

High-performance Computing for the Geodynamo

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Outline

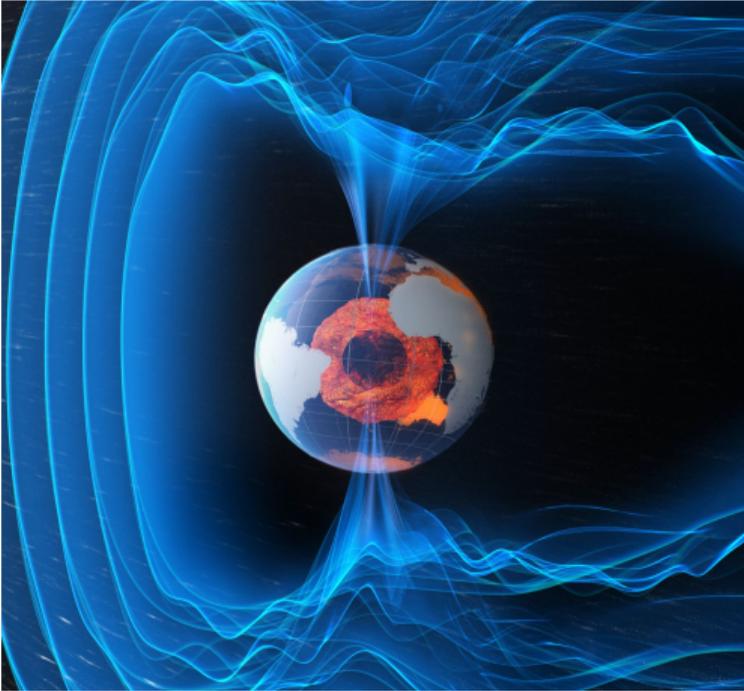
The geodynamo

Solution method

State-of-the-art simulations

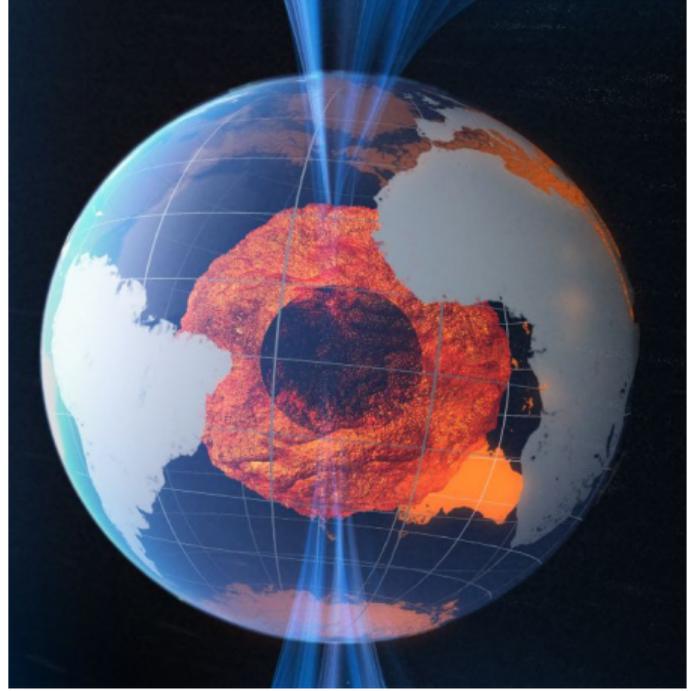
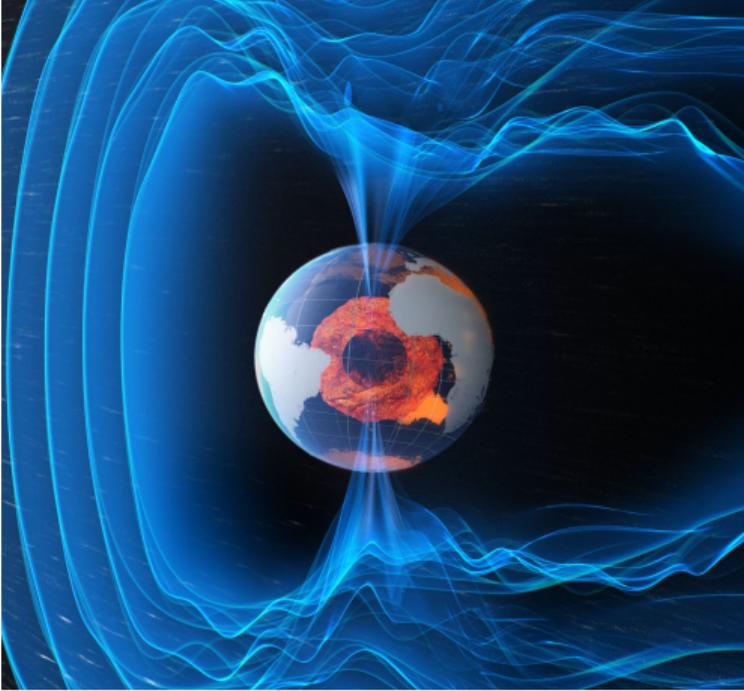
Reversals

The Earth's interior and the geomagnetic field



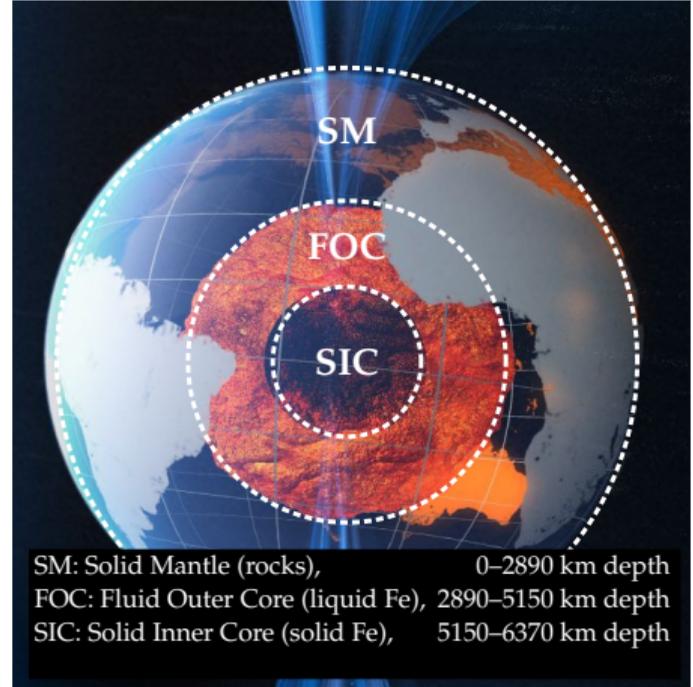
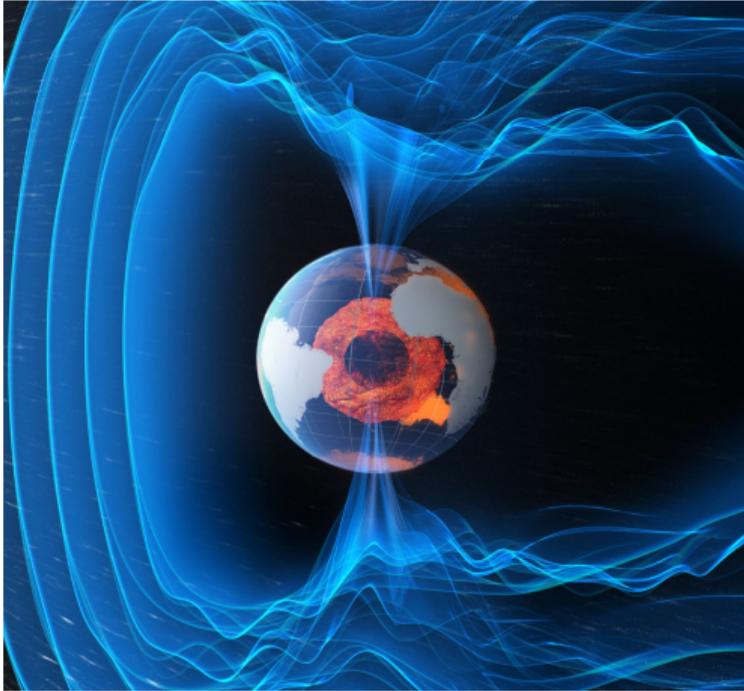
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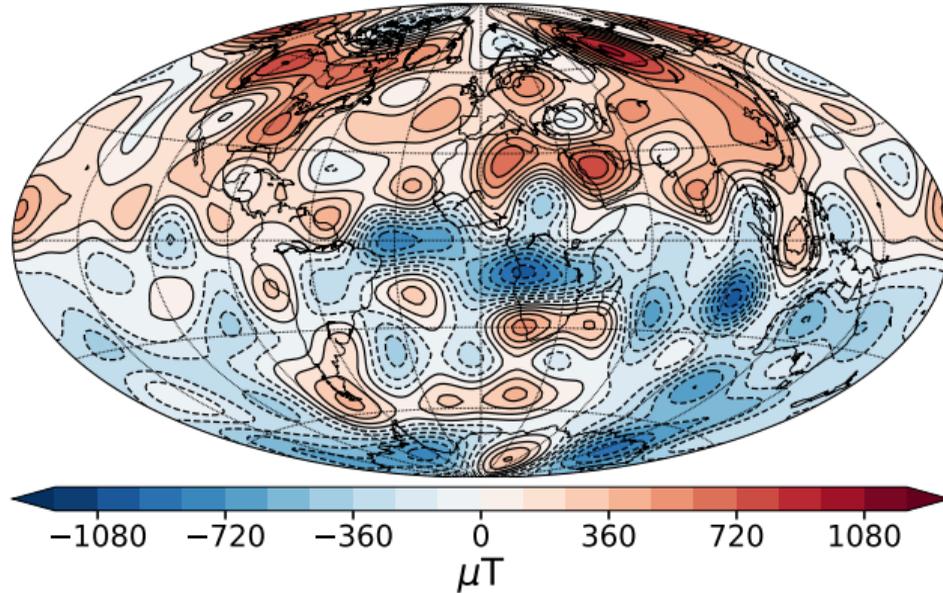


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The geomagnetic field: a sparse record (in space and time)

A short-sighted view

- ▶ dipole-dominated
- ▶ small scales of dynamo field concealed by the small scales of the crustal field
- ▶ even if perfect sampling: $\ell \lesssim 13$ (lateral resolution of ~ 1500 km at the core surface)



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Time variations : constraints provided by geomagnetism (observatory and satellite data)

- ▶ Smooth decadal variations punctuated by rapid (interannual) impulses (geomagnetic jerks)

Constraints provided by paleomagnetism

- ▶ The strength of the field varies on secular, millennial and geological time scales
- ▶ The further in the past we look, the cruder our description of the field (axial dipole)
- ▶ The field reverses its polarity every once in a while ($\approx 4 \text{ Myr}^{-1}$ over the past 25 Myr)
- ▶ Last one 780 ka, poorly constrained transitional field

First-principle simulations can complement observations

Numerical models of the geodynamo – the problem at hand

The Earth's dynamo is powered by convection. In its simplest Boussinesq form, using the codensity formalism (Braginsky and Roberts, 1995), the problem reads

$$\nabla \cdot \mathbf{u} = 0,$$

$$\rho_0 \partial_t \mathbf{u} = \mathbf{F}_p + \mathbf{F}_C + \mathbf{F}_i + \mathbf{F}_L + \mathbf{F}_v + \mathbf{F}_b,$$

$$\partial_t C = -\mathbf{u} \cdot \nabla C + \kappa \nabla^2 C,$$

$$\partial_t \mathbf{B} = \nabla \times (\mathbf{u} \times \mathbf{B}) + \lambda \nabla^2 \mathbf{B},$$

$$\nabla \cdot \mathbf{B} = 0.$$

Forces

- ▶ \mathbf{F}_p pressure
- ▶ \mathbf{F}_C Coriolis (lin. in \mathbf{u})
- ▶ \mathbf{F}_i inertia (quad. in \mathbf{u})
- ▶ \mathbf{F}_L Lorentz (quad. in \mathbf{B})
- ▶ \mathbf{F}_v viscous (lin. in \mathbf{u})
- ▶ \mathbf{F}_b buoyancy (lin. in C)

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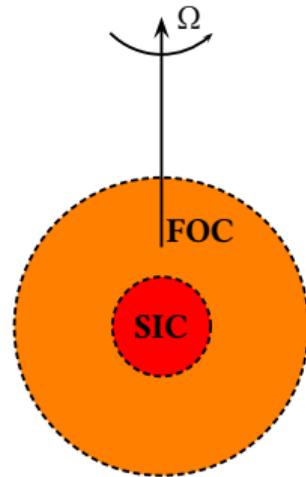
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$$\nabla \cdot \mathbf{B} = 0.$$

+ initial and boundary conditions: no-slip at CMB and ICB, insulating BC at CMB, conducting inner core, Neumann or Dirichlet conditions for \mathbf{C} .



FOC: Fluid Outer Core
SIC: Solid Inner Core

2890–5150 km depth
5150–6370 km depth

Solution method - spatial discretization

Pioneered by [Glatzmaier \(1984\)](#) for the solar dynamo, still adopted by most codes 35 years later ([Matsui et al., 2016](#))

- ▶ Poloidal-toroidal decomposition of solenoidal fields

$$\mathbf{u}(\mathbf{r}, t) = \nabla \times \nabla \times [\mathcal{P}^u(\mathbf{r}, t)\mathbf{r}] + \nabla \times [\mathcal{T}^u(\mathbf{r}, t)\mathbf{r}], \quad \mathbf{B}(\mathbf{r}, t) = \nabla \times \nabla \times [\mathcal{P}^B(\mathbf{r}, t)\mathbf{r}] + \nabla \times [\mathcal{T}^B(\mathbf{r}, t)\mathbf{r}]$$

- ▶ The horizontal dependency is handled by means of spherical harmonics, e. g.

$$\mathcal{P}^u(\mathbf{r}, t) \approx \sum_{\ell=0}^{\ell=\ell_{\max}} \sum_{m=-m_{\max}}^{m=m_{\max}} \mathcal{P}_{\ell m}^u(r, t) \mathcal{Y}_{\ell}^m(\theta, \varphi)$$

- ▶ Radial dependency: finite-difference or Chebyshev polynomials

Solution method - temporal discretization

One ends up with the following generic equation to time step

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}_L(\mathbf{x}) + \mathbf{f}_{NL}(\mathbf{x}),$$

in which \mathbf{x} is the complex-valued state vector.

Implicit-Explicit (IMEX) scheme

- ▶ Implicit for $\mathbf{f}_L(\mathbf{x})$
- ▶ Explicit for $\mathbf{f}_{NL}(\mathbf{x})$ (computed in physical space – pseudo-spectral approach), one round-trip per evaluation of $\mathbf{f}_{NL}(\mathbf{x})$
- ▶ Most codes resort to second order IMEX (CNAB2, CNAB3) with adaptive time-stepping

What the ideal geodynamo simulation should achieve

- ▶ produce a geomagnetic secular variation similar to the observed one
- ▶ generate a dipole-dominated field whose morphology at the CMB is similar to that of the recent geomagnetic field up to degree 13
- ▶ operate in a strong-field regime (magnetic energy \gg kinetic energy)
- ▶ produce a scale separation between \mathbf{B} (large-scale) and \mathbf{u} (small-scale)
- ▶ account for interannual geomagnetic impulses observed in the recent record
- ▶ produce irregular reversals of polarity over geological time scales

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This is contingent upon honoring the following separation of time scales

τ_{Ω}		τ_A		τ_{adv}		τ_{λ}
rotation	\ll	Alfvén	\ll	advection	\ll	mag diffusion
1 day		1 yr		100 yr		10^5 yr

over a simulation time spanning several million years (τ_{\oplus})

What current geodynamo simulations can achieve

- ✓ produce a geomagnetic secular variation similar to the observed one
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Christensen et al. (2010): The Earth-likeness is controlled by 2 ratios of 3 time scales

$$E_\lambda = \frac{\tau_\Omega}{\tau_\lambda}$$
$$Rm = \frac{\tau_\lambda}{\tau_{adv}}$$

$Rm = O(1000)$ for Earth

What state-of-the-art geodynamo simulations can achieve

- ✓ operate in a strong-field regime (magnetic energy \gg kinetic energy)
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Schaeffer et al. (2017): current state-of-the-art for DNS

- ▶ $(Nr, \ell_{\max}, m_{\max}) = (1280, 1000, 893)$
- ▶ 10 million core hours
- ▶ $O(8000)$ cores
- ▶ Integration length: $8 \tau_{\text{adv}}$ (~ 1000 yr)

The XSHELLS code

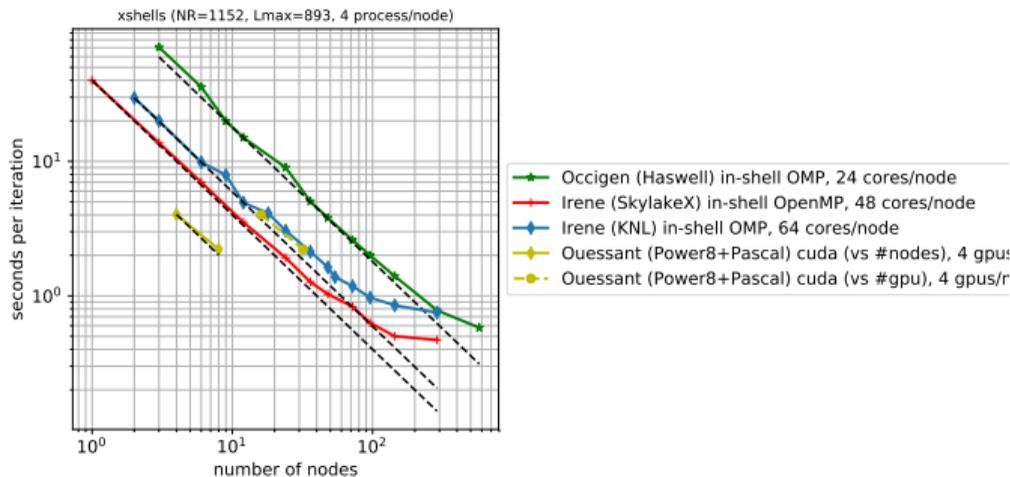
- ▶ FD in r , SH in (θ, φ)
- ▶ hybrid MPI/OpenMP parallelization
- ▶ Order 2 IMEX time scheme
- ▶ Uses the SHTns SH library (Schaeffer, 2013)
- ▶ open-source, available at <https://bitbucket.org/nschaeff/xshells>

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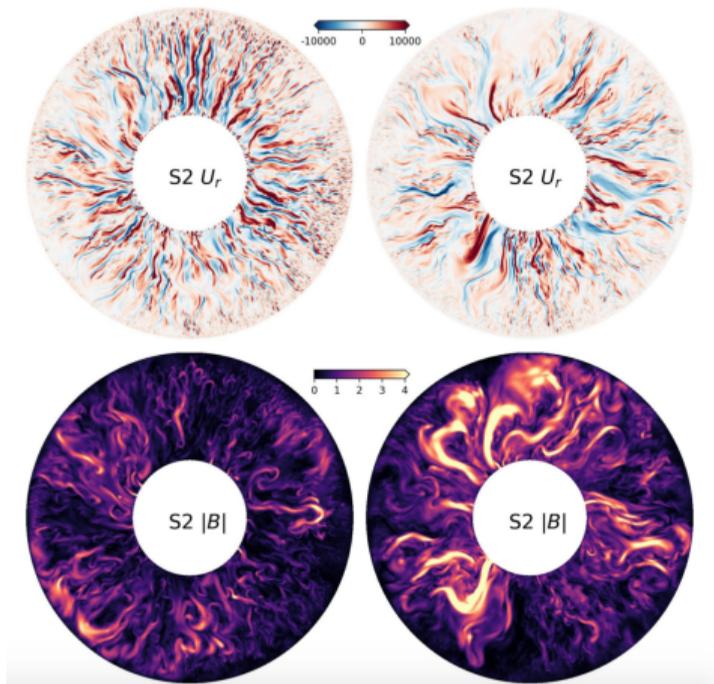
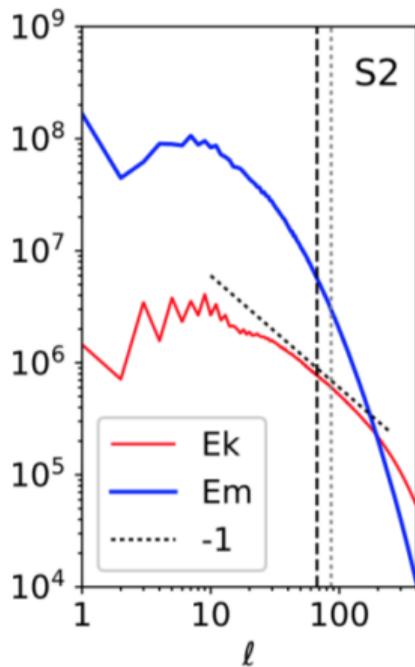
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What state-of-the-art geodynamo simulations can achieve

- ✓ account for interannual geomagnetic impulses observed in the recent record: simulation exhibits waves of various kinds (torsional Alfvén waves, Magneto-Coriolis waves) thanks to reduced diffusivities

Torsional waves:

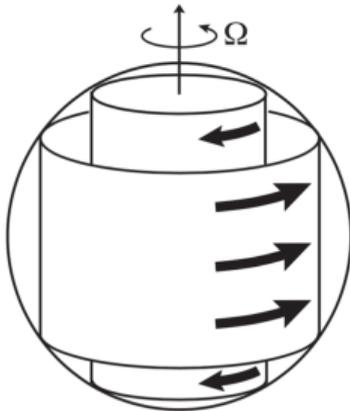
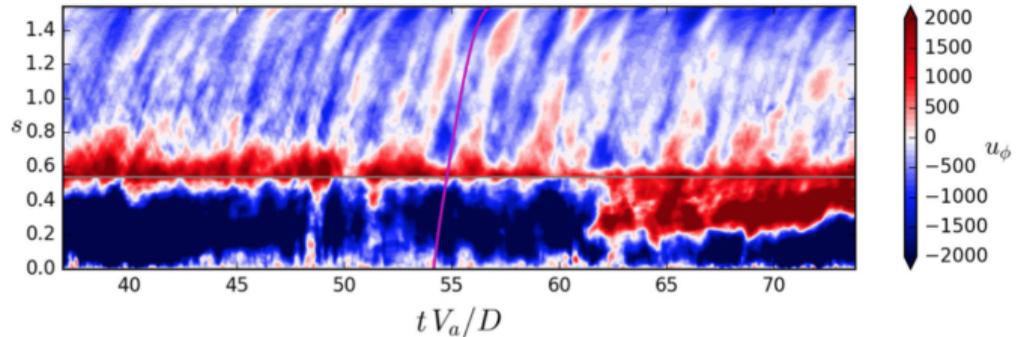


Figure 1. The geometry of the zonal flows in Earth's outer core which carry angular momentum. The depicted time varying zonal flows consist in either free Alfvén waves or forced accelerations.



Schaeffer et al. (2017)

More and Dumberry (2017)

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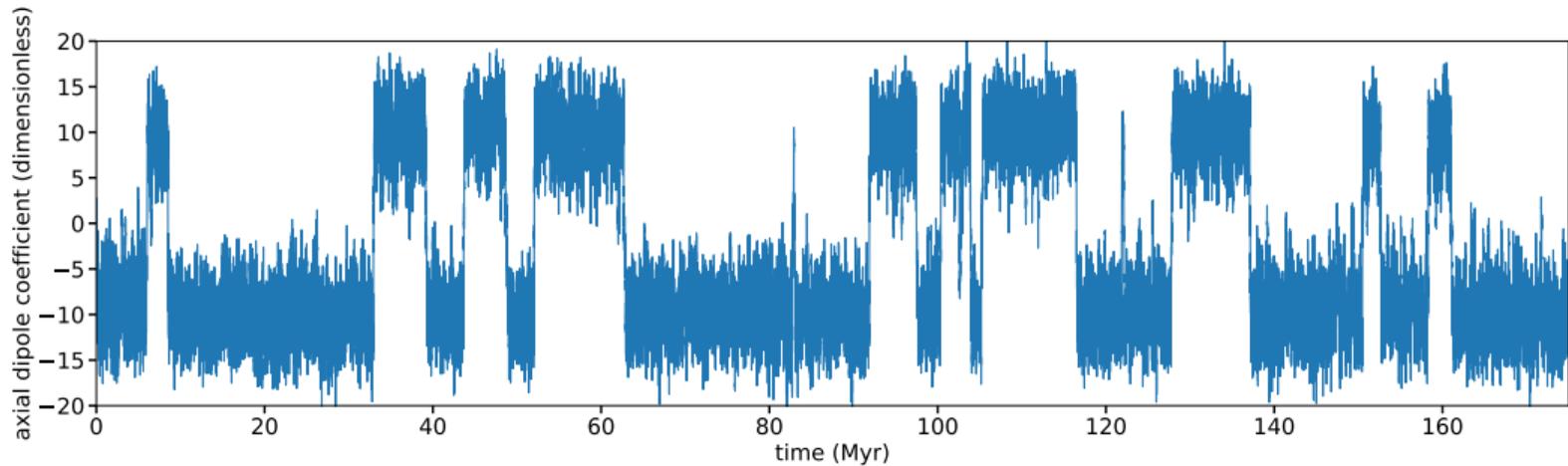
$$\tau_{\Omega} \quad \tau_A \quad \tau_{\text{adv}} \quad \tau_{\lambda}$$

rotation < Alfvén < advection < mag diffusion

over a simulation time spanning several million years (τ_{\oplus}) τ_{adv}

Low-resolution reversal simulations

$(N_r, \ell_{\max}, m_{\max}) = (144, 79, 63)$ (3 orders of magnitude more viscous than state-of-the-art)



(600,000 core hours)

Low-resolution reversal simulations

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Low-resolution reversal simulations

$(N_r, \ell_{\max}, m_{\max}) = (144, 79, 63)$ (3 orders of magnitude more viscous than state-of-the-art)

Issues

- ▶ kinetic energy \sim magnetic energy
- ▶ laminar, large-scale flow: no scale separation
- ▶ F_v and F_i too important in force balance
- ▶ Are those reversals relevant?

What to improve

Longer integration times with less viscous dynamos require a shorter time to solution.

Two possible options to explore

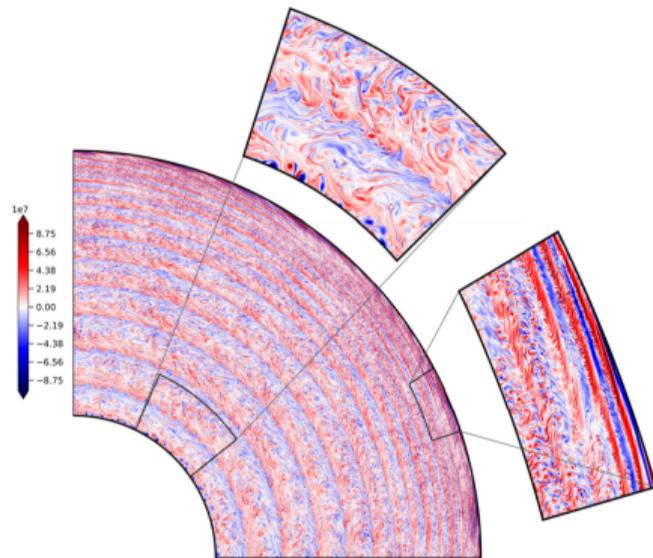
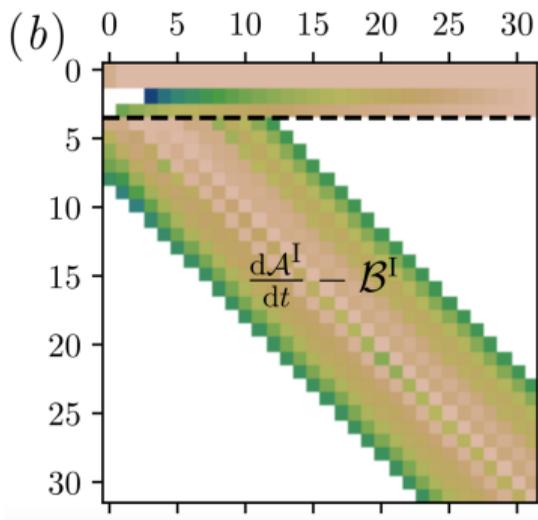
- ▶ Spatial discretization: sparse spectral representation in r
- ▶ Parallel in Time (PinT) approach

Sparse spectral representation

Goal: to benefit from spectral convergence in r while decreasing the memory imprint and improving the efficiency of a standard collocation approach

How: by generating (almost) banded matrices (Julien and Watson, 2009; Olver and Townsend, 2013; Marti et al., 2016).

Applied by Gastine (2019) to 2D spherical quasi-geostrophic convection



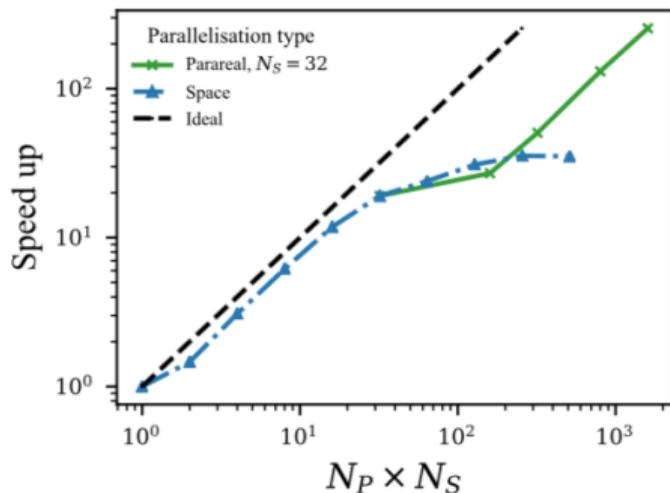
<https://github.com/magic-sph/pizza>

$(N_r, N_m) = (6145, 6144)$

Idea: enable extra domain decomposition when spatial parallelization is exhausted.

Possibilities: Parareal (Lions et al., 2001), PFASST (parallel full approximation scheme in space and time) (Emmett and Minion, 2012), ...

Clarke et al. (2019): application of Parareal to kinematic Cartesian dynamos



Galloway-Proctor flow, $Rm = 300$

N_S : # of procs. in space

N_P : # of procs. for parareal

Conclusion

The Geodynamo and HPC

- ▶ Current geodynamo simulations can run up to $O(10,000)$ cores (optimized SH transform library, MPI/OpenMP parallelization)
- ▶ Fair level of geophysical realism
- ▶ “turbulent state-of-the-art”: time integration too short for reversals

Room for improvement: decrease time to solution

- ▶ sparse spectral methods
- ▶ PinT

Have to be assessed for the geodynamo problem

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The internal field

Spherical harmonic analysis

$\mathbf{B} = -\nabla V$ in a current-free region; with internal sources,

$$V(r, \theta, \varphi, t) = a \sum_{\ell, m} \left(\frac{a}{r}\right)^{\ell+1} [g_{\ell}^m(t) \cos m\varphi + h_{\ell}^m(t) \sin m\varphi] P_{\ell}^m(\cos \theta),$$

$$B_r(r, \theta, \varphi, t) = \sum_{\ell, m} \left(\frac{a}{r}\right)^{\ell+2} [g_{\ell}^m(t) \cos m\varphi + h_{\ell}^m(t) \sin m\varphi] P_{\ell}^m(\cos \theta).$$



Connection between surface observations and the field at the CMB

(CMB: Core-Mantle Boundary)

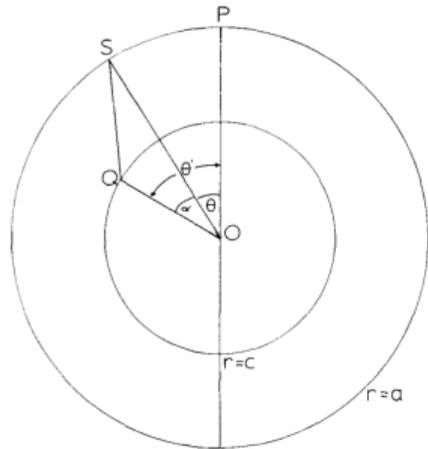
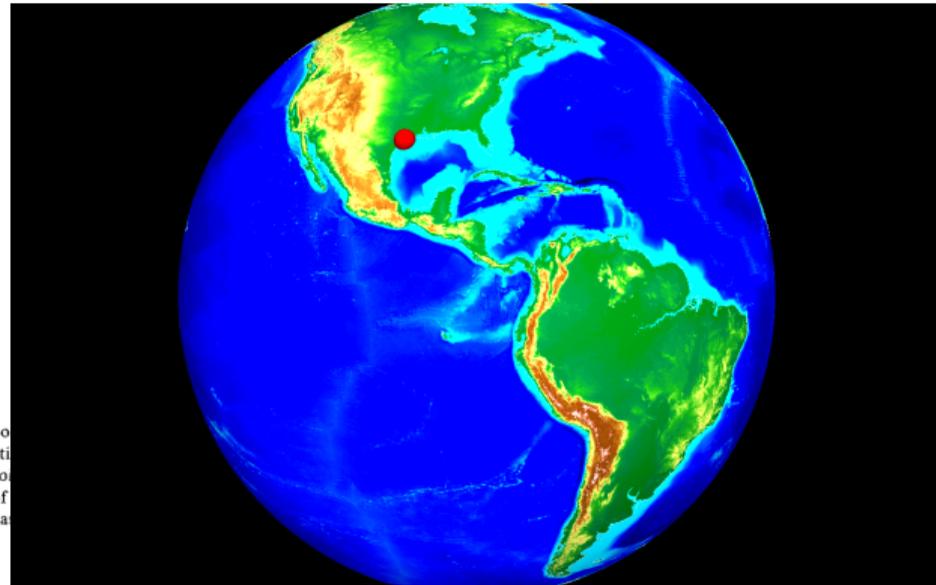


Figure 1. Geometry for the superposition integral (3). O is the origin of a system of spherical coordinates with pole P . The site is at $S(\theta, \phi)$ on the surface of the Earth. The Green's function $N(Y, \theta, \phi; \theta', \phi')$, is the potential at S due to a singularity of unit strength in the radial field at pole (θ', ϕ') on the core-mantle boundary. N is symmetric about the axis OS and is a function only of the angular distance between Q and S . N is a maximum when Q is immediately beneath S , and decreases monotonically with increasing angular distance α .



Gubbins and Roberts (1983)

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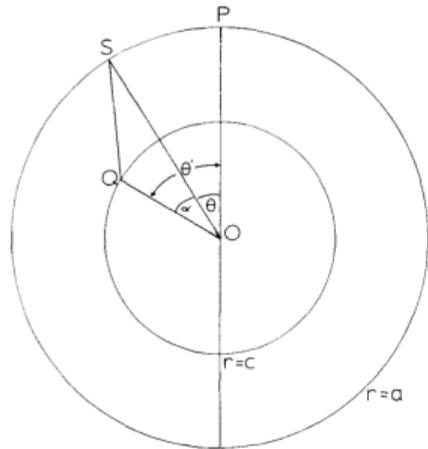
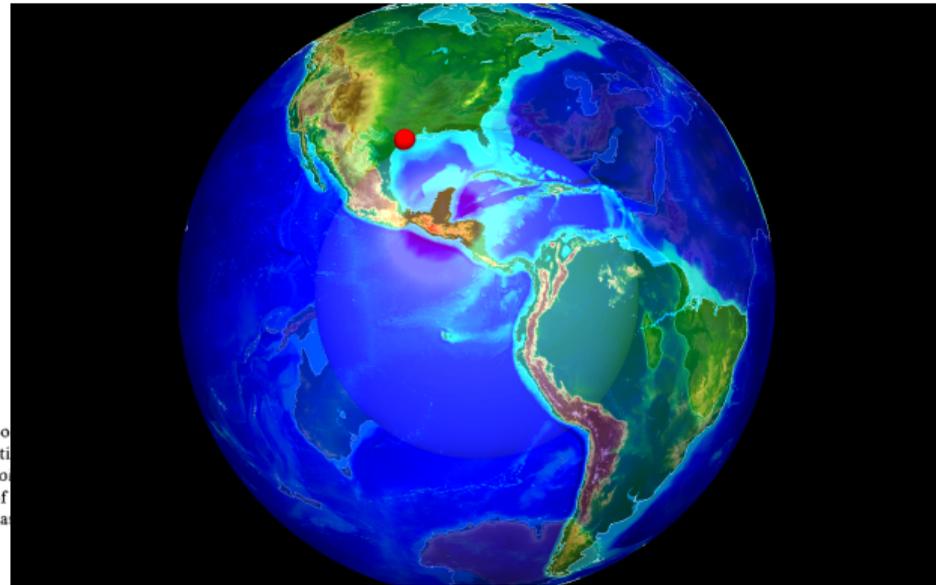


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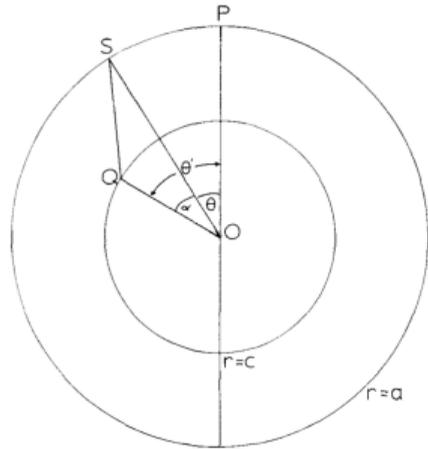
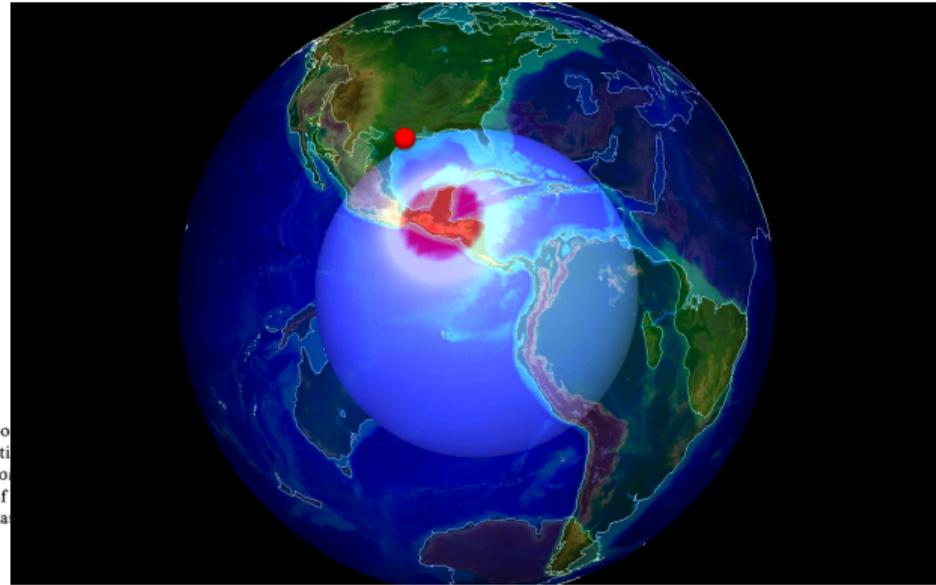


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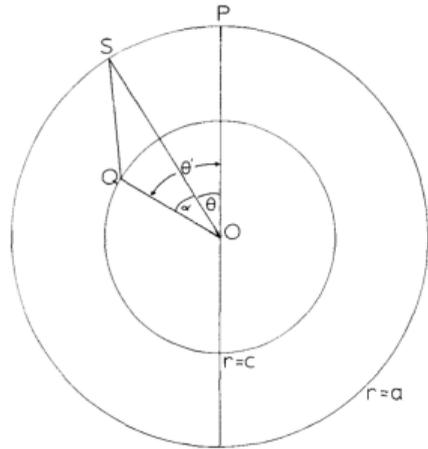
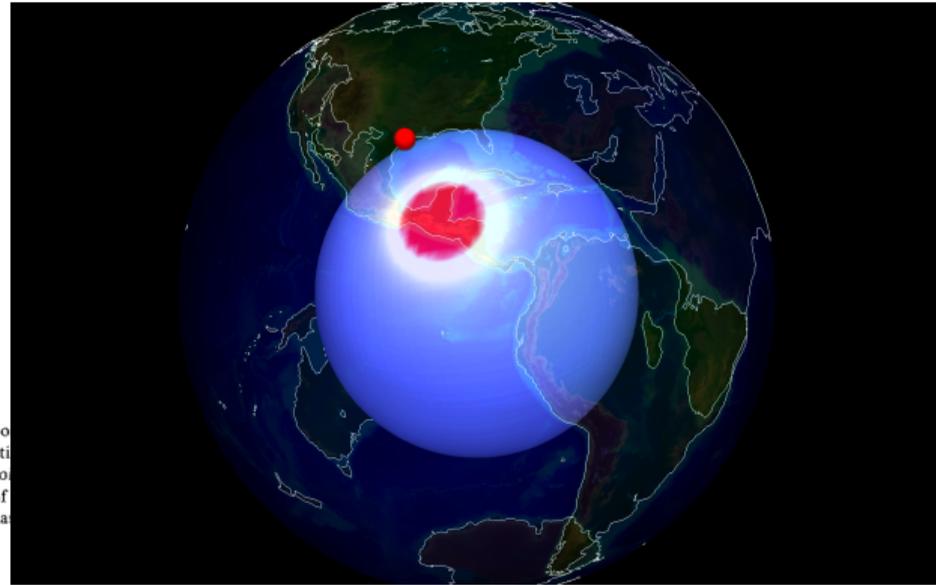


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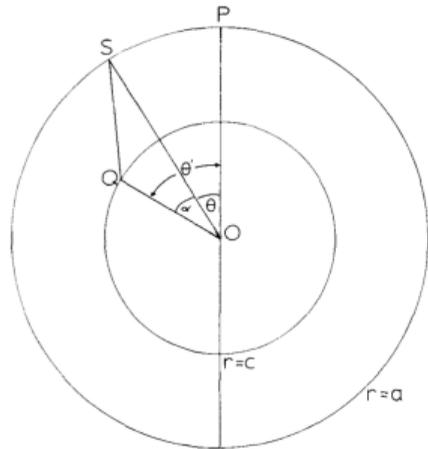
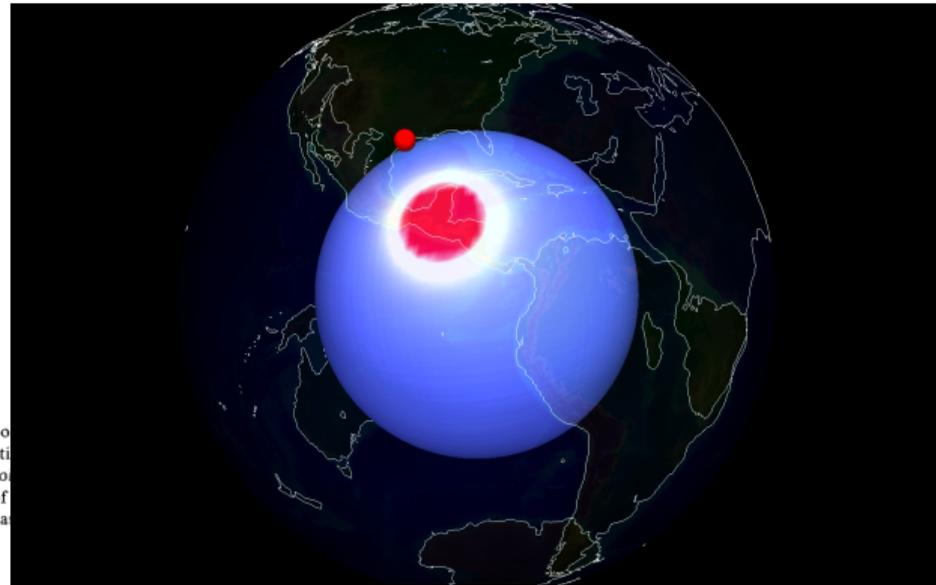
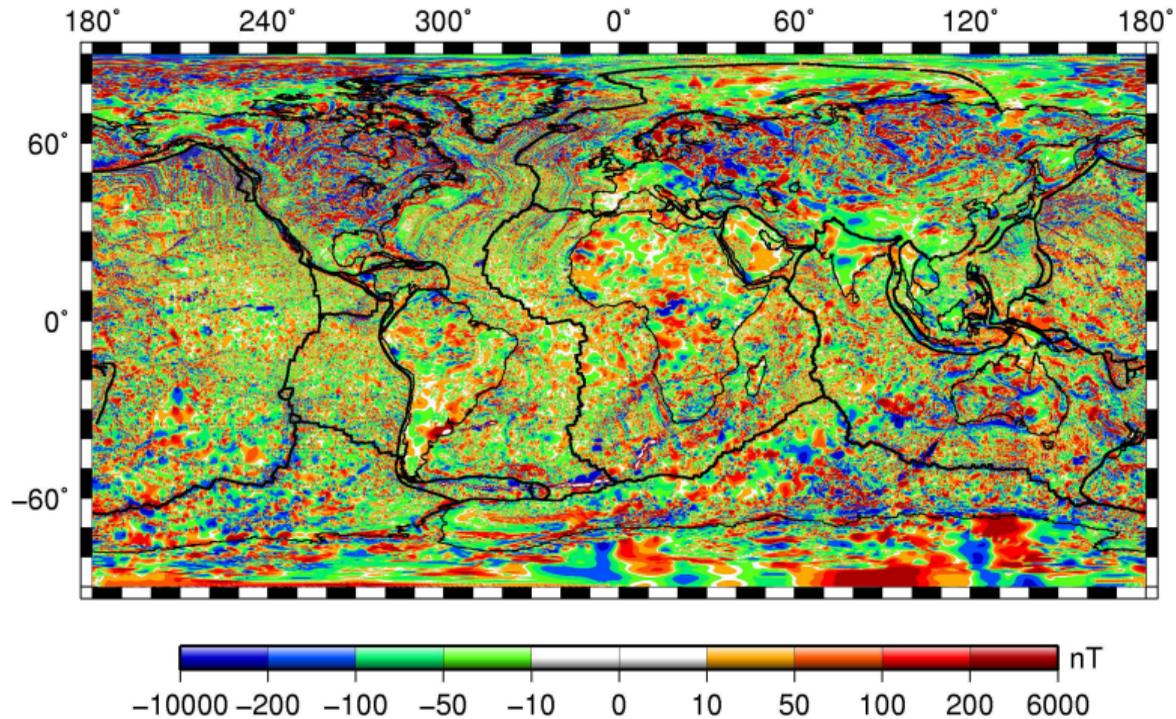


Figure 1. Geometry for the superposition integral (3). O is the origin of a system of spherical coordinates with pole P . The site is at $S(\theta, \phi)$ on the surface of the Earth. The Green's function $N(Y, \theta, \phi; \theta', \phi')$, is the potential at S due to a singularity of unit strength in the radial field at pole (θ', ϕ') on the core-mantle boundary. N is symmetric about the axis OS and is a function only of the angular distance between Q and S . N is a maximum when Q is immediately beneath S , and decreases monotonically with increasing angular distance α .



Gubbins and Roberts (1983)

The lithosphere is magnetized

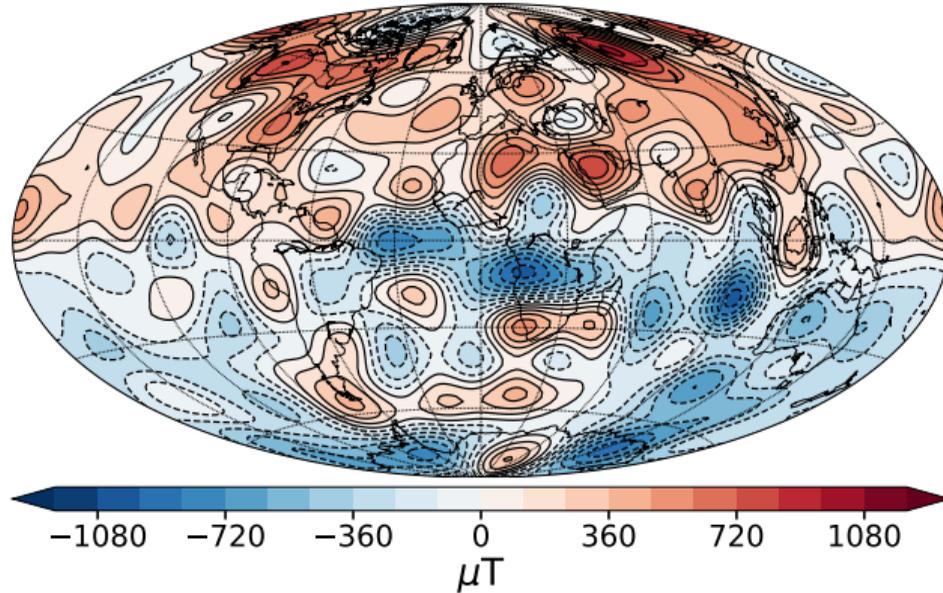


World Digital Magnetic Anomaly Map consortium

The geomagnetic field: a sparse record (in space and time)

A short-sighted view

- ▶ dipole-dominated
- ▶ small scales of dynamo field concealed by the small scales of the crustal field
- ▶ even if perfect sampling: $\ell \lesssim 13$ (lateral resolution of ~ 1500 km at the core surface)



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Time variations : constraints provided by geomagnetism (observatory and satellite data)

- ▶ Smooth decadal variations punctuated by rapid (interannual) impulses (geomagnetic jerks)

Constraints provided by paleomagnetism

- ▶ The strength of the field varies on secular, millennial and geological time scales
- ▶ The further in the past we look, the cruder our description of the field (axial dipole)
- ▶ The field reverses its polarity every once in a while ($\approx 4 \text{ Myr}^{-1}$ over the past 25 Myr)
- ▶ Last one 780 ka, poorly constrained transitional field

First-principle simulations can complement observations

Spherical harmonics: Pros and cons

Pros

- ▶ No pole problem
- ▶ Spectral convergence
- ▶ No need to solve for the exterior magnetic problem (Robin condition on the $\mathcal{P}_{\ell m}^B$)

$$\frac{d\mathcal{P}_{\ell m}^B}{dr} = -\frac{\ell}{r}\mathcal{P}_{\ell m}^B \text{ at } r = r_{\text{CMB}}$$

Cons

- ▶ No operational fast Legendre transform: $O(\ell_{\text{max}}^2)$ cost
- ▶ Global basis: parallelization is not straightforward

The SHTns library

Schaeffer (2013)

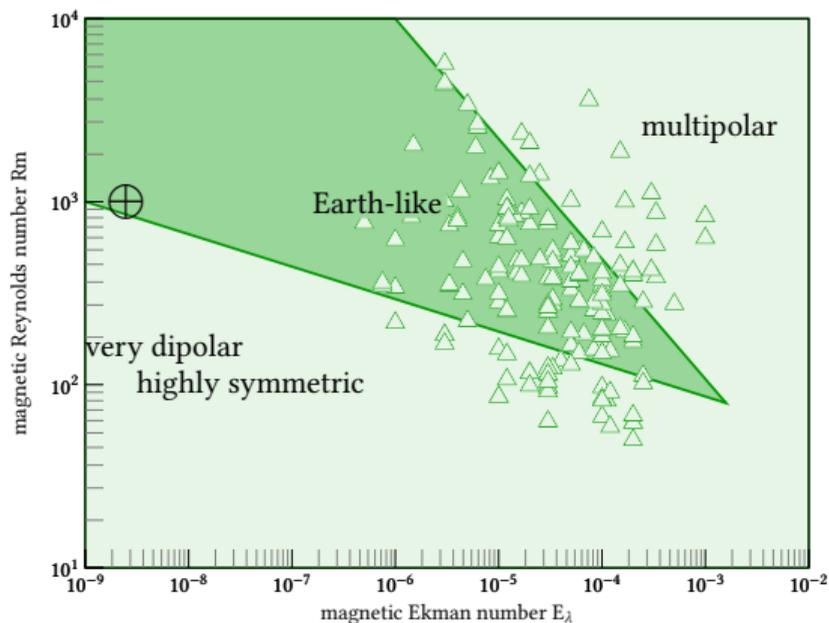
- ▶ **Matrix-free algorithm:** computing recurrence on-the-fly is faster than reading from memory [unless maybe matrix-matrix product is used], and you save a lot of memory too.
- ▶ **Hand vectorized**, yet easily portable (currently supports Intel SSE2, AVX, AVX2+FMA, AVX512, CUDA).
- ▶ SHTns performance scales with microarchitecture: x2 for SSE2, x4 for AVX, x8 for AVX2+FMA, x16 for AVX512 (for large enough transforms).
It also means the gap between classic implementations and SHTns will increase.
- ▶ Efficient **OpenMP parallelization**.
- ▶ Reaches 80% to 90% of peak performance on Intel SandyBridge.
- ▶ Accurate up to spherical harmonic degree $\ell = 16383$ (at least).
- ▶ **Free software:** <https://bitbucket.org/nschaeff/shtns>

What current geodynamo simulations can achieve

- ✓ produce a geomagnetic secular variation similar to the observed one
- ✓ generate a dipole-dominated field whose morphology at the CMB is similar to that of the recent geomagnetic field up to degree 13

Christensen et al. (2010): The Earth-likeness is controlled by 2 ratios of 3 time scales

$$E_\lambda = \frac{\tau_\Omega}{\tau_\lambda}$$
$$Rm = \frac{\tau_\lambda}{\tau_{adv}}$$



data courtesy U. Christensen