Code construction – 1: coordinate grid points and relating parts.

Generate coordinate grid points for the spherical coordinate (r, θ, ϕ), and tables for functions that is used in the integration of Green's formula.

- An elliptic PDE, $\overset{\circ}{\Delta}\,\phi = S(x)$, is written in the integral form,

$$\phi(x) = -\frac{1}{4\pi}\int_V G(x,x')S(x')dV + \frac{1}{4\pi}\int_{\partial V}\left[G(x,x')\nabla\phi(x') - \phi(x')\nabla G(x,x')\right]\cdot dS,$$

Green's funciton without the boundary is expanded in the multipoles,

$$G(x,x') = \frac{1}{|x-x'|} \quad = \quad \sum_{\ell=0}^{\infty} g_\ell(r,r') \sum_{m=0}^{\ell} \epsilon_m \frac{(\ell-m)!}{(\ell+m)!} P_\ell{}^m(\cos\theta)\, P_\ell{}^m(\cos\theta')$$

$$\times(\cos m\varphi \cos m\varphi' + \sin m\varphi \sin m\varphi').$$

$$\epsilon_m := \begin{cases} 1 & \text{for } m=0 \\ 2 & \text{for } m = 1,\, 2,\, \cdots \end{cases} \qquad g_\ell(r,r') := \begin{cases} \dfrac{r^\ell}{r'^{\ell+1}} & \text{for } r \le r' \\ \dfrac{r'^\ell}{r^{\ell+1}} & \text{for } r' \le r \end{cases}$$

subroutine coordinate_patch_kit

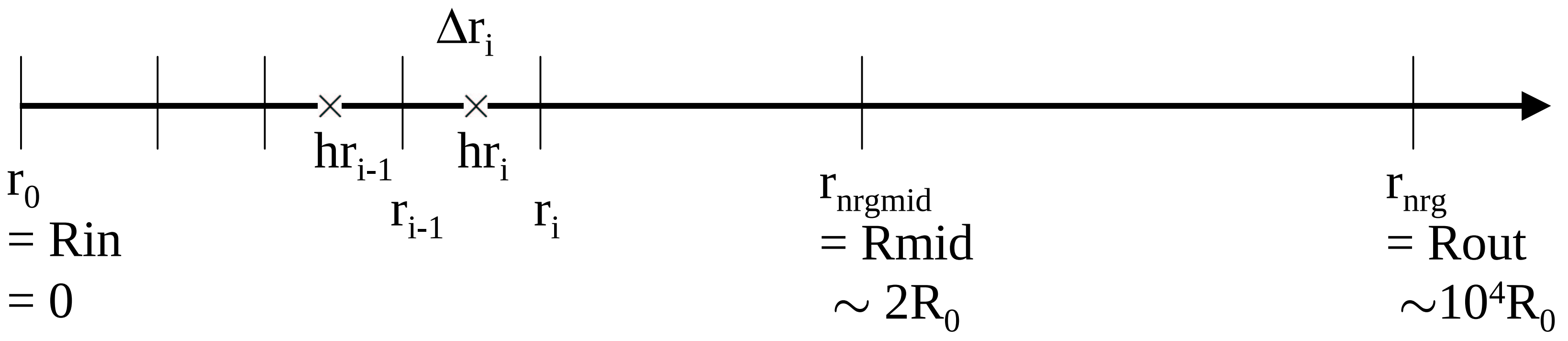
Radial coordinate grid is non-equidistant, angular grids are equidistant.
We use the mid-point rule for the quadrature formula.

Radial coordinate input parameters: nrg, nrgin, Rin, Rmid, Rout.

Rin < Rmid < Rout : $r \in$ [Rin, Rout], the grid spacing rule is changed at Rmid.

nrg : Total number of radial grid points (-1).
nrgmid : Number of radial grid points from Rin to Rmid (-1).

rg(ir), ir = 0, nrg : Radial coordinate grid points r_i .
hrg(ir) : Mid-point of radial grids.
drg(ir) : Radial grid spacing $\Delta r_i := r_i - r_{i-1}$.



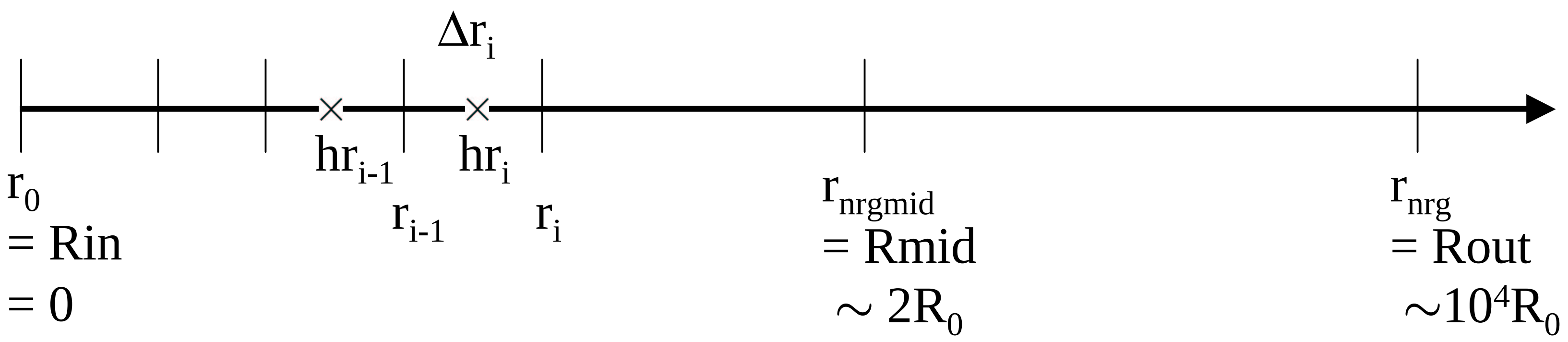
Grid spacing : $r \in$ [Rin, Rmid], equidistant or let $\Delta r_1 \sim 1/4 \Delta r_{nrgmid}$ etc.
$r \in$ [Rmid, Rout], $\Delta r_{i+1} = k \Delta r_i$.

Radial Green's function $g_\ell(r, r') := \begin{cases} \dfrac{r^\ell}{r'^{\ell+1}} & \text{for } r \le r' \\ \dfrac{r'^\ell}{r^{\ell+1}} & \text{for } r' \le r \end{cases}$

nrg, rg(ir), hrg(ir), lgmax are used.
lgmax: a number of the largest multipole

Since mid-point rule is used for the numerical integration, r' is hrg(irr).

$$\text{hgfn\_nb(irr,il,ir)} = \begin{cases} \dfrac{rg(ir)^{il}}{hrg(irr)^{il+1}} & \text{for } rg(ir) \le hrg(irr) \\ \dfrac{hrg(irr)^{il}}{rg(ir)^{il+1}} & \text{for } hrg(irr) \le rg(ir) \end{cases}$$



θ coordinate input parameter: ntg.

$\theta \in [0, \pi]$, the grid spacing is equidistant.

ntg : Total number of θ grid points (-1).

thg(it), it = 0, ntg : θ grid points θ_i .
hthg(it) : Mid-point of θ grids $\theta_{i+1/2}$.
dthg : θ grid spacing $\Delta\theta$.

Functions associated with θ coordinate input parameters: lgmax.

Trigonometric funcitons.
sinthg(it), it = 0, ntg : $\sin\theta_i$. hsinthg(it) : $\sin\theta_{i+1/2}$ sin at mid-point of θ grids.
costhg(it), it = 0, ntg : $\cos\theta_i$. hcosthg(it) : $\cos\theta_{i+1/2}$ cosin at mid-point of θ grids.

Associated Legendre funcitons $P_\ell{}^m(\cos\theta)$ $P_\ell{}^m(\cos\theta_i)$ $P_\ell{}^m(\cos\theta_{i+1/2})$
plmg(it,il,im), it = 0, ntg , il = 0, lgmax , im = 0, lgmax : at each grid point θ_i
hplmg(it,il,im), it = 1, ntg , il = 0, lgmax , im = 0, lgmax :
at each half grid point $\theta_{i+1/2}$

Since mid-point rule is used for the numerical integration,
we need hplmg(it,il,im) at half grid points $\theta_{i+1/2}$.

ϕ coordinate input parameter: npg.

$\phi \in [0, 2\pi]$, the grid spacing is equidistant.

npg : Total number of ϕ grid points (-1).

phig(ip), ip = 0, npg : ϕ grid points ϕ_i .
hphig(ip) : Mid-point of ϕ grids $\phi_{i+1/2}$.
dphig : ϕ grid spacing $\Delta\phi$.

Functions associated with ϕ coordinate input parameters: mgmax = lgmax.

Trigonometric funcitons.
sinphig(ip), ip = 0, npg : $\sin\phi_i$. hsinphig(ip) : $\sin\phi_{i+1/2}$ sin at mid-point of ϕ grids.
cosphig(ip), ip = 0, npg : $\cos\phi_i$. hcosphig(ip): $\cos\phi_{i+1/2}$ cos at mid-point of ϕ grids.

Trigonometric funcitons with the angle $m\phi$.
sinmpg(im,ip), im = 0, mgmax , ip = 0, npg : at each grid point ϕ_i
cosmpg(im,ip), im = 0, mgmax , ip = 0, npg : at each grid point ϕ_i
hsinmpg(im,ip), im = 0, mgmax , ip = 1, npg : at each half grid point $\phi_{i+1/2}$
hcosmpg(im,ip), im = 0, mgmax , ip = 1, npg : at each half grid point $\phi_{i+1/2}$

Weight for the integration: assigned at the mid-points.

wrg(irr) = hrg(irr)^2 drg(irr) : weight for the radial integratoin $r_i^2 \Delta r_i$
wtg(itt) = hsintheg(itt) dtg : weight for the θ integratoin $\sin\theta_i \Delta\theta_i$
wpg(ipp) = dpg : weight for the ϕ integratoin $\Delta\phi_i$

Weights for the numerical integration formula of mid-point rule is included in the above (which is 1 at all points).

Other parts in the Green's formula input parameters: lgmax = mgmax.

faclmg(il,im) = $\dfrac{(il - im)!}{(il + im)!}$ il = 0, lgmax, im = 0, mgmax. $\dfrac{(\ell - m)!}{(\ell + m)!}$

epsig(im) = $\epsilon_m := \begin{cases} 1 & \text{for } m = 0 \\ 2 & \text{for } m = 1, 2, \cdots \end{cases}$

end subroutine coordinate_patch_kit