The spherical MHD code MagIC

Fundamentals

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Outline

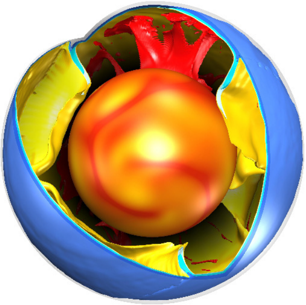
1 Introduction
- What for? How?
- Introducting MagIC

2 MHD problem

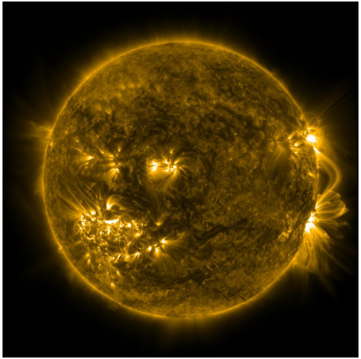
3 Installing and running the code

4 Postprocessing

What for?



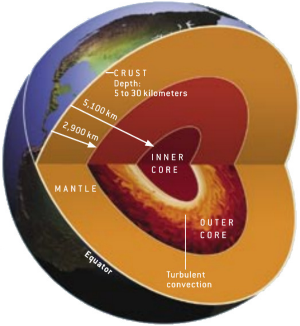
Crameri (2014)



VERIS (2013)

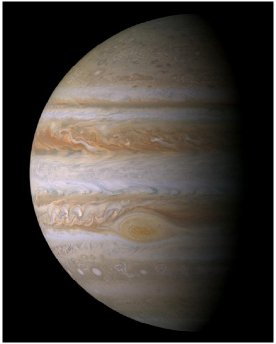
Earth's mantle **Solar convective zone**

What for?



Glatzmaier & Olson (2005)

Earth's core



Cassini

Jupiter

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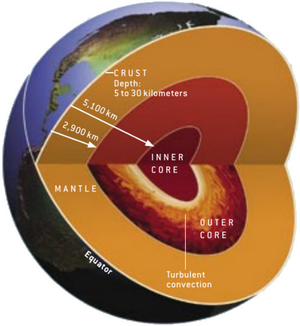

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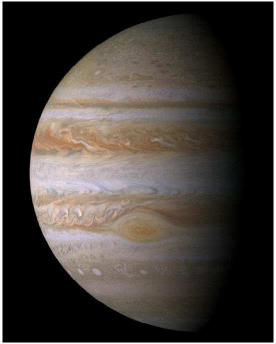

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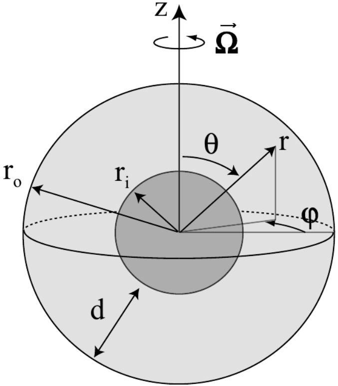
Jupiter

Spherical geometry is more natural for studying rotating convection in astrophysical and geophysical objects!

The setup



Rotating spherical shell

Frame of reference rotating with system rotation Ω

How?

Local methods = finite differences, volume, elements?

- **PROS**: easier to implement, more straightforward to parallelise, grid refinements possible
- **CONS**: anisotropic grids, pole instability, problem with vacuum magnetic boundary condition, more points required to get same accuracy

How?

Spectral methods =expansion as complete sets of functions?

- **PROS**: derivatives easier to calculate with high accuracy, magnetic boundary condition is straightforward, lower number of grid points required
- **CONS**: parallelisation harder to implement and more communications

How?

To date spectral methods are more suitable!

"Local methods [...] need longer elapsed times than spectral methods to achieve the same accuracy with the same number of processors. Spherical harmonic expansion methods [...] offer the best assurance of efficiency for geodynamo simulations" (Matsui *et al.* 2016)

Some milestones...

1. **Chandrasekhar (1960s)**: poloidal/toroidal decomposition, onset of convection in spherical shells

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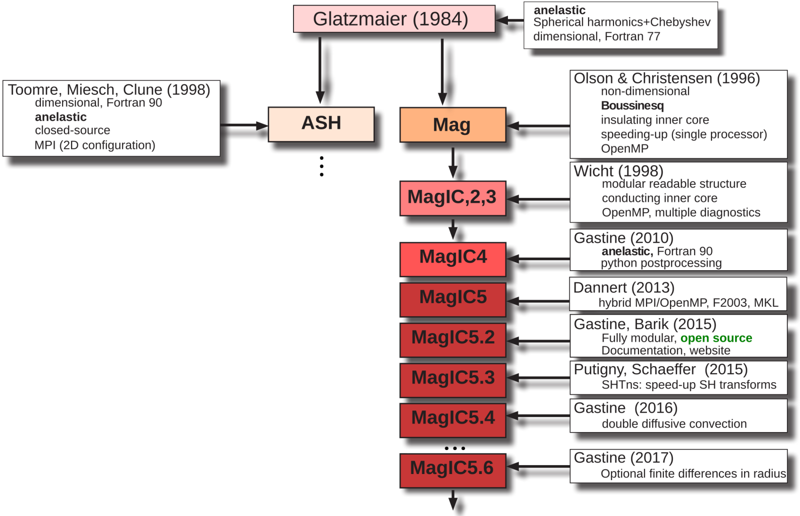
4. **Glatzmaier & Gilman (1980)**: onset of compressible convection in a spherical shell
5. **Glatzmaier (1984)**: **pseudo-spectral MHD code in a spherical shell geometry**

Pseudo-spectral? What does it mean?

Pseudo-spectral codes

- **The linear terms are expanded as complete sets of functions** (e.g. spherical harmonics, Chebyshev polynomials, Fourier functions, ...)
- **Nonlinear terms treated in grid space** rather than spectral space = numerical transformations between spectral and spatial representations

MagIC heritage



MagIC in words

- 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
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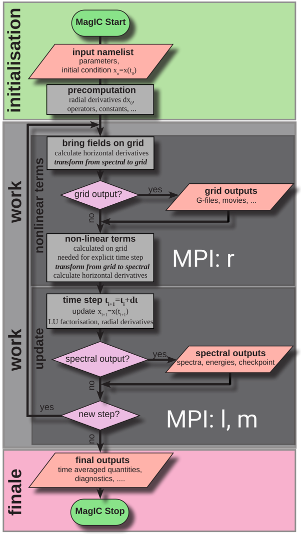
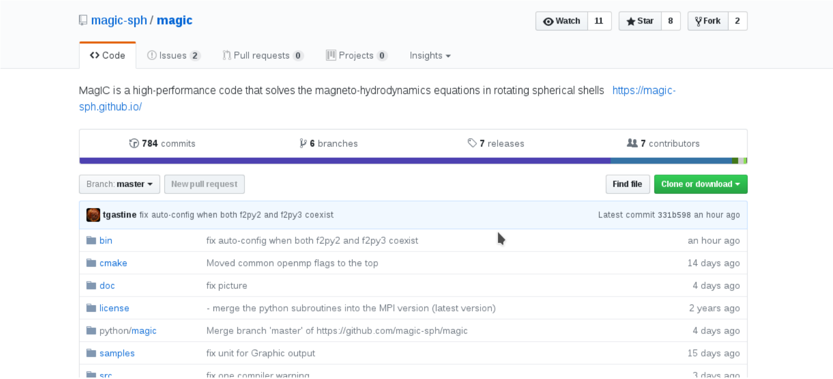
- The code relies on a hybrid parallelisation scheme (MPI/OpenMP)

Stucture of the code



Website and documentation

- Since 2015: MagIC is a hosted on https://github.com/magic-sph/magic



- **Online documentation**: https://magic-sph.github.io

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2 MHD problem
- Fully compressible equations
- From fully compressible to anelastic
- Dimensionless anelastic equations

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Equation of motion for a compressible fluid

Continuity equation

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0$$

Navier Stokes equation:

$$\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} + 2\boldsymbol{\Omega} \times \boldsymbol{u} \right) = -\boldsymbol{\nabla} p + \rho \, \boldsymbol{g} + \frac{1}{\mu_0} (\boldsymbol{\nabla} \times \boldsymbol{B}) \times \boldsymbol{B} + \boldsymbol{\nabla} \cdot \mathsf{S}$$

with the rate-of-strain tensor expressed by

$$\mathsf{S}_{ij} = \nu \rho \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \, \boldsymbol{\nabla} \cdot \boldsymbol{u} \right)$$

Energy equation for a compressible fluid

$$\rho T \left(\frac{\partial s}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} s \right) = \boldsymbol{\nabla} \cdot (k_T \boldsymbol{\nabla} T) + \Phi_\nu + \lambda (\boldsymbol{\nabla} \times B)^2 + \epsilon_T$$

with the viscous heating Φ_ν expressed by

$$\Phi_\nu = 2\rho \left[e_{ij} e_{ji} - \frac{1}{3} (\boldsymbol{\nabla} \cdot \boldsymbol{u})^2 \right]$$

If in addition to that, compositional changes are also considered another equation for the chemical composition ξ reads

$$\rho \left(\frac{\partial \xi}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \xi \right) = \boldsymbol{\nabla} \cdot (k_\xi \boldsymbol{\nabla} \xi) + \epsilon_\xi$$

Induction equation

Non-relativistic Maxwell equations provide

$$\frac{\partial \boldsymbol{B}}{\partial t} = \boldsymbol{\nabla} \times (\boldsymbol{u} \times \boldsymbol{B} - \lambda \boldsymbol{\nabla} \times \boldsymbol{B})$$

with $\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$

When λ is homogeneous, one simply gets

$$\frac{\partial \boldsymbol{B}}{\partial t} = \boldsymbol{\nabla} \times (\boldsymbol{u} \times \boldsymbol{B}) + \lambda \boldsymbol{\Delta} \boldsymbol{B}$$

Equation of state

In general:

$$p = f(\rho, T, \xi)$$

or

$$\frac{1}{\rho}\partial\rho = -\alpha\,\partial T + \beta\,\partial p + \delta\partial\xi$$

where

$$\text{Thermal expansivity: } \alpha = -\frac{1}{\rho}\left(\frac{\partial\rho}{\partial T}\right)_{\xi,p}$$

$$\text{Compressibillity: } \beta = \frac{1}{\rho}\left(\frac{\partial\rho}{\partial p}\right)_{\xi,\rho}$$

$$\text{Chemical coefficient: } \delta = \frac{1}{\rho}\left(\frac{\partial\rho}{\partial\xi}\right)_{p,\rho}$$

From fully compressible to anelastic and Boussinesq

Reference state

MHD equations

MagIC either uses the **anelastic** or the **Boussinesq** approximation of the Navier Stokes equation

Anelastic approximation = small disturbance (prime) around an **adiabatic** reference state (tilde):

$$\epsilon \sim \frac{s'}{c_p} \sim \frac{T'}{\tilde{T}} \sim \frac{\rho'}{\tilde{\rho}} \sim \frac{p'}{\tilde{p}} \sim \frac{\xi'}{\tilde{\xi}}$$

The reference state is **hydrostatic, adiabatic, and non magnetic**:

$$\boldsymbol{\nabla} \tilde{p} = \tilde{\rho}\, \boldsymbol{g}; \quad \boldsymbol{\nabla} \tilde{T} = \frac{\alpha \tilde{T}}{c_p} \boldsymbol{g}; \quad \boldsymbol{\nabla} \tilde{\xi} = 0$$

Anelastic continuity equation

Using $\rho = \tilde{\rho} + \rho'$ yields

$$\underbrace{\frac{\partial \tilde{\rho}}{\partial t}}_{=0} + \frac{\partial \rho'}{\partial t} + \boldsymbol{\nabla} \cdot (\tilde{\rho} \boldsymbol{u}) + \underbrace{\boldsymbol{\nabla} \cdot (\rho' \boldsymbol{u})}_{\mathcal{O}(\epsilon^2)} = 0$$

Estimate of the ratio

$$\frac{\partial \rho' / \partial t}{\boldsymbol{\nabla} \cdot (\tilde{\rho} \boldsymbol{u})} \sim \frac{\rho'}{\tilde{\rho}} \sim \epsilon$$

The first order anelastic equation thus reads

$$\boxed{\boldsymbol{\nabla} \cdot (\tilde{\rho} \boldsymbol{u}) = 0}$$

Anelastic equations

Navier-Stokes equation:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} + 2\boldsymbol{\Omega} \times \boldsymbol{u} = -\boldsymbol{\nabla} \frac{p'}{\tilde{\rho}} - \frac{\tilde{\alpha} \tilde{T}}{c_p} s' \boldsymbol{g} + \frac{1}{\mu_0 \tilde{\rho}} (\boldsymbol{\nabla} \times \boldsymbol{B}) \times \boldsymbol{B} + \frac{1}{\tilde{\rho}} \boldsymbol{\nabla} \cdot \mathsf{S}$$

Energy equation:

$$\tilde{\rho} \tilde{T} \left(\frac{\partial s'}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} s' \right) = \boldsymbol{\nabla} \cdot \left(k_T \boldsymbol{\nabla} T' \right) + \Phi_\nu + \lambda \left(\boldsymbol{\nabla} \times B \right)^2 + \epsilon_T$$

Induction equation:

$$\frac{\partial \boldsymbol{B}}{\partial t} = \boldsymbol{\nabla} \times \left(\boldsymbol{u} \times \boldsymbol{B} - \lambda \boldsymbol{\nabla} \times \boldsymbol{B} \right)$$

Boundary conditions

- **Mechanical boundary conditions**:

$$\text{Stress-free: } \boldsymbol{n} \times (\mathsf{S} \cdot \boldsymbol{n}) = \boldsymbol{0}, \quad \text{or no-slip: } \boldsymbol{u} = \boldsymbol{0}, \quad r = r_i, r_o$$

- **Magnetic boundary conditions**:

$$\text{Vacuum: } \boldsymbol{\Delta B} = \boldsymbol{0}, \quad r = r_i, r_o$$

- **Thermal boundary conditions**:

$$\text{Flux: } \frac{\partial T'}{\partial r} = 0, \quad \text{or temperature: } T' = 0, \quad r = r_i, r_o$$

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A dimensionless formulation of the anelastic MHD equation

MHD equations

MagIC uses a **dimensionless form** of the anelastic MHD equations

In MagIC, the viscous diffusion time is assumed to be the **reference timescale** and the spherical shell gap the **reference lengthscale**:

$$[\tilde{\rho}] = \tilde{\rho}(r = r_o); \quad [\tilde{T}] = \tilde{T}(r = r_o); \quad [r] = r_o - r_i;$$
$$[t] = \frac{d^2}{\nu}; \quad [u] = \frac{\nu}{d}; \quad [B] = \sqrt{\mu_0 \lambda \tilde{\rho} \Omega}; \quad [p'] = \tilde{\rho}(r = r_o)\frac{\nu^2}{d^2}$$

This implies that the velocity is expressed in **Reynolds number** unit, and the magnetic field in **Elsasser number** unit.

Dimensionless anelastic MHD equations

In the case of an ideal gas with homogeneous kinematic viscosity ν, thermal diffusivity κ and magnetic diffusivity λ, one gets:

$$
\begin{aligned}
\boldsymbol{\nabla} \cdot (\tilde{\rho} \boldsymbol{u}) &= 0 \\
\boldsymbol{\nabla} \cdot \boldsymbol{B} &= 0 \\
\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} + \frac{2}{E} \boldsymbol{e_z} \times \boldsymbol{u} &= -\boldsymbol{\nabla} \frac{p'}{\tilde{\rho}} + \frac{Ra}{Pr} g(r)\, s' \boldsymbol{e_r} + \frac{1}{\tilde{\rho}\, E\, Pm} (\boldsymbol{\nabla} \times \boldsymbol{B}) \times \boldsymbol{B} + \frac{1}{\tilde{\rho}} \boldsymbol{\nabla} \cdot \mathsf{S} \\
\frac{\partial \boldsymbol{B}}{\partial t} &= \boldsymbol{\nabla} \times (\boldsymbol{u} \times \boldsymbol{B}) + \frac{1}{Pm} \boldsymbol{\Delta} \boldsymbol{B} \\
\tilde{\rho} \tilde{T} \left(\frac{\partial s'}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} s' \right) &= \frac{1}{Pr} \boldsymbol{\nabla} \cdot (\tilde{\rho} \boldsymbol{\nabla} T') + \frac{Di\, Pr}{Ra} \left[\Phi_\nu + \frac{1}{Pm^2\, E} (\boldsymbol{\nabla} \times B)^2 \right]
\end{aligned}
$$

N.B. In case of compositional convection, another equation and two additional control parameters are required.

Dimensionless Boussinesq MHD equations

In the Boussinesq limit, $Di \to 0$, then

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} + \frac{2}{E} \boldsymbol{e_z} \times \boldsymbol{u} = -\boldsymbol{\nabla} p' + \frac{Ra}{Pr} g(r)\, T' \boldsymbol{e_r} + \frac{1}{E\ Pm} (\boldsymbol{\nabla} \times \boldsymbol{B}) \times \boldsymbol{B} + \boldsymbol{\Delta} \boldsymbol{u}$$

$$\frac{\partial \boldsymbol{B}}{\partial t} = \boldsymbol{\nabla} \times (\boldsymbol{u} \times \boldsymbol{B}) + \frac{1}{Pm} \boldsymbol{\Delta} \boldsymbol{B}$$

$$\frac{\partial T'}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} T' = \frac{1}{Pr} \boldsymbol{\Delta} T'$$

From physical properties to dimensionless numbers

Ekman number: $E = \dfrac{\nu}{\Omega\, d^2}$

Rayleigh number: $Ra = \dfrac{\alpha T_o g_o d^3 \Delta s}{c_p \nu \kappa}$

Prandtl number: $Pr = \dfrac{\nu}{\kappa}$

Magnetic Prandtl number: $Pm = \dfrac{\nu}{\lambda}$

Dissipation number: $Di = \dfrac{\alpha T_o g_o}{c_p}$

Radius ratio: $\eta = \dfrac{r_i}{r_o}$

N.B. when $Di \rightarrow 0$, the Boussinesq limit is recovered.

The (astro/geo)physical regime

Parameter	Earth's core	Giant planets	Sun
E	10^{-15}	10^{-18}	10^{-15}
Ra	10^{27}	10^{30}	10^{24}
Pr	0.1	0.1	10^{-6}
Pm	10^{-6}	10^{-7}	10^{-3}
Λ (Lorentz/Coriolis)	1	1	?
Ro_ℓ (Inertia/Coriolis)	10^{-2}	10^{-3}	1
Rm (adv./diff.)	1000	10^{5}	10^{9}
Re (adv./diff.)	10^{9}	10^{12}	10^{12}

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Re (adv./diff.)	10^{9}	10^{12}	10^{12}

What does it actually implies? Is it possible to reach these parameters with my numerical dynamo model?

Reynolds number: the range of length-scale

$$Re = \frac{u_{rms}\, d}{\nu} = \frac{d}{\ell_d} \quad \text{where} \quad \ell_d = \frac{\nu}{u_{rms}}$$

$$\ell_d = \frac{d}{Re}$$

Reynolds number: the range of length-scale

$$Re = \frac{u_{rms}\, d}{\nu} = \frac{d}{\ell_d} \quad \text{where} \quad \ell_d = \frac{\nu}{u_{rms}}$$

$$\ell_d = \frac{d}{Re}$$

- In natural objects, $l_d \sim 10^{-9}\, d$
- In other words, the ratio of the bigger length-scale to the smallest one is 10^9.
- **You might need 10^9 grid points in each direction**. This implies $Re_{mesh} = 1$.

Ekman number: the range of time-scales

$$E = \frac{\nu}{\Omega\, d^2} = \frac{P_{rot}}{\tau_\nu} \quad \text{where} \quad \tau_\nu = \frac{d^2}{\nu}$$

τ_ν is the viscous diffusion time, P_{rot} the rotation period.

$$\tau_\nu = \frac{P_{rot}}{E}$$

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τ_ν is the viscous diffusion time, P_{rot} the rotation period.

$$\tau_\nu = \frac{P_{rot}}{E}$$

- In natural objects, $\tau_\nu \sim 10^{15}\, P_{rot}$
- In other words, the ratio of the longest time-scale to the smallest one is 10^{15}!
- **You might need 10^{15} time steps to model the problem**

Summary

Parameter	Earth's core	Tractable	Hard limit (2015)
E	10^{-15}	$\geq 10^{-6}$	10^{-7}
Ra	10^{27}	$\leq 10^{12}$	10^{13}
Pr	0.1	$0.1 - 10$	1
Pm	10^{-6}	0.1	6×10^{-2}
Λ (Lorentz/Coriolis)	1	1	1
Ro_ℓ (Inertia/Coriolis)	10^{-2}	$10^{-3} - 10^{-1}$	10^{-1}
Rm (adv./diff.)	1000	1000	1000
Re (adv./diff.)	10^{9}	$100 - 1000$	7000

Two complementary approaches

- In the **“tractable” regime**: parameter studies are possible
- In the **“hard-limit” regime**, only one single run is possible

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3 Installing and running the code
- Requirements and compilation
- Executing MagIC

4 Postprocessing

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Requirements to compile MagIC

Requirements

Mandatory Fortran and C compilers

Suggested git (https://git-scm.com/) to clone the code repository

Suggested CMake (https://cmake.org) to build the code

Suggested MPI library: rather use intelMPI or MPICH for full support for hybrid MPI/OpenMP

Optional LAPACK or MKL

Optional SHTns for spherical harmonics transforms

Data visualisation and post processing

Requirements

Post-processing functions are python based. You need to install the following libraries:

Python libraries required

Mandatory `matplotlib` (https://matplotlib.org): plotting functions

Mandatory `scipy` (https://www.scipy.org): scientific libraries

Suggested `ipython` (https://ipython.org): interactive shell

Optional `basemap` (https://matplotlib.org/basemap/): additional map projections

Get the code and compile it

1. **Install requirements**:

```
$ module load gcc-6 gfortran-6 libopenmpi cmake git
$ module load python27 python-scipy  ipython  python-matplotlib
```

2. **Clone the code from** `github`

```
$ git clone https://github.com/magic-sph/magic.git
```

3. **Set-up the environment variables**

```
$ cd magic
$ source sourceme.sh # (or sourceme.csh)
```

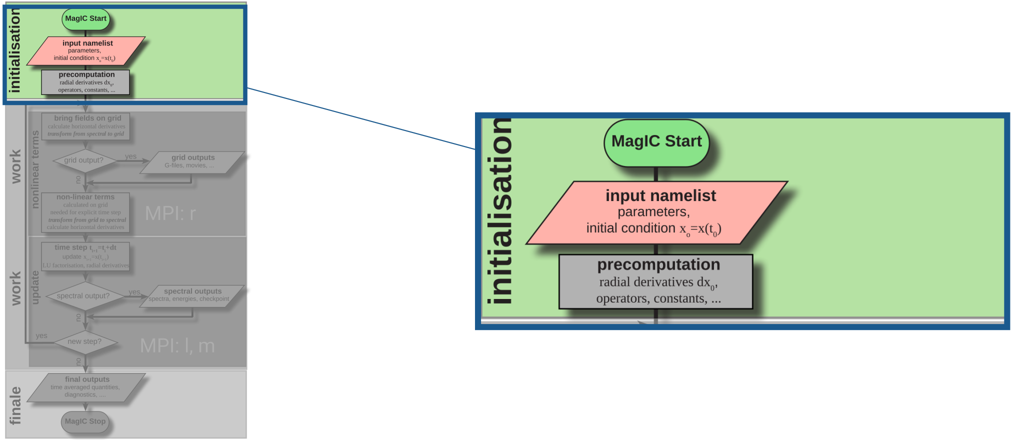
4. **Define the Fortran and C compilers**

```
$ export FC=mpif90 # replace by your compiler
$ export CC=mpicc
```

5. **Create a build directory and compile**

```
$ mkdir build; cd build
$ cmake $MAGIC_HOME -DUSE_MPI=yes -DUSE_OMP=no
$ make -j
```

MagIC structure



Run MagIC

Run with 8 CPUs:

```
$ export OMP_NUM_THREADS=1
$ mpiexec -n 8 magic.exe input.nml
```

`input.nml` contains all the input informations required to run the code!

Documentation

Input namelist (1/3)

```
&grid
 n_r_max      =33,  ! Radial resolution
 n_cheb_max   =31,  ! Number of Chebyshev polynomials
 n_phi_tot    =192, ! Azimuthal resolution
 minc         =1,   ! Azimuthal symmetry
/
&control
 mode         =0,       ! Magnetic, non-magnetic, ...
 tag          ="test",  ! Extension of the output files
 n_time_steps=40000,    ! Number of timesteps
 dtmax        =1.0D-4,  ! Maximum timestep
 runHours     =02,      ! Run-time
 runMinutes   =00,
/
```

Input namelist (2/3)

```
&phys_param
 ra          =1.1D5,  ! Rayleigh number
 ek          =1.0D-3, ! Ekman number
 pr          =1.0D0,  ! Prandtl number
 prmag       =5.0D0   ! Magnetic Prandtl number
 radratio    =0.35D0, ! Radius ratio r_i/r_o
 ktops       =1,      ! BC: fixed-temperature at the top
 ktopv       =2,      ! BC: rigid wall at the top
/
&start_field
 l_start_file=.false.,                ! Start from a check point?
 start_file  ="checkpoint_end.start", ! Name of the check point
 init_b1     =3,                      ! Init. mag. field: dipole
 amp_b1      =1,                      ! Amplitude \Lambda=1
 init_s1     =0404,                   ! Init. temperature perturbation
 amp_s1      =0.03,                   ! Amplitude of the init. pert.
/
```

Input namelist (3/3)

```
&output_control
 n_log_step  =50,    ! Output every n_log_step
 n_graphs    =3,     ! Number of graphic files
 n_rsts      =1,     ! Number of restart files
 n_stores    =0,
 n_specs     =1,     ! Number of spectra
/
&mantle
 nRotMa      =0
/
&inner_core
 sigma_ratio =1.d0,   ! Conducting inner-core
 nRotIC      =1,      ! Rotating inner core
/
```

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log.TAG file

`log.TAG` **provides all the important information about the run**:

- All parameters and other inputs including default values
- Information on parallelization, run time etc
- Log of important events: important output files, changing time step, ...
- Some important time averaged quantities, measures ...

Documentation

Plotting time series

`e_kin.TAG` **is always produced. It contains the time evolution of kinetic energy. To plot it:**

- Open ipython and load the python modules

```
ipython --matplotlib=gtk (or ipython --pylab)
>>> from magic import *
>>> ts = MagicTs(field='e_kin') # Read e_kin.TAG file in $PWD
>>> pdoc MagicTs # Gives you the documentation
```

- Plot the time evolution of magnetic energy

```
>>> ts = MagicTs(field='e_mag_oc') # Read e_mag_oc.TAG file in $PWD
```

- Manipulate the data

```
>>> print(ts.time, ts.emagoc_pol)
```

▸ Documentation

Loading and plotting snapshots

`G_#.TAG` **files contain 3-D arrays on the grid**:

- Load the `G_1.TAG` file:

```
>>> from magic import *
>>> s = Surf(ivar=1)
```

- Plot the radial velocity u_r in the equatorial plane:

```
>>> s.equat(field='vr')
```

- Plot the ϕ-averaged azimuthal flow u_ϕ:

```
>>> s.avg(field='vp', cm='seismic', levels=33)
```

- Plot the radial cut of B_r at $r = 0.75\, r_o$:

```
>>> s.surf(field='Br', r=0.75) # Hammer projection
```

▸ Documentation

Data visualisation and post processing

Additional outputs

- Plot spectra kin_spec_1.TAG

```
>>> # Plot kin_spec_1.TAG
>>> sp = MagicSpectrum(field='kin', ispec=1)
```

Documentation

- Plot the time-averaged radial profile of magnetic energy eMagR.TAG

```
>>> # Plot eMagR.TAG
>>> r = MagicRadial(field='eMagR')
```

Documentation

- And more...

```
>>> # Movie files (time evolution of 2D slices)
>>> m = Movie()
```

Documentation

Data visualisation and post processing

3-D visualisation with paraview

Requirements

Install a vtk-friendly software: here `paraview` but `VisIt` or `mayavi` should also work fine.

1. Read the graphic file you want to convert

```
>>> from magic import MagicGraph
>>> gr = MagicGraph(ivar=1) # Load G_1.TAG
```

2. Convert it to a file format readable by `paraview`

```
>>> # Produce output.vts
>>> Graph2Vtk(gr, filename='output')
```

3. Load `output.vts` with `paraview`

```
$ paraview output.vts
```

Documentation