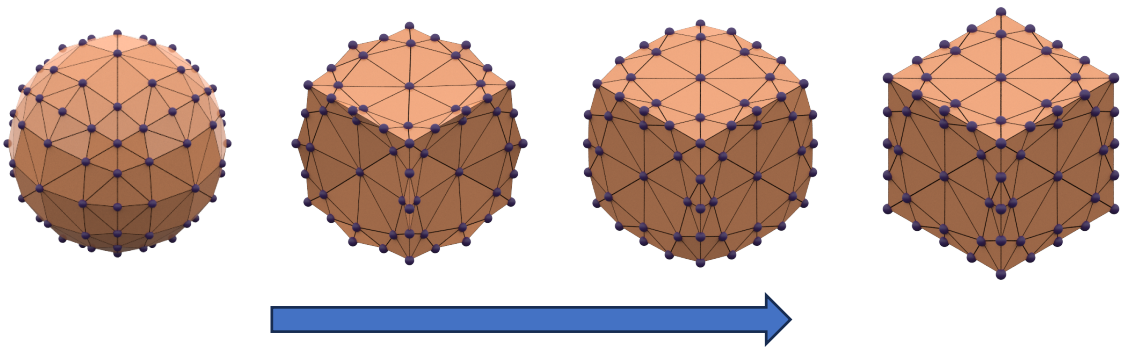
Nanoparticle Shape Optimization using Differentiable Total Scattering

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Accurately determining the three-dimensional shape of nanoparticles from powder diffraction data constitutes a challenging inverse problem. While high fidelity methods like the Debye scattering equation [1] offer model independent accuracy, their O(N^2) scaling with the number of atoms precludes their use in large scale optimization. Consequently, standard workflows rely on manually testing discrete shape models, a trial-and-error process limited by predefined geometries. To address this, we present a fully end-to-end differentiable framework for total scattering analysis. A key innovation of this work is a method that connects particle shape directly to diffraction intensity in a differentiable manner, allowing continuous shape meshes to be optimized via backpropagation. We validate this framework by successfully reconstructing shapes from simulated and experimental datasets, demonstrating a pathway for automated morphological characterization from powder diffraction profiles.



Optimization Progress

References

[1] Leonardi, A., & Bish, D. L. J. Appl. Crystallogr., **2016**, 49(5), 1593–1608.

Acknowledgements. This work was supported by Deutsche Forschungsgemeinschaft under grant No. LE4543/2-1.