

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

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## Software

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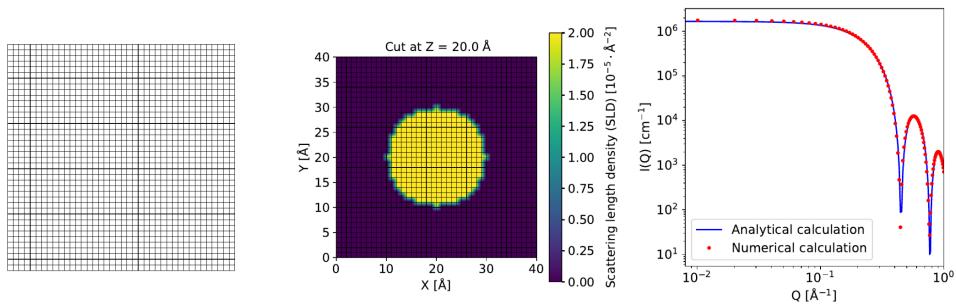
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## <sup>9</sup> Summary

<sup>10</sup> Cont2SAS facilitates the calculation of Small Angle Scattering (SAS) parameters from simulated  
<sup>11</sup> Continuum (Cont) nanostructures. Cont2SAS is built on the existing software solution Sassaena  
<sup>12</sup> – known for calculating scattering patterns from simulated atomic structures (Lindner, 2012,  
<sup>13</sup> 2017; Lindner & Smith, 2012; Majumdar et al., 2024; Majumdar & Lindner, 2023). Cont2SAS  
<sup>14</sup> can calculate SAS patterns and the effective scattering cross-section ( $\sigma_{\text{eff}}$ ). SAS patterns  
<sup>15</sup> contain a SAS intensity ( $I$ ) vs. scattering vector magnitude ( $Q$ ). The  $\sigma_{\text{eff}}$  is the count rate  
<sup>16</sup> of scattered radiation per incident unit flux. The time evolution of  $\sigma_{\text{eff}}$  is calculated from  
<sup>17</sup> SAS patterns at different time steps. Through the comparison of calculated and measured  
<sup>18</sup> SAS parameters, simulations and SAS experiments can be used complementarily for different  
<sup>19</sup> purposes, such as validating simulations, tuning simulation parameters, and analyzing SAS  
<sup>20</sup> data obtained from experiments (Dorrell et al., 2020; Majumdar et al., 2024; Reich et al.,  
<sup>21</sup> 2022).

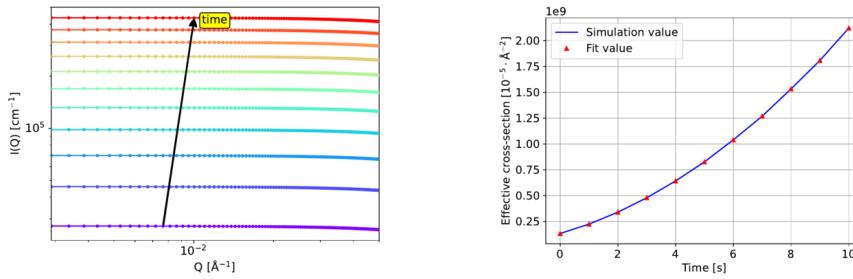
## <sup>22</sup> Statement of need

<sup>23</sup> The simulation of material structure at the nanometer length scale can be performed using  
<sup>24</sup> atomistic simulations and continuum simulations. Continuum simulations have the advantage  
<sup>25</sup> over atomistic ones that they can simulate bigger volumes for a larger time. However, continuum  
<sup>26</sup> simulations are less accurate than the atomistic simulations. Cont2SAS is created to check the  
<sup>27</sup> accuracy of continuum simulations by validating them against SAS experiments, such as Small  
<sup>28</sup> Angle Neutron Scattering (SANS) and Small Angle X-ray Scattering (SAXS). The validation  
<sup>29</sup> is performed by comparing SAS parameters calculated using Cont2SAS with measured ones. A  
<sup>30</sup> validated simulation can also be used to retrieve nanostructure from SAS data because a direct  
<sup>31</sup> retrieval of nanstructure from SAS data is not possible (Billinge & Levin, 2007). Alternatively  
<sup>32</sup> to simulating continuum nanostructures based on physics-based equations, they can also be  
<sup>33</sup> simulated based on the user's knowledge of the sample to retrieve nanostructures from SAS  
<sup>34</sup> data.



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

Both physics- and knowledge-based simulated structures are expected to output either Scattering Length Density (SLD) ( $\beta$ ) values or a set of variables (e.g. local molar density ( $\rho_m$ ) and composition ( $\chi$ )) 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 ( $\sigma_{\text{eff}}$ ) calculation: [left] Calculated SAS pattern at different time steps, [right]  $\sigma_{\text{eff}}$  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 ( $\sigma_{\text{eff}}$ ), and can be calculated using Cont2SAS. [Figure 2](#) demonstrates such a calculation from a series of SAS patterns. The calculated  $\sigma_{\text{eff}}$  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.

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