High-Performance PIC-BCA for Plasma-Material Interactions

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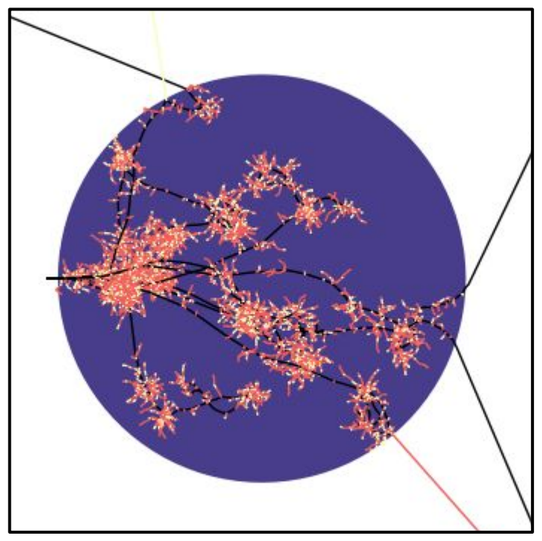
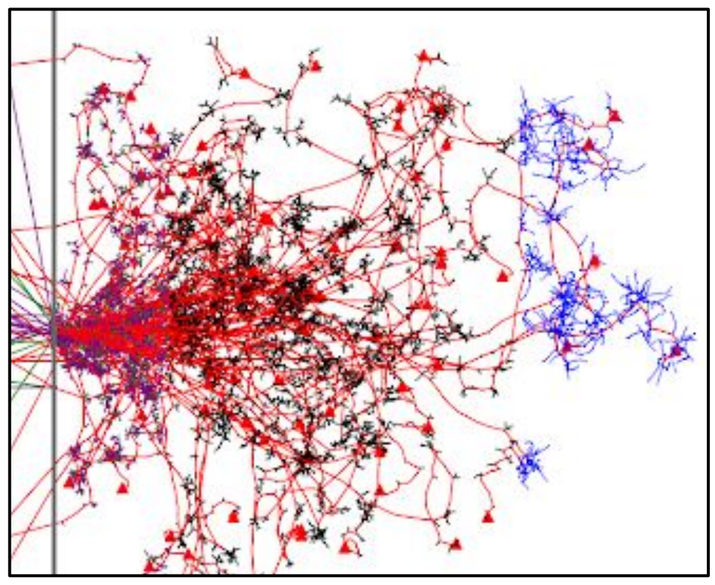
rustBCA

A new, open-source, Binary Collision Approximation code for Ion-Material Interactions:

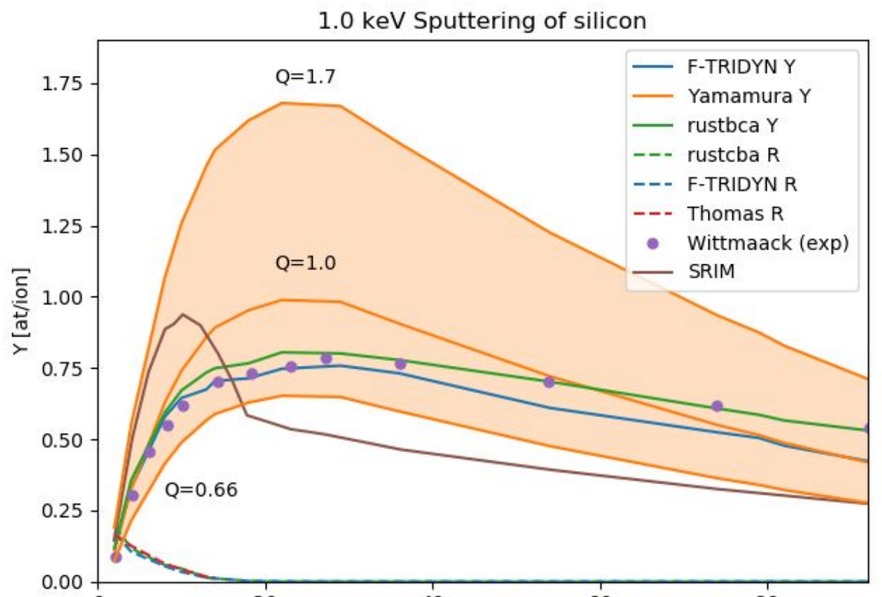
https://github.com/lcpp-org/RustBCA/wiki





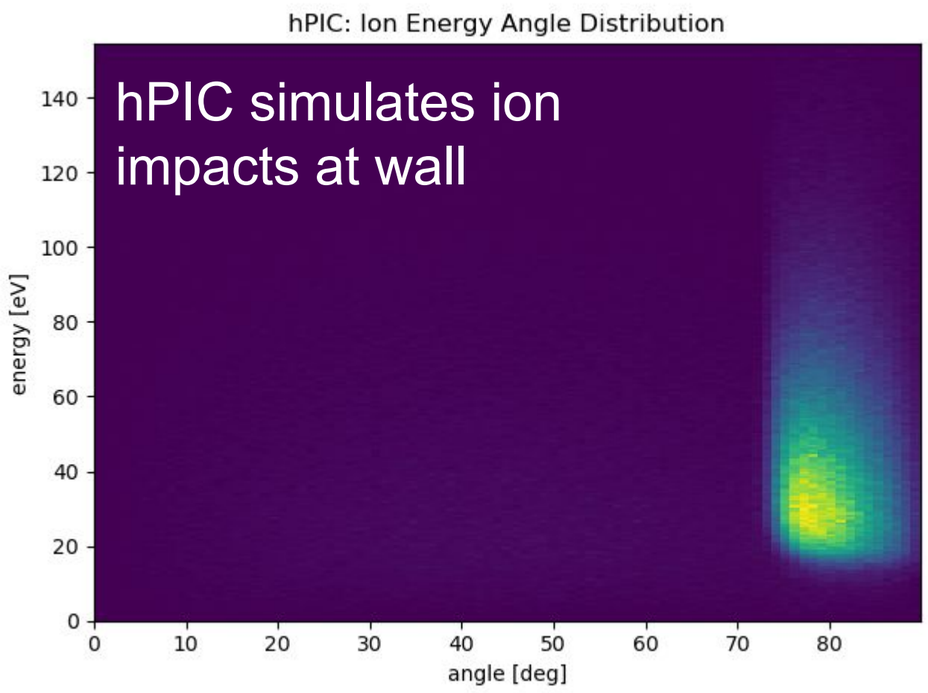
- Reflection, implantation, sputtering
- Multithreaded
- Modern programming techniques
- Energies from eV to ~GeV per nucleon
- Kr-C, Moliere, ZBL, Lennard-Jones, Morse, & cubic spline interaction potentials
- Arbitrary 2D geometry and inhomogeneous composition
- Human and machine-readable TOML format input file
- Can be compiled as a library for in-memory coupling

rustBCA has been benchmarked against experimental data, legacy BCA codes and empirical formulas and reproduces expected results

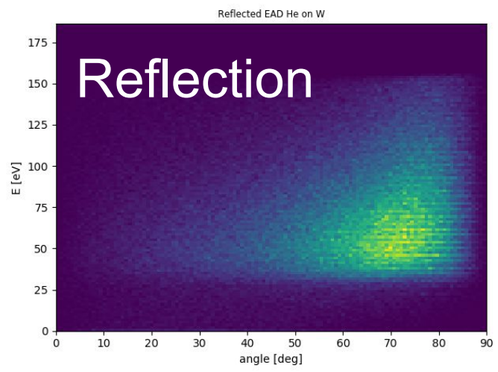


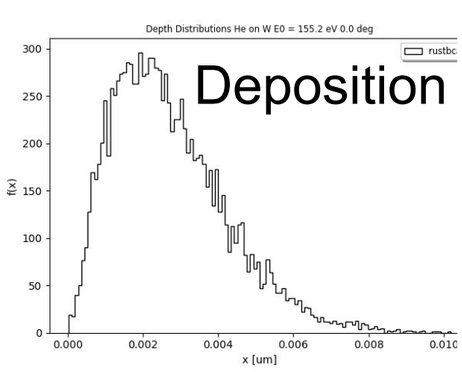
Above: benchmarking rustBCA sputtering results

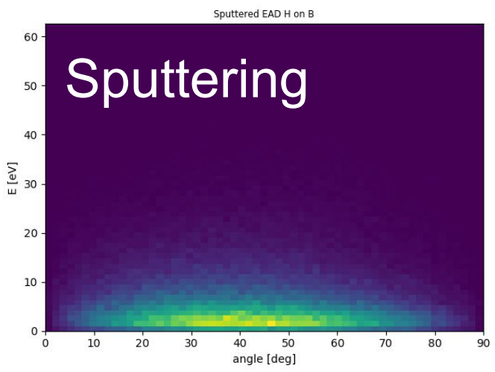
hPIC[1] and PIC-BCA coupling



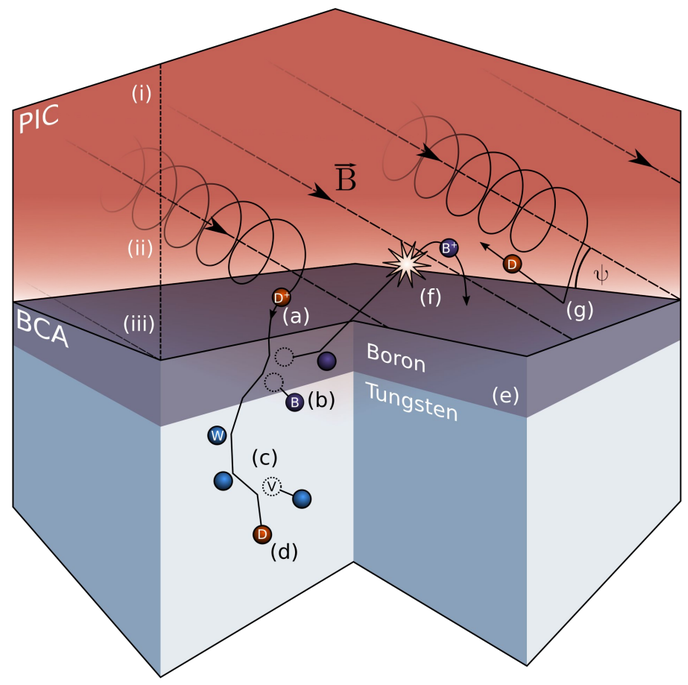
rustBCA simulation



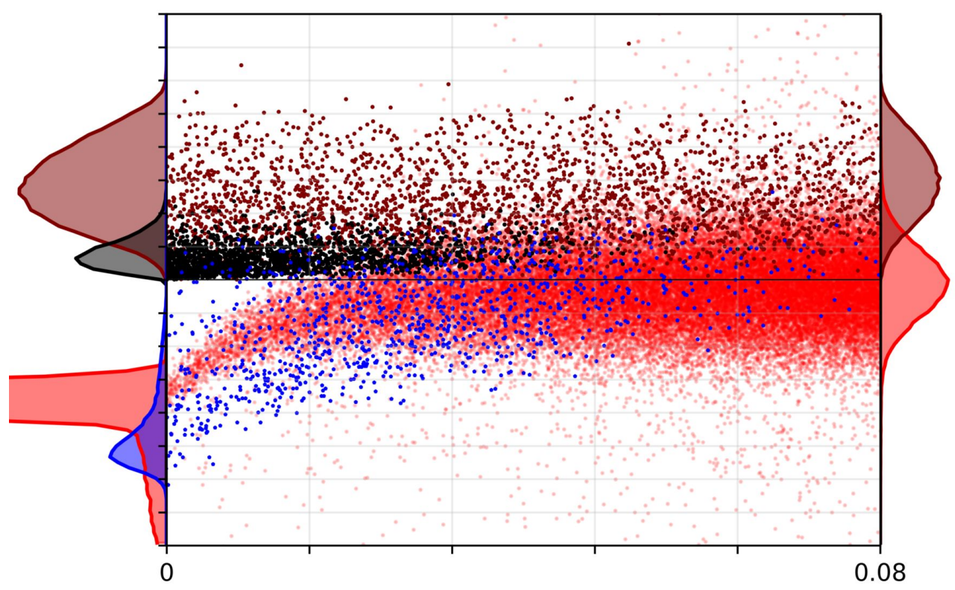




- File-based, one way coupling is complete
- hPIC provides ion distributions at wall
- Full PIC-BCA simulations using Python prototype have been successful



Above: PIC-BCA coupling with an oblique magnetic field
Below: x, v distributions in prototype PIC-BCA



[1] R. Khaziev, D. Curreli, CPC (2018) https://doi.org/10.1016/j.cpc.2018.03.028; This work was supported by the US Department of Energy through contract DOE-DE-SC0008658 as part of the PSI2-SciDAC Project.