

Approximation of data on a spherical grid for numerical climatology

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A brief history

- 1922: Lewis Fry Richardson published *Weather Prediction by Numerical Process*, introducing a numerical method for weather forecasting.
- Before computers existed, he proposed manual calculations in a 'Weather Forecasting Factory'.

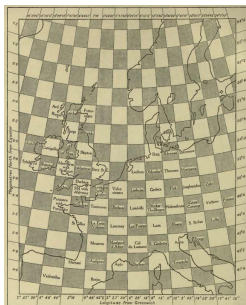
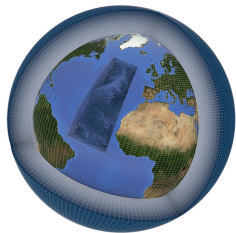


Figure: Left: Richardson's grid section. Right: the Weather Forecasting Factory (Illustration by S. Conlin, The Irish Times).

- The numerical method is based finite differences and the use of measure on nodes on a long-lat grid to solve Navier-Stokes equation.

- Richardson process useless in practice :
 - Computational cost (64000 people required);
 - No filtering on data;
 - Stability issues:
 - ▶ CFL condition introduced for linear PDEs (*On the Partial Difference Equations of Mathematical Physics* – 1928)
 - ▶ Stability formalized by J. G. Charney, R. Jörtoft, J. von Neumann (*Numerical Integration of the Barotropic Vorticity Equation* – 1950).
- Some key ideas still used today for numerical calculations on a spherical Earth.



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Figure: Illustration of ocean, atmospheric, and continental surface model grids. © CEA/CNRS/Meteo France/Animea

Introduction

In this talk, we consider **advection and diffusion** as a toy model for a (time dependant) of Munk equation:

$$\frac{\partial \psi}{\partial t} + \underbrace{c(x, t) \cdot \nabla_T \psi}_{\text{advection}} + \underbrace{\nu \Delta_T^2 \psi}_{\text{bi-diffusion}} = 0.$$

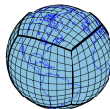
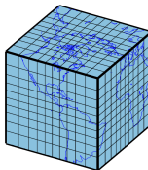
- $\psi : \mathbb{S}_a^2 \times \mathbb{R}^+ \mapsto \mathbb{R}$, the streamfunction,
- $\psi_0 : \mathbb{S}_a^2 \mapsto \mathbb{R}$ is the initial state,
- $c \in \mathbb{TS}_a^2$ a tangential velocity field with $\nabla_T \cdot c = 0$ (related to Coriolis force),
- ν the diffusion parameter,

Remark : Equation is (numerically) difficult to solve if $\frac{\|c\|_\infty}{\nu} \gg 1$ and presence of a boundary layer.

Spherical grid to compute numerical solution:

- Consider the equiangular Cubed-Sphere $\mathcal{CS}_N$ ($\bar{N} = 6N^2 + 2$ nodes).
- Let a grid function $(\psi_j) \in \mathbb{R}^{\mathcal{CS}_N}$ (related to spherical data).
- Compute a function $\psi : \mathbb{S}_a^2 \rightarrow \mathbb{R}$ such that

$$\psi(\mathbf{x}_j) \approx \psi_j \quad 1 \leq j \leq \bar{N}.$$



Roadmap:

- ▷ Determine a framework to find ψ as a Spherical Harmonic,
- ▷ Effective calculation of ψ ,
- ▷ Compute $\Delta_T \psi$ and $\nabla_T \psi$.
- ▷ Numerical solver for the diffusion and the advection PDEs.

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

Spherical Harmonics on $\mathcal{CS}_N$

Spherical Harmonics Y_n^m

- Spherical harmonic are harmonic polynom restricted to a sphere and eigenfunction of Laplacian.
- Let $n \in \mathbb{N}$ **the degree**, $|m| \leq n$ and define

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

(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 $\psi \in L^2(\mathbb{S}_a^2)$ we have

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

- 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.

The Vandermonde matrix

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

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

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

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

$$[\psi(\mathbf{x}_j)] = \mathbf{A}_D [\hat{\psi}].$$

Interpolation and least squares processes : deduce $\hat{\Psi} = [\psi_\ell] \in \mathbb{R}^{(D+1)^2}$ from the vector of data $\Psi = [\psi_j] \in \mathbb{R}^{\bar{N}}$ such that

$$\mathbf{A}_D \hat{\Psi} \approx \Psi.$$

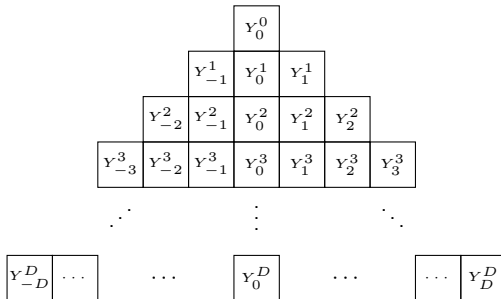
Interpolation

Interpolation

Interpolation : deduce $\hat{\Psi} = [\hat{\psi}_{m,n}]$ from the vector of data $\Psi = [\psi_j] \in \mathbb{R}^{\bar{N}}$ such that

$$\mathbf{A}_D \hat{\Psi} = \Psi.$$

- $\bar{N} = 6N^2 + 2$ values on each node,
- $(D+1)^2$ coefficients to compute.



Remark : Because $(D+1)^2 \neq \bar{N}$ and $\mathbf{A}_D$ properties, the system is either underdetermined or overdetermined, and may not admit a unique solution.

Proposition: There exist a smallest degree $D \in \mathbb{N}$ such that

- A_D has row full rank,
- Interpolation problem has a solution in $\bigoplus_{n \leq D} \mathbb{Y}_n$.

Remark :

- This gives the existence of interpolation.
- If we consider all spherical harmonics $(Y_k^m)_{|m| \leq n \leq D}$, there are *a priori* several solution to the interpolation problem.

Uniqueness

Consider the orthogonal decomposition

$$\mathbb{Y}_n = Y_n \oplus^\perp Y'_n$$

where $Y'_n = \left\{ f \in \mathbb{Y}_n : \exists g \in \bigoplus_{k \leq n-1} \mathbb{Y}_k \text{ such that } f(x_j) = g(x_j) \text{ for all } 1 \leq j \leq \bar{N} \right\}$.

- Y'_n is composed with undersampled spherical harmonics.
- Y_n corresponds to the functions correctly represented on the grid.

Then, we deduce the following theorem :

Proposition: The interpolation problem has an unique solution in

$$\mathcal{Y}'_D = \bigoplus_{n \leq D} Y_n.$$

The matrix A_D will give us information about $\mathcal{Y}'_D$.

Theorem: Let $n \in \mathbb{N}$. The matrix $\mathbf{A}_n$ can be factorized in the form

$$\mathbf{A}_n = \mathbf{V}_n \mathbf{E}_n \mathbf{U}_n^T$$

where

- $\mathbf{U}_n \in \mathcal{M}_{(n+1)^2}(\mathbb{R})$ and $\mathbf{V}_n \in \mathcal{M}_{\bar{N}}(\mathbb{R})$ are orthogonal matrices;
- $\mathbf{E}_n \in \mathcal{M}_{\bar{N}, (n+1)^2}(\mathbb{R})$ is a row echelon matrix.

In particular, $\text{rank}(\mathbf{E}_n) = \text{rank}(\mathbf{A}_n)$.

Remark :

- Proof is constructive (proof by induction) and based on singular value decomposition of suitable matrices.
- Matrix $\mathbf{U}_n$ is block diagonal and $\mathbf{U}_n = \begin{bmatrix} \mathbf{U}_{n-1} & (0) \\ (0) & \mathbf{U}_n \end{bmatrix}$.
- An orthogonal basis of $\mathcal{Y}_D$ is encoded into $\mathbf{U}_n(:, 1 : g_n)$ where $g_n = \text{rank}(\mathbf{A}_n) - \text{rank}(\mathbf{A}_{n-1})$.

Explicit solution

Let define

$$\tilde{U}_n = \begin{bmatrix} U_0(1:1, 1:g_0) & & \\ & \ddots & \\ & & U_n(1:2n+1, 1:g_n) \end{bmatrix} \in \mathcal{M}_{(n+1)^2, \text{rank}(\mathbf{A}_n)}(\mathbb{R})$$

$$\mathbf{R}_n = \mathbf{E}_n \begin{bmatrix} \text{Id}(1:1, 1:g_0) & & \\ & \ddots & \\ & & \text{Id}(1:2n+1, 1:g_n) \end{bmatrix} \in \mathcal{M}_{\text{rank}(\mathbf{A}_n), \bar{N}}(\mathbb{R})$$

So we deduce:

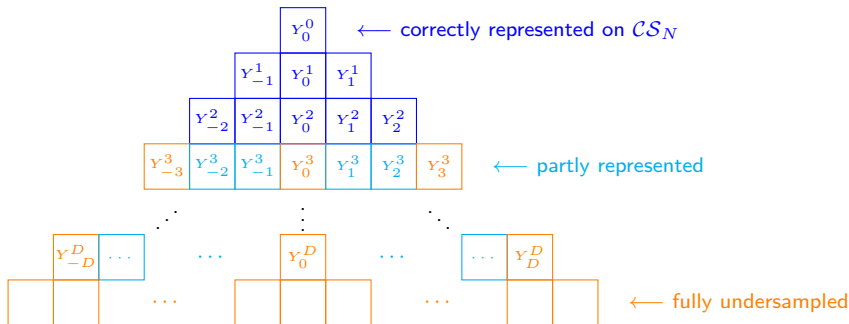
$$\mathbf{A}_n \tilde{U}_n = \mathbf{V}_n \mathbf{R}_n.$$

Theorem:

- The subspace $\mathcal{Y}'_D$ is unisolvent for the Lagrange interpolation problem,
- The interpolant $p(x)$ is expressed in the basis (Y_n^m) by

$$\psi(x) = [Y_n^m(x)]_{|m| \leq n \leq D}^T \hat{\Psi} \quad \text{and} \quad \hat{\Psi} = \tilde{U}_D \mathbf{R}_D^{-1} \mathbf{V}_D^T \Psi.$$

- Subspace $\mathcal{Y}'_D$ is construct thanks a **matrix factorization** of A_D (see [Bellet, Brachet, and Croisille 2023](#)).
- Key idea:** exclude iteratively exclude undersampled Spherical Harmonics (if restricted to the grid).



Numerical observation : $\bigoplus_{n \leq N'} \mathbb{Y}_n \subset \mathcal{Y}'_D$ with $N' = 2N - 1$.

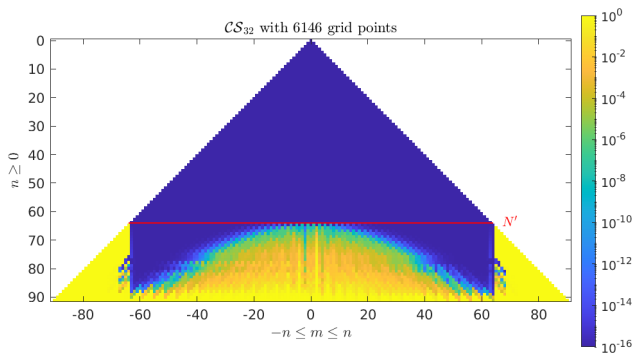


Figure: Distance between $\mathcal{Y}'_D$ and Y_m^n a spherical harmonics for CS_{32} .

Numerical Illustration

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

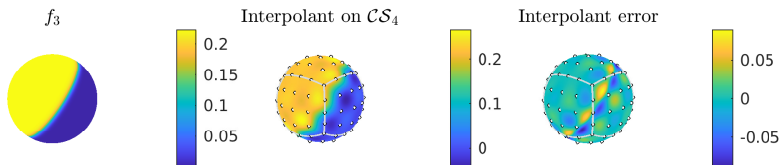


Figure: Interpolation on $\mathcal{CS}_4$.

Problems with the Interpolation approach

- Oscillations between nodes,
- Computational cost to factorise A_D ,
- Matrices involved have poor condition number

Least Square Approximation

Least Squares approximation

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

$$\mathcal{J}(\hat{\Psi}) = \left\| \Omega^{1/2} (\mathbf{A}_D \hat{\Psi} - \Psi) \right\|_2^2 = \sum_{x_j \in \mathcal{CS}_N} \omega(x_j) |\psi(x_j) - \hat{\psi}_j|^2$$

where the matrix $\Omega = \text{diag}(\omega(x_1), \dots, \omega(x_{\bar{N}}))$ contains the weights $\omega(x_j) > 0$.

- The vector $\hat{\Psi}$ satisfies

$$\mathbf{A}_D^T \Omega_N \mathbf{A}_D \hat{\Psi} = \mathbf{A}_D^T \Omega_N \Psi$$

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

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

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 $\hat{\Psi}$.
- Which weights $(\omega(x_j))$ to choose?

Uniqueness and stability

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

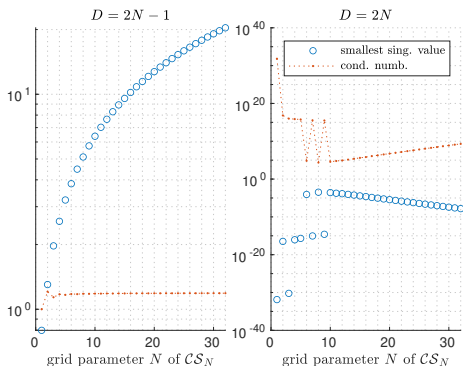


Figure: Smallest singular values and condition number of $\mathbf{A}_D$

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

Efficient solver

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

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

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

$$\mathbf{A}_D^T \Omega_N \mathbf{A}_D \hat{\Psi} = \mathbf{A}_D^T \Omega_N \Psi$$

Some weights considered :

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

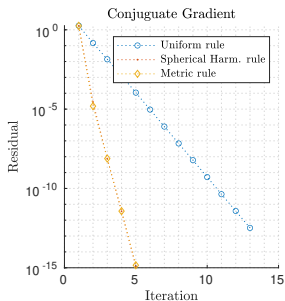


Figure: Residual of conjugate gradient to solve WLS with $D = 2N - 1$ (test case with $N = 6146$ nodes).

Numerical illustration

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

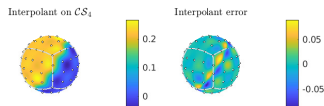


Figure: Interpolation on CS_4 .

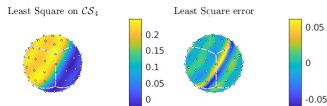


Figure: Weighted Least Squares on CS_4 .

- 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.

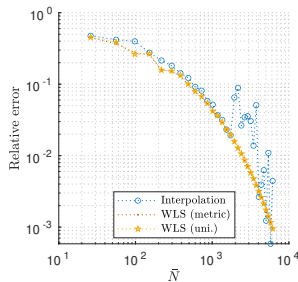


Figure: Relative error evaluated on long/lat grid with 10^5 nodes.

Advection-bidiffusion PDE

Diffusion PDE

Let the **diffusion equation** :

$$\frac{\partial \psi}{\partial t} = -\nu \Delta_T^2 \psi$$

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

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

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

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

$$\psi(\mathbf{x}, t) = \sum_{n=0}^D \sum_{m=-n}^n \hat{\psi}_{m,n}^0 e^{-\nu t \left(\frac{n(n+1)}{a^2} \right)^2} Y_n^m(\mathbf{x}) \in \bigoplus_{n \leq D} \mathbb{Y}_n.$$

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

Consider a radial initial function on earth $\mathbb{S}_a^2$ with $a = 6371.22 \cdot 10^3 \text{m}$ and $\nu = 10^{-7} a^4$ (test case inspired from [Skiba 2015](#)).

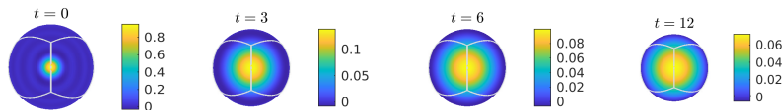


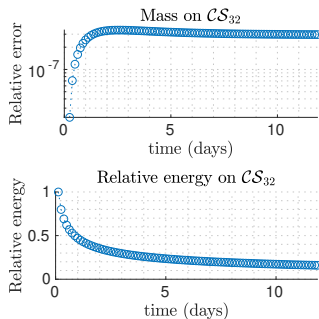
Figure: Diffusion PDE. Solution with $\Delta t = 3 \times 3600 \text{s}$ on $\mathcal{CS}_{32}$.

Property: Mass conservation

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

Property: Energy dissipation

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



Advection PDE

Consider the **advection equation** :

$$\frac{\partial \psi}{\partial t} + \mathbf{c} \cdot \nabla_T \psi = 0$$

with $\psi^0 = \sum_{n=0}^D \sum_{m=-n}^n \hat{u}_{m,n}^0 Y_n^m$ and the velocity field $\mathbf{c} : (\mathbf{x}, t) \mapsto \mathbf{c}(\mathbf{x}, t) \in \mathbb{TS}_a^2$.

Use spherical harmonics to compute $\mathbf{c} \cdot \nabla_T \psi$ but $\mathbf{c} \cdot \nabla_T Y_n^m \notin \bigoplus_{n \leq D} \mathbb{Y}_n$.

We consider the approximation : $\mathbf{c} \cdot \nabla_T Y_n^m \approx \mathcal{I}_{\mathcal{CS}_N}^D [\mathbf{c} \cdot \nabla_T Y_n^m |_{\mathcal{CS}_N}] \in \bigoplus_{n \leq D} \mathbb{Y}_n$.

Then

$$\mathbf{c} \cdot \nabla_T \psi \approx \mathcal{I}_{\mathcal{CS}_N}^D [\mathbf{c} \cdot \nabla_T \psi |_{\mathcal{CS}_N}] = \sum_{n=0}^D \sum_{m=-n}^n \hat{\psi}_{m,n} \mathcal{I}_{\mathcal{CS}_N}^D [\mathbf{c} \cdot \nabla_T Y_n^m].$$

Advection equation

Consider the **advection equation** :

$$\frac{\partial \psi}{\partial t} + \mathbf{c} \cdot \nabla_T \psi = 0$$

Time integrator :

Let the (modified) initial state: $\psi^{(0)} = \mathcal{I}_{\mathcal{CS}_N}^D[\psi_0] \in \bigoplus_{n \leq D} \mathbb{Y}_n$.

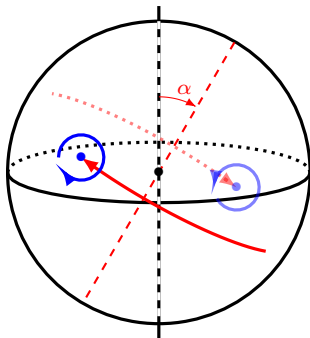
For $k = 0, \dots$,

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

★ 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 :

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

with $\nabla_T \cdot \mathbf{c} = 0$ and $\mathbf{c} \in \mathbb{TS}_a^2$.

- Solution given by

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

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

Advection PDE

- The initial state corresponds to two phases that will roll up around each other over time.

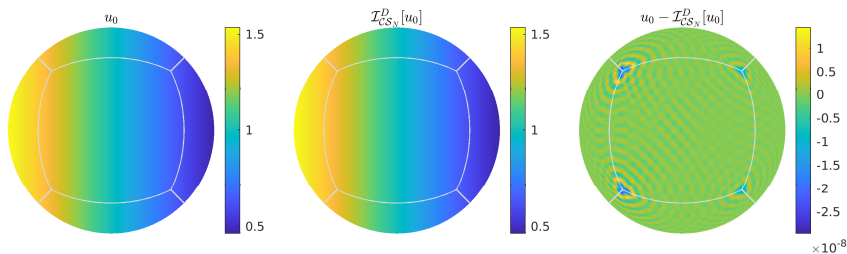


Figure: ψ_0 , $\mathcal{I}_{CS_{32}}^D[\psi_0]$ and $\psi_0 - \mathcal{I}_{CS_{32}}^D[\psi_0]$

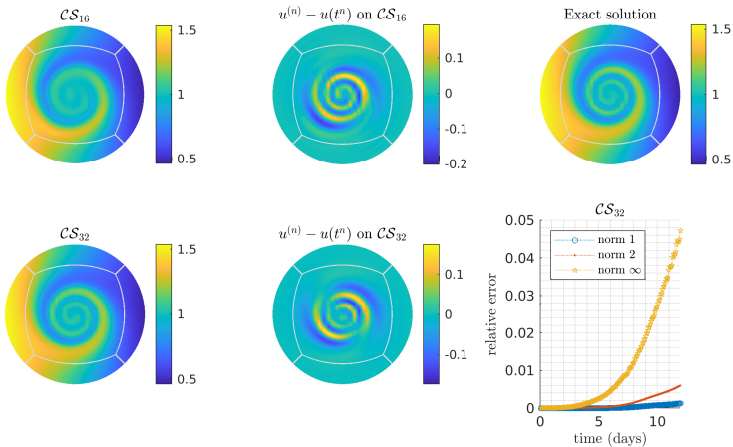


Figure: Results for Moving vortices test cases on $\mathcal{CS}_{16}$ ($\Delta t = 189\text{min}$) and $\mathcal{CS}_{32}$ ($\Delta t = 94.5\text{min}$) with $\alpha = \pi/4$.

Advection Diffusion equation

Let the partial differential equation

$$\frac{\partial \psi}{\partial t} + \mathbf{c} \cdot \nabla_T \psi + \nu^2 \Delta_T \psi = 0$$

Theoretical continuous properties.

Mass conservation :

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

Energy stability :

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

Strang splitting integrator : $\psi^{(k+1)} = \mathcal{D}_{\Delta t/2} \circ \mathcal{A}_{\Delta t} \circ \mathcal{D}_{\Delta t/2} \psi^{(k)}.$

Let $\psi^{(0)} = \mathcal{I}_{CS_N}^D[\psi_0].$

For $k = 0, 1, \dots$

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

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

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

Consider the following advection-diffusion test case (based on [Williamson et al. 1992](#) where it is considered without any diffusion):

- $\mathbf{c} = \mathbf{c}_s(\mathbf{x}) \in \mathbb{TS}_a^2$ the solid body velocity ($\alpha = \pi/4$) and $\nu = 10^{-10}a^4(\text{m}^4 \cdot \text{s}^{-1})$,
- $\psi_0 \in \mathcal{C}^1(\mathbb{S}_a^2, \mathbb{R})$ a radial function centred on $(\lambda_0, \theta_0) = (\pi/4, \pi/4)$.

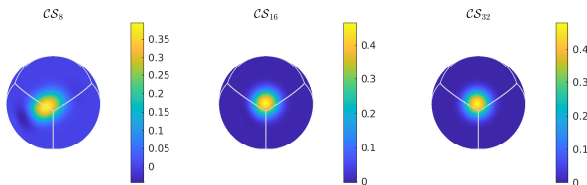


Figure: Solution at $t = 36$ days obtained on CS_8 ($\Delta t = 6.26\text{h}$), CS_{16} ($\Delta t = 3.15\text{h}$) and CS_{32} ($\Delta t = 1.57\text{h}$).

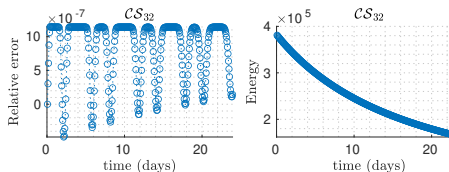


Figure: Mass error and energy history obtained on CS_{32} ($\Delta t = 1.57\text{h}$) using quadrature formula.

Conclusion

Conclusion and perspectives

Conclusion :

- Data set on $\mathcal{CS}_N$ are approximated by a spherical harmonics function.
- Process could be applied to other spherical grid.
- The SH function is used to solve advection and diffusion PDEs.

Perspectives

- VanDerMonde matrix A_D is expensive to compute and/or factorize. A fast method should be required but not obtained yet.
- Many theoretical and modelisation 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.
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