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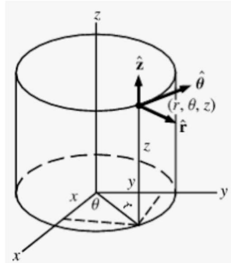
Numerical Methods for Differential Equations in Physics

Curvilinear Coordinates

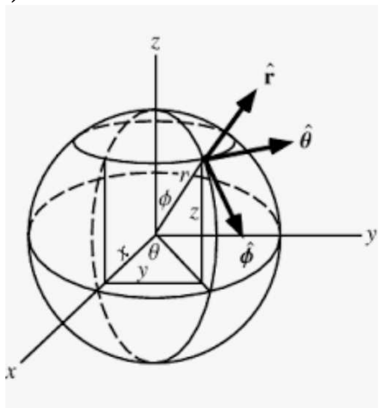
Cylindrical coordinates (r, θ, z) (sometimes called (ρ, θ, z))

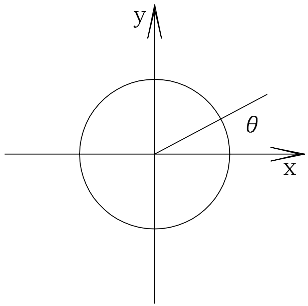
$$x = r\cos\theta \qquad r^2 = x^2 + y^2$$
$$y = r\sin\theta \qquad \theta = \mathbf{atan2}(y, x)$$
$$z = z \qquad z = z$$

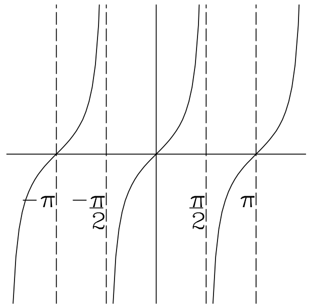


Spherical coordinates (r, θ, ϕ) (sometimes called (r, ϕ, θ))

$$x = r\sin\theta\cos\phi \qquad r^2 = x^2 + y^2 + z^2$$
$$y = r\sin\theta\sin\phi \qquad \theta = \mathbf{atan2}(\sqrt{x^2 + y^2}, z)$$
$$z = r\cos\theta \qquad \phi = \mathbf{atan2}(y, x)$$







Range of atan is $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right]$

Range of atan2 is $(-\pi, \pi]$

Differential operators in cylindrical coordinates contain $\frac{1}{r}$

$$\nabla f = \frac{\partial f}{\partial r}\mathrm{e_r} + \frac{1}{r}\frac{\partial f}{\partial \theta}\mathrm{e}_\theta + \frac{\partial f}{\partial z}\mathrm{e_z}$$

$$\nabla \cdot f = \frac{1}{r}\frac{\partial r f_r}{\partial r} + \frac{1}{r}\frac{\partial f_\theta}{\partial \theta} + \frac{\partial f_z}{\partial z}$$

$$\nabla \times f = \left(\frac{1}{r}\frac{\partial f_z}{\partial \theta} - \frac{\partial f_\theta}{\partial z}\right)\mathrm{e_r} + \left(\frac{\partial f_r}{\partial z} - \frac{\partial f_z}{\partial r}\right)\mathrm{e}_\theta + \frac{1}{r}\left(\frac{\partial r f_\theta}{\partial r} - \frac{\partial f_r}{\partial \theta}\right)\mathrm{e_z}$$

$$\Delta f = \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2}$$

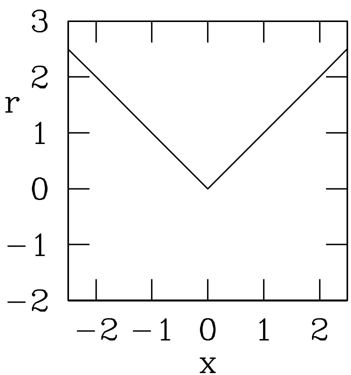
Tensor product

$$f(x,y) = \sum_{k,n} f_{k,n} x^k y^n \quad \text{or, better} \quad f(x,y) = \sum_{k,n} f_{k,n} T_k(x) T_n(y)$$

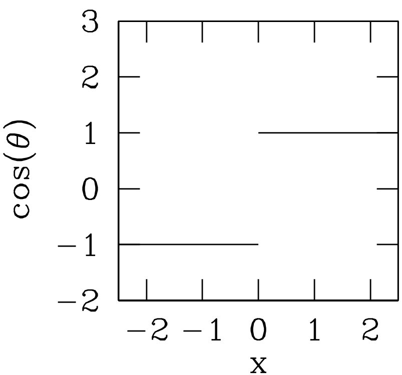
Cylindrical coordinates

$$f(r,\theta) = \sum_{k,m} f_{k,m} r^k e^{im\theta}$$

Despite their seemingly innocuous form, these are not analytic at the origin!



$f(r,\theta) = r$



$f(r,\theta) = \cos(\theta)$

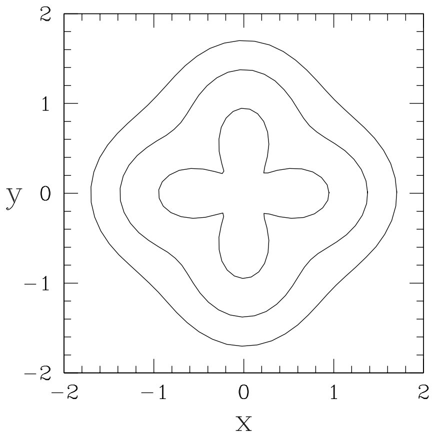
$$
\begin{aligned}
x^k y^n &= (r\cos\theta)^k (r\sin\theta)^n \\
&= r^{k+n}\left(\frac{e^{i\theta}+e^{-i\theta}}{2}\right)^k \left(\frac{e^{i\theta}-e^{-i\theta}}{2i}\right)^n \\
&= \left(\frac{r}{4}\right)^{k+n} (-i)^n \sum_{k'=0}^{k} \binom{k}{k'} e^{ik'\theta} e^{-i(k-k')\theta} \\
&\qquad\qquad \sum_{n'=0}^{n} \binom{n}{n'} e^{in'\theta} (-1)^{n-n'} e^{-i(n-n')\theta} \\
&= \left(\frac{r}{4}\right)^{k+n} (-i)^n \sum_{k'=0}^{k} \sum_{n'=0}^{n} \binom{k}{k'} \binom{n}{n'} (-1)^{n-n'} e^{i(2k'-k+2n'-n)\theta}
\end{aligned}
$$

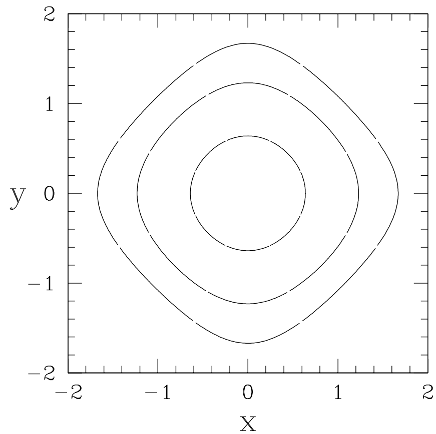
Wavenumber in θ multiplying r^{k+n} is same parity and restricted to

$$
-(k+n) \le 2k' - k + 2n' - n \le k+n
$$

$$
f(r,\theta) = \sum_{j=0}^{\infty} \sum_{\substack{m=-j \\ j+m \text{ even}}}^{j} f_{jm} r^j e^{im\theta} = \sum_{m=-\infty}^{\infty} \sum_{\substack{j=|m| \\ j+m \text{ even}}}^{\infty} f_{jm} r^j e^{im\theta}
$$

$f = r^2 + \frac{1}{2}\cos(4\theta)$ $\times$ **NO** $f = r^2 - \frac{1}{10}r^4\cos(4\theta)$ ✓ **OK**





Trigonometric functions with wavenumber m contain m oscillations. As r decreases, oscillations are compressed over decreasing circumference. Requirement that radial function multiplying $e^{im\theta}$ begin with r^m (that it have an m-th order zero) leads to sufficiently fast damping of oscillation amplitude near origin.

Same result can be demonstrated via differentiation:

$$\frac{\partial}{\partial x}(x^k y^n) = k x^{k-1} y^n$$

Not singular at $x = 0$, since $k - 1 < 0 \to k = 0$. But:

$$\begin{aligned}\nabla\left(r^j e^{im\theta}\right) &= \left(\mathrm{e}_r \frac{\partial}{\partial r} + \mathrm{e}_\theta \frac{1}{r}\frac{\partial}{\partial \theta}\right)\nabla\left(r^j e^{im\theta}\right)\\ &= (\mathrm{e}_r j + \mathrm{e}_\theta i m) r^{j-1} e^{im\theta}\end{aligned}$$

Singular at $r = 0$ for $j = 0, m \neq 0$. (Require $j \geq m$.)

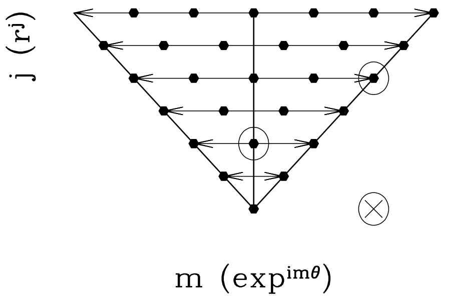
$$\begin{aligned}\Delta\left(r^j e^{im\theta}\right) &= \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right)\left(r^j e^{im\theta}\right)\\ &= \left(j(j-1) + j - m^2\right) r^{j-2} e^{im\theta}\\ &= \left(j^2 - m^2\right) r^{j-2} e^{im\theta} \Longrightarrow \textbf{need } \ m = \pm j \ \textbf{ for } \ j = 0, 1\end{aligned}$$

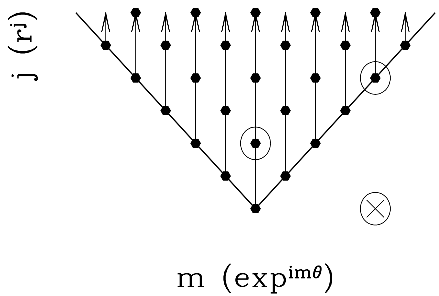
$$\Delta^2\left(r^j e^{im\theta}\right) = (j^2 - m^2)((j-2)^2 - m^2)\, r^{j-4} e^{im\theta}$$

Need $m = \pm j$ or $m = \pm(j-2)$ for $j \leq 4$. Etc.

For f to be infinitely differentiable, require

$$f(r,\theta) = \sum_{j=0}^{\infty} \sum_{\substack{m=-j \\ j+m \text{ even}}}^{j} f_{jm} r^j e^{im\theta} = \sum_{m=-\infty}^{\infty} \sum_{\substack{j=|m| \\ j+m \text{ even}}}^{\infty} f_{jm} r^j e^{im\theta}$$





$$r^j \left(e^{\pm ij\theta} + e^{\pm i(j-2)\theta} + \ldots\right) \qquad e^{im\theta} \left(r^{|m|} + r^{|m|+2} + \ldots\right)$$

• We know that monomials r^j are a badly conditioned basis. They are small almost everywhere in the interior. Matrix transforming between $f(r_j)$ and monomial coeffcients is badly conditioned.

• What about $r^m T_j(r)$ (called Roberts functions)?

$$f(r,\theta) = \sum_{m=-\infty}^{\infty} \sum_{\substack{j=0 \\ j+m \text{ even}}}^{\infty} r^m f_{jm} T_j(r) e^{im\theta}$$

Also badly behaved, again because r^m exaggerate the boundary.

• Bessel functions:

$$\left\{ \begin{array}{c} J_m \\ I_m \end{array} \right\} (\lambda r) = \left(\frac{\lambda r}{2}\right)^m \sum_{j=0}^{\infty} \frac{(\mp \lambda r/2)^{2j}}{j!\,\Gamma(m+j+1)}$$

Eigenfunctions of the Laplacian: $\Delta J_m(\lambda r) e^{im\theta} = -\dfrac{\lambda^2}{r^2} J_m(\lambda r) e^{im\theta}$
Correct relations between r exponent $m+2j$ and θ wavenumber m.
But convergence rate of coefficients in Bessel series is only algebraic.

• **One-sided Jacobi basis** $W_j^m(r)e^{im\theta} = r^m P^{0,m}_{(j-m)/2}(2r^2-1)$
Has good propreties, but too difficult to deal with.

• **Instead, impose only parity** $\Longrightarrow f$ **not analytic:**

$$f(r,\theta) = \sum_{m=-\infty}^{\infty} \sum_{\substack{j=0 \\ j+m \text{ even}}}^{\infty} f_{jm} T_j(r) e^{im\theta}$$

($f, \nabla f$ **regular but** $\Delta f \sim e^{2i\theta}/r^2$)

Turns out to be wasteful but not harmful.
Coefficient of non-analytic functions are carried around and computed but do not mix with the coefficients of the analytic basis functions. This is even true if parity is not imposed. (Then 3/4 of the functions are non-analytic.)

If using finite differences in r, require at $r = 0$

for m even $\quad f_m = a + cr^2 + \ldots$ **(no linear term)** $\quad \Longrightarrow \quad \dfrac{df_m}{dr}(r=0) = 0$

for m odd $\quad f_m = br + \ldots$ **(no constant term)** $\quad \Longrightarrow \quad f_m(r=0) = 0$

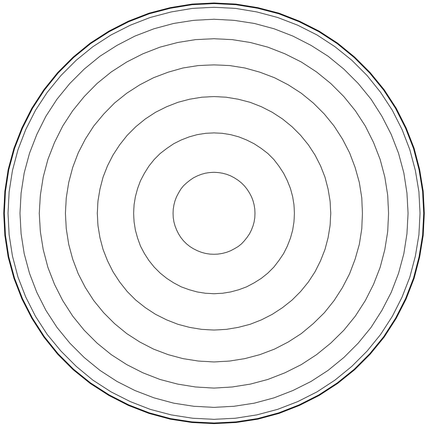
How to incorporate BCs at $r = r_0 = 0$ into finite difference operator?

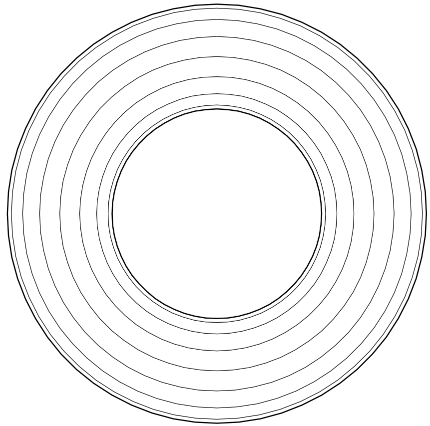
$$\frac{d^2 f}{dr^2}(r_2) \approx \alpha f(r_3) + \beta f(r_2) + \gamma f(r_1)$$

$$\frac{d^2 f}{dr^2}(r_1) \approx \alpha f(r_2) + \beta f(r_1) \qquad\qquad f(r_0) = 0$$

$$\frac{d^2 f}{dr^2}(r_1) \approx \alpha f(r_2) + (\beta + \gamma) f(r_1) \qquad\qquad f'(r_0) = 0 \Longrightarrow f(r_0) = f(r_1)$$

Can use Cartesian five or nine-point finite-difference stencil at $r = 0$, polar coordinates elsewhere. Or omit point at $r = 0$.





Full disk

BC at r_{out} and regularity at r_{in}

Cluster points at outer boundary, not at the origin

Either $r \in [0, 1]$ and $\theta \in [0, 2\pi]$ or $r \in [-1, 1]$ and $\theta \in (0, \pi]$

Annulus: no singularity

Use finite differences or Chebyshev polynomials in r and Fourier series in θ

Map $[r_{\text{in}}, r_{\text{out}}]$ to $[-1, 1]$

BCs at $r_{\text{in}}, r_{\text{out}}$.

What about vector components (u^r, u^θ, u^z)?
All of (u^x, u^y, u^z) are like scalars and must obey rules above.

$$\begin{aligned} u^r &= \cos(\theta) u^x + \sin(\theta) u^y \\ u^\theta &= -\sin(\theta) u^x + \cos(\theta) u^y \end{aligned}$$

Expanding u^x and u^y leads to

$$u^{r,\theta} = \sum_{j=0}^{\infty} \sum_{\substack{m=-|j+1| \\ j+m \text{ odd}}}^{|j+1|} u_{jm}^{r,\theta} r^j e^{im\theta} = \sum_{m=-\infty}^{\infty} \sum_{\substack{j=|m-1| \\ j+m \text{ odd}}}^{\infty} u_{jm}^{r,\theta} r^j e^{im\theta}$$

Vector Laplacian couples u^r and u^θ:

$$\vec{\Delta}\begin{bmatrix} u^r \\ u^\theta \\ u^z \end{bmatrix} \equiv \begin{bmatrix} \Delta - \frac{1}{r^2} & -\frac{2}{r^2}\partial_\theta & 0 \\ \frac{2}{r^2}\partial_\theta & \Delta - \frac{1}{r^2} & 0 \\ 0 & 0 & \Delta \end{bmatrix}\begin{bmatrix} u^r \\ u^\theta \\ u^z \end{bmatrix} = \begin{bmatrix} g^r \\ g^\theta \\ g^z \end{bmatrix}$$

Diagonalize the two-by-two block:

$$u^\pm \equiv u^r \pm i u^\theta \qquad E \equiv \begin{bmatrix} I & iI \\ I & -iI \end{bmatrix} \qquad \begin{bmatrix} u^+ \\ u^- \end{bmatrix} = E\begin{bmatrix} u^r \\ u^\theta \end{bmatrix}$$

$$E\,\vec{\Delta}\,E^{-1} = \begin{bmatrix} \Delta - \frac{1}{r^2} + \frac{2i}{r^2}\partial_\theta & 0 \\ 0 & \Delta - \frac{1}{r^2} - \frac{2i}{r^2}\partial_\theta \end{bmatrix}$$

$$\vec{\Delta}\begin{bmatrix} u^r \\ u^\theta \end{bmatrix} = \begin{bmatrix} g^r \\ g^\theta \end{bmatrix}$$

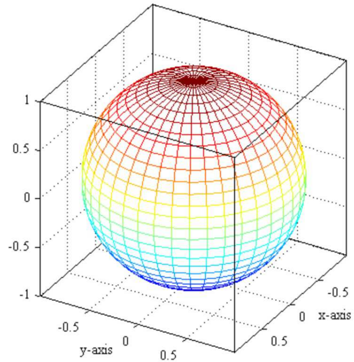
$$E\,\vec{\Delta}E^{-1}\,E\begin{bmatrix} u^r \\ u^\theta \end{bmatrix} = E\begin{bmatrix} g^r \\ g^\theta \end{bmatrix}$$

$$\begin{bmatrix} \Delta - \frac{1}{r^2} + \frac{2i}{r^2}\partial_\theta & 0 \\ 0 & \Delta - \frac{1}{r^2} - \frac{2i}{r^2}\partial_\theta \end{bmatrix}\begin{bmatrix} u^+ \\ u^- \end{bmatrix} = \begin{bmatrix} g^+ \\ g^- \end{bmatrix}$$

Spherical Coordinates and Spherical Harmonics

Spherical harmonics:

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



Behavior near poles:

$$P_\ell^m(\cos\theta) \sim \sin^m\theta$$

Spherical θ at poles is like r near center of disk: polar cap

Many useful relations, such as: $\Delta Y_{\ell,m} = \dfrac{-\ell(\ell+1)}{r^2} Y_{\ell,m}$

$$P_\ell^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\ell^0(x)$$

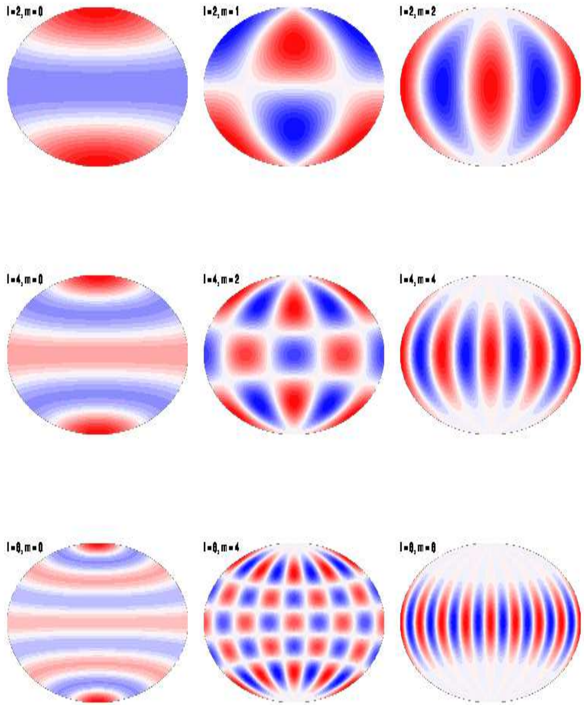
$$(1-x^2)\frac{d}{dx}P_\ell^m = \frac{1}{2\ell+1}\left[(\ell+1)(\ell+m)P_{\ell-1}^m - \ell(\ell-m+1)P_{\ell+1}^m\right]$$

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

$\ell = 2$

$\ell = 4$

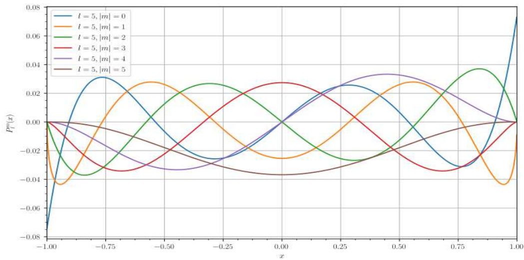
$\ell = 8$

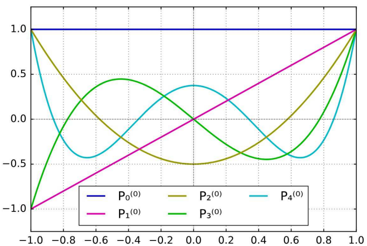


$m = 0$	$m \neq 0, \ell$	$m = \ell$
zonal	**tesseral**	**sectoral**

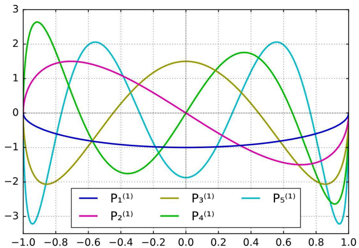
$$P_\ell^m(\cos\theta)$$

$\ell = 5 \quad \rightarrow$

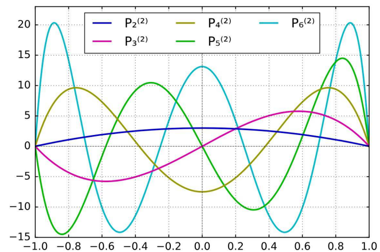




$m = 0$



$m = 1$



$m = 2$

As m increases, roots/extrema/variation of polynomials concentrate at origin (equator). Counteracts accumulation of longitude lines ($e^{im\phi}$) at poles.

$\Longrightarrow$ Areas sampled equally over entire sphere via oscillations of P_ℓ^m

Pseudospectral method: transform to grids

$$f(\theta,\phi) = \sum_{\ell=0}^{N} \sum_{m=-\ell}^{\ell} f_\ell^m P_\ell^m(\cos\theta) e^{im\phi} = \sum_{m=-N}^{N} \underbrace{\left(\sum_{\ell=|m|}^{N} f_\ell^m P_\ell^m(\cos\theta) \right)}_{f_m(\theta)} e^{im\phi}$$

$$f_m(\theta) = \int_0^{2\pi} f(\theta,\phi)\, e^{-im\phi} d\phi \approx \sum_{j=1}^{N_\phi} f(\theta,\phi_j)\, e^{-im\phi_j} \Delta\phi$$

$$f_\ell^m = \int_0^{\pi} f_m(\theta)\, P_\ell^m(\cos\theta)\, \sin\theta\, d\theta \approx \sum_{j=1}^{N_{\theta(m)}} f_m(\theta_j)\, P_\ell^m(\cos\theta_j)\, \underbrace{\sin\theta_j\, \frac{2\pi j}{N_{\theta(m)}}}_{\Delta\theta_j}$$

Transform to physical grid via $\begin{cases} \textbf{FFT in } \phi \textbf{ direction} \\ \textbf{weighted sum (matrix mult) in } \theta \textbf{ direction} \end{cases}$

Grid is equally spaced in ϕ but more concentrated in θ near equator.

Optimal grid for each m would be $N_{\theta(m)}$ roots of $P_\ell^m(\cos\theta)/\sin^m\theta$,
but want same θ grid for each m, so use N roots of Legendre poly P_N^0.
Retain f_ℓ^m for $\ell \in [m, N]$

Orientation and role of m

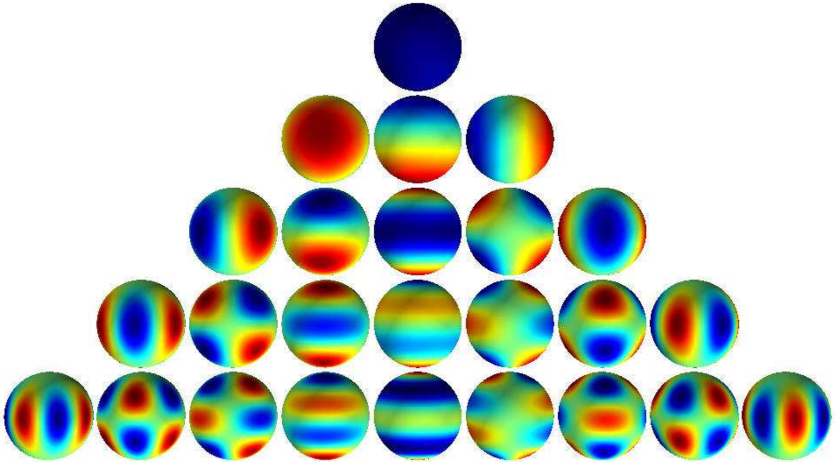
$\ell = 0$

$\ell = 1 \rightarrow$

$\ell = 2$

$\ell = 3$

$\ell = 4$



$$Y_1^{\pm 1} = -N e^{\pm i\phi} \sin\theta = N\,\frac{\mp x - iy}{r} \qquad \tfrac{1}{2}\left(Y_1^{-1} - Y_1^{1}\right) = N\frac{x}{r}$$

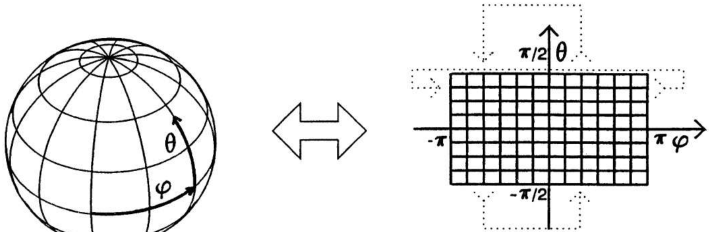
$$Y_1^{0} = N\sqrt{2}\cos\theta = N\sqrt{2}\,\frac{z}{r} \qquad \pm\tfrac{1}{\sqrt{2}}Y_1^{0} + \tfrac{1}{2}\left(Y_1^{-1} + Y_1^{1}\right) = N\frac{\pm z - iy}{r}$$

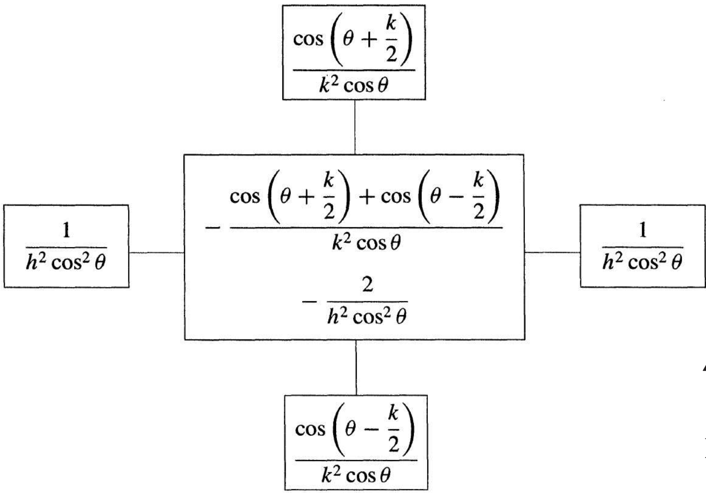
So m depends on orientation w.r.t. z-axis as well as on variation, unlike ℓ.

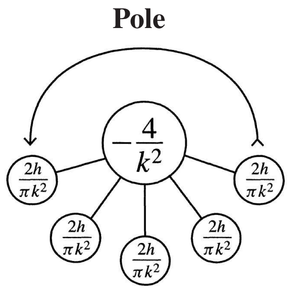
Rotating $(z, x) \rightarrow (-x, z)$ changes m, but $\Delta Y_\ell^m = \frac{-\ell(\ell+1)}{r} Y_\ell^m \quad \forall m$

Distinguished choice of z axis if there is rotation.

Fornberg: finite differences on an equally spaced grid







$$\Delta_{\text{surface}} f = \frac{1}{\cos\tilde{\theta}} \frac{\partial}{\partial\tilde{\theta}} \left(\cos\tilde{\theta} \frac{\partial f}{\partial\tilde{\theta}} \right) + \frac{1}{\cos\tilde{\theta}} \frac{\partial^2 f}{\partial\phi^2}$$

Here $\tilde{\theta}$ is latitude, measured from equator

$$h \equiv \Delta\phi, k \equiv \Delta\tilde{\theta}$$

Solve Poisson's equation with finite differences on equispaced (θ, ϕ) grid

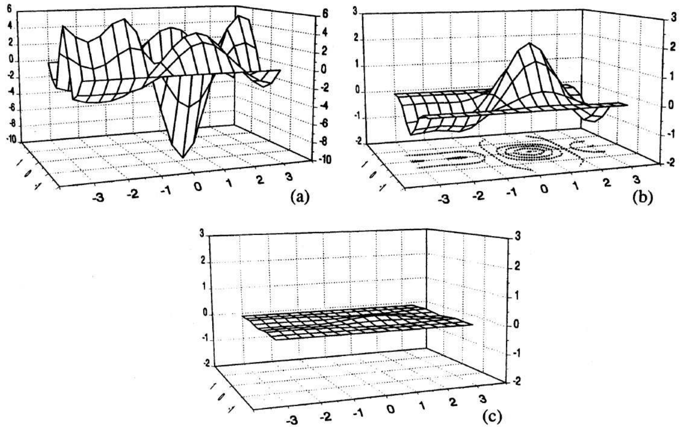


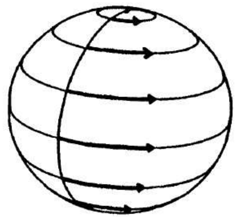
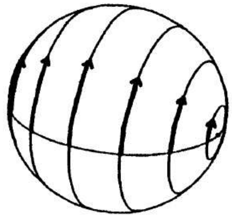
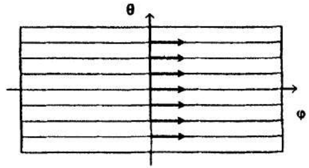
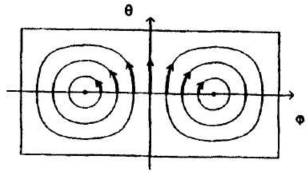
FIG. 8. *Solution of Poisson's equation on a sphere using second-order finite differences.* (a) *Function* $f(\varphi, \theta) = -\cos^2\theta[(\sin\varphi + \cos\varphi)(20\cos^2\theta - 15) + \sin 2\varphi(10\cos^2\theta - 6)]$ *shown on domain* $\varphi \times \theta = [-\pi, \pi] \times \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$. (b) *Numerical solution to Poisson's equation* $\frac{\partial^2 u}{\partial \theta^2} - \tan\theta \frac{\partial u}{\partial \theta} + \frac{1}{\cos^2\theta} \frac{\partial^2 u}{\partial \varphi^2} = f(\varphi, \theta)$ *obtained by second-order FD on the displayed grid.* (c) *Error in the numerical solution above – difference to the analytic solution* $u(\varphi, \theta) = \cos^4\theta \left[\sin\varphi + \cos\varphi + \frac{1}{2}\sin(2\varphi)\right]$ *(displayed on the same scale as the numerical solution).*

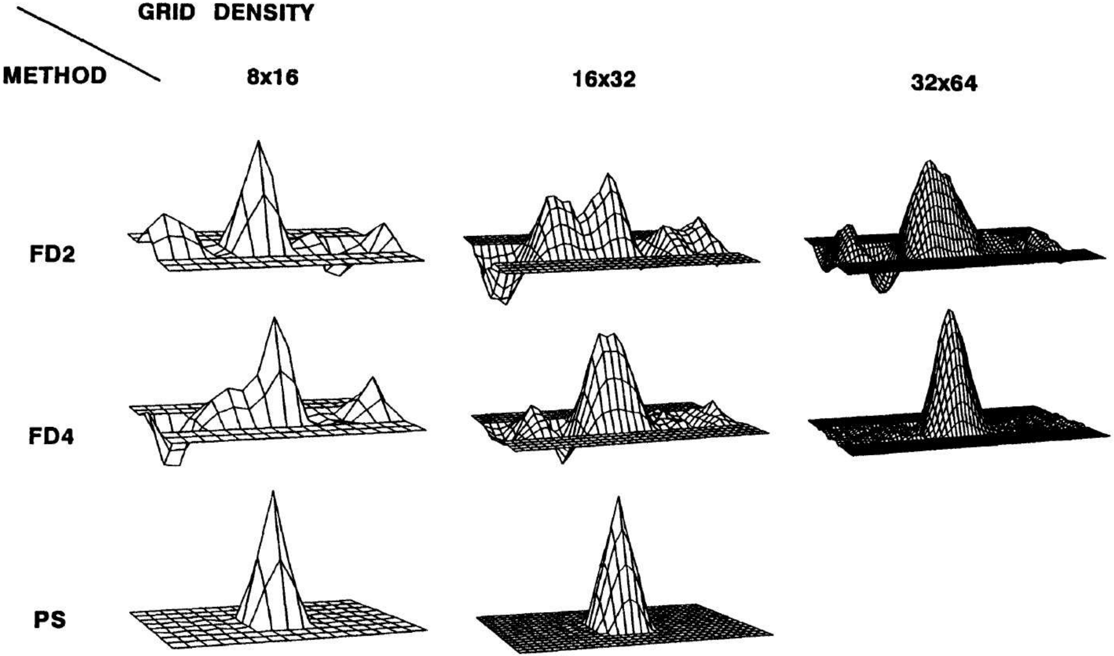
$$u(\tilde{\theta}, \phi) = \cos^4\tilde{\theta}[\sin\phi + \cos\phi + \tfrac{1}{2}\sin(2\phi)]$$

$$\Delta_{\text{surface}} u = -\cos^2\tilde{\theta}(\sin\phi + \cos\phi)(20\cos^2\tilde{\theta} - 15) + \sin(2\phi)(10\cos^2\tilde{\theta} - 6)$$

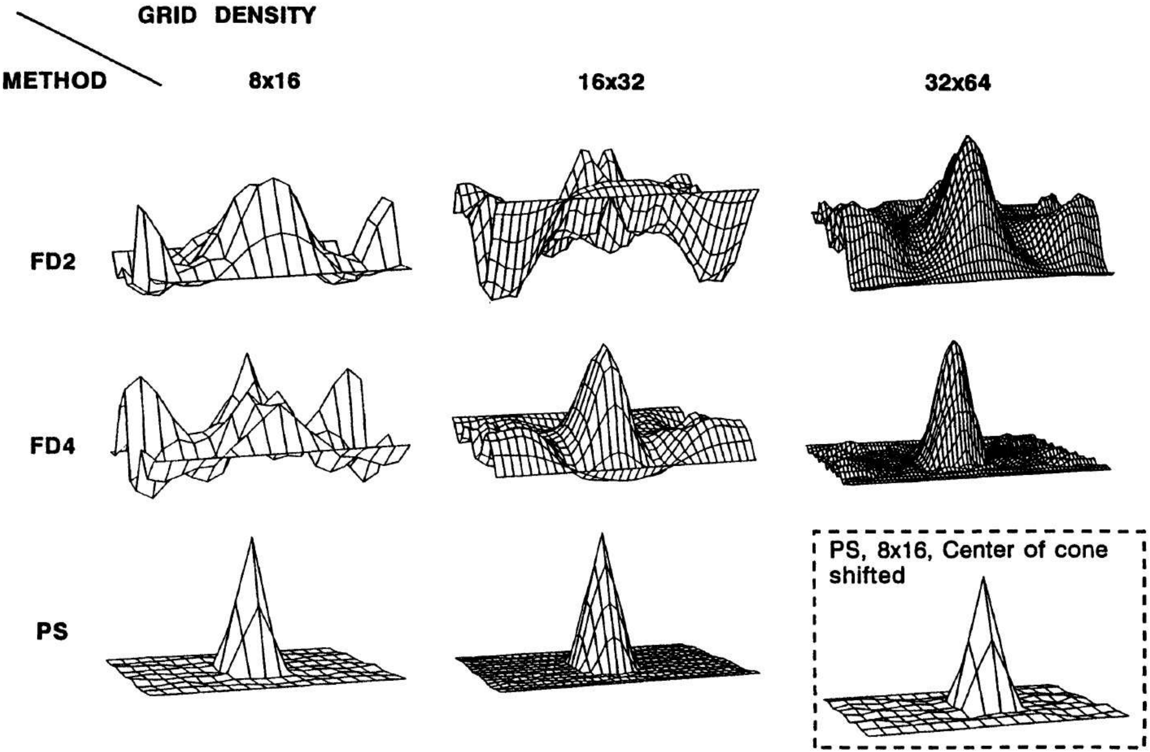
Start with u, calculate $f \equiv \Delta_{\text{surface}} u$, then test.

Fornberg: Fourier-Fourier for wave equation

	CASE 1	CASE 2
DIRECTION OF CHARACTERISTICS (SOLID-BODY ROTATION) ON SPHERICAL SURFACE		
IN (φ, θ)–PLANE (AXES AS IN FIGURE 3)		
GOVERNING EQUATION IN (φ, θ)-PLANE $\frac{\partial u}{\partial t} = a(\varphi,\theta)\frac{\partial u}{\partial \varphi} + b(\varphi,\theta)\frac{\partial u}{\partial \theta}$	$a(\varphi,\theta) = -1$ $b(\varphi,\theta) = 0$	$a(\varphi,\theta) = -\sin\varphi \quad \tan\theta$ $b(\varphi,\theta) = -\cos\varphi$
EQUATIONS FOR CHARACTERISTICS IN (φ, θ)-PLANE, PARAMETERIZED THROUGH TIME $= t$.	$\varphi(t) = t$ $\theta(t) = \theta_0$	$\varphi(t) = \arctan(\tan\varphi_0 / \cos t)$ $\theta(t) = \arcsin(\cos\varphi_0 \times \sin t)$



East-West wave (along equator)



North-South wave (over pole)

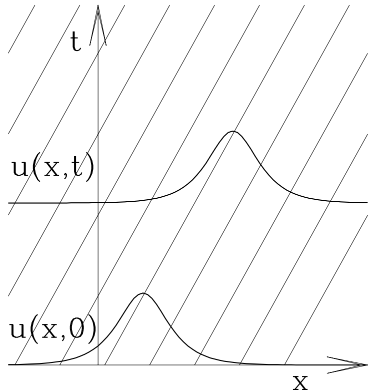
Hyperbolic Equations: Characteristics

First-order wave equation:

$$u_t = c u_x$$

Analytic solution: traveling wave

$$u(x,t) = u(x + ct, 0)$$



The wave equation <u>carries</u> the initial condition through time.

$$\textbf{Generalization: } 0 = u_t + g(x,t,u)u_x$$

$$0 = u_t + \frac{dx}{dt} u_x$$

u is constant along curve $x(t)$ such that $\frac{dx}{dt} = g(x,t,u)$:

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{dx}{dt} = 0$$

Burger’s equation: $u_t + uu_x = 0$