Numerical solution of Laplace's equation in spherical finite volumes

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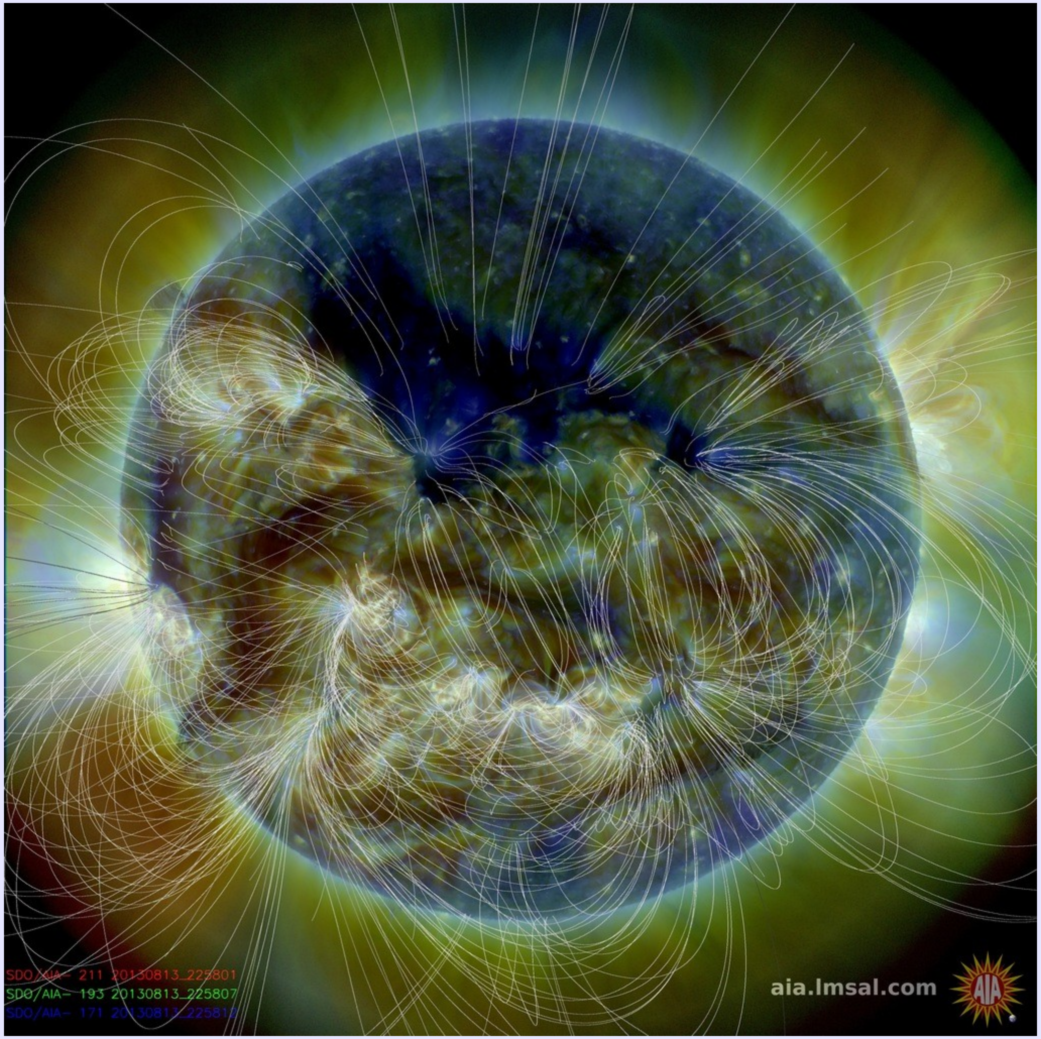
Outline

- Introduction – Magnetic helicity
- Solution method description + validation
- Concluding remarks

Introduction



Solar studies

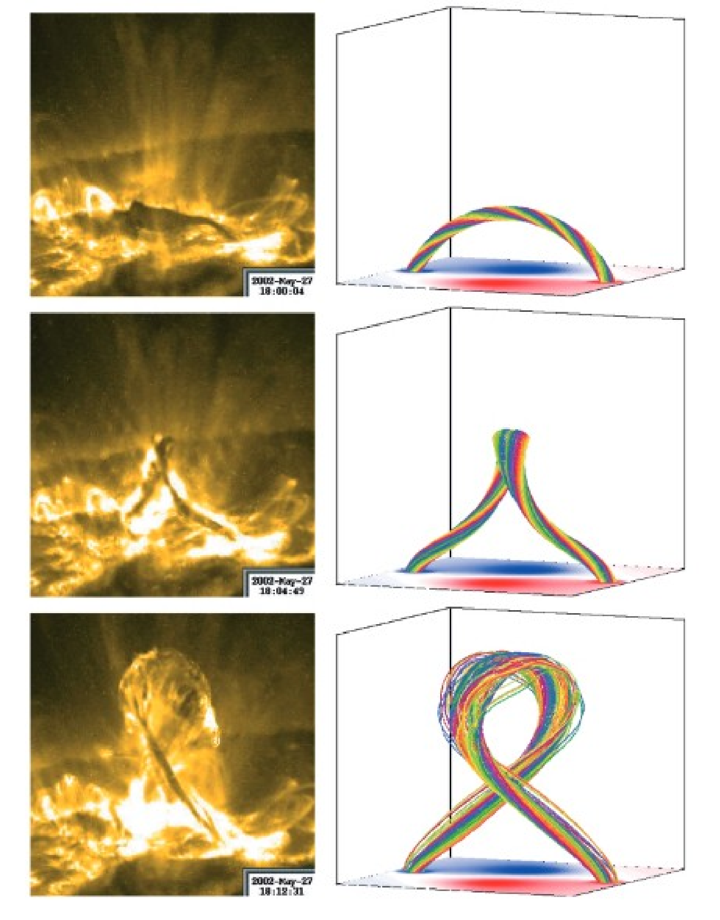
- Eruptive phenomena (solar flares, coronal mass ejections)
- Fundamental role of the magnetic field
- Spherical geometry

Magnetic helicity

- Signed scalar quantity (right (+), or left (-) handed)
- Helicity measures the twist and writhe of mfls, and the amount of flux linkages between pairs of lines (Gauss linking number)

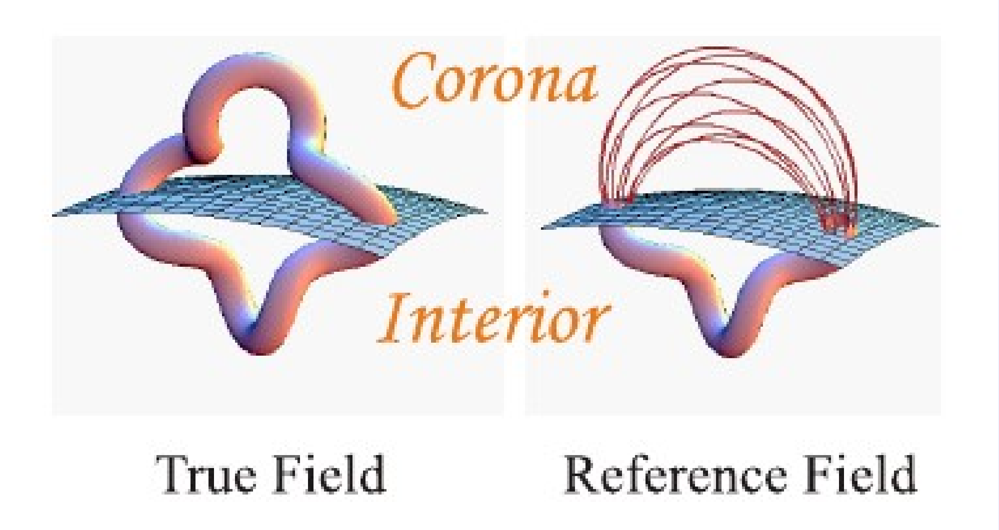
$$H = \int_V \boldsymbol{A} \cdot \boldsymbol{B} \, dV \qquad \boldsymbol{B} = \nabla \times \boldsymbol{A}$$

- Conserved in the standard paradigm of solar study (ideal magnetohydrodynamics, MHD)
- Coronal mass ejections are caused by the need to expel the excess helicity accumulated in the corona (Rust 1994)



Török & Kliem 2005

Relative magnetic helicity



Berger & Field 1984, Finn & Antonsen 1985

relative magnetic helicity

$$H = \int_V (\boldsymbol{A} + \boldsymbol{A}_p) \cdot (\boldsymbol{B} - \boldsymbol{B}_p)\, dV$$

gauge invariant for closed
(and solenoidal) $\boldsymbol{B} - \boldsymbol{B}_p$

$$\hat{n} \cdot \boldsymbol{B}|_{\partial V} = \hat{n} \cdot \boldsymbol{B}_p|_{\partial V}$$

∂V: the whole boundary

Finite volume computation

$$H = \int_V (\boldsymbol{A} + \boldsymbol{A}_p) \cdot (\boldsymbol{B} - \boldsymbol{B}_p)\, dV$$

1. given $\boldsymbol{B}$ find $\boldsymbol{B}_p$
2. given $\boldsymbol{B}$, $\boldsymbol{B}_p$ find $\boldsymbol{A}$, $\boldsymbol{A}_p$

Potential field calculation

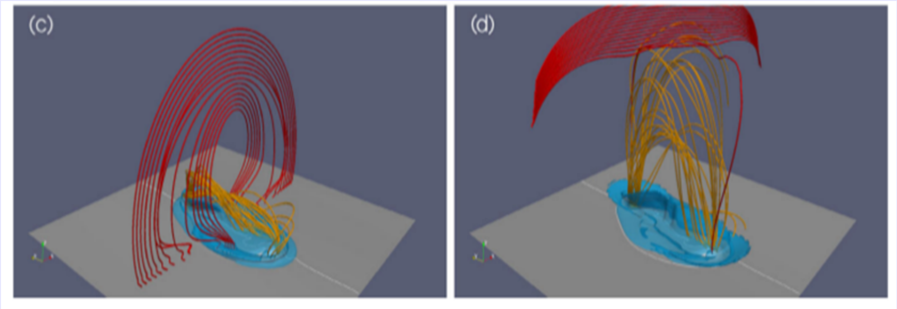
Potential magnetic field satisfying condition $\mathbf{B}_{\mathrm{P}} = \nabla\Phi$

$$\hat{n}\cdot \boldsymbol{B}_{\boldsymbol{p}}\big|_{\partial V} = \hat{n}\cdot \boldsymbol{B}\big|_{\partial V}$$

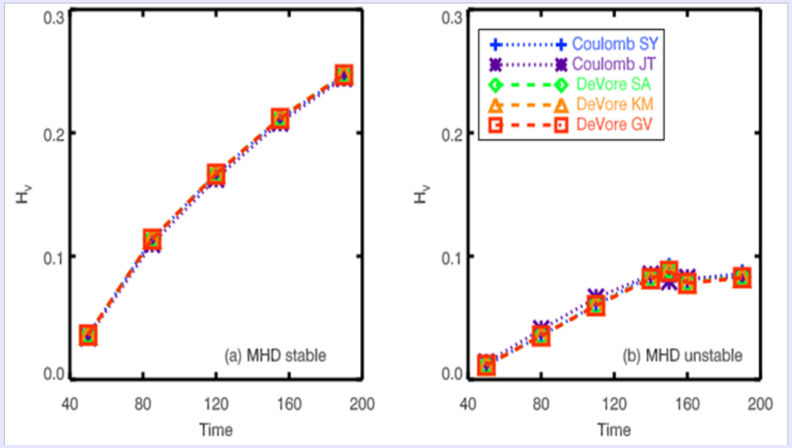
→ solution of Laplace's equation $\nabla^2\Phi = 0$

$$\left.\frac{\partial\Phi}{\partial\hat{n}}\right|_{\partial V} = \hat{n}\cdot\mathbf{B}|_{\partial V}$$

under Neumann BCs



Leake et al. 2013, 2014



Valori et al. 2016

In Cartesian coordinates:

- Many methods to solve (eg FFT)
- Not considering all 6 boundaries of the volume (eg, considering only the bottom boundary) can lead to incorrect helicity values, and even to opposite sign (Valori et al. 2012)

Potential field calculation – Spherical geometry

Potential magnetic field satisfying condition

$$\mathbf{B}_{\mathrm{p}} = \nabla\Phi$$

$$\hat{n}\cdot\boldsymbol{B}\big|_{\partial V} = \hat{n}\cdot\boldsymbol{B}_{\boldsymbol{p}}\big|_{\partial V}$$

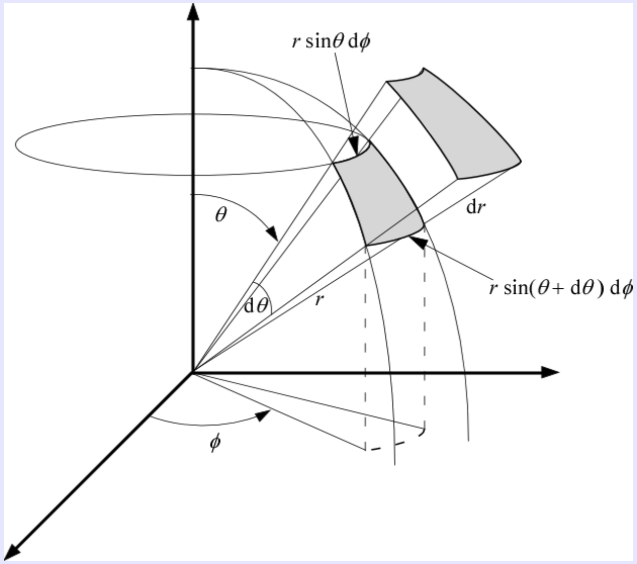
→

$$\nabla^2\Phi = 0$$

$$\left.\frac{\partial\Phi}{\partial\hat{n}}\right|_{\partial V} = \hat{n}\cdot\mathbf{B}|_{\partial V}$$

solution of Laplace's equation

under Neumann BCs



$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin\theta^2}\frac{\partial^2\Phi}{\partial\phi^2} = 0$$

$$\left.\frac{\partial\Phi}{\partial\hat{n}}\right|_{\partial V} = \hat{n}\cdot\mathbf{B}|_{\partial V}$$

in the spherical finite volume (wedge)

$$V=\{(r,\theta,\varphi): r\in[r_{min}, r_{max}], \theta\in[\theta_{min}, \theta_{max}], \varphi\in[\varphi_{min}, \varphi_{max}]\}$$

BVP well defined only for flux-balanced 3D field $\int_{\partial V}\mathbf{B}\cdot\mathrm{d}\mathbf{S} = 0$

Solution methods

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right)+\frac{1}{r^2\sin\theta^2}\frac{\partial^2\Phi}{\partial\phi^2}=0$$

$$\left.\frac{\partial\Phi}{\partial\hat{n}}\right|_{\partial V}=\left.\hat{n}\cdot\mathbf{B}\right|_{\partial V}$$

$$V=\{(r,\theta,\varphi):r\in[r_{min},r_{max}],\theta\in[\theta_{min},\theta_{max}],\varphi\in[\varphi_{min},\varphi_{max}]\}$$

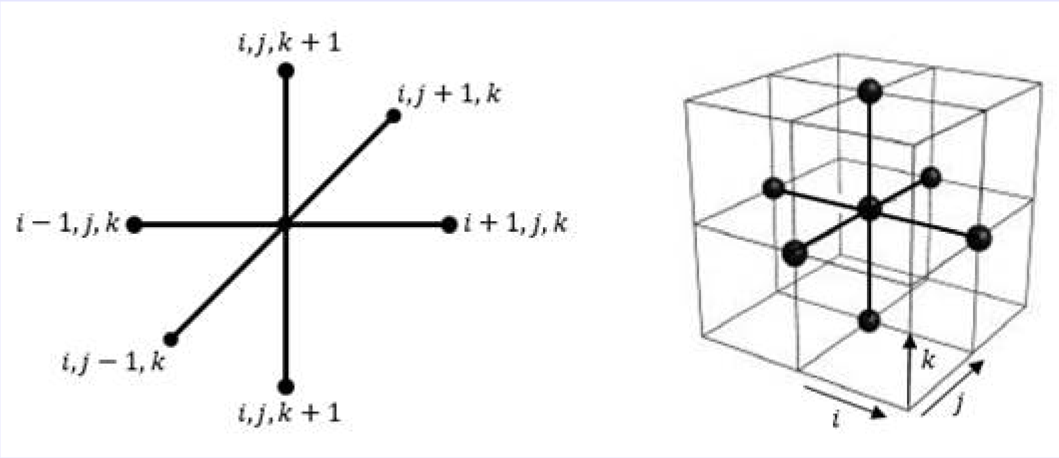
Finite difference discretization of the volume and the equation

$$r_i,\ i=0,\ldots,N_r-1$$
$$\theta_j,\ j=0,\ldots,N_\theta-1$$
$$\phi_k,\ k=0,\ldots,N_\phi-1$$

results in the large linear system of N_rxN_θxN_φ equations

Lu=*f*

with *L* a block tridiagonal matrix

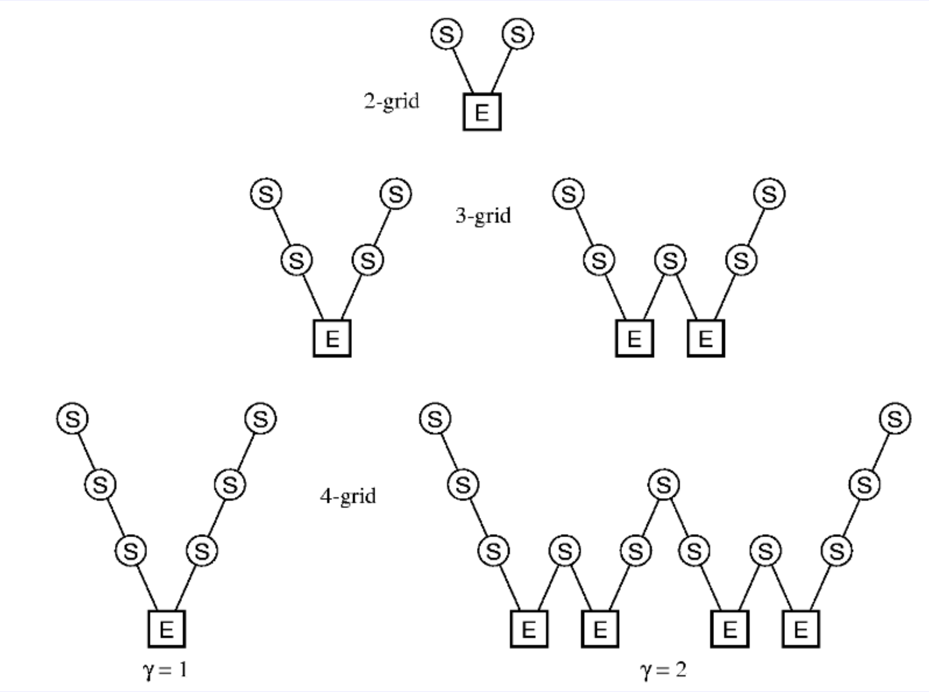


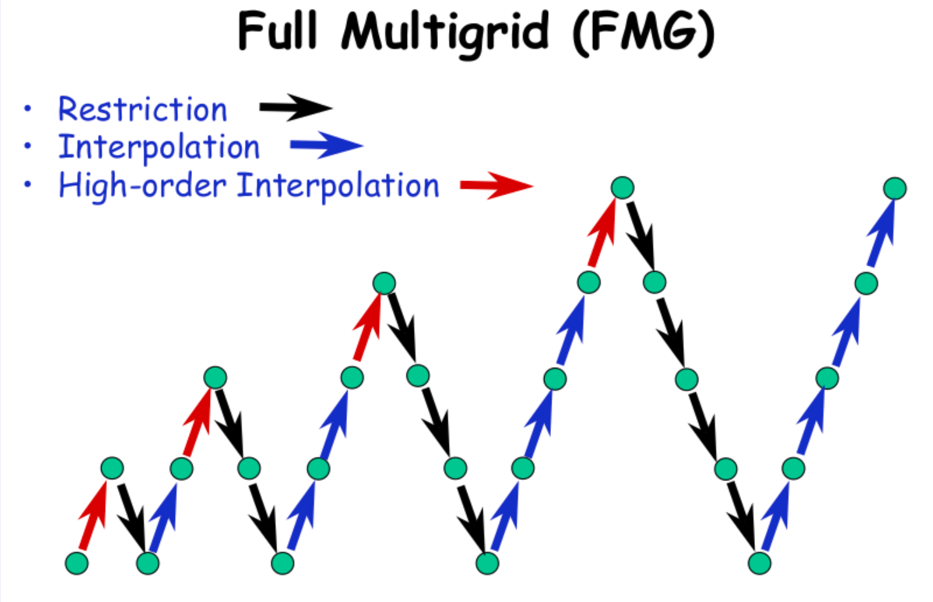
Direct
Gauss elimination
Factorization

Iterative
Jacobi
Gauss-Seidel
Conjugate gradient
Multigrid

Multigrid technique

exact $Lu=f$
approximate $Lv=f$
error $e=u-v$, residual $d=Lv-f$
$Le=-d$
Relaxation (smoothing) – Restriction – Prolongation (interpolation)





Solution method

We use the FORTRAN (F77/F90) routine **mud3sa** from the MUDPACK* library (NCAR)
mud3sa automatically discretizes and attempts to compute the 2nd order conservative finite difference approximation to the 3D linear, non-separable, self-adjoint, elliptic PDE

$$\frac{\partial}{\partial x}\left(g_x \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(g_y \frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(g_z \frac{\partial u}{\partial z}\right)+\lambda u=S$$

on the rectangle $[x_1,x_2]\times[y_1,y_2]\times[z_1,z_2]$

$$x \rightarrow r \quad y \rightarrow \theta \quad z \rightarrow \varphi \quad g_x \rightarrow r^2 \sin(\theta) \quad g_y \rightarrow \sin(\theta) \quad g_z \rightarrow 1/\sin(\theta) \quad \lambda = S = 0$$

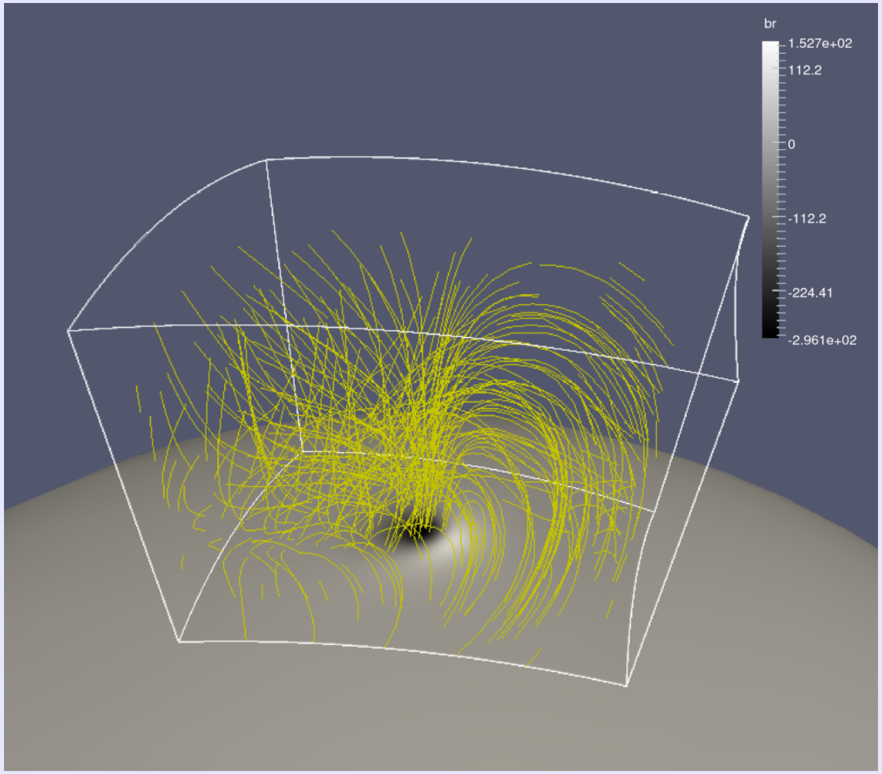
- Uniform (*dx*=const., *dy*=const., *dz*=const.), non-homogenous (*dx*≠*dy*≠*dz*) grid
- Routine is called twice: discretization call/approximation call; error checking
- **Input to the routine**
- functions g_x, g_y, g_z, S, and parameter λ
- N_r, N_θ, N_φ ($a*2^{b-1}+1$, so that multigrid is efficient; if not interpolate) (11,13,17,21,25,33,41,49,65,81,97,129,161,193,257,321,385,513,641,769,1025)
- r_{min}, r_{max}, θ_{min}, θ_{max}, φ_{min}, φ_{max}
- type of BCs (periodic, Dirichlet, or mixed derivative)
- rhs of BCs $\left.\frac{\partial \Phi}{\partial \hat{n}}\right|_{\partial V} = \hat{n}\cdot\mathbf{B}|_{\partial V}$
- solver options: # of relaxation sweeps before/after a fine-coarse-fine cycle, v-, w-, or k-cycles, FMG or not, multilinear/multicubic prolongation, relaxation method (Gauss-Seidel, linear/planar relaxation)
- **Output** Φ

*www2.cisl.ucar.edu/resources/legacy/mudpack

Solution method

Grid Size	Storage	T0	Ts	Mflop	Error
25 X 9 X 17	0.056 Mwords	0.13 sec	0.02 sec	16	0.17e-2
49 X 17 X 33	0.388 Mwords	0.86 sec	0.09 sec	32	0.40e-3
97 X 33 X 65	2.895 Mwords	6.63 sec	0.39 sec	57	0.99e-4
193 X 65 X 129	22.351 Mwords	51.61 sec	1.91 sec	91	0.25e-4

Method validation



- semi-analytical, force-free fields of Low & Lou 1990
- LL parameters: *n*=*m*=1, *l*=0.3, *Φ*=π/4
- angular size: 20°x20° on the Sun, or ~200Mm x ~200Mm
- AR height: 200Mm
- resolution:
  129x129x129 grid points
  257x257x257 grid points
- Test for:
  resolution + solenoidality

field	grid	$\langle \|f_i\| \rangle$	$\epsilon_{\rm flux}$	ξ	E	$E_{\rm c}/E$	$E_{\rm div}/E$	$s_{\rm max}$
$\mathbf{B}$	129	$2.21\,10^{-4}$	$1.70\,10^{-3}$	$1.99\,10^{-2}$	45.3	0.262	$1.10\,10^{-3}$	$7.9\,10^{-3}$
$\mathbf{B_p}$		$1.15\,10^{-4}$	$1.83\,10^{-3}$	$1.81\,10^{-4}$	33.4			
$\mathbf{B}$	257	$2.16\,10^{-4}$	$2.15\,10^{-3}$	$3.67\,10^{-2}$	45.2	0.261	$2.51\,10^{-3}$	$5.1\,10^{-3}$
$\mathbf{B_p}$		$2.14\,10^{-4}$	$2.23\,10^{-3}$	$3.59\,10^{-4}$	33.4			

Conclusions

the physical problem

$$\nabla^2 \Phi = 0 \text{ in } V \qquad \qquad \nabla \times \boldsymbol{X} = \nabla \cdot \boldsymbol{X} = 0 \text{ in } V$$

$$\Rightarrow$$

$$\frac{\partial \Phi}{\partial \hat{n}} = \text{ given in } \partial V \qquad \qquad \hat{n} \cdot \boldsymbol{X} = \text{ given in } \partial V$$

the numerical problem

- Solution of linear elliptic PDEs in various forms (real/complex, 2D/3D, separable/non-separable, …), with various types of BCs, in any coordinate system, BUT only uniform grids, and additionally:
- Ease of input
- Automatic discretization to 2nd/4th order approximation
- Many choices for multigrid options and relaxation methods
- Error control
- Flagging of errors
- OpenMP parallelization
- +many more (output of minimal workspace requirements, documentation, test programs)