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A GPU-Accelerated Open-Source Python Package for Rapid Calculation of the Debye Scattering Equation: Applications in Small-Angle Scattering, Powder Scattering, and Total Scattering with Pair Distribution Function Analysis

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Abstract

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Introduction

The Debye scattering equation, derived in 1915 by P. Debye, is commonly used to calculate the scattering intensities considering the position of each atom in the structure:[debye1915zerstreuung; Scardi et al. (2016)]

$$I(Q) = \sum_{i=1}^{N} \sum_{j=1}^{N} f_i(Q) f_j(Q) \frac{\sin(Q r_{ij})}{Q r_{ij}} \tag{1}$$

In this equation, Q is the scattering vector, r_ij is the distance between atom-pair, i and j, and f is the atomic scattering factor. The Debye scattering equation can be used to compute the scattering pattern of any atomic structure and is commonly used to study both crystalline and non-crystalline materials with a range of scattering techniques like powder diffraction (PD), total scattering (TS) with pair distribution function (PDF) and small-angle scattering (SAS).(Scardi et al., 2016) Although the Debye scattering equation is extremely versatile, its applicability has been limited by the double sum of the atoms in the structure which makes the equation computationally expensive to calculate. With the advancement in computing technology,[schaller1997moore] new horizons have opened up for applying the Debye scattering equation to larger materials. Modern central processing Units (CPUs), ranging from tenths to hundreds of cores, offer an opportunity to parallelise the computation, significantly enhancing the computational efficiency. This parallel architecture allows for the distribution of the double sum calculations across multiple cores. Graphics processing units (GPUs) further expand computational possibilities, consisting of hundreds or even thousands of smaller, more efficient cores designed for parallel processing.[garland2008parallel] Unlike traditional CPUs, GPUs are ideally suited for calculations like the Debye scattering equation, where many computations can be performed simultaneously. By leveraging GPU acceleration, researchers can achieve computational speeds that are orders of magnitude faster than even the most advanced

multi-core CPUs. We introduce a GPU-accelerated open-source Python package for rapid calculation of the scattering intensity from a xyz-file using the Debye scattering equation. The xyz-file format describes the atomic structure with the atomic identify and its xyz-coordinates and is commonly used in materials chemistry. We further calculate the PDF as described in Underneath the Bragg Peaks.[egami2003underneath] We show that our software can simulate the PD, TS, SAS and PDF data orders of magnitudes faster than on the CPU, while being open-source and easy assessable by other scientists.

Results & Discussion:

Table: Pseudo-code incl. profiling (times)

Figure 1: Q and r-space comparison ours and DiffPy-CMI on two systems: (evt. Topas??) - Monoatomic system (metal) - Diatomic system (metal oxide)

Figure 2: CPU vs. GPU (in Q and in r-space) (+ batching)

Figure 3: GPU time vs. size and #atoms

Conclusions

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We acknowledge contributions from Brigitta Sipocz, Syrtis Major, and Semyeong Oh, and support from Kathryn Johnston during the genesis of this project.

References

Mathematics

Single dollars ($) are required for inline mathematics e.g. $f(x) = e^{\pi/x}$

Double dollars make self-standing equations:

$$\Theta(x) = \begin{cases} 0 \text{ if } x < 0 \\ 1 \text{ else} \end{cases}$$

You can also use plain LaTeXfor equations

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} f(x) e^{i\omega x} dx \tag{2}$$

and refer to Equation 2 from text.

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Figures

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Scardi, P., Billinge, S. J., Neder, R., & Cervellino, A. (2016). Celebrating 100 years of the debye scattering equation. In *Acta Crystallographica Section A: Foundations and Advances* (No. 6; Vol. 72, pp. 589–590). International Union of Crystallography.