

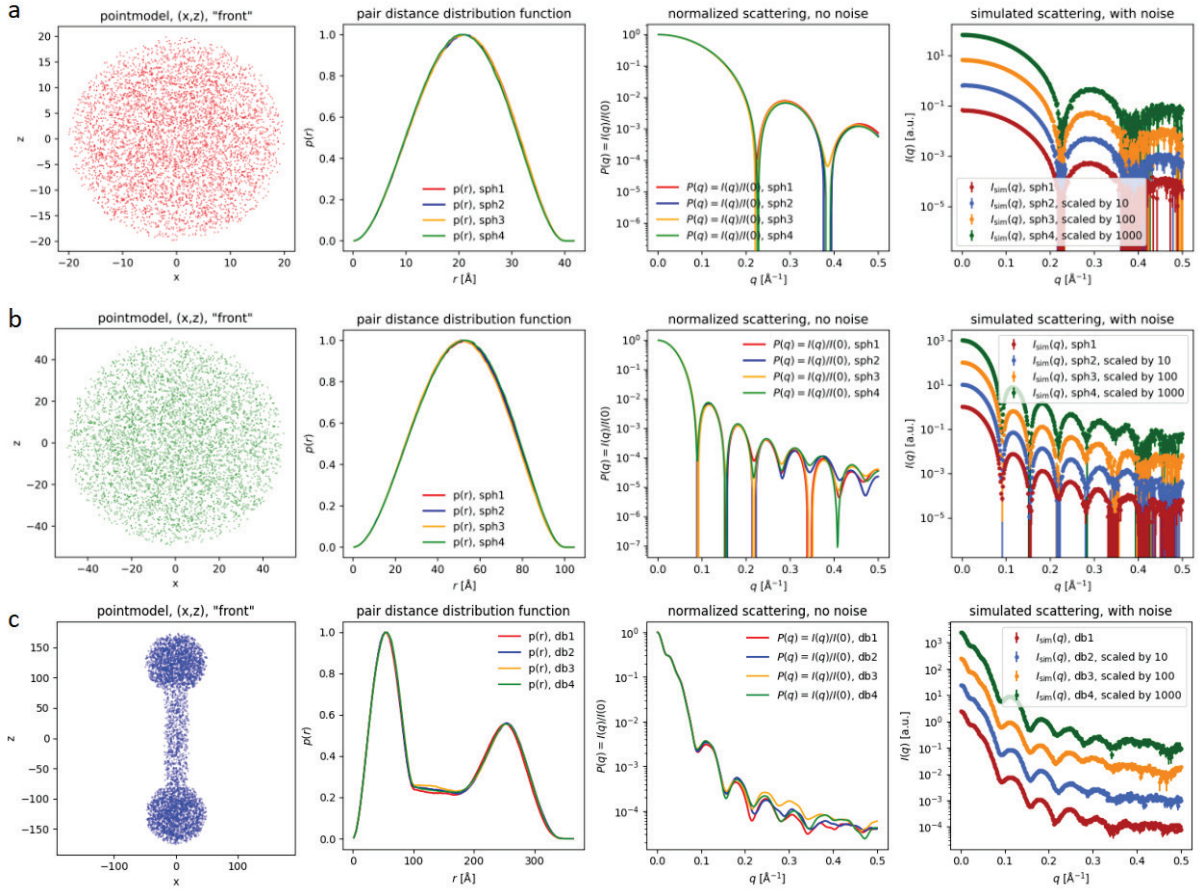


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**Supporting information for article:**

***Shape2SAS: a web application to simulate small-angle scattering data and pair distance distributions from user-defined shapes***

**Andreas Haahr Larsen, Emre Brookes, Martin Cramer Pedersen and Jacob Judas Kain Kirkensgaard**



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2 **Figure S1.** Precision of Shape2SAS when using 5000 points. Calculated pair distance  
3 distribution and intensity for five repeated simulations. (a) Sphere with radius 20 Å. (b)  
4 Sphere with radius 50 Å. (c) Dumbbell composed of a cylinder with radius 20 Å and length  
5 200 Å, and two spheres of radius 50 Å, with their center of mass shifted  $\pm 125$  Å.

**a**

q min [ $1/\text{\AA}$ ] 0.001  
q max [ $1/\text{\AA}$ ] 0.5  
Number of points in q 400  
Relative exposure time [a.u.] 100  
Number of points in p(r) 100  
Number of simulated points 5000

Calculate scattering for Model 1

Name of Model 1 sph\_excl\_on  
Exclude overlap regions   
Number of subunits 2

subunit type	a	b	c	$\Delta\text{SLD}$	x_com	y_com	z_com
Sphere	50			1	-15	0	0
Sphere	50			-1	15	0	0

Relative polydispersity 0  
Structure factor None  
Volume fraction (conc) 0.02  
Interface roughness [ $\text{\AA}$ ] 0

Calculate scattering for Model 2

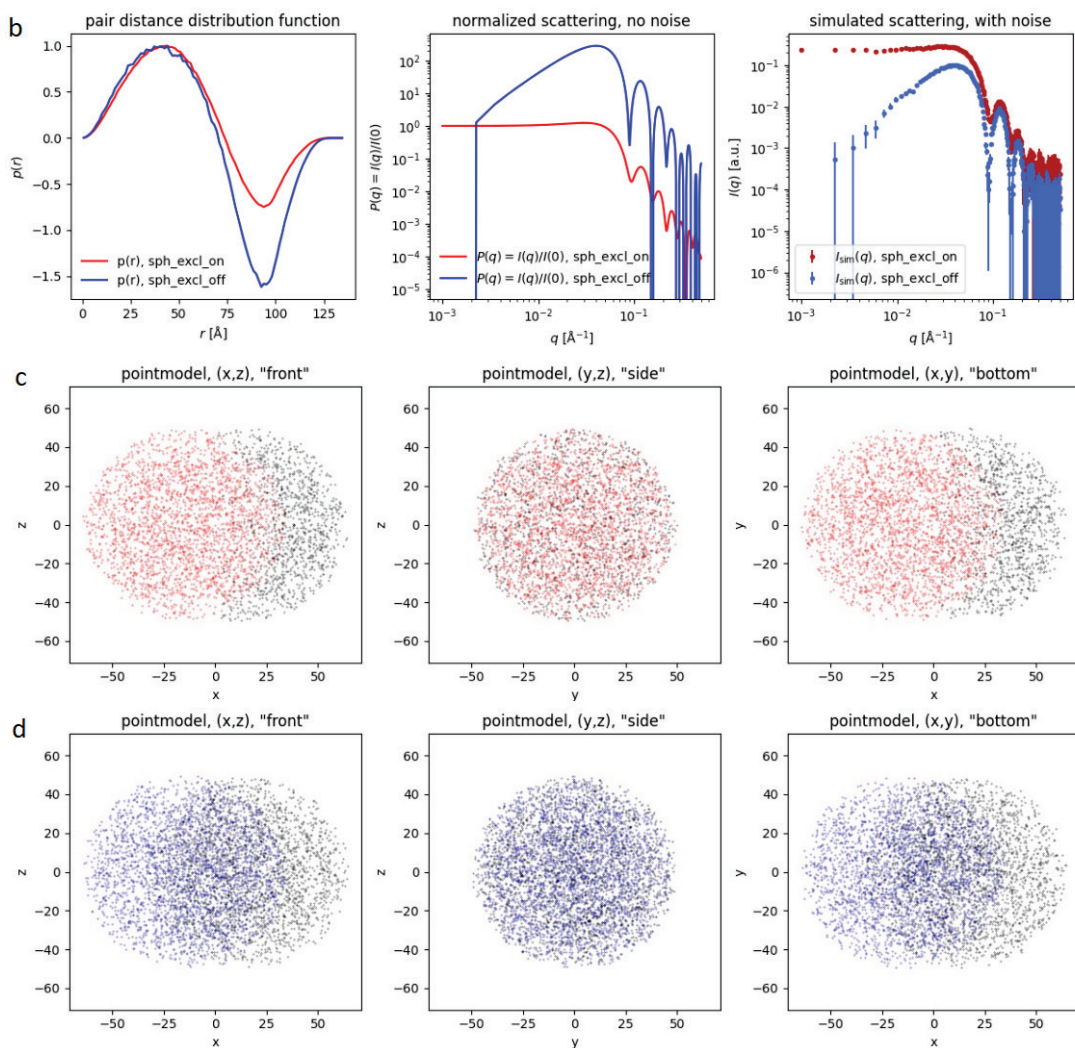
Name of Model 2 sph\_excl\_off  
Exclude overlap regions   
Number of subunits 2

subunit type	a	b	c	$\Delta\text{SLD}$	x_com	y_com	z_com
Sphere	50			1	-15	0	0
Sphere	50			-1	15	0	0

Relative polydispersity 0  
Structure factor None  
Volume fraction (conc) 0.02  
Interface roughness [ $\text{\AA}$ ] 0

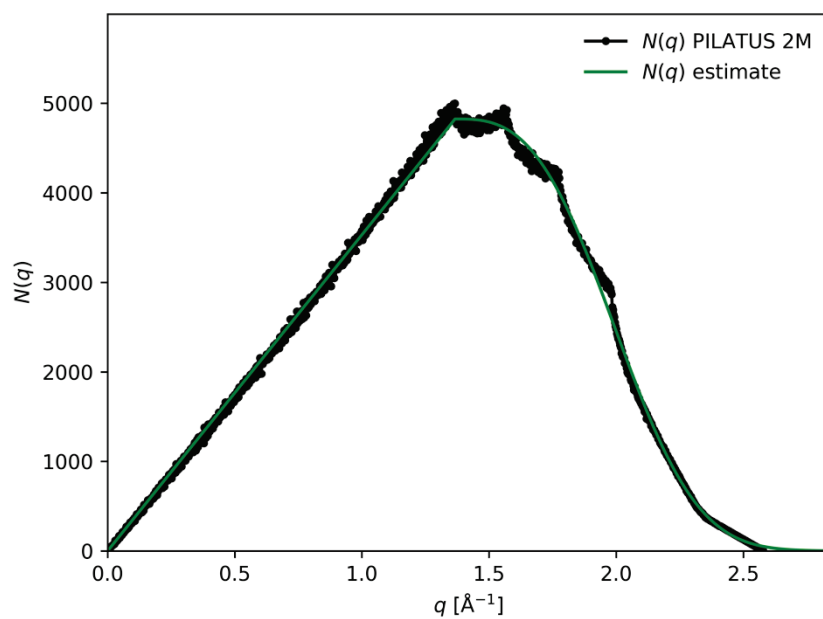
Calculate scattering for Model 3

Calculate scattering for Model 4



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7 **Figure S2.** Illustration of 2 models with exclusion of regions enables (red) or disables (blue).  
8 (a) Input. (b) Output pair distance distribution and scattering. (c-d) 2D projections of the  
9 particles. Red/blue for positive contrast, black for negative.

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 12 **Figure S3.** Numerical approximation (black) of the number of pixels per  $q$  bin, obtained by  
 13 simulating a SAXS setup with a PILATUS 2M detector (centered beam, pixel size 172x172  
 14  $\mu\text{m}$ , 1475x1679 pixels,  $\lambda = 1.0 \text{ \AA}$ , sample-detector distance 0.5 m, 1000 bins in the  $N(q)$   
 15 histogram). Analytical approximation (green) plotted on top.

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	<b>McSim</b>	<b>Shape2SAS version 1.2</b>	
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19	Language	Fortran77+Gnuplot	Python3
20	Installation	compile from source code	no installation required
21	GUI	none*	web-application
22	Max number of models	1	4
23	Max number of subunits	10	15
24	Visualization of model(s)	2D projections	2D projections, 3D visualization
25	Documentation	source code	source code, current paper, web app.
26		----- <i>Additional options</i> -----	
27	Polydispersity	yes (Gaussian)	yes (Gaussian)
28	Interface roughness	no	yes
29	Structure factors	none	hard-sphere, aggregation (2D fractal)
30		----- <i>Simulated data</i> -----	
31	Error model	$\sigma(q) = aI(q) + b$	empirical model (Appendix A)
32	Forward scattering	$I(0) = 1$	depends on contrast, volume and conc.

33 **Table S1:** comparison of McSim and Shape2SAS. \*There used to be a web interface for  
34 McSim [1], but this is no longer available.

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37 **References for supplemental information**

- 38 1. Hansen, S. Update for BayesApp : A Web Site for Analysis of Small-Angle Scattering  
39 Data. *J. Appl. Crystallogr.* **2014**, *47*, 1469–1471, doi:10.1107/S1600576714013156.

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