

# <sup>1</sup> Cont2SAS: A python package for calculating SAS parameters from continuum nanostructures

<sup>3</sup> **Arnab Majumdar**  <sup>1,3</sup>, **Martin Müller** <sup>1,2,3</sup>, and **Sebastian Busch**  <sup>1¶</sup>

<sup>4</sup> 1 German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ),  
<sup>5</sup> Helmholtz-Zentrum Hereon GmbH, Lichtenbergstr. 1, 85748 Garching, Germany 2 Institute of Materials  
<sup>6</sup> Physics, Helmholtz-Zentrum Hereon GmbH, Max-Planck-Str. 1, 21502 Geesthacht, Germany 3 Institut  
<sup>7</sup> für Experimentelle und Angewandte Physik (IEAP), Christian-Albrechts-Universität zu Kiel, Leibnizstr.  
<sup>8</sup> 19, 24098 Kiel, Germany ¶ Corresponding author

DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

## Software

- [Review](#) 
- [Repository](#) 
- [Archive](#) 

---

Editor: [Open Journals](#) 

Reviewers:

- [@openjournals](#)

Submitted: 01 January 1970

Published: unpublished

## License

Authors of papers retain copyright and release the work under a

Creative Commons Attribution 4.0 International License ([CC BY 4.0](#))

## <sup>9</sup> Summary

<sup>10</sup> Cont2SAS is a software tool built around the existing software solution Sassen - known for calculating scattering patterns from simulated atomic structures. The goal of Cont2SAS is to provide a software similar to Sassen, but for calculating Small Angle Scattering (SAS) data from simulated Continuum (Cont) nanostructures. Cont2SAS can calculate SAS patterns, i.e. SAS intensity ( $I$ ) vs. scattering vector magnitude ( $Q$ ) using a novel numerical method. Cont2SAS can also calculate effective cross-section ( $\sigma_{\text{eff}}$ ), i.e. the count rate of scattered radiation per incident unit flux.  $\sigma_{\text{eff}}$  is calculated by integrating instrument-agnostic SAS patterns taking instrument geometry into account. Cont2SAS can be used for different purposes, such as validating simulations, tuning simulation parameters, and analyzing SAS data.

## <sup>18</sup> Statement of need

Small Angle Scattering (SAS) experiments with neutrons (SANS) and X-rays (SAXS) are useful techniques for probing material nanostructures (Chen et al., 2012). With the Time Resolved (TR) variant of SAS, the time evolution of nanostructures can also be probed (Hollamby, 2013). However, a direct retrieval of nanostructure from SAS data is not possible due to the so-called phase problem (Billinge & Levin, 2007). Therefore, it is fruitful to combine SAS data with simulations to study nanostructures (Majumdar et al., 2024). This approach is also useful for validating theories underlying simulations (Reich et al., 2022).

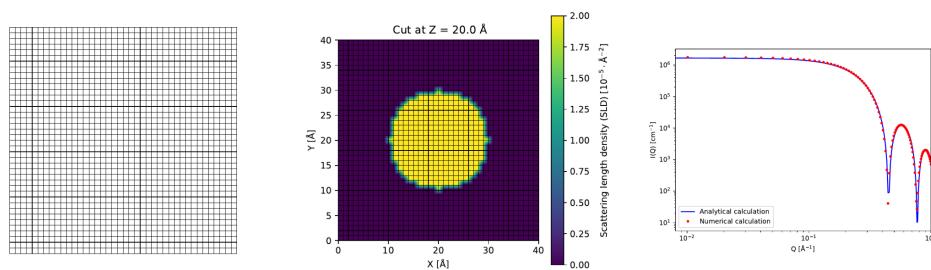
Simulated structures in real space can be generated using atomistic and continuum simulation. However, continuum simulation is the only option when the nanostructure evolution is influenced by bigger features or the SAS data is recorded for long time period, as atomistic simulation can not simulate large structures for long time (Ghavanloo et al., 2019). Despite this indispensability, there is no software available for calculating SAS data from continuum simulations. Cont2SAS aims to fill this void by providing a tool that offers fast and error-free comparison of continuum simulations and SAS data. The ultimate goal is to study nanomaterials and validating theories using SAS data, particularly when length-scales and time-scales, inaccessible to atomistic simulations, need to be simulated.

## <sup>36</sup> State of the field

<sup>37</sup> From atomistic simulations, different software such as nMoldyn (Hinsen, 2023; Rög et al., 2003), MDANSE (Goret et al., 2017; Neutron & Facility, 2023), LiquidLib (Walter et al., 2018; Z-laboratory, 2023), and Sassen (Lindner, 2012, 2017; Lindner & Smith, 2012; Majumdar et

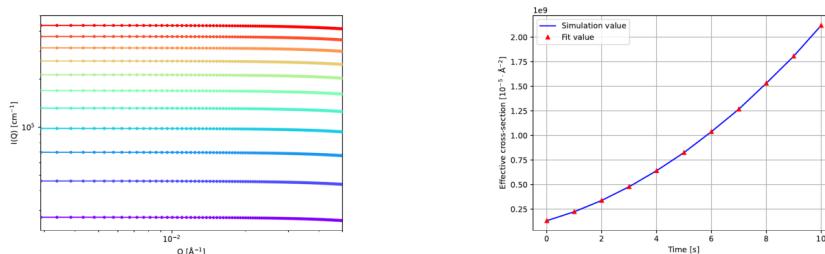
40 al., 2024; Majumdar & Lindner, 2023) can calculate SAS patterns but they can not calculate  
 41 the same from continuum simulations. An in-house code is available for continuum simulations  
 42 but it was built for a 2D membrane system lacking generality (Dorrell et al., 2020). Hence,  
 43 Cont2SAS is built using Sassena as a backend calculator. Sassena was chosen over other  
 44 software due to its notable computation speed and robustness (Majumdar et al., 2024).

## 45 Software features



**Figure 1:** Workflow of SAS pattern calculation: [left] Mesh generation, [middle] SLD assignment, [right] SAS pattern calculation.

46 Cont2SAS calculates SAS patterns taking simulated nanostructures as an input. The simulated  
 47 structure must provide either Scattering Length Density (SLD) ( $\beta$ ) values or a set of variables  
 48 from which SLD values can be calculated. The simulated input is processed to a data taylor-  
 49 made for Sassena. Sassena calculates the SAS intensity ( $I$ ) as a function of scattering vector  
 50 magnitude ( $Q$ ), i.e. SAS pattern, for different time steps (see Figure 1).



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

51 Cont2SAS can also calculate the time evolution of effective cross-section ( $\sigma_{\text{eff}}$ ), which is defined  
 52 as the count rate per incident unit flux. This feature was not available in the in-house code  
 53 (Dorrell et al., 2020) or Sassena (Majumdar & Lindner, 2023). The time evolution of count  
 54 rate is useful when the chemical composition changes over time instead of the nanostructure,  
 55 e.g. while storing hydrogen in ball-milled powder sample (Aslan et al., 2019). Figure 2  
 56 demonstrates the workflow of such calculation from a series of SAS patterns. The calculated  
 57  $\sigma_{\text{eff}}$  must be multiplied by an empirical factor before comparing with measured count rate.

## 58 Conclusion

59 Cont2SAS provides a software platform for calculating SAS pattern from continuum simulations  
60 of nanostructures. The addition of effective cross-section in the software package further  
61 enables the analysis of count rate. Cont2SAS can be used for analyzing SAS data and validating  
62 simulations to study nanomaterials.

## 63 Acknowledgements

64 This publication was written in the context of the work of the consortium DAPHNE4NFDI  
65 in association with the German National Research Data Infrastructure (NFDI) e.V. NFDI is  
66 financed by the Federal Republic of Germany and the 16 federal states and the consortium  
67 is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) -  
68 project number 460248799. The authors would like to thank for the funding and support.  
69 Furthermore, thanks go to all institutions and actors who are committed to the association  
70 and its goals.

## 71 References

- 72 Aslan, N., Horstmann, C., Metz, O., Kotlyar, O., Dornheim, M., Pistidda, C., Busch, S.,  
73 Lohstroh, W., Müller, M., & Pranzas, K. (2019). High-pressure cell for in situ neutron  
74 studies of hydrogen storage materials. *Journal of Neutron Research*, 21(3-4), 125–135.  
75 <https://doi.org/10.3233/JNR-190116>
- 76 Billinge, S. J., & Levin, I. (2007). The problem with determining atomic structure at the  
77 nanoscale. *Science*, 316(5824), 561–565. <https://doi.org/10.1126/science.1135080>
- 78 Chen, Z. H., Kim, C., Zeng, X., Hwang, S. H., Jang, J., & Ungar, G. (2012). Characterizing size  
79 and porosity of hollow nanoparticles: SAXS, SANS, TEM, DLS, and adsorption isotherms  
80 compared. *Langmuir*, 28(43), 15350–15361. <https://doi.org/10.1021/la302236u>
- 81 Dorrell, M. W., Beaven, A. H., & Sodt, A. J. (2020). A combined molecular/continuum-  
82 modeling approach to predict the small-angle neutron scattering of curved membranes.  
83 *Chemistry and Physics of Lipids*, 233, 104983. <https://doi.org/10.1016/j.chemphyslip.2020.104983>
- 85 Ghavanloo, E., Rafii-Tabar, H., & Fazelzadeh, S. A. (2019). *Computational continuum  
86 mechanics of nanoscopic structures*. Springer. <https://doi.org/10.1007/978-3-030-11650-7>
- 87 Goret, G., Aoun, B., & Pellegrini, E. (2017). MDANSE: An interactive analysis environment  
88 for molecular dynamics simulations. *Journal of Chemical Information and Modeling*, 57(1),  
89 1–5. <https://doi.org/10.1021/acs.jcim.6b00571>
- 90 Hinsen, K. (2023). *nMOLDYN3*—version 3.0.12. <https://github.com/khinsen/nMOLDYN3/>.
- 91 Hollamby, M. J. (2013). Practical applications of small-angle neutron scattering. *Phys. Chem.  
92 Chem. Phys.*, 15, 10566–10579. <https://doi.org/10.1039/C3CP50293G>
- 93 Lindner, B. (2012). *Towards a unification of supercomputing, molecular dynamics simulation  
94 and experimental neutron and x-ray scattering techniques* [PhD thesis]. University of  
95 Tennessee, United States.
- 96 Lindner, B. (2017). *Sassena*. <https://github.com/camm/sassena>.
- 97 Lindner, B., & Smith, J. C. (2012). Sassena—x-ray and neutron scattering calculated from  
98 molecular dynamics trajectories using massively parallel computers. *Computer Physics  
99 Communications*, 183(7), 1491–1501. <https://doi.org/10.1016/j.cpc.2012.02.010>
- 100 Majumdar, A., & Lindner, B. (2023). *Sassena*. <https://codebase.helmholtz.cloud/>

- 101        [DAPHNE4NFDI/sassena](https://doi.org/10.5281/zenodo.10037485). <https://doi.org/10.5281/zenodo.10037485>
- 102        Majumdar, A., Müller, M., & Busch, S. (2024). Computation of x-ray and neutron scattering  
103        patterns to benchmark atomistic simulations against experiments. *International Journal of  
104        Molecular Sciences*, 25(3), 1547. <https://doi.org/10.3390/ijms25031547>
- 105        Neutron, U. S. I., & Facility, M. (2023). *MDANSE-version 1.5.2*. [https://github.com/  
106        ISISNeutronMuon/MDANSE/](https://github.com/ISISNeutronMuon/MDANSE/).
- 107        Reich, V., Majumdar, A., Müller, M., & Busch, S. (2022). Comparison of molecular dynamics  
108        simulations of water with neutron and x-ray scattering experiments. *EPJ Web of  
109        Conferences*, 272, 01015. <https://doi.org/10.1051/epjconf/20227201015>
- 110        Rög, T., Murzyn, K., Hinsen, K., & Kneller, G. R. (2003). nMoldyn: A program package  
111        for a neutron scattering oriented analysis of molecular dynamics simulations. *Journal of  
112        Computational Chemistry*, 24(5), 657–667. <https://doi.org/10.1002/jcc.10243>
- 113        Walter, N. P., Jaiswal, A., Cai, Z., & Zhang, Y. (2018). LiquidLib: A comprehensive  
114        toolbox for analyzing classical and ab initio molecular dynamics simulations of liquids and  
115        liquid-like matter with applications to neutron scattering experiments. *Computer Physics  
116        Communications*, 228, 209–218. <https://doi.org/10.1016/j.cpc.2018.03.005>
- 117        Z-laboratory. (2023). *Liquidlib-version 1.0*. [https://github.com/Z-Laboratory/LiquidLib/tree/  
118        master](https://github.com/Z-Laboratory/LiquidLib/tree/master).

DRAFT