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Cont2SAS: A python package for calculating SAS parameters from continuum nanostructures

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DOI: 10.xxxxxx/draft

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Submitted: 01 January 1970
Published: unpublished

Summary

Cont2SAS facilitates the calculation of Small Angle Scattering (SAS) parameters from simulated Continuum (Cont) nanostructures. Cont2SAS is built on the existing software solution Sassena – known for calculating scattering patterns from simulated atomic structures (Lindner, 2012, 2017; Lindner & Smith, 2012; Majumdar et al., 2024; Majumdar & Lindner, 2023). Cont2SAS can calculate SAS patterns and the effective scattering cross-section (σ_{eff}). SAS patterns contain a SAS intensity (I) vs. scattering vector magnitude (Q). The σ_{eff} is the count rate of scattered radiation per incident unit flux. The time evolution of σ_{eff} is calculated from SAS patterns at different time steps. Through the comparison of calculated and measured SAS parameters, simulations and SAS experiments can be used complementarily for different purposes, such as validating simulations, tuning simulation parameters, and analyzing SAS data obtained from experiments (Dorrell et al., 2020; Majumdar et al., 2024; Reich et al., 2022).

Statement of need

The simulation of material structure at the nanometer length scale can be performed using atomistic simulations and continuum simulations. Continuum simulations have the advantage over atomistic ones that they can simulate bigger volumes for a larger time. However, continuum simulations are less accurate than the atomistic simulations. Cont2SAS is created to check the accuracy of continuum simulations by validating them against SAS experiments, such as Small Angle Neutron Scattering (SANS) and Small Angle X-ray Scattering (SAXS). The validation is performed by comparing SAS parameters calculated using Cont2SAS with measured ones. A validated simulation can also be used to retrieve nanostructure from SAS data because a direct retrieval of nanstructure from SAS data is not possible (Billinge & Levin, 2007). Alternatively to simulating continuum nanostructures based on physics-based equations, they can also be simulated based on the user's knowledge of the sample to retrieve nanostructures from SAS data.

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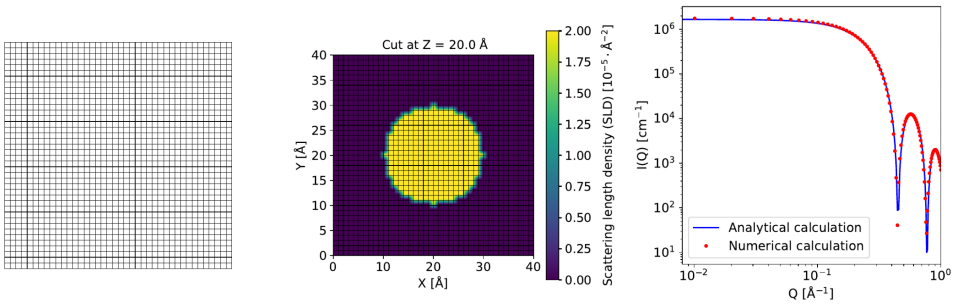

Figure 1: Workflow of SAS pattern calculation: [left] Mesh generation, [middle] SLD assignment, [right] numerical calculation of SAS pattern. The numerical calculation matches well with the known analytical formula for spherical nanoparticles (Guinier et al., 1955).

Both physics- and knowledge-based simulated structures are expected to output either Scattering Length Density (SLD) (β) values or a set of variables (e.g. local molar density (ρ_m) and composition (χ)) from which SLD values can be calculated. `Cont2SAS` creates a mesh, assigns SLD based on the simulated values, and calculates SAS pattern from them, as shown in Figure 1.

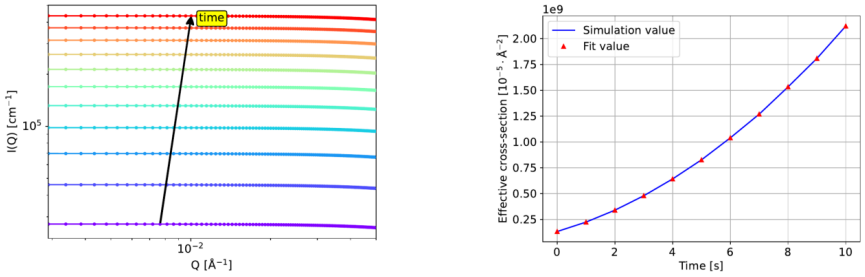

Figure 2: Workflow of effective cross-section (σ_{eff}) calculation: [left] Calculated SAS pattern at different time steps, [right] σ_{eff} calculated from SAS patterns at different time steps: .

For some materials, the nanostructure does not change over time but the chemical composition does (e.g., ball-milled hydrogen storage materials). For such a scenario, the time evolution of the count rate is a useful parameter (Aslan et al., 2019). This count rate per incident unit flux is named `effective cross-section` (σ_{eff}), and can be calculated using `Cont2SAS`. Figure 2 demonstrates such a calculation from a series of SAS patterns. The calculated σ_{eff} must be multiplied by an empirical factor before comparing with measured neutron count rate.

Conclusion

`Cont2SAS` provides the much needed software platform for calculating SAS pattern from continuum simulations of nanostructures. The addition of effective cross-section in the software package is going be helpful for analyzing powder-like structures. One can also retrieve continuum nanostructures from SAS data using simulated structures.

Acknowledgements

This publication was written in the context of the work of the consortium DAPHNE4NFDI in association with the German National Research Data Infrastructure (NFDI) e.V. NFDI is

financed by the Federal Republic of Germany and the 16 federal states and the consortium is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - project number 460248799. The authors would like to thank for the funding and support. Furthermore, thanks go to all institutions and actors who are committed to the association and its goals.

References

Aslan, N., Horstmann, C., Metz, O., Kotlyar, O., Dornheim, M., Pistidda, C., Busch, S., Lohstroh, W., Müller, M., & Pranzas, K. (2019). High-pressure cell for in situ neutron studies of hydrogen storage materials. *Journal of Neutron Research*, *21*(3-4), 125–135. https://doi.org/10.3233/JNR-190116

Billinge, S. J., & Levin, I. (2007). The problem with determining atomic structure at the nanoscale. *Science*, *316*(5824), 561–565.

Dorrell, M. W., Beaven, A. H., & Sodt, A. J. (2020). A combined molecular/continuum-modeling approach to predict the small-angle neutron scattering of curved membranes. *Chemistry and Physics of Lipids*, *233*, 104983. https://doi.org/10.1016/j.chemphyslip.2020.104983

Guinier, A., Fournet, G., Walker, C. B., & Yudowitch, K. L. (1955). *Small-angle scattering of x-rays*. Wiley New York.

Lindner, B. (2012). *Towards a unification of supercomputing, molecular dynamics simulation and experimental neutron and x-ray scattering techniques* [PhD thesis]. University of Tennessee, United States.

Lindner, B. (2017). *Sassena*. https://github.com/camm/sassena.

Lindner, B., & Smith, J. C. (2012). Sassena—x-ray and neutron scattering calculated from molecular dynamics trajectories using massively parallel computers. *Computer Physics Communications*, *183*(7), 1491–1501. https://doi.org/10.1016/j.cpc.2012.02.010

Majumdar, A., & Lindner, B. (2023). *Sassena*. https://codebase.helmholtz.cloud/DAPHNE4NFDI/sassena. https://doi.org/10.5281/zenodo.10037485

Majumdar, A., Müller, M., & Busch, S. (2024). Computation of x-ray and neutron scattering patterns to benchmark atomistic simulations against experiments. *International Journal of Molecular Sciences*, *25*(3), 1547. https://doi.org/10.3390/ijms25031547

Reich, V., Majumdar, A., Müller, M., & Busch, S. (2022). Comparison of molecular dynamics simulations of water with neutron and x-ray scattering experiments. *EPJ Web of Conferences*, *272*, 01015. https://doi.org/10.1051/epjconf/202227201015