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Supporting information for article:

Calculation of two-dimensional scattering patterns for oriented systems

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Supplementary information

The possibilities and also the limits of **Polygen2D** are demonstrate in this supplementary part. In figure S1 the subunit size is varied. In this case, the subunit size of model must be smaller than the resolution of the scattering pattern $d_{\text{sub}} < \pi/q_{\text{max}}$. Four different subunit sizes are used using 1.0 Å, 2.0 Å, 6.5 Å and 7.0 Å. The corresponding bi-dimensional scattering pattern are shown in panels A-D. The results show that if the size of subunit is at least two times smaller than π/q_{max} a good description of the expected scattering image is obtained.

To calculate the scattering pattern from very anisometric oriented objects with main axis perpendicular to incident beam, it is necessary use very small bin sizes on the histogram of the projections. This is necessary, in cases where the density of subunits is very high, and there are many projections around 90°, so there are many small projections of pairs distances around value 0.0, equation (13). The increase of step of histogram of the projections increases linearly the time of the simulation. Thus, to optimize the calculation time, it is possible to use two different bin sizes in histogram of the projections, decreasing the size of bin used in small projection (angles between two subunits around 90° produce short distance), and using other bigger step to most large distance projection. The results from this point are available in figures S2 and S3.

One example demonstrating the use of subunits with different scattering length densities is shown in figure S4.

The possibilities showed in section 2.3 *Introducing Polydispersity in Orientations* and 2.4 *Generation of 3D scattering space for the particle* are presented in figures S5 and S6, respectively.

To show the influence of angular step used in calculation of two-dimensional scattering pattern, four different angular steps was used, 0.1°, 1.0°, 2.0° and 5.0°. The four images simulated, figure S7, show good relative agreement, and large angular steps could be used to make fast tests, until the target pattern is obtained. There are deviations, mainly at high angles, due to the fact that if there are pixels without a computed value, the program calculates the average of neighboring pixels, according to the angle and distance of center. Thus, if the angular step is large, it is necessary to calculate more pixel values using the values of neighborhood pixel.

Typical calculation times, varying the number of cores used on the parallelization procedure, are shown in Figure S8. Examples for hen egg lysozyme (4NY5.PDB), collagen model peptide (2CUO.PDB) and rod model (see Figure 2) are shown. This example shows that the parallelization can speed up the calculation up to 4 times. These calculations were performed on a laptop machine, with 8M of RAM equipped with processor Intel® Core™ i7-3610QM CPU 2.30GHz × 8.

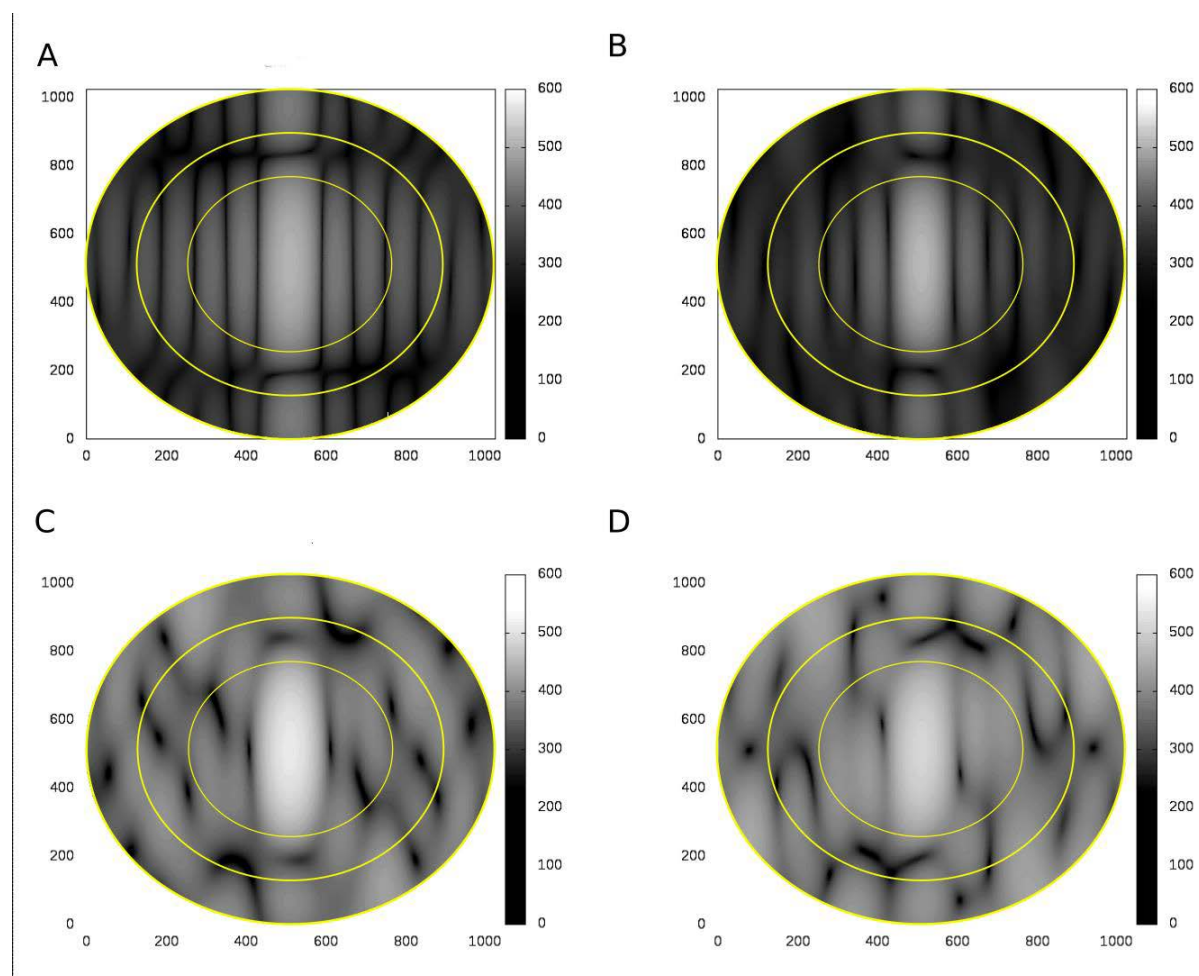


Figure S1 Computation of test example for parallelepiped, modeled using different subunit radius.
(A) Image calculated using subunit radius: (A) 1.0 Å, (B) 2.0 Å, (C) 6.5 Å and (D) 7.0 Å.

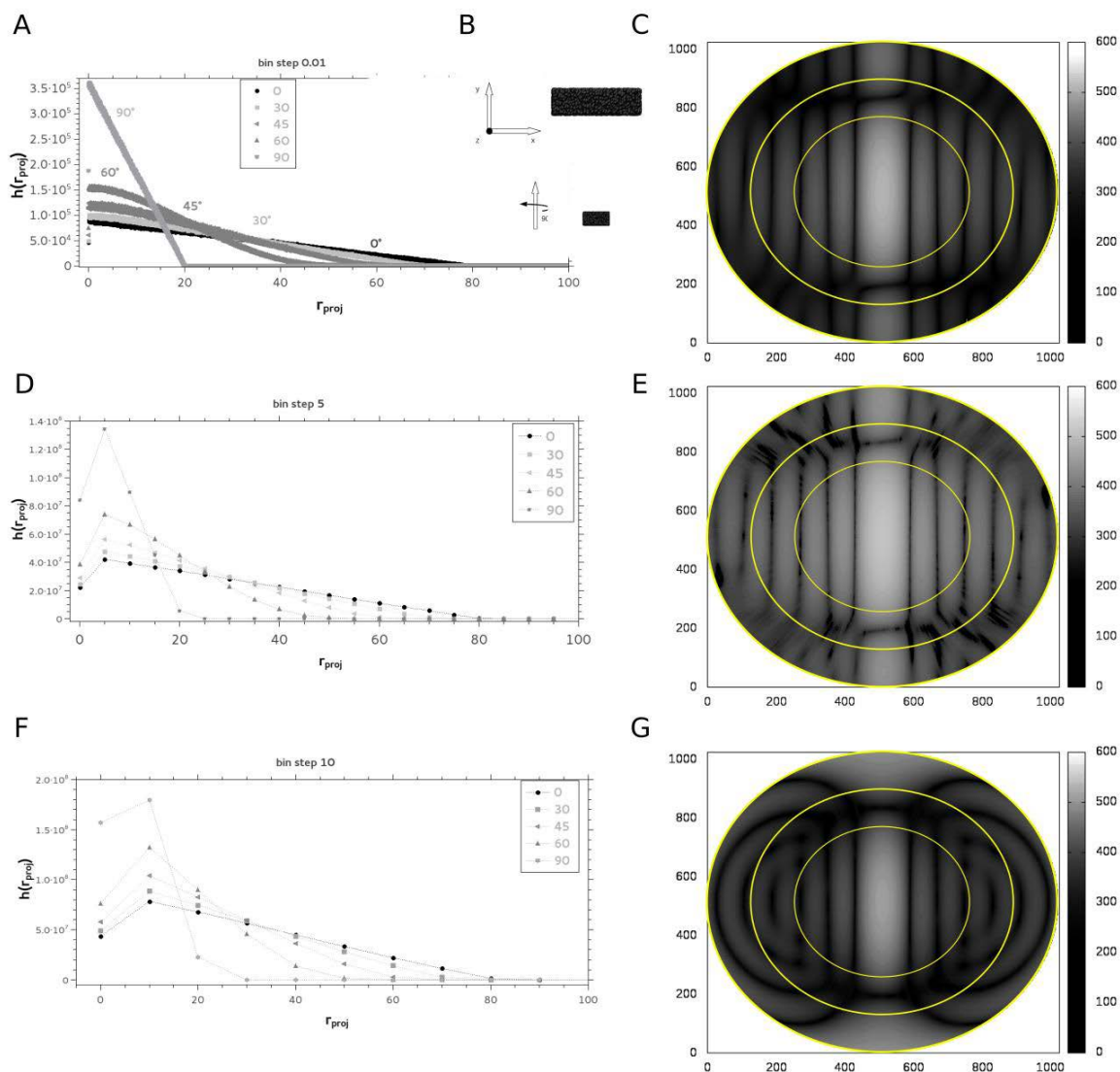


Figure S2 Computation of test example for parallelepiped, using different number of channels in the histogram (bin step), equation (13). The bin step used in histogram calculation: (A) 0.01, (D) 5.0 and (F) 10 Å. (B) Model of parallelepiped used to simulate the images: (C) bin step: 0.01, (E) bin step: 5.0 and (G) bin step: 10.0 Å. The pale rings corresponds to a radius of 0.25, 0.375 and 0.5 (\AA^{-1}).

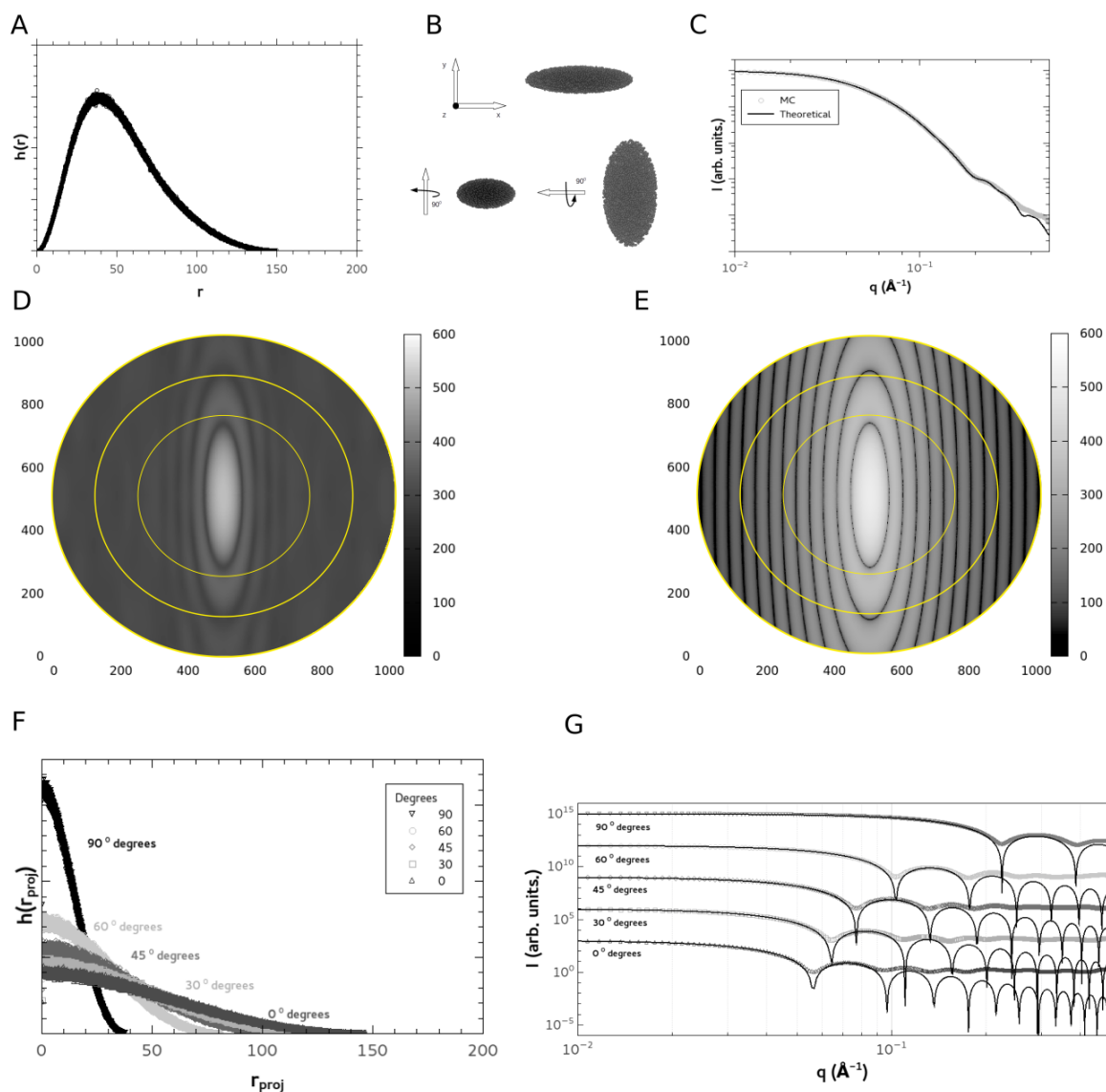


Figure S3 Computation of test example for parallelepiped, using different number of channels (bin step) in the same the histogram, equation (13). The different bin steps used in histogram calculation: (A) bin step (in \AA): 0.001 (from 0.000 to 10.000) and bin step: 0.01 (from 10.00 to 100.00). (C) Simulated images using the histograms (A). (B) Model of parallelepiped used to simulate the 2D image of scattering. (D) Bin step: 1.0 (from 0.0 to 100.0). (E) Simulated images using the histogram (D). (F) Bin step: 0.001 (from 0.001 to 10.000) and bin step: 1.0 (from 10.0 to 100.0). (G) Simulated images using the histogram (F). The yellow rings corresponds to a radius of 0.25, 0.375 and 0.5 (\AA^{-1}).

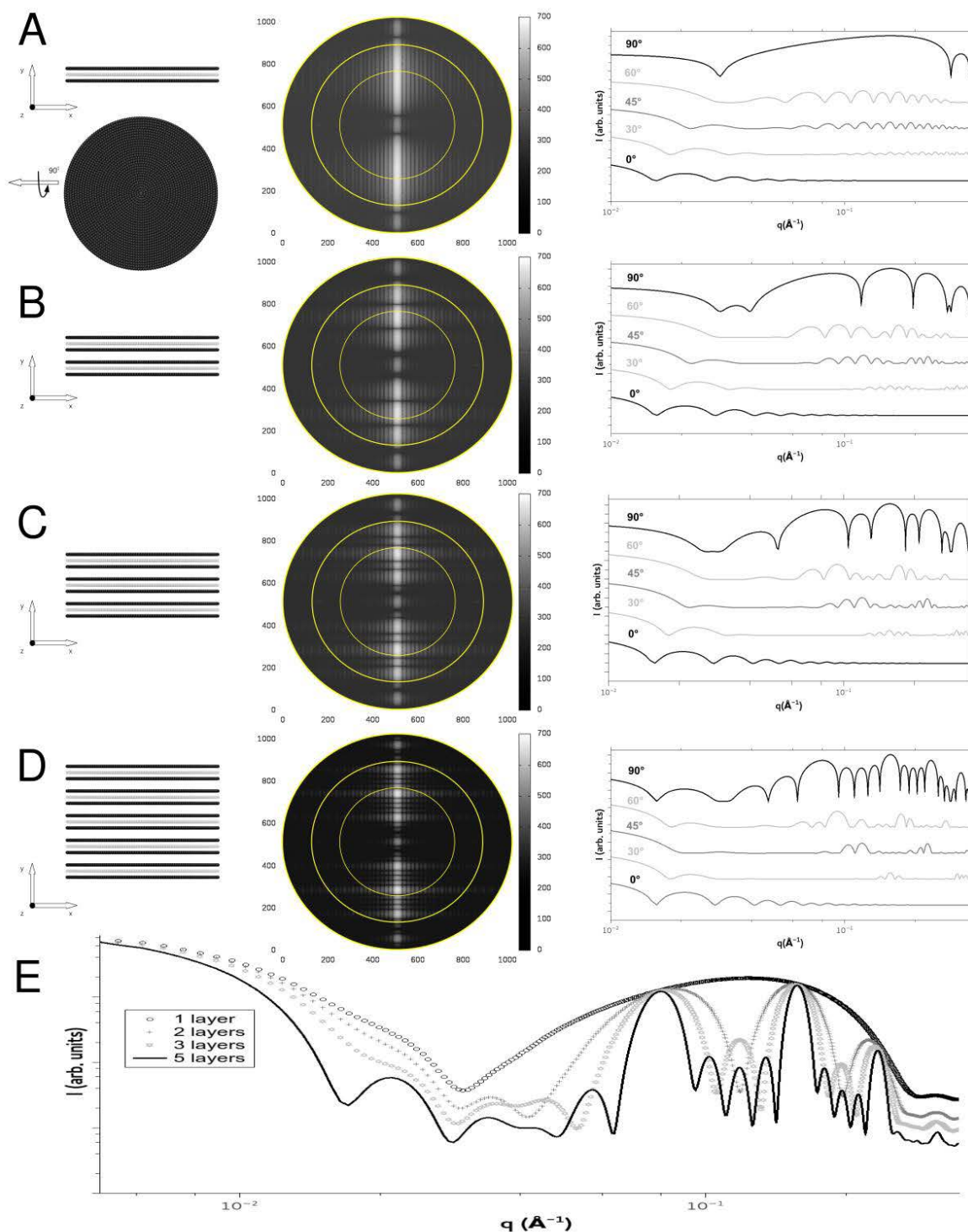


Figure S4 Computation of test example for systems with variable scattering length density for the subunits. The model is composed of three parallel circular plates (bilayer) with radius of 250 Å, separated by a distance of 20 Å. Copies of this bilayer are then separated by a distance of 60 Å. The dummy atoms in the external layer (dark atoms) have scattering factor equal to 0.6 and dummy atoms in the internal layer (grey atoms) -1.0. For (A-D): (left) model; (center) 2D scattering pattern simulated for the model oriented as in the side view. The pale rings corresponds to a radius of 0.17, 0.26 and 0.35

(\AA^{-1}). (right) One-dimensional cuts in the image in five directions of q . (A) (left) bilayer model in top and side view. (B) (left) Two bilayer model (side view). (C) (left) Three bilayer model (side view). (D) (left) Five bilayer model (side view). (E) The simulation of scattered intensity of the all bilayers models randomly oriented.

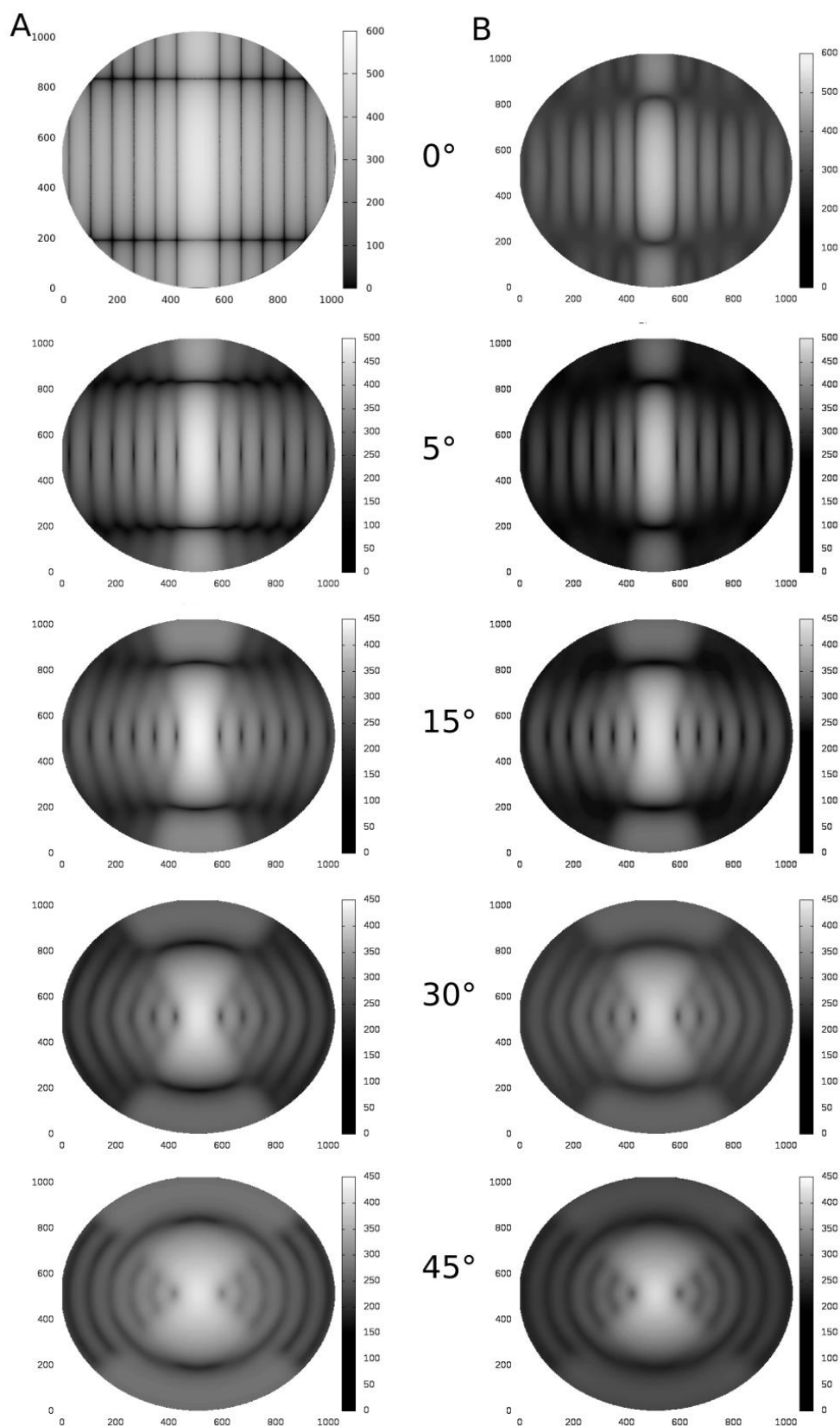


Figure S5 Computation of test example for parallelepiped introducing polydispersity in orientations, using a uniform distribution. (A) Image calculated with semi-analytic expression for parallelepiped

introducing dispersity in orientations of angles, from top to bottom: 0° (without introducing dispersity), -5° to 5° , -15° to 15° , 30° to 30° and -45° to 45° . (B) Simulation of image of scattered intensity introducing dispersity in orientations of the range, from top to bottom: 0° (without introducing dispersity), -5° to 5° , -15° to 15° , -30° to 30° and -45° to 45° .

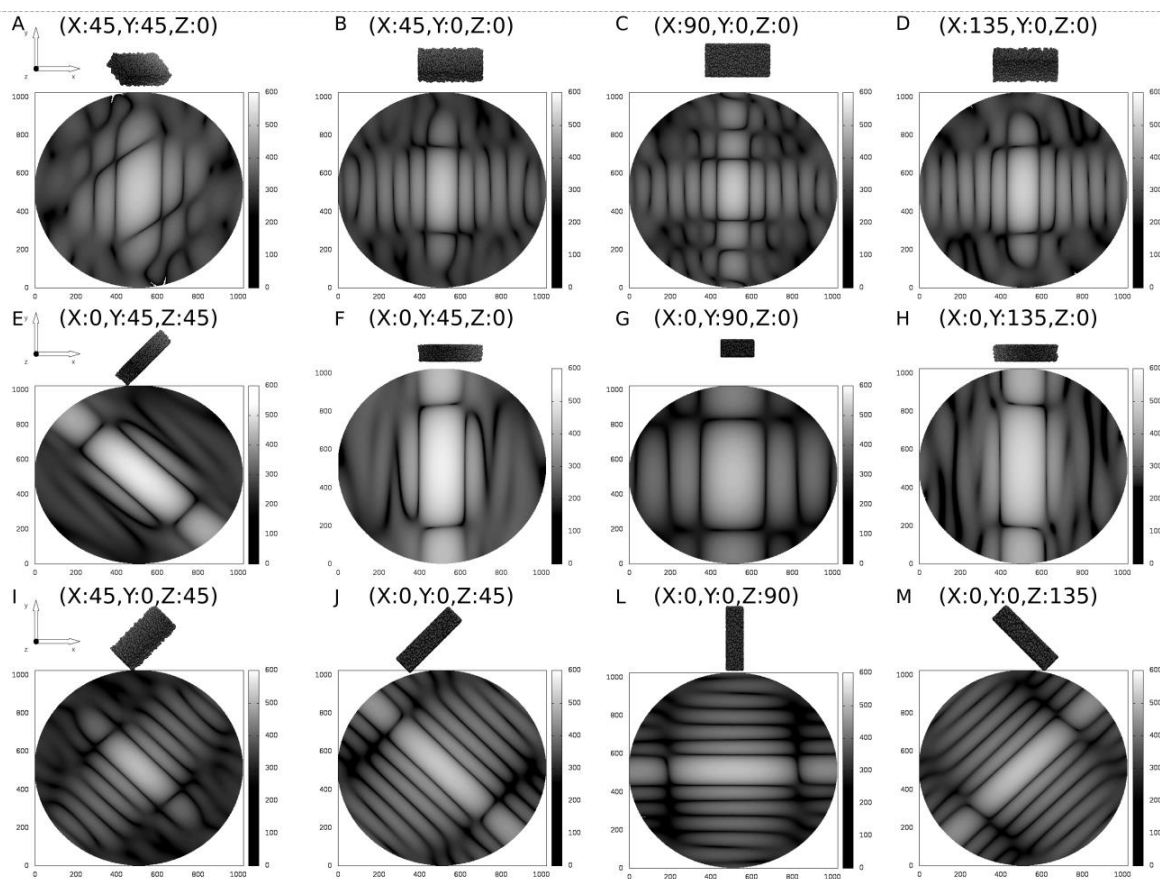


Figure S6 Computation of test example for parallelepiped, in different positions rotated. The different models was rotated by the following sorted angles (in degrees): (A) X:45, Y:45, Z:0. (B) X:45, Y:0, Z:0. (C) X:90, Y:0, Z:0. (D) X:135, Y:0, Z:0. (E) X:0, Y:45, Z:45. (F) X:0, Y:45, Z:0. (G) X:0, Y:90, Z:0. (H) X:0, Y:135, Z:0. (I) X:45, Y:0, Z:45. (J) X:0, Y:0, Z:45. (L) X:0, Y:0, Z:90. (M) X:0, Y:0, Z:135.

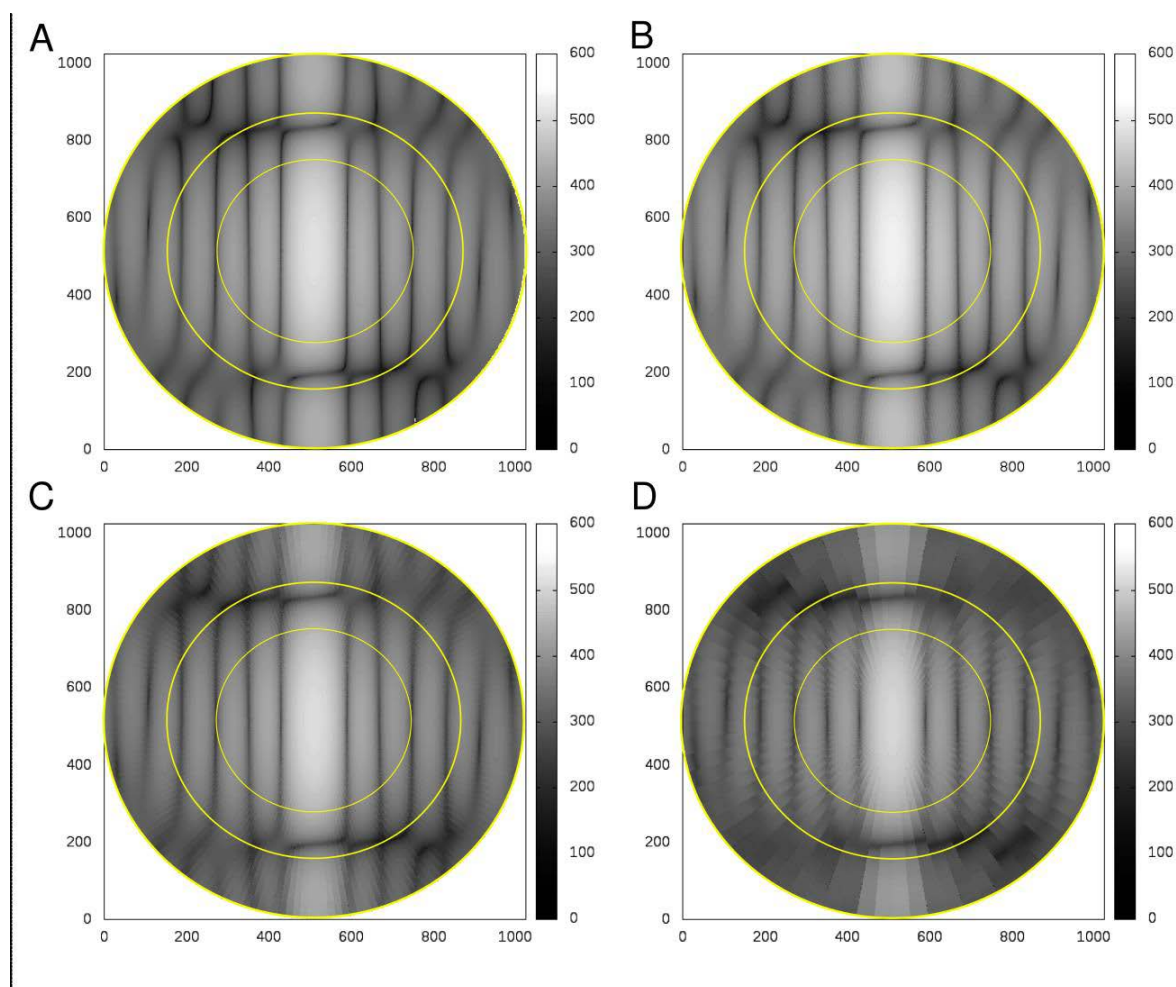


Figure S7 Computation of test example using parallelepiped model (the same used in figure S5), introducing different step angles to calculate the scattering pattern. Simulation of image of scattered intensity with different angles steps: (A) 0.1° , (B) 1.0° (C) 2.0° and (D) 5.0° . The pale rings corresponds to a radius of 0.25, 0.375 and 0.5 (\AA^{-1}).

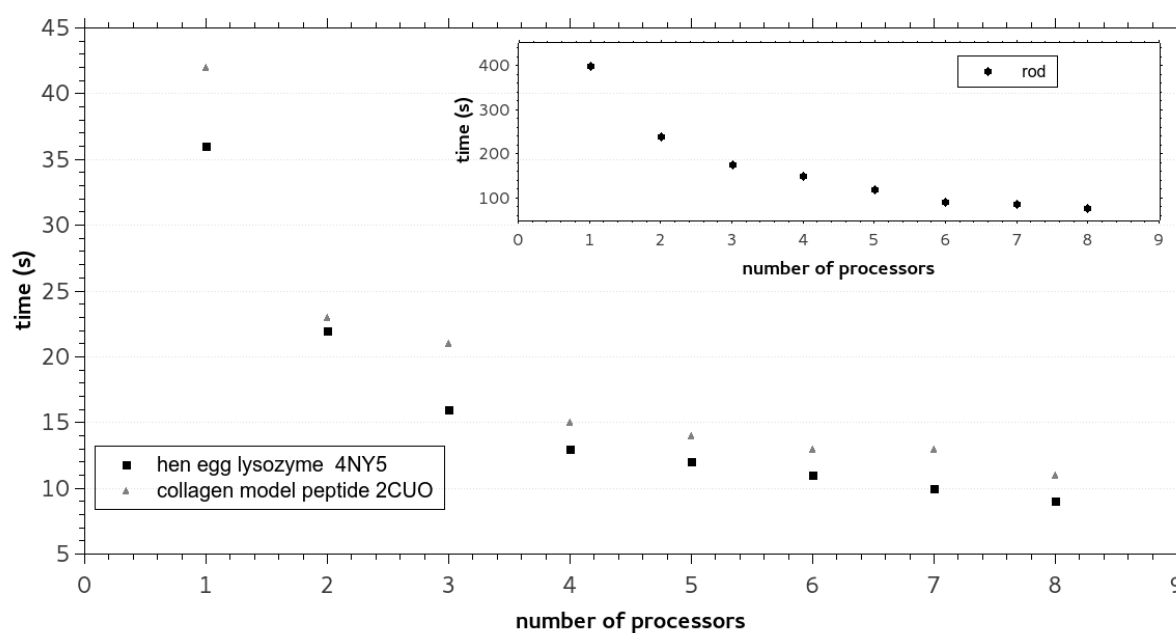


Figure S8 Typical computation times for intensity calculation varying the number of processors used in the parallelization. The values for the hen egg lysozyme (4NY5.PDB) collagen model peptide (2CUO.PDB) and rod (insert) are shown. These calculations were performed on a laptop machine, with 8M of RAM equipped with processor Intel® Core™ i7-3610QM CPU 2.30GHz × 8.