Pencil-code in Spherical Polar Coordinates

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

- Gradient of a scalar:

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

\[ \nabla f = e_r \partial_r f + e_\theta \partial_\theta f + e_\phi \partial_\phi f \]
Divergence in non-cartesian coordinate

- Vectors need to parallel transported to take derivatives. Hence derivatives are to be replaced by covariant derivatives:

- In Cartesian: \( \text{div} \vec{A} = \partial_\alpha A_\alpha = A_{\alpha,\alpha} \)

- Include scaling factors:
  \( A_{\hat{\alpha},\hat{\theta}} = \frac{1}{r} \partial_\theta A_{\hat{\alpha}} \)

- Co-variant derivative of a vector
  \( A_{\hat{\alpha};\hat{\beta}} = A_{\hat{\alpha},\hat{\beta}} - \Gamma_{\hat{\alpha}\hat{\beta}}^{\hat{\gamma}} A_{\hat{\gamma}} \)

- 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 differential operators in non-cartesian coordinate

- \( \text{curl} \ \vec{\mathbf{A}} = \epsilon_{\hat{\alpha} \hat{\beta} \hat{\gamma}} A_{\hat{\gamma} ; \hat{\beta}} \)

- Second co-variant derivatives:

\[
A_{\alpha ; \beta \gamma} = (A_{\alpha , \beta} - \Gamma^\sigma_{\alpha \beta} A_\sigma) ; \gamma = (A_{\alpha , \beta}) ; \gamma - (\Gamma^\sigma_{\alpha \beta} A_\sigma) ; \gamma
\]

WRONG!

\[
A_{\alpha ; \beta \gamma} = (A_{\alpha ; \beta}) ; \gamma - \Gamma^\sigma_{\alpha \gamma} A_{\sigma ; \beta} - \Gamma^\sigma_{\beta \gamma} A_{\alpha ; \sigma}
\]

RIGHT
Example: Laplacian

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

- Spherical polar co-ordinate system:

\[ \nabla^2 \hat{A}_r = \hat{A}_{r, \hat{\mu} \hat{\mu}} = \hat{A}_{r, \hat{\mu} \hat{\mu}} + \frac{2}{r} \left[ \hat{A}_{r, r} - \hat{A}_{\hat{\theta}, \hat{\theta}} - \hat{A}_{\hat{\phi}, \hat{\phi}} \right] \]

\[ \frac{\cot(\theta)}{r} \hat{A}_{r, \hat{\theta}} - \frac{2}{r^2} \hat{A}_r - \frac{2 \cot(\theta)}{r^2} A_\theta \]
Implementation in pencil-code

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

- Introduce parameters:
  
  ```fortran
  cdata.f90 lspherical_coords, r1_mn ..
  ```

- Calculate them
  
  ```fortran
  register.f90 initialize_modules
  ```
Implementation (contd.)

- Add “connection-terms” in file sub.f90

```fortran
subroutine div_mn(aij,b,a)
    if (lspherical_coords) then
        b=b+2.*r1_mn*a(:,1)+r1_mn*cotth(m)*a(:,2)
    endif
endif
```

- Similarly for gi_j etc ..

- Changed in only a few places:

```
src > grep lspherical *.f90 | wc -l
81
```
Other modifications

- Boundary conditions:
  \[ \frac{d}{dr}(rA_r) = 0; r_{i-j}A_{i-j} = r_{i+j}A_{i+j}; j = 1,2,3 \]

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(l1:12)**2 &
  (r1_mn*dy_1(m))**2 + (r1_mn*sinlth(m)*dz_1(n))**2
```

Averages

- Right volume element to be included:

```fortran
subroutine sum_mn(a,res)
if(lspherical_coords) then
  do isum=l1,l2
    res = res +
    x(isum) *x(isum)*sintth(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:

<table>
<thead>
<tr>
<th>no. of proc</th>
<th>cartesian</th>
<th>spherical</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>1.95</td>
<td>2.97 (64^3)</td>
</tr>
<tr>
<td>8</td>
<td>0.945</td>
<td>1.41 (64^3)</td>
</tr>
<tr>
<td>16</td>
<td>0.679</td>
<td>0.867 (64^3)</td>
</tr>
<tr>
<td>16</td>
<td>0.503</td>
<td>0.733 (256^3)</td>
</tr>
<tr>
<td>32</td>
<td>0.303</td>
<td>0.421</td>
</tr>
</tbody>
</table>

- 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.