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# In-Situ Void detection in Large-Scale Molecular Dynamics Simulations: A Case Study on Tantalum Spall Fracture.

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## Abstract

Advancements in computational power have enabled molecular dynamics (MD) simulations to model billions of particles, providing unprecedented insights into crystal defects, phase transformations, and void dynamics. These simulations generate vast data, creating challenges for storage, post-processing, and analysis. On-the-fly methods address these challenges by enabling real-time data processing, though their implementation is non-trivial. This work compares a recent on-the-fly analysis technique with the established software OVITO, focusing on void detection and volume quantification. We validate and assess uncertainties in both methods, introducing an empirical scaling law to correlate analysis parameters with measurement errors. While results for single voids align, significant disparities arise in large-scale spall fracture simulations. The study highlights challenges in defining "true" outcomes, underscoring the need for robust parametric studies to interpret physical phenomena effectively.

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