

A time-stepping dynamically-consistent spherical-shell dynamo code

D. J. Ivers*

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Abstract

A pseudo-spectral dynamo code, developed as a computational laboratory, is described. The magnetic, heat and Boussinesq Navier-Stokes equations, with inertia, non-linear advection, buoyancy with asymmetric gravity, Coriolis, viscous and Lorentz forces, are solved numerically in a rotating conducting fluid shell. The convection is thermally driven by prescribed boundary temperatures. The equations are discretised using toroidal-poloidal fields, Chebychev collocation in radius and spherical harmonic expansion in angles. Derivatives are performed spectrally. Products are evaluated in physical space for efficiency. Fields are transformed between physical and spectral spaces by fast Fourier and Gauss-Legendre methods. Linear terms are time-stepped

*School of Mathematics & Statistics, University of Sydney, AUSTRALIA.
<mailto:D.Ivers@maths.usyd.edu.au>

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implicitly and product terms explicitly using an Adams predictor/corrector. Results are presented for two benchmark models.

Contents

1	Introduction	C401
2	Numerical methods	C405
2.1	Spectral equations	C406
2.2	Discrete symmetries	C411
2.3	Spatial discretisation	C412
2.3.1	Angular discretisation	C412
2.3.2	Radial discretisation	C415
2.4	Time-stepping	C415
2.5	Solution of the linear systems	C417
3	Benchmark models	C418
3.1	Model 0: no-slip rotating thermal convection . . .	C419
3.2	Model 1: dynamo with insulating inner-core . . .	C420
4	Concluding remarks	C421
	References	C421

1 Introduction

The main magnetic fields of the larger planets — Uranus, Neptune, Saturn, Jupiter, the Earth, possibly Mercury and the Sun are generated by motion in the electrically-conducting fluid cores or shells. Motions which are sufficiently vigorous and asymmetric can act as

self-exciting dynamos. Attempts are also underway by several research groups to develop laboratory rotating fluid dynamos liquid sodium and gallium; see [1] for recent articles. A pseudo-spectral dynamo code, which has been developed as a computational laboratory primarily to study planetary dynamos and the different parameter regimes of dynamical dynamos generally, is described herein. The ultimate aim is to develop realistic dynamical models of planetary main magnetic fields.

The Earth is composed of an electrically-conducting core, consisting of a solid inner core and a liquid outer core, surrounded by a solid poorly conducting mantle. This motivates the prototype model underlying the code, which consists of an electrically-conducting rotating fluid spherical shell, $V : r_i < r < r_o$, enclosing a rigid inner core and surrounded by an electrically-insulating rigid mantle with an insulating exterior. Core and mantle are uniformly and rapidly co-rotating. The Boussinesq approximation is made, in which density variations are retained only in the buoyancy force. The convection is thermally driven by prescribed temperatures at the inner and outer core boundaries. The gravitational field may be asymmetric. The dynamo action of the flow in the liquid outer core is self-exciting, since the magnetic field vanishes at infinity.

The magnetic field \mathbf{B} , velocity \mathbf{v} and temperature Θ in the liquid spherical shell are governed by the magnetic induction equation, the Boussinesq Navier-Stokes momentum equation in a reference frame uniformly rotating at rate Ω , with inertia, non-linear advection, Coriolis, buoyancy, viscous and magnetic Lorentz forces and the heat equation with advection and thermal diffusion. The magnetic field and the velocity are solenoidal. The magnetic, viscous and thermal diffusivities, η , ν and κ , respectively, are constant. The spherical radius, co-latitude and east-longitude are denoted r , θ and ϕ , with the z axis ($\theta = 0$) orientated along the rotation

axis. Physical quantities are non-dimensionalised using the length scale $\mathcal{L} = r_o - r_i$, viscous diffusion time scale \mathcal{L}^2/ν , viscous velocity scale ν/\mathcal{L} , magnetic induction scale $\sqrt{\rho\Omega\mu_0\eta}$ and temperature scale $\Theta_o^0 - \Theta_i^0$, where Θ_o^0 and Θ_i^0 are typical temperatures on inner and outer shell boundaries. The dimensionless equations are thus

$$\frac{\partial \mathbf{B}}{\partial t} - \text{Pm}^{-1} \nabla^2 \mathbf{B} = \nabla \times (\mathbf{v} \times \mathbf{B}), \quad (1)$$

$$E \left(\frac{\partial \mathbf{v}}{\partial t} + \boldsymbol{\omega} \times \mathbf{v} - \nabla^2 \mathbf{v} \right) + \mathbf{1}_z \times \mathbf{v} \\ = -\nabla P - \text{Ra} \Theta \mathbf{g} + (2\text{Pm})^{-1} \mathbf{J} \times \mathbf{B}, \quad (2)$$

$$\frac{\partial \Theta}{\partial t} - \text{Pr}^{-1} \nabla^2 \Theta = -\mathbf{v} \cdot \nabla \Theta + Q, \quad (3)$$

$$\nabla \cdot \mathbf{v} = 0, \quad \nabla \cdot \mathbf{B} = 0, \quad (4)$$

where the vorticity $\boldsymbol{\omega} = \nabla \times \mathbf{v}$, $P = p + \frac{1}{2} \mathbf{v}^2$ is the modified pressure, g is the gravitational acceleration, Ra is the modified Rayleigh number, $\mathbf{J} = \nabla \times \mathbf{B}$, $E = \nu/2\Omega\mathcal{L}^2$ is the Ekman number, $\text{Pr} = \nu/\kappa$ is the Prandtl number and $\text{Pm} = \nu/\eta$ is the magnetic Prandtl number.

The shell differential equations are complemented by boundary and matching conditions. The mantle and inner-core are rigid and stationary in the uniformly rotating reference frame, and the velocity is continuous across the inner and outer shell boundaries. Thus

$$\mathbf{v} = \mathbf{0}, \quad \text{at } r = r_i, r_o. \quad (5)$$

Thermal convection is driven by prescribed temperatures at the inner and outer shell boundaries,

$$\Theta = \Theta_o, \quad \text{at } r = r_o; \quad \Theta = \Theta_i, \quad \text{at } r = r_i. \quad (6)$$

The inner-core V_i , the mantle and the exterior \widehat{V} are electrically-insulating, and the magnetic field is solenoidal,

$$\nabla \times \mathbf{B} = \mathbf{0}, \quad \nabla \cdot \mathbf{B} = 0, \quad \text{in } V_i, \widehat{V}, \quad (7)$$

the magnetic field is continuous across the inner and outer shell boundaries,

$$[\mathbf{B}] = \mathbf{0}, \quad \text{at } r = r_i, r_o \quad (8)$$

and there are no sources of magnetic field at infinity,

$$\mathbf{B} = \mathcal{O}(r^{-3}), \quad \text{as } r \rightarrow \infty. \quad (9)$$

Dynamo codes using a variety of methods have been developed [3, 5, 4, 6]. The numerical solution of the full dynamical dynamo problem is extremely difficult and the codes are complicated, so a variety of codes implementing the same and different numerical methods is absolutely essential to provide quantitative checks. The code described herein solves the equations using a pseudo-spectral method, which is Galerkin in the angles and Chebychev collocation in the radius. The code differs from previous work either in the use of the poloidal momentum equation rather than the radial and horizontal divergence momentum equations [3], the use of radial Chebychev collocation rather than Chebychev tau [6] or finite-differences [5], the implicit time-stepping of the Coriolis terms rather than explicit time-stepping [4], or the exploitation of problem symmetries. It should be noted that descriptions of these large codes is often incomplete or unclear in the literature.

In §2 the numerical methods, which are used in the code, are described. In §3 results are presented for two benchmark models [2]: a non-magnetic thermal convection model and a convective dynamo model, both with mantle and inner-core uniformly co-rotating. Concluding remarks are made in §4.

2 Numerical methods

There are several substantial difficulties in the numerical solution of the equations (1)–(9). The system has widely differing time- and length-scales; stiffness; geometrical complications due to the spherical boundaries and the non-local magnetic matching condition with an insulating exterior, but the preferred axis of (rapid) rotation; and the non-linearity of the advection terms in the momentum and heat equations, the Lorentz force and the Faraday induction term of the magnetic induction equation. The axisymmetric, toroidal flow and planar flow antidynamo theorems imply that the solution must be essentially three-dimensional, both in the number of independent variables and vector field directions.

The potentials of the poloidal-toroidal representations of the magnetic field and the velocity, together with the temperature, are expanded in spherical harmonics in θ and ϕ , and Chebychev polynomials in r . There are five scalar fields: the temperature, and the toroidal and poloidal potentials of the magnetic field and the velocity. The associated angular spectral forms of the linear terms in the governing equations, isolated on the left sides of (1)–(3), are also given. The discrete symmetries of the problem exploited in the code to reduce the problem size are outlined. The spectral equations are truncated and evaluated at the interior collocation points. Differentiations are performed spectrally. For efficiency the vector fields are calculated on an (r, θ, ϕ) -grid and the product terms on the right sides of (1)–(3), are evaluated. The results are transformed back to angular-spectral/radial space using fast Fourier and Gauss-Legendre methods. The time-stepping method uses the implicit two-step Adams-Moulton method for the linear diffusion terms and the Coriolis force, and an Adams three-step predictor/two-step corrector method for the product and non-linear terms. The solution of the linear algebraic systems uses banded Gaussian elimination.

2.1 Spectral equations

A vector field \mathbf{F} has the scaloidal-poloidal-toroidal representation,

$$\begin{aligned}\mathbf{F} &= \mathbf{R}\{R\} + \mathbf{S}\{S\} + \mathbf{T}\{T\}, & \mathbf{R}\{R\} &= \nabla R, \\ \mathbf{S}\{S\} &= \nabla \times \mathbf{T}\{S\}, & \mathbf{T}\{T\} &= \nabla \times T\mathbf{r},\end{aligned}$$

in a spherical shell concentric with the origin. If \mathbf{F} is solenoidal, then the scaloidal field $\mathbf{R}\{R\}$ can be omitted. In component form

$$\begin{aligned}F_r &= \partial_r R - \frac{L^2 S}{r}, \\ F_\theta &= \frac{\partial_\theta R}{r} + \frac{\partial_\theta \partial_r (rS)}{r} + \frac{\partial_\phi T}{\sin \theta}, \\ F_\phi &= \frac{\partial_\phi R}{r \sin \theta} + \frac{\partial_\phi \partial_r (rS)}{r \sin \theta} - \partial_\theta T.\end{aligned}$$

Thus the velocity and magnetic field, which are solenoidal by (4), and the temperature gradient have the representations,

$$\begin{aligned}\mathbf{v} &= \mathbf{S}\{s\} + \mathbf{T}\{t\}, & \text{in } V; \\ \mathbf{B} &= \mathbf{S}\{S\} + \mathbf{T}\{T\}, & \text{in } E^3; \\ \nabla \Theta &= \mathbf{R}\{\Theta\}, & \text{in } V.\end{aligned}$$

The poloidal and toroidal potentials, s , t , S and T , of the velocity and the magnetic field are expanded in terms of mean-normalised (surface) spherical harmonics of degree $n \in \mathbb{N}$ and order $m = -n, \dots, n$ defined by

$$\begin{aligned}Y_n^m(\theta, \phi) &= P_n^m(\cos \theta) e^{im\phi}, & m \geq 0; \\ Y_n^m &= (-)^m (Y_n^{-m})^*, & m < 0;\end{aligned}\tag{10}$$

where the asterisk denotes the complex conjugate and the associated Legendre functions are defined by

$$P_n^m(z) = (-)^{n+m} (1-z^2)^{m/2} \frac{\sqrt{2n+1}}{2^n n!} \sqrt{\frac{(n-m)!}{(n+m)!}} \frac{d^{n+m}(1-z^2)^n}{dz^{n+m}}. \quad (11)$$

These spherical harmonics are orthonormal with respect to the inner-product,

$$(f, g) := \frac{1}{4\pi} \oint f g^* d\Omega. \quad (12)$$

It is useful to define the spherical harmonic transform of a scalar function f by $\mathcal{Y}_n^m\{f\} := (f, Y_n^m)$. Y_n^m is symmetric (antisymmetric) about the equator if $n-m$ is even (odd),

$$Y_n^m(\pi - \theta, \phi) = (-)^{n-m} Y_n^m(\theta, \phi). \quad (13)$$

The expansions of the poloidal and toroidal potentials in spherical harmonics in V or E^3 are thus given by

$$f = \sum_{n=1}^{\infty} \sum_{m=-n}^n f_n^m Y_n^m, \quad f = s, t, S, T, \quad (14)$$

where the coefficients $s_n^m, t_n^m, S_n^m, T_n^m$ are functions of r and the time t . The n -sum has the lower limit $n = 1$, since poloidal and toroidal vector fields are invariant under addition of an arbitrary function of r to the potential. The temperature has the expansion,

$$\Theta = \sum_{n=0}^{\infty} \sum_{m=-n}^n \Theta_n^m Y_n^m. \quad (15)$$

The inverse scaloidal-poloidal-toroidal transform from the spherical harmonic (spectral) coefficients of the scaloidal, poloidal and

toroidal potentials to the physical vector fields is required to construct \mathbf{B} , \mathbf{v} and $\nabla\Theta$ from S_n^m , T_n^m , s_n^m , t_n^m and Θ_n^m :

$$\begin{aligned}
 R &= \sum_{n=0}^{\infty} \sum_{m=-n}^n R_n^m Y_n^m, \\
 S &= \sum_{n=1}^{\infty} \sum_{m=-n}^n S_n^m Y_n^m, \\
 T &= \sum_{n=1}^{\infty} \sum_{m=-n}^n T_n^m Y_n^m, \\
 \mathbf{F} &= F_0^0 \mathbf{1}_r + \sum_{n=1}^{\infty} \sum_{m=-n}^n \{F_{rn}^m \mathbf{1}_r + F_{\theta n}^m \mathbf{1}_\theta + F_{\phi n}^m \mathbf{1}_\phi\},
 \end{aligned}$$

where $F_0^0 = \partial_r R_0^0$ and

$$\begin{aligned}
 F_{rn}^m &= \left\{ \frac{\partial_r R_n^m}{n(n+1)} + \frac{S_n^m}{r} \right\} n(n+1) Y_n^m \\
 F_{\theta n}^m &= \left\{ \frac{R_n^m}{r} + \frac{\partial_r (r S_n^m)}{r} \right\} \partial_\theta Y_n^m + T_n^m \frac{\partial_\phi Y_n^m}{\sin \theta} \\
 F_{\phi n}^m &= \left\{ \frac{R_n^m}{r} + \frac{\partial_r (r S_n^m)}{r} \right\} \frac{\partial_\phi Y_n^m}{\sin \theta} - T_n^m \partial_\theta Y_n^m.
 \end{aligned}$$

The poloidal-toroidal transform from a physical solenoidal field \mathbf{F} to the spectral coefficients of its poloidal and toroidal potentials is defined by

$$\mathcal{T}_n^m \{\mathbf{F}\} := \frac{1}{4\pi n(n+1)} \oint Y_n^{m*} \mathbf{r} \cdot \nabla \times \mathbf{F} d\Omega \tag{16}$$

$$\mathcal{D}\mathcal{S}_n^m \{\mathbf{F}\} := -\frac{1}{4\pi n(n+1)} \oint Y_n^{m*} \mathbf{r} \cdot \nabla \times \nabla \times \mathbf{F} d\Omega. \tag{17}$$

In particular, applying (16) and (17) to $\mathbf{F} = \mathbf{T}\{T\} + \mathbf{S}\{S\}$ gives $\mathcal{T}_n^m \{\mathbf{F}\} = T_n^m$ and $\mathcal{D}\mathcal{S}_n^m \{\mathbf{F}\} = S_n^m$, where $r^2 D_n := r^2 \partial_{rr} + 2r \partial_r -$

$n(n+1)$. The transform is used to extract the spectral poloidal and toroidal momentum and magnetic induction equations.

The spectral toroidal and poloidal momentum equations are given by the poloidal-toroidal transform of the momentum equation,

$$E(\partial_t - D_n)t_n^m - c_n^m \frac{n-1}{n} d_{1-n} s_{n-1}^m - c_{n+1}^m \frac{n+2}{n+1} d_{n+2} s_{n+1}^m - \frac{imt_n^m}{n(n+1)} = \mathcal{T}_n^m \{\mathbf{F}\} \quad (18)$$

$$E(\partial_t - D_n)D_n s_n^m + c_n^m \frac{n-1}{n} d_{1-n} t_{n-1}^m + c_{n+1}^m \frac{n+2}{n+1} d_{n+2} t_{n+1}^m - \frac{imD_n s_n^m}{n(n+1)} = \mathcal{D}\mathcal{S}_n^m \{\mathbf{F}\}, \quad (19)$$

where

$$\begin{aligned} \mathbf{F} &= -E\boldsymbol{\omega} \times \mathbf{v} + (2\text{Pm})^{-1} \mathbf{J} \times \mathbf{B} - \text{Ra}\Theta \mathbf{g}, \\ c_n^m &= \sqrt{(n^2 - m^2)/(4n^2 - 1)}, \\ d_n &= \partial_r + n/r. \end{aligned}$$

Equations (18) and (19) are equivalent to the spherical harmonic transform of the radial components of the vorticity equation and its curl. The pressure is eliminated reducing the number of dependent fields from six to five, at the expense of increasing the order of the differential system. The poloidal and toroidal coefficients are coupled on the left sides of the equations (18) and (19) by the Coriolis force.

The spectral magnetic induction equations are obtained by applying the poloidal-toroidal transform to the magnetic vector potential equation,

$$\frac{\partial \mathbf{A}}{\partial t} - \text{Pm}^{-1} \nabla^2 \mathbf{A} = \mathbf{v} \times \mathbf{B} - \nabla \Phi,$$

where \mathbf{A} is the vector potential, $\mathbf{B} = \nabla \times \mathbf{A}$, and Φ is the electrostatic potential. Thus

$$\begin{aligned} (\partial_t - \text{Pm}^{-1} D_n) S_n^m &= T_n^m \{ \mathbf{v} \times \mathbf{B} \}, \\ (\partial_t - \text{Pm}^{-1} D_n) T_n^m &= -S_n^m \{ \mathbf{v} \times \mathbf{B} \}. \end{aligned} \quad (20)$$

Note the toroidal transform produces the poloidal induction equation (20) and conversely. The poloidal and toroidal coefficients are decoupled on the left sides of the equations.

The spectral heat equation is the spherical harmonic transform of the heat equation (3):

$$(\partial_t - \text{Pr}^{-1} D_n) \Theta_n^m = -\mathcal{Y}_n^m \{ \mathbf{v} \cdot \nabla \Theta \}. \quad (21)$$

At the inner and outer shell boundaries the spectral coefficients of the velocity satisfy the no-slip conditions by (5):

$$s_n^m = 0, \quad \partial_r s_n^m = 0, \quad t_n^m = 0, \quad \text{at } r = r_i, r_o. \quad (22)$$

The magnetic induction matches continuously to a potential field in the insulating inner core, mantle and exterior by (7), (8) and (9):

$$\begin{aligned} d_{-n} S_n^m &= 0, \quad \text{at } r = r_i; \\ d_{n+1} S_n^m &= 0, \quad \text{at } r = r_o; \\ T_n^m &= 0, \quad \text{at } r = r_i, r_o; \end{aligned} \quad (23)$$

and the temperature is fixed by (6):

$$\Theta_n^m = \Theta_{in}^m, \quad \text{at } r = r_i; \quad \Theta_n^m = \Theta_{on}^m, \quad \text{at } r = r_o. \quad (24)$$

In the models considered in §3 the temperature is constant at the inner and outer boundaries, $\Theta_{i0}^0 = 1$, $\Theta_{in}^m = 0$ for $n > 0$ and $\Theta_{on}^m = 0$ for $n \geq 0$.

2.2 Discrete symmetries

There are two symmetries of the problem, which are exploited to reduce its size. Whether such symmetries are stable under small perturbations must be investigated on a case by case basis.

The first is symmetry under reflection in the equatorial plane or parity, giving odd/even scalar fields and dipole/quadrupole vector fields.

- A scalar field f is odd if $f(r, \theta, \phi) = -f(r, \pi - \theta, \phi)$; and even if $f(r, \theta, \phi) = f(r, \pi - \theta, \phi)$.
- A vector field \mathbf{F} is dipole if $F_r(r, \theta, \phi) = -F_r(r, \pi - \theta, \phi)$, $F_\theta(r, \theta, \phi) = F_\theta(r, \pi - \theta, \phi)$ and $F_\phi(r, \theta, \phi) = -F_\phi(r, \pi - \theta, \phi)$.
- A vector field \mathbf{F} is quadrupole if $F_r(r, \theta, \phi) = F_r(r, \pi - \theta, \phi)$, $F_\theta(r, \theta, \phi) = -F_\theta(r, \pi - \theta, \phi)$ and $F_\phi(r, \theta, \phi) = F_\phi(r, \pi - \theta, \phi)$.

Let o, e, d and q denote odd, even, dipole and quadrupole, respectively. If initially, the velocity is quadrupole, $\mathbf{v}_d = \mathbf{0}$, the magnetic field is purely dipolar or quadrupolar, $\mathbf{B}_q = \mathbf{0}$ or $\mathbf{B}_d = \mathbf{0}$, the pressure is even, $P_o = 0$, gravity is quadrupole, $\mathbf{g}_d = \mathbf{0}$, the temperature is even, $\Theta_o = 0$, and the heat source is even, $Q_o = 0$, then the fields and equations split into two sets which evolve independently: the dipole set $(\mathbf{v}_q, \boldsymbol{\omega}_d, \mathbf{B}_d, \mathbf{J}_q, P_e, \Theta_e)$ and the quadrupole set $(\mathbf{v}_q, \boldsymbol{\omega}_d, \mathbf{B}_q, \mathbf{J}_d, P_e, \Theta_e)$. Using the parity property (13) of spherical harmonics, a scalar field f is odd/even, if its coefficients f_n^m vanish, when $n - m$ is even/odd. A vector field is dipole/quadrupole, if its toroidal potential is even/odd, and its poloidal and scaloidal potentials are odd/even.

The second symmetry is rotational symmetry about the z -axis. If the highest common factor of the orders m , which occur in the

initial conditions, is m_{hcf} , then the only spherical harmonic coefficients, which are generated subsequently are multiples of m_{hcf} .

The code exploits both symmetries, since they can reduce the problem size by factors 2 and m_{hcf} , respectively.

2.3 Spatial discretisation

The spectral equations (18)–(21) are discretised in angle by truncating and in radius by collocating. As described below, product terms are evaluated on an (r, θ, ϕ) -grid and then transformed to angular-spectral/radial space using a discrete form of the poloidal-toroidal transform.

2.3.1 Angular discretisation

Triangular truncation of the spherical harmonic expansions is used. Thus the degree- or n -sums in the expansions (14)–(15) of the velocity and magnetic potentials, and the temperature, are truncated at $n = N_n$. The maximum order is also N_n , that is, $m = -N_n, \dots, N_n$. Other truncations are possible, but this particular truncation is used, since there is no orientation-preferred length scale and Y_n^m is mapped to a linear combination of $\{Y_n^{-n}, \dots, Y_n^n\}$ under any rotation of the coordinate system.

Angular discretisation is performed on a finite grid,

$$\{(\theta_k, \phi_\ell) \mid k = 1, \dots, N_\theta, \ell = 0, \dots, N_\phi\} \quad (25)$$

where $\{\mu_k := \cos \theta_k \mid k = 1, \dots, N_\theta\}$ are the nodes of the N_θ -point Gauss-Legendre quadrature rule with weights w_k and $\{\phi_\ell =$

$2\pi\ell/N_\phi \mid \ell = 0, \dots, N_\phi\}$ are the nodes for the N_ϕ -panel trapezoidal rule.

For a real function f the discrete spherical harmonic transform (DSHT) is

$$\begin{aligned}\tilde{\mathcal{Y}}_n^m\{f\} &= \sum_{k=1}^{N_\theta} f^m(\theta_k) P_n^m(\theta_k) \frac{w_k}{2}, \\ f^m(\theta_k) &= \frac{1}{N_\phi} \sum_{\ell=0}^{N_\phi-1} f(\theta_k, \phi_\ell) e^{-im\phi_\ell}.\end{aligned}\quad (26)$$

The ℓ -summation, which is the discrete Fourier transform (DFT) in ϕ , can be performed using a fast Fourier transform (FFT). If the k -summation is done first an FFT cannot be used, since P_n^m depends on m . If the SH expansion of f is finite and the summations in (14) and (15) truncate at $n = N_n$ and $|m| = N_n$, then the DSHT (26) gives the exact coefficients f_n^m , if $2N_n \leq 2N_\theta - 1$ and $2N_n + 1 \leq N_\phi$, since the DFT is then m -orthogonal with no aliasing, N_θ -point Gaussian quadrature is exact for polynomials of degree $2N_\theta - 1$ and fP_n^m is a polynomial in μ of degree $\leq 2N_n$. [Note $P_{n_1}^m P_n^m$ is a polynomial in μ of degree $n_1 + n$.] The DSHT also preserves parity about the equator $\mu = 0$.

If f is a product $f = gh$, where g and h have finite SH-expansions truncated at $n = N_n$ and $|m| = N_n$, then fP_n^m is polynomial of degree $\leq 3N_n$ in μ , since it is a linear combination of polynomials $P_{n_1}^{m_1} P_{n_2}^{m_2} P_n^m$ of degree $n_1 + n_2 + n$ in μ , noting $m = m_1 + m_2$ since the DFT is m -orthogonal with no aliasing. In this case the DSHT is exact if $3N_n \leq 2N_\theta - 1$ and $4N_n + 1 \leq N_\phi$. This result is true with some further justification in the application of the DSHT to the term $\mathbf{v} \cdot \nabla\Theta$ in the heat equation.

The inverse discrete scaloidal-poloidal-toroidal transform is required to construct \mathbf{B} , \mathbf{J} , \mathbf{v} , $\boldsymbol{\omega}$ and $\nabla\Theta$ on the grid (25) for the

product terms. It is

$$F_\xi(\theta_k, \phi_\ell) = \sum_{m=-N_n}^{N_n} F_\xi^m(\theta_k) e^{im\phi_\ell}, \quad \xi = r, \theta, \phi,$$

where

$$\begin{aligned} F_r^m(\theta_k) &= \sum_{n=m}^{N_\theta} \left\{ \frac{\partial_r R_n^m}{n(n+1)} + \frac{S_n^m}{r} \right\} n(n+1) P_n^m(\theta_k) \\ F_\theta^m(\theta_k) &= \sum_{n=m}^{N_\theta} \left\{ \left[\frac{R_n^m}{r} + \frac{\partial_r(rS_n^m)}{r} \right] \partial_\theta P_n^m(\theta_k) + T_n^m \frac{imP_n^m(\theta_k)}{\sin \theta_k} \right\} \\ F_\phi^m(\theta_k) &= \sum_{n=m}^{N_\theta} \left\{ \left[\frac{R_n^m}{r} + \frac{\partial_r(rS_n^m)}{r} \right] \frac{imP_n^m(\theta_k)}{\sin \theta_k} - T_n^m \partial_\theta P_n^m(\theta_k) \right\}. \end{aligned}$$

The ϕ -DFT's are evaluated using real FFT's.

The discrete poloidal-toroidal transform is

$$\tilde{\mathcal{T}}_n^m \{\mathbf{F}\} = - \sum_{k=1}^{N_\theta} \left\{ F_\theta^m(\theta_k) \frac{imP_n^m(\theta_k)}{n(n+1)\sin \theta_k} + F_\phi^m(\theta_k) \frac{\partial_\theta P_n^m(\theta_k)}{n(n+1)} \right\} \frac{w_k}{2} \quad (27)$$

$$\begin{aligned} \mathcal{D}\tilde{\mathcal{S}}_n^m \{\mathbf{F}\} &= \sum_{k=1}^{N_\theta} \left\{ -\frac{F_r^m(\theta_k)}{r} P_n^m(\theta_k) + \frac{\partial_r[rF_\theta^m(\theta_k)]}{r} \frac{\partial_\theta P_n^m(\theta_k)}{n(n+1)} \right. \\ &\quad \left. - \frac{\partial_r[rF_\phi^m(\theta_k)]}{r} \frac{imP_n^m(\theta_k)}{n(n+1)\sin \theta_k} \right\} \frac{w_k}{2}. \quad (28) \end{aligned}$$

The five combinations of the associated Legendre function and its derivatives, which occur, are precomputed and stored.

2.3.2 Radial discretisation

The radial discretisation is performed by expanding the spherical harmonic coefficients of the temperature and the poloidal-toroidal potentials of the velocity and the magnetic field in N_T Chebychev polynomials of the first kind, $T_j(x) := \cos(j \cos^{-1} x)$, $-1 \leq x \leq 1$, $j = 0, \dots, N_T - 1$, where $r = (r_i + r_o)/2 - x(r_o - r_i)/2$. Thus

$$f_n^m(r, t) = \sum_{j=0}^{N_T-1} f_{n,j}^m T_j(x), \quad f = \Theta, s, t, S, T,$$

where the primes denote $\frac{1}{2}$ factors in the $j = 0$ and $j = N_T - 1$ terms. The Chebychev collocation points, $x_j = \cos[j\pi/(N_T - 1)]$, $j = 0, \dots, N_T - 1$ are used. This permits the use of the fast cosine transform. The differential equations (18)–(21) are satisfied at the interior points, x_j , $j = 1, \dots, N_T - 2$, and the boundary conditions (22)(c)–(24) are satisfied at the endpoints, x_j , $j = 0, N_T - 1$. The poloidal momentum equation (28) is satisfied at the interior points, x_j , $j = 2, \dots, N_T - 3$, and the boundary conditions (28)(a,b) are satisfied at the points, x_j , $j = 0, 1, N_T - 2, N_T - 1$.

2.4 Time-stepping

The spatially discretised momentum, magnetic and heat equations and boundary conditions are of the form

$$\mathbf{A} \frac{d\mathbf{x}}{dt} = \mathbf{L}\mathbf{x} + \mathbf{N}(t, \mathbf{x}). \quad (29)$$

where $\mathbf{x} = (\mathbf{x}_B, \mathbf{x}_v, \mathbf{x}_\Theta)^T$, in which the column vectors \mathbf{x}_B , \mathbf{x}_v and \mathbf{x}_Θ represent the spatially discretised fields S , T , s , t and Θ . The

matrices \mathbf{A} , \mathbf{L} and the vector-valued non-linear function \mathbf{N} have the structure,

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_B & 0 & 0 \\ 0 & \mathbf{A}_v & 0 \\ 0 & 0 & \mathbf{A}_\Theta \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} \mathbf{L}_B & 0 & 0 \\ 0 & \mathbf{L}_v & 0 \\ 0 & 0 & \mathbf{L}_\Theta \end{bmatrix},$$

$$\mathbf{N} = \begin{bmatrix} \mathbf{N}_B(B, v) \\ \mathbf{N}_v(B, v, \Theta) \\ \mathbf{N}_\Theta(v, \Theta) \end{bmatrix}.$$

The matrices \mathbf{A} and \mathbf{L} are independent of t . Equation (29) is replaced by the system,

$$\mathbf{A}\mathbf{x} = \mathbf{y} + \mathbf{z}, \quad \frac{d\mathbf{y}}{dt} = \mathbf{L}\mathbf{x}, \quad \frac{d\mathbf{z}}{dt} = \mathbf{N}(t, \mathbf{x}), \quad (30)$$

to split off the non-linear terms, and the ordinary differential systems (30)(b,c) are time-stepped using the one-step Adams-Moulton method and a two-step Adams-Bashforth /one-step Adams-Moulton predictor/corrector (PC) method, respectively. The time-stepping equations are thus the predictor schemes with step-size h :

$$\mathbf{M}_B^0 B_{n+1}^P = \mathbf{M}_B^1 B_n + \frac{1}{2}h\{3\mathbf{N}_B(B_n, v_n) - \mathbf{N}_B(B_{n-1}, v_{n-1})\}, \quad (31)$$

$$\mathbf{M}_v^0 v_{n+1}^P = \mathbf{M}_v^1 v_n + \frac{1}{2}h\{3\mathbf{N}_v(B_n, v_n, \Theta_n) - \mathbf{N}_v(B_{n-1}, v_{n-1}, \Theta_{n-1})\}, \quad (32)$$

$$\mathbf{M}_\Theta^0 \Theta_{n+1}^P = \mathbf{M}_\Theta^1 \Theta_n + \frac{1}{2}h\{3\mathbf{N}_\Theta(v_n, \Theta_n) - \mathbf{N}_\Theta(v_{n-1}, \Theta_{n-1})\}, \quad (33)$$

and the single-iteration corrector schemes:

$$\mathbf{M}_B^0 B_{n+1} = \mathbf{M}_B^1 B_n + \frac{1}{2}h\mathbf{N}_B(B_{n+1}^P, v_{n+1}^P) + \frac{1}{2}h\mathbf{N}_B(B_n, v_n), \quad (34)$$

$$\mathbf{M}_v^0 v_{n+1} = \mathbf{M}_v^1 v_n + \frac{1}{2}h\mathbf{N}_v(B_{n+1}^P, v_{n+1}^P, \Theta_{n+1}^P) + \frac{1}{2}h\mathbf{N}_v(B_n, v_n, \Theta_n), \quad (35)$$

$$\mathbf{M}_\Theta^0 \Theta_{n+1} = \mathbf{M}_\Theta^1 \Theta_n + \frac{1}{2}h\mathbf{N}_\Theta(v_{n+1}^P, \Theta_{n+1}^P) + \frac{1}{2}h\mathbf{N}_\Theta(v_n, \Theta_n), \quad (36)$$

where

$$\mathbf{M}_B^0 = \mathbf{A}_B - \frac{1}{2}h\mathbf{L}_B, \quad \mathbf{M}_v^0 = \mathbf{A}_v - \frac{1}{2}h\mathbf{L}_v, \quad \mathbf{M}_\Theta^0 = \mathbf{A}_\Theta - \frac{1}{2}h\mathbf{L}_\Theta, \quad (37)$$

$$\mathbf{M}_B^1 = \mathbf{A}_B + \frac{1}{2}h\mathbf{L}_B, \quad \mathbf{M}_v^1 = \mathbf{A}_v + \frac{1}{2}h\mathbf{L}_v, \quad \mathbf{M}_\Theta^1 = \mathbf{A}_\Theta + \frac{1}{2}h\mathbf{L}_\Theta. \quad (38)$$

2.5 Solution of the linear systems

Only three different matrices, \mathbf{M}_B^0 , \mathbf{M}_v^0 and \mathbf{M}_Θ^0 , must be inverted to solve the six linear systems (31)–(36). Once model parameters are fixed, these matrices depend only on the time-step h , so the linear systems (31)–(36) are solved by using the LU -decomposition of \mathbf{M}_B^0 , \mathbf{M}_v^0 and \mathbf{M}_Θ^0 , which is computed prior to time-stepping. Time-step change, which is not implemented, would require recomputation of the LU -decompositions at each step change. The equations and fields for $m < 0$ are omitted since the physical fields are real.

The largest and most difficult linear systems to solve are the velocity systems (32) and (35). By exploiting the dipole-quadrupole parity \mathbf{M}_v^0 and the axisymmetry of the coefficients on the left side of the momentum equation (2), and the real nature of the velocity, the matrix \mathbf{M}_v^0 can be split into $2(N_n + 1)$ irreducible matrices, one dipole and one quadrupole matrix for each $m = 0, \dots, N_n$. Moreover, these matrices are block tridiagonal, if the different radial (row) and Chebychev (column) entries for given m and n are blocked together. The two matrices for $m = 0$ are real and $N_n N_r \times N_n N_T$; for $m > 0$ the matrices are complex and $(N_n - m + 1)N_r \times (N_n - m + 1)N_T$. The velocity is stored in two real and two complex arrays, which have the structure,

$$v_q^0 = (t_1^0, s_2^0, t_3^0, s_4^0, \dots), \quad v_q = (s_1^1, t_2^1, s_3^1, t_4^1, \dots, s_2^2, t_3^2, s_4^2, t_5^2, \dots),$$

for the quadrupole field and

$$v_d^0 = (s_1^0, t_2^0, s_3^0, t_4^0, \dots), \quad v_d = (t_1^1, s_2^1, t_3^1, s_4^1, \dots, t_2^2, s_3^2, t_4^2, s_5^2, \dots),$$

for the quadrupole field, where each entry is itself an array of Chebyshev coefficients, $t_1^0 = (t_{1,0}^0, \dots, t_{1,N_T-1}^0)$, etc., real for $m = 0$ and complex for $m > 0$.

The matrix \mathbf{M}_B^0 appearing in the magnetic induction equations (31) and (34), decomposes into $4N_n$ irreducible real matrices of size $N_r \times N_T$ independently of m , for the odd/even poloidal/toroidal potentials. The magnetic field is stored in four real arrays, which have the structure,

$$\begin{aligned} S_o &= (S_1^0, S_3^0, \dots, S_2^{1r}, S_2^{1i}, S_4^{1r}, S_4^{1i}, \dots, S_3^{2r}, S_3^{2i}, S_5^{2r}, S_5^{2i}, \dots) \\ T_e &= (T_2^0, T_4^0, \dots, T_1^{1r}, T_1^{1i}, T_3^{1r}, T_3^{1i}, \dots, T_2^{2r}, T_2^{2i}, T_4^{2r}, T_4^{2i}, \dots), \end{aligned}$$

for the dipole field and

$$\begin{aligned} S_e &= (S_2^0, S_4^0, \dots, S_1^{1r}, S_1^{1i}, S_3^{1r}, S_3^{1i}, \dots, S_2^{2r}, S_2^{2i}, S_4^{2r}, S_4^{2i}, \dots) \\ T_o &= (T_1^0, T_3^0, \dots, T_2^{1r}, T_2^{1i}, T_4^{1r}, T_4^{1i}, \dots, T_3^{2r}, T_3^{2i}, T_5^{2r}, T_5^{2i}, \dots), \end{aligned}$$

for the quadrupole field. Note that S_1^{1r} and S_1^{1i} denote the real and imaginary parts of S_1^1 , etc.

The heat equation and the temperature are analogous to the magnetic potentials, except the $n = 0$ terms must be included,

$$\begin{aligned} \Theta_e &= (\Theta_2^0, \Theta_4^0, \dots, \Theta_1^{1r}, \Theta_1^{1i}, \Theta_3^{1r}, \Theta_3^{1i}, \dots, \Theta_2^{2r}, \Theta_2^{2i}, \Theta_4^{2r}, \Theta_4^{2i}, \dots) \\ \Theta_o &= (\Theta_1^0, \Theta_3^0, \dots, \Theta_2^{1r}, \Theta_2^{1i}, \Theta_4^{1r}, \Theta_4^{1i}, \dots, \Theta_3^{2r}, \Theta_3^{2i}, \Theta_5^{2r}, \Theta_5^{2i}, \dots). \end{aligned}$$

3 Benchmark models

The code has been tested against two benchmark models given in [2]. After an initial transient of large amplitude the solution settles down

to a steady drift state with four identical rolls, which drift eastward in Model 0 and westward in Model 1. The velocity components, the temperature and, in Model 1, the magnetic field components are of the form $v_{r,\theta,\phi} = v'_{r,\theta,\phi}(r, \theta)f(\phi - \omega t)$, $\Theta = \Theta'(r, \theta)f(\phi - \omega t)$, $B_{r,\theta,\phi} = B'_{r,\theta,\phi}(r, \theta)f(\phi - \omega t)$, where ω is the drift rate. The benchmark values are the average kinetic E_v and shell magnetic E_B energy densities,

$$E_v = \frac{1}{2V_s} \int_V \mathbf{v}^2 dV, \quad E_B = \frac{1}{4E \text{ Pm } V_s} \int_V \mathbf{B}^2 dV,$$

and the values of v_ϕ , Θ and B_θ at $r = (r_o + r_i)/2$ and $\theta = \pi/2$, where the value of ϕ is given by $v_r = 0$ and $\partial_\phi v_r > 0$.

3.1 Model 0: no-slip rotating thermal convection

The magnetic field and its associated terms, equations and boundary conditions are ignored. The velocity and temperature boundary conditions are (31) and (33). The initial ($t = 0$) fields in $r_i \leq r \leq r_o$ are $s_n^m = 0$, $t_n^m = 0$,

$$\Theta_0^0 = r_o r_i / r - r_i, \quad \Theta_4^4 = \frac{1}{40\sqrt{\pi}}(1 - 3x^2 + 3x^4 - x^6), \quad x = 2r - r_i - r_o,$$

and all other $\Theta_n^m = 0$, $m \geq 0$. The parameter values are $r_i = 7/13$, $r_o = 20/13$, $E = 5 \times 10^{-4}$, $\text{Pr} = 1$ and $\text{Ra} = 50$. Results are shown in Table 1, including the benchmark values. The agreement is accurate to three significant figures.

TABLE 1: Results for Models 0 & 1.

	Model 0	Benchmark 0	Model 1		Benchmark 1
dt	10^{-4}		10^{-4}	10^{-4}	
t_{\max}	1.2		5	5	15
N_r	25		25	25	65
N_θ	48		36	48	128
N_ϕ	65		49	65	
N_n	32		18	32	
E_v	58.348	$58.348 \pm .050$	30.50	30.42	$30.773 \pm .020$
E_B			625.09	621.53	$626.41 \pm .40$
Θ	0.4287	$0.42812 \pm .00012$		0.3972	$0.37338 \pm .00040$
v_ϕ	-10.139	$-10.1571 \pm .0020$		-8.181	$-7.6250 \pm .0060$
B_θ				-4.799	$-4.9289 \pm .0060$
ω	0.18234	$0.1824 \pm .0050$		-3.0341	$-3.1017 \pm .0040$

3.2 Model 1: dynamo with insulating inner-core

The boundary conditions are (31)–(33). The initial ($t = 0$) fields in $r_i \leq r \leq r_o$ are $s_n^m = 0$, $t_n^m = 0$,

$$\Theta_0^0 = r_o r_i / r - r_i, \quad \Theta_4^4 = \frac{1}{40\sqrt{\pi}}(1 - 3x^2 + 3x^4 - x^6), \quad x = 2r - r_i - r_o,$$

all other $\Theta_n^m = 0$, $m \geq 0$,

$$S_1^0 = -(5/8\sqrt{3})(3r^2 - 4rr_o + r_i^4/r^2), \quad T_2^0 = 2\sqrt{5}/3 \sin \pi(r - r_i).$$

all other $S_n^m = 0$ and $T_n^m = 0$, $m \geq 0$. The parameter values are $r_i = 7/13$, $r_o = 20/13$, $E = 5 \times 10^{-4}$, $\text{Pr} = 1$, $\text{Ra} = 50$ and $\text{Pm} = 5$. Results are shown in Table 1, including the benchmark values. Here the agreement is accurate to about two significant figures. The disagreement is most probably due to the lower truncation levels used in the present work. The computing resources necessary to

achieve the higher truncation levels of the benchmark and the longer integration time are not available for the present work.

4 Concluding remarks

In summary, the dynamical dynamo equations have been solved in a spherical shell for two benchmark models, thermal convection with fixed inner-core and a convective dynamo with insulating fixed inner-core. Higher truncation level should improve agreement with the benchmarks. The code has been extended to incorporate an electrically-conducting, no-slip inner-core, which can rotate freely about the rotation axis of the mantle under the control of the axial viscous and magnetic torques at the inner-core boundary. A related code is being developed for spherical conducting region. Work is also actively underway to incorporate anisotropic diffusivities [7].

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