The spherical MHD code MagIC Advanced (2/2)

Thomas Gastine

Institut de Physique du Globe de Paris

6th July 2017





Time integration ●00000000000	Parallelisation strategy 00000	Resolution check	Science with MagIC	Bibliography 0000
Outline				

- 2 Parallelisation strategy
- 3 Resolution check
- 4 Science with MaglC

5 Bibliography

- MagIC simulates rotating fluid dynamics in a spherical shell
- It solves for the coupled evolution of Navier-Stokes equation, MHD equation, temperature (or entropy) equation and an equation for chemical composition under both the anelastic and the Boussinesq approximations
- A dimensionless formulation of the equations is assumed
- MagIC is a free software (GPL), written in Fortran
- Post-processing relies on python libraries
- Poloidal/toroidal decomposition is employed
- MagIC uses spherical harmonic decomposition in the angular directions
- Chebyshev polynomials or finite differences are employed in the radial direction
- MagIC uses a mixed implicit/explicit time stepping scheme
- The code relies on a hybrid parallelisation scheme (MPI/OpenMP)

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
0000000000	00000	0000000		0000
Spectral poloida	al dynamo equation	า		

Equation for each spherical harmonic degree and order

$$\frac{\ell(\ell+1)}{r^2} \left[\left(\frac{\partial}{\partial t} + \frac{1}{Pm} \frac{\ell(\ell+1)}{r^2} \right) \mathcal{C}_n - \frac{1}{Pm} \mathcal{C}_n'' \right] g_{\ell n}^m = \mathcal{N}_{\ell}^m$$

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
0000000000	00000	0000000		0000
Spectral poloid:	al dynamo equation	า		

Equation for each spherical harmonic degree and order

$$\frac{\ell(\ell+1)}{r^2} \left[\left(\frac{\partial}{\partial t} + \frac{1}{Pm} \frac{\ell(\ell+1)}{r^2} \right) \mathcal{C}_n - \frac{1}{Pm} \mathcal{C}_n'' \right] g_{\ell n}^m = \mathcal{N}_{\ell}^m$$

How to deal with the time integration, i.e. discretisation in time?

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
000●0000000	00000	0000000		0000
Strategy				

Strong non linearities = stiff problem. Usually, higher-order schemes (RK4), or multi-step algorithms are employed (BDF).

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
000●00000000	00000	0000000		0000
Strategy				

- Strong non linearities = stiff problem. Usually, higher-order schemes (RK4), or multi-step algorithms are employed (BDF).
- BUT Courant condition gives:

$$\delta t < C \frac{\mathrm{d}r^2}{\nu} \quad o \quad$$
 Small time steps!

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
000●00000000	00000	0000000		0000
Strategy				

- Strong non linearities = stiff problem. Usually, higher-order schemes (RK4), or multi-step algorithms are employed (BDF).
- BUT Courant condition gives:

 $\delta t < C \frac{\mathrm{d}r^2}{\nu} \quad o \quad$ Small time steps!

Implicit schemes offer increased stability and allow larger timesteps

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
000●00000000	00000	0000000		0000
Strategy				

- Strong non linearities = stiff problem. Usually, higher-order schemes (RK4), or multi-step algorithms are employed (BDF).
- BUT Courant condition gives:

 $\delta t < C \frac{\mathrm{d}r^2}{\nu} \quad o \quad$ Small time steps!

- Implicit schemes offer increased stability and allow larger timesteps
- BUT fully implicit schemes couple all spherical harmonic modes → huge memory imprint

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
000●00000000	00000	0000000		0000
Strategy				

- Strong non linearities = stiff problem. Usually, higher-order schemes (RK4), or multi-step algorithms are employed (BDF).
- BUT Courant condition gives:

 $\delta t < C \frac{\mathrm{d}r^2}{\nu} \quad o \quad$ Small time steps!

- Implicit schemes offer increased stability and allow larger timesteps
- BUT fully implicit schemes couple all spherical harmonic modes → huge memory imprint

Adopted strategy

Most authors adopt a mixed implicit/explicit algorithm

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
00000000000	00000	0000000		0000
Semi-implicit so	cheme			

Generic evolution equation with terms $\mathcal{I}(x, t)$ to be treated **implicitly** and $\mathcal{E}(x, t)$ to be treated explicitly:

$$\frac{\partial x}{\partial t} + \mathcal{I}(x,t) = \mathcal{E}(x,t)$$

Time integration 00000000000	Parallelisation strategy 00000	Resolution check	Science with MagIC	Bibliography 0000
Semi-implicit so	cheme			

Generic evolution equation with terms $\mathcal{I}(x, t)$ to be treated **implicitly** and $\mathcal{E}(x, t)$ to be treated explicitly:

$$rac{\partial x}{\partial t} + \mathcal{I}(x,t) = \mathcal{E}(x,t)$$

Glatzmaier's (1984) time integration scheme (2nd order): Implicit **Crank-Nicolson** scheme:

$$\left(\frac{x(t+\delta t)-x(t)}{\delta t}\right)_{\mathcal{I}}=-\alpha\,\mathcal{I}(x,t+\delta t)-(1-\alpha)\,\mathcal{I}(x,t)$$

Explicit 2nd order Adams-Bashforth scheme:

$$\left(rac{x(t+\delta t)-x(t)}{\delta t}
ight)_{\mathcal{E}}=rac{3}{2}\,\mathcal{E}(x,t)-rac{1}{2}\,\mathcal{E}(x,t-\delta t)$$

N.B. Other schemes are used in some pseudo-spectral codes: BDF/AB or predictor-corrector

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
00000000000	00000	0000000	00000000000000	0000
Time stepping s	scheme			

$$\frac{x(t+\delta t)}{\delta t} + \alpha \mathcal{I}(x,t+\delta t) = \frac{x(t)}{\delta t} - (1-\alpha)\mathcal{I}(x,t) + \frac{3}{2}\mathcal{E}(x,t) - \frac{1}{2}\mathcal{E}(x,t-\delta t)$$

- When $\alpha = 0.5$, this is pure CN/AB2 implicit/explicit 2nd order scheme
- Glatzmaier (1984) reported an improved stability when $\alpha = 0.6$ (see MagIC's input namelist)

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
00000000000	00000	0000000	00000000000000	0000
Treatment of C	oriolis force			

As an example, Coriolis force that enters the $\ensuremath{\mathcal{W}}$ equation:

$$2\tilde{\rho}\,\mathbf{e}_{\mathbf{r}}\cdot(\mathbf{u}\times\mathbf{e}_{\mathbf{z}})=2\sin\theta\,\tilde{\rho}u_{\phi}=\frac{2}{r}\left(\frac{\partial^{2}W}{\partial r\partial\phi}-\sin\theta\frac{\partial Z}{\partial\theta}\right)$$

This yields:

$$\operatorname{Cor}_{\ell n}^{m} = \frac{2}{r} \left[\operatorname{im} \mathcal{C}_{n}^{\prime} W_{\ell n}^{m} - (\ell - 1) c_{\ell}^{m} \mathcal{C}_{n} Z_{\ell - 1, n}^{m} + (\ell + 2) c_{\ell + 1}^{m} \mathcal{C}_{n} Z_{\ell + 1, n}^{m} \right]$$

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
00000000000	00000	0000000	00000000000000	0000
Treatment of C	oriolis force			

As an example, Coriolis force that enters the W equation:

$$2\tilde{\rho}\,\mathbf{e}_{\mathbf{r}}\cdot(\mathbf{u}\times\mathbf{e}_{\mathbf{z}})=2\sin\theta\,\tilde{\rho}u_{\phi}=\frac{2}{r}\left(\frac{\partial^{2}W}{\partial r\partial\phi}-\sin\theta\frac{\partial Z}{\partial\theta}\right)$$

This yields:

$$\operatorname{Cor}_{\ell n}^{m} = \frac{2}{r} \left[im \mathcal{C}_{n}^{\prime} W_{\ell n}^{m} - (\ell - 1) c_{\ell}^{m} \mathcal{C}_{n} Z_{\ell - 1, n}^{m} + (\ell + 2) c_{\ell + 1}^{m} \mathcal{C}_{n} Z_{\ell + 1, n}^{m} \right]$$

Implicit treatment?

- (ℓ, m) mode coupled with $(\ell + 1, m)$ and $(\ell 1, m)$ modes
- Poloidal and toroidal equations coupled
- Implicit treatment of Coriolis force = much larger matrix
- In MagIC, Coriolis force is treated explicitly...

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
000000000000	00000	0000000		0000
Poloidal magne	tic field time stepp	ing		

Again equation for poloidal magnetic field:

$$\frac{\ell(\ell+1)}{r^2} \left[\left(\frac{\partial}{\partial t} + \frac{1}{Pm} \frac{\ell(\ell+1)}{r^2} \right) \mathcal{C}_n - \frac{1}{Pm} \mathcal{C}_n'' \right] g_{\ell n}^m = \mathcal{N}_\ell^m$$

0000000000			
Doloidol morno	tic field time stone	100	

Poloidal magnetic field time stepping

Again equation for poloidal magnetic field:

$$\frac{\ell(\ell+1)}{r^2} \left[\left(\frac{\partial}{\partial t} + \frac{1}{Pm} \frac{\ell(\ell+1)}{r^2} \right) \mathcal{C}_n - \frac{1}{Pm} \mathcal{C}_n'' \right] g_{\ell n}^m = \mathcal{N}_\ell^m$$

Using the CN/AB2 scheme yields the following linear problem

$$\begin{bmatrix} A_{kn} + \alpha G_{kn} \end{bmatrix} g_{\ell n}^{m}(t + \delta t) = \begin{bmatrix} A_{kn} - (1 - \alpha) G_{kn} \end{bmatrix} g_{\ell n}^{m}(t) \\ + \frac{3}{2} D_{kn}(t) - \frac{1}{2} D_{kn}(t - \delta t)$$

with

$$\begin{split} A_{kn} &= \frac{\ell(\ell+1)}{r_k^2} \frac{\mathcal{C}_n(r_k)}{\delta t}; \quad G_{kn} = \frac{\ell(\ell+1)}{r_k^2} \frac{1}{Pm} \left[\frac{\ell(\ell+1)}{r_k^2} \mathcal{C}_n(r_k) - \mathcal{C}_n''(r_k) \right]; \\ D_{kn} &= \mathcal{N}_\ell^m(r_k) \end{split}$$

Parallelisation strategy 00000 Resolution check

Science with MagIC

Bibliography 0000

Some comments on the time-stepping

- $C_n(r_k)$, $C'_n(r_k)$, $C''_n(r_k)$ are **full matrices**: costly **LU factorisations** required ($\mathcal{O}(N_r^2)$) and possibly large memory imprints
- BUT as long as δt does not change, the left hand-side operator does not change
- Finite differences in radius yield sparse matrices: less memory, faster solve (at the price of reduced accuracy though)...

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
000000000●00	00000	0000000		0000
Courant condit	ion			

- Explicit treatment of Coriolis force: $\delta t \leq 0.1 E$
- δt should be smaller than the advection between two grid points:

$$\delta t_r \leq \min\left[\frac{\delta r}{|u_r|}
ight]; \ \delta t_H \leq \min\left[\left(\frac{r^2}{\ell_{\max}(\ell_{\max}+1)(u_{ heta}^2+u_{\phi}^2)}
ight)^{1/2}
ight]$$

Hence

$$\delta t = C \min(\delta t_r, \delta t_H)$$

In presence of a magnetic field, another condition on the Alvén velocity is required

Parallelisation strategy 00000

Resolution check

Science with MagIC

Bibliography 0000

Time integration: summary

Take-away messages on time stepping

- Most of the pseudo-spectral codes assume a mixed implicit/explicit scheme (most of the time 2nd order)
- At each time step a linear system needs to be solved
- For Chebyshev-based code: **LU factorisations** $\rightarrow O(\ell_{\max}^2 N_r^2)$ (matrix can be saved as long as δt does not change though)
- Finite difference are cheaper here: sparse matrix, less memory, faster inversion

Documentation





Time integration	Parallelisation strategy ●0000	Resolution check 0000000	Science with MagIC	Bibliography 0000
Outline				

2 Parallelisation strategy

- 3 Resolution check
- 4 Science with MaglC

5 Bibliography

- MagIC simulates rotating fluid dynamics in a spherical shell
- It solves for the coupled evolution of Navier-Stokes equation, MHD equation, temperature (or entropy) equation and an equation for chemical composition under both the anelastic and the Boussinesq approximations
- A dimensionless formulation of the equations is assumed
- MagIC is a free software (GPL), written in Fortran
- Post-processing relies on python libraries
- Poloidal/toroidal decomposition is employed
- MagIC uses spherical harmonic decomposition in the angular directions.
- Chebyshev polynomials or finite differences are employed in the radial direction
- MagIC uses a mixed implicit/explicit time stepping scheme
- The code relies on a hybrid parallelisation scheme (MPI/OpenMP)

Parallelisation strategy

Resolution check

Science with MagIC

Bibliography 0000

Hybrid configuration used in MagIC

MPI:

- Ist part of the code: calculation of the nonlinear terms and SH transforms = radial levels can be treated independently: r is distributed over N_p MPI ranks
- 2nd part of the code: time advance of the equations = linear solve = all the (ℓ, m) modes can be treated independently: (ℓ, m) is distributed over N_p MPI ranks (pairing needed to ensure the load balancing
- In between: costly mpi_all_to_all(...) calls are required. For large truncations, this becomes a bottleneck...

OpenMP:

- **1st part of the code**: N_t OpenMP threads can be used over the θ blocks for the SH transforms and computation of nonlinear terms
- **1st part of the code**: N_t OpenMP tasks are used over (ℓ, m)

Time	integration	

Parallelisation strategy

Resolution check

Science with MagIC

Bibliography 0000

MagIC structure



Parallelisation strategy

Resolution check

Science with MagIC

Bibliography 0000

Possible improvements: 2D-MPI configuration



Taken from Calypso's documentation

Time integration	Parallelisation strategy 00000	Resolution check	Science with MagIC 00000000000000	Bibliography 0000
Outline				

- 2 Parallelisation strategy
- 3 Resolution check
- 4 Science with MaglC

5 Bibliography



 $E = 3 \times 10^{-4}, Ra = 3 \times 10^{6}$

 Obvious signatures of under-resolution: small-scale structures of comparable size than the grid, "eyes", aliases (sudden localized changes of polarities)



• Look at **spectra** and check the dissipation:



- Rule of thumb: 2 orders of magnitude between the injection scale and the dissipation scale
- Additional diagnostics of under-resolution: heat flux conservation, power budget



- Under-resolution might be an issue: it really depends what you are looking at...
- Let's take another example of under-resolution



A lot of localised "eyes"



- Under-resolution might be an issue: it really depends what you are looking at...
- Let's take another example of under-resolution



- A lot of localised "eyes"
- **Solution**: multiply the angular resolution by 3



Possible impacts of under-resolution (2/2)



- At first glance, you would better trash the under-resolved case
- But, the largest scales contributions are reasonably captured
- Surprisingly, some global quantities might still be OK!

Time integration	Parallelisation strategy 00000	Resolution check 0000000	Science with MagIC	Bibliography 0000
Is it that bad?				

Parameter	Under-resolved	Resolved
Volum	e-averaged quant	ities
Rm	1000	1000
٨	16	16
Surfac	e-averaged quant	ities
$\Lambda(r = r_o)$	53	34
$Nu(r = r_o)$	1.55	1.3
$Nu(r = r_i)$	1.3	1.3

Results

■ Global volume-integrated quantities are still good!

_

- But surface-averaged and local quantities are completely wrong
- Be careful with what you are doing!

Parallelisation strategy

Resolution check

Science with MagIC

Bibliography 0000

How much does it cost?



1024³-class simulation: 10^7 CPU hours

Schaeffer et al. (2017)

Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
୦୦୦୦୦୦୦୦୦୦	00000	000000●	00000000000000	0000

Summary: little recipes for MagIC

- **I** Good resolution: no localised "eyes" or aliases clean spectra
- 2 Bad resolution: aliasing, pile-up of energy, no proper dissipation
- 3 At some point the simulation will crash (hopefully)...
- But some compromises are possible: slightly under-resolved cases can still provide good volume-integrated quantities (numerically cheap)
- **5** Be careful though: local properties (heat transfer, scaling laws) are likely wrong
- 6 Don't over-do it! Large resolution are computationally expensive
- Why not running first a smaller and cheaper truncation for transients and possibly refining the grid later on?

Time integration	Parallelisation strategy 00000	Resolution check	Science with MagIC ●000000000000000	Bibliography 0000
Outline				

- 2 Parallelisation strategy
- 3 Resolution check
- 4 Science with MagIC



Time integration	Parallelisation strategy	Resolution check	Science with MagIC	Bibliography
	00000	0000000	000000000000000000000000000000000000	0000
List of publicat	ions			

To date, around **90 publications** in more than 10 different peer-reviewed journals have been produced using MagIC:



Parallelisation strateg

Resolution check

Science with MagIC

Bibliography 0000

International dynamo benchmark Christensen *et al.*, PEPI, 2001

- Earth-like setup
- Boussinesq
- $r_i/r_o = 0.35$
- Weakly-supercritical laminar dynamo
- Code validation



Parallelisation strategy 00000 Resolution check

Science with MagIC

Bibliography 0000

Modelling the Jovian zonal jets Heimpel *et al.*, Nature, 2005

- Jupiter-like zonal jets in a thin convective shell
- Boussinesq
- Non-magnetic
- Stress-free boundaries
- $r_i/r_o=0.9$
- low *E*, large *Ra*



Anelastic, non-magnetic model with a stably-stratified atmosphere.



Parallelisation strateg

Resolution check

Science with MagIC

Bibliography 0000

Explaining chaos terrain on Europa Soderlund *et al.*, Nat. Geo., 2014

- Europa's ocean
- Thin convective shell
- Boussinesq
- Non-magnetic
- ∎ large *Ra*
- stronger equatorial heat flux



 Time integration
 Parallelisation strategy
 Resolution check

 00000000000
 00000
 000000

Science with MagIC

Bibliography 0000

Explaining inner core anisotropy Aubert *et al.*, Nature, 2008

- Geodynamo simulation
- Boussinesq
- Tomographic CMB heat flux pattern
- Inner core anisotropy



Parallelisation strategy

Resolution check

Science with MagIC

Bibliography 0000

Explaining the Martian crustal field anisotropy Dietrich & Wicht, PEPI, 2013

- Increased southern heat flux
- Boussinesq
- Anistropic flow and field



Parallelisation strateg

Resolution check

Science with MagIC

Bibliography 0000

Inertial modes in spherical Couette flows $_{\rm Wicht,\ JFM,\ 2014}$

- Spherical Couette
- Boussinesq
- Non-magnetic
- Comparison with Maryland's experiment



Parallelisation strategy

Resolution check

Science with MagIC

Bibliography 0000

Rayleigh-Bénard convection in spherical shells Gastine *et al.*, JFM, 2015

- Non-rotating
- Boussinesq
- Non-magnetic
- high *Ra*



Parallelisation strateg

Resolution check

Science with MagIC

Bibliography 0000

Explaining Saturn's peculiar magnetic field Cao *et al.*, Icarus, 2012

Slightly supercritical spherical Taylor-Couette dynamo



Parallelisation strategy

Resolution check

Science with MagIC

Bibliography 0000

Jupiter hosts two dynamos? Gastine *et al.*, GRL, 2014

- Jovian-like reference state
- Anelastic
- Magnetic
- low E high Ra



Parallelisation strategy

Resolution check

Science with MagIC

Bibliography 0000

Formation of polar spots on rapidly-rotating cool stars Yadav *et al.*, ApJ, 2015

- fully convective M dwarf
- Anelastic
- Magnetic
- Large density contrast



Parallelisation strateg

Resolution check

Science with MagIC

Bibliography 0000

MRI in radiative zones of A-type stars Jouve *et al.*, A&A, 2015

- Incompressible fluid
- Magnetic instabilities (MRI & Tayler)
- Here MRI





Fully convective, anelastic, rapidly-rotating dynamo (M dwarf)



Time integration	Parallelisation strategy 00000	Resolution check	Science with MagIC 00000000000000	Bibliography 0000
What is coming	g next?			

?!

It is up to you now!

Time integration	Parallelisation strategy 00000	Resolution check 0000000	Science with MagIC	Bibliography ●000
Outline				

- 2 Parallelisation strategy
- 3 Resolution check
- 4 Science with MaglC



000000000000	00000	0000000	000000000000000000000000000000000000000			
Selected references I						

J. P. Boyd.

Chebyshev and Fourier spectral methods. Dover Publications, 2001.

C. Canuto, M. Y. Hussaini, A. M. Quarteroni, and T. A. Zang. Spectral methods. Springer, 2006.

S. Chandrasekhar.

Hydrodynamic and Hydromagnetic Stability. Oxford University Press, 1961.

T. C. Clune, J. R. Elliott, M. S. Miesch, J. Toomre, and G. A. Glatzmaier. Computational aspects of a code to study rotating turbulent convection in spherical shells. *Parallel Computing*, 25:361–380, 1999.

00000000000	00000		000000000000000	0000		
Selected references II						

G. A. Glatzmaier.

Numerical simulations of stellar convective dynamos. I - The model and method. *Journal of Computational Physics*, 55:461–484, September 1984.

G. A. Glatzmaier.

Introduction to modeling convection in planets and stars: Magnetic field, density stratification, rotation.

Princeton University Press, 2013.

🔋 R. Hollerbach.

A spectral solution of the magneto-convection equations in spherical geometry. International Journal for Numerical Methods in Fluids, 32:773–797, April 2000.

C. A. Jones, P. Boronski, A. S. Brun, G. A. Glatzmaier, T. Gastine, M. S. Miesch, and J. Wicht. Anelastic convection-driven dynamo benchmarks.

Icarus, 216:120-135, November 2011.

Time integration	Parallelisation strategy 00000	Resolution check	Science with MagIC 00000000000000	Bibliography ○●●●
Selected referer	nces III			

H. Matsui, E. Heien, J. Aubert, J. M. Aurnou, M. Avery, and et al.

Performance benchmarks for a next generation numerical dynamo model. *Geochemistry, Geophysics, Geosystems*, 17:1586–1607, May 2016.

S. A. Orszag.

On the Elimination of Aliasing in Finite-Difference Schemes by Filtering High-Wavenumber Components.

Journal of Atmospheric Sciences, 28:1074–1074, September 1971.

N. Schaeffer.

Efficient spherical harmonic transforms aimed at pseudospectral numerical simulations. *Geochemistry, Geophysics, Geosystems*, 14:751–758, March 2013.

A. Tilgner.

Spectral methods for the simulation of incompressible flows in spherical shells. *International Journal for Numerical Methods in Fluids*, 30:713–724, July 1999.