Code construction – 2: Poisson solver.

- The multipole expansion is a consequence of the separation of variables on the spherical coordinate (r, θ, ϕ), and it decreases the number of floating operations drastically.
- Integrations in three coordinates r', θ', ϕ' are performed first. We then have multipole components $S_{\ell m}$ and sum up the multipoles ℓ and m . The number of floating operation can be minimized as one choose the order of integration and sums in multipoles appropriately.

- Recall the integral form; we consider the volume integral

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

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

$$S(x') = S(r',\theta',\phi'), \qquad dV = r'^2 dr' \sin\theta' d\theta' d\phi'$$

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

subroutine greens_formula_volume

1. Integarte in ϕ'.

$$S(r',\theta',\phi')\left\{\begin{array}{c}\sin m\phi'\\ \cos m\phi'\end{array}\right\} r'^2 dr' \sin\theta d\theta' d\phi' \;\rightarrow\; \left\{\begin{array}{c}S^{1s}(r',\theta',m)\\ S^{1c}(r',\theta',m)\end{array}\right\}$$

2. Integarte in θ'.

$$\left\{\begin{array}{c}S^{1s}(r',\theta',m)\\ S^{1c}(r',\theta',m)\end{array}\right\} \epsilon_m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(\cos\theta') \;\rightarrow\; \left\{\begin{array}{c}S^{2s}(r',\ell,m)\\ S^{2c}(r',\ell,m)\end{array}\right\}$$

3. Integarte in r'.

$$\left\{\begin{array}{c}S^{2s}(r',\ell,m)\\ S^{2c}(r',\ell,m)\end{array}\right\} g_\ell(r,r') \;\rightarrow\; \left\{\begin{array}{c}S^{3s}(r,\ell,m)\\ S^{3c}(r,\ell,m)\end{array}\right\}$$

4. Sum in multipole ℓ.

$$\left\{\begin{array}{c}S^{3s}(r,\ell,m)\\ S^{3c}(r,\ell,m)\end{array}\right\} P_\ell^m(\cos\theta) \;\rightarrow\; \left\{\begin{array}{c}S^{4s}(r,\theta,m)\\ S^{4c}(r,\theta,m)\end{array}\right\}$$

5. Sum in multipole m. $\cdots$ and done.

$$\left\{\begin{array}{c}S^{4s}(r,\theta,m)\sin m\phi\\ S^{4c}(r,\theta,m)\cos m\phi\end{array}\right\} \rightarrow \left\{\begin{array}{c}S^{5s}(r,\theta,\phi)\\ S^{5c}(r,\theta,\phi)\end{array}\right\} \rightarrow \phi^{(\mathrm{vol})} = -\frac{1}{4\pi}\left(S^{5s}+S^{5c}\right)$$

end subroutine greens_formula_volume

- Surface integral is calculated in the same way, so it is not written here. Integration in r’ is not necessary in the surface integrals. Instead r’ is replaced by the radius of the boundary.

subroutine Poisson_solver

call greens_formula_volume

call greens_formula_surface

$$\phi^{(\mathrm{new})} = \phi^{(\mathrm{vol})} + \phi^{(\mathrm{surf})}$$

end subroutine Poisson_solver

- $\phi^{(\mathrm{new})}$ is not use as it is for the next iteration. To avoid a divergence of iterations, we introduce a convergence factor λ in the following way

subroutine update_grfield

$$\phi^{(\mathrm{N+1})} = \lambda\phi^{(\mathrm{new})} + (1-\lambda)\phi^{(\mathrm{N})}, \qquad (\lambda \sim 0.2 - 0.5)$$

end subroutine update_grfield

$\phi^{(\mathrm{N})}$ is the field value at the Nth iteration.