GPU Clusters for Large-Scale Analysis of X-ray Scattering Data

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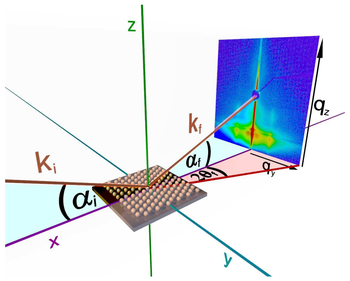
X-RAY SCATTERING is a valuable tool for measuring the structural properties of materials used in the design and fabrication of energy-relevant nanodevices that are key to the reduction of carbon emissions. Although today's X-ray scattering detectors can provide raw information on structural properties of nanoparticles, a primary challenge remains in the analysis of this data due to its size. We are developing novel high-performance computing algorithms and codes for such analyses. Here we present two such HPC advances:

1. **a flexible Grazing Incidence Small Angle Scattering (GISAXS) simulation code** based on the **Distorted Wave Born Approximation (DWBA)** theory. This code can compute the scattered light intensity from any given sample in all directions of space.
2. **an efficient inverse modeling code for structural fitting problems** using **Reverse Monte Carlo (RMC) simulation** algorithm.

Distorted Wave Born Approximation

- Studying complex nanostructures requires solving for **form factors** in a high-resolution Q-grid resulting in matrices with $\sim 10^7$ to 10^{10} q-points.
- This time-consuming and memory-demanding step is a major bottleneck in GISAXS simulations.



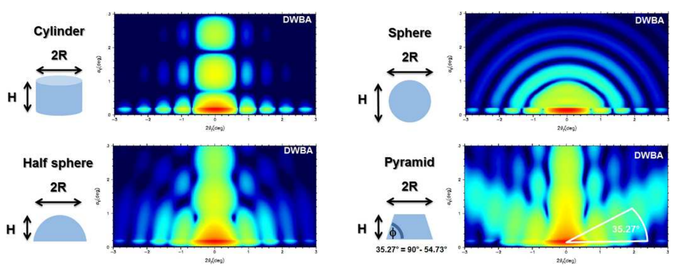
DWBA is the only theoretical framework which models the GISAXS process. It defines scattering intensity of the X-rays as:

$$I(\vec{\mathbf{q}}) \quad \propto \quad |F(\vec{\mathbf{q}})|^2$$

$F(\vec{\mathbf{q}})$ is the form factor of a q-point $\vec{\mathbf{q}}$, computed as an integral over the shape function $S(\vec{r})$ of the nanoparticles. For computational purposes, the shape surface is triangulated and the form factor is approximated as a summation over resulting N triangles, with surface area of triangle $t = s_t$:

$$F(\vec{\mathbf{q}}) \quad = \quad \int_{S(\vec{r})} e^{i\vec{\mathbf{q}}\cdot\vec{r}} d\vec{r} \quad \approx \quad \sum_{t=1}^{N} e^{i\vec{\mathbf{q}}\cdot\vec{r}} s_t$$

Below are analytically computed example form factor intensity images for simple shapes.

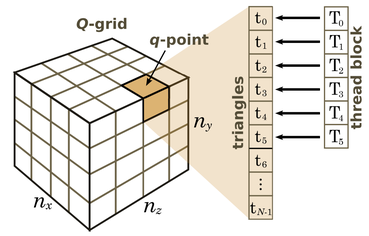


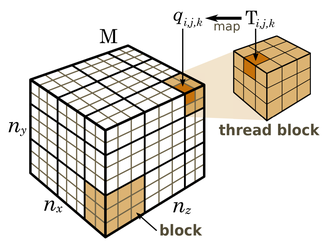
Computing Form Factors on GPUs

- **Given:** A 3-D Q-grid of resolution $n_x \times n_y \times n_z$, triangulated shape surface (set of N triangles.)
- **Task:** Generate 3-D matrix M of size $n_x \times n_y \times n_z$ where each $M(i,j,k) = F(q_i, q_j, q_k) = F(\vec{\mathbf{q}}_{i,j,k})$

Phase 1

- Compute inner term, $F_{t_l}(\vec{\mathbf{q}}) = e^{i\vec{q}\cdot\vec{r}} s_{t_l}$ for each triangle t_l.
- Store in a 4-D matrix M_I of size $n_x \times n_y \times n_z \times N$.
- Decompose computations along triangles: each thread mapped to a unique triangle.



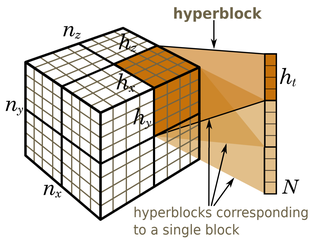


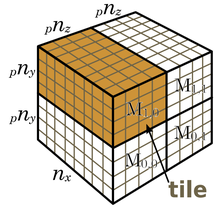
Phase 2

- Decompose M into a grid of 3-D **blocks**, M_b, each corresponding to a CUDA thread block.
- For each q-point $\vec{\mathbf{q}}_{i,j,k}$, a thread $T_{i,j,k}$ computes $M_b(i,j,k) = F(\vec{\mathbf{q}}) = \sum_{l=1}^{N} F_{t_l}(\vec{\mathbf{q}}_{i,j,k})$, generating M_b.

Handling Memory Limitations

- Decompose M_I along all dimensions into 4-D **hyperblocks**, M_h.
- Each hyperblock results in a partial sum in M. All partial sums for a block are reduced later.



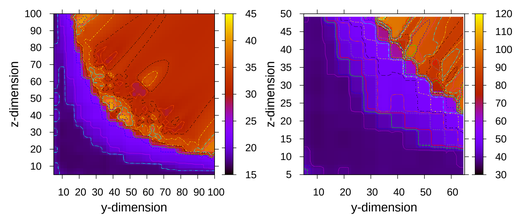


Utilizing Cluster of GPUs

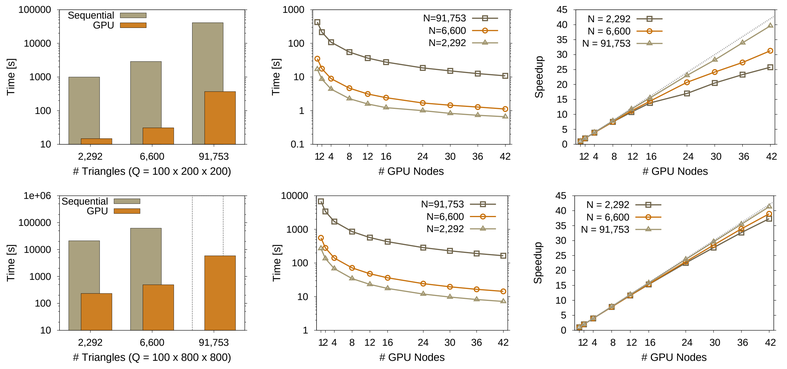
- Decompose M along y and z into **tiles**, as a higher level of parallelism.
- Use MPI across GPU nodes.
- Tile $M_{i,j}$ is assigned to processor $P_{i,j}$.

Choosing Hyperblock Size

- Crucial for performance: demonstrated by heat maps of runtimes (seconds) with varying sizes.
- Q-grid size is $100 \times 200 \times 200$, and $N_1 = 2,292$ and $N_2 = 91,753$, respectively.

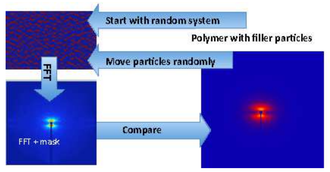


Performance Results



Reverse Monte Carlo Modeling on GPU

- Information on material structure from Small Angle X-ray Scattering (SAXS) data, consisting of 2-D images, is extracted using RMC.
- Involves $\sim 10^6$ iterations, each with $\sim 10^4$ Fourier transformations.

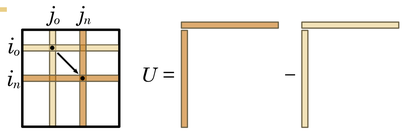


- **Given:** SAXS image as $N \times N$ array I, and random particle array A.
- **Task:** Compute structure factor F_n^2 fitting input image.

Initialization: Compute $F_0 = \text{FFT}(A)$, $F_0^2 = \texttt{cws}(F)$.

Simulation Steps

1. Randomly move a particle from (i_o, j_o) to (i_n, j_n).
2. Compute update to the Fourier transform, new structure factor, and χ^2 error (D = DFT matrix, cws = component-wise square):



$$U = \texttt{dft2}(i_o, j_o, i_n, j_n) = D(j, i_n) \cdot D(j_n, i) - D(j, i_o) \cdot D(j_o, i),$$
$$F_n = F_{n-1} + U, \qquad F_n^2 = \texttt{cws}(F_n), \qquad \chi_n^2 = \sum_{i,j} (I(i,j) - F_n^2(i,j))$$

- Decompose array computations into 1-D grid of thread blocks, each thread computing one element in the $N \times N$ matrices.
- Observed about 900x speedup over a sequential Matlab code.

Acknowledgements

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