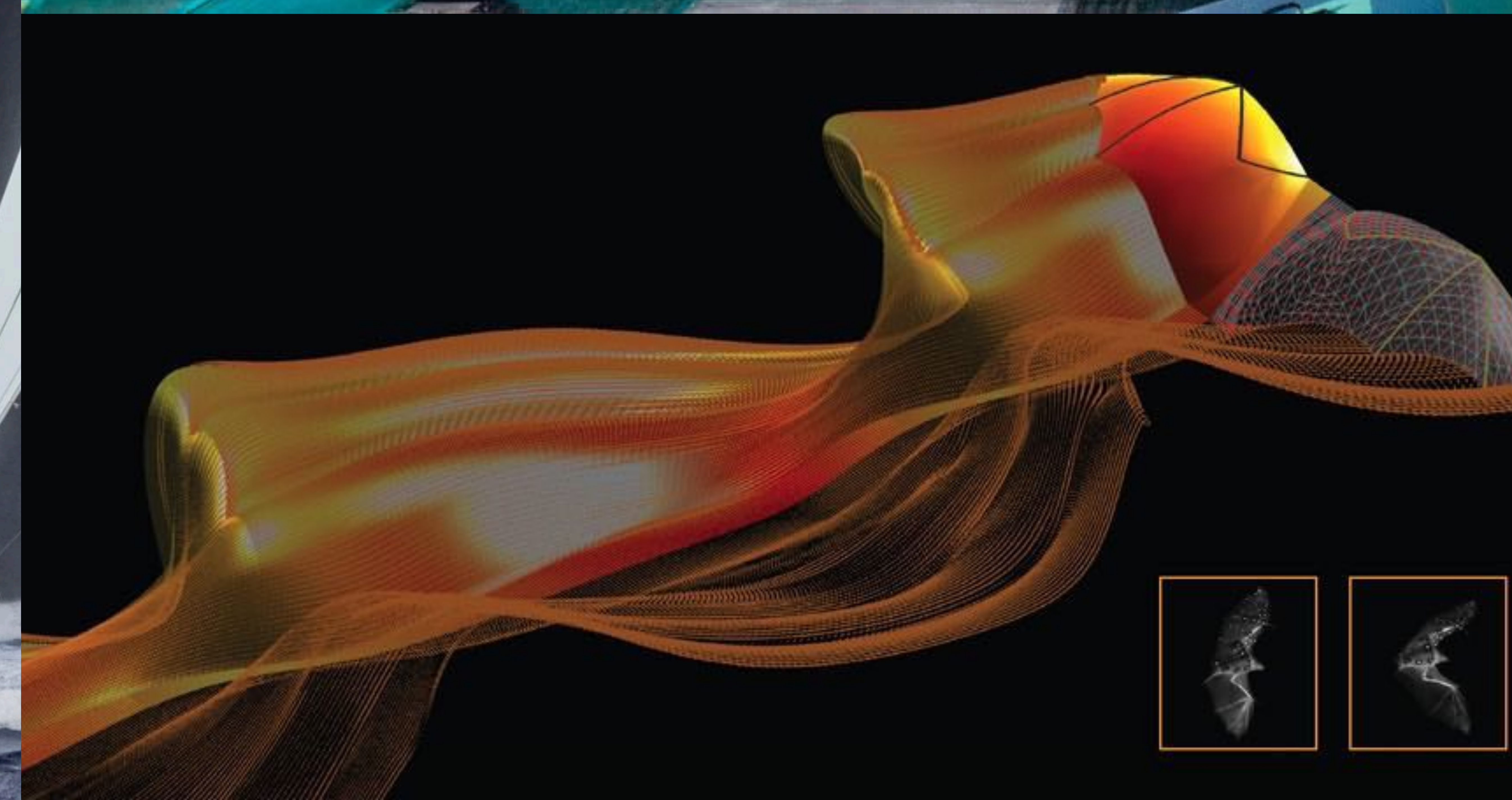
Introduction to Spectral Methods & Dedalus

Keaton Burns

BPM Summer School 2023

PDEs across science & engineering

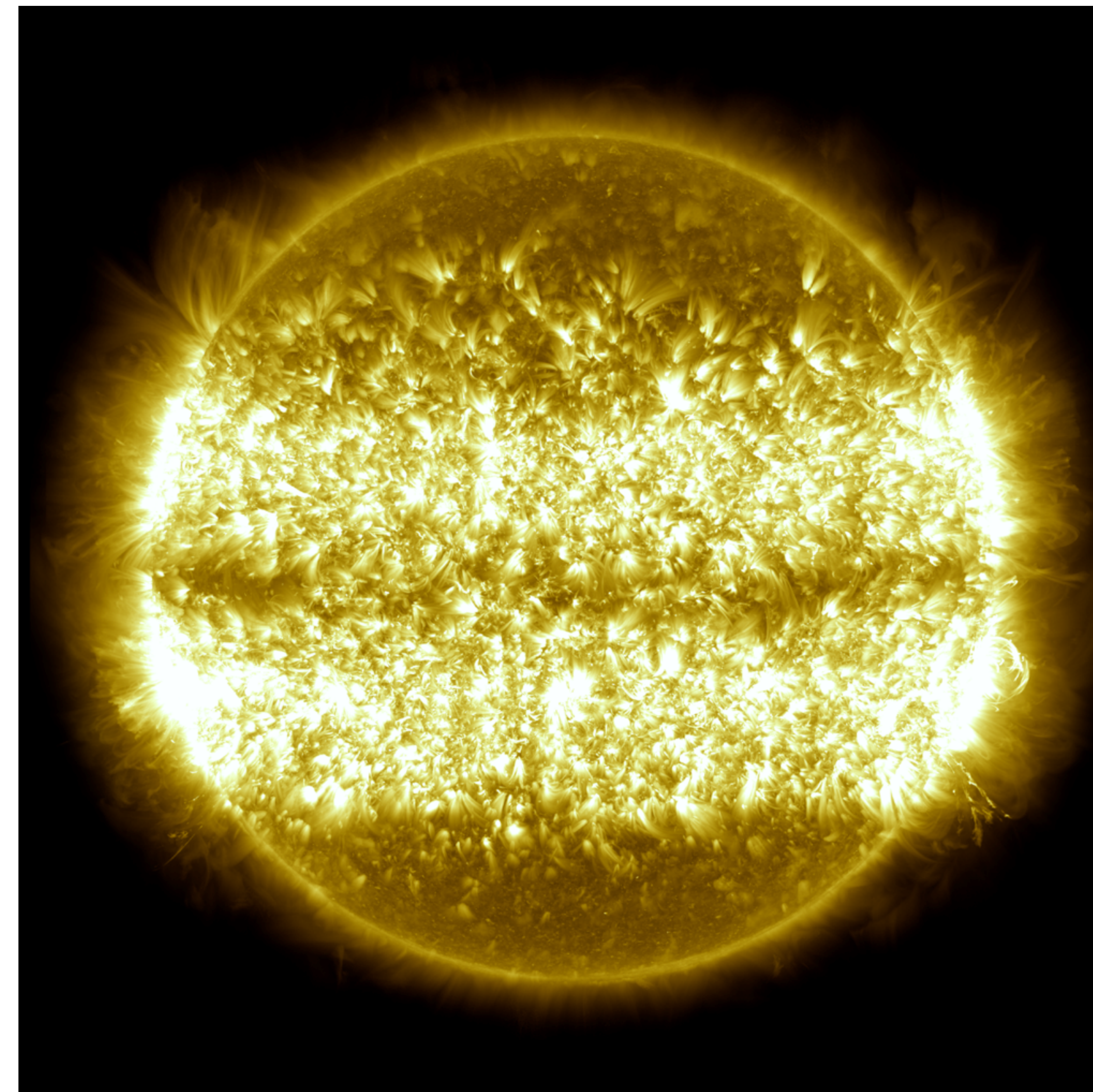


PDEs across science & engineering

Belousov–Zhabotinsky reaction

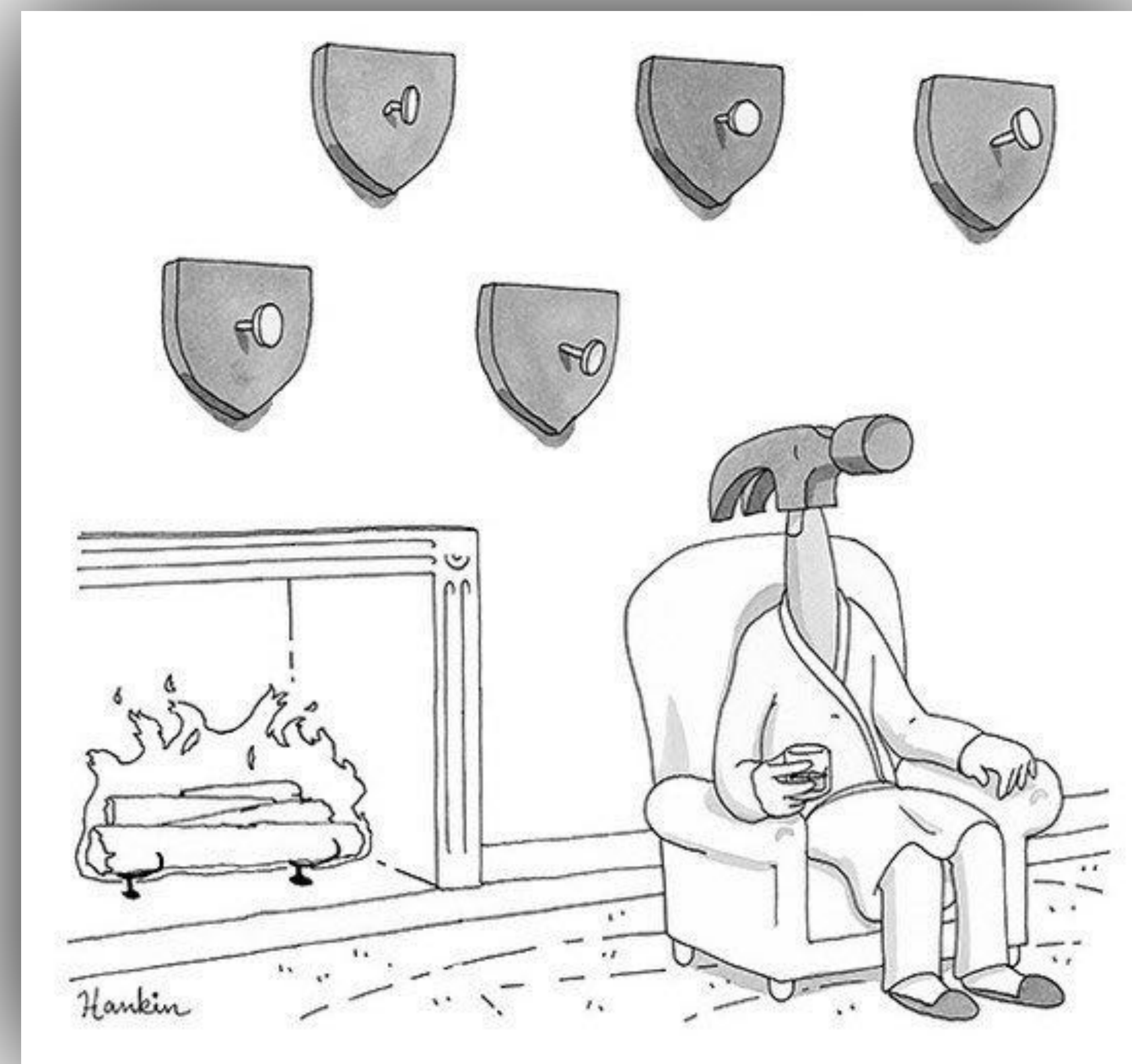
(Stephen Morris)

Solar convection



(NASA/SDO)

Challenge: high-order & flexible methods at scale



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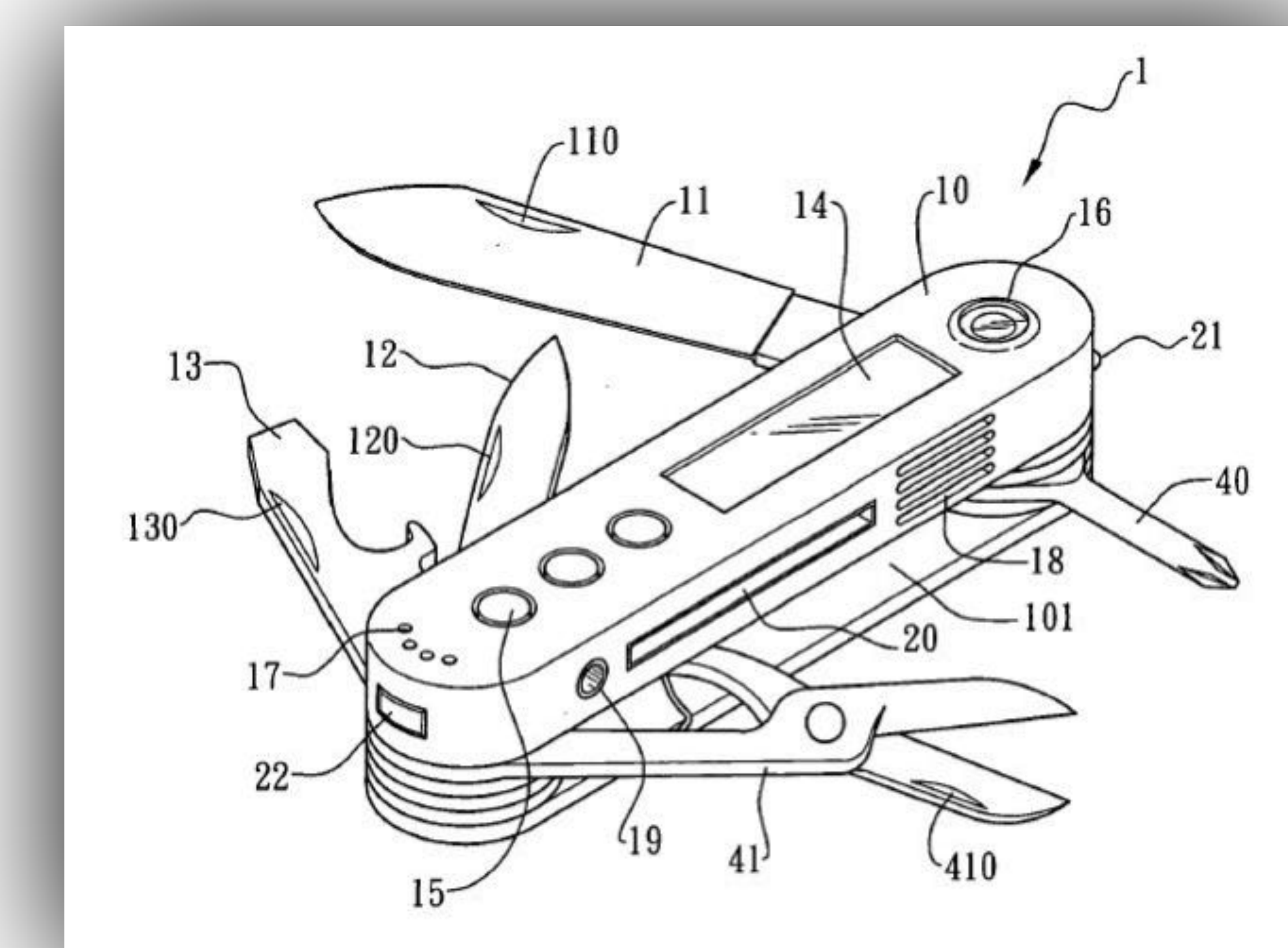
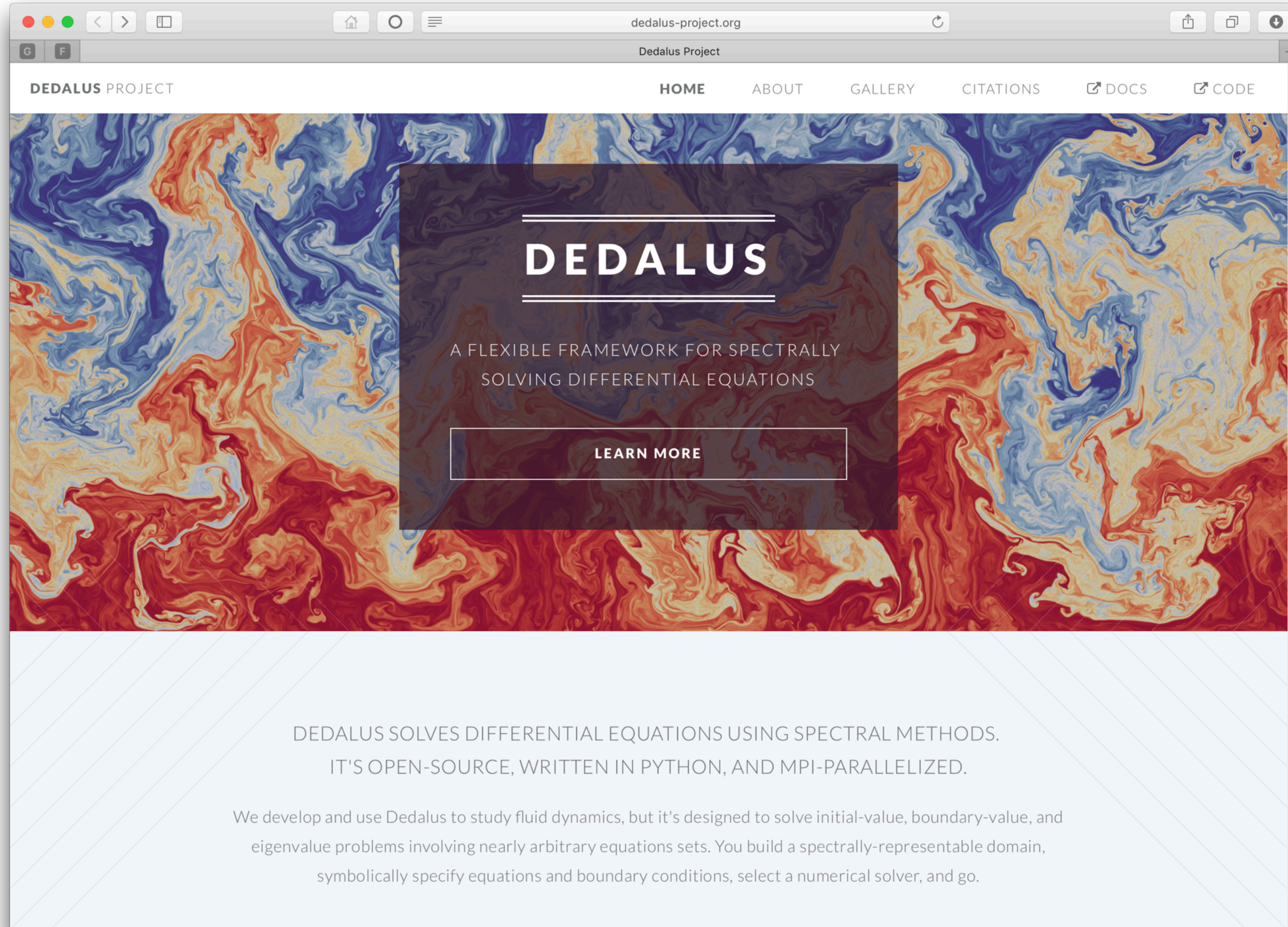
Performance & Scalability



Accuracy & Flexibility

Dedalus Project

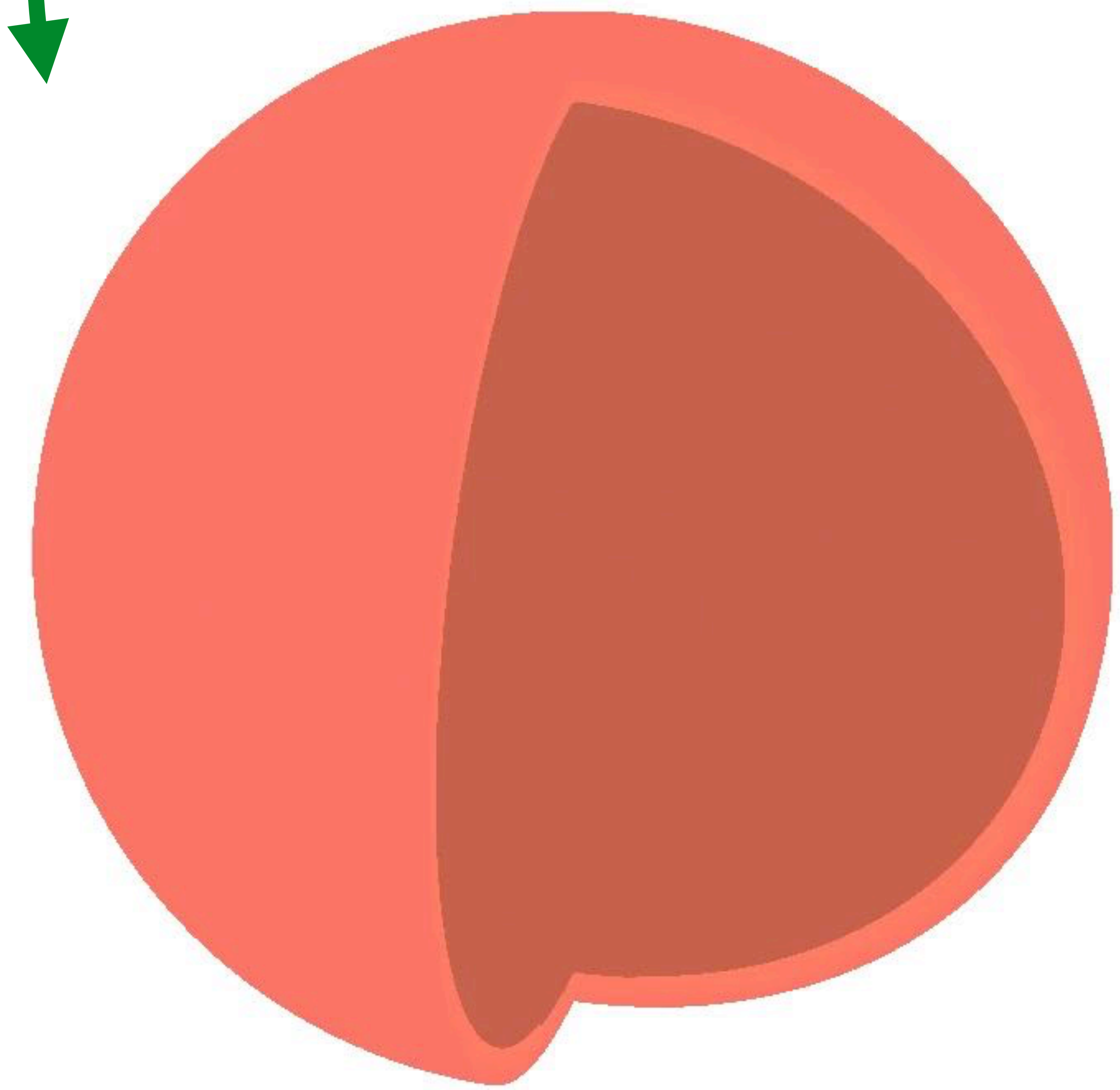


Dedalus Project

```
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

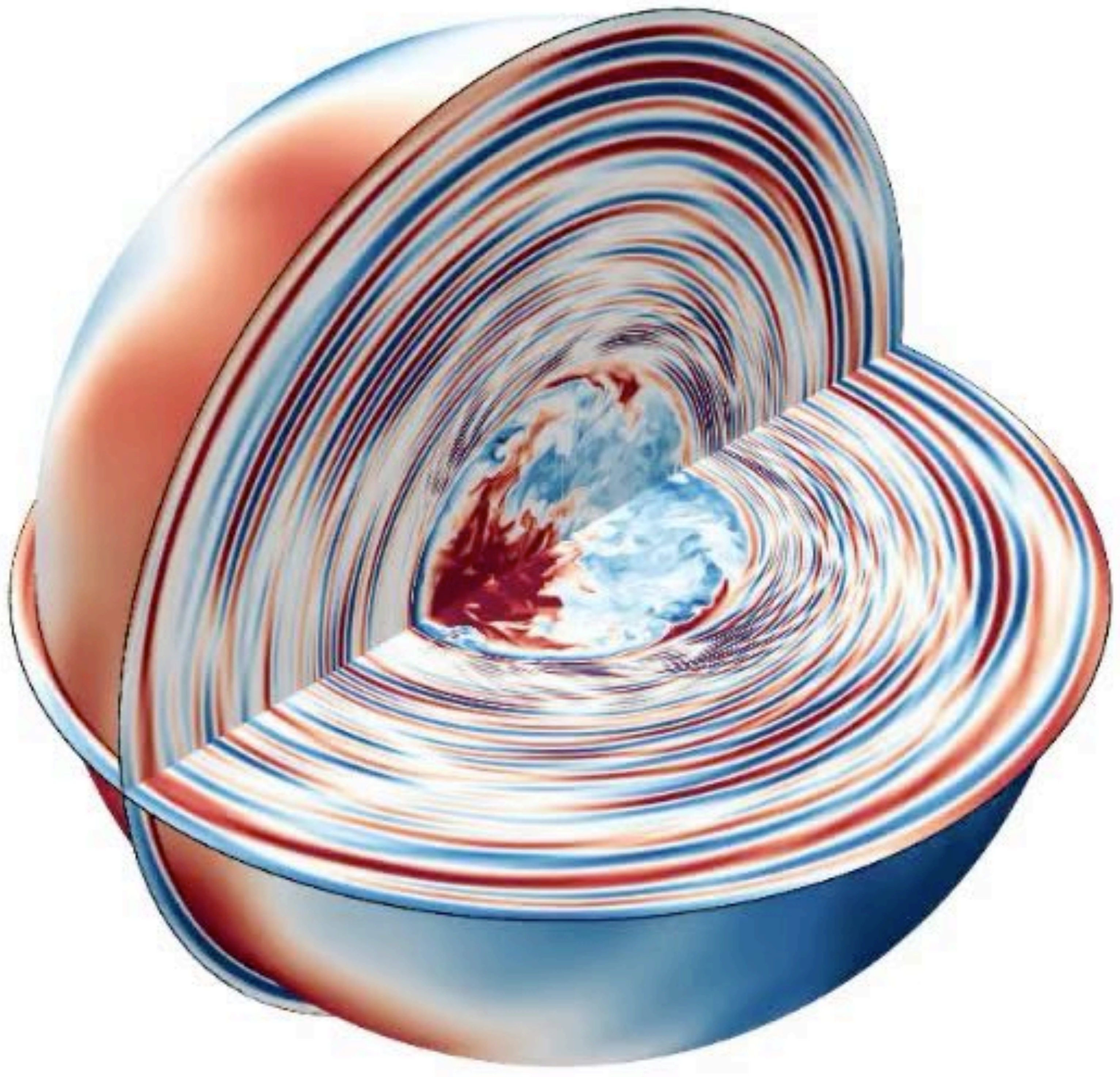


Flexible equations

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:

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

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

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

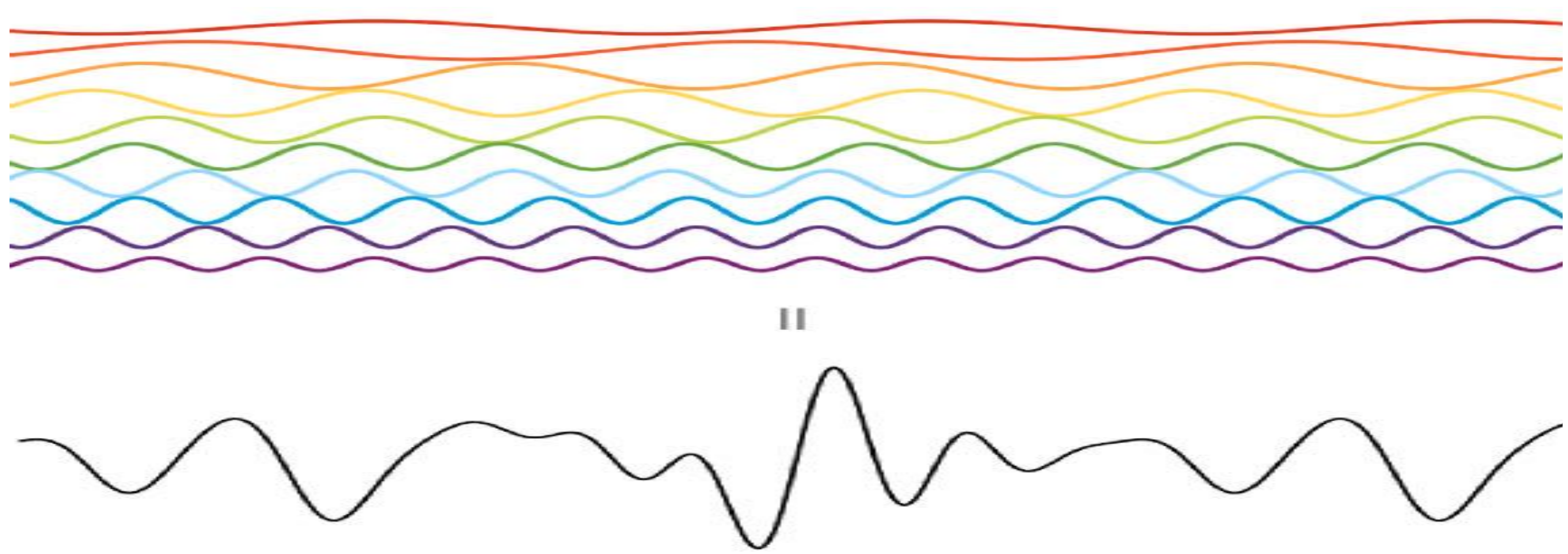
- Easy to adapt to different equations
- **Exponential convergence** for smooth functions
- Only possible in **simple geometries**
- **Fast** if discretized operators are **sparse**
- RHS terms require **spectral transforms**

Fourier spectral methods

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

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

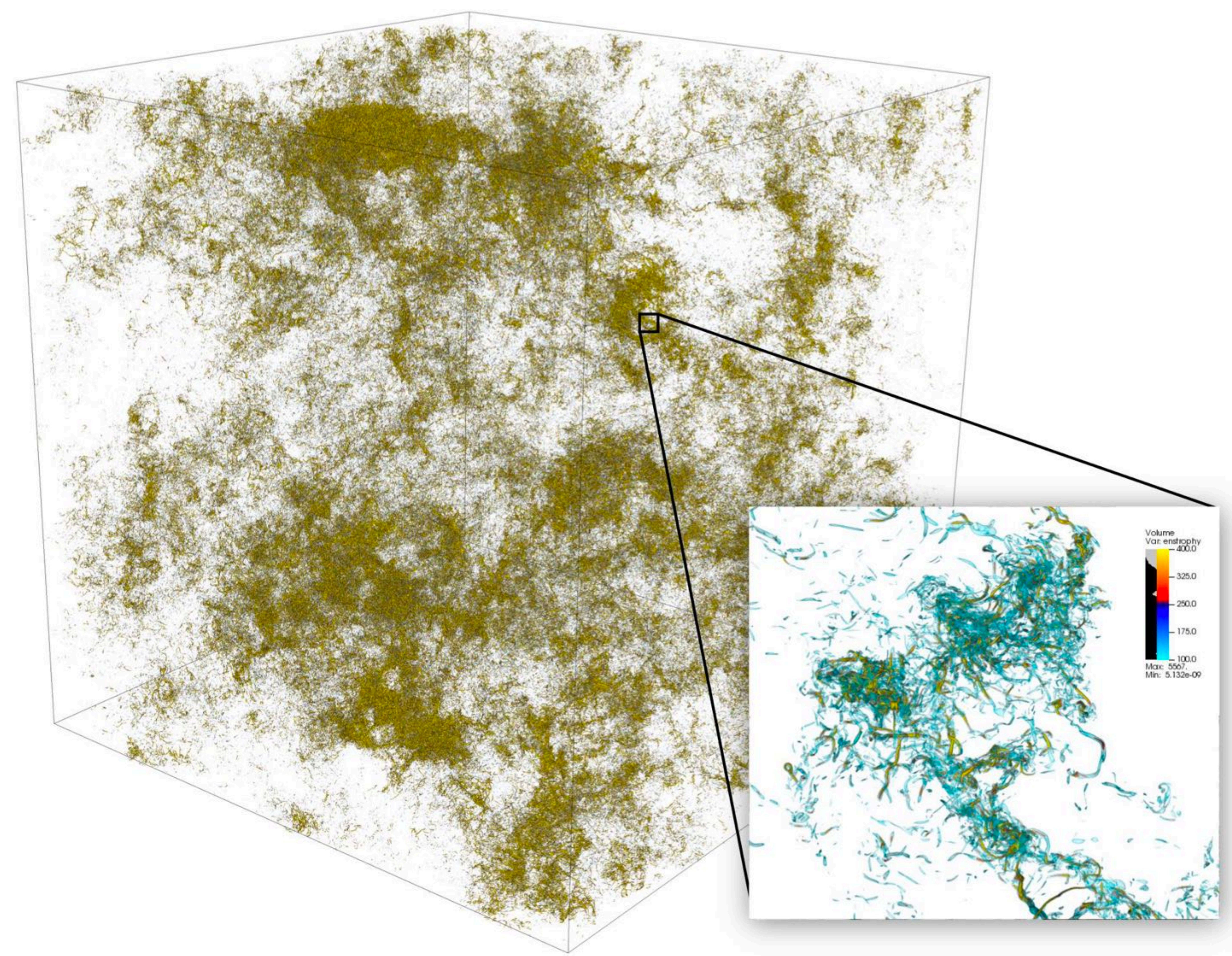
$$\langle \phi_m | \partial_x \phi_n \rangle = in\delta_{m,n}$$



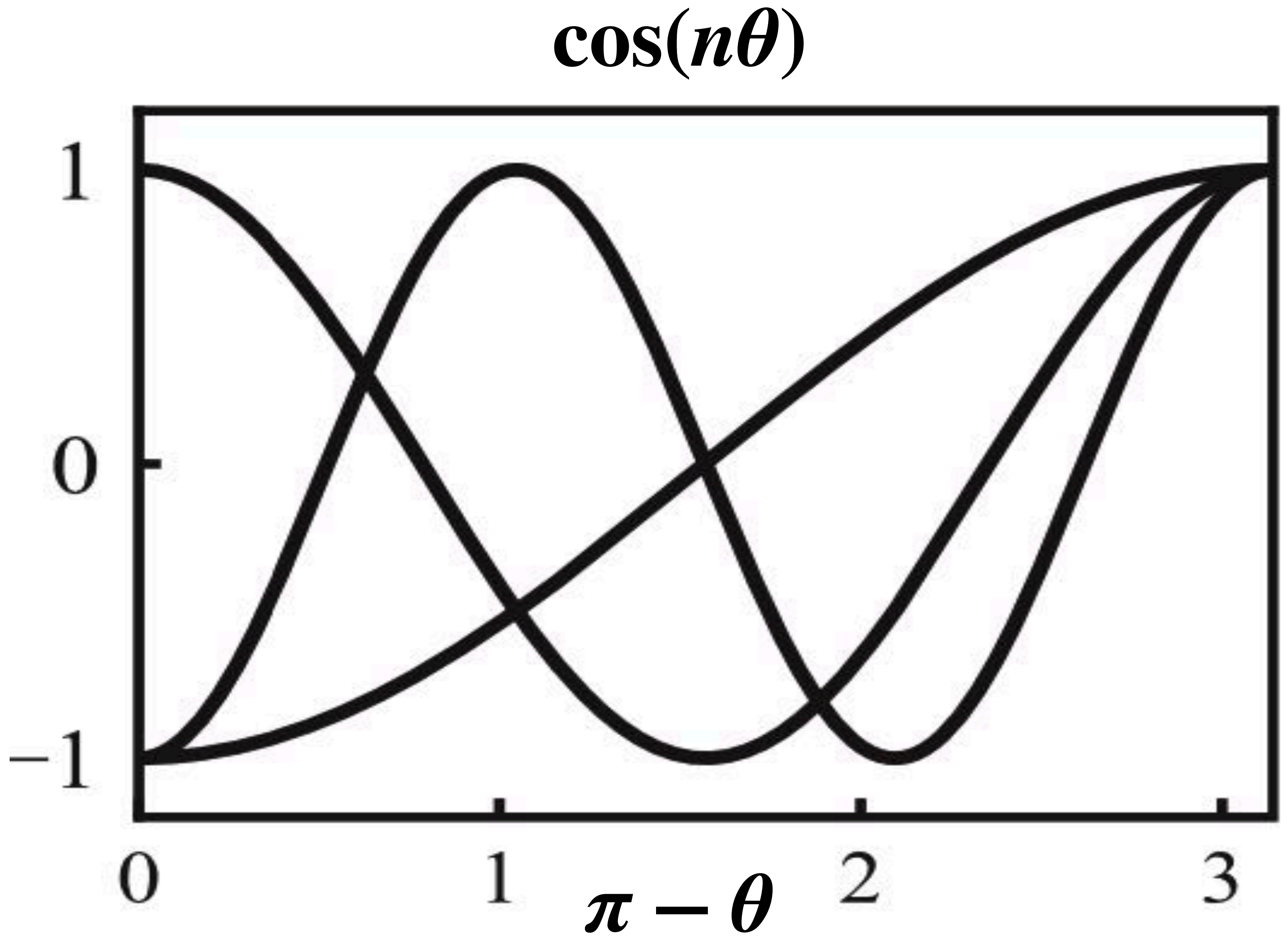
World’s largest turbulence simulations

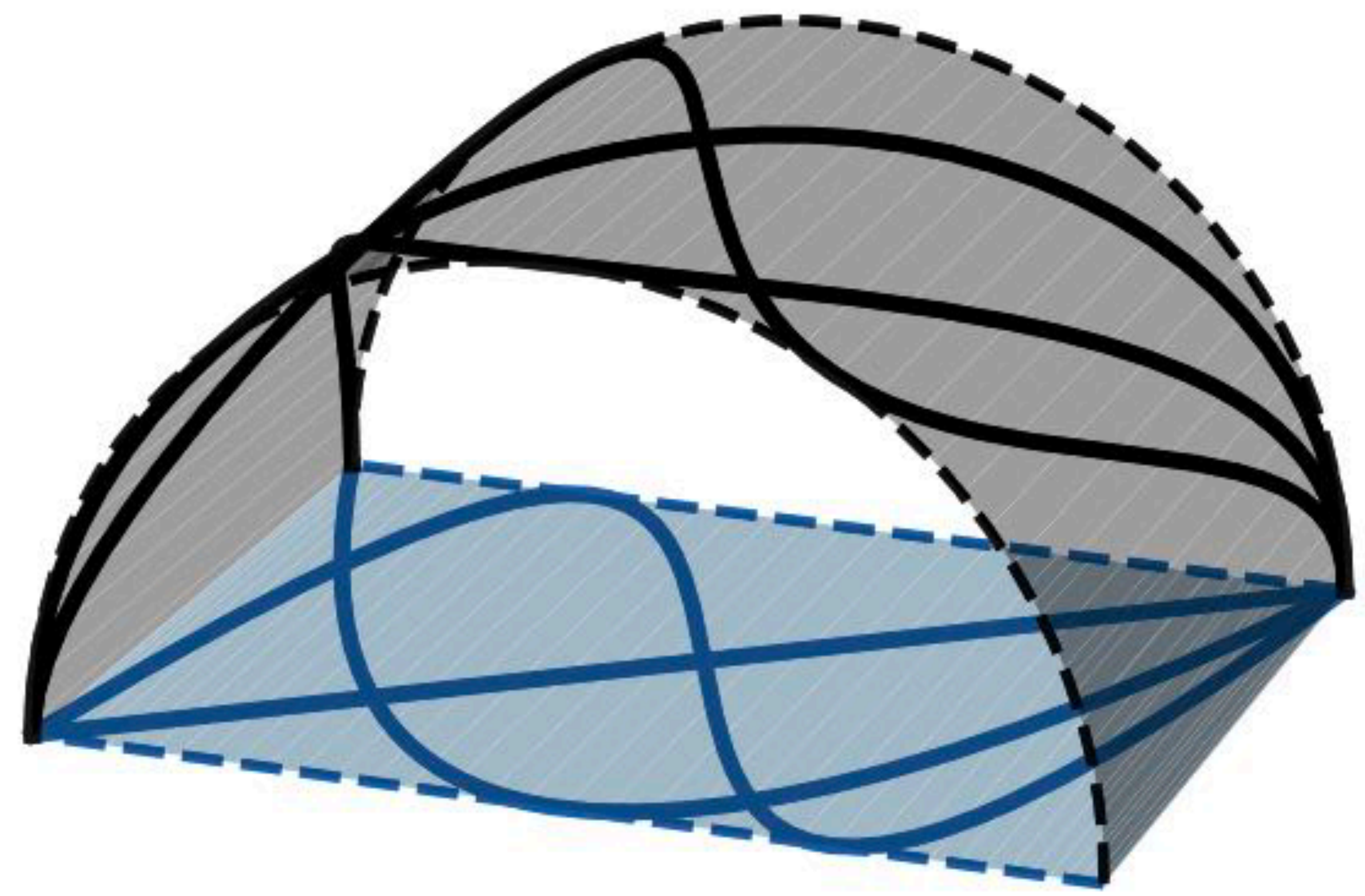
Yeung & Ravikumar, Phys. Rev. Fluids (2021)

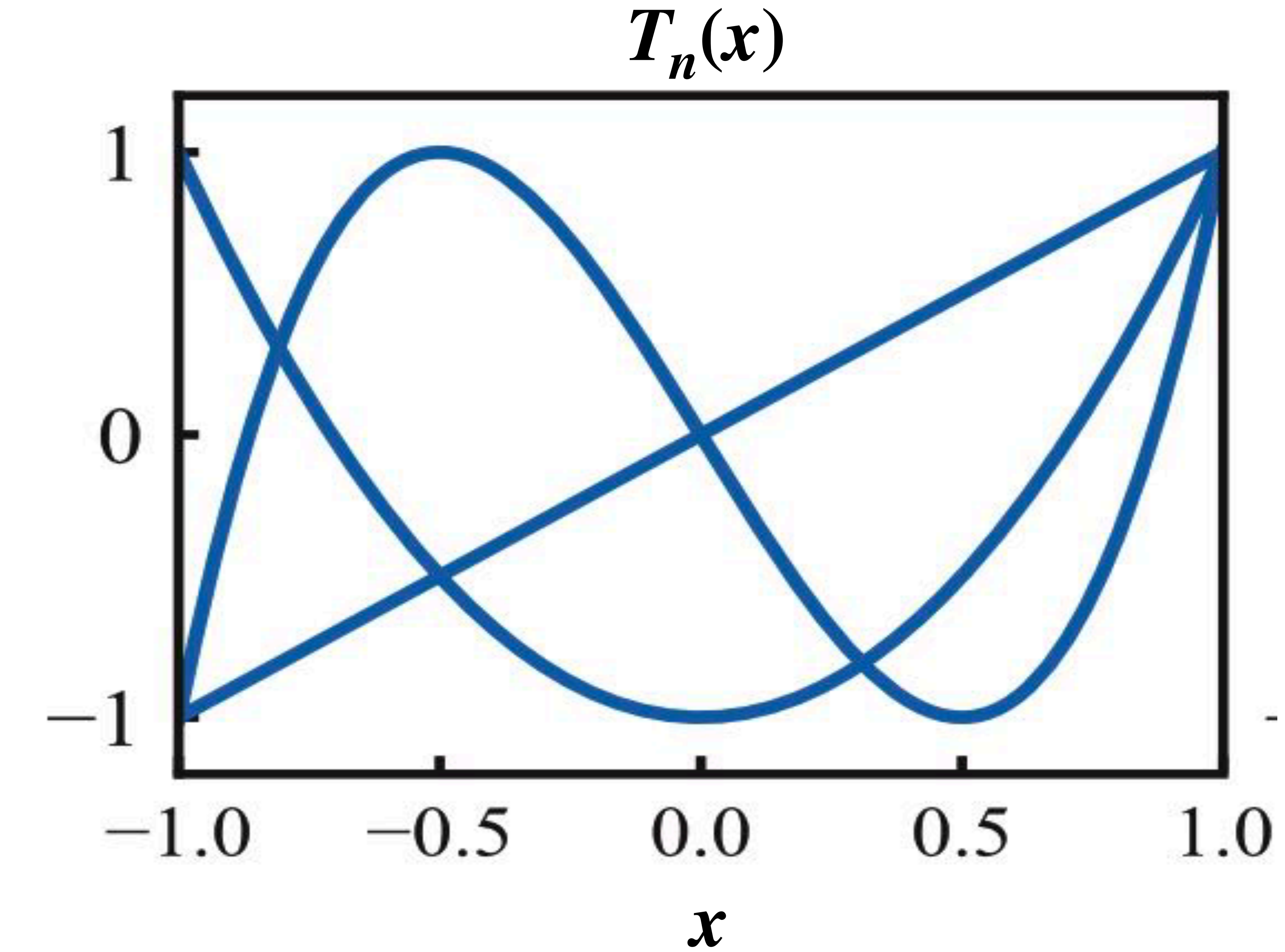
- Fourier pseudospectral method (not Dedalus)
- $18{,}432^3$ grid points
- 18,432 GPUs



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 $(\alpha = \beta = 0)$ $P_n(x)$

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

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

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

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

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

Classical Chebyshev Methods

Same trial & test functions:

E.g. Collocation

$$u(x) = \sum_{i=0}^{N} u(x_i) L_i(x)$$

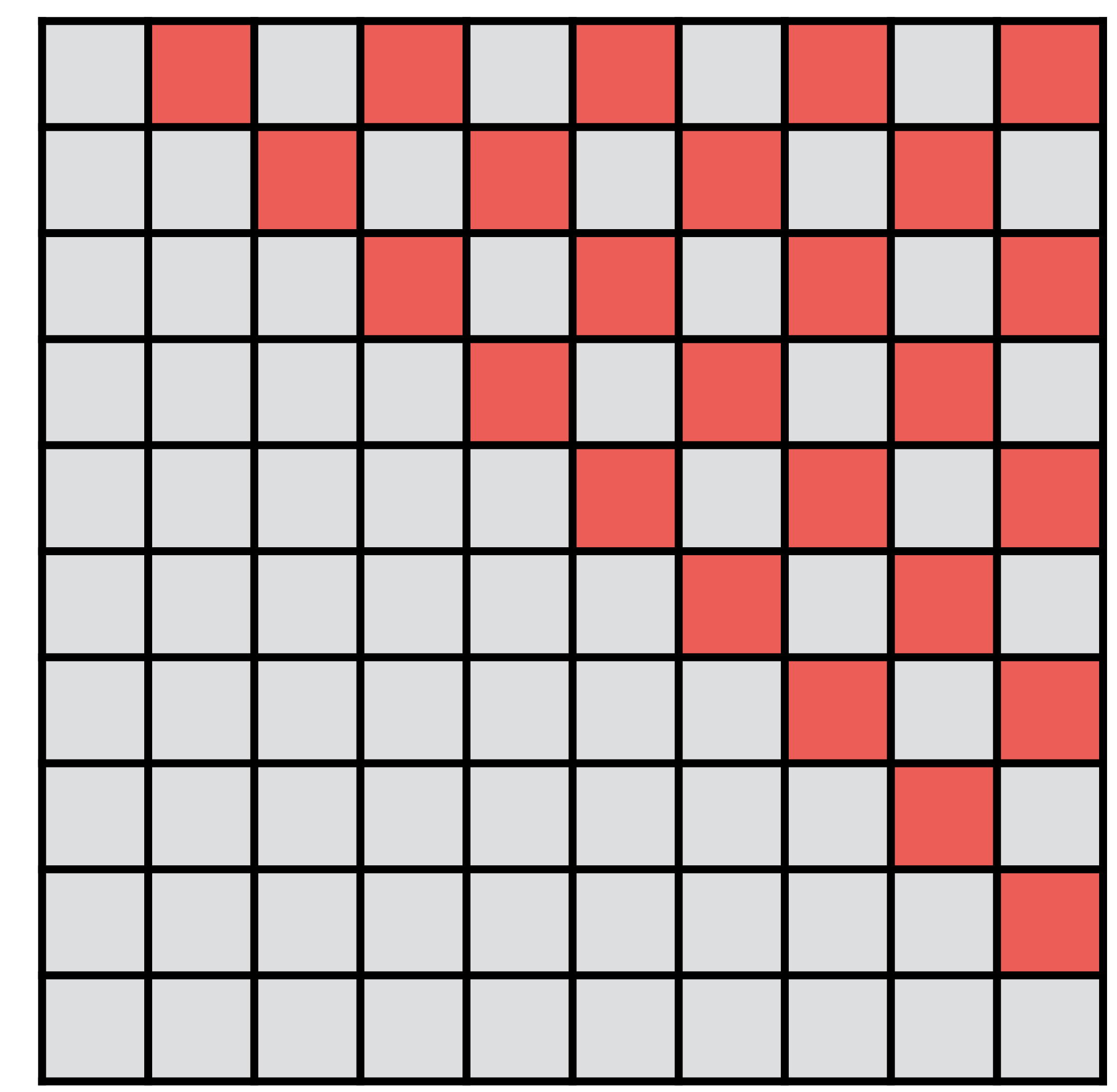
$$L_i(x) = \prod_{j \neq i} \frac{x - x_j}{x_i - x_j}$$

E.g. Chebyshev-tau

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

Differentiation:

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



- Dense matrices
- Poor conditioning

Lanczos, Liu, Ortiz, Gottlieb, Hussaini, Orszag, Trefethen

Sparse Chebyshev Methods

Chebyshev trial functions:

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

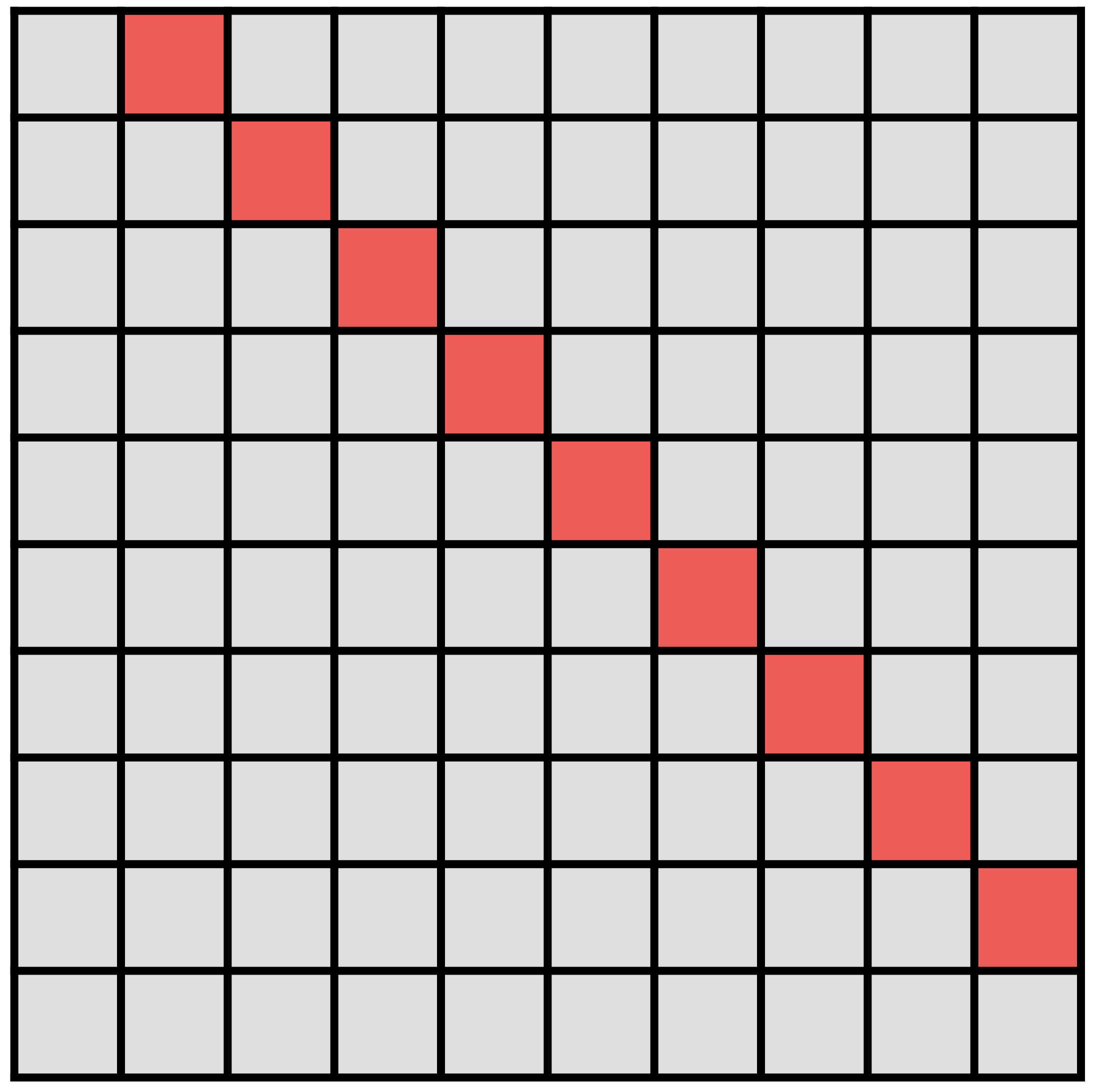
Ultraspherical test functions:

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

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

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**
   - Rapidly convergent approximations

$$\{\phi_i(x)\}$$

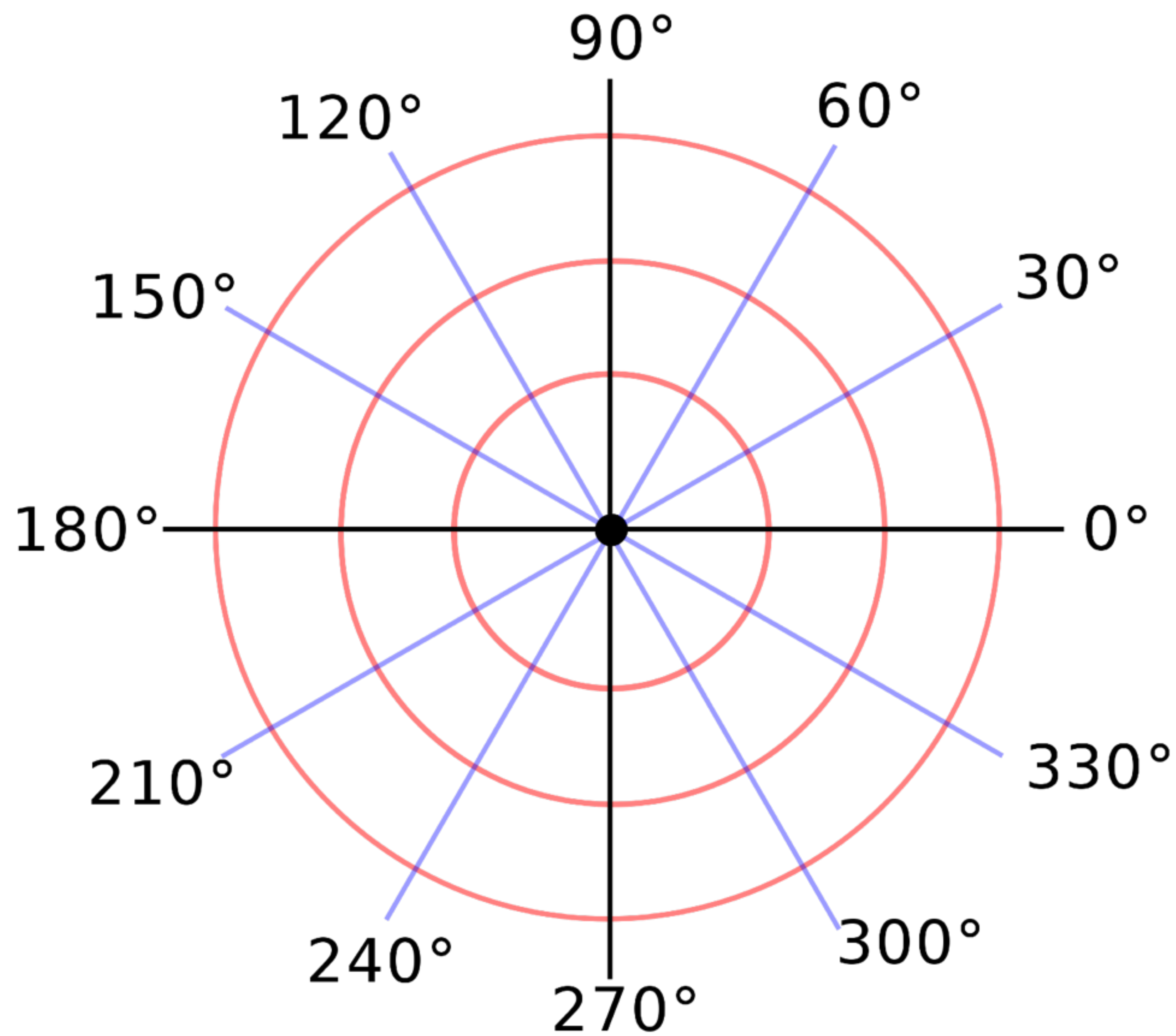
2. **Sparse differential operators**
   - Fast operator evaluation
   - Fast direct solvers for LHS

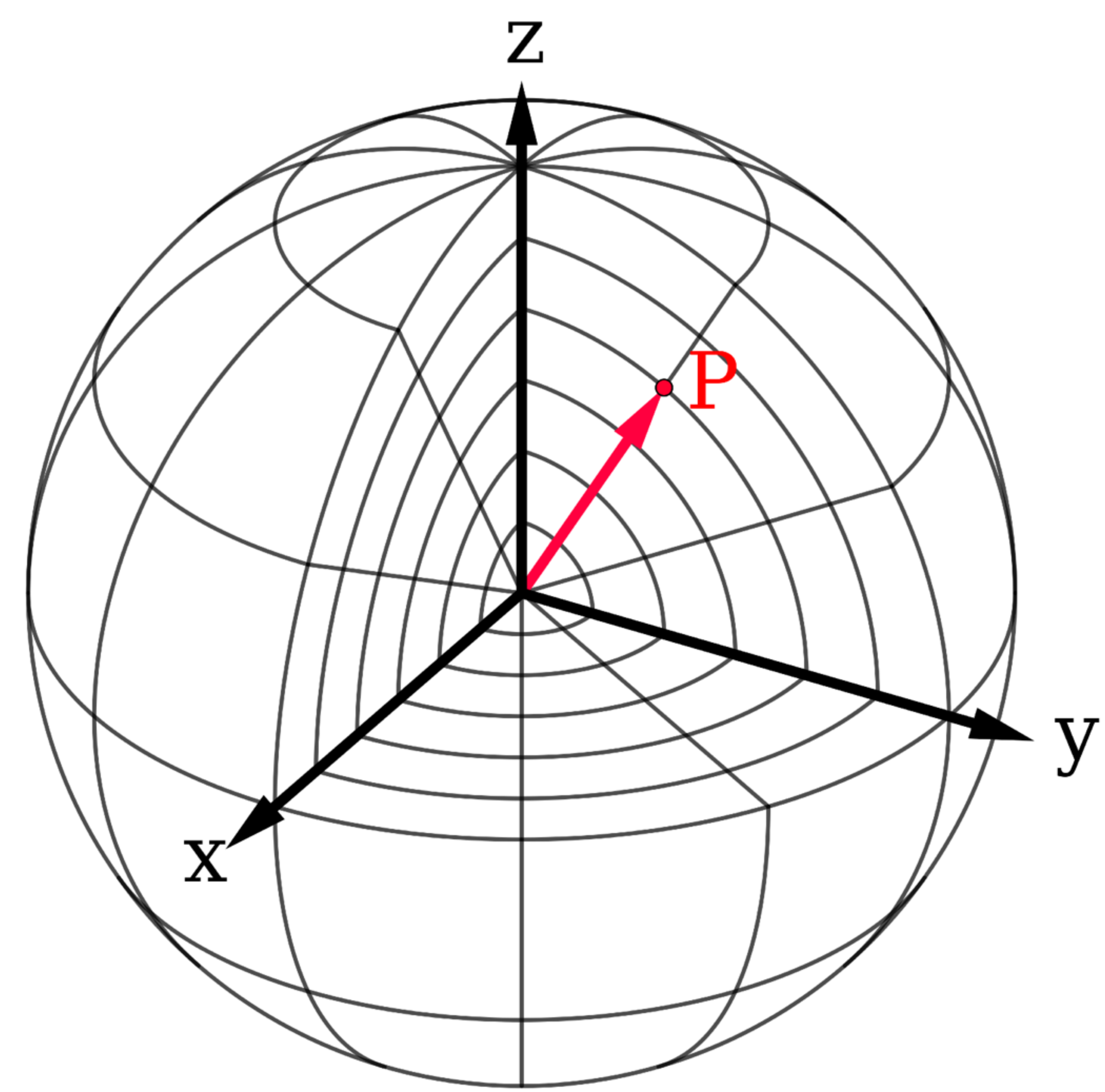
$$\langle \psi_i | H \phi_j \rangle$$

3. **Fast spectral transforms**
   - Fast evaluation of nonlinear RHS

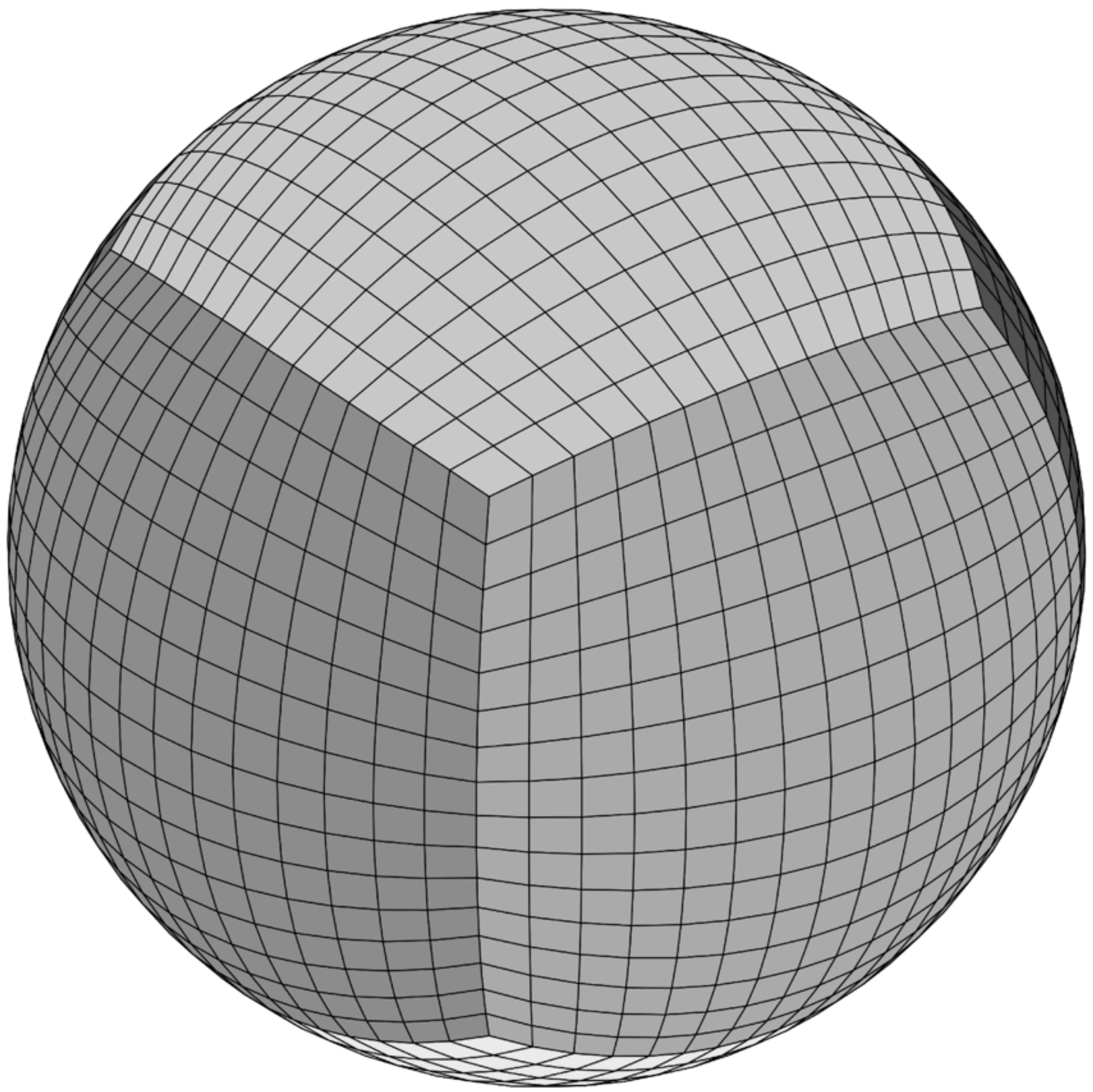
$$F(X)$$

Polar & spherical coordinate singularities

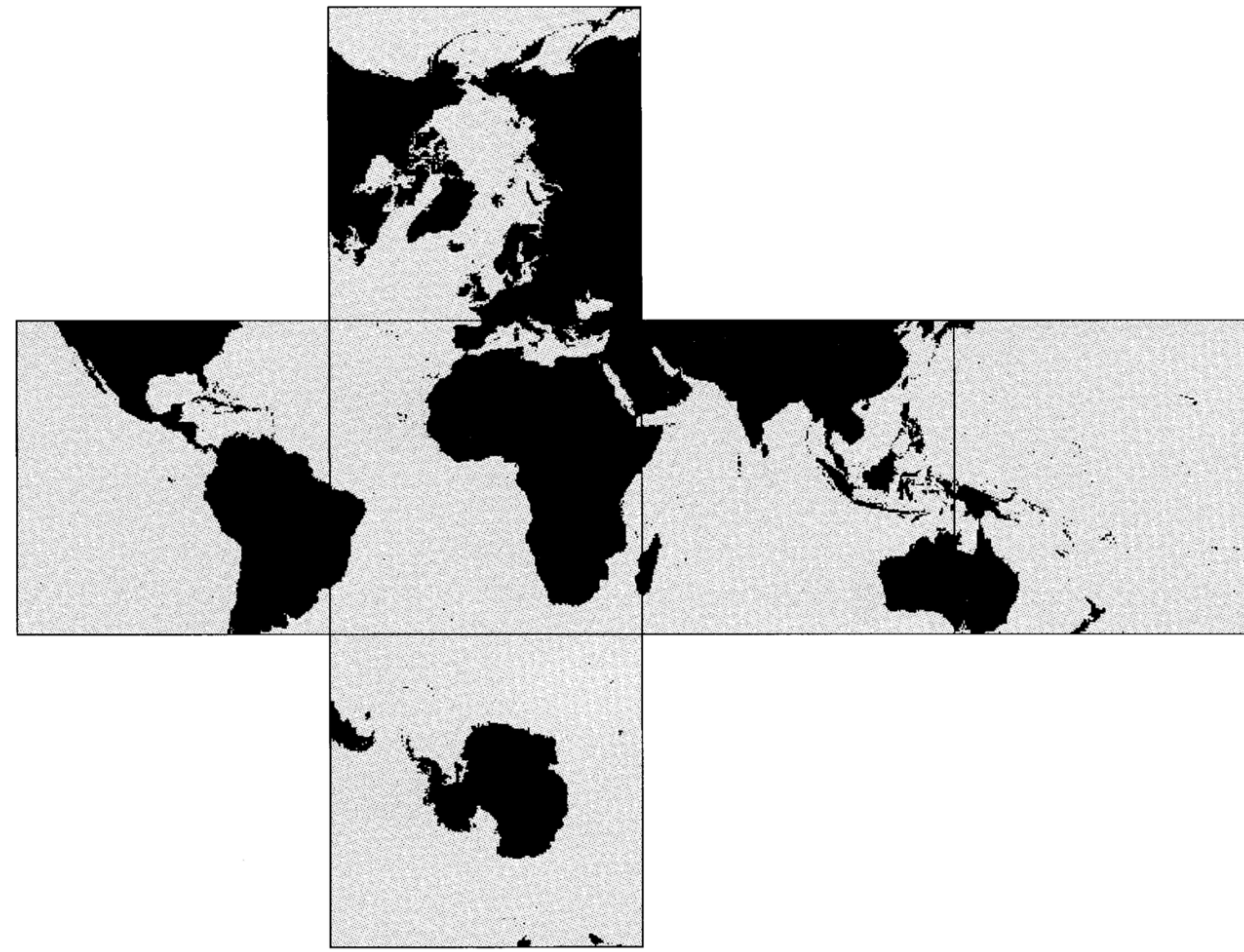




The “cubed sphere” avoids the poles



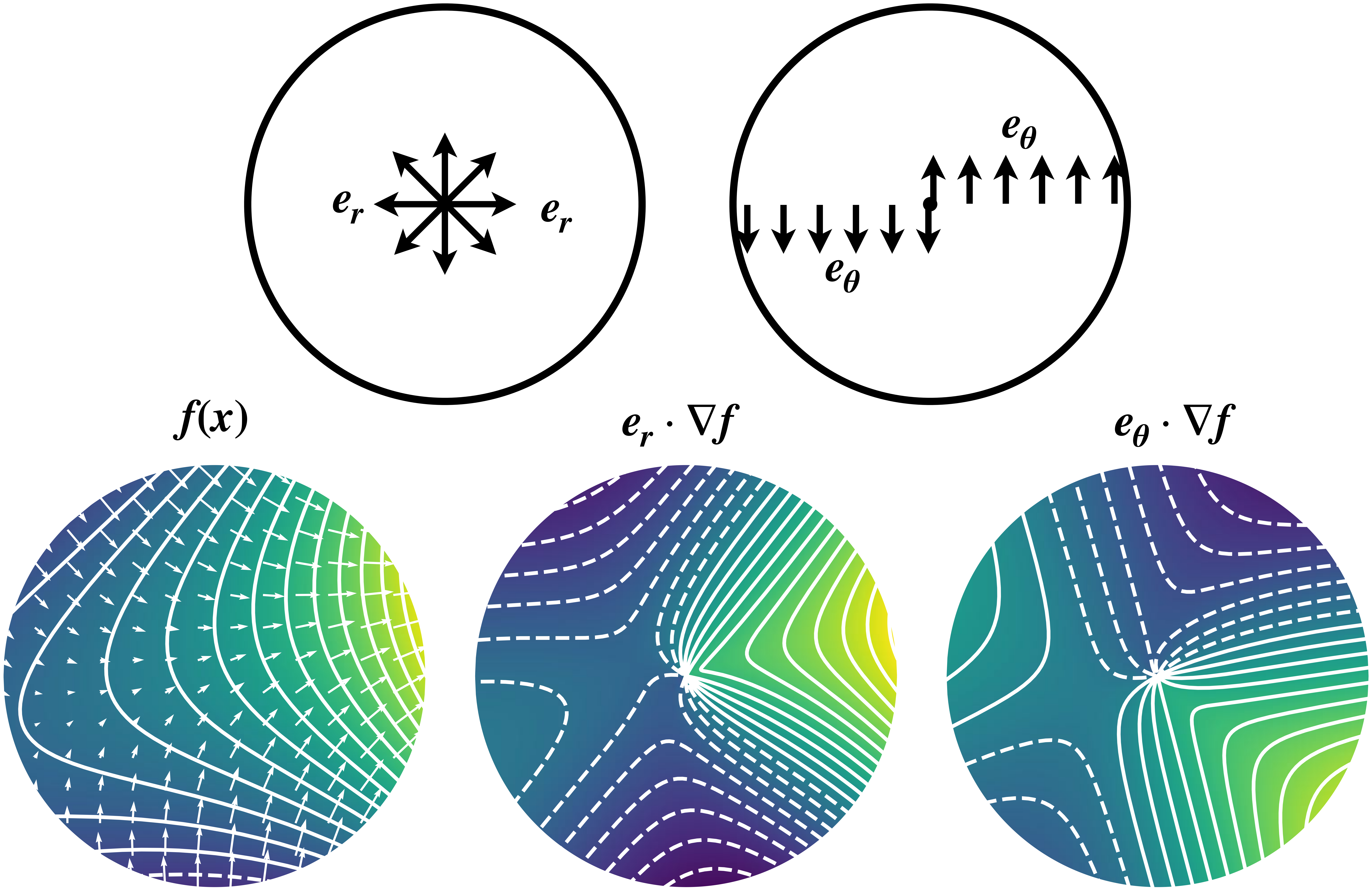
Ullrich (2014)



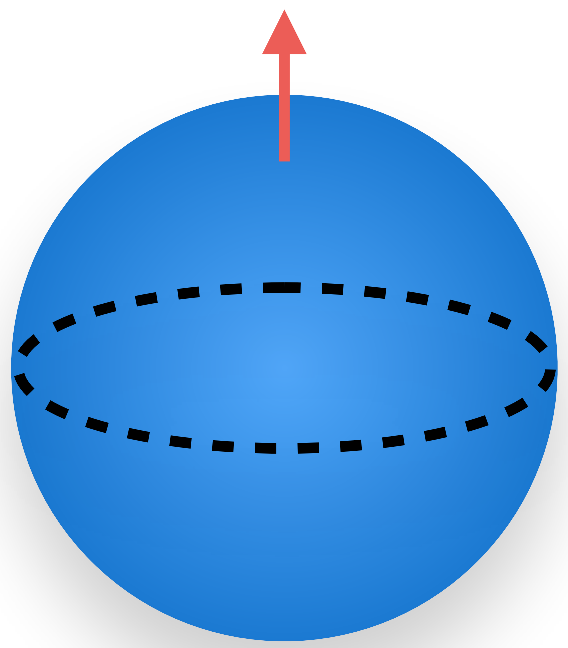
Rochi (1996)

Most codes also cut out the origin

Components of smooth tensors become singular

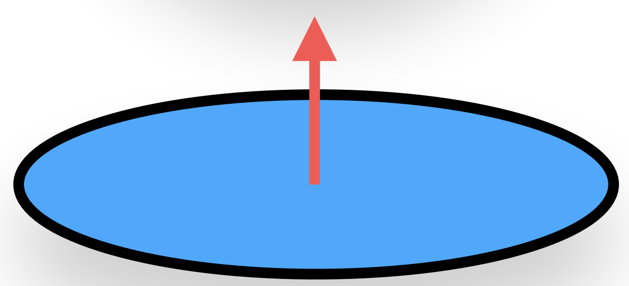


Regularity-aware curvilinear trial functions



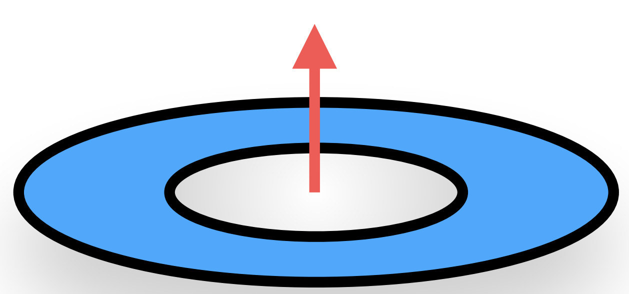
Spheres*: spin-weighted spherical harmonics $\quad Y^{s}_{l,m}(\phi,\theta)$

Newman & Penrose, JMP (1966)



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

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

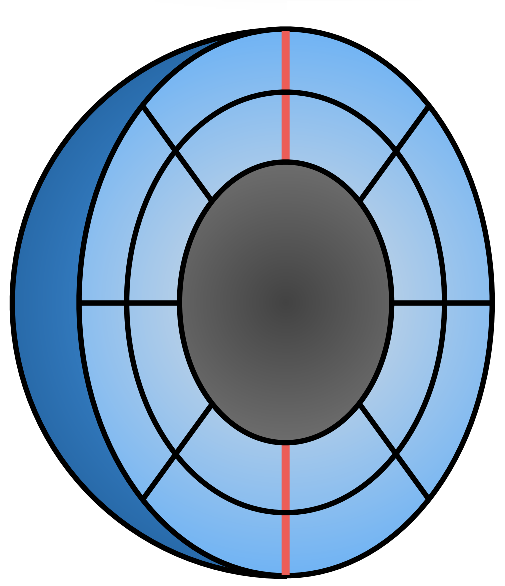


Ar $\quad e^{im\phi}\, r^{-k}\, T_n(r')$

Spectral accuracy for arbitrary tensor fields

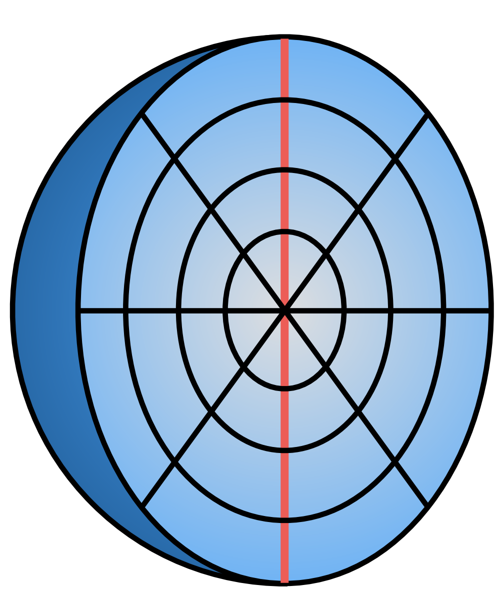
Sparse tensor calculus

No fast transforms*



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

Dedalus collab (+KB)., in prep.



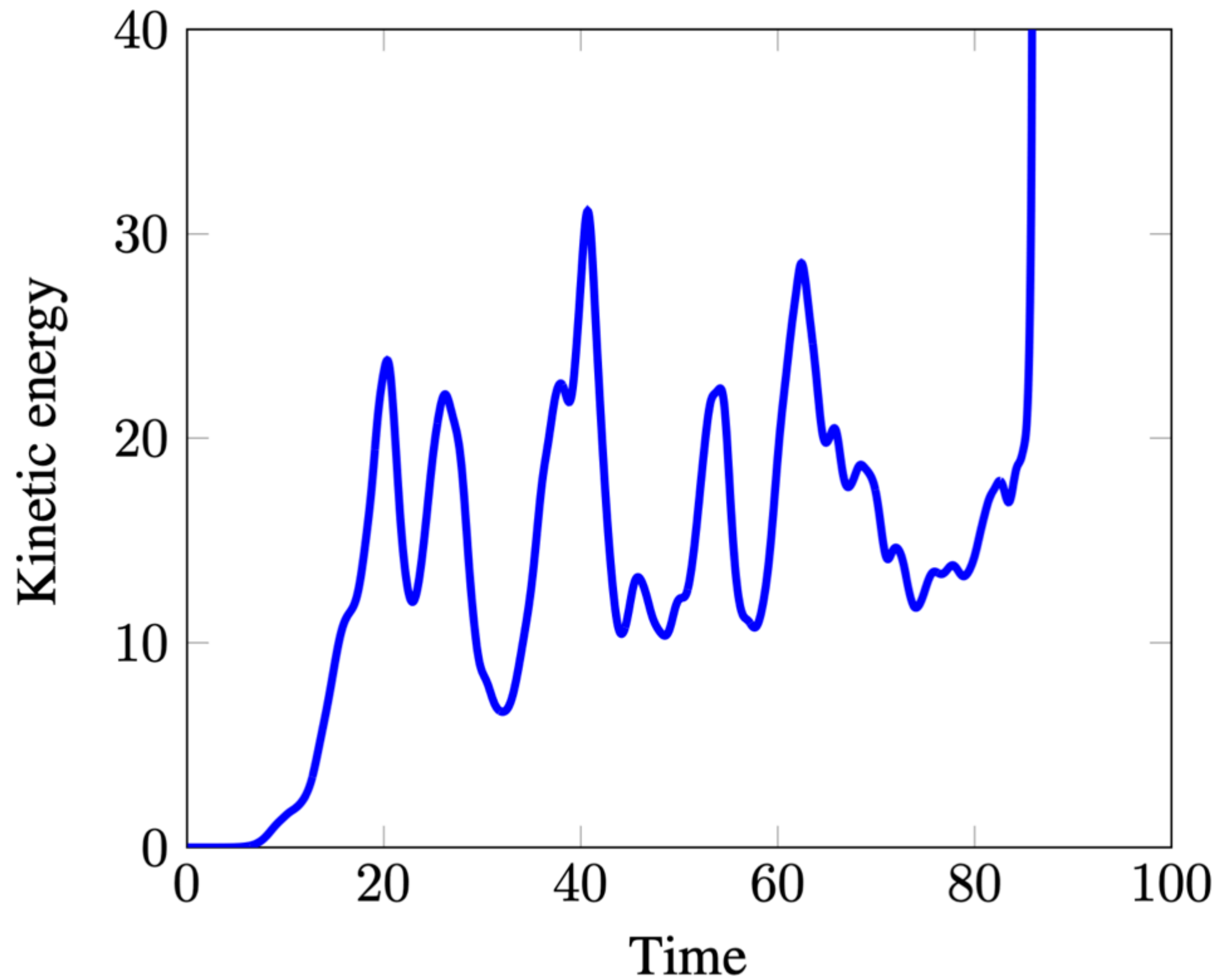
Balls: SWSH + one-sided Jacobi polynomials $\quad Y^{s}_{l,m}\, Q_l^{s,a}\, r^{l+a}\, P_n^{(k,l+a+1/2)}(r')$

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

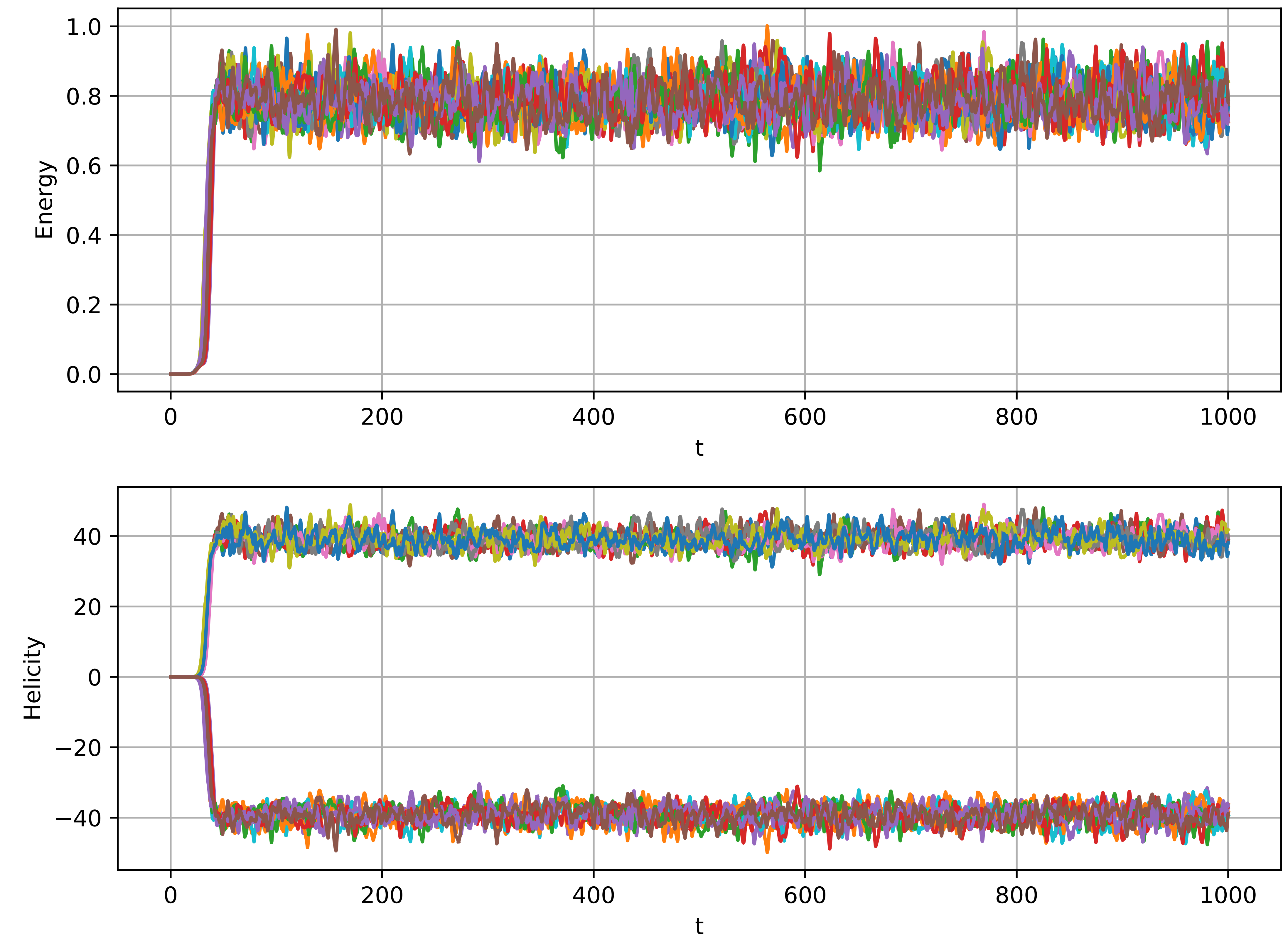
Confined active turbulence

Partial regularity (“Double Fourier”)

Boullé et al. 2021



Exact regularity (Dedalus)



w/ Nico Romeo

Dedalus Project

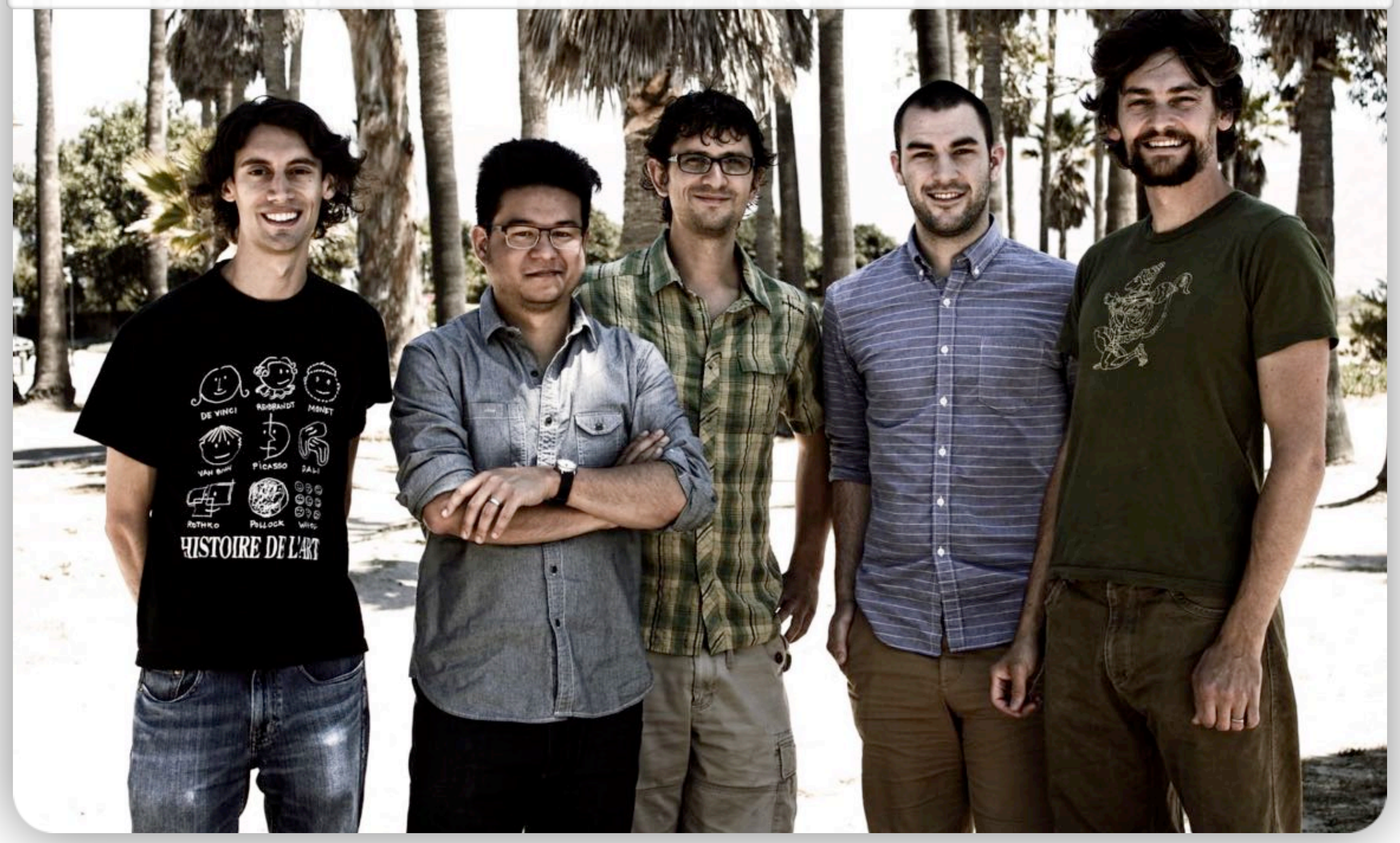
Dedalus Project

Community

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

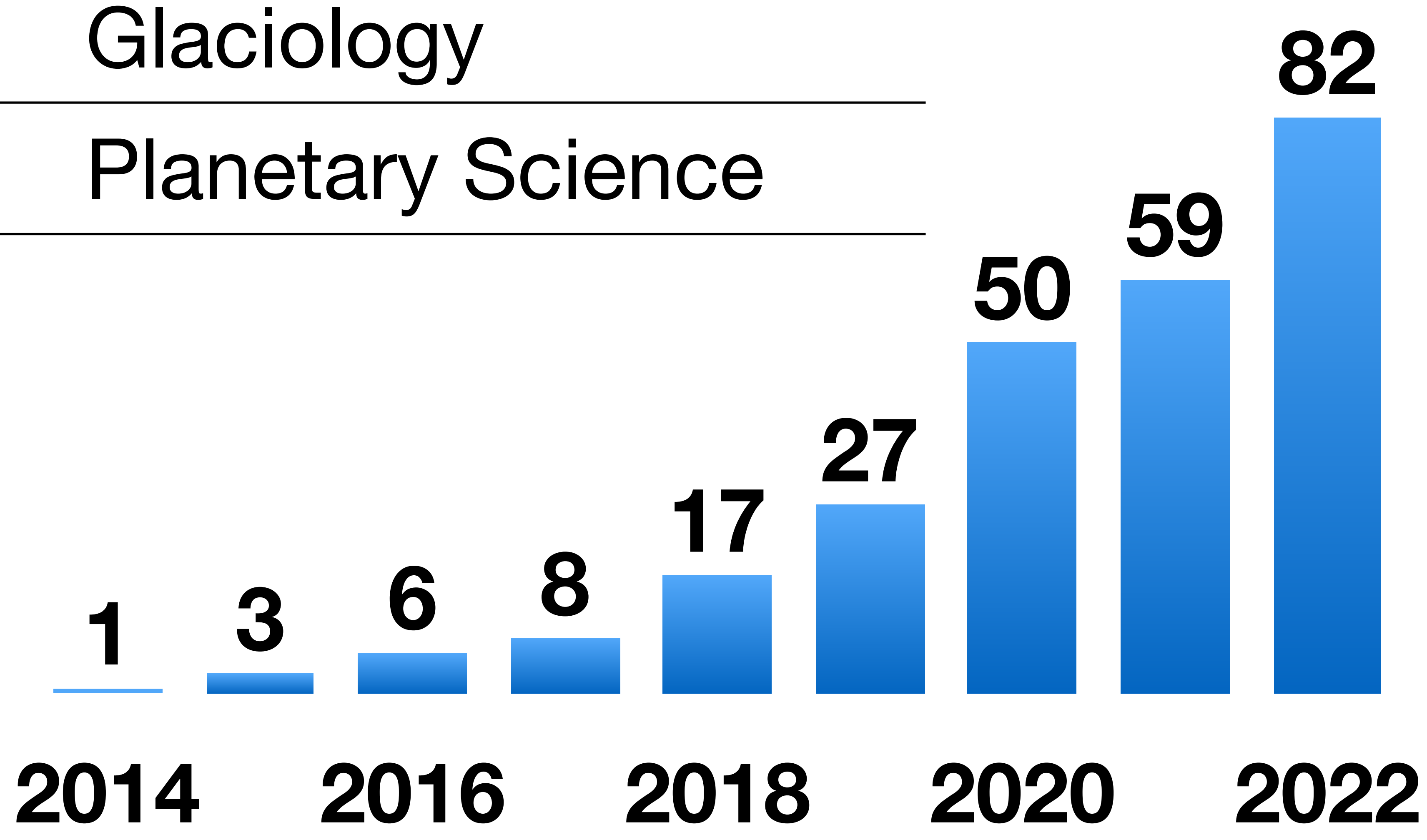
Core developers

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



Publications (300+)

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



Parsing systems of equations

E.g wave equation: $\partial_t^2 u = c^2 \partial_x^2 u \longrightarrow \boxed{\begin{aligned} u_t &= \partial_t u \\ u_x &= \partial_x u \\ \partial_t u_t &= c^2 \partial_x u_x \end{aligned}}$

Operator form: $$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \partial_t \begin{bmatrix} u \\ u_t \\ u_x \end{bmatrix} + \begin{bmatrix} 0 & -1 & 0 \\ \partial_x & 0 & -1 \\ 0 & 0 & -c^2 \partial_x \end{bmatrix} \begin{bmatrix} u \\ u_t \\ u_x \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Matrix form: $$\boxed{\begin{bmatrix} I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & I & 0 \end{bmatrix} \partial_t \begin{bmatrix} u \\ u_t \\ u_x \end{bmatrix} + \begin{bmatrix} 0 & -I & 0 \\ D_x & 0 & -I \\ 0 & 0 & -c^2 D_x \end{bmatrix} \begin{bmatrix} u \\ u_t \\ u_x \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}}$$

$$(D_x)_{ij} = \langle \psi_i | \partial_x \phi_j \rangle$$
$$(I)_{ij} = \langle \psi_i | \phi_j \rangle$$

Maximize sparsity

General form: $$\mathcal{M} \cdot \partial_t \mathcal{X} + \mathcal{L} \cdot \mathcal{X} = \boxed{\mathcal{F}(\mathcal{X})}$$

Evaluated pseudospectrally

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

Vector-invariant PDE specification

```
# Bases
coords = SphericalCoords('phi', 'theta', 'r')
dist = Distributor(coords, mesh=64)
basis = SphereBasis(coords, shape=(1024, 512))

# Fields
p = ScalarField(dist, basis)
u = VectorField(dist, basis)

# Problem
problem = IVP(variables=[p, u])
problem.parameters['Re'] = 1e4
problem.add_equation("dt(u) - Lap(u)/Re + grad(p) = - u@grad(u)")
problem.add_equation("div(u) + integ(p) = 0")

# Solver
solver = problem.build_solver(timestepper='RK443')
solver.step(dt=1e-3)
```

Automatically MPI parallelized

No reduction to scalar potentials
Extends to compressible flows

LHS parsed into sparse system for implicit integration of stiff terms & constraints

Incompressible hydrodynamics

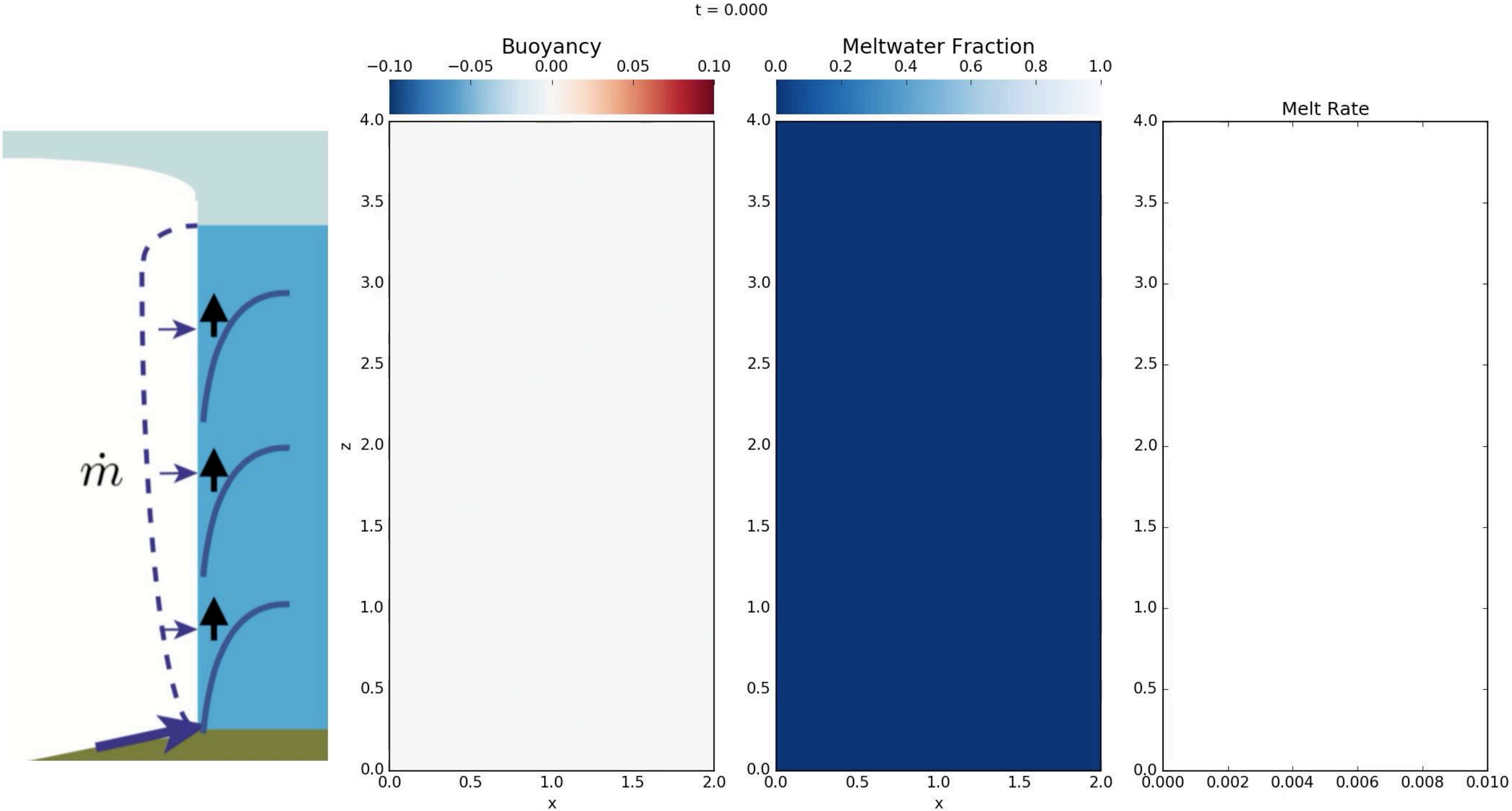
$$\mathcal{M} \cdot \partial_t \mathcal{X} + \mathcal{L} \cdot \mathcal{X} = \mathcal{F}(\mathcal{X})$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \partial_t \begin{bmatrix} u \\ v \\ p \end{bmatrix} + \begin{bmatrix} -\nu\nabla^2 & 0 & \partial_x \\ 0 & -\nu\nabla^2 & \partial_y \\ \partial_x & \partial_y & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ p \end{bmatrix} = \begin{bmatrix} -\vec{u} \cdot \nabla u \\ -\vec{u} \cdot \nabla v \\ 0 \end{bmatrix}$$

Directly coupled formulation:

- Explicitly enforce divergence constraint
- Pressure determined as Lagrange multiplier
- No splitting / pressure boundary conditions
- Allows for high-order DAE timesteppers

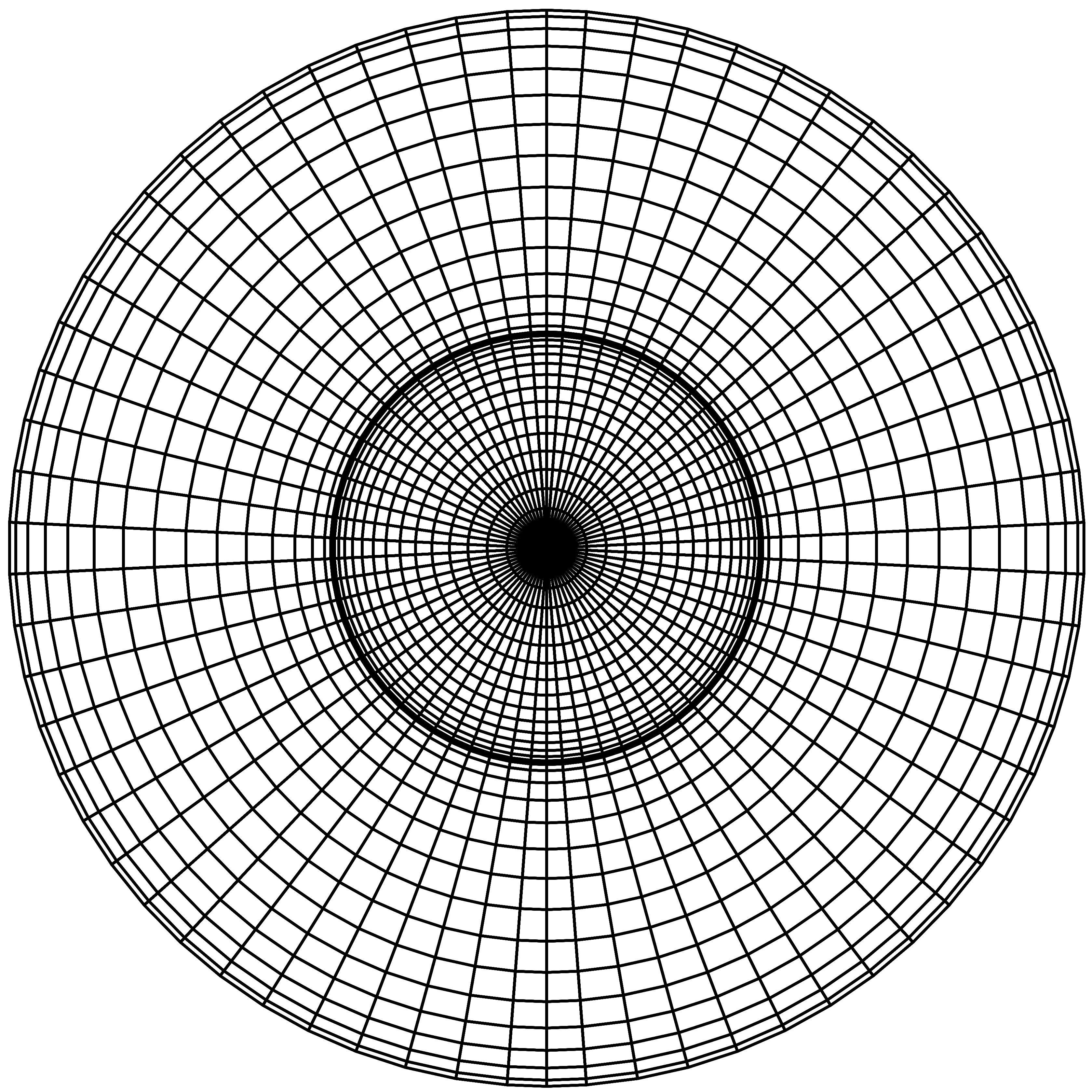
Turbulent enhancement of glacier melting

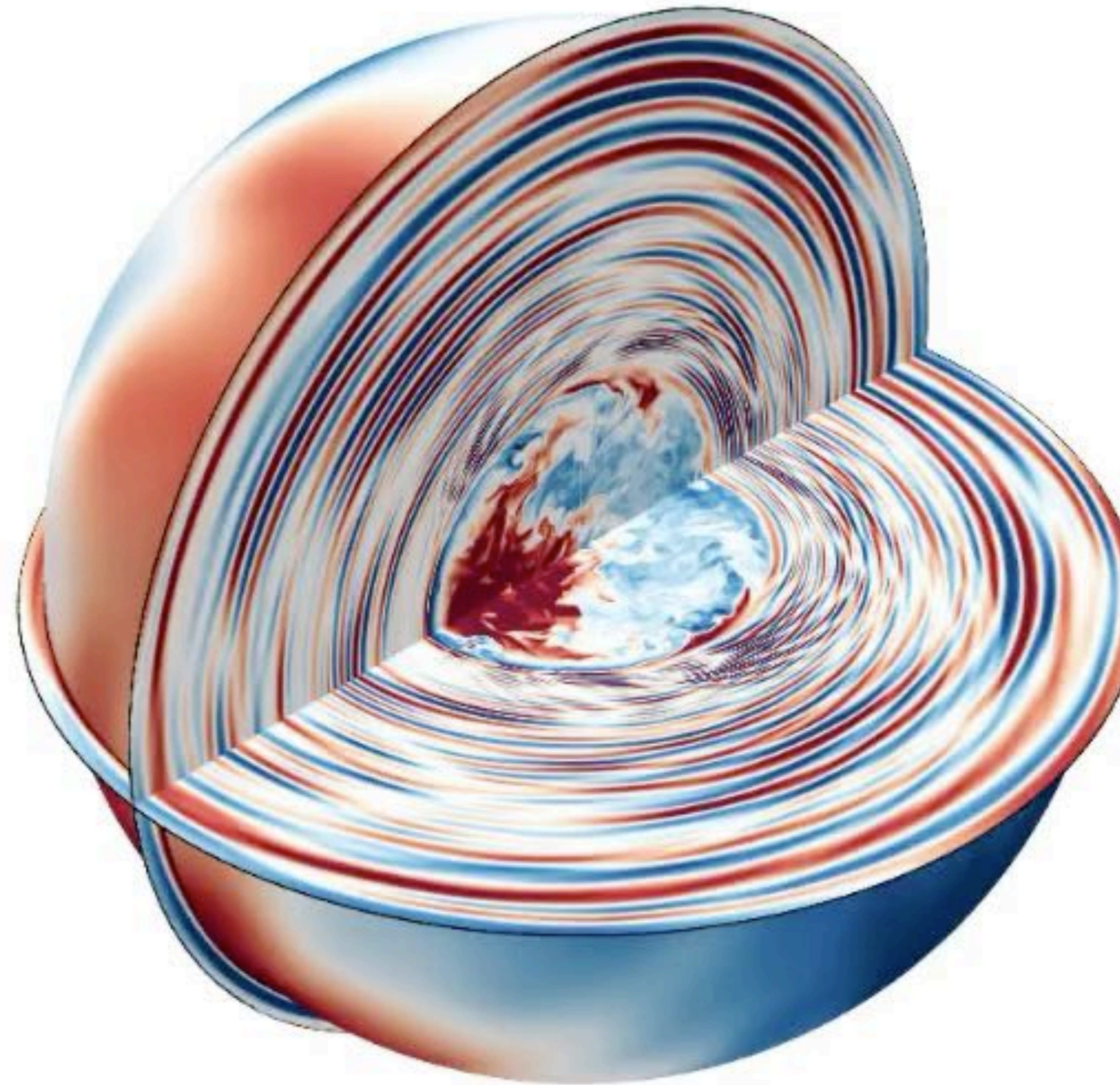


Burns (2018)

High-*p* spherical spectral elements

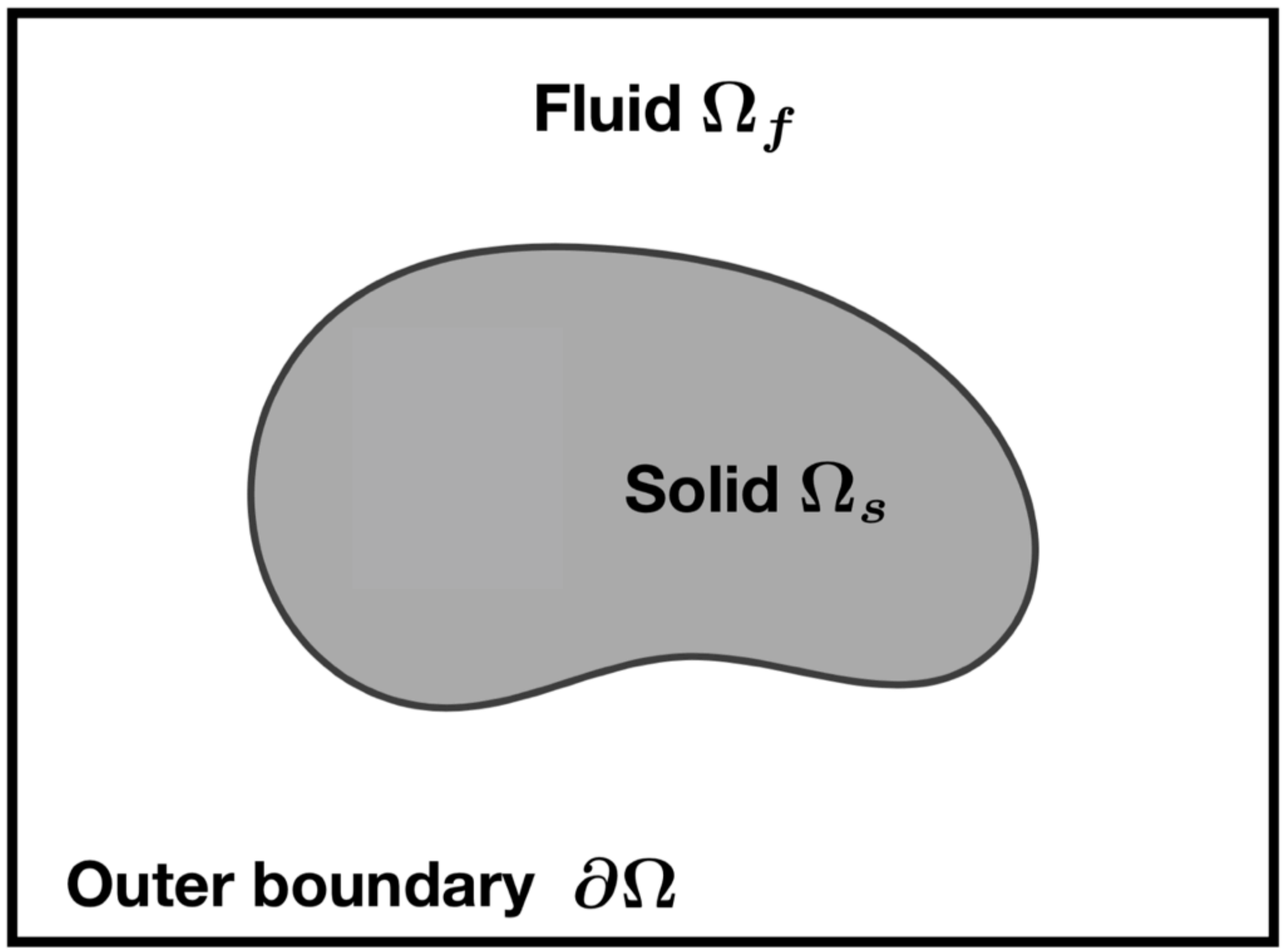
- Stacked ball and spherical shell bases
- Resolves internal/material boundaries





w/ Evan Anders

Immersed boundary methods



Volume penalization:

Damp solution to reference

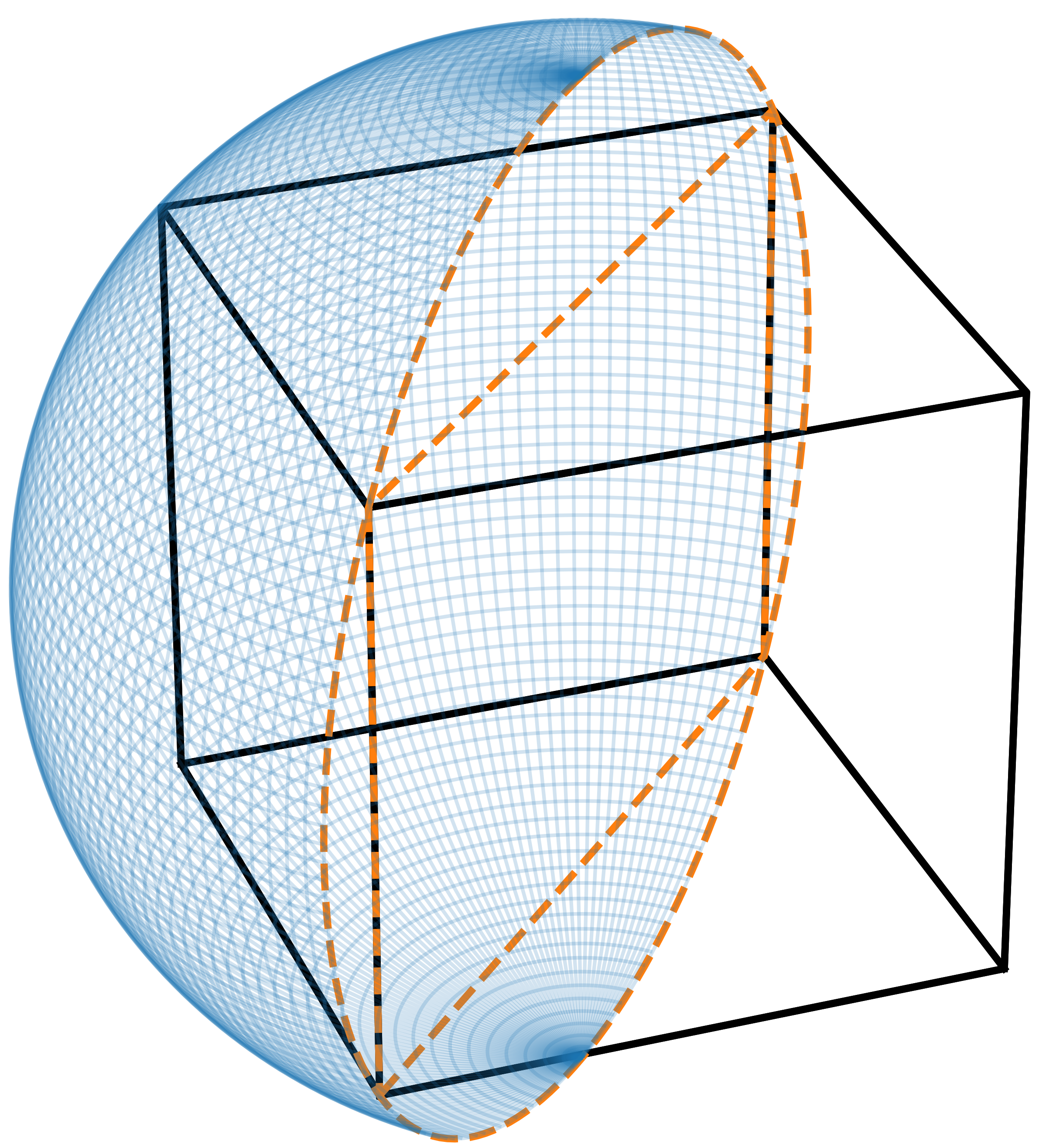
$$\partial_t \vec{u} = \ldots - \gamma M(\vec{x})(\vec{u} - \vec{u}_{\mathrm{ref}})$$

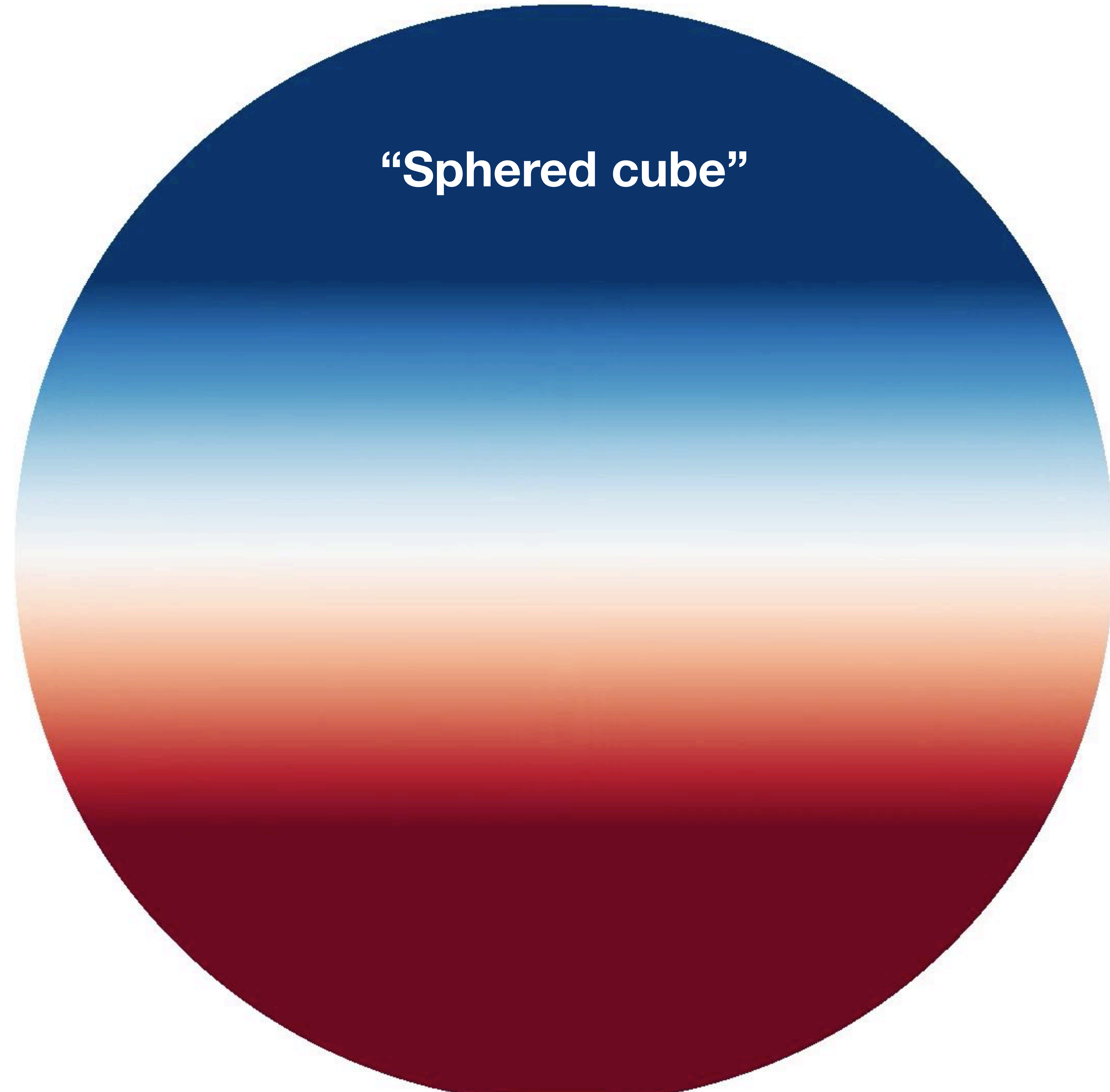
Dedalus: easily add forcing, modify mask

Recent work: optimize mask/damping for 2nd order convergence (*Hester et al. 2020)*

Convection in a cube

Immersed boundaries





Burns et al. (2019)

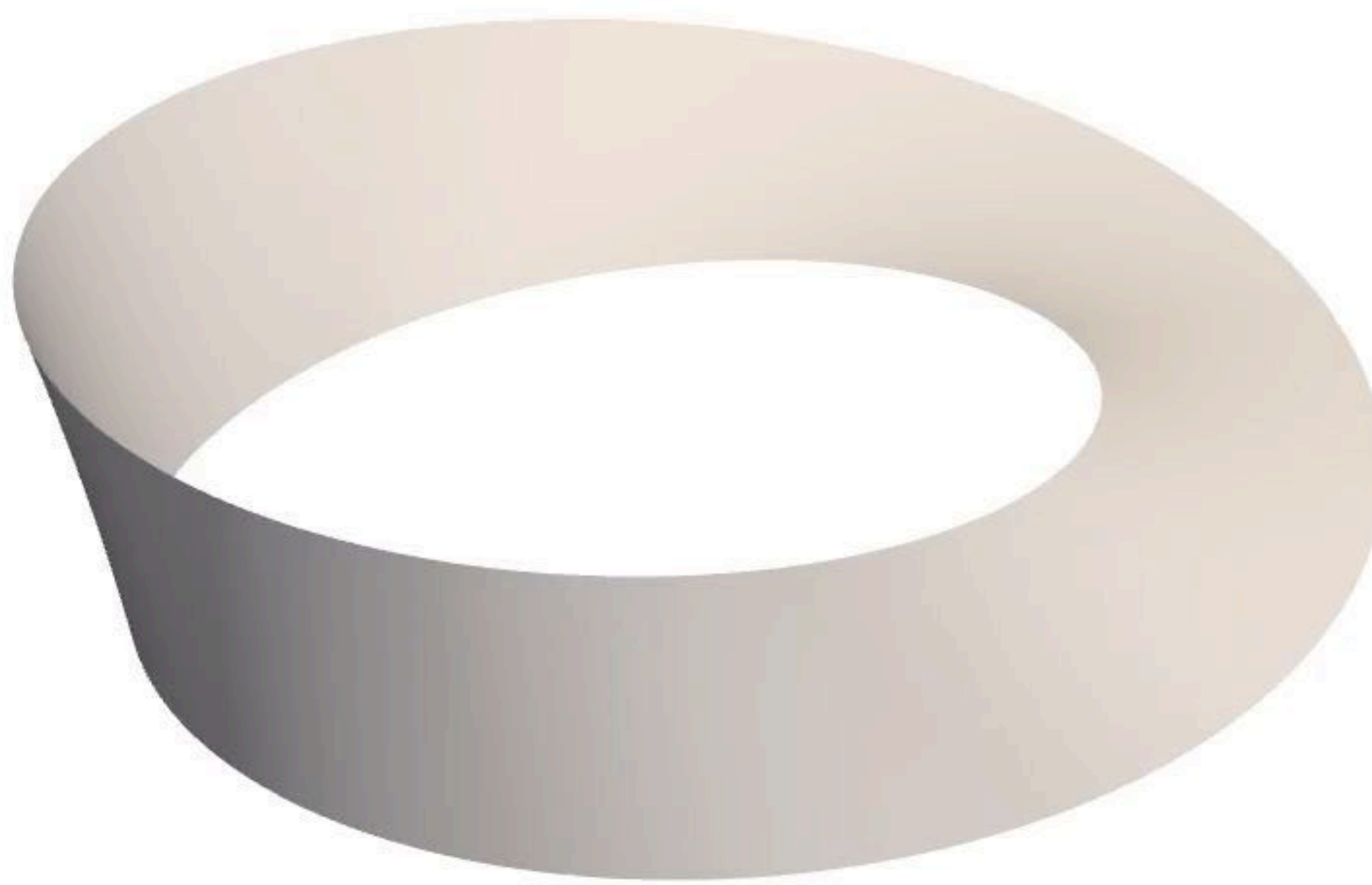
Quantum graphs

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

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