Carnegie Mellon University

(S)TEM Simulations Tutorial + Examples

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For the CMU MCF TEM user group
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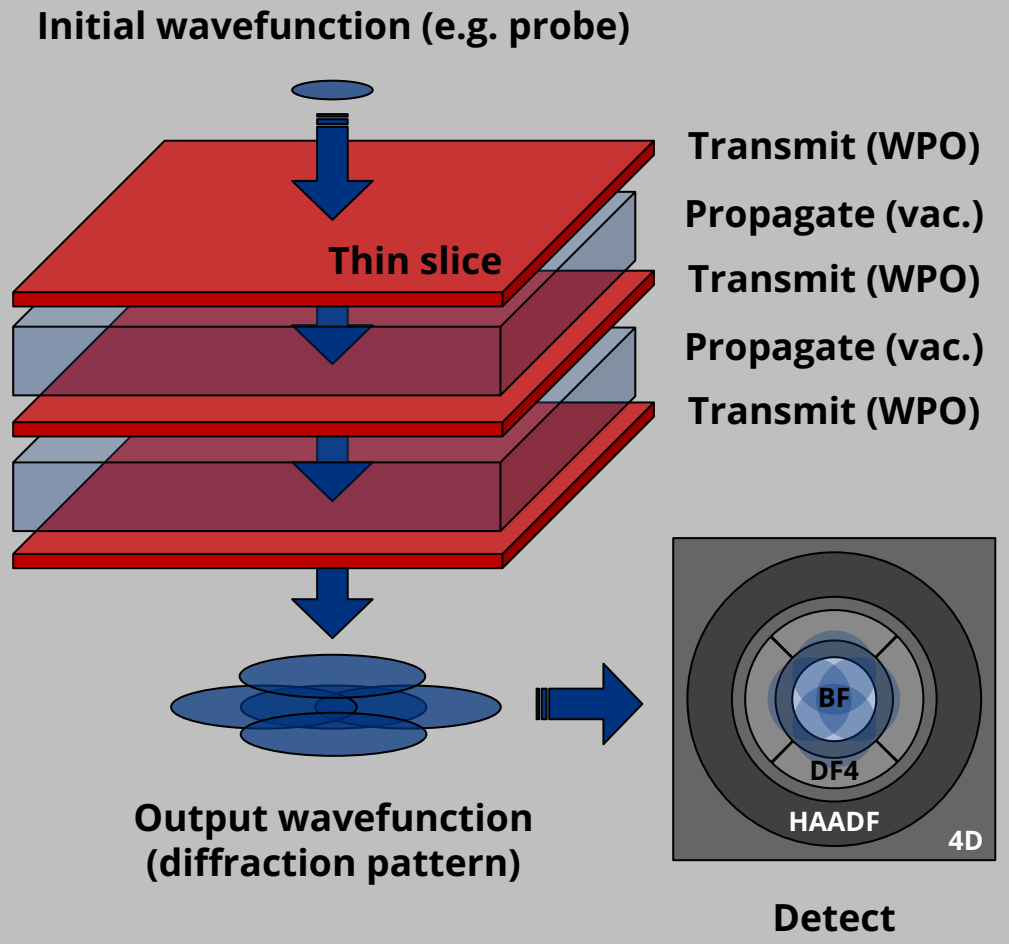
Contents

Background

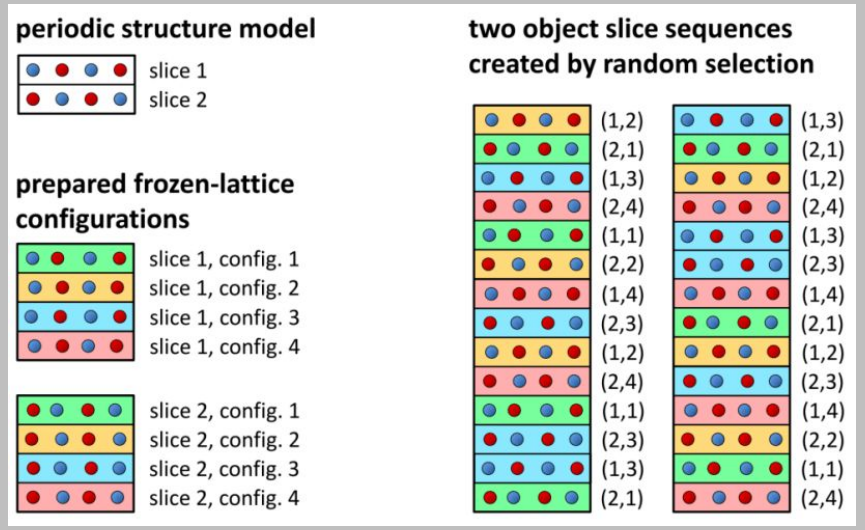
The Multislicce Algorithm

- Thin samples are fairly easy to solve (WPO), but this is not the case for thick samples
- Solution: divide a thick sample up into thin slices and treat them separately
- Transmit the wavefunction through the thin sample, then propagate it through vacuum

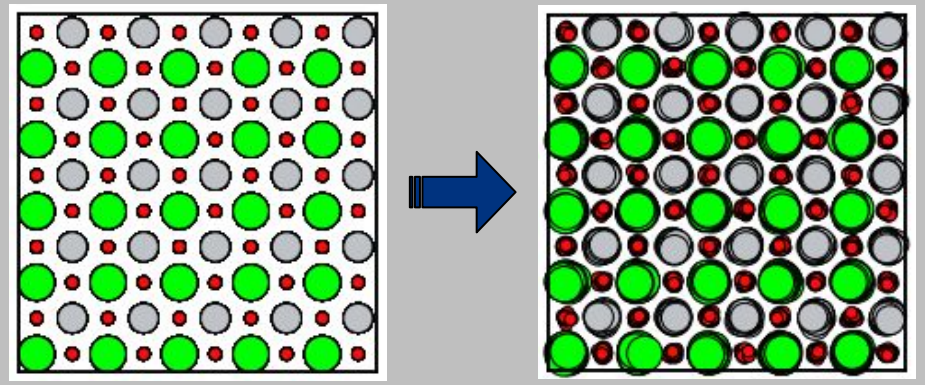


Frozen Phonons

- To get accurate simulated images (especially HAADF), thermal vibrations need to be taken into account
- Tricky to do directly, so we use frozen phonons (a Monte-Carlo approach)
- Run several simulations with atoms shifted by small amounts (U_{iso}) and average
- Alternative: MD trajectory



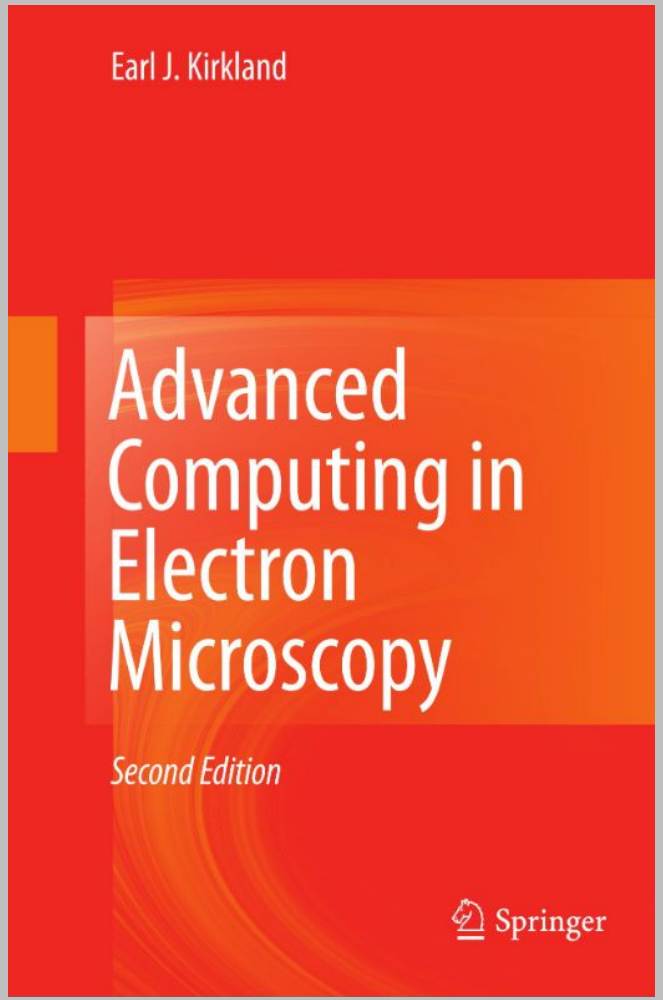
Dr Probe



abTEM

For More Theory…

- *Advanced Computing in Electron Microscopy*, Kirkland 2010
  - CMU has PDF access through Springer's site
- 6.4: multislice
- 7.4: frozen phonons
- Lots of details, other techniques (e.g. Bloch wave)



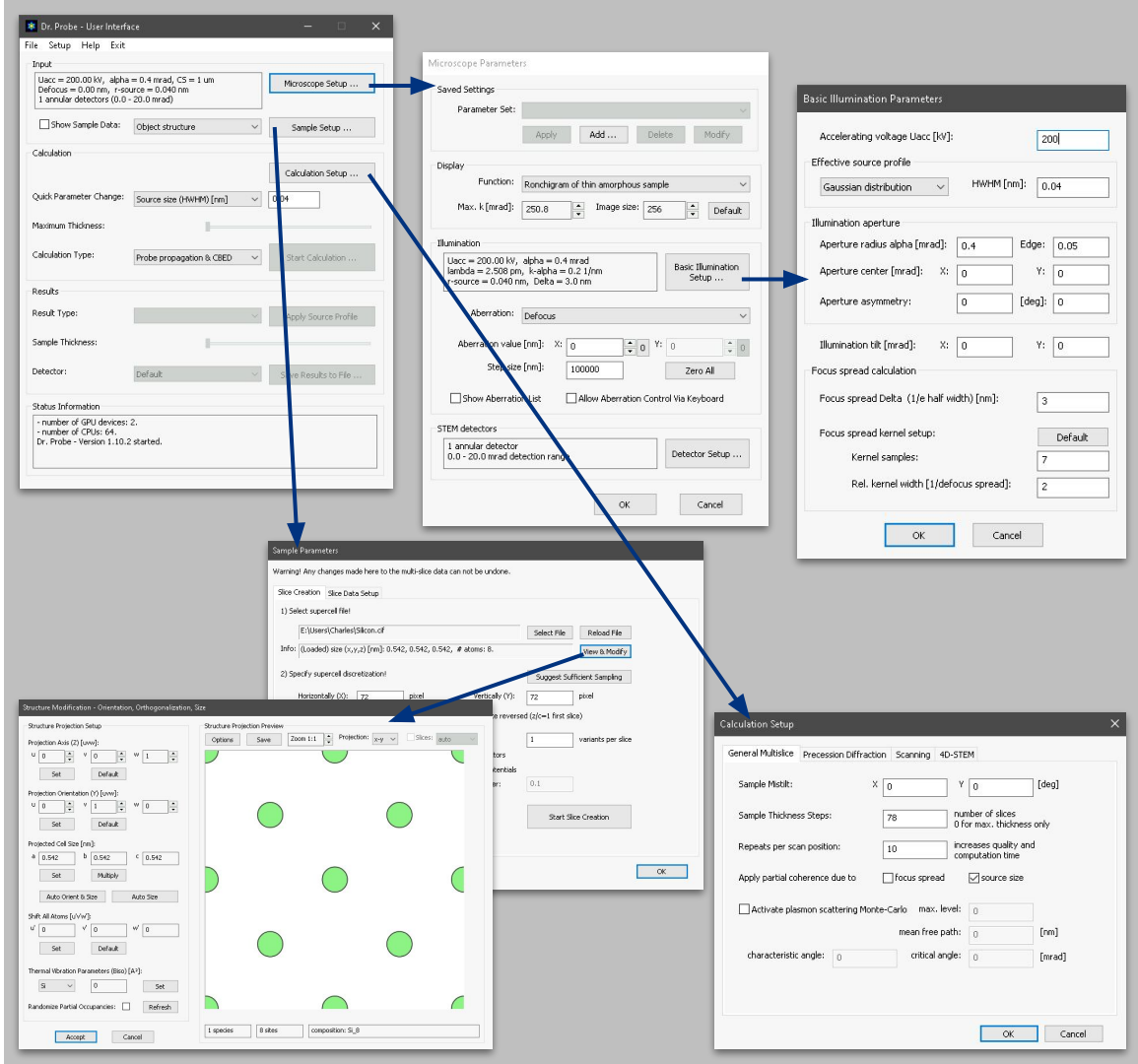
Dr Probe

Background

- STEM simulation software maintained by J. Barthel
  - Website: https://er-c.org/barthel/drprobe/
  - Paper: 10.1016/j.ultramic.2018.06.003
- GUI focused, with supporting CLI tools (optional)
- Quick to pick up, capable, free (for academic use), open source
- Multi-threading + GPU, exclusively multislice

Basic Workflow

- Setup microscope params (voltage, aperture, detectors, aberrations, etc)
- Setup sample (import, orient, slice, etc)
- Setup calculation (scan reps, sampling, etc)



Dr Probe Live Demo

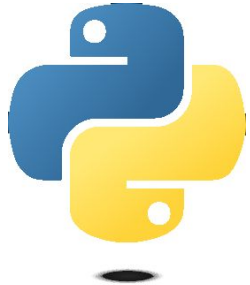
Quick Tips

- Dr Probe uses .cif or .cel files (GitHub page has a script to convert .xyz to .cel)
- You can duplicate slices instead of slicing a huge model
- Make sure you set the D-W factors (especially for HAADF simulations)
- PACBED .dat file is raw 32-bit real formatted
- Check out the online documentation (examples)

abTEM (Python)

Background

- Python package for STEM simulation maintained by J. Madsen
  - Website: https://github.com/abTEM
  - Paper: 10.12688/openreseurope.13015.2
- No dedicated GUI
- Quick to pick up (if you know python), extremely flexible, open source & permissive license (GPL)
- Implements both multislice & PRISM



abTEM Live Demo

Quick Tips

- The documentation is split between GitHub and Read the Docs
- abTEM supports GPU & parallel computation
- For very large models, PRISM is much faster with some tradeoffs (read the documentation)
- Includes a PlaneWave class that can be used to simulate HRTEM image
- It's a good idea to pickle your results so you don't need to rerun if you want to look at them again (especially for long simulations)