The Spherical MHD Code MagIC, Fundamentals

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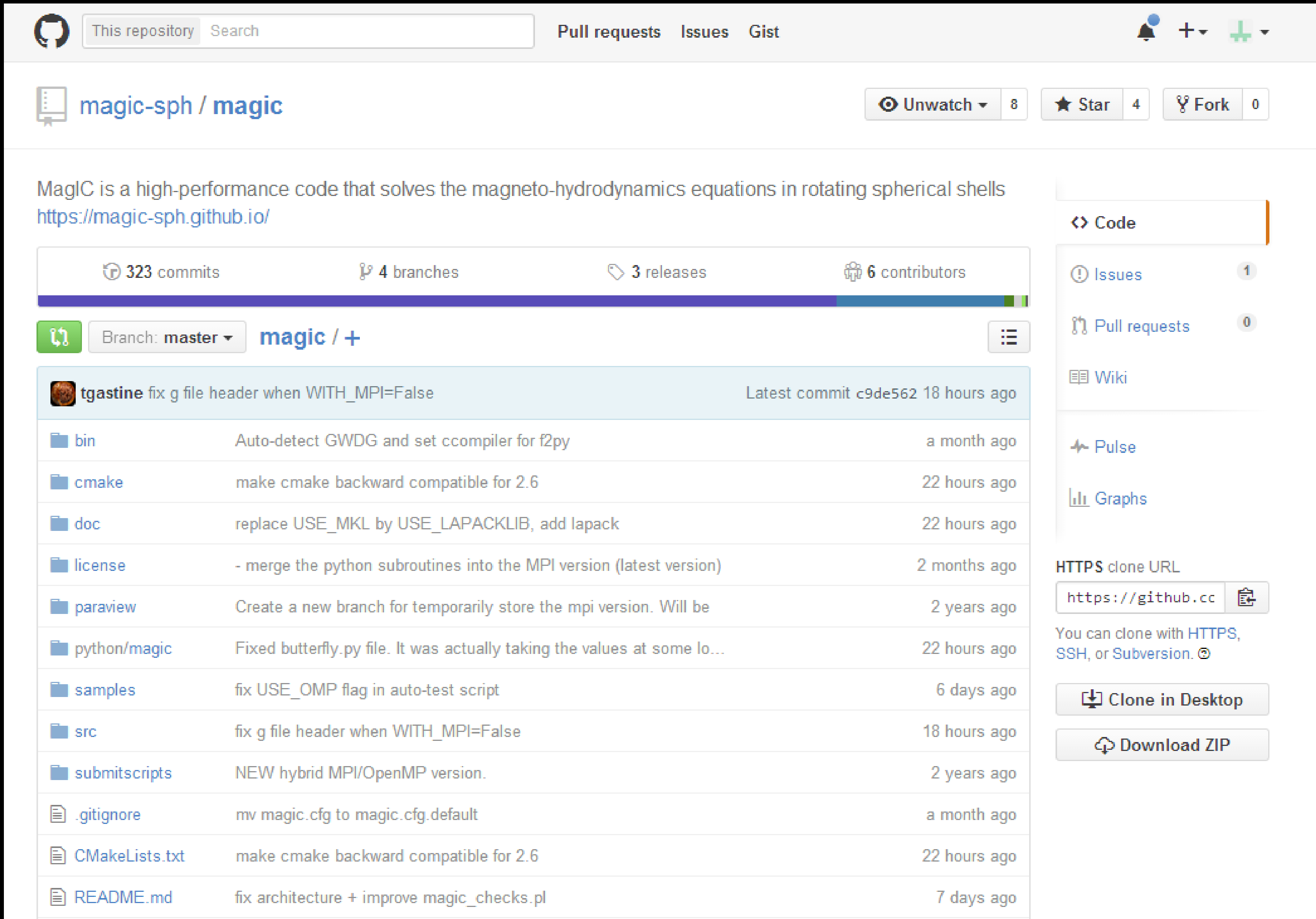
MagIC in Words

- MagIC solves for thermodynamic evolution, fluid flow and magnet field generation
- Domain = spherical shell
- Region below and above domain treated as boundary conditions or parametrized
- Frame of reference rotating with system rotation Ω
- MagIC uses a dimensionless formulation
- Poloidal/toroidal decomposition in employed
- MagIC is a pseudo spectral code
- MagIC uses a mixed impicite, explicite time stepping

MagIC github



MagIC homepage

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Welcome

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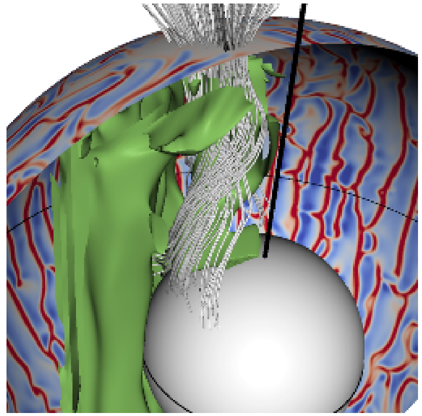
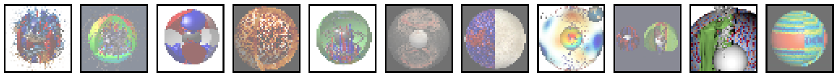
Yadav, R. et al., A&A, 2015





MagIC is a numerical code that can simulate fluid dynamics in a spherical shell. MagIC solves for the Navier-Stokes equation including Coriolis force, optionally coupled with an induction equation for Magneto-Hydro Dynamics (MHD) and a temperature (or entropy) equation under both the anelastic and the Boussinesq approximations.

MagIC uses Chebyshev polynomials in the radial direction and spherical harmonic decomposition in the azimuthal and latitudinal directions. The time-stepping scheme relies on a semi-implicit Crank-Nicolson for the linear terms of the MHD equations and a Adams-Bashforth scheme for the non-linear terms and the Coriolis force.

MagIC is written in Fortran and designed to be used on supercomputing clusters. It thus relies on a hybrid

Spectral and Grid Representation

MagIC

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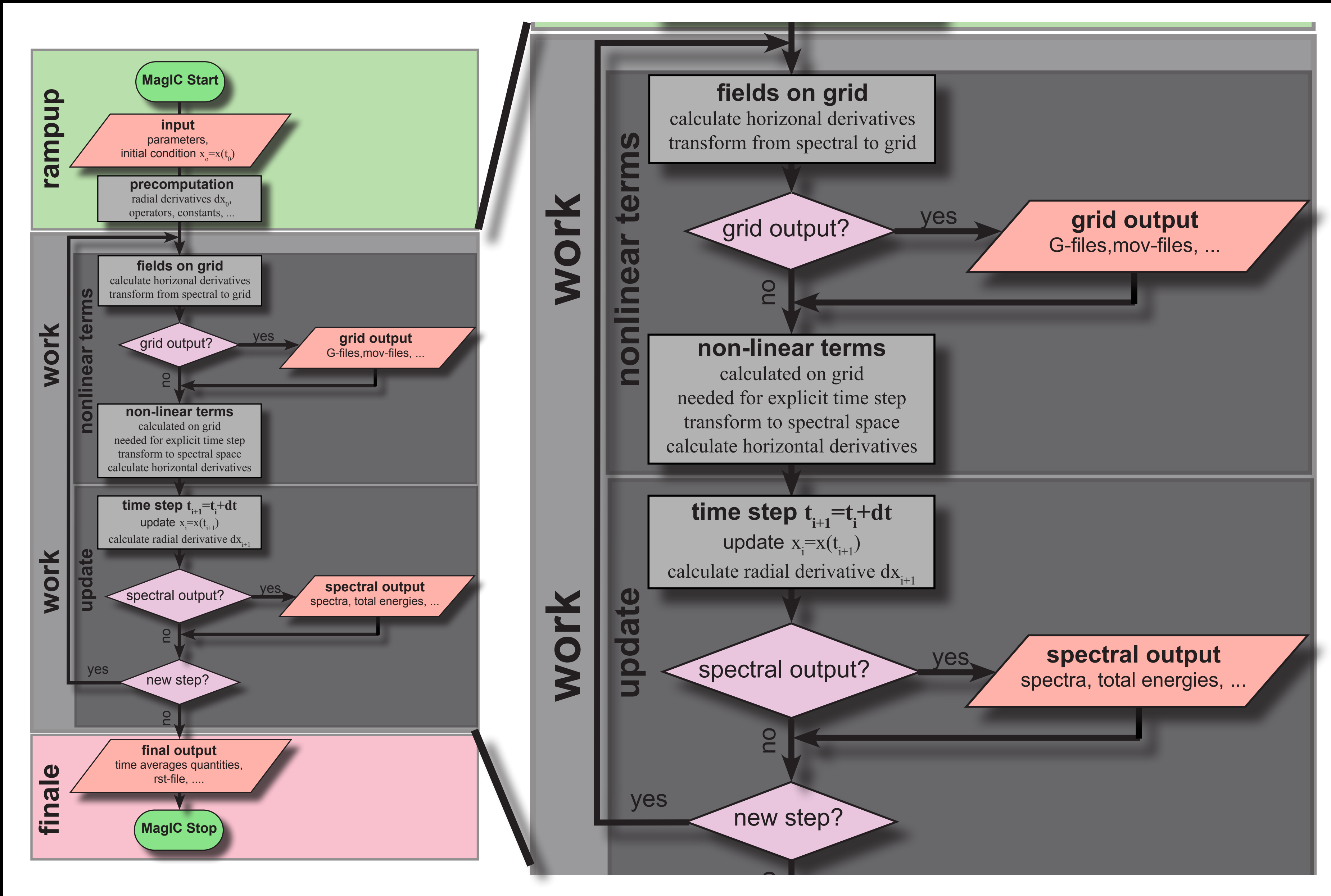
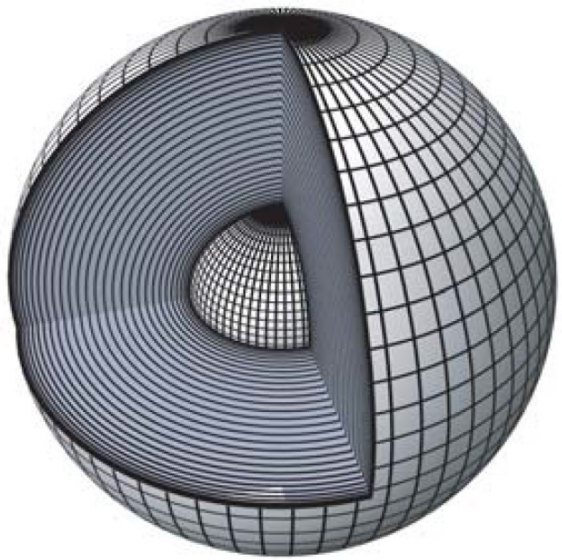
MagIC Structure



Numerical Grid

- Non-linear terms calculated on local grid



- Gauss-Legendre grid points in latitude
- evenly spaced grid points in logitude for FFT
- special grid points in radius for FFT

$$C_{nk} = C_n(x_k) = \cos\left(\pi \frac{n(k-1)}{N_r - 1}\right)$$

Horizontal Representation

- Spherical surface harmonics in longitude and latitude:

$$Y_\ell^m(\theta,\phi) = P_\ell^m(\cos\theta)\, e^{im\phi}$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, Y_\ell^m(\theta,\phi)\, Y_{\ell'}^{m'}(\theta,\phi) \;=\; \delta_{\ell\ell'}\delta^{mm'}$$

- Grid representation:

$$g(r,\theta,\phi) = \sum_{\ell=0}^{\ell_{max}} \sum_{m=-\ell}^{\ell} g_{\ell m}(r)\, Y_\ell^m(\theta,\phi)$$

With degree and order up to ℓ_{max}

- Spectral representation:

$$g_{\ell m}(r) = \frac{1}{\pi} \int_0^{\pi} d\theta \sin\theta \; g_m(r,\theta)\; P_\ell^m(\cos\theta)$$

$$g_m(r,\theta) = \frac{1}{2\pi} \int_0^{2\pi} d\phi\; g(r,\theta,\phi)\; e^{-im\phi}.$$

Horizontal Transforms

1) FFT for $\phi \rightarrow m$ and $m \rightarrow \phi$.
with $N_\phi = 2N_\theta$ azimuthal grid points

2) Gauss-Legendre integration for $\theta \rightarrow \ell$.

$$g_{\ell m}(r) = \frac{1}{N_\theta} \sum_{j=1}^{N_\theta} w_j \, g_m(r,\theta_j) \; P_\ell^m(\cos\theta_j)$$

with N_θ azimuthal grid points

Clever vector multiplication $\ell \rightarrow \theta$.
Recently both azimuthal transforms changed to SHTns.

3) Full dealiasing with $\ell_{max} = [\min(2N_\theta, N_\phi) - 1]/3$

Horizontal Derivatives, two Examples

1) Horizontal Laplacian:

$$\Delta_H Y_\ell^m = -\frac{\ell(\ell+1)}{r^2}\, Y_\ell^m$$

2) Latitudinal derivative:

$$\vartheta_2 = \sin\theta \frac{\partial}{\partial\theta}$$

$$\vartheta_2 P_\ell^m(\cos\theta) = \ell\, c_{\ell+1}^m\, P_{\ell+1}^m(\cos\theta) - (\ell+1)\, c_\ell^m\, P_{\ell-1}^m(\cos\theta)$$

with

$$c_\ell^m = \sqrt{\frac{(\ell+m)(\ell-m)}{(2\ell-1)(2\ell+1)}}$$

so that

$$\int_0^\pi d\theta\, \sin\theta\, P_\ell^m \vartheta_2 \sum_{\ell'} f_{\ell'}^m P_{\ell'}^m = (\ell-1)\, c_\ell^m\, f_{\ell-1}^m - (\ell+2)\, c_{\ell+1}^m\, f_{\ell+1}^m$$

Radial Representation

1) Chebychev polynomials up to degree

$$g_{\ell m}(r) = \sum_{n=0}^{N} g_{\ell m n}\, \mathcal{C}_n(r)$$

with

$$\mathcal{C}_n(x) = \cos\left[n\ \arccos(x)\right] \qquad -1 \le x \le 1$$

2) Grid points are the N$_r$ extrema of $\mathcal{C}_{N_r-1}$:

$$x_k = \cos\left(\pi \frac{(k-1)}{N_r-1}\right) \quad , \quad k = 1, 2, \ldots, N_r$$

so that

$$\mathcal{C}_{nk} = \mathcal{C}_n(x_k) = \cos\left(\pi \frac{n(k-1)}{N_r-1}\right)$$

3) Thus fast cosine transforms can be

4) Dealiasing for $N_r > N$.

Spectral Poloidal Dynamo Equation

1) Take radial component of the dynamo equation

$$\boldsymbol{e_r}\cdot\left(\frac{\partial \boldsymbol{B}}{\partial t}\right) = \frac{\partial}{\partial t}(\boldsymbol{e_r}\cdot\boldsymbol{B}) = -\Delta_H \frac{\partial g}{\partial t}$$

2) Plug in horizontal spectral representation of g . Multiply with spherical hamonic, integrate over spherical surface and use orthogonal relations:

radial diffusion

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

$$= \mathcal{N}^g_{\ell m} = \int d\Omega\, Y_\ell^{m\star}\mathcal{N}^g = \int d\Omega\, Y_\ell^{m\star}\,\boldsymbol{e_r}\cdot\boldsymbol{D}$$

nonlinear dynamo term

Solving the Nonlinear Term

1) Calculate horizontal components of EMF $\mathcal{F} = \boldsymbol{u} \times \boldsymbol{B}$ on grid:

$$\mathcal{F}_\theta = u_\phi B_r - u_r B_\phi, \quad \mathcal{F}_\phi = u_r B_\theta - u_\theta B_r$$

so that

$$\mathcal{N}^g = \boldsymbol{e_r} \cdot [\boldsymbol{\nabla} \times (\boldsymbol{u} \times \boldsymbol{B})] = \frac{1}{r \sin\theta} \left[\frac{\partial (\sin\theta \mathcal{F}_\phi)}{\partial \theta} - \frac{\partial \mathcal{F}_\theta}{\partial \phi} \right]$$

2) Transform these to spectral space: ${\mathcal{F}_\theta}_\ell^m \quad {\mathcal{F}_\phi}_\ell^m$

3) Calculate curl in spectral space using recurrence relations:

$$\mathcal{N}^g_{\ell m} = (\ell+1)\, c_\ell^m\, {\mathcal{F}_\phi}_{\ell-1}^m - \ell\, c_{\ell+1}^m\, {\mathcal{F}_\phi}_{\ell+1}^m - im\, {\mathcal{F}_\theta}_\ell^m$$

How does that look like in the code?

Calculating Nonlinear terms

0) Master: `rIterThetaBlocking_seq.f90`

1) `transform_to_grid_space` in `rIterThetaBlocking.f90`

2) Legendre transform: `legTFG` in `legendre_spec_to_grid.f90`

```
do mc=1,n_m_max
   dm =D_mc2m(mc)
   lmS=lStop(mc)
   vrES    =zero
   vrEA    =zero
   dvrdtES=zero
   dvrdtEA=zero
   cbrES   =zero
   cbrEA   =zero
   !--- 8 add/mult, 29 dble words
   do lm=lStart(mc),lmS-1,2
      vrES    =vrES    + leg_helper%dLhw(lm)*   Plm(lm,nThetaNHS)
      dvrdtEA =dvrdtEA + leg_helper%dLhw(lm)*  dPlm(lm,nThetaNHS)
```

3) FFT (internal or MKL) called in `rIterThetaBlocking.f90`

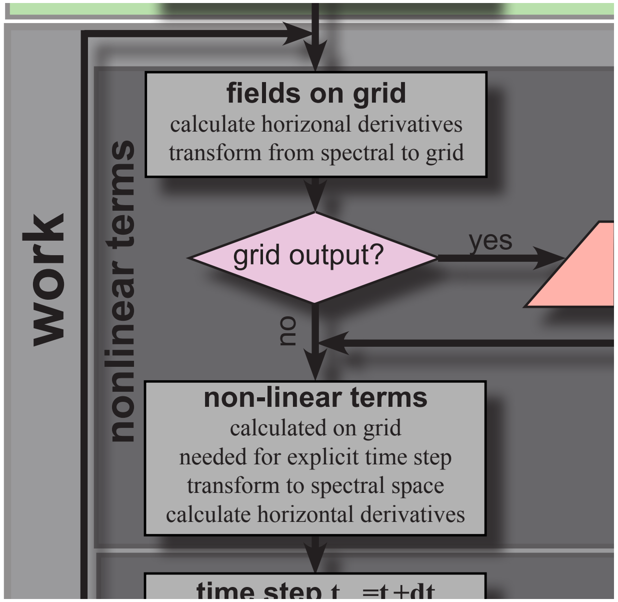
```
if ( this%nBc == 0 ) then
   call fft_thetab(gsa%vrc,1)
   call fft_thetab(gsa%vtc,1)
```

Calculating Nonlinear terms

4) Calculate nonlinear terms on grid:

`get_nl.f90`

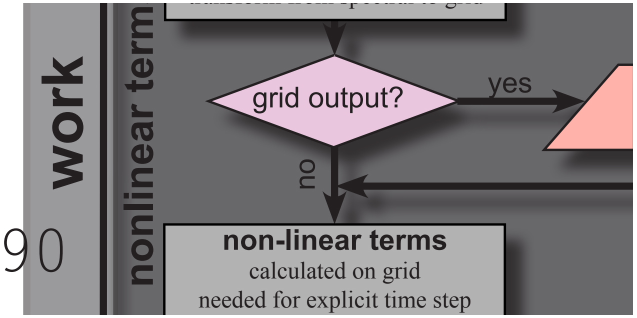
$$\mathcal{F}_\theta = u_\phi B_r - u_r B_\phi, \quad \mathcal{F}_\phi = u_r B_\theta - u_\theta B_r$$




```
nTheta=nThetaLast
do nThetaB=1,sizeThetaB
   nTheta    =nTheta+1
   nThetaNHS=(nTheta+1)/2
   or4sn2=or4(nR)*osn2(nThetaNHS)

  do nPhi=1,n_phi_max
     this%VxBt(nPhi,nThetaB)=  orho1(nR)*or4sn2 * (          &
           this%vpc(nPhi,nThetaB)*this%brc(nPhi,nThetaB) - &
           this%vrc(nPhi,nThetaB)*this%bpc(nPhi,nThetaB)  )
  end do
```

Back Transform to Spectral Space

5) `transfrom_to_lm_space` in `rIterThetaBlocking.f90`



6) Gauss-Legendre back transform: `legTFG` in `legendre_spec_to_grid.f90`

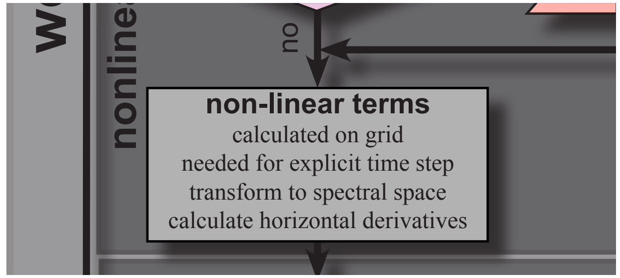
```
do nThetaB1=nThetaMin,sizeThetaB/2,2
   nThetaB2=nThetaB1+1
   nTheta1 =nTheta1+2
   nTheta2 =nTheta1+1

   do mc=1,n_m_max
      lmS=lStopP(mc)
      f1ES1=f1ES(mc,nThetaB1)
      f1ES2=f1ES(mc,nThetaB2)
      f1EA1=f1EA(mc,nThetaB1)
      f1EA2=f1EA(mc,nThetaB2)
      do lm=lStartP(mc),lmS-1,2
         f1LM(lm)   =f1LM(lm)   +f1ES1*wPlm(lm,nTheta1)+f1ES2*wPlm(lm,nTheta2)
         f1LM(lm+1)=f1LM(lm+1)+f1EA1*wPlm(lm+1,nTheta1)+f1EA2*wPlm(lm+1,nTheta2)
      end do
```

7) FFT back transform (internal or MKL) called in `rIterThetaBlocking.f90`

```
call fft_thetab(gsa%VxBt,-1)
call fft_thetab(gsa%VxBp,-1)
```

Finish off Induction Term in Spetral Space

8) Calculate extra derivatives in `get_td.F90` called by `rIterThetaBlocking.f90`



$$\mathcal{N}^{g}_{\ell m} = (\ell+1)\, c^{m}_{\ell}\, \mathcal{F}_{\phi}{}^{m}_{\ell-1} - \ell\, c^{m}_{\ell+1}\, \mathcal{F}_{\phi}{}^{m}_{\ell+1} - im\, \mathcal{F}_{\theta}{}^{m}_{\ell}$$

```
do lm=1,lm max
    if ( l > m ) then
       dbdt(lm)=  dTheta1S(lm)*this%VxBpLM(lmPS) &
            &    -dTheta1A(lm)*this%VxBpLM(lmPA) &
            &    -dPhi(lm)    *this%VxBtLM(lmP)
    else if ( l == m ) then
       dbdt(lm)= -dTheta1A(lm)*this%VxBpLM(lmPA) &
            &    -dPhi(lm)    *this%VxBtLM(lmP)
    end if
```

9) Output is called `dbdt(k,lm)` where `k` numbers the radial grid points and `lm` the spherical harmonic modes.

Everything in Spherical Harmonic Space!

Equations for each radial grid point and spherical harmonic mode!
No spatial derivatives left!

$$\frac{\ell(\ell+1)}{r^2}\left[\left(\frac{\partial}{\partial t}+\frac{1}{Pm}\lambda\,\frac{\ell(\ell+1)}{r^2}\right)\mathcal{C}_n-\frac{1}{Pm}\lambda\,\mathcal{C}_n''\right]\,g_{\ell mn}$$

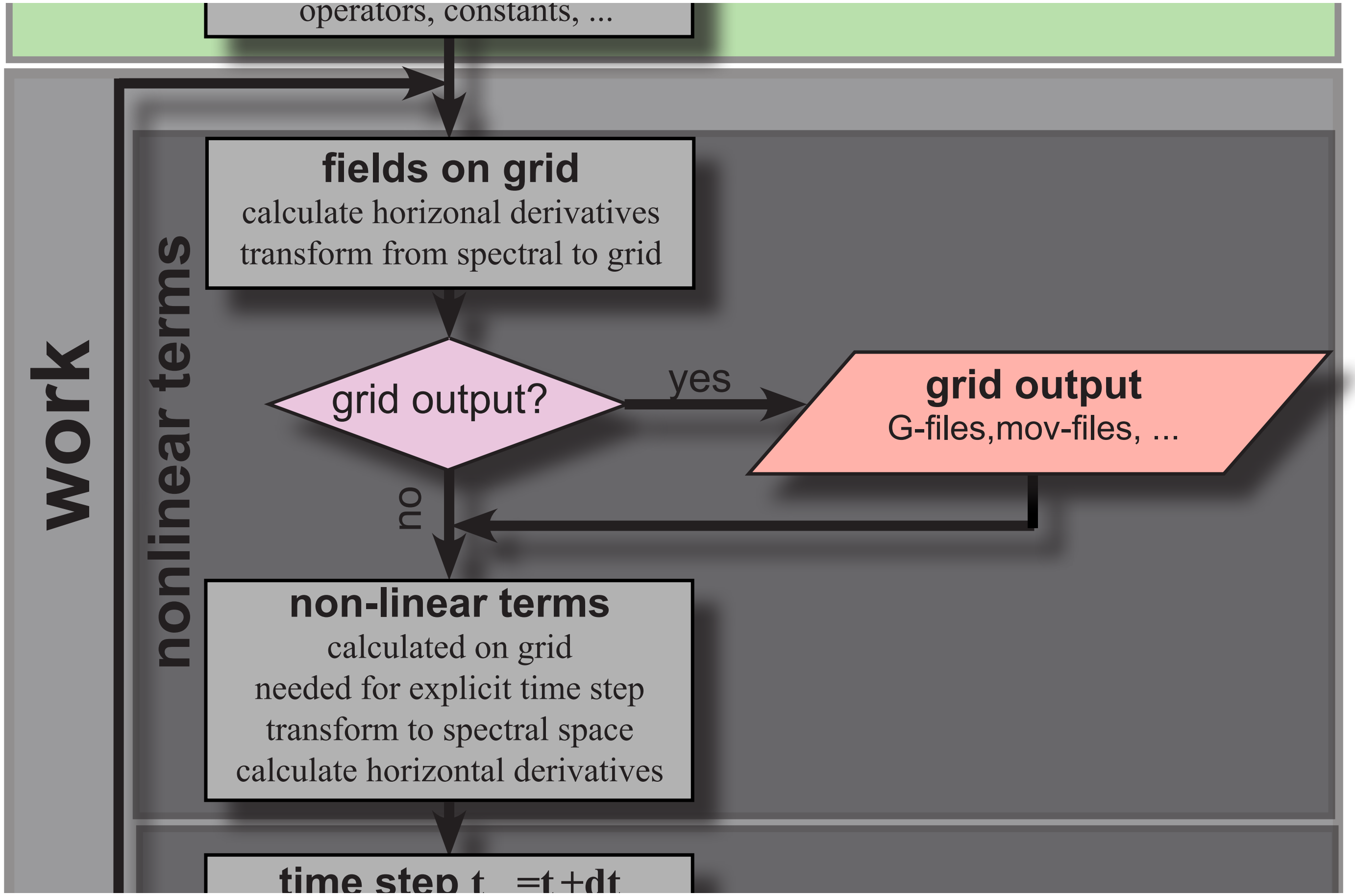
$$=\mathcal{N}^g_{\ell m}=\int d\Omega\,Y_\ell^{m\star}\,\mathcal{N}^g=\int d\Omega\,Y_\ell^{m\star}\,\boldsymbol{e_r}\cdot\boldsymbol{D}$$

nonlinear dynamo term

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

MagIC Structure

The most time consuming part of the code!



Time Stepping Scheme

Generic evolutions equation with
terms $\mathcal{I}(x,t)$ to be treated implicitely and
terms $\mathcal{E}(x,t)$ to be treated explicitely.

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

Implicite Crank-Nicolson type time step:

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

Explicite Adams-Bashforth type time step:

$$\left(\frac{x(t+\delta t) - x(t)}{\delta t} \right)_E = \frac{3}{2}\, \mathcal{E}(x,t) - \frac{1}{2}\, \mathcal{E}(x, t-\delta t)$$

Mixed time step:

$$\frac{x(t+\delta t)}{\delta t} + \alpha\, \mathcal{I}(x, t+\delta t) =$$

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

Poloidal Magnetic Potential Time Stepping

$$\left(\mathcal{A}_{kn} + \alpha\,\mathcal{I}_{kn}\right)\; g_{\ell mn}(t+\delta t) = \left(\mathcal{A}_{kn} - (1-\alpha)\,\mathcal{I}_{kn}\right)\; g_{\ell mn}(t) + \frac{3}{2}\,\mathcal{E}_{k\ell m}(t) - \frac{1}{2}\,\mathcal{E}_{k\ell m}(t-\delta t)$$

with

$$\mathcal{A}_{kn} = \frac{\ell(\ell+1)}{r_k^2}\,\frac{1}{\delta t}\mathcal{C}_{nk}$$

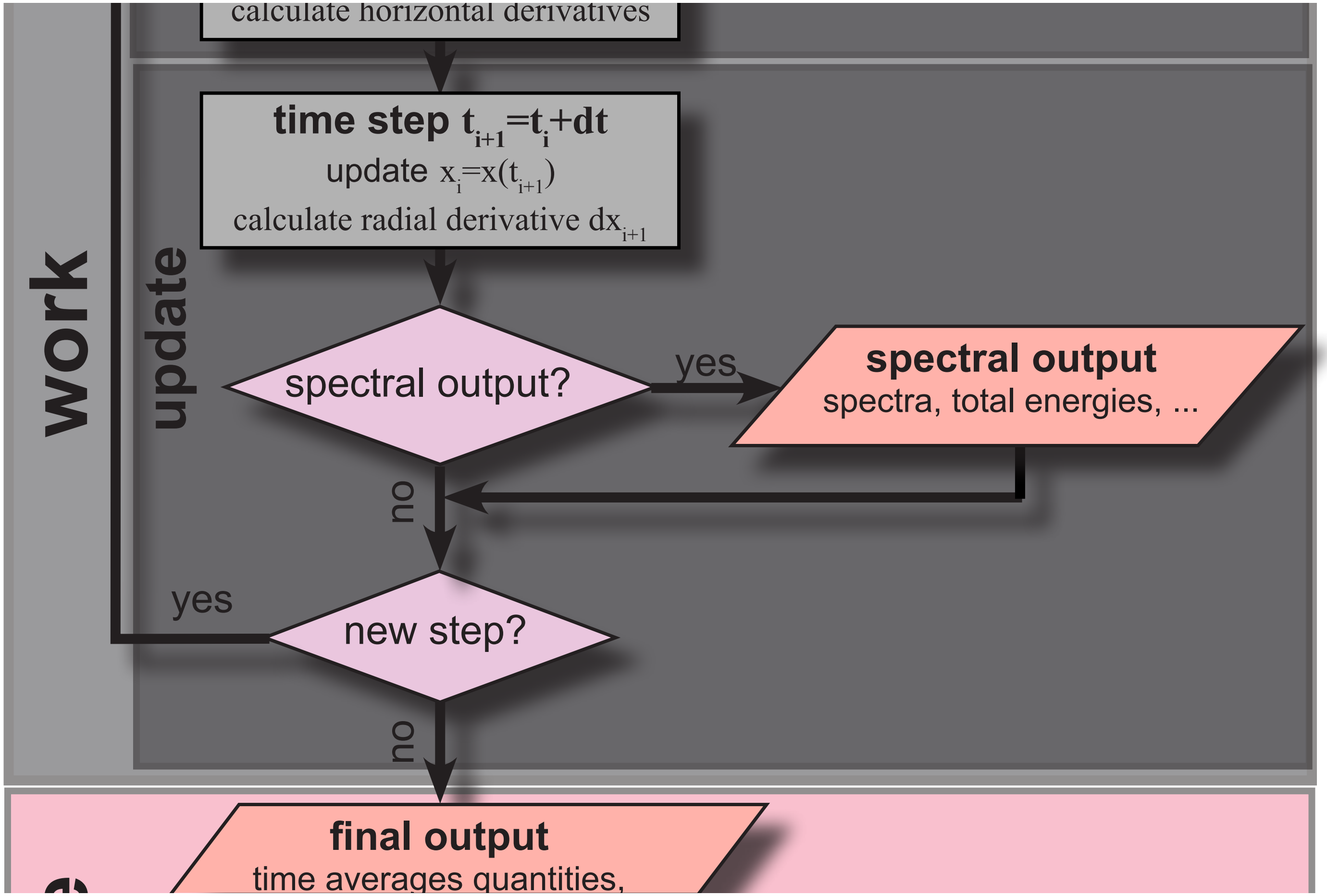
$$\mathcal{I}_{kn} = \frac{\ell(\ell+1)}{r_k^2}\,\frac{1}{Pm}\left(\frac{\ell(\ell+1)}{r_k^2}\,\mathcal{C}_{nk} - \mathcal{C}''_{nk}\right)$$

$$\mathcal{E}_{k\ell m}(t) = \mathcal{N}^g_{k\ell m} = \int d\Omega\; Y_\ell^{m\star}\; \boldsymbol{e_r}\cdot\boldsymbol{D}(t, r_k, \theta, \phi)$$

How does that look like in the code?

MagIC Structure

The most important part of the code!



Poloidal Magnetic Potential Time Stepping

We already know how the nonlinear terms is calculated

$$\texttt{dbdt}(k,\ell m) = \mathcal{E}_{k\ell m}$$

The time stepping matrix is

$$\texttt{bmat}(k,n,\ell) = A_{kn} + \alpha \mathcal{I}_{kn}$$

Information from previous time steps:

$$\texttt{dbdtLast}(k,lm) = -\frac{1}{2}\,\mathcal{E}_{k\ell m}(t-\delta t) - (1-\alpha)\,\mathcal{I}_{kn}\,g_{\ell mn}(t)$$

Also used are the following expressions

$$\texttt{w1} = -1/2\frac{\delta t}{\delta t_{old}}\ ,\quad \texttt{w2} = 1 - \texttt{w2}$$

$$\texttt{Odt} = 1/\delta t\ ,\quad \texttt{dLh}(\ell) = \ell(\ell+1)\ ,\quad \texttt{Or2}(k) = 1/r_k^2$$

Update Routine

Putting it all together:

$$\texttt{bmat}(k,n,\ell)\star \texttt{b}_{i+1}(n,\ell m) = \texttt{w1}\star\texttt{dbdt}(k,\ell m)+\texttt{w2}\star\texttt{dbdtLast}(k,\ell m)+ \texttt{Odt}\star\texttt{dLh}(\ell)\star\texttt{Or2}(k)\star\texttt{b}_i(n,\ell m) = \texttt{rhs}(k,\ell m)$$

The time stepping matrix is stored in an LU-decomposed form.

All done in module `updateB.f90`:

1) Defining the rhs:

```
do nR=2,n_r_max-1
   if ( nR<=n_r_LCR ) then
      rhs1(nR,lmB,threadid)=0.0_cp
      rhs2(nR,lmB,threadid)=0.0_cp
   else
      rhs1(nR,lmB,threadid)= ( w1*dbdt(lm1,nR)+w2*dbdtLast(lm1,nR) )
        &         + O_dt*dLh(st_map%lm2(l1,m1))*or2(nR)*b(lm1,nR)
      rhs2(nR,lmB,threadid)= ( w1*djdt(lm1,nR)+w2*djdtLast(lm1,nR) )
        &         + O_dt*dLh(st_map%lm2(l1,m1))*or2(nR)*aj(lm1,nR)
   end if
end do
```

Update Routine

2) Solving the linear equation system:

```
call cgeslML(bMat(:,:,l1),n_r_tot,n_r_real, &
     bPivot(:,l1),rhs1(:,lmB0+1:lmB,threadid),2*n r max,lmB-lmB0)
```

3) Result is in Cheb-space!

4) Calculate and store radial derivatives in Cheb-space:

```
call get_ddr(b,db,ddb,ulmMag-llmMag+1,start_lm-llmMag+1, &
     &       stop_lm-llmMag+1,n_r_max,n_cheb_max,        &
     &       dbdtLast,djdtLast,chebt_oc,drx,ddrx)
```

5) Calculate and store $\texttt{dbdtLast}(k, \ell m)$ for next time step:

```
do nR=n_r_cmb,n_r_icb-1
   do lm1=lmStart_00,lmStop
      l1=lm2l(lm1)
      m1=lm2m(lm1)
      dbdtLast(lm1,nR)= dbdt(lm1,nR) -                        &
           coex*opm*lambda(nR)*hdif_B(st_map%lm2(l1,m1))*  &
                      dLh(st_map%lm2(l1,m1))*or2(nR)  *  &
           ( ddb(lm1,nR) - dLh(st_map%lm2(l1,m1))*or2(nR)*b(lm1,nR) )
```

Mode Methods

- Adaptive time step according to modified Courant-Friedrich-Levy criterium.
- Coriolis force treated explicitely.
- Transform on cylindrical grid for output possible.