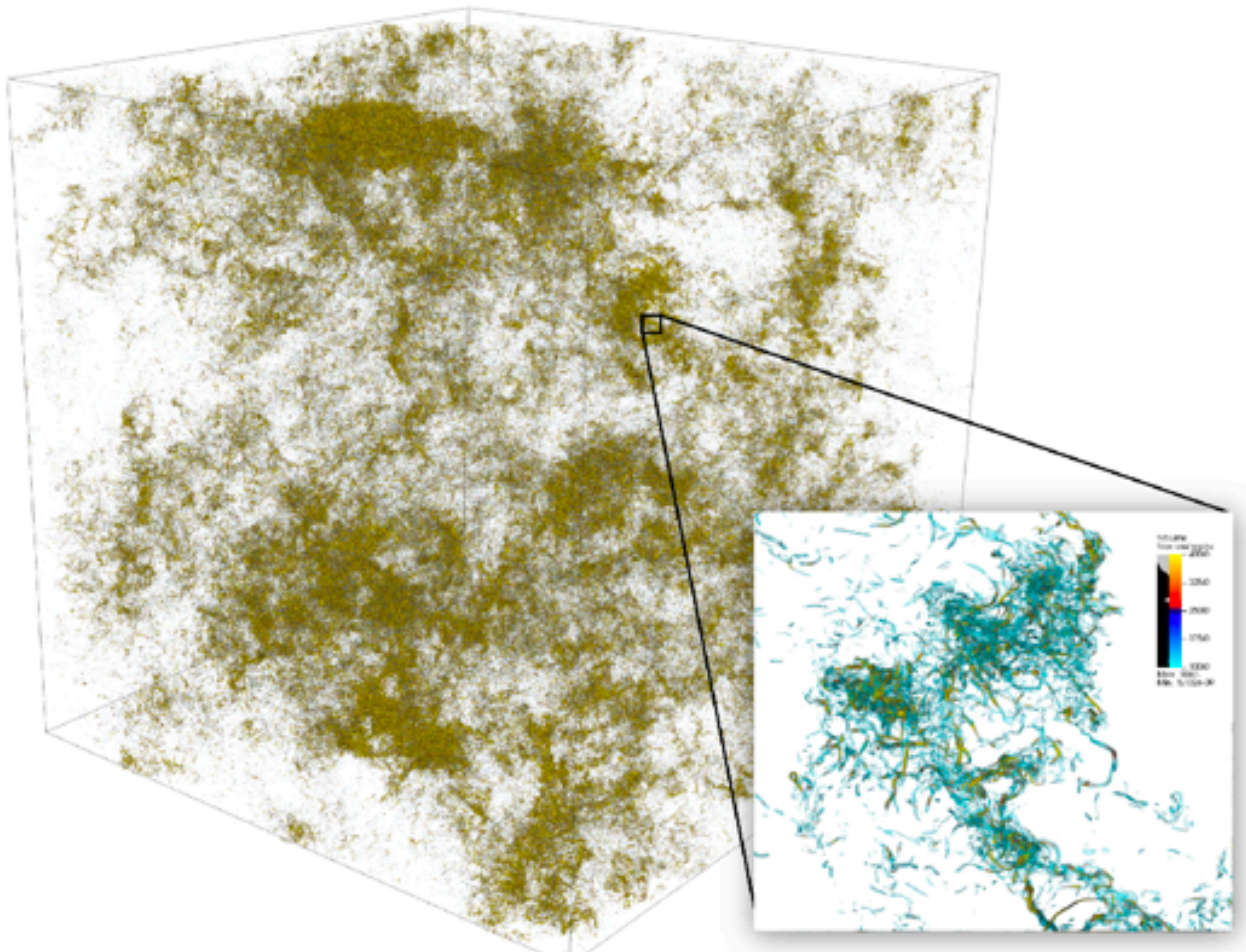
$$\langle \phi_m | \partial_x \phi_n \rangle = in\delta_{m,n}$$



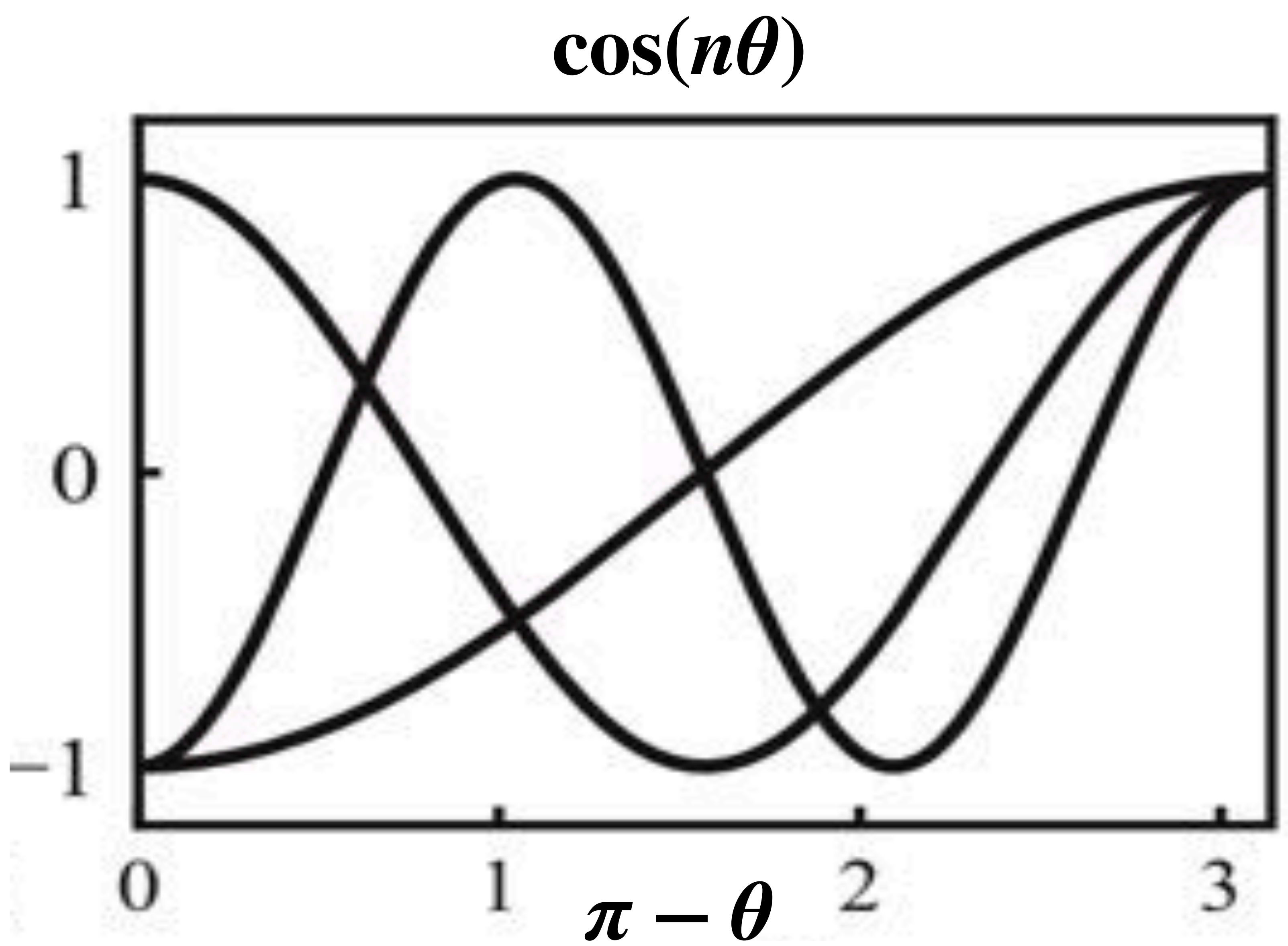
World’s largest turbulence simulations

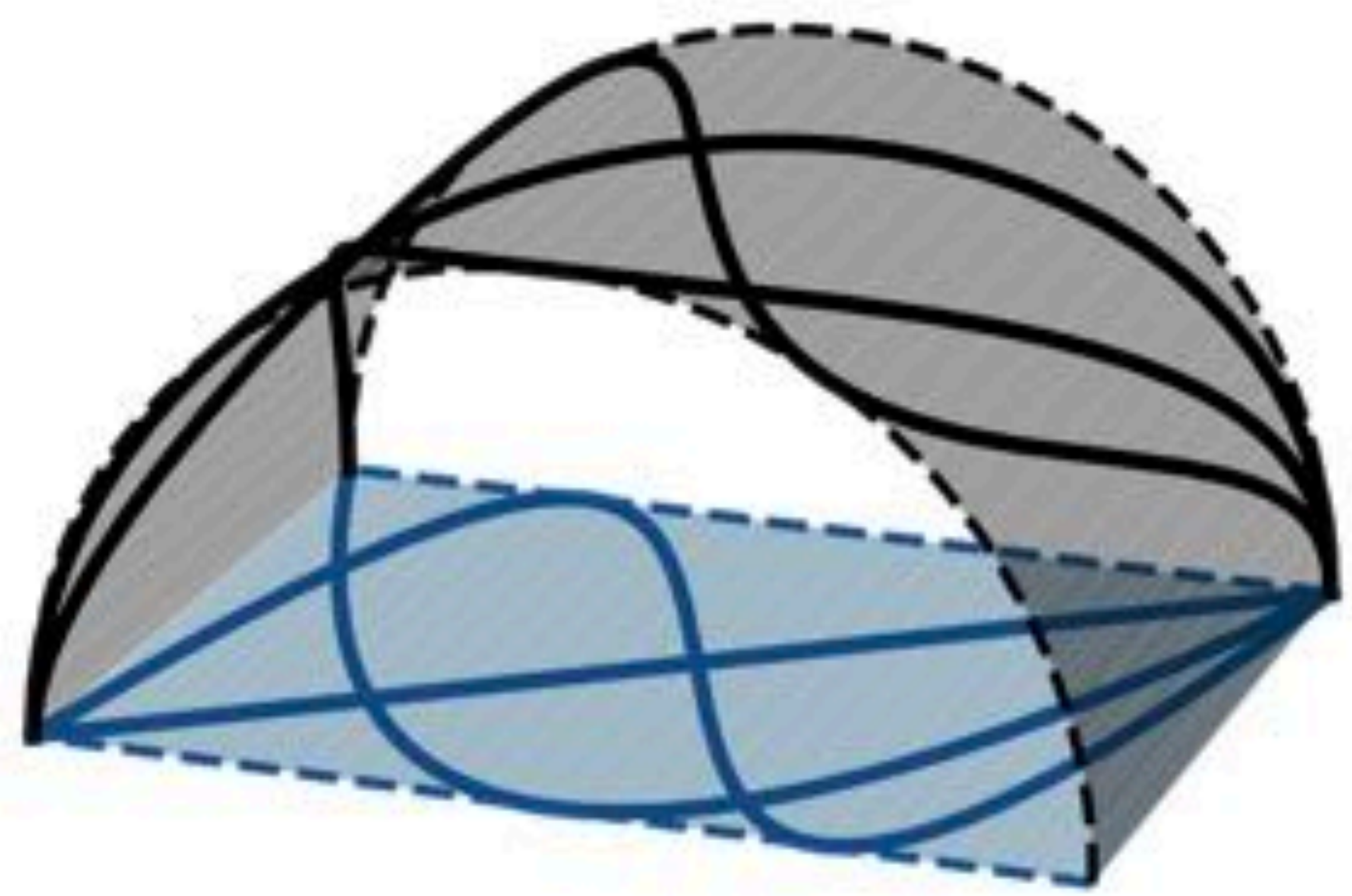
Yeung & Ravikumar, Phys. Rev. Fluids (2021)

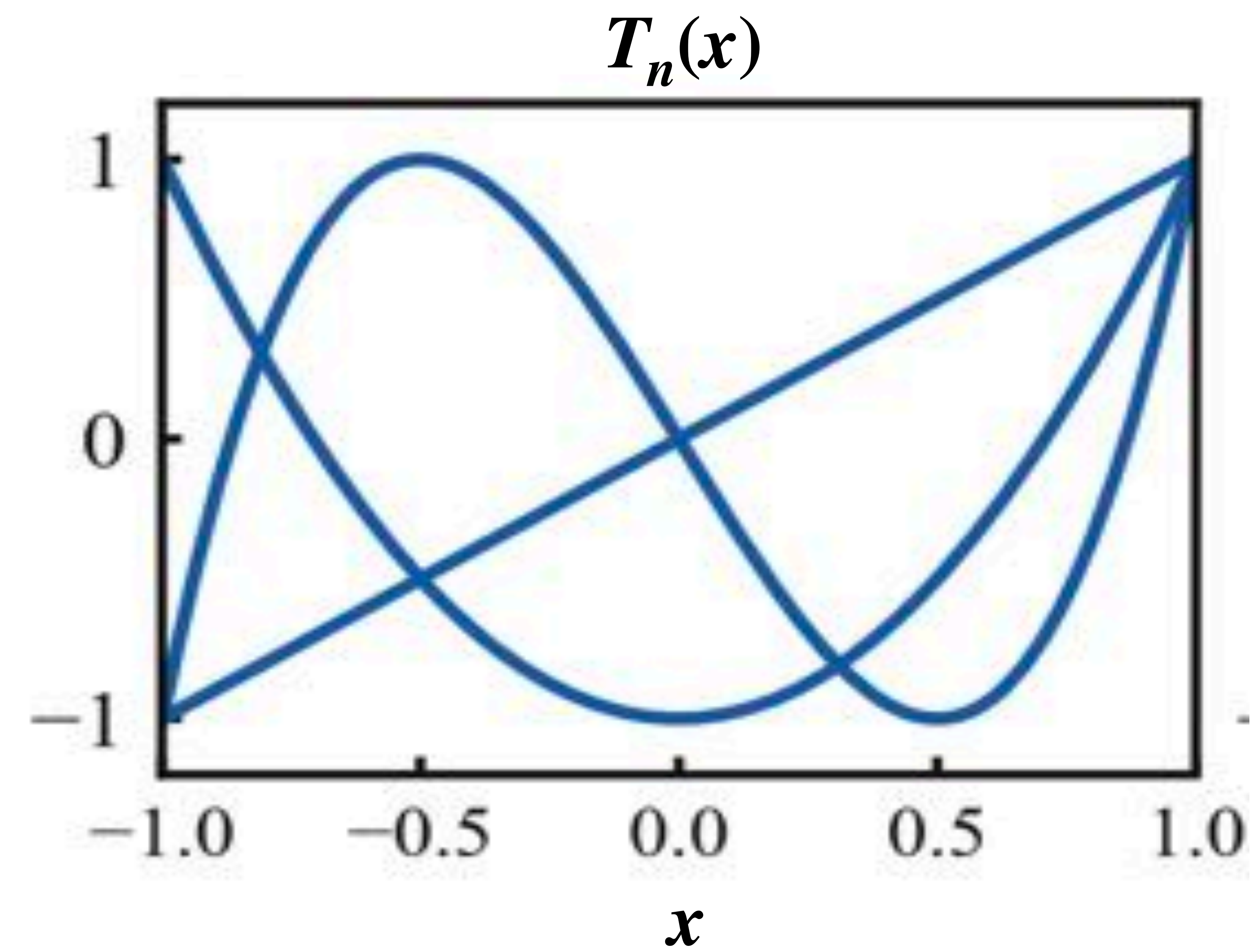
- Fourier pseudospectral method (not Dedalus)
- $18{,}432^3$ grid points
- 18,432 GPUs



Chebyshev polynomials: cosines in disguise







Orthogonal polynomials for non-periodic intervals

Jacobi polynomials $P_n^{(\alpha,\beta)}(x) \in \Pi_n$

- Orthogonal under weight: $w(x) = (1-x)^\alpha(1+x)^\beta$
- Closed under differentiation: $\partial_x^k P_n^{(\alpha,\beta)} \propto P_{n-k}^{(\alpha+k,\beta+k)}$
- **Exponential convergence** for smooth functions on [-1, 1]

1) Legendre polynomials $(\alpha = \beta = 0) \quad P_n(x)$

- **Best L2 approximations** $w(x) = 1$

2) Chebyshev polynomials $(\alpha = \beta = -1/2) \quad T_n(x)$

- **Fast transforms** (DCT) for computing coefficients

3) Ultraspherical / Gegenbauer polynomials $(\alpha = \beta = k - 1/2) \quad C_n^{(k)}(x)$

- ***k***-th derivatives of Chebyshev polynomials

Classical Chebyshev Methods

Same trial & test functions:

E.g. Legendre-tau

$$u(x) = \sum_{n=0}^{N} u_n P_n(x)$$

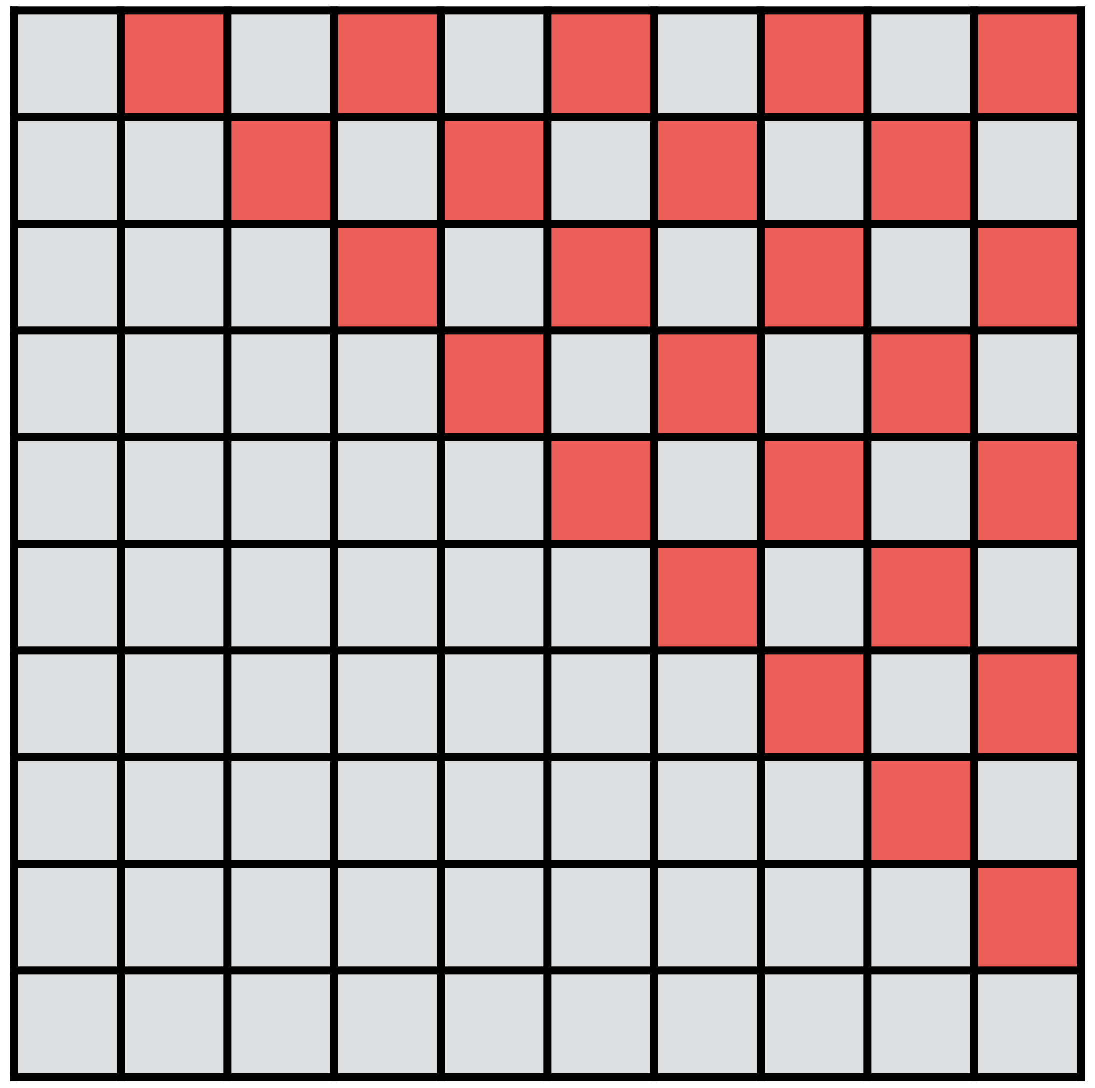
E.g. Chebyshev-tau

$$u(x) = \sum_{n=0}^{N} u_n T_n(x)$$

$$u_n = \mathrm{DCT}(u(x_i))$$

Differentiation:

$$\mathscr{D}_{m,n} = \langle T_m \,|\, \partial_x T_n \rangle$$



- Dense matrices
- Poor conditioning

Lanczos, Liu, Ortiz

Ultraspherical Method

Chebyshev trial functions:

$$u(x) = \sum_{n=0}^{N} u_n T_n(x)$$

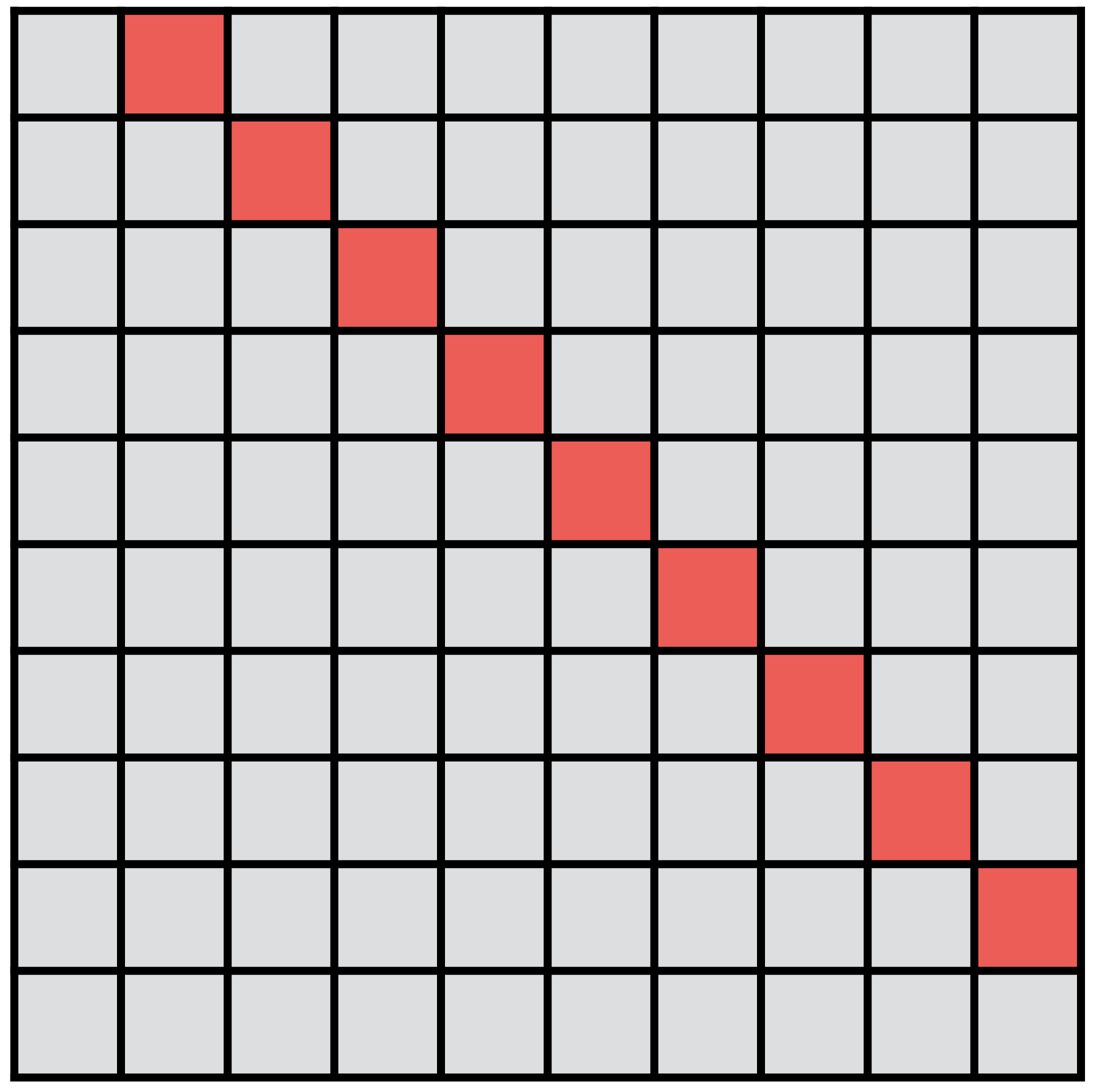
Ultraspherical test functions:

$$\alpha = \beta = k - 1/2$$

$$C_n^{(k)}(x) \propto \partial_x^k T_{n+k}(x)$$

Differentiation:

$$\mathcal{D}_{m,n} = \langle C_m^{(1)} | \partial_x T_n \rangle$$



- Banded
- Well conditioned

Clenshaw, Orszag, Greengard, Julien, Coutsias, Olver, Townsend

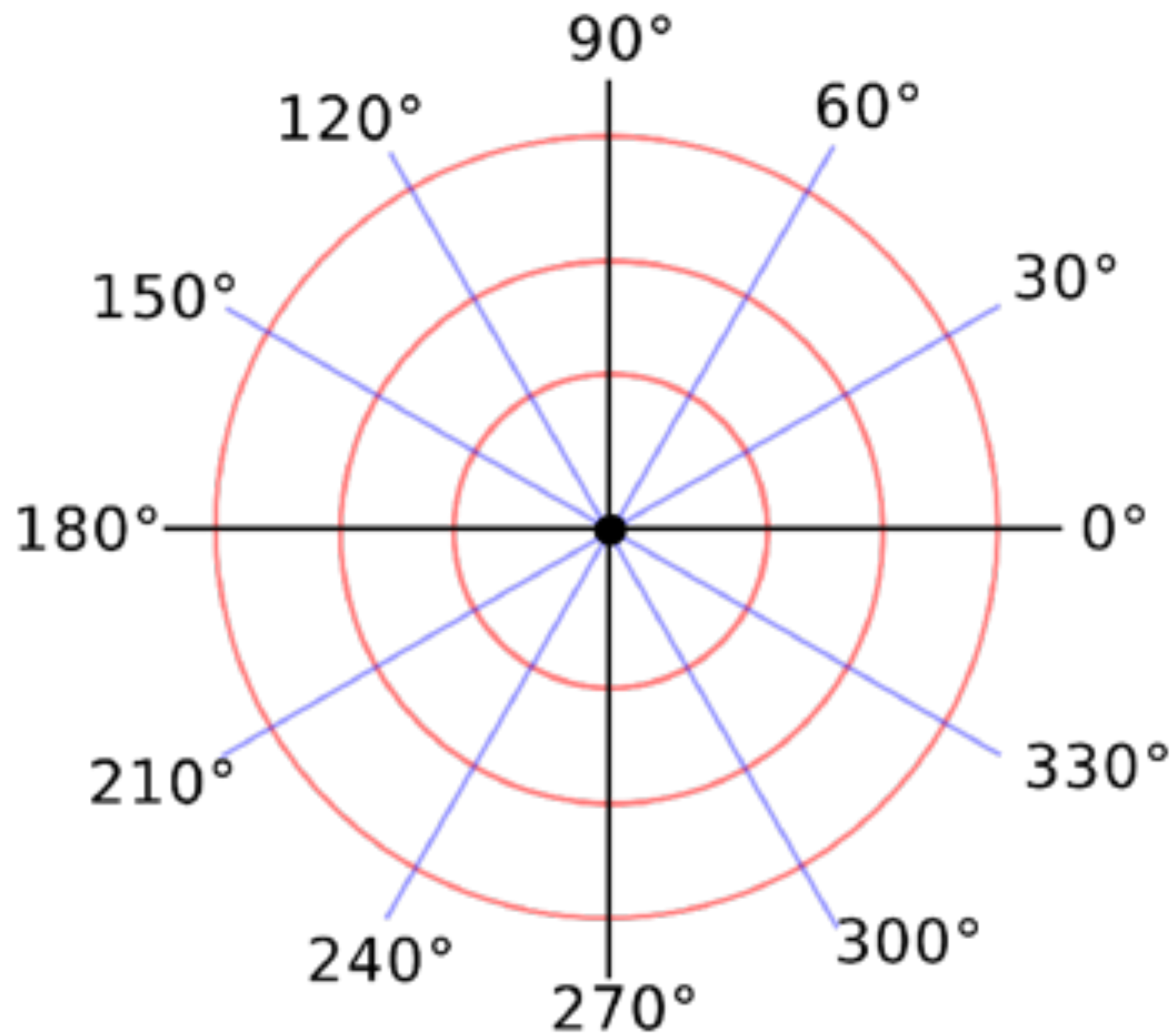
Key points for efficient spectral solvers

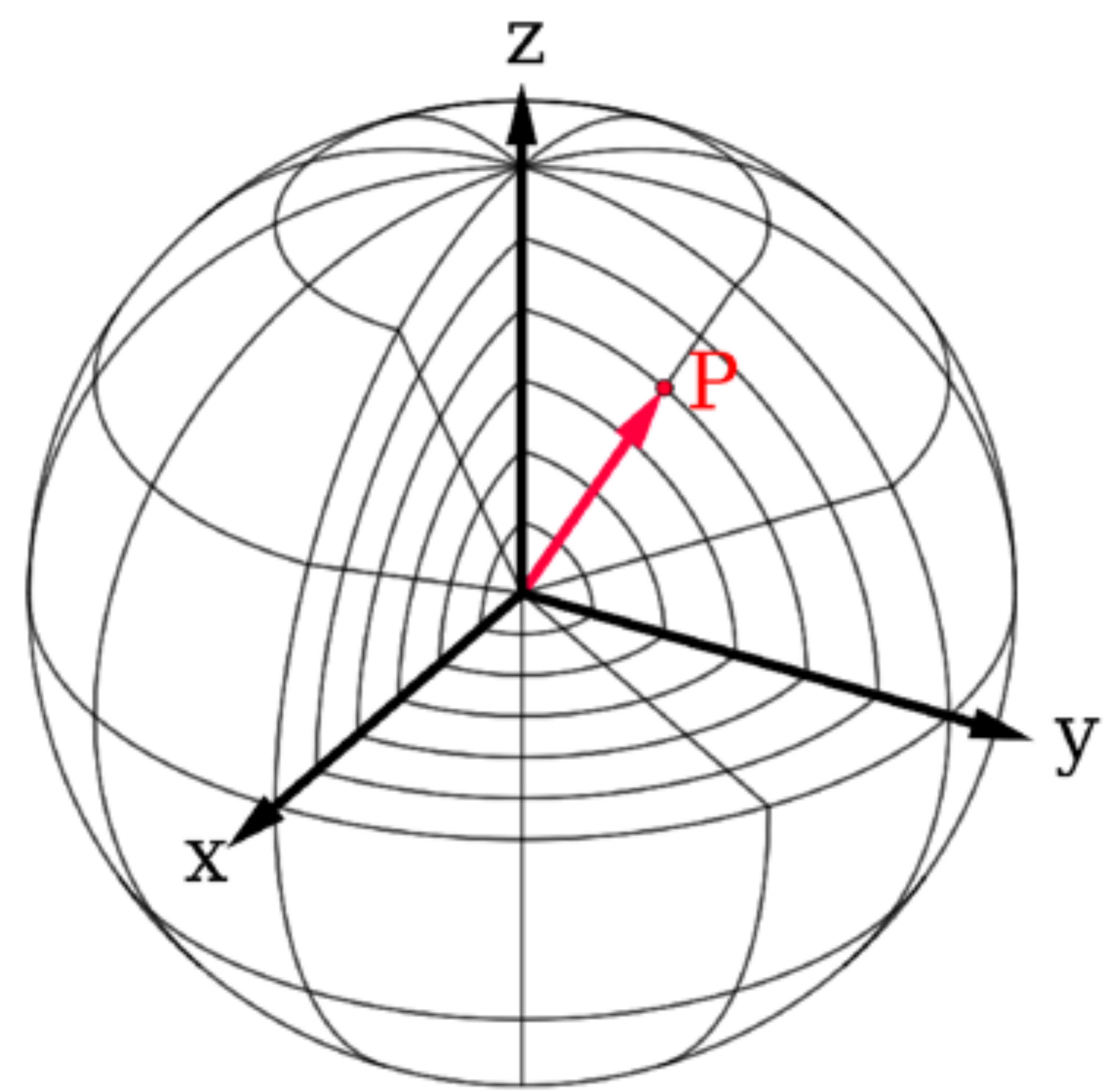
1. **Spectrally accurate bases** $\{\phi_i(x)\}$
   - Rapidly convergent approximations

2. **Sparse differential operators** $\langle\psi_i|H\phi_j\rangle$
   - Fast operator evaluation
   - Fast direct solvers for LHS

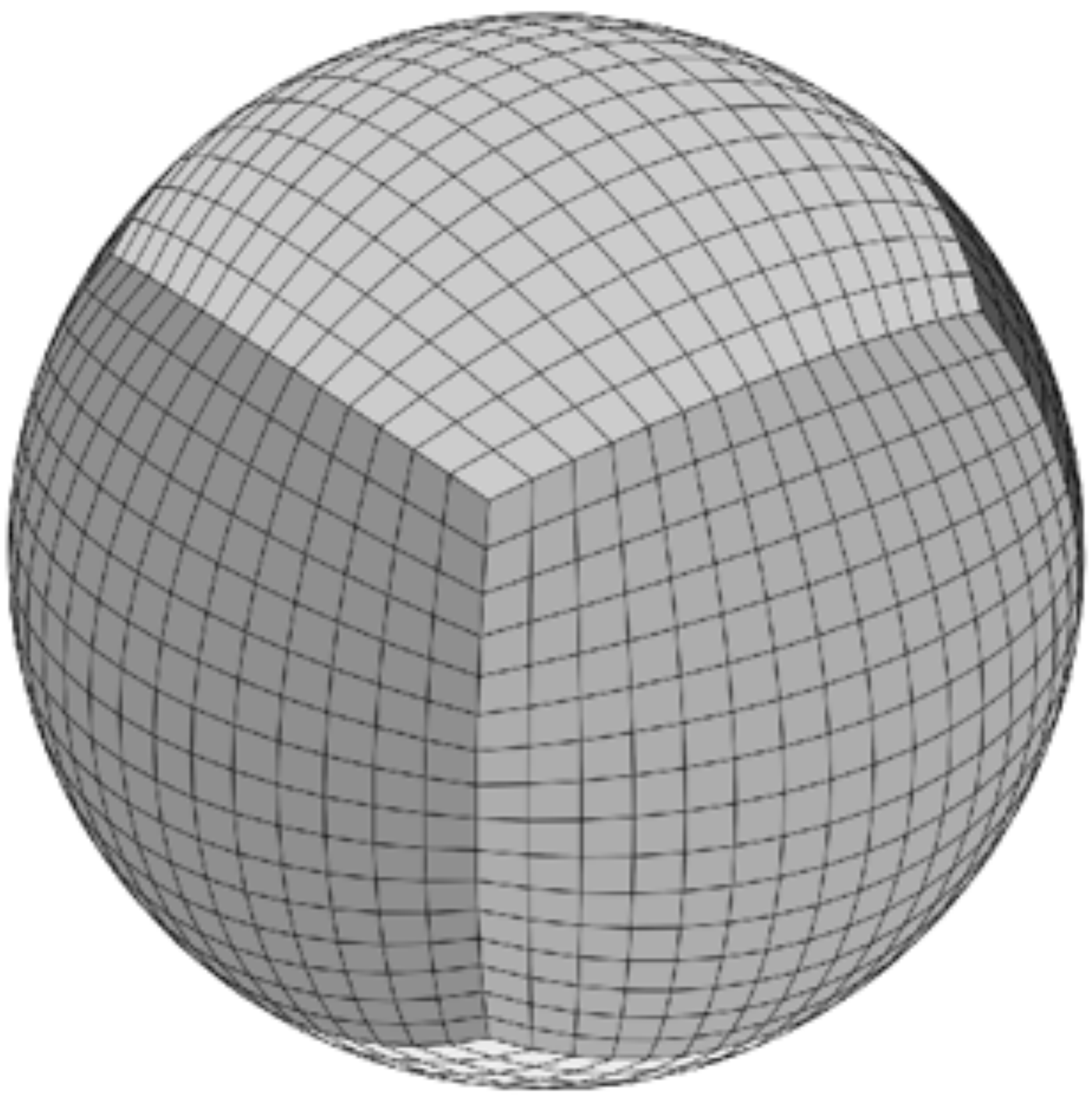
3. **Fast spectral transforms** $F(X)$
   - Fast evaluation of nonlinear RHS

Polar & spherical coordinate singularities

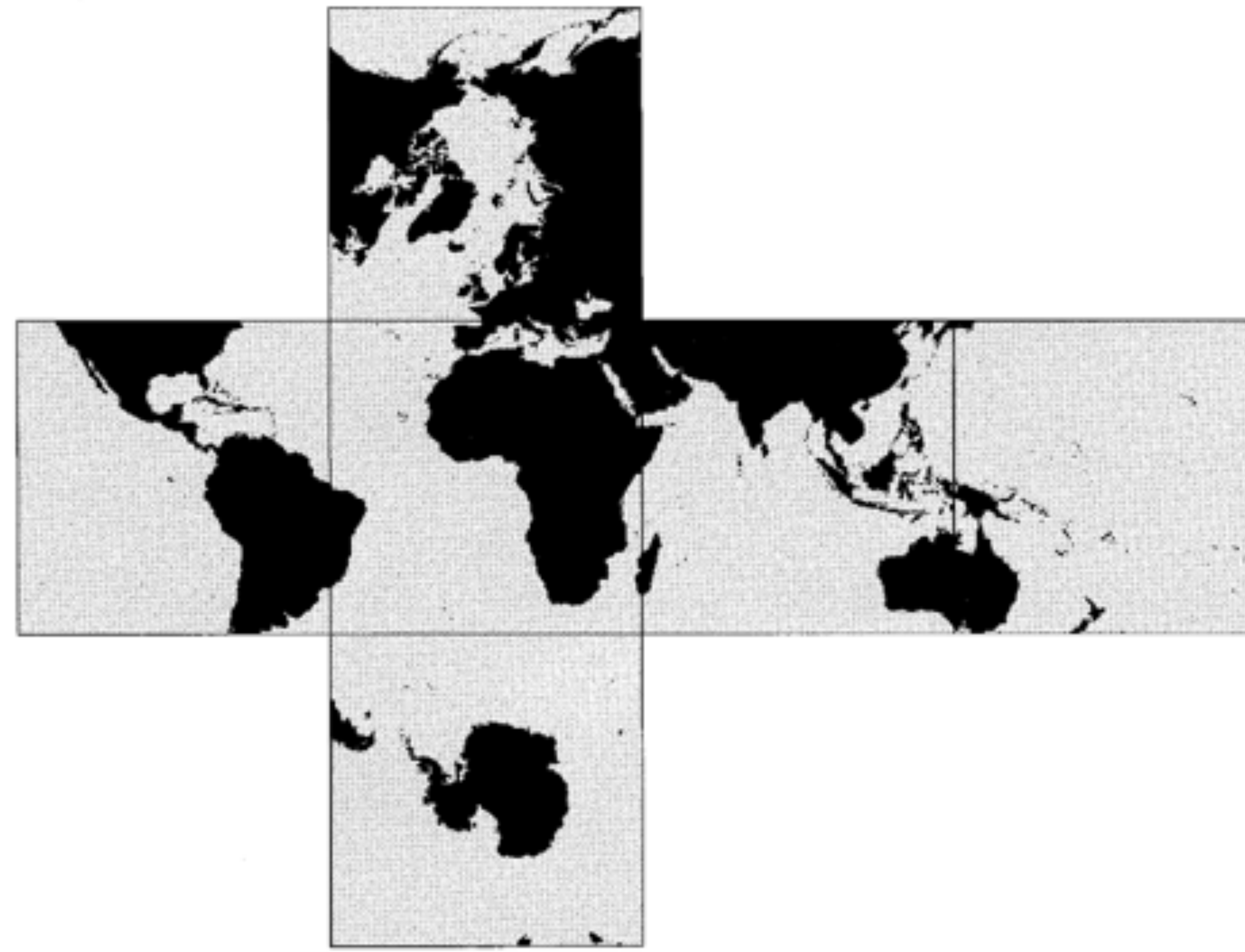




The “cubed sphere” avoids the poles



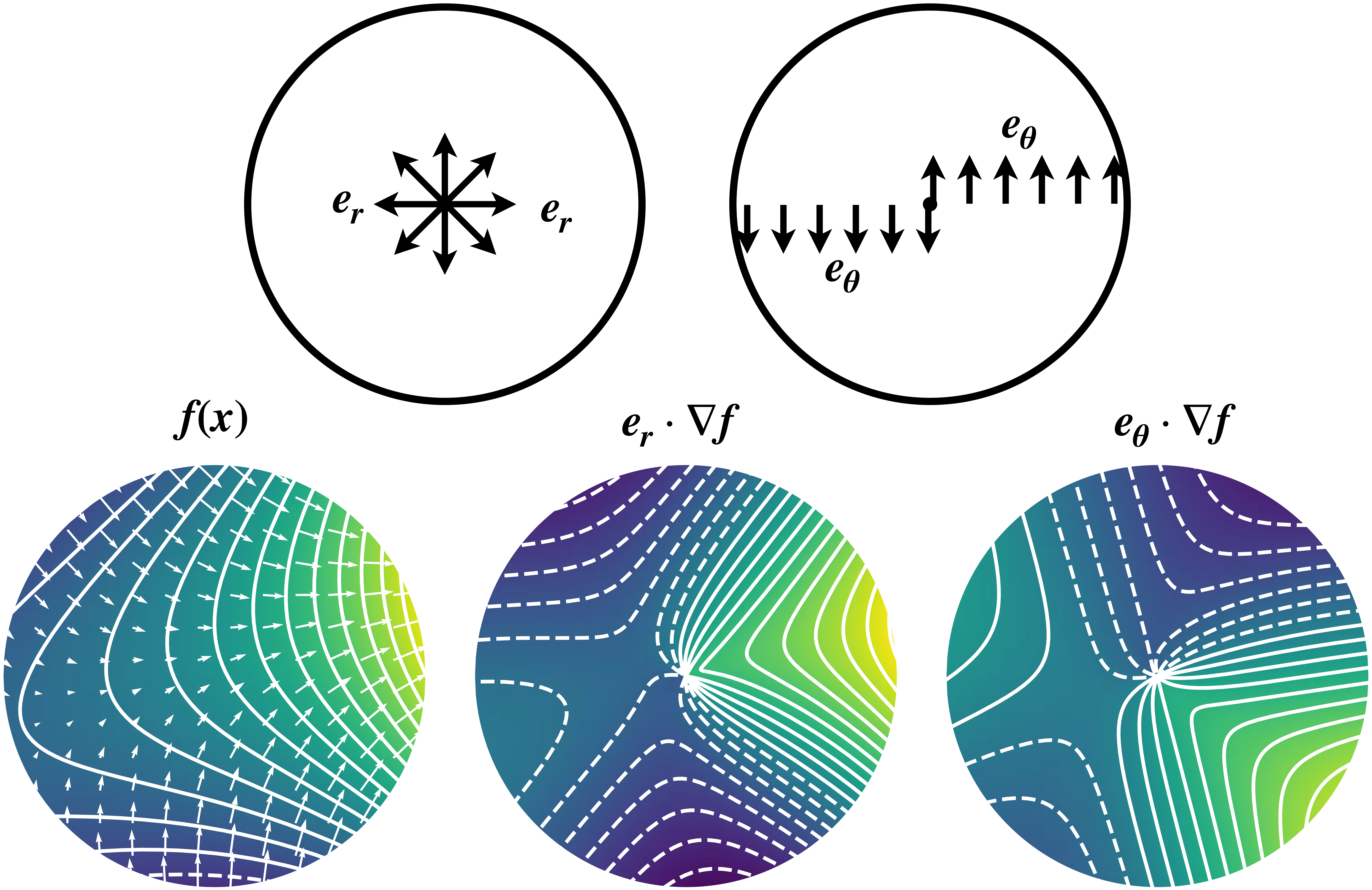
Ullrich (2014)



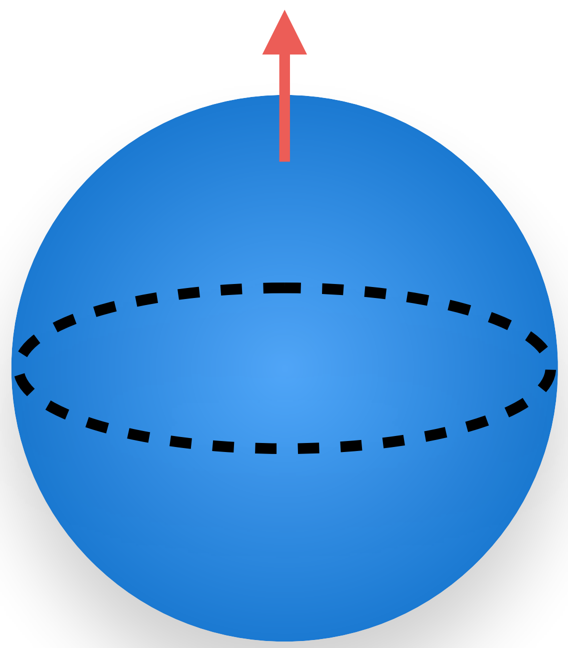
Rochi (1996)

Most codes also cut out the origin

Components of smooth tensors become singular

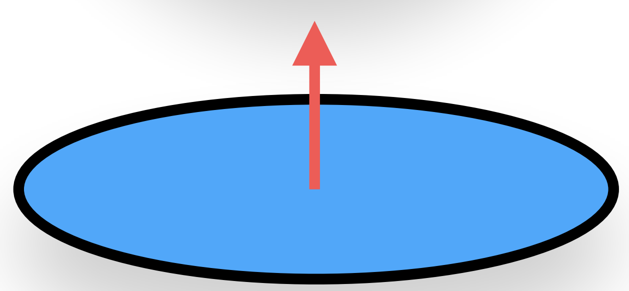


Regularity-aware curvilinear trial functions



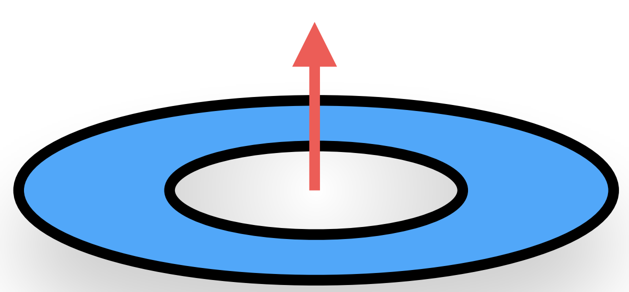
Spheres*: spin-weighted spherical harmonics $Y^s_{l,m}(\phi,\theta)$

Newman & Penrose, JMP (1966)



Disks: Fourier + generalized Zernike polynomials $e^{im\phi}\, r^{m+s}\, P_n^{(k,m+s)}(r')$

Vasil et al (+KB)., JCP (2016)

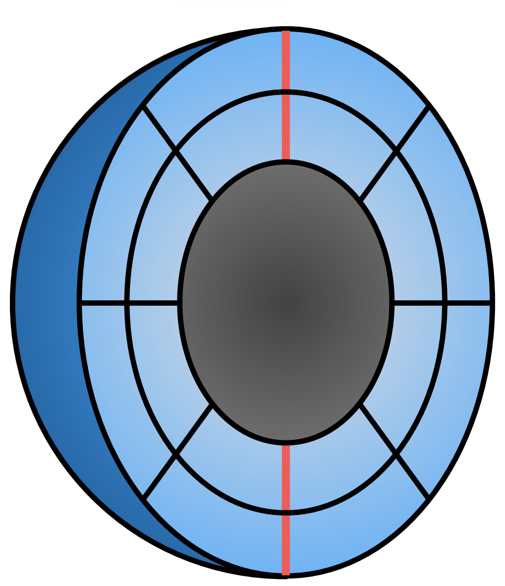


Ar $e^{im\phi}\, r^{-k}\, T_n(r')$

Spectral accuracy for arbitrary tensor fields

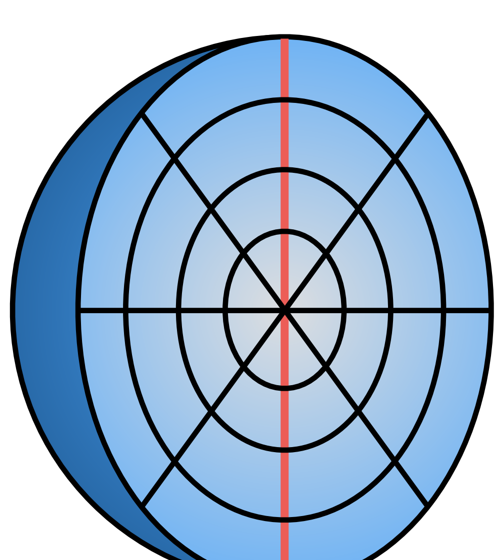
Sparse tensor calculus

No fast transforms*



Spherical shells: SWSH + rational Chebyshev $Y^s_{l,m}\, r^{-k}\, T_n(r')$

Dedalus collab (+KB)., in prep.



Balls: SWSH + one-sided Jacobi polynomials $Y^s_{l,m}\, Q_l^{s,a}\, r^{l+a}\, P_n^{(k,l+a+1/2)}(r')$

Vasil et al (+KB)., JCPX (2019)

Dedalus Project

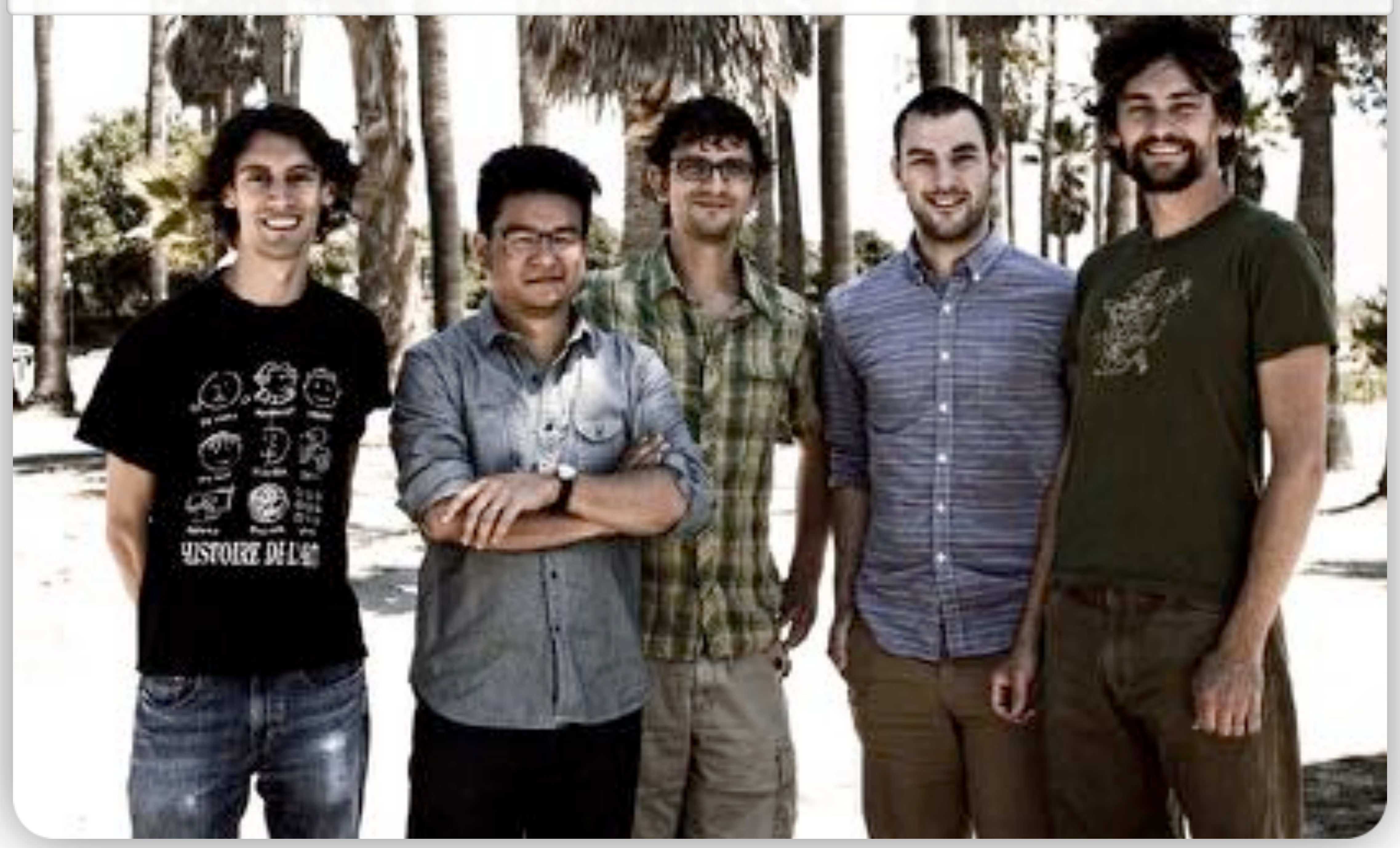
Dedalus Project

Community

- 350+ members on user mailing list
- 19 contributors on GitHub
- NASA *High-value Open Source Tools* project

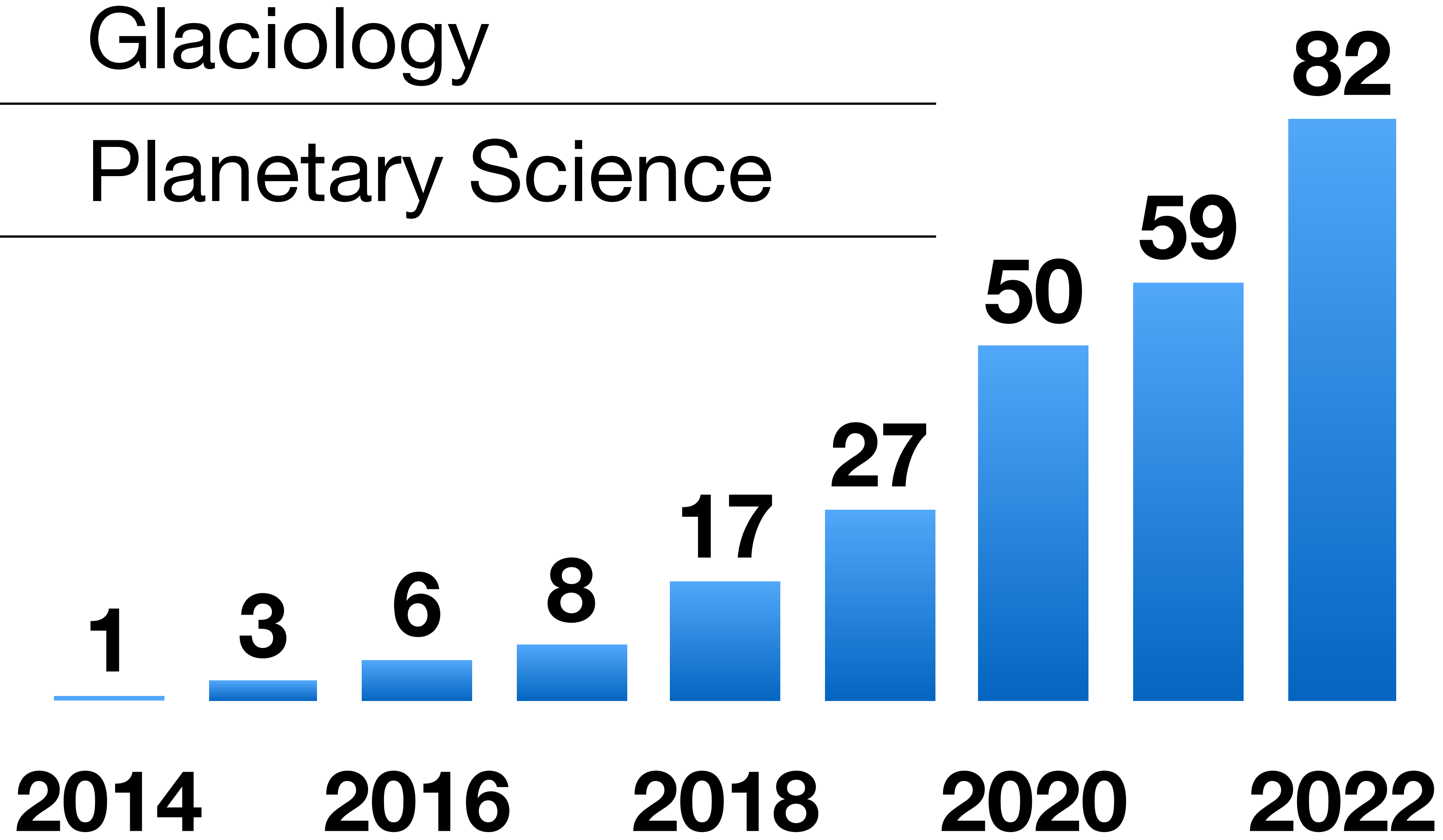
Core developers

Daniel Lecoanet, Jeff Oishi, Geoff Vasil, Keaton Burns, Ben Brown



Publications (250+)

25%	Fluid Dynamics
22%	Astrophysics
13%	Numerical analysis
10%	Plasma Physics
9%	Oceanography
6%	Atmospheric Science
5%	Biology
4%	Condensed Matter
3%	Glaciology
3%	Planetary Science



Supported problem types

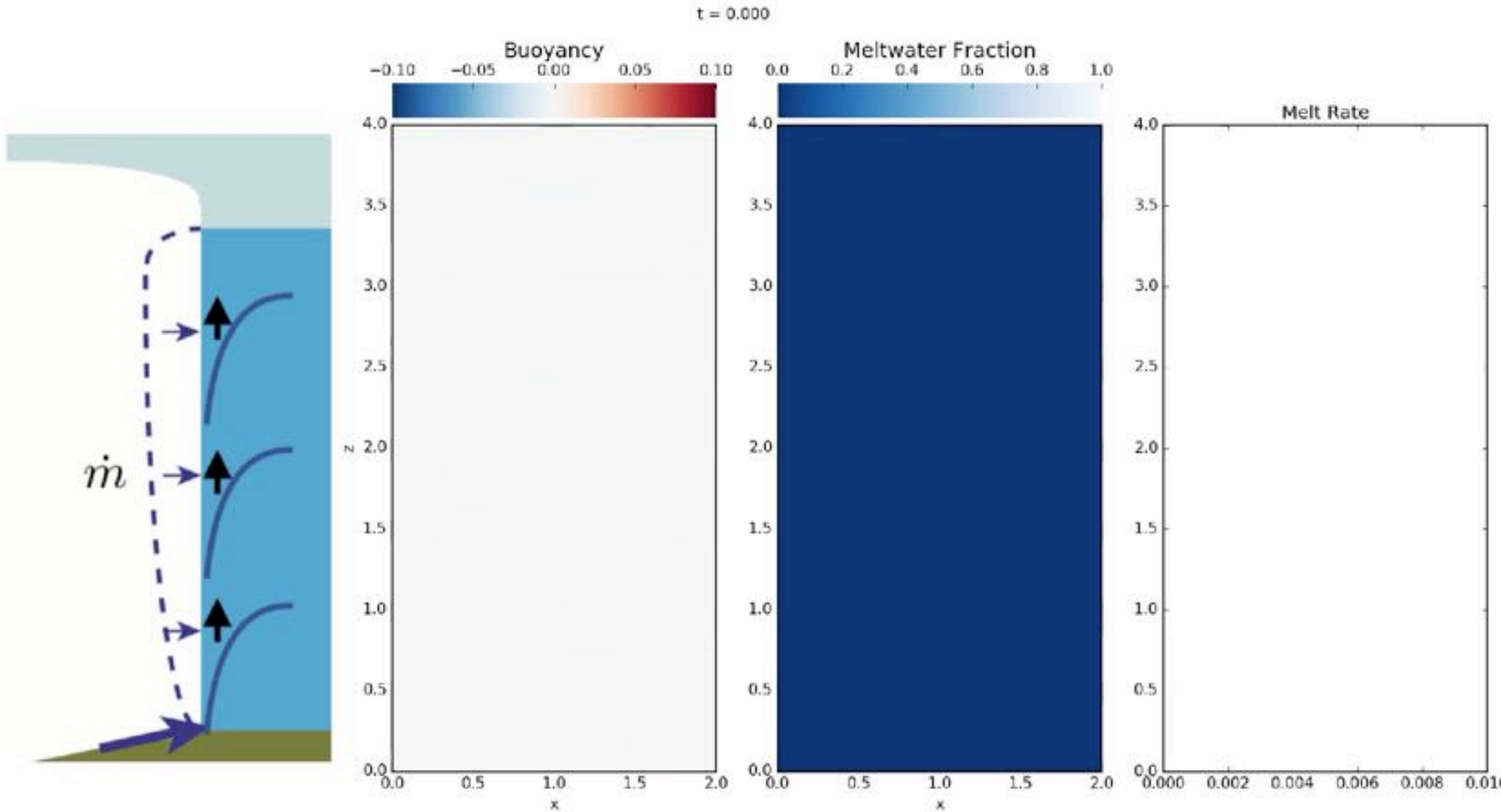
Initial value problems: $$\mathcal{M} \cdot \partial_t \mathcal{X} + \mathcal{L} \cdot \mathcal{X} = \mathcal{F}(\mathcal{X})$$

Nonlinear boundary value problems: $$\mathcal{L} \cdot \mathcal{X} = \mathcal{F}(\mathcal{X})$$

Eigenvalue problems: $$\sigma \mathcal{M} \cdot \mathcal{X} + \mathcal{L} \cdot \mathcal{X} = 0$$

Pseudospectra:
(Eigentools package)
$$\sigma \mathcal{M} \cdot \mathcal{X} + (\mathcal{L} + \mathcal{N}) \cdot \mathcal{X} = 0, \quad ||\mathcal{N}|| \leq \epsilon$$

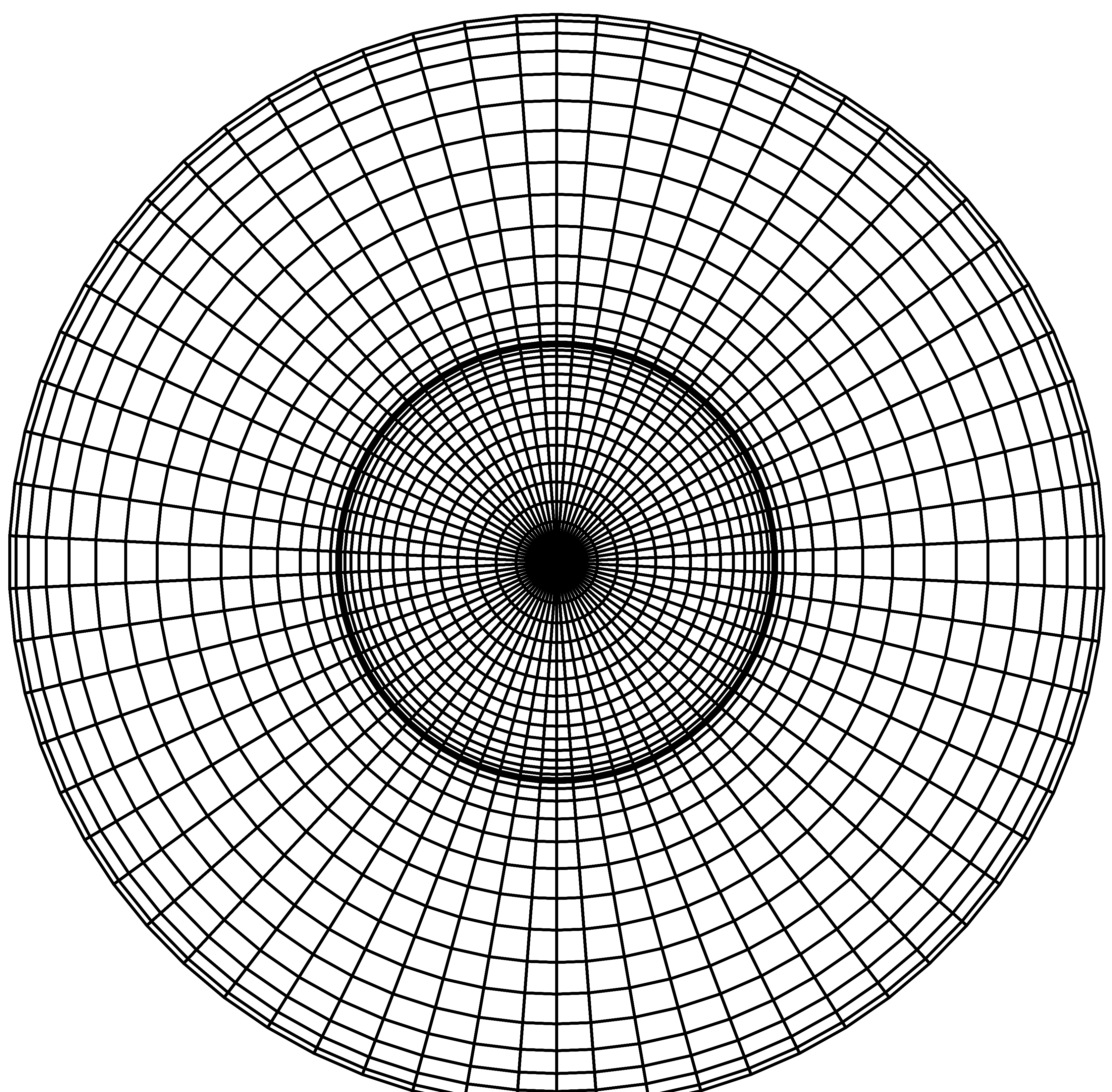
Turbulent enhancement of glacier melting

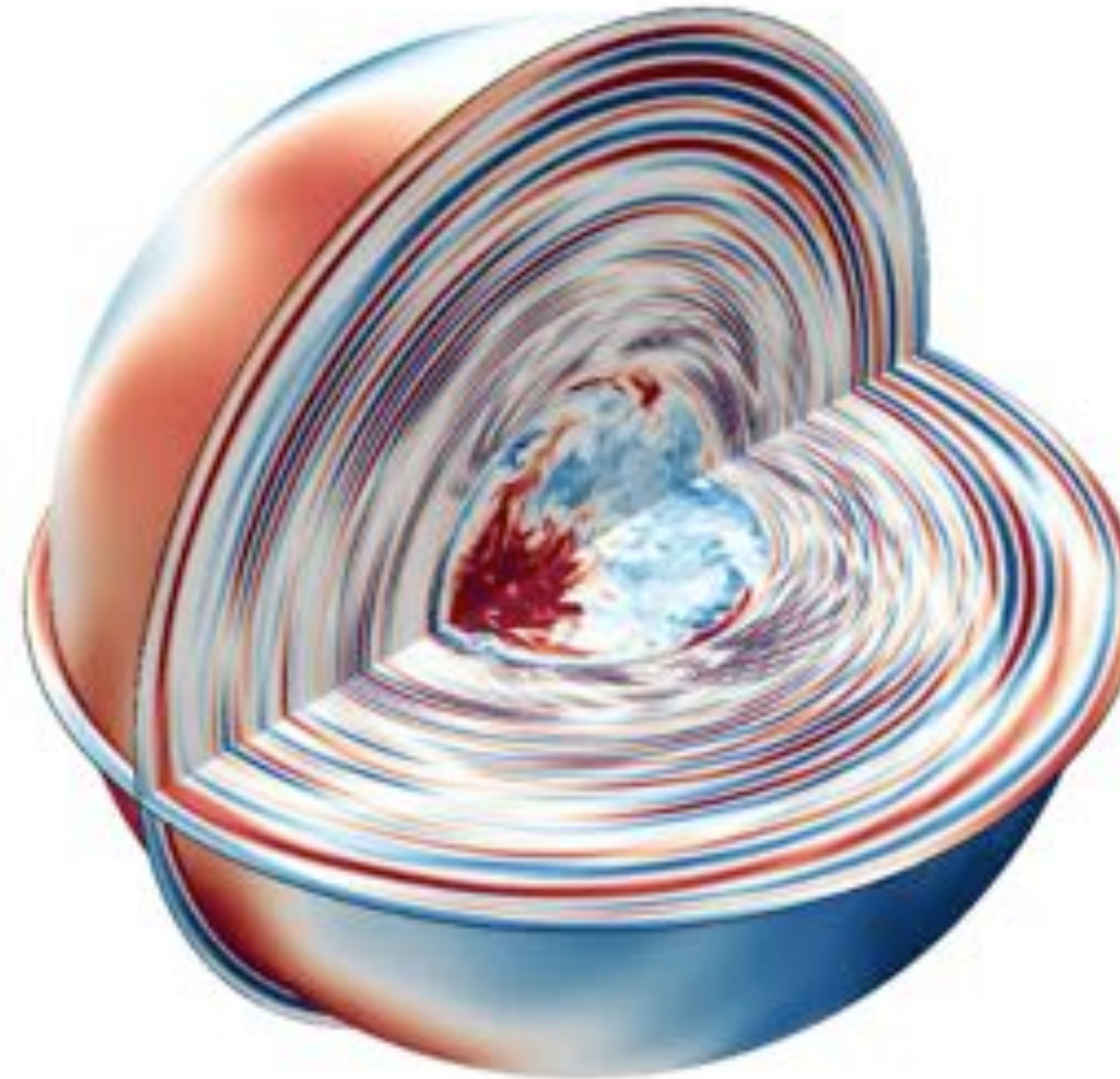


Burns (2018)

High-*p* spherical spectral elements

- Stacked ball and spherical shell bases
- Resolves internal/material boundaries





w/ Evan Anders

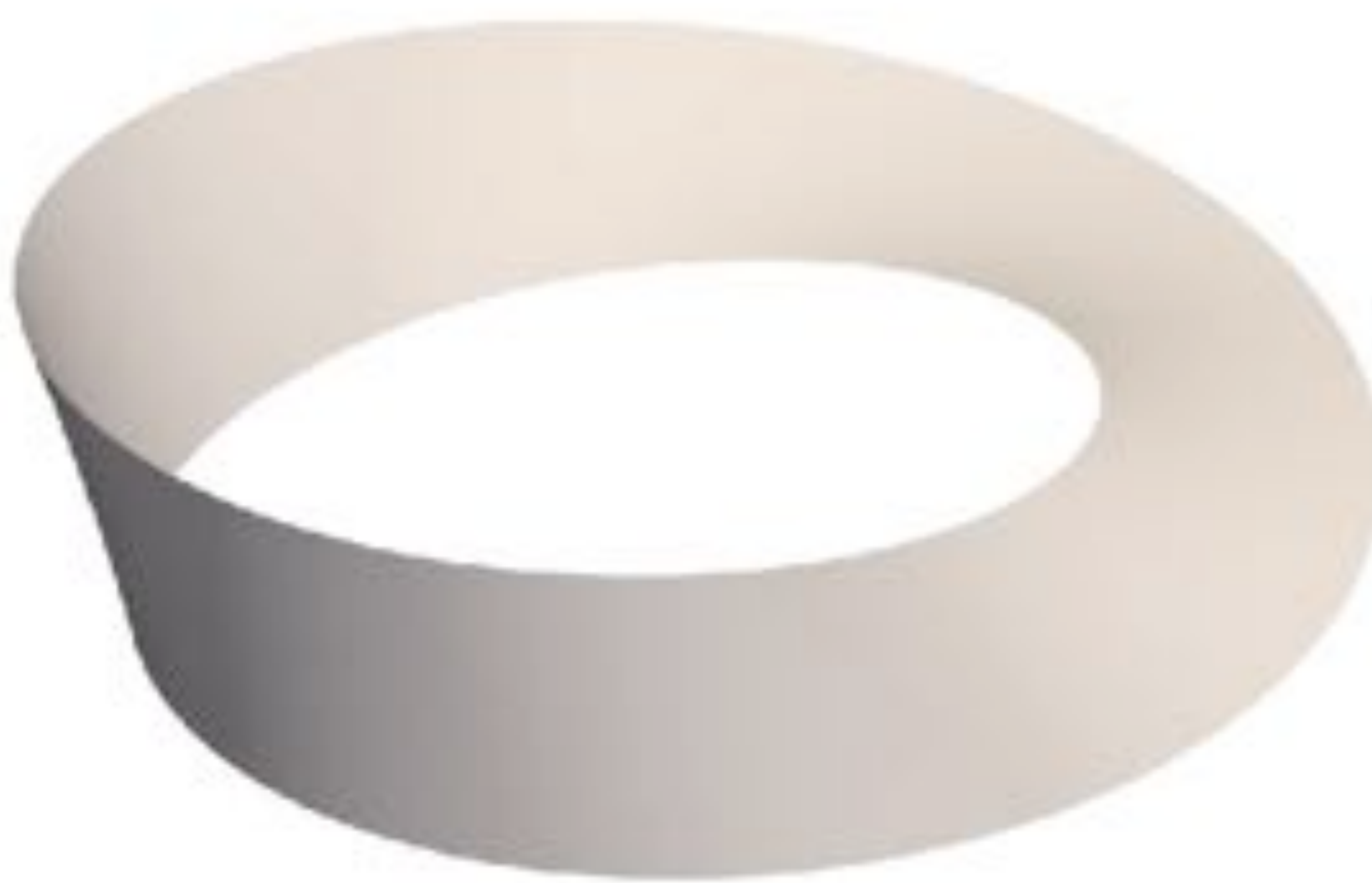
Quantum graphs

$$i\partial_t\psi + \frac{1}{2}\partial_x^2\psi = -|\psi|^2\psi$$

Burns et al., PRR (2020)

Non-orientable & symplectic manifolds

Mobius strip



Klein bottle

Real projective plane

Goals:

- Double-cover domains with exact symmetries
- Symplectic manifolds / phase-space simulations