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A faster image simulation algorithm for scanning transmission electron microscopy

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Image simulations are an integral part of research in scanning transmission electron microscopy (STEM), yet large-scale simulations can still require extended simulation times, and can quickly become infeasible.

As machine learning is becoming increasingly important in electron microscopy, speedups in simulation time would allow for the generation of larger ground-truth datasets required for training larger and more powerful neural network models, or even on-the-fly generation of large datasets.

Recently, the plane-wave reciprocal space interpolated scattering matrix (PRISM) algorithm [1,2] has achieved speedups of > 10x for STEM simulations compared to traditional multi-slice calculations [3] with negligible loss of accuracy. It achieves this speedup by using Fourier interpolation to reduce the number of input beams sampled in the scattering matrix for large fields of view (FOV), and consequently the number of multi-slice simulations needed to calculate exit-waves for each input beam. Given a Fourier interpolation factor *f*, the PRISM algorithm achieves a speedup ranging from f^2 to f^4, compared to the traditional multi-slice algorithm for STEM simulations.

In this talk, we introduce an additional interpolation concept to reduce the number of calculated input beams further and, therefore, the computation time and memory requirements with negligible loss of accuracy.

Fig. 1 a) walks through the concepts step-by-step: After determining the Fourier-space sampling of the probe, we determine an overcomplete basis of the condenser aperture by first choosing several/subset of parent beams in a pseudo-hexagonal pattern and then computing the natural neighbor interpolation weights for each non-parent beam in the aperture. Panel 1 displays the weights associated with each parent beam. We call these per-beam weight distributions ‘beamlets’, inspired by the wavelet concept used in the signal processing literature [4]. Panel 2 Shows the generated beamlets in real space, corresponding to spatially confined plane-waves coming from different incident angles. For each of the parent beams, we calculate an exit wave with the multi-slice algorithm. Exit waves for each probe position are then generated by first multiplying the beamlets with the corresponding parent-beam exit waves and performing a coherent sum over all beamlet exit waves. We call the resulting algorithm enhanced PRISM (ePRISM). Combining beam partitioning with Fourier interpolation would facilitate simulations with previously inaccessibly large FOVs. Figs. 1b),c), and d) show five different beam partitions and corresponding diffraction patterns for a platinum nanoparticle on an amorphous carbon substrate. The ePRISM partitionings for 1, 7, 19, 61, and 217 beams for an S-matrix of 7377 beams provide a speedup of 7377x, 1053x, 388x, 121x, 34x, respectively, compared to the PRISM algorithm with f=1. For the moderate speedup of 34x, all relative diffraction-space intensity errors compared to multi-slice simulations are less at the 0.1% level.

Fig. 2 shows timing results for a large-scale STEM simulation of the polycrystalline particle with different simulation algorithms. While the multislice simulation with 500^2 probe positions takes an estimated 3.1 days, ePRISM with 6 partitioned rings and 127 beams took 10 hours, PRISM with f=5 took 1 hour and ePRISM with f=5 and 3 rings took only 15 minutes on the CPU.

The reduction in the size of the scattering matrix also means that larger FOVs can be simulated with the same amount of available memory.[5]

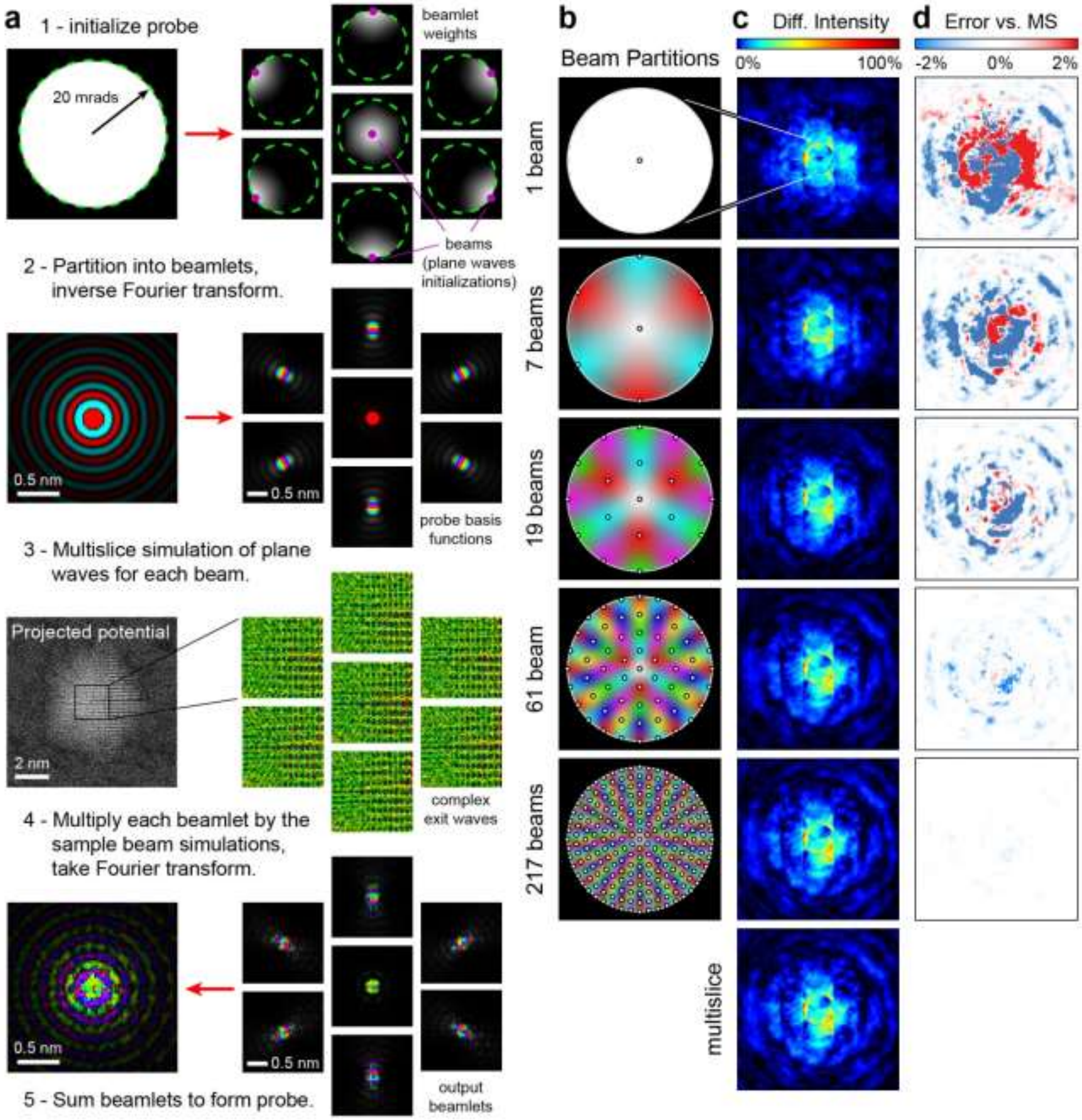

Figure 1. Fig. 1: a) Steps in the PRISM algorithm with beam partitioning: 1) Left: determine the probe sampling and the number of beams from the given convergence angle, sampling and field of view

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parameters. Right: given the number of angular and radial beam partitions, create a beamlet basis spanning the angles in the condenser aperture. 2) Right: Inverse Fourier transform the beamlets to create the probe basis in real space. Left: The full probe is the coherent sum of all real-space beamlets. 3) Perform a multi-slice simulation for each parent beam in the illumination aperture. 4) Multiply parent-beam exit waves with real-space beamlets and 5) coherently sum all exit wavesb) 5 examples of beam partitioning with a pseudo-hexagonal layout for even distribution of the parent beams. c) Example diffraction intensity for the beam partitioning layout to the left. d) Relative error with respect to a full multislice simulation.

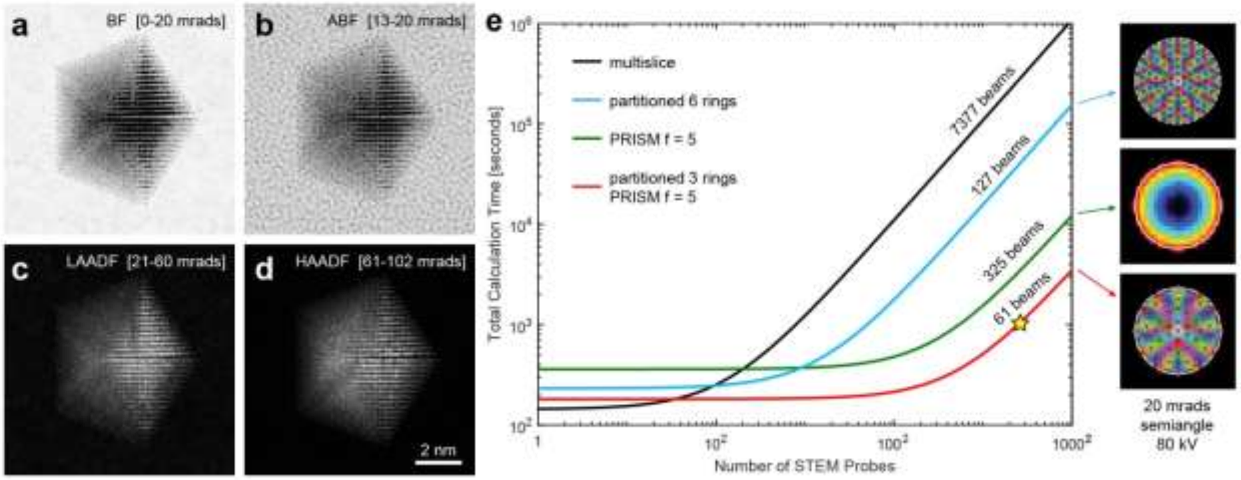

Figure 2. Fig. 2: a)-d) STEM images generated in 15 minutes on CPU with the ePRISM algorithm and 61 parent beams. e) timing chart for different methods as a function of computed probes. The timing for the images on the left is indicated with a star.

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