Pencil-code in Spherical Polar Coordinates

Axel Brandenburg, Dhrubaditya Mitra, David Moss and Reza Tavakol



- Differential operators in non-cartesian coordinates
- Boundary conditions
- Averaged quantities
- Performance
- Preliminary results

Differential operators in non-cartesian coordinates

• Gradient of a scalar:

$$\nabla f(r,\theta,\phi) = e_r \frac{\partial}{\partial r} f + e_\theta \frac{1}{r} \frac{\partial}{\partial \theta} f + e_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} f$$

$$\nabla \boldsymbol{f} = \boldsymbol{e}_r \partial_{\hat{r}} \boldsymbol{f} + \boldsymbol{e}_{\theta} \partial_{\hat{\theta}} \boldsymbol{f} + \boldsymbol{e}_{\phi} \partial_{\hat{\phi}} \boldsymbol{f}$$

Divergence in non-cartesian coordinate

- Vectors need to parallel transported to take derivatives. Hence derivatives are to be replaced by covariant derivatives:
- In Cartesian: $\vec{divA} = \partial_{\alpha} A_{\alpha} = A_{\alpha}$
- Include scaling factors :

$$\mathbf{A}_{\hat{\alpha},\hat{\theta}} = \frac{1}{r} \partial_{\theta} \mathbf{A}_{\hat{\alpha}}$$

Co-variant derivative of a vector

$$\boldsymbol{A}_{\hat{\alpha}\,;\hat{\beta}} = \boldsymbol{A}_{\hat{\alpha}\,,\hat{\beta}} - \boldsymbol{\Gamma}_{\hat{\alpha}\,\hat{\beta}}^{\hat{\gamma}} \,\boldsymbol{A}_{\hat{\gamma}}$$

• Contract indices:

$$A_{\hat{\alpha};\hat{\alpha}} = A_{\hat{\alpha},\hat{\alpha}} + \frac{2}{r}A_r + \frac{1}{r}\cot\theta A_{\theta}$$

Connection coefficients

- In "hatted" basis : metric tensor is unit tensor.
- The "usual" symmetry of connection coefficients is not true.
- In spherical polar coordinate system:

$$\Gamma_{\hat{r}\hat{\theta}}^{\hat{\theta}} = \Gamma_{\hat{\phi}\hat{r}}^{\hat{\phi}} = -\Gamma_{\hat{\theta}\hat{\theta}}^{\hat{r}} = -\Gamma_{\hat{\phi}\hat{\phi}}^{\hat{r}} = \frac{1}{r}$$

$$\Gamma_{\hat{\theta}\hat{\phi}}^{\hat{\phi}} = -\Gamma_{\hat{\phi}\hat{\phi}}^{\hat{\theta}} = \frac{\cot(\theta)}{r}$$

Other differental operators in noncartesian coordinate

$$curl\,ec{{\mathsf A}}{=}\epsilon_{{\hatlpha}\,{\hateta}\,{\hat y}}\,{\mathsf A}_{{\hat y}\,{};{\hateta}}$$

Second co-variant derivatives:

$$\boldsymbol{A}_{\alpha;\beta\gamma} = (\boldsymbol{A}_{\alpha,\beta} - \boldsymbol{\Gamma}_{\alpha\beta}^{\sigma} \boldsymbol{A}_{\sigma})_{;\gamma} = (\boldsymbol{A}_{\alpha,\beta})_{;\gamma} - (\boldsymbol{\Gamma}_{\alpha\beta}^{\sigma} \boldsymbol{A}_{\sigma})_{;\gamma}$$

WRONG !

$$\boldsymbol{A}_{\alpha;\beta\gamma} = (\boldsymbol{A}_{\alpha;\beta})_{\gamma} - \boldsymbol{\Gamma}_{\alpha\gamma}^{\sigma} \boldsymbol{A}_{\sigma;\beta} - \boldsymbol{\Gamma}_{\beta\gamma}^{\sigma} \boldsymbol{A}_{\alpha;\sigma}$$

RIGHT

Example: Laplacian

$$\nabla^2 A_{\alpha} = \partial_{\beta\beta} A_{\alpha} = A_{\alpha,\beta\beta}$$

• Spherical polar co-ordinate system:

$$\nabla^{2} A_{\hat{r}} = A_{\hat{r};\hat{\mu}\hat{\mu}} = A_{\hat{r},\hat{\mu}\hat{\mu}} + \frac{2}{r} [A_{\hat{r},\hat{r}} - A_{\hat{\theta},\hat{\theta}} - A_{\hat{\phi},\hat{\phi}}]$$
$$\frac{cot(\theta)}{r} A_{\hat{r},\hat{\theta}} - \frac{2}{r^{2}} A_{\hat{r}} - \frac{2 cot(\theta)}{r^{2}} A_{\theta}$$

Implementation in pencil-code

- Change in subroutine der_main in file deriv.f90 to include the right scaling factors: if (lspherical_coords) df=df*r1_mn
- Introduce parameters :

cdata.f90 lspherical_coords, r1_mn ..

Calculate them

register.f90 initialize_modules

Implementation (contd.)

• Add "connection-terms" in file sub.f90

subroutine div_mn(aij,b,a)

- if (lspherical_coords) then
- b=b+2.*r1_mn*a(:,1)+r1_mn*cotth(m)*a(:,2)
 endif
- Similarly for gij_etc ..
- Changed in only a few places:
- src > grep lspherical *.f90 | wc -l

Other modifications

• Boundary conditons:

$$\frac{d}{dr}(rA_{r})=0;r_{i-j}A_{i-j}=r_{i+j}A_{i+j};j=1,2,3$$

Instead of the a condition, we need slo condition with unit slope.

• Estimation of CFL time-step: equ.f90

if(lspherical_coords) then &

dxyz_2 = dx_1(l1:l2)**2+ &
 (r1_mn*dy_1(m))**2+(r1_mn*sin1th(m)*dz_1(n)
)**2

Averages

• Right volume element to be included:

```
subroutine sum mn(a,res)
if(lspherical_coords) then
  do isum=11,12
    res = res +
      x(isum) *x(isum)*sinth(m)*a(isum)
  enddo
else
  res=sum(a)
endif
```

Performance

 Same MHD code is roughly 1.5 times slower in spherical coordinate system compared to cartesian coordinate system:

no. of proc 4 8	cartesian	spherical
	1.95	2.97 (64^3)
	0.945	1.41 (64^3)
16	0.679	0.867 (64^3)
16	0.503	0.733 (256^3)
32	0.303	0.421

 I expect cylindrical coordinate system will be somewhere in the middle.

Turbulent MHD dynamo

- Perfect conductor boundary versus open vertical (radial) field boundary.
- Results are very similar to what obtained in Cartesian coordinate system earlier.
- No convection, but helical forcing.



Plot of magnetic and kinetic energy as a function of time. Left : open (radial) field bc Right: Perfect conductor bc

Plot of magnetic vector potential in meridional plane



Plot of magnetic field in meridional plane



Limitations

- Helical forcing in spherical polar coordinate system is difficult to implement (involves allocation of one system size array and calculation of spherical bessel functions and spherical harmonics) but the cartesian helical forcing seems to work perfectly well.
- We cannot work at the axis, numerical singularity, too small time step needed.