A fast and accurate SAS calculation from MD simulations

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Our talk will focus on the calculation of SAXS (and SANS) profiles from molecular dynamics simulations. Applications to globular and membrane proteins along with DNA and RNA will show that SAXS calculations can be used to probe and validate force fields for bio-molecular systems in solution. The SAXS method that we have developed uses 3D fast Fourier transforms (FFTs) and particle meshing interpolation, similar to the one used in smooth particle mesh Ewald for electrostatic energies and forces, combined with a uniform solvent density FFT padding scheme to obtain a convenient SAXS spectral resolution. As a FFT's approach, our method scales favorably for systems of increasing size and is devoid of many of the artifacts of other approaches proposed so far in the literature.