Spherical Harmonics Least Squares Approximation on the Cubed-Sphere

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Introduction

Consider **advection and diffusion** of neutral pollutant on the sphere. This is modelled by

$$\frac{\partial u}{\partial t} + \underbrace{\boldsymbol{c}(x,t) \cdot \nabla_T u}_{\text{advection}} - \underbrace{\nu \Delta u}_{\text{diffusion}} = 0.$$

- $u : \mathbb{S}_a^2 \times \mathbb{R}^+ \mapsto \mathbb{R}$ a pollutant concentration,
- $u_0 : \mathbb{S}_a^2 \mapsto \mathbb{R}$ is the initial concentration,
- $\boldsymbol{c}$ ($\mathrm{m} \cdot \mathrm{s}^{-1}$) a velocity field with $\nabla_T \cdot \boldsymbol{c} = 0$,
- ν ($\mathrm{m}^2 \cdot \mathrm{s}^{-1}$) the diffusion parameter,

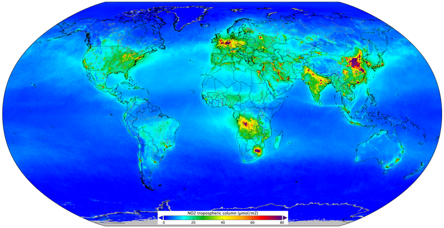


Figure: Nitrogen concentration in the troposphere 2018 (Source: `ESA.int`).

Consider a **spherical grid** to compute numerical solution.

- Consider the equiangular Cubed-Sphere $\mathcal{CS}_N$ ($\bar{N} = 6N^2 + 2$ nodes).
- Let a grid function $(\mathfrak{u}_j) \in \mathbb{R}^{\mathcal{CS}_N}$.
- Compute a function u such that

$$u(\boldsymbol{x}_j) \approx \mathfrak{u}_j \qquad 1 \leq j \leq \bar{N}.$$

Key ideas:

- ▷ Determine a framework to find u as a Spherical Harmonic,
- ▷ Effective calculation of u,
- ▷ Compute Δu and $\nabla_T u$ to solve the diffusion and the advection PDEs.

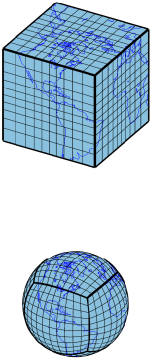


Figure: The Equiangular Cubed-Sphere $\mathcal{CS}_N$ contains $\bar{N} = 6N^2 + 2$ nodes.

Spherical Harmonics Y_n^m

- Let $n \in \mathbb{N}$ **the degree** and $|m| \leq n$:

$$Y_n^m(\boldsymbol{x}(\lambda,\theta)) = C_{n,m} P_n^{|m|}(\sin(\theta)) \begin{cases} \sin(|m|\lambda) & \text{if } m < 0 \\ 1/\sqrt{2} & \text{if } m = 0 \\ \cos(m\lambda) & \text{if } m > 0 \end{cases}$$

  (λ,θ) are longitude-latitude coordinates, $C_{n,m} \in \mathbb{R}$ is a constant and $P_n^{|m|}$ is an associated Legendre function.

- (Y_n^m) is an orthogonal Hilbert basis of $L^2(\mathbb{S}_a^2)$
- For all $u \in L^2(\mathbb{S}_a^2)$ we have

$$u = \sum_{n=0}^{+\infty} \sum_{m=-n}^{n} \hat{u}_{m,n} Y_n^m.$$

- Let $\mathbb{Y}_n = \text{Span}(Y_n^m, \quad |m| \leq n)$.
- $(Y_n^m)_{|m|\leq n \leq D}$ is a good candidate to generate u and approximate grid function $(\mathfrak{u}_j)_{1\leq j\leq \bar{N}}$.

The Vandermonde matrix

Approximation properties are encoded in the **Vandermonde matrix kind** :

$$\boldsymbol{A}_D = \left[Y_k^m(\boldsymbol{x}_j) \right]_{1 \le j \le \bar{N}; |m| \le k \le D}$$

where each column corresponds to a SH function Y_n^m.

Let $u = \sum_{n=0}^{D} \sum_{m=-n}^{n} \hat{u}_{m,n} Y_n^m$, then we have $[u(\boldsymbol{x}_j)] = \boldsymbol{A}_D [\hat{u}]$.

Least Squares and interpolation process : deduce $\hat{U} = [\hat{u}_j]$ from the vector of data $U = [\mathfrak{u}_j]$ such that

$$\boldsymbol{A}_D \hat{U} \approx U.$$

Remarks

- If D is large enough, it is possible to interpolate data on the grid.
- If D is small, interpolating function does not exist but least squares approximation can be use.

Since Bellet, Brachet, and Croisille 2023, we know how to interpolate data on $\mathcal{CS}_N$ using Spherical Harmonics and the factorization of the Vandermonde matrix.

Example : interpolation of $f(x, y, z) = \frac{1}{9}(1 + \tanh(-9x - 9y + 9z))$ on $\mathcal{CS}_4$.

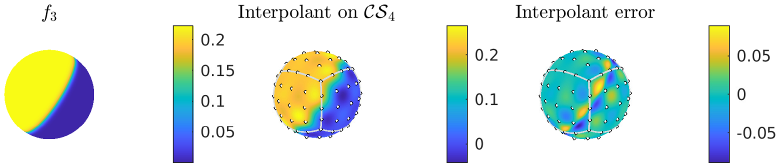


Figure: Interpolation on $\mathcal{CS}_4$.

Problems with the Interpolation approach

- Oscillations between nodes,
- Computational cost to factorise $\boldsymbol{A}_D$,
- Matrices involved have poor condition number

Least Squares approximation

- Compute $\hat{U} = [\hat{u}_{m,n}]$ that minimises

$$\mathcal{J}(\hat{U}) = \left\|\Omega^{1/2}(\boldsymbol{A}_D \hat{U} - U)\right\|_2^2 = \sum_{\boldsymbol{x}_j \in \mathcal{CS}_N} \omega(\boldsymbol{x}_j)|u(\boldsymbol{x}_j) - \mathfrak{u}_j|^2$$

where the matrix $\Omega = \mathrm{diag}(\omega(\boldsymbol{x}_1), \cdots, \omega(\boldsymbol{x}_{\bar{N}}))$ contains the weights $\omega(\boldsymbol{x}_j) > 0$.

- The vector $\hat{U}$ satisfies

$$\boldsymbol{A}_D^T \Omega_N \boldsymbol{A}_D \hat{U} = \boldsymbol{A}_D^T \Omega_N U$$

- The weighted least squares approximation is $\mathcal{I}_{\mathcal{CS}_N}^D[\mathfrak{u}]$ and

$$\mathcal{I}_{\mathcal{CS}_N}^D[\mathfrak{u}](\boldsymbol{x}) = \sum_{n=0}^{D} \sum_{m=-n}^{n} \hat{u}_{m,n} Y_n^m(\boldsymbol{x}).$$

Questions :

- How to select the degree D (as a function of the grid parameter N) such that there are a (satisfactory) solution?
- Effective computation of $\hat{U}$.
- Which weights $(\omega(\boldsymbol{x}_j))$ to choose?

Uniqueness and stability

- Uniqueness is satisfied if $\boldsymbol{A}_D$ in injective (then 0 is not a singular value).
- Stability is represented by $\mathrm{cond}_2(\boldsymbol{A}_D)$.

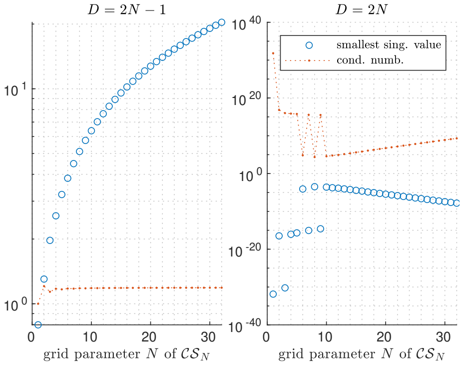


Figure: Smallest singular values and condition number of $\boldsymbol{A}_D$

★ $D = 2N - 1$ gives satisfactory results (existence, uniqueness and stability) and is chosen in the experiments hereafter.

Efficient solver

Let the weights $(\omega(\boldsymbol{x}_j))_j$ come from a quadrature rule. Then, we have

$$\boldsymbol{A}_D^T \Omega_N \boldsymbol{A}_D = \left[\sum_{\boldsymbol{x}_j \in \mathcal{CS}_N} \omega(\boldsymbol{x}_j) Y_n^m(\boldsymbol{x}_j) Y_{n'}^{m'}(\boldsymbol{x}_j)\right] \approx \left[\int_{\mathbb{S}_a^2} Y_n^m(\boldsymbol{x}) Y_{n'}^{m'}(\boldsymbol{x}) d\sigma(\boldsymbol{x})\right] = a \mathsf{I}_{(D+1)^2}$$

Conjugate gradient solver (CG) is used to compute $\hat{U}$ (and thus $(\hat{u}_j)$) :

$$\boldsymbol{A}_D^T \Omega_N \boldsymbol{A}_D \hat{U} = \boldsymbol{A}_D^T \Omega_N U$$

Some weights considered :

- Uniform rule : $\omega(\boldsymbol{x}) = \frac{4\pi a}{\bar{N}}$,
- Spherical Harm. rule : based on exact integration of interpolating function Bellet, Brachet, and Croisille 2022,
- Metric rule : $\omega(\boldsymbol{x}) = \frac{\pi^2}{4N^2} \sqrt{|\det(\boldsymbol{G}(\boldsymbol{x}))|}$ where $\boldsymbol{G}(\boldsymbol{x})$ is the metric tensor (see Brachet 2018)

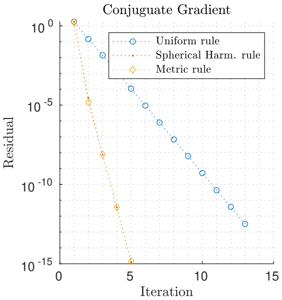


Figure: Residual of conjuguate gradient to solve WLS with $D = 2N - 1$ (test case with $\bar{N} = 6146$ nodes).

Numerical illustration

Consider $f(x,y,z) = \frac{1}{9}(1 + \tanh(-9x - 9y + 9z))$ approximated by interpolation and WLS.

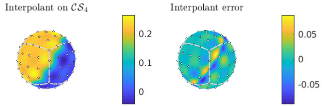


Figure: Interpolation on $\mathcal{CS}_4$.

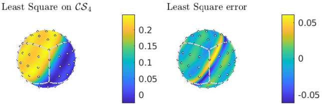


Figure: Weighted Least Squares on $\mathcal{CS}_4$.

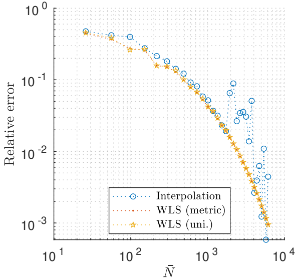


Figure: Relative error evaluated on long/lat grid with 10^5 nodes.

- The poor accuracy for interpolation can be related to the condition number.
- WLS is satisfactory.

★ The metric rule gives satisfactory results and is chosen for in the numerical experiments hereafter.

Diffusion PDE

Let the **diffusion equation** :

$$\frac{\partial u}{\partial t} = \nu \Delta u$$

with $u^0 = \sum_{n=0}^{D} \sum_{m=-n}^{n} \hat{u}^0_{m,n} Y_n^m$.

Spherical harmonics $(Y_n^m)_{0\le|m|\le n}$ are eigenfunction of Δ:

$$\Delta Y_n^m = -\frac{n(n+1)}{a^2} Y_n^m$$

Assuming $u^0 = \sum_{n=0}^{D} \sum_{m=-n}^{n} \hat{u}^0_{m,n} Y_n^m$ then we have

$$u(\boldsymbol{x}, t) = \sum_{n=0}^{D} \sum_{m=-n}^{n} \hat{u}^0_{m,n} e^{-\nu t^{n(n+1)/a^2}} Y_n^m(\boldsymbol{x}) \in \bigoplus_{n\le D} \mathbb{Y}_n.$$

★ It corresponds to an exponential integrator denoted by $\mathcal{D}_t$.

Consider a radial initial function on earth $\mathbb{S}_a^2$ with $a = 6371.22 \cdot 10^3$m and $\nu = 10^7$m $\cdot$ s^{-2} (test case inspired from Skiba 2015).

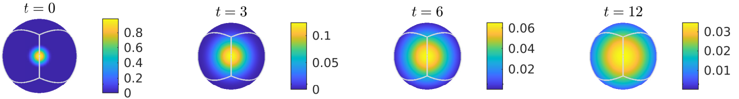
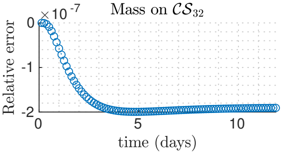


Figure: Diffusion PDE. Solution with $\Delta t = 3 \times 3600$s

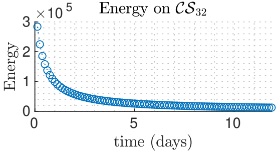
Property: Mass conservation

$$\frac{d}{dt}\int_{\mathbb{S}_a^2} u(\boldsymbol{x},t)d\sigma(\boldsymbol{x}) = 0$$



Property: Energy dissipation

$$\frac{d}{dt}\int_{\mathbb{S}_a^2} \left|u(\boldsymbol{x},t)\right|^2 d\sigma(\boldsymbol{x}) \leq 0.$$



Advection equation

Consider the **advection equation** :

$$\frac{\partial u}{\partial t} + \boldsymbol{c} \cdot \nabla_T u = 0$$

Advection operator approximation :

- Use spherical harmonics to compute $\boldsymbol{c} \cdot \nabla_T u$ but $\boldsymbol{c} \cdot \nabla_T Y_n^m \notin \bigoplus_{n \leq D} \mathbb{Y}_n$.
- Consider the approximation $\boldsymbol{c} \cdot \nabla_T Y_n^m \approx \mathcal{I}_{\mathcal{CS}_N}^D \left[\boldsymbol{c} \cdot \nabla_T Y_n^m |_{\mathcal{CS}_N} \right] \in \bigoplus_{n \leq D} \mathbb{Y}_n$.

Time integrator :

Let the (modified) initial state: $u^{(0)} = \mathcal{I}_{\mathcal{CS}_N}^D [u_0] \in \bigoplus_{n \leq D} \mathbb{Y}_n$.

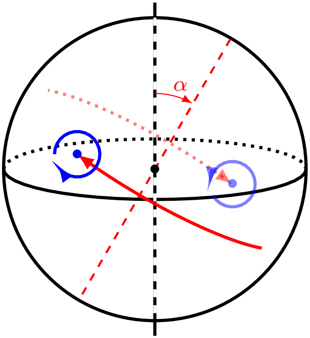
For $k = 0, \cdots$,

$$\begin{aligned}
K_1 &= -\mathcal{I}_{\mathcal{CS}_N}^D \left[\boldsymbol{c} \cdot \nabla_T u^{(k)} |_{\mathcal{CS}_N} \right] \\
K_2 &= -\mathcal{I}_{\mathcal{CS}_N}^D \left[\boldsymbol{c} \cdot \nabla_T \left(u^{(k)} + \tfrac{\Delta t}{2} K_1 \right) |_{\mathcal{CS}_N} \right] \\
K_3 &= -\mathcal{I}_{\mathcal{CS}_N}^D \left[\boldsymbol{c} \cdot \nabla_T \left(u^{(k)} + \tfrac{\Delta t}{2} K_2 \right) |_{\mathcal{CS}_N} \right] \\
K_4 &= -\mathcal{I}_{\mathcal{CS}_N}^D \left[\boldsymbol{c} \cdot \nabla_T \left(u^{(k)} + \Delta t K_3 \right) |_{\mathcal{CS}_N} \right] \\
u^{(k+1)} &= u^{(k)} + \tfrac{\Delta t}{6} (K_1 + 2K_2 + 2K_3 + K_4).
\end{aligned}$$

★ We consider RK4 time discretization (denote $\mathcal{A}_t$ the solver).

Vortex in rotation

Moving vortices on the sphere test case introduced in Nair and Jablonowski 2008.



- Velocity :

$$\boldsymbol{c}(\boldsymbol{x},t) = \underbrace{\boldsymbol{c}_s(\boldsymbol{x})}_{\text{solid vel.}} + \underbrace{\boldsymbol{c}_r(\boldsymbol{x},t)}_{\text{vortex vel.}}$$

with $\nabla_T \cdot \boldsymbol{c} = 0$.

- Solution given by

$$u(\lambda', \theta', t) = 1 - \tanh\left(\frac{\rho}{\gamma}(\lambda' - \omega_r t)\right)$$

with (λ', θ') the rotated long/lat coordinates on $\mathbb{S}^2_a$.

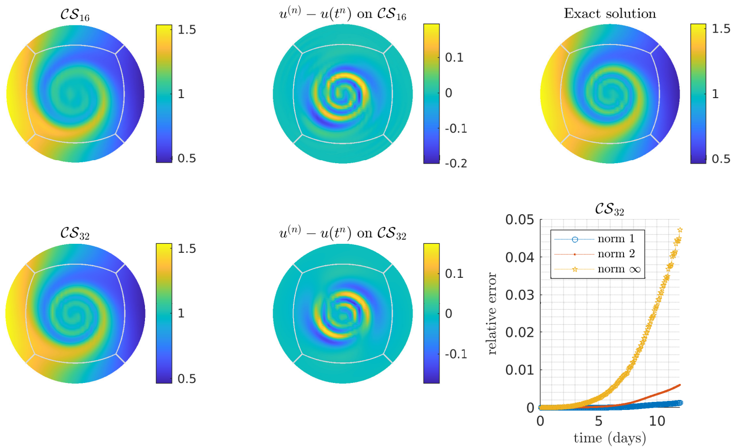


Figure: Results for Moving vortices test cases on $\mathcal{CS}_{16}$ ($\Delta t = 189$min) and $\mathcal{CS}_{32}$ ($\Delta t = 94.5$min) with $\alpha = {}^{\pi}/_{4}$.

Advection Diffusion equation

Let the partial differential equation

$$\frac{\partial u}{\partial t} + \boldsymbol{c} \cdot \nabla_T u - \nu \Delta u = 0$$

Theoretical continuous properties.

Mass conservation :

$$\frac{d}{dt} \int_{\mathbb{S}_a^2} u(t, \boldsymbol{x}) d\sigma(\boldsymbol{x}) = 0.$$

Energy stability :

$$\frac{d}{dt} \int_{\mathbb{S}_a^2} u(t, \boldsymbol{x})^2 d\sigma(\boldsymbol{x}) \leq 0.$$

Strang splitting integrator : $u^{(k+1)} = \mathcal{D}_{\Delta t/2} \circ \mathcal{A}_{\Delta t} \circ \mathcal{D}_{\Delta t/2} u^{(k)}$.
Let $u^{(0)} = \mathcal{I}^{D}_{\mathcal{CS}_N}[u_0]$.
For $k = 0, 1, \cdots$

$$u^{(*)} = \mathcal{D}_{\Delta t/2} u^{(k)} \qquad \text{(Exponential)}$$

$$u^{(**)} = \mathcal{A}_{\Delta t} u^{(*)} \qquad \text{(RK4)}$$

$$u^{(k+1)} = \mathcal{D}_{\Delta t/2} u^{(**)} \qquad \text{(Exponential)}$$

Consider the following advection-diffusion test case (based on Williamson et al. 1992):

- $\boldsymbol{c} = \boldsymbol{c}_s(\boldsymbol{x})$ the solid body velocity ($\alpha = \pi/4$) and $\nu = 2 \times 10^5 \mathrm{m} \cdot \mathrm{s}^{-2}$,
- $u_0 \in \mathcal{C}^1(\mathbb{S}^2_a, \mathbb{R})$ a radial function centred on $(\lambda_0, \theta_0) = (\pi/4, \pi/4)$.

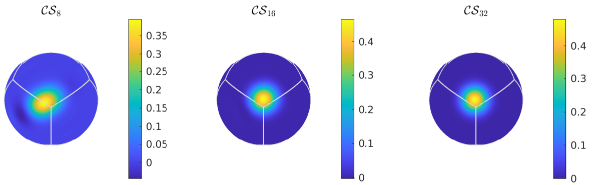


Figure: Solution at $t = 36$ days obtained on $\mathcal{CS}_8$ ($\Delta t = 6.26$h), $\mathcal{CS}_{16}$ ($\Delta t = 3.15$h) and $\mathcal{CS}_{32}$ ($\Delta t = 1.57$h).

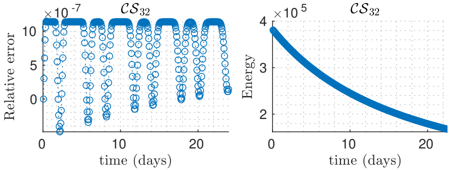


Figure: Mass error and energy history obtained on $\mathcal{CS}_{32}$ ($\Delta t = 1.57$h).

Conclusion and perspectives

Conclusion :

- Data are approximated by a function in spherical harmonics using WLS.
- Weights have an influence on the solver convergence but not a significantly one on the approximation.
- The SH function are used to solve advection and diffusion PDEs.

Perspectives

- VanDerMonde matrix $\boldsymbol{A}_D$ is expensive to compute. A fast method should be required but not obtained yet.
- Many theoretical problems remain open.
- Irregular geometries (coasts) embedded on the Cubed-Sphere?

- Bellet, Jean-Baptiste, Matthieu Brachet, and Jean-Pierre Croisille (2022). "Quadrature and symmetry on the Cubed Sphere". In: *Journal of Computational and Applied Mathematics* 409, p. 114142.
- – (2023). "Interpolation on the cubed sphere with spherical harmonics". In: *Numerische Mathematik* 153.2, pp. 249–278.
- – (2025). "Spherical Harmonics collocation: A computational intercomparison of several grids". In: *hal-04895616*.
- Bellet, Jean-Baptiste and Jean-Pierre Croisille (2023). "Least squares spherical harmonics approximation on the Cubed Sphere". In: *Journal of Computational and Applied Mathematics* 429, p. 115213.
- Brachet, Matthieu (2018). "Schémas compacts hermitiens sur la Sphère: applications en climatologie et océanographie numérique". PhD thesis. Université de Lorraine.
- Nair, Ramachandran D and Christiane Jablonowski (2008). "Moving vortices on the sphere: A test case for horizontal advection problems". In: *Monthly Weather Review* 136.2, pp. 699–711.
- Skiba, Yuri N (2015). "A non-iterative implicit algorithm for the solution of advection–diffusion equation on a sphere". In: *International Journal for Numerical Methods in Fluids* 78.5, pp. 257–282.
- Williamson, David L et al. (1992). "A standard test set for numerical approximations to the shallow water equations in spherical geometry". In: *Journal of computational physics* 102.1, pp. 211–224.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