

Timofey Kruglov, CR/RTO-RU

External task

Calculate overlap between spherical harmonics analytically

Robert Bosch OOO
Affiliated Office in Saint
Petersburg
Shvetsova str. 41, bld. 15
198095 Saint Petersburg
Russia
Tel +7 812 449 9710
Fax +7 812 313 9323
www.bosch.ru

Motivation:

Porous and powder-based medias are modelled as ensembles of particles of various shapes. The simplest ones are spheres. The shape of the next level of complexity is a spherocylinder. The core algorithm, which allows to model media, composed of such particles in a framework of DEM (discrete element method), is calculation of overlap between two particles with a given shape. Overlap of spheres and spherocylinders is known analytically. When it comes to ellipsoid, the analytical expression for overlap does not exist. There is however, a chance that an analytical expression may exist for shapes defined by spherical harmonics. If it does, than any shape can be decomposed onto a limited (similar to Fourier transform) number of such harmonics, starting from sphere. That might open a way to use multipole shape decomposition to characterise particulate matter and apply this approach to solve transport equations for batteries, supercapacitors, fuel cell etc. This may also have implications in cavitation problems, when it comes to deviations from spherical shape.

Contact:

Timofey.kruglov@ru.bosch.com

Task formulation:

Find analytical expression for closest points between surfaces of spherical harmonics 1 and 2, which centers are separated by the distance Δr and axes are oriented at Eulerian angles Θ_1, Φ_1, Ψ_1 and Θ_2, Φ_2, Ψ_2 correspondingly. Spherical harmonics are $Y_{l_1}^{m_1}(\vartheta_1, \varphi_1)$ and $Y_{l_2}^{m_2}(\vartheta_2, \varphi_2)$ and the answer should be given in a form of two vector functions $\mathbf{r}_1(\Delta r, \Theta_1, \Phi_1, \Psi_1, \Theta_2, \Phi_2, \Psi_2)$ and $\mathbf{r}_2(\Delta r, \Theta_1, \Phi_1, \Psi_1, \Theta_2, \Phi_2, \Psi_2)$. If they overlap each other, the degree of overlap has to be found. The latter is the shortest shift vector, which removes the overlap. Overlap is to be considered infinitesimally small.

Hint: The whole system can be reoriented in such a way that $\Theta_1 = \Phi_1 = \Psi_1 = 0$.

