Radial distribution functions

gmx rdf

The *radial distribution function* (RDF) or pair correlation function $g_{AB}(r)$ between particles of type A and B is defined in the following way:

$$\begin{aligned} g_{AB}(r) &= \frac{\langle \rho_B(r) \rangle}{\langle \rho_B \rangle_{local}} \\ &= \frac{1}{\langle \rho_B \rangle_{local}} \frac{1}{N_A} \sum_{i \in A}^{N_A} \sum_{j \in B}^{N_B} \frac{\delta(r_{ij} - r)}{4 \pi r^2} \end{aligned} \tag{435}$$

with $\langle \rho_B(r) \rangle$ the particle density of type B at a distance r around particles A, and $\langle \rho_B \rangle_{local}$ the particle density of type B averaged over all spheres around particles A with radius r_{max} (see Fig. 52 C).

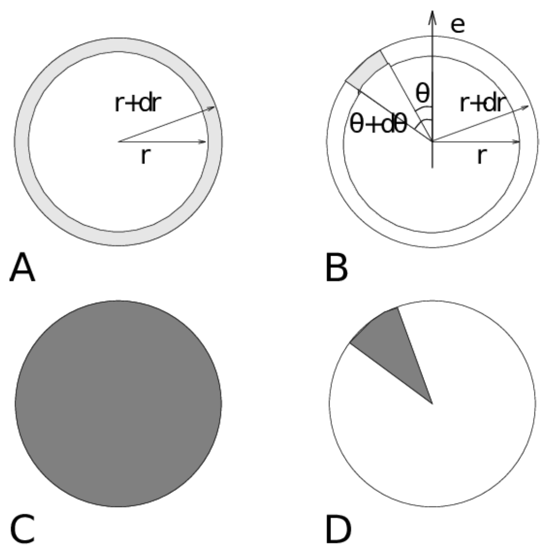
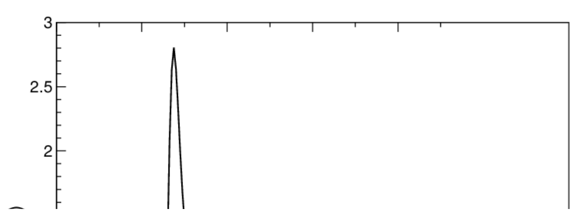


Fig. 52 Definition of slices in gmx rdf: A. $g_{AB}(r)$. B. $g_{AB}(r, \theta)$. The slices are colored gray. C. Normalization $\langle \rho_B \rangle_{local}$. D. Normalization $\langle \rho_B \rangle_{local,\ \theta}$. Normalization volumes are colored gray.

Usually the value of r_{max} is half of the box length. The averaging is also performed in time. In practice the analysis program gmx rdf divides the system into spherical slices (from r to $r + dr$, see Fig. 52 A) and makes a histogram in stead of the δ-function. An example of the RDF of oxygen-oxygen in SPC water 80 is given in Fig. 53



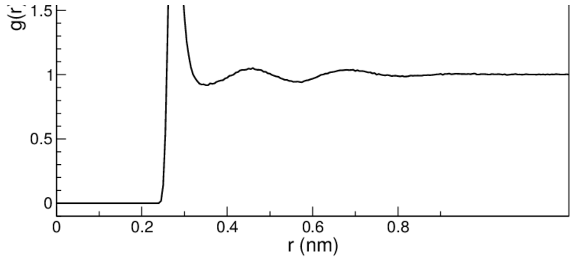


Fig. 53 $g_{OO}(r)$ for Oxygen-Oxygen of SPC-water.

With gmx rdf it is also possible to calculate an angle dependent rdf $g_{AB}(r,\theta)$, where the angle θ is defined with respect to a certain laboratory axis $\mathbf{e}$, see Fig. 52 B.

$$g_{AB}(r,\theta) = \frac{1}{\langle\rho_B\rangle_{local,\,\theta}} \frac{1}{N_A} \sum_{i\in A}^{N_A} \sum_{j\in B}^{N_B} \frac{\delta(r_{ij}-r)\delta(\theta_{ij}-\theta)}{2\pi r^2 sin(\theta)} \tag{436}$$

$$cos(\theta_{ij}) = \frac{\mathbf{r}_{ij}\cdot\mathbf{e}}{\|r_{ij}\|\;\|e\|} \tag{437}$$

This $g_{AB}(r,\theta)$ is useful for analyzing anisotropic systems. **Note** that in this case the normalization $\langle\rho_B\rangle_{local,\,\theta}$ is the average density in all angle slices from θ to $\theta + d\theta$ up to r_{max}, so angle dependent, see Fig. 52 D.