

SCACS

Simulator Collection for Atomic-to-Continuum Scales

Value Proposition

Built on novel atomic-site-projected conductivity methods and accelerated through graph neural networks, SCACS predicts spatially varying, direction-dependent thermal and electrical transport across large million-atom systems, giving material design engineers a physics-grounded view of where hot-spots will form in materials, how defects will steer current and which microstructural choices will make or break performance.

Technology Readiness Level 4

IP Information for S-196281

U.S. Patent pending; Related software: T5032

Contact Information

licensing@lanl.gov

Overview

The SCACS Toolkit is an AI-driven multiscale simulation platform designed to accelerate the development and deployment of advanced materials. Today, materials innovation is slowed by a fundamental gap: High-fidelity physics models (e.g., molecular dynamics) are too computationally expensive for real-world design, while the engineering-scale tools rely on simplified assumptions that limit predictive accuracy. This disconnect leads to costly trial-and-error development cycles and unexpected material failures in critical systems.

SCACS bridges this gap by embedding machine-learned physics directly into engineering-scale

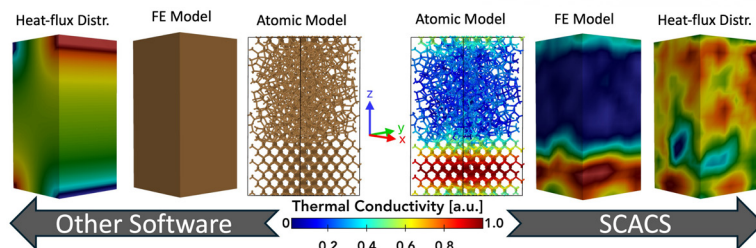


Fig. 1. Most simulation tools rely on a single averaged conductivity value, missing the microstructural variation that produces hot spots, unexpected transport pathways, and early failures in real materials.

simulations. Its core technology uses proprietary models Site-Projected Thermal Conductivity (SPTC-AI) and Site-Projected Electronic Conductivity (SPEC-AI) to translate first-principles insights into spatially resolved transport properties that can be used within standard finite element workflows. This approach enables accurate prediction of heat and electrical behavior in complex, heterogeneous materials at practical scales.

The platform has broad commercial relevance across industries where thermal and electrical performance are critical, including semiconductors, energy systems, and advanced manufacturing. By reducing development time, improving reliability and lowering testing costs, SCACS offers a pathway to faster material qualification and more efficient product design, positioning it as a high-impact enabling technology for next-generation hardware innovation.

Advantages

- Reveals localized hot-spots and transport pathways that conventional continuum models routinely miss
- Cuts simulation runtimes from days on high-performance computing clusters down to minutes, without sacrificing atomic-scale fidelity
- Scales predictions from small atomistic cells up to million-atom microstructures previously out of reach for direct atomistic methods
- Captures anisotropy and spatial variation in both

Continued on reverse

Advantages continued

thermal and electrical conductivity, giving engineers a directionally accurate picture of material behavior

- Easily Integrates with existing finite-element solvers, such as Abaqus

Technology Description

At its core, SCACS is a computational suite that links atomistic simulations to continuum finite-element models through two integrated modules: SPTC-AI for thermal transport and SPEC-AI for electronic transport. The Site-Projected Thermal Conductivity (SPTC) and Space-Projected Electronic Conductivity (SPEC) methods decompose a material's bulk conductivity into per-atom contributions, revealing how individual phases, defects and interfaces locally steer the flow of heat or charge. A machine-learning graph neural network then learns these atomic-scale contributions from a curated training set and scales the predictions up to representative volume elements suitable for finite-element analysis. The companion solver modules called `sptc2fem` and `spec2fem`, built on FEniCSx, ingest the resulting thermal and electronic conductivity fields, respectively, and produce temperature/current maps, heat-flux/current density distributions and direction-resolved effective conductivities under realistic boundary conditions. This result preserves the atomic-scale anisotropy upstream that other methods would wash out.

The end-to-end workflow delivers atomistic fidelity at device-relevant length scales. HPC runtimes drop from days to seconds, hot-spots and localized transport pathways become visible at the design stage, and engineers can interrogate how microstructural features will influence thermal and electrical performance before a single component is fabricated. By coarse-graining atom-resolved conductivity into spatially varying fields rather than collapsing them to a single bulk value, the technology preserves the heterogeneity, interfaces and defect populations that conventional finite-element treatments tend to hide behind an averaged scalar input.

Market Applications

- **Semiconductor advanced packaging** (3D integrated circuits, chiplet thermal management, package reliability analysis)
- **Fusion energy systems** (divertor and first-wall plasma-facing components, refractory metal joining qualification)
- **Aerospace and space systems** (spacecraft thermal analysis, radiation-exposed materials, mission reliability modeling)
- **Computer-aided engineering software** (constitutive model inputs for industry-standard simulation platforms)
- **Battery and energy storage** (thermal management of cells, modules and packs)
- **Thermoelectrics and biosensors** (materials discovery, device-level transport characterization)
- **Quantum device manufacturing** (cryogenic cooling design, qubit thermal isolation)