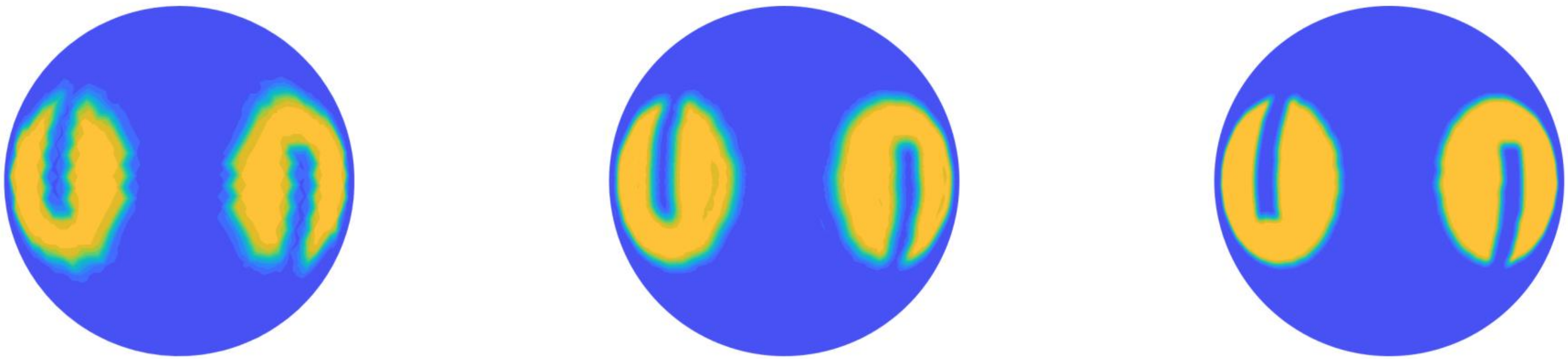

Atmospheric Dynamics with Polyharmonic Spline RBFs

Greg Barnett

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Outline

- Polyharmonic Spline (PHS) RBFs with Polynomials
  - 1D Example
- Interpolation and Differentiation Weights
  - Interpolation/Weights in 2D
  - Weights on the Sphere
- Semi-Lagrangian Transport
  - Governing Equations
  - Limiter/Fixer
  - Test Cases
  - Results
- Eulerian Shallow Water Model
  - Governing Equations
  - Test Cases
  - Results
- Conclusions and Future Work

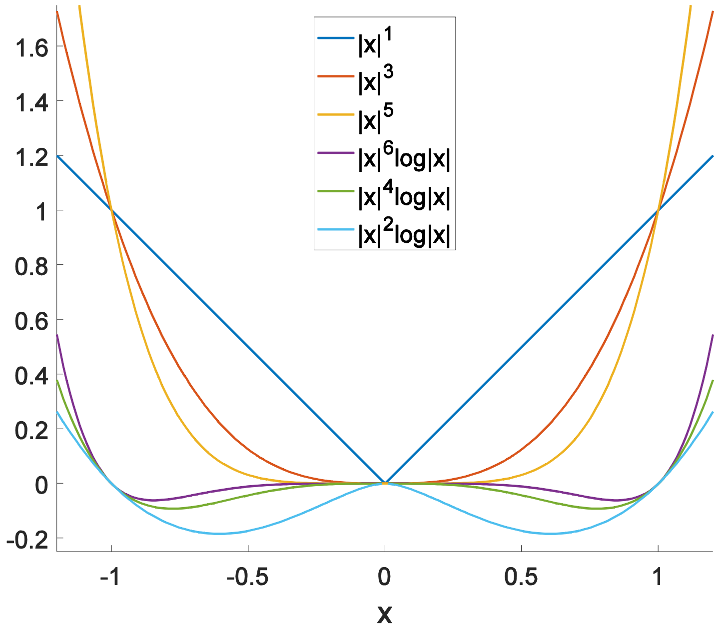
Table of RBFs

$\phi(\boldsymbol{x}), \boldsymbol{x} \in \mathbb{R}^d, \varepsilon \in \mathbb{R}$	Name (acronym)
$\sqrt{1+(\varepsilon\|\boldsymbol{x}\|)^2}$	Multiquadric (MQ)
$\dfrac{1}{1+(\varepsilon\|\boldsymbol{x}\|)^2}$	Inverse Quadratic (IQ)
$\dfrac{1}{\sqrt{1+(\varepsilon\|\boldsymbol{x}\|)^2}}$	Inverse Multiquadric (IMQ)
$e^{-(\varepsilon\|\boldsymbol{x}\|)^2}$	Gaussian (GA)
$\|\boldsymbol{x}\|^{2k+1}$ $\|\boldsymbol{x}\|^{2k}\log\|\boldsymbol{x}\|, k \in \mathbb{N}$	Polyharmonic Spline (PHS)

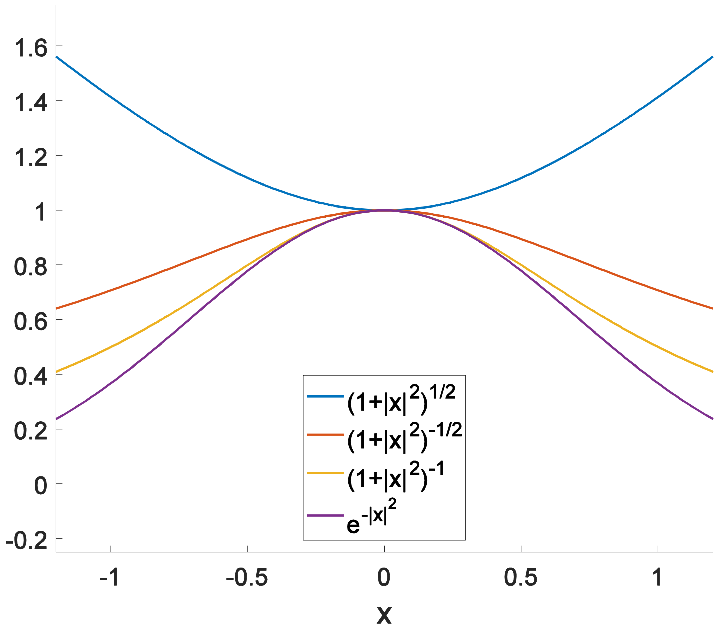
$$\|\cdot\| = \|\cdot\|_2$$

Some RBFs in 1D

Polyharmonic Spline RBFs

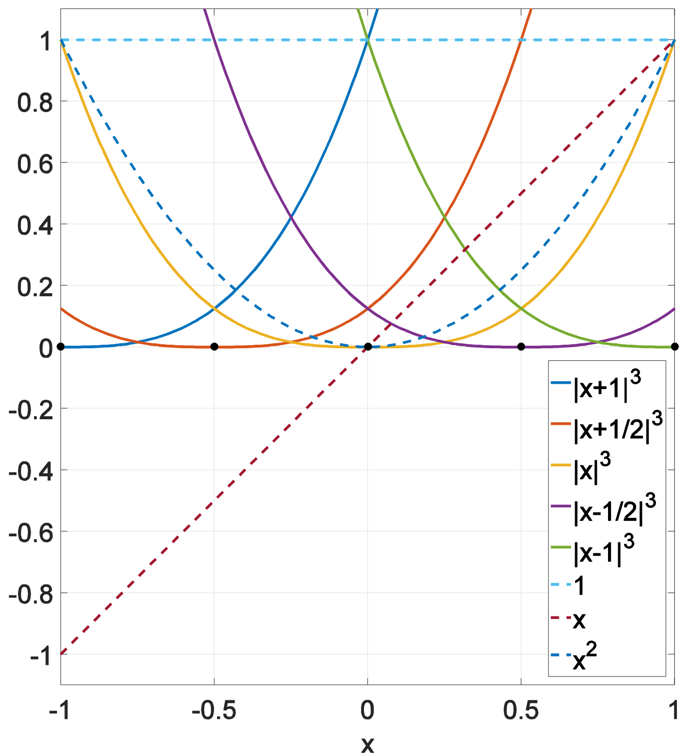


Infinitely Differentiable RBFs

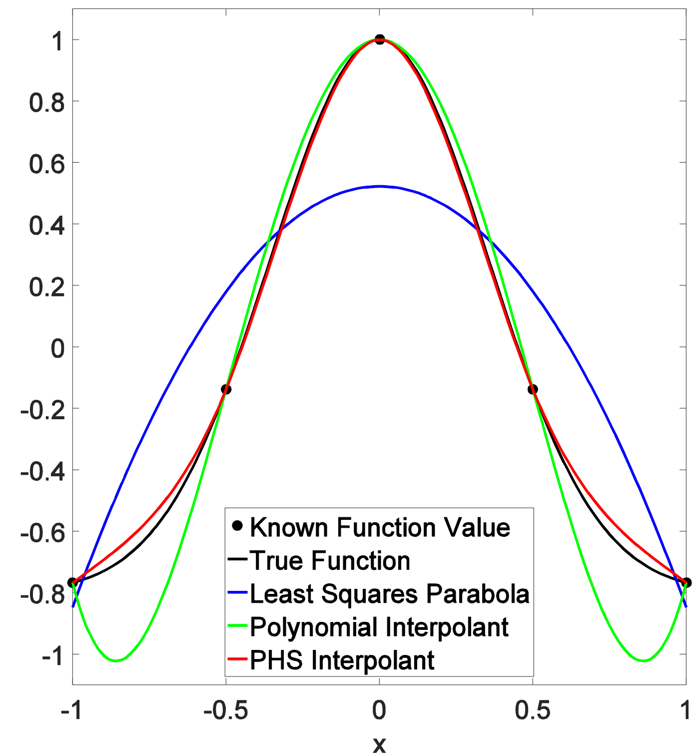


Example: Equi-spaced Interpolation in 1D

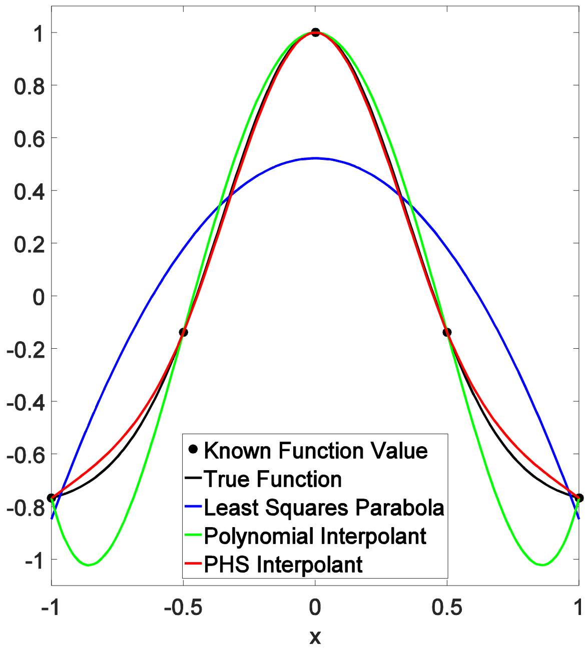
PHS Basis Functions



Approximation



Structure of the Linear System



Least Squares Parabola:
$\mu_1 + \mu_2 x + \mu_3 x^2$

$$\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ 1 & x_4 & x_4^2 \\ 1 & x_5 & x_5^2 \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix}$$

Polynomial Interpolant:
$\mu_1 + \mu_2 x + \mu_3 x^2 + \mu_4 x^3 + \mu_5 x^4$

$$\begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & x_1^4 \\ 1 & x_2 & x_2^2 & x_2^3 & x_2^4 \\ 1 & x_3 & x_3^2 & x_3^3 & x_3^4 \\ 1 & x_4 & x_4^2 & x_4^3 & x_4^4 \\ 1 & x_5 & x_5^2 & x_5^3 & x_5^4 \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \\ \mu_5 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix}$$

PHS Interpolant:
$$\sum_{j=1}^{5} \lambda_j \left|x - x_j\right|^3 + \mu_1 + \mu_2 x + \mu_3 x^2$$

$$\left[\begin{array}{ccccc|ccc} 0 & |x_1 - x_2|^3 & |x_1 - x_3|^3 & |x_1 - x_4|^3 & |x_1 - x_5|^3 & 1 & x_1 & x_1^2 \\ |x_2 - x_1|^3 & 0 & |x_2 - x_3|^3 & |x_2 - x_4|^3 & |x_2 - x_5|^3 & 1 & x_2 & x_2^2 \\ |x_3 - x_1|^3 & |x_3 - x_2|^3 & 0 & |x_3 - x_4|^3 & |x_3 - x_5|^3 & 1 & x_3 & x_3^2 \\ |x_4 - x_1|^3 & |x_4 - x_2|^3 & |x_4 - x_3|^3 & 0 & |x_4 - x_5|^3 & 1 & x_4 & x_4^2 \\ |x_5 - x_1|^3 & |x_5 - x_2|^3 & |x_5 - x_3|^3 & |x_5 - x_4|^3 & 0 & 1 & x_5 & x_5^2 \\ \hline 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ x_1 & x_2 & x_3 & x_4 & x_5 & 0 & 0 & 0 \\ x_1^2 & x_2^2 & x_3^2 & x_4^2 & x_5^2 & 0 & 0 & 0 \end{array}\right] \left[\begin{array}{c} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \hline \mu_1 \\ \mu_2 \\ \mu_3 \end{array}\right] = \left[\begin{array}{c} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ \hline 0 \\ 0 \\ 0 \end{array}\right]$$

Properties of Polyharmonic Splines

- PHS basis includes both RBFs and polynomials
  - RBFs improve performance and allow the use of irregular nodes
  - polynomials give convergence to smooth solutions (no saturation error)
- The interpolation problem is guaranteed to have a unique solution provided that polynomials are included up to the required degree, and the nodes are unisolvent. For $k = 1,2,3,\ldots$
  - $\phi(\boldsymbol{x}) = \|\boldsymbol{x}\|^{2k} \log\|\boldsymbol{x}\|$
    - Polynomials up to degree k or higher
  - $\phi(\boldsymbol{x}) = \|\boldsymbol{x}\|^{2k+1}$
    - Polynomials up to degree k or higher
  - Rule of thumb for modest polynomial degrees: Twice as many RBFs as polynomials
- Condition number of PHS A-matrix is invariant under rotation, translation, and uniform scaling
- No need to search for optimal shape parameter

Interpolation in 2D $[\boldsymbol{x} = (x, y)]$

Given nodes $\{(x_i, y_i)\}_{i=1}^{n}$ and corresponding function values $\{f_i\}_{i=1}^{n}$, find a linear combination of RBF and polynomial basis functions that matches the data exactly.

1. Assume the appropriate form of the underlying approximation:

$$\Phi(x, y) = \sum_{j=1}^{n} \lambda_j \phi_j(x, y) + \sum_{k=1}^{m} \mu_k p_k(x, y)\,,$$
$$\text{where } \phi_j(x, y) = \phi\left(x - x_j, y - y_j\right).$$

2. Require Φ to match the data at each node:

$$\Phi(\, x_i, y_i) = \sum_{j=1}^{n} \lambda_j \phi_j(x_i, y_i) + \sum_{k=1}^{m} \mu_k p_k(x_i, y_i) = f_i, \qquad i = 1,2,3, \dots, n.$$

3. Enforce regularity conditions on the coefficients $\{\lambda_j\}$:

$$\sum_{j=1}^{n} \lambda_j p_k\left(x_j, y_j\right) = 0, \qquad k = 1,2,3, \dots, m.$$

4. Solve the symmetric linear system for $\{\lambda_j\}$ and $\{\mu_k\}$.

Differentiation Weights in 2D

Interpolation Problem:

$$\begin{bmatrix} \mathbf{A} & \mathbf{P} \\ \mathbf{P}^T & \mathbf{O} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\mu} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{O} \end{bmatrix},$$

$$a_{ij} = \phi_j(x_i, y_i) = \phi\left(x_i - x_j, y_i - y_j\right), \qquad i, j = 1,2,3, \dots, n,$$
$$p_{ik} = p_k(x_i, y_i), \qquad i = 1,2,3, \dots, n, \qquad k = 1,2,3, \dots, m.$$

Use $[L\Phi](\tilde{x}, \tilde{y})$ to approximate $[Lf](\tilde{x}, \tilde{y})$:

$$[L\Phi](\tilde{x}, \tilde{y}) = \sum_{j=1}^{n} \lambda_j \left[L\phi_j\right](\tilde{x}, \tilde{y}) + \sum_{k=1}^{m} \mu_k [Lp_k](\tilde{x}, \tilde{y})$$
$$= [\boldsymbol{b} \quad \boldsymbol{c}] \begin{bmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\mu} \end{bmatrix} = \underbrace{\left([\boldsymbol{b} \quad \boldsymbol{c}] \begin{bmatrix} \mathbf{A} & \mathbf{P} \\ \mathbf{P}^T & \mathbf{O} \end{bmatrix}^{-1} \right)}_{\text{weights}} \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{O} \end{bmatrix},$$

$$b_j = \left[L\phi_j\right](\tilde{x}, \tilde{y}), \qquad j = 1,2,3, \dots, n,$$
$$c_k = [Lp_k](\tilde{x}, \tilde{y}), \qquad k = 1,2,3, \dots, m.$$

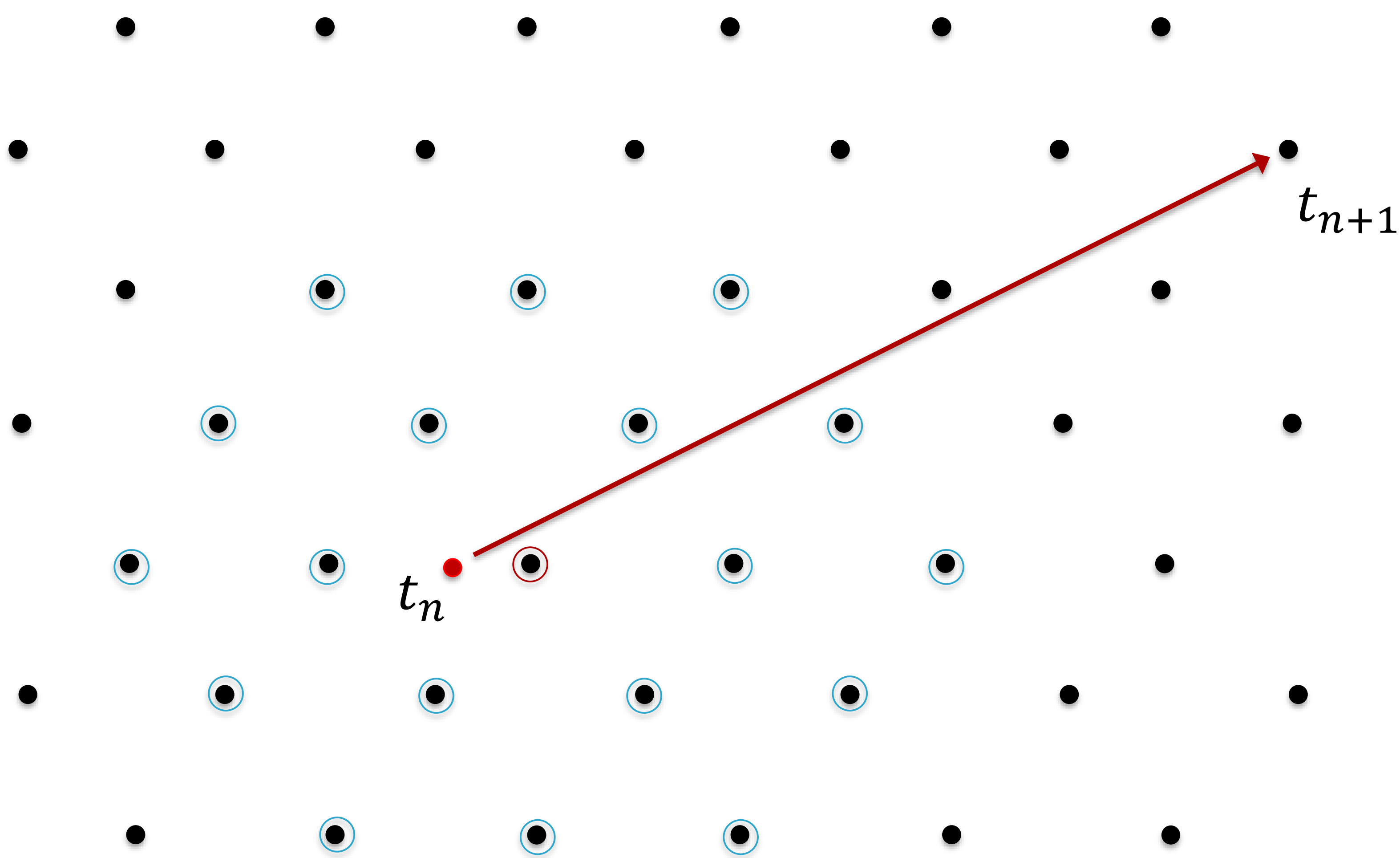
Derivative Approximation on the Sphere

- Given: nodes $[\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}]$ on the sphere and function values $\boldsymbol{f}$
- Find: differentiation matrices (DMs) $\mathbf{W}_x$, $\mathbf{W}_y$, $\mathbf{W}_z$ to approximate $\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}$
- Method: Use the fact that $\nabla f(\tilde{x}, \tilde{y}, \tilde{z})$ is tangent to the sphere at $(\tilde{x}, \tilde{y}, \tilde{z})$
  - For each node, get orthogonal unit vectors $\boldsymbol{e}_{\hat{x}}$ and $\boldsymbol{e}_{\hat{y}}$ tangent to the sphere
  - Use 2D method to get matrices $\mathbf{W}_{\hat{x}}$ and $\mathbf{W}_{\hat{y}}$ that approximate $\frac{\partial}{\partial \hat{x}}$ and $\frac{\partial}{\partial \hat{y}}$
  - $\nabla f = \boldsymbol{e}_{\hat{x}} \frac{\partial f}{\partial \hat{x}} + \boldsymbol{e}_{\hat{y}} \frac{\partial f}{\partial \hat{y}}$
  - $\frac{\partial f}{\partial x} = (\nabla f)_1 = (\boldsymbol{e}_{\hat{x}})_1 \frac{\partial f}{\partial \hat{x}} + \left(\boldsymbol{e}_{\hat{y}}\right)_1 \frac{\partial f}{\partial \hat{y}} = \left\{(\boldsymbol{e}_{\hat{x}})_1 \frac{\partial}{\partial \hat{x}} + \left(\boldsymbol{e}_{\hat{y}}\right)_1 \frac{\partial}{\partial \hat{y}}\right\} f$
    - $\mathbf{W}_x = \operatorname{diag}\{(\boldsymbol{e}_{\hat{x}})_1\}\mathbf{W}_{\hat{x}} + \operatorname{diag}\left\{\left(\boldsymbol{e}_{\hat{y}}\right)_1\right\}\mathbf{W}_{\hat{y}}$
    - $\mathbf{W}_y = \operatorname{diag}\{(\boldsymbol{e}_{\hat{x}})_2\}\mathbf{W}_{\hat{x}} + \operatorname{diag}\left\{\left(\boldsymbol{e}_{\hat{y}}\right)_2\right\}\mathbf{W}_{\hat{y}}$
    - $\mathbf{W}_z = \operatorname{diag}\{(\boldsymbol{e}_{\hat{x}})_3\}\mathbf{W}_{\hat{x}} + \operatorname{diag}\left\{\left(\boldsymbol{e}_{\hat{y}}\right)_3\right\}\mathbf{W}_{\hat{y}}$

Semi-Lagrangian Transport

- Governing Equations (velocity $\boldsymbol{u}$ is a known function)
  - $\frac{\partial \rho}{\partial t} = -\boldsymbol{u} \cdot \nabla \rho - \rho \nabla \cdot \boldsymbol{u}$, (Eulerian, short time-steps)
  - $\frac{Dq}{Dt} = \left(\frac{\partial}{\partial t} + \boldsymbol{u} \cdot \nabla\right) q = 0.$ (Semi-Lagrangian, long time-steps)
- Quasi-Monotone Limiter for q (const. along flow trajectories)
  - $m_k = \min_{\ell} \left\{ q_{k_\ell}^{(n)} \right\}$ and $M_k = \max_{\ell} \left\{ q_{k_\ell}^{(n)} \right\}$
  - Set $q_k^{(n+1)} = \min \left\{ q_k^{(n+1)}, M_k \right\}$
  - Set $q_k^{(n+1)} = \max \left\{ q_k^{(n+1)}, m_k \right\}$
- Mass Fixer $\left(\text{tracerMass} \equiv \sum_{k=1}^{N} \rho_k q_k V_k\right)$
  - If tracerMass < initialMass, add mass in cells with $q_k < M_k$
  - If tracerMass > initialMass, subtract mass from cells with $q_k > m_k$

Semi-Lagrangian Transport



Pre-Processing

- Get DMs $\mathbf{W}_x$, $\mathbf{W}_y$, and $\mathbf{W}_z$ for the continuity equation
- Find index of the n nearest neighbors to each node
- For each node $\boldsymbol{x}_k = (x_k, y_k, z_k)$, write its n neighbors in terms of two orthogonal unit vectors $\left(\boldsymbol{e}_{\hat{x}}, \boldsymbol{e}_{\hat{y}}\right)$ tangent to the sphere at $\boldsymbol{x}_k$, and one unit vector $\boldsymbol{e}_{\hat{z}}$ normal to the sphere at $\boldsymbol{x}_k$, so that

$$\boldsymbol{x}_{k_\ell} = \hat{x}_{k_\ell}\boldsymbol{e}_{\hat{x}} + \hat{y}_{k_\ell}\boldsymbol{e}_{\hat{y}} + \hat{z}_{k_\ell}\boldsymbol{e}_{\hat{z}}, \qquad \ell = 1,2,3,\dots,n.$$

- Set $\mathbf{C}_k = \begin{bmatrix} \mathbf{A}_k & \mathbf{P}_k \\ \mathbf{P}_k^T & \mathbf{O}_{6\times 6} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{I}_n \\ \mathbf{O}_{6\times n} \end{bmatrix}$, where

$$(\mathbf{A}_k)_{ij} = \phi\left(\hat{x}_{k_i} - \hat{x}_{k_j}, \hat{y}_{k_i} - \hat{y}_{k_j}\right), \qquad i,j = 1,2,3,\dots,n,$$

$$\mathbf{P}_k = \left[\mathbf{1}, \hat{\boldsymbol{x}}_k, \hat{\boldsymbol{y}}_k, \hat{\boldsymbol{x}}_k^2, \hat{\boldsymbol{x}}_k\hat{\boldsymbol{y}}_k, \hat{\boldsymbol{y}}_k^2\right].$$

Time Stepping

1. Step $\frac{\partial \rho}{\partial t} = -\boldsymbol{u} \cdot \nabla \rho - \rho \nabla \cdot \boldsymbol{u}$ from t_n to t_{n+1} using several explicit Eulerian time steps (RK3)
2. Step $\boldsymbol{x}' = -\boldsymbol{u}$ from t_{n+1} to t_n to get departure points (RK4)
3. Find the nearest fixed neighbor to each departure point
4. Use the corresponding pre-calculated cardinal coefficients $\{\mathbf{C}_k\}$ and the newly formed row-vectors $\{\boldsymbol{b}_k\}$ to get rows of the interpolation matrix $\mathbf{W}$ $(\mathbf{W}_{k\cdot} = \boldsymbol{b}_k \mathbf{C}_k)$
5. Update q on fixed nodes using weights $\mathbf{W}$
6. Cycle quasi-monotone limiter and mass-fixer until the tracer mass is nearly equal to the initial tracer mass (diff<1e-13)
7. Repeat

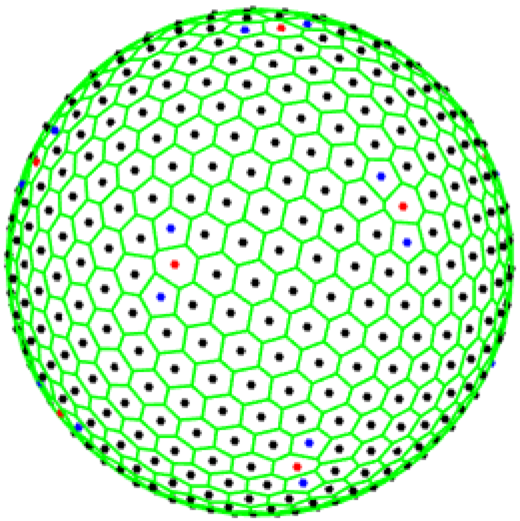
Hyperviscosity

- Add a small dissipative term to the continuity equation
  - $\frac{\partial \rho}{\partial t} = -\boldsymbol{u} \cdot \nabla \rho - \rho \nabla \cdot \boldsymbol{u} + \gamma \max\|\boldsymbol{u}\| \, (\Delta x)^{2K-1} \Delta^K \rho$
- Reduce high-frequency noise while keeping order of convergence intact
- Achieve stability in time using explicit time-stepping
- PHS are ideal for hyperviscosity, because applying the Laplace operator to a PHS returns another PHS
  - $\phi(x, y) = (x^2 + y^2)^{m/2}$
  - $[\Delta\phi](x, y) = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = m^2 (x^2 + y^2)^{(m-2)/2}$
- Parameter $\gamma \in \mathbb{R}$ is determined experimentally at low resolution, and remains unchanged as resolution increases

Transport Test Cases on the Sphere

- Initial Condition q_0 ($\rho_0 = 1$ in all cases)
  - Taken from Nair and Lauritzen, 2010 (NL2010)
    - Gaussian Hills (infinitely differentiable)
    - Cosine Bells (once continuously differentiable)
    - Slotted Cylinders (not continuous)
- Velocity Field (NL2010)
  - Case 1: Translating, vorticity-dominated flow $\left(\mathrm{CFL}_{\max} = \frac{\max\|\boldsymbol{u}\|\Delta t}{\Delta x} \approx 8\right)$
  - Case 2: Translating, divergence-dominated flow $(\mathrm{CFL}_{\max} \approx 5)$
- Spatial Approximations (Minimum Energy (ME) Nodes)
  - Number of nodes $N = 24^2(576)$, $48^2(2304)$, $96^2(9216)$, $192^2(36864)$
  - Interpolation (semi-Lagrangian tracer transport)
    - $\|\boldsymbol{x}\|^3 + p1 + n19$
  - Derivative Approximation (Eulerian continuity equation)
    - $\|\boldsymbol{x}\|^2 \log\|\boldsymbol{x}\| + p5 + n42$
- Time-stepping from $t = 0$ to $t = 5$ (one revolution)

Nodes and Initial Conditions for q

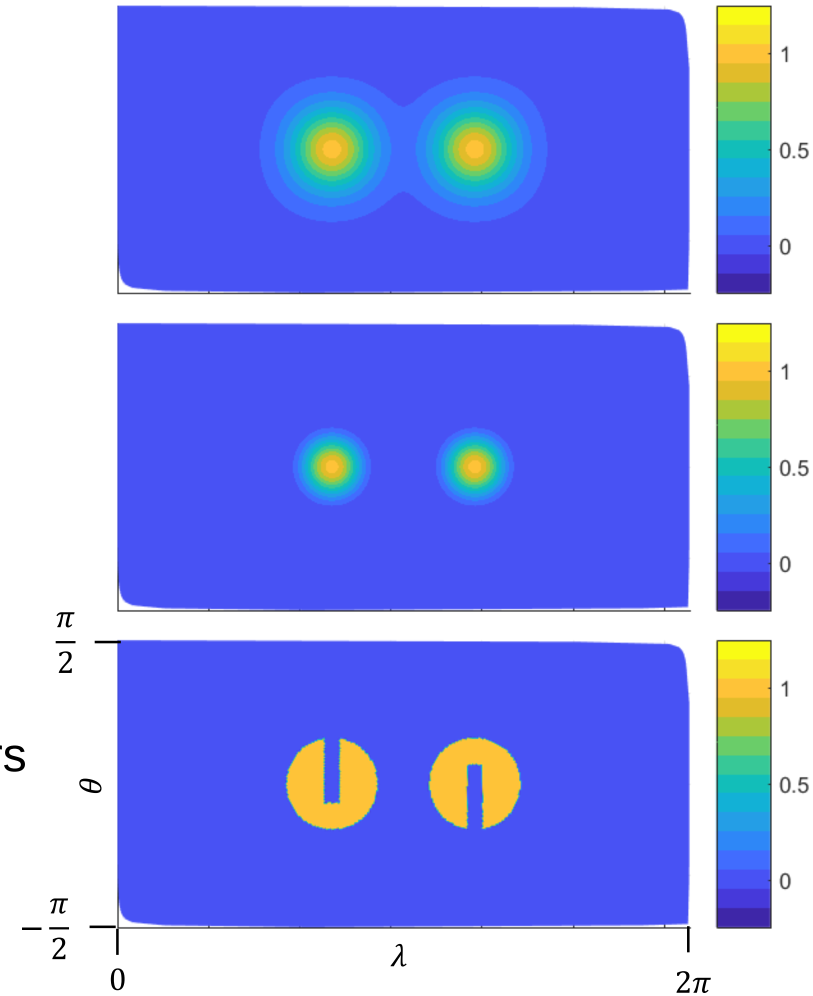


$N = 24^2 = 576$
ME nodes

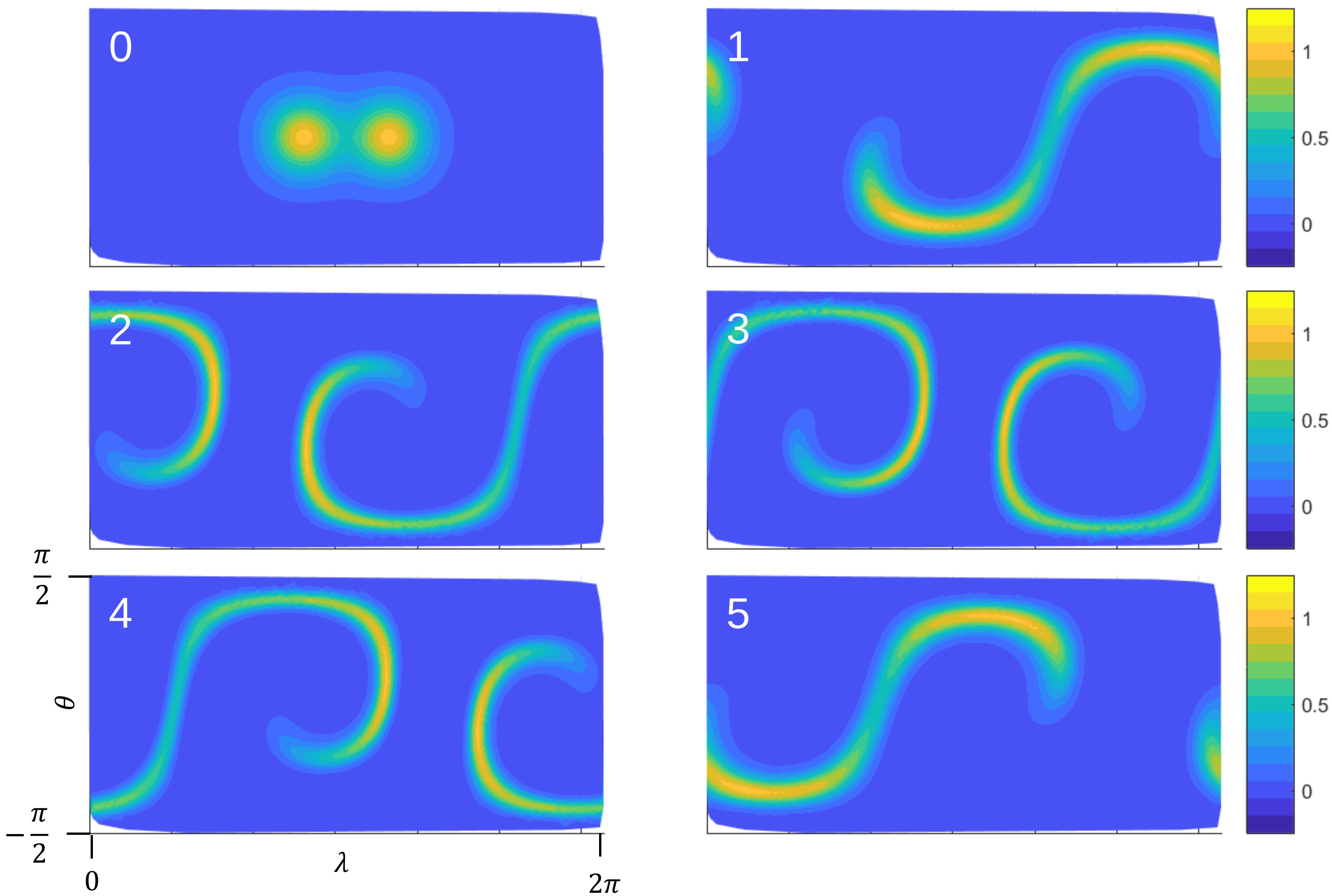
Gaussian Hills
(GH)

Cosine Bells
(CB)

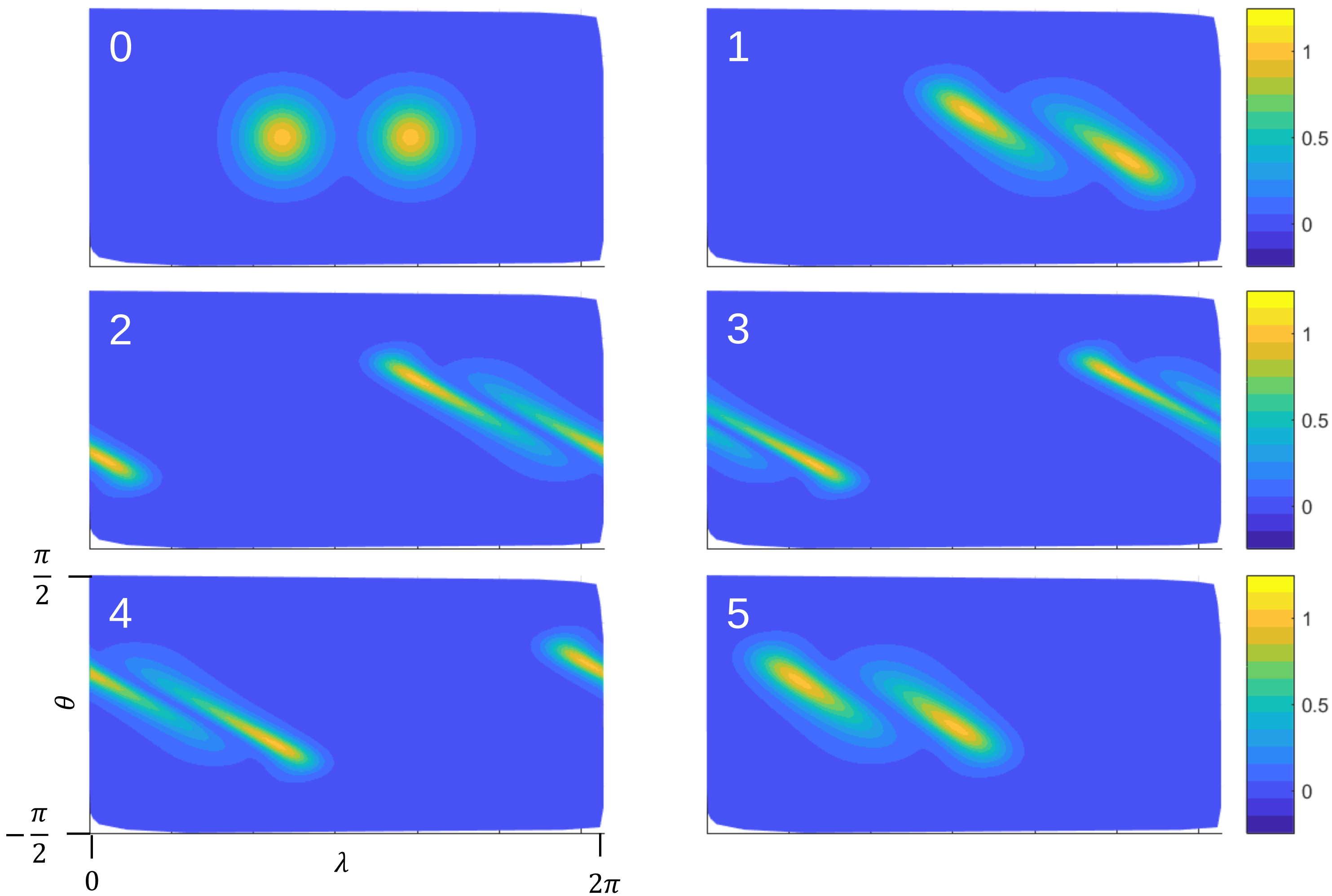
Slotted Cylinders
(SC)



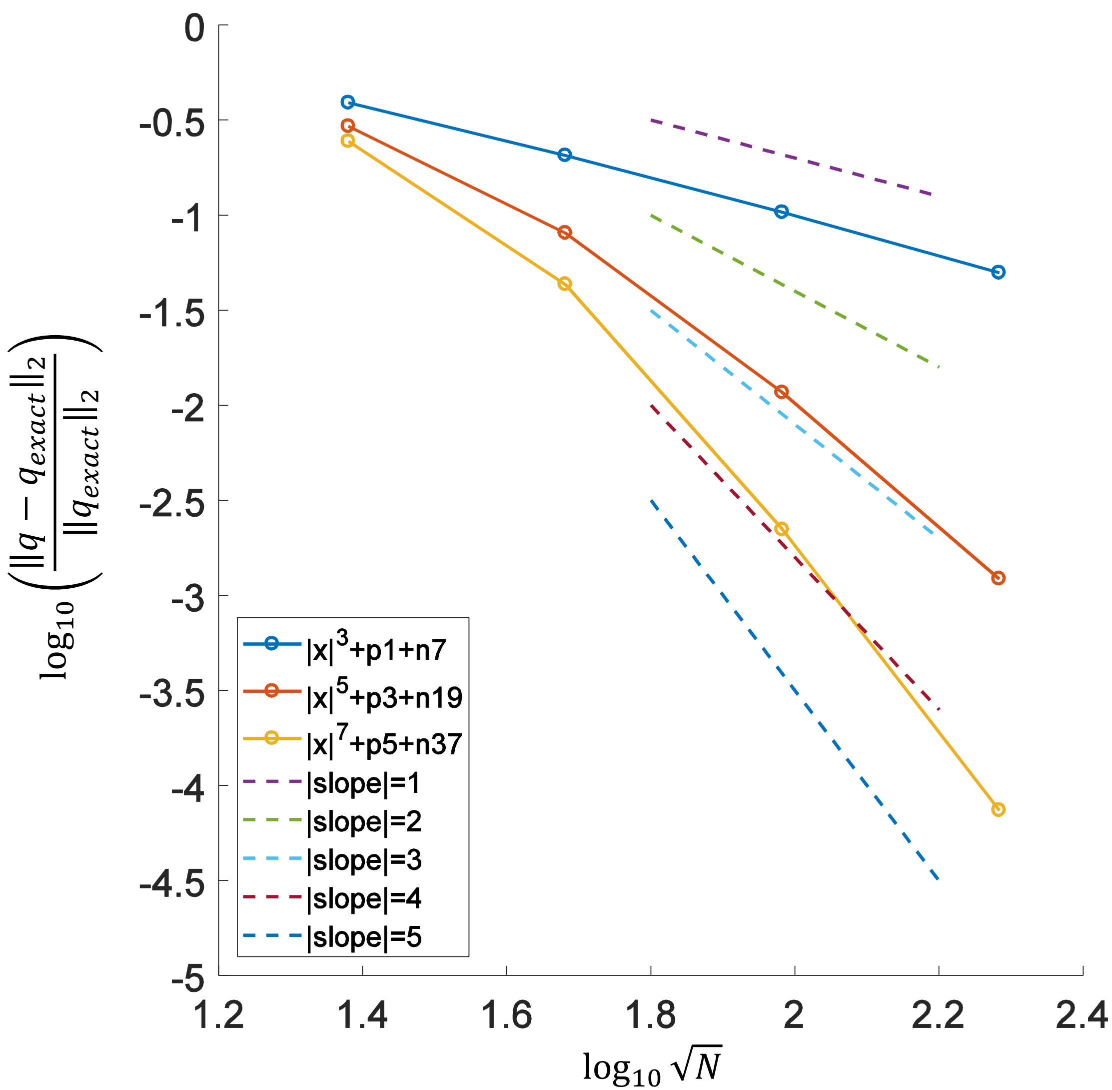
Time Snapshots, Velocity Case 1



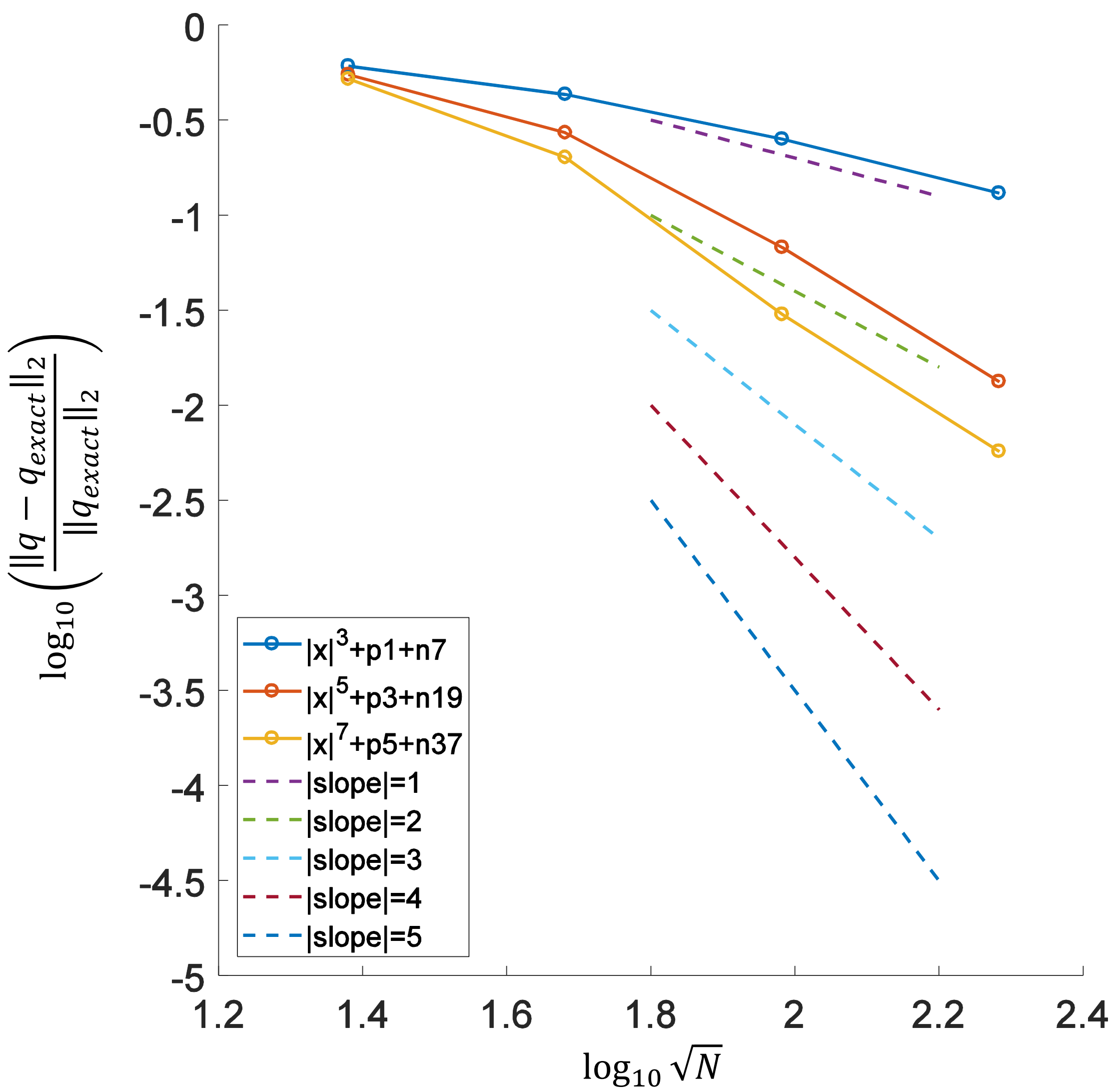
Time Snapshots, Velocity Case 2



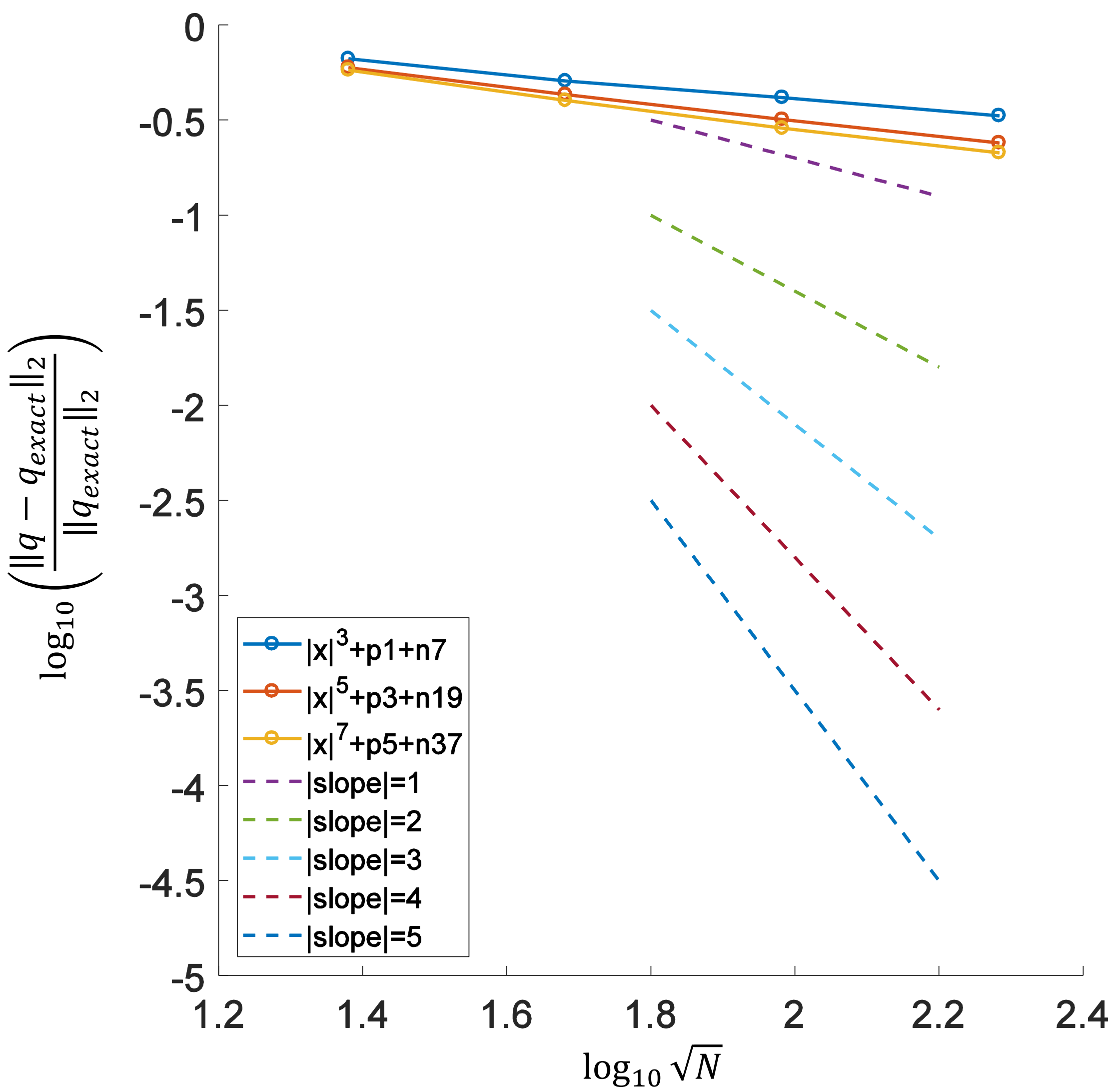
GH, Velocity Case 1, Unlimited



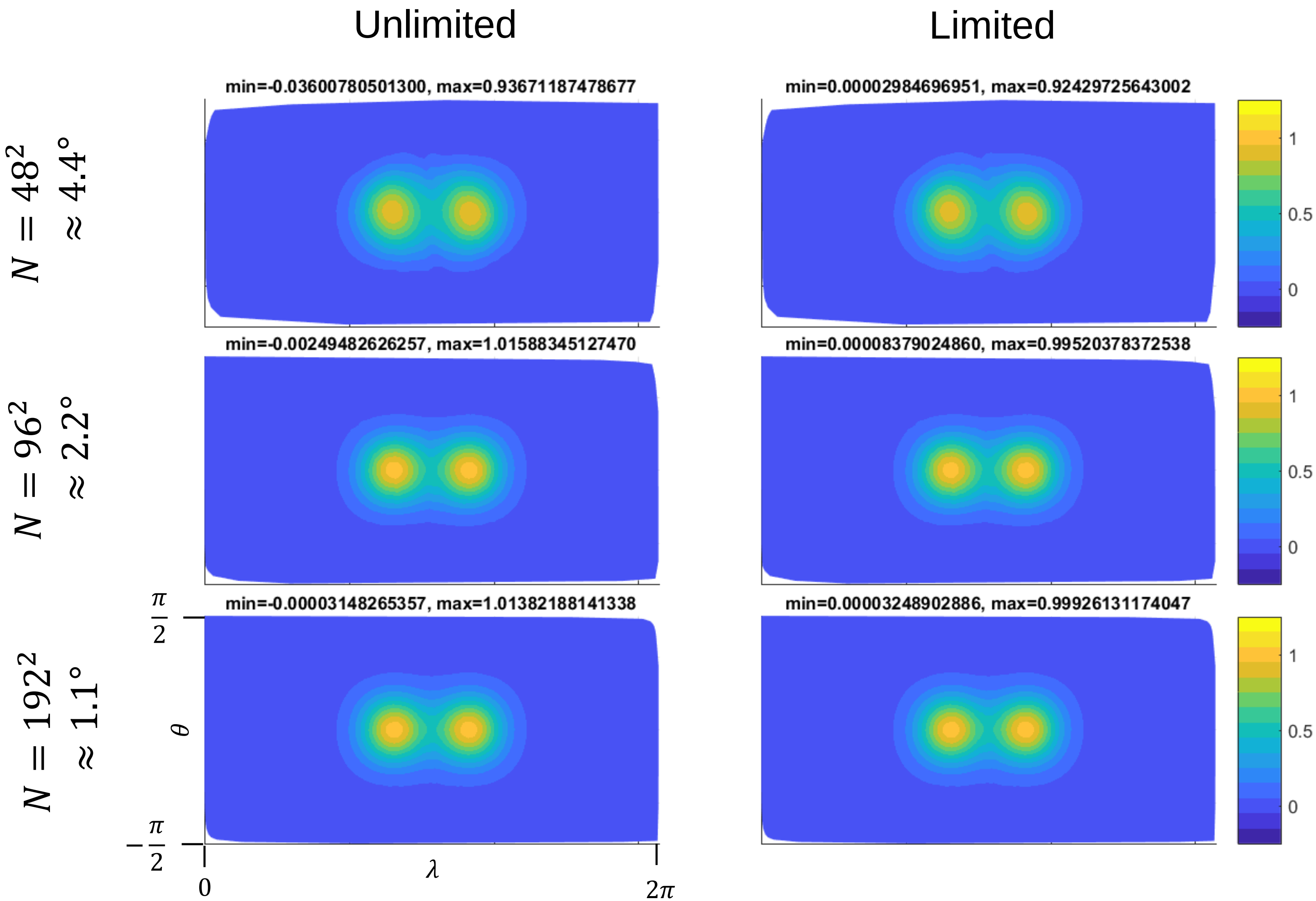
CB, Velocity Case 1, Unlimited



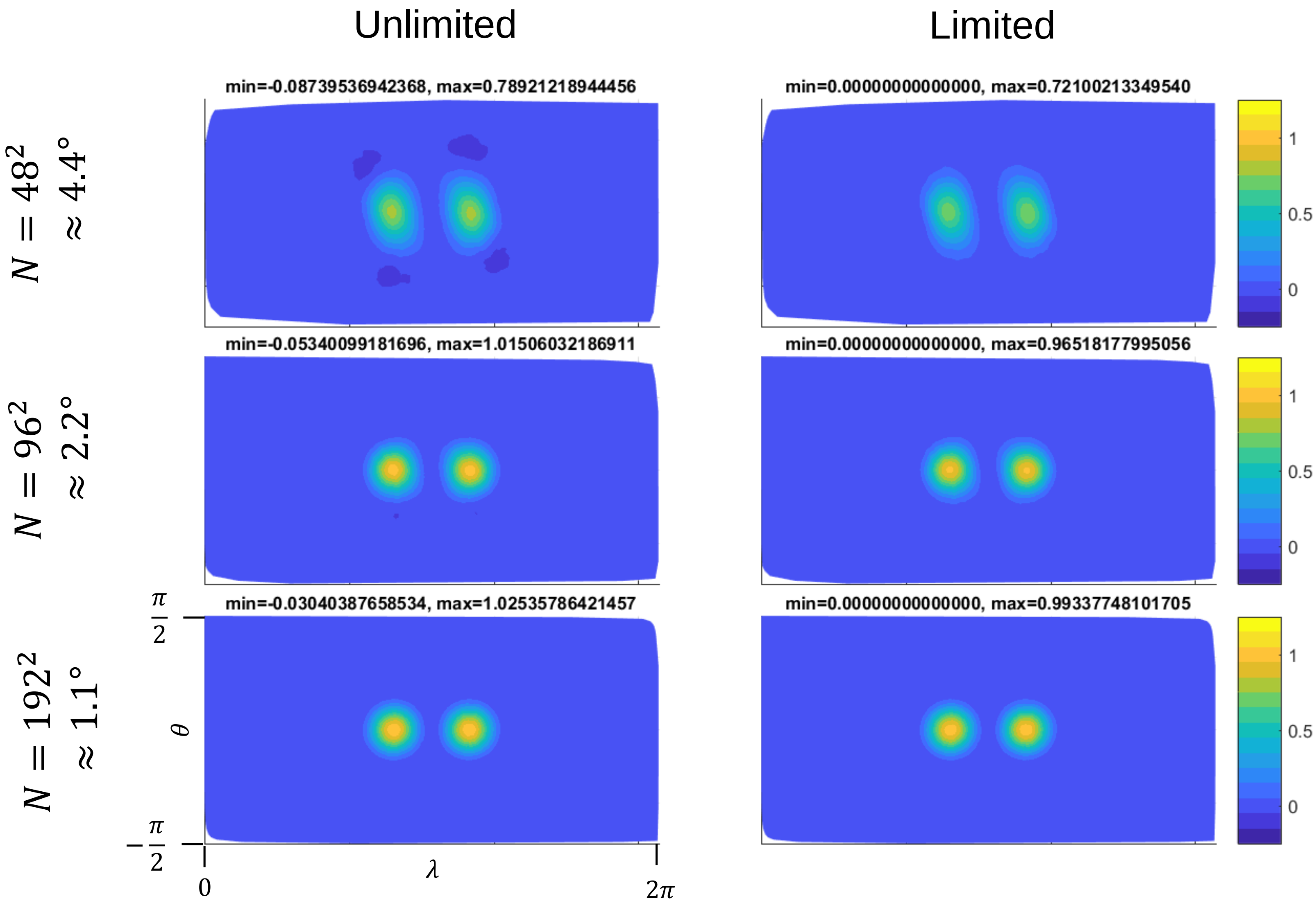
SC, Velocity Case 1, Unlimited



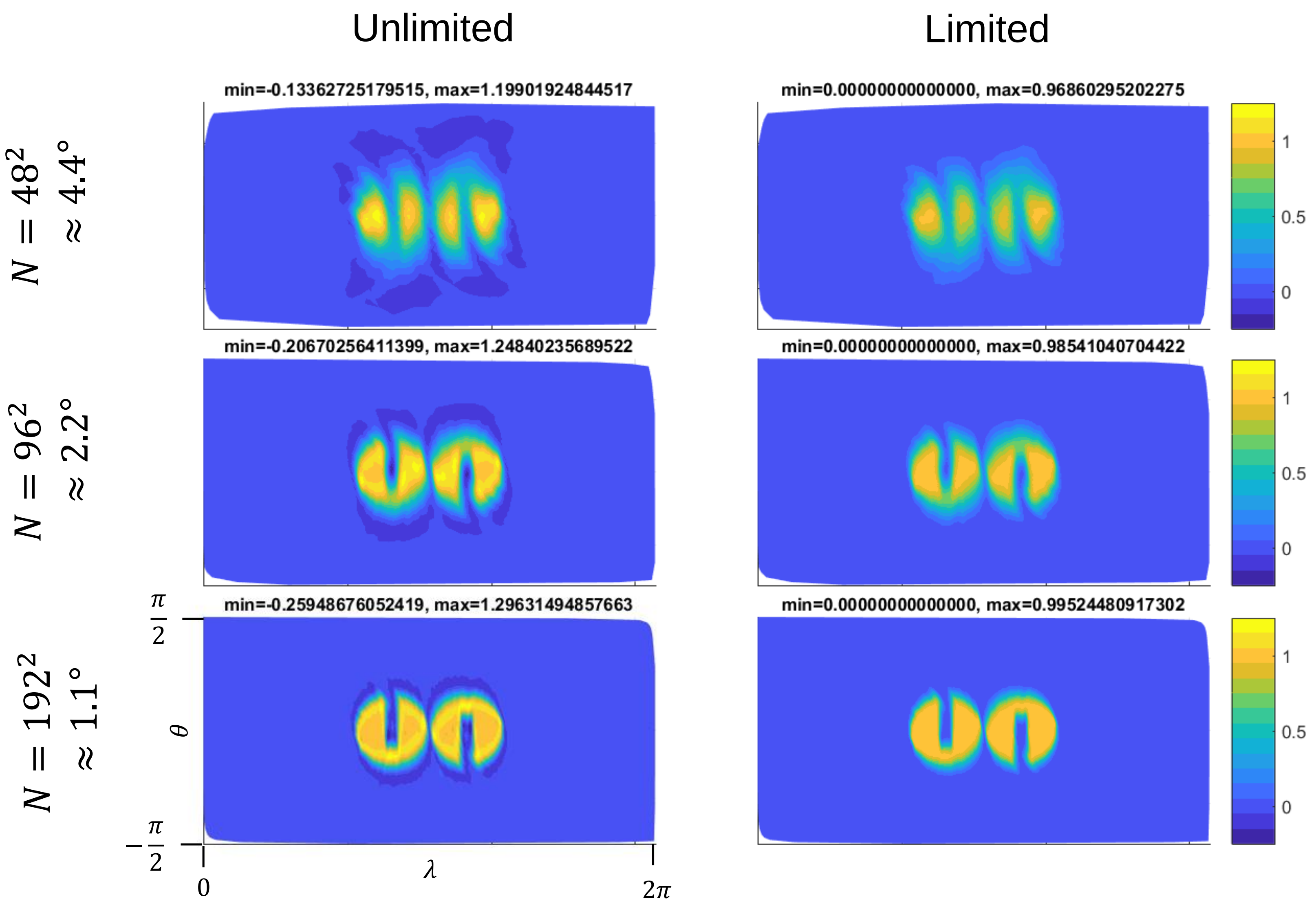
GH, Velocity Case 1



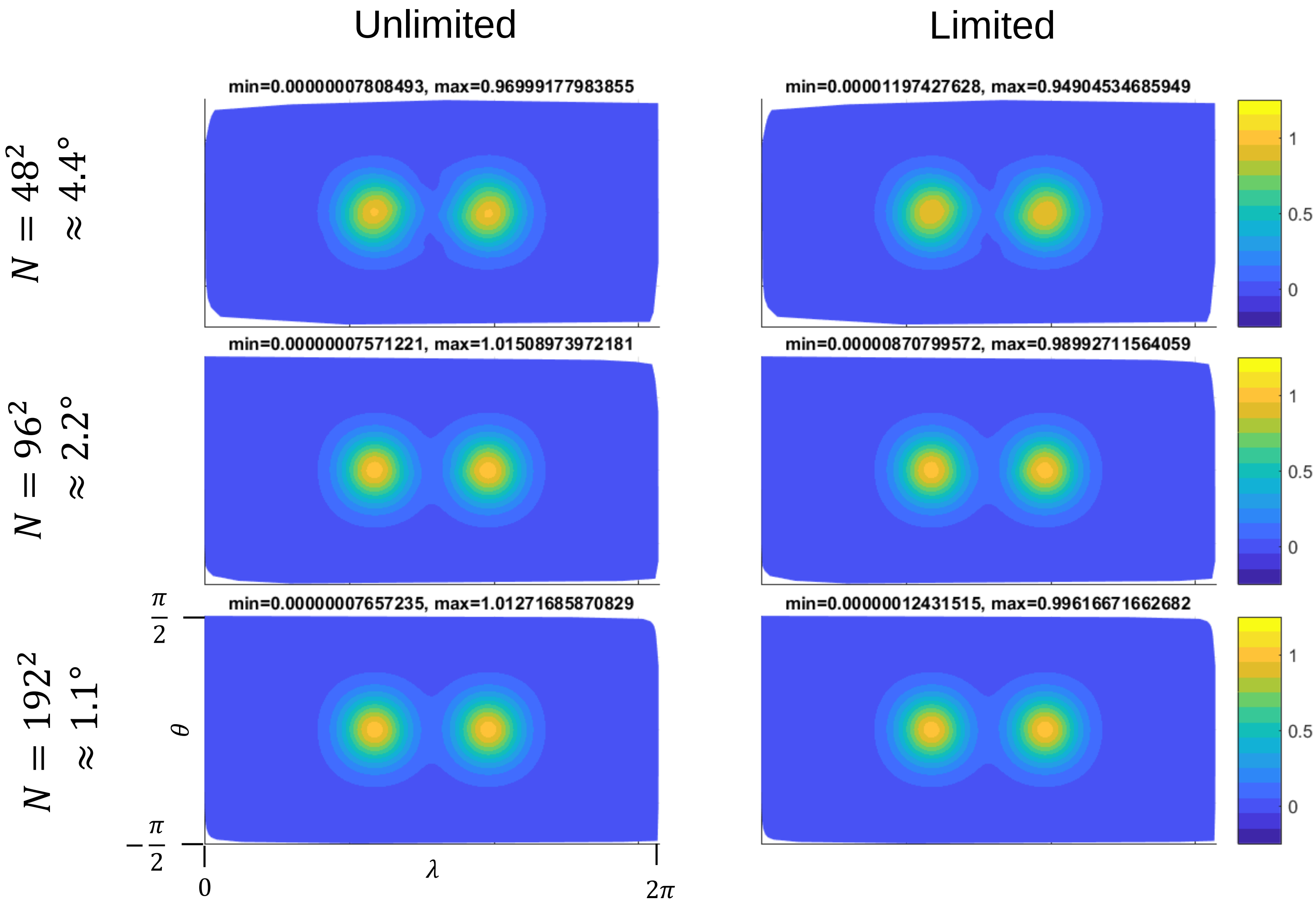
CB, Velocity Case 1



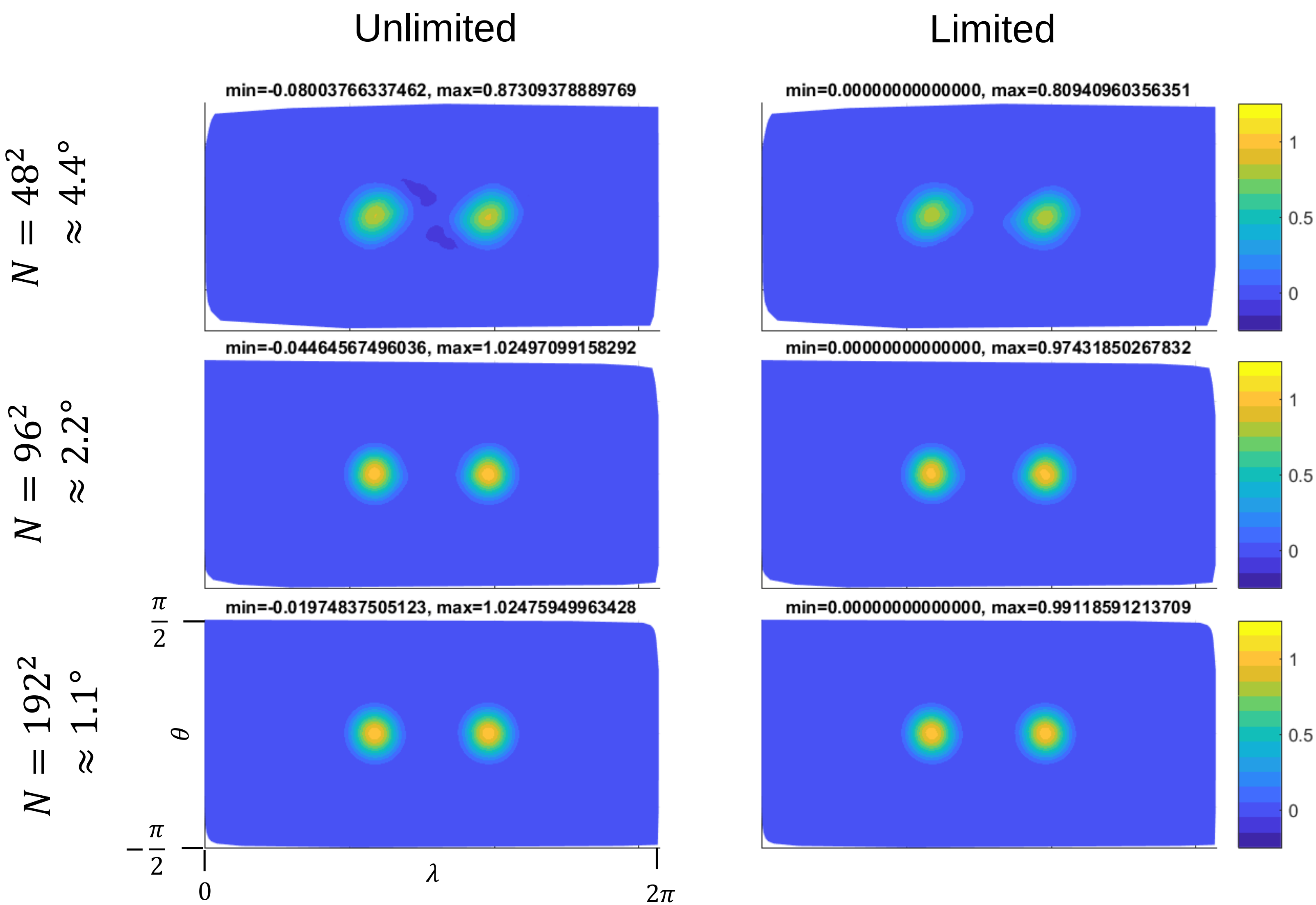
SC, Velocity Case 1



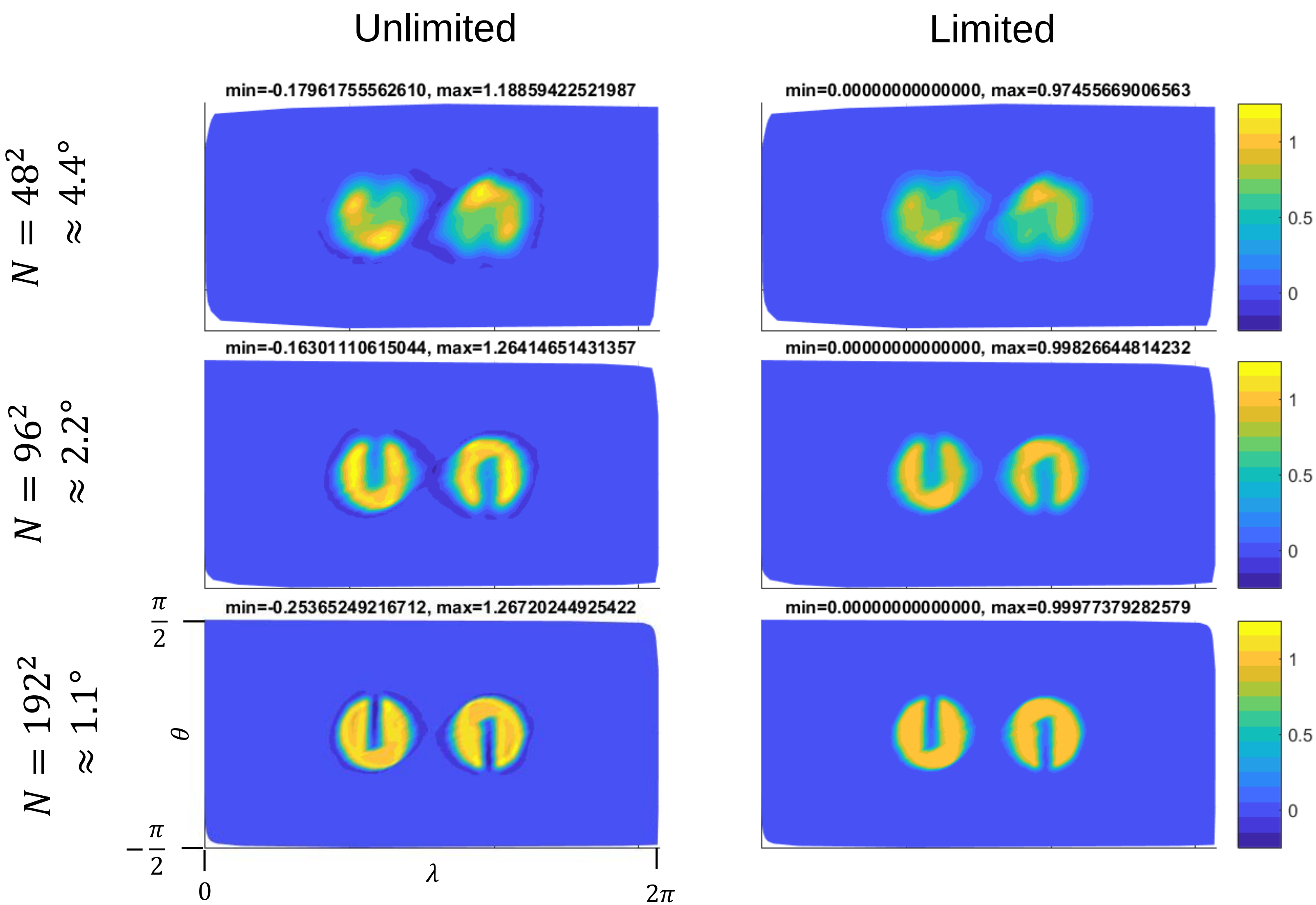
GH, Velocity Case 2



CB, Velocity Case 2



SC, Velocity Case 2



Advantages of Semi-Lagrangian Transport

- Large Time steps $\left(\frac{\max\|\boldsymbol{u}\|\Delta t}{\Delta x} \gg 1\right)$
- Simple governing equation and solution algorithm
  - $\frac{Dq}{Dt} = 0 \qquad \left(\frac{D}{Dt} = \frac{\partial}{\partial t} + \boldsymbol{u} \cdot \nabla\right)$
    - q is constant along flow trajectories
    - No spatial derivatives
  - (1) time-step for departure points, (2) interpolate for new values of q
- No need for hyperviscosity
  - High frequencies automatically damped by repeated interpolation
  - Numerical solutions remain bounded even if the node set is poorly distributed
- Simple limiter to reduce oscillations and preserve bounds

Shallow Water Model

Governing Equations:

$$\frac{\partial \boldsymbol{u}}{\partial t} = -\boldsymbol{u} \cdot \nabla \boldsymbol{u} - f\left(\widehat{\boldsymbol{k}} \times \boldsymbol{u}\right) - g\nabla h,$$

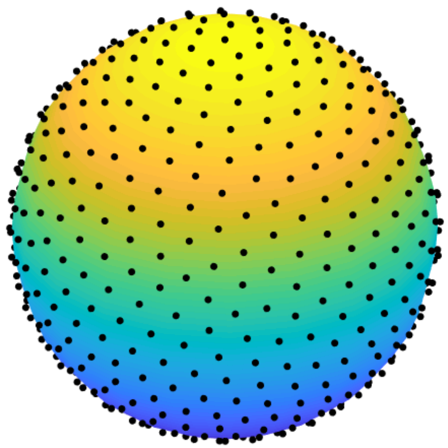
$$\frac{\partial h^*}{\partial t} = -\boldsymbol{u} \cdot \nabla h^* - h^*(\nabla \cdot \boldsymbol{u}).$$

- $f = 2\Omega \sin \theta$, where $\Omega =$ angular velocity of Earth, $\theta =$ latitude
- $\widehat{\boldsymbol{k}}$ is the unit normal to the sphere
- g is gravitational acceleration
- $h = h_s(x, y, z) + h^*(x, y, z, t)$ is the depth of the fluid

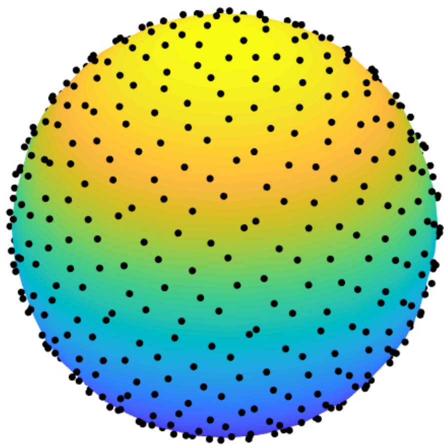
Note: The velocity $\boldsymbol{u}$ is adjusted after every Runge-Kutta stage to remain tangent to the sphere $\left(\boldsymbol{u} \leftarrow \boldsymbol{u} - \left(\boldsymbol{u} \cdot \widehat{\boldsymbol{k}}\right)\widehat{\boldsymbol{k}}\right)$

Nodes

Maximum Determinant (MD)



Hammersley



Shallow Water Test Cases

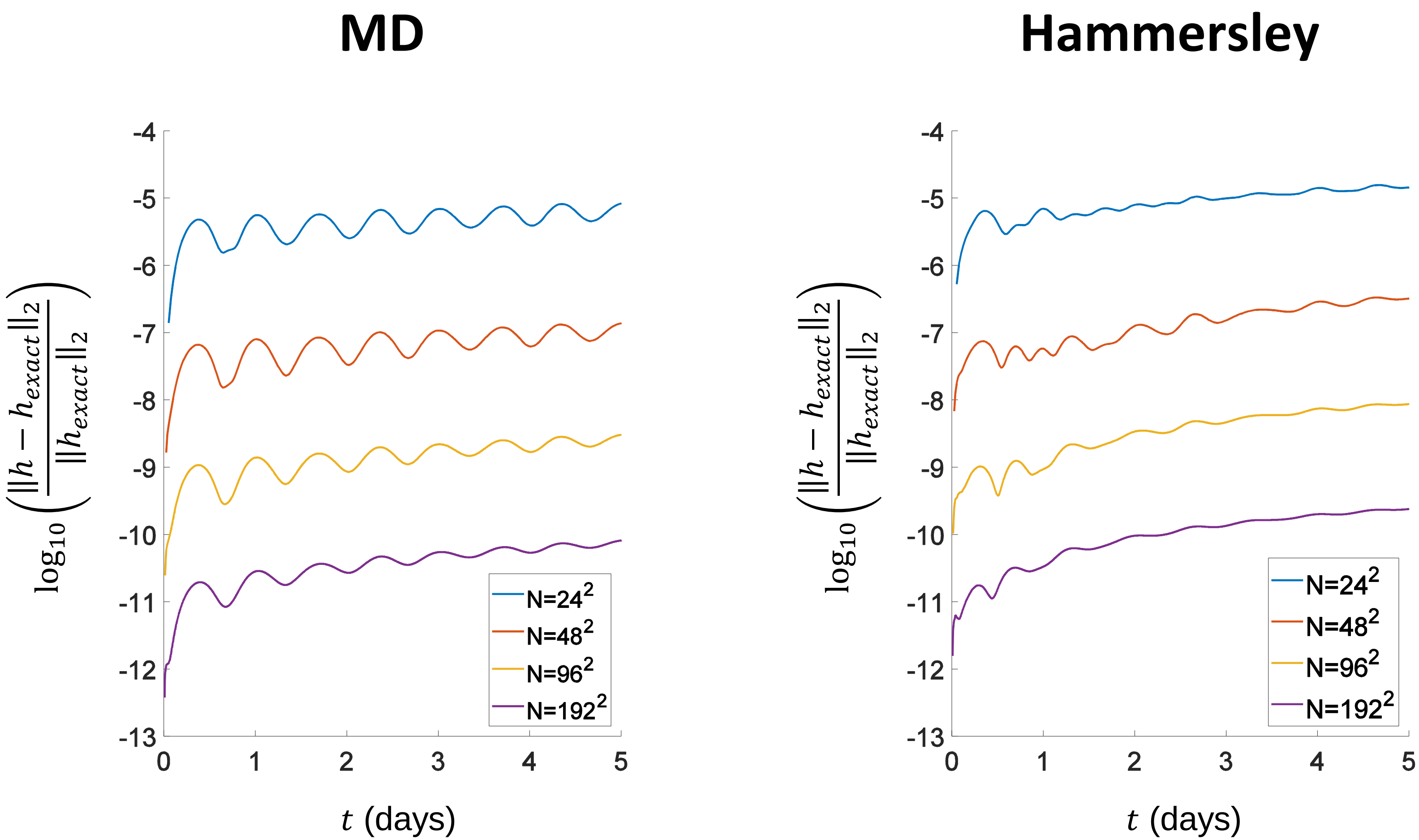
- Taken from Williamson et al, JCP 1992
  - Steady-state smooth flow
    - $h_s = 0$
    - Exact solution known
  - Flow over an isolated mountain
    - h_s is a cone-shaped mountain centered at $(\lambda, \theta) = \left(-\frac{\pi}{2}, \frac{\pi}{6}\right)$
    - Exact solution unavailable
  - Rossby-Haurwitz Wave
    - $\boldsymbol{u}_0$ and h_0 satisfy the barotropic vorticity equations
    - $h_s = 0$
    - Exact solution unavailable

Parameters for Shallow Water Tests

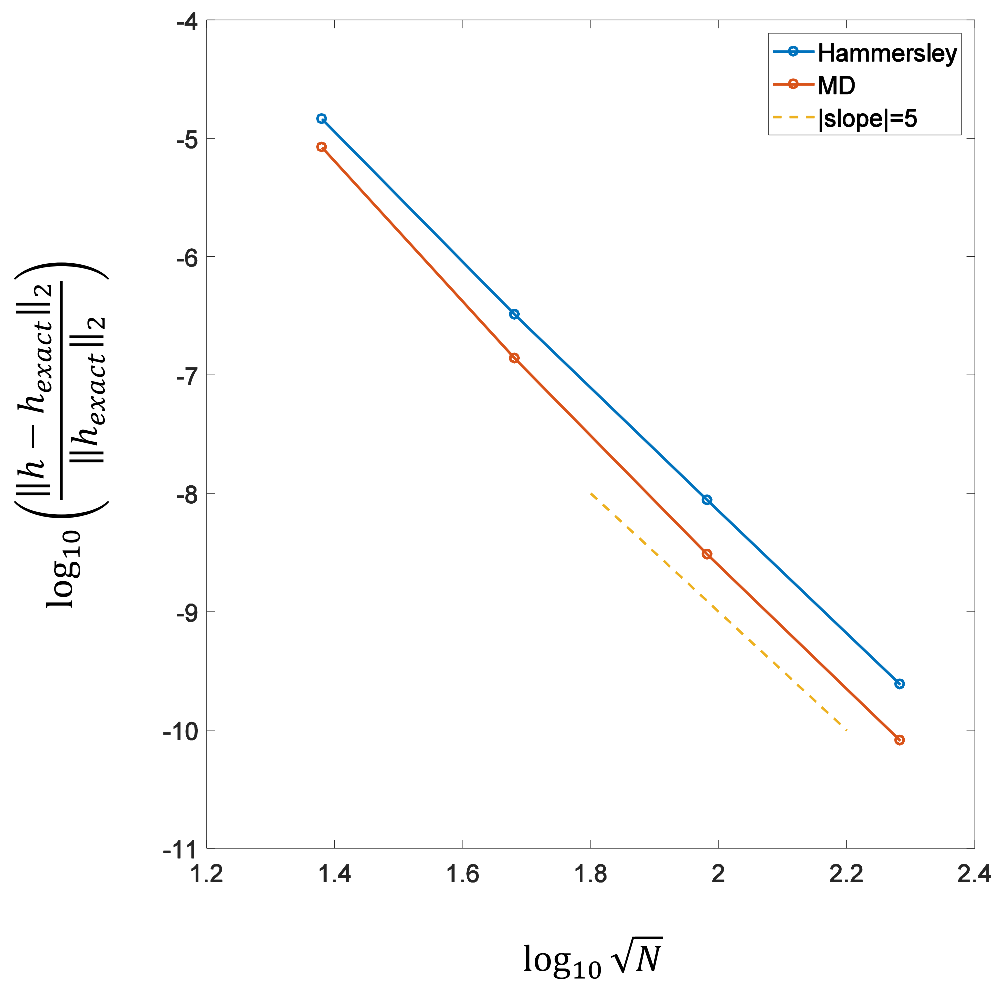
- Derivative approximations $\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$
  - $\phi(\underline{x}) = \|\underline{x}\|^2 \log\|\underline{x}\|$
  - Polynomials up to degree 5
  - Stencil size 42 (twice as many RBFs as polynomials)
- Hyperviscosity (Δ^3)
  - $\phi(\underline{x}) = \|\underline{x}\|^7$
  - Polynomials up to degree 5
  - Stencil size 42
  - Parameter $\gamma = 2^{-12} \approx 2.4 \times 10^{-4}$
- Time Stepping (3 stage, 3rd order Runge-Kutta)

	$N = 24^2$	$N = 48^2$	$N = 96^2$	$N = 192^2$
Δt (minutes)	36	18	9	4.5

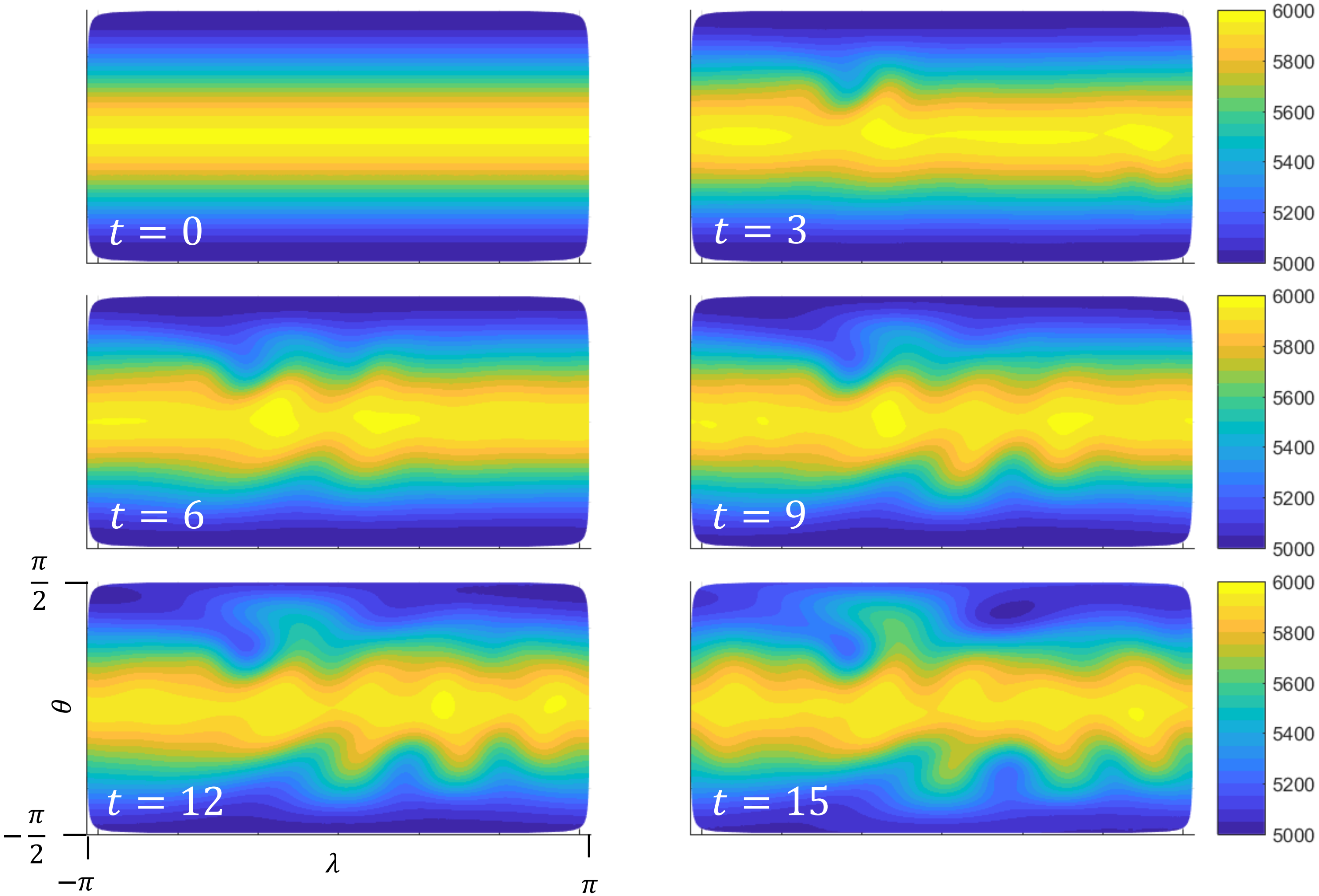
Error Growth in Time



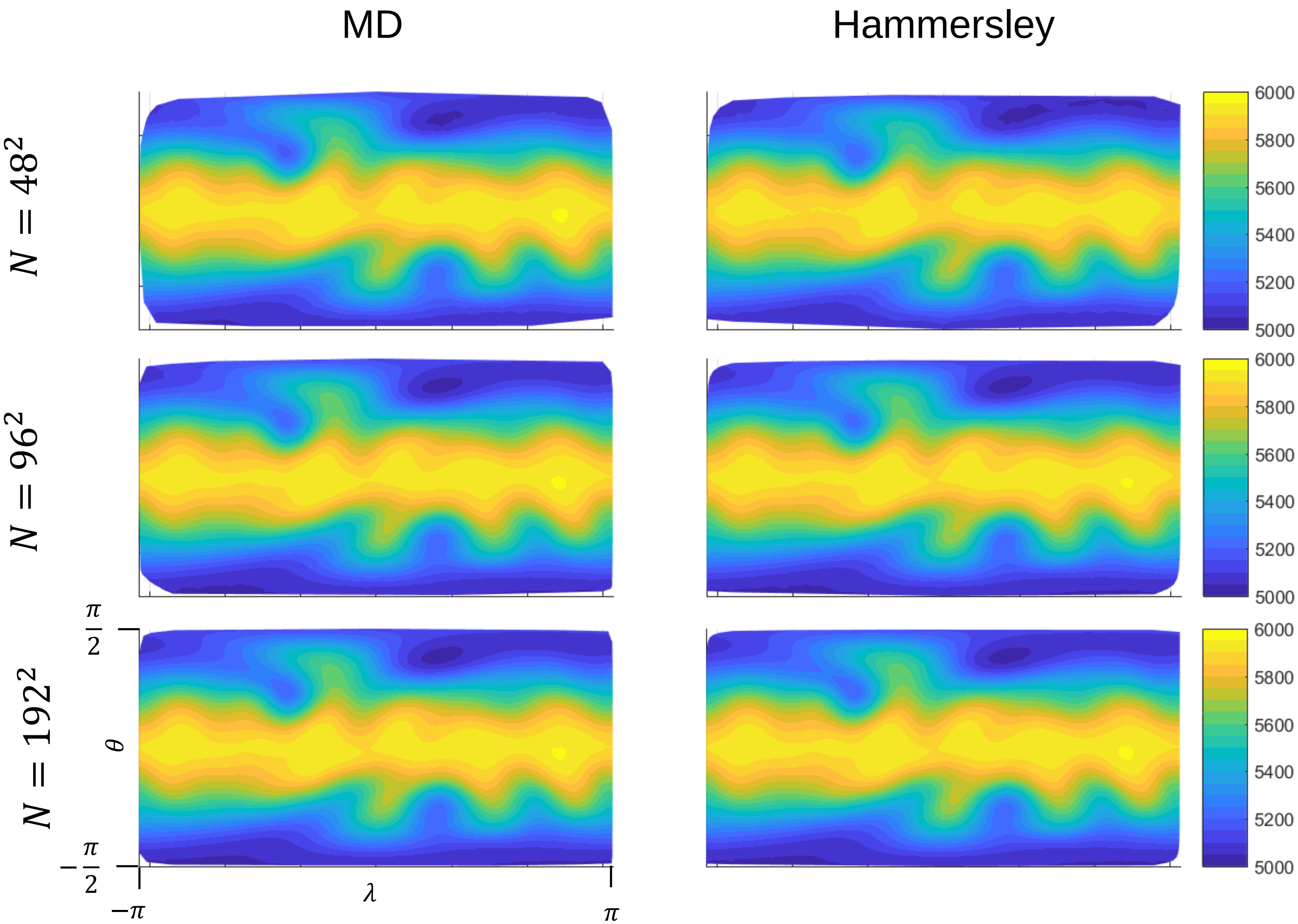
Convergence Verification ($t = 5$)



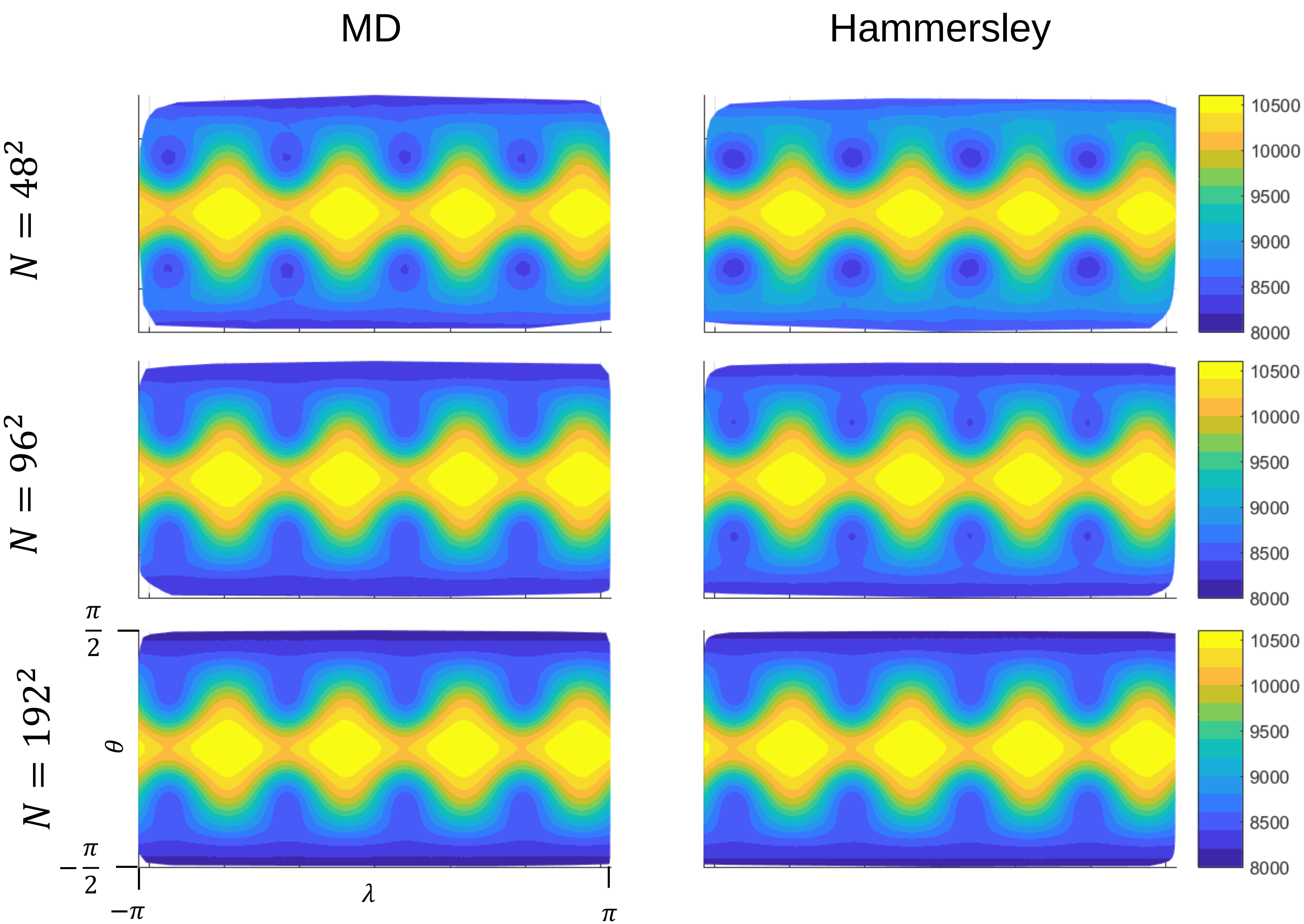
Time Snapshots, Isolated Mountain



Flow over Mountain, $t = 15$



Rossby-Haurwitz, $t = 14$



Strengths of PHS RBF-FD

- Simple and accurate on the sphere
- Local and well suited for parallel computations
- Free from coordinate singularities
  - Discretize directly from Cartesian equations
- Geometrically flexible
  - Does not require a mesh
  - Static Node Refinement
  - Dynamic Node Refinement
- Robust
  - Same configuration (basis, stencil-size, hyperviscosity parameter) runs on a wide variety of node-sets and test problems
    - $||\boldsymbol{x}||^2 \log||\boldsymbol{x}|| + \mathrm{p}5 + n42$ for first derivative approximations

Future Work

- Transport
  - 3D test cases on spherical shell (DCMIP test cases)
  - More sophisticated fixer/limiter procedure
    - Reduce parallel communication
- Shallow water equations
  - Quantitative comparison to other methods
  - Additional tests on the sphere from Williamson et al, JCP 1992
    - Forced nonlinear system with a translating Low
    - Evolution of highly nonlinear wave
- Nonhydrostatic Dynamical Core for climate/weather
  - 2D benchmarks in Cartesian geometry with topography
  - Fully 3D without using a terrain-following coordinate transformation
  - Eulerian dynamics, semi-Lagrangian transport with fixer/limiter

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