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From Grains to Gigabytes: Generating Massive Virtual Specimens for Irradiation Damage Study

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In nuclear fusion environments, structural materials must withstand severe thermal loads and high-energy particle bombardment. Accurately simulating these conditions requires large-scale atomistic models capable of capturing complex grain and interface arrangements. PolyPal provides a *big* solution by generating massive polycrystalline specimens—scaling to tens of billions of atoms—in only a few minutes.

Existing atomic structure generators typically operate in serial and thus can handle just a few million atoms, limiting their capacity to represent realistic microstructural features. In contrast, PolyPal runs in parallel and supports flexible memory configurations, offering virtually unlimited scalability. The code also features a fully parallelized file I/O scheme for seamless integration with large-scale molecular dynamics (MD) simulations. Its domain-preserving file format removes the need for time-consuming atom sorting during MD initialization, an operation that can otherwise take hours for extremely large virtual specimens.

In tungsten and other fusion-relevant alloys, grain boundaries and solute distributions significantly influence defect migration, damage clustering, and embrittlement phenomena. PolyPal accommodates polycrystalline structures at the micrometer scale, allowing precise control over grain size distribution, crystallographic orientation, and compositional variations. This capability enables systematic exploration of how different microstructures may either enhance or diminish material performance under fusion conditions. Notably, such versatility enables more realistic multi-PKA simulations, transient thermal shock analyses, and other advanced MD studies relevant to reactor component design.

In this presentation, we will describe the computational framework underlying PolyPal, highlighting its parallel I/O architecture, performance benchmarks, and customizable microstructure settings. We will also explore its potential application to cutting-edge fusion-material research.

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