PROJECT SUMMARY

Overview

We will establish a particle-resolved open-source ecosystem (OSE) that unifies: (i) FAME (ML-augmented thermal CFD for AM), (ii) DEM+ (high-speed radiative heat transfer for granular media), and (iii) a GPU-based DEM dynamic library with a stable C-ABI for portable coupling to any CFD solver. The OSE emphasizes reproducibility (versioned APIs & conformance tests), portability (dynamic-library interfaces), and performance (GPU-first kernels).

Intellectual Merit

The project advances multi-physics modeling by tightly coupling particle-scale radiation and dynamics to continuum thermal CFD, enabling credible melt/sinter predictions and radiatively heated particle-bed studies. Phase I focuses on scoping: ecosystem discovery (I-Corps-for-POSE), governance and contributor pathways, an openly reviewed coupling spec, and feasibility exercises with minimal adapters—laying the foundation for a sustainable OSE.

Broader Impacts

Open, reproducible tools and tutorials will reduce time/cost for AM part qualification and improve TES/CSP design. Public conformance tests and example cases will accelerate workforce training and technology transfer across universities, national labs, and industry. Results and training materials will be disseminated via open repositories, documentation, and conference tutorials.

Keywords: ENG; additive manufacturing; thermal energy storage; radiative heat transfer; DEM/CFD coupling.

POSE Phase I: Enabling an Open Ecosystem for Thermo-Fluid Computational Intelligence in Manufacturing and Energy Systems

Overview

This Phase-I research aims at a structured transition of FAME (https://github.com/neoceph/FAME), a machine learning (ML) augmented finite-volume based thermal CFD solver, into a sustainable, distributed Open-Source Ecosystem (OSE) for Additive Manufacturing (AM) and supercritical (sCO_2) researchers. FAME is available to researchers under an open-source license on GitHub and has been validated against NIST metal AM experiments [1], attracting limited academic research users. The proposed OSE will provide targeted training and illustrative use cases, covering topics such as the design and analysis of AM processes and the production of sCO_2-based energy systems. Phase I activities will include: 1) formalizing the managing organization; 2) developing an effective governance model; 3) identifying and expanding the external developer and user community; and 4) designing the onboarding, outreach, licensing, and sustainability strategies for tool support. Tool development and support are led by Dr. Abdullah A. Amin and Dr. Andrew J. Schrader from the Mechanical and Aerospace Engineering Department at the University of Dayton. These researchers bring domain expertise in the design, optimization, and application of AM and Energy Systems, directly responding to the broader need for open, reproducible, and extensible infrastructure in manufacturing and energy research and development. This proposal focuses on building the foundation for a sustainable and community-driven OSE for manufacturing and energy research.

Intellectual Merit

This project will advance the FAME framework into a sustainable, community-driven open-source ecosystem (OSE) that supports high-fidelity thermal-fluid simulations for additive manufacturing (AM) and sCO_2-based thermal management. Emphasizing reproducibility, modularity, and extensibility, FAME integrates data-augmented modeling with ray-tracing-based radiative heat transfer to accurately capture beam-powder interactions and phase change dynamics key to understanding defect formation, microstructure evolution, and thermal system performance. Designed for heterogeneous CPU/GPU architectures, the framework supports scalable simulations and enables rapid iteration. By coupling physics-based solvers with modern ML libraries, it provides a rigorous platform to develop and validate AI/ML methods for surrogate modeling, real-time optimization, and intelligent process control. The project will formalize a flexible architectural design and foster a distributed contributor base to sustain long-term innovation. Integrated training resources will support the onboarding of new users, reducing entry barriers while enabling participation in advancing computational methods for intelligent manufacturing and energy systems.

Context of OSE

Long-term vision. Establish a sustainable, *particle-resolved* Open-Source Ecosystem (OSE) that unifies: (i) **FAME** (ML-augmented thermal CFD for AM), (ii) **DEM+** (high-speed radiative heat transfer for granular media), and (iii) a **GPU-based DEM** dynamic library for portable particle dynamics. The OSE's guiding principles are: reproducibility (versioned APIs, conformance tests), portability (stable C-ABI/dynamic library coupling to *any* CFD solver), and performance (GPU-first implementations).

Societal/national need. Particle-resolved thermo-fluid modeling shortens AM part qualification cycles and improves TES/CSP design by accurately predicting melt/sinter transitions and radiative heating in granular media. The OSE lowers cost-to-validate and increases transparency versus proprietary tools, supporting U.S. competitiveness in advanced manufacturing and energy systems.

Anticipated broader impacts. Faster design iteration and reduced experimental costs in LPBF AM; improved TES efficiency via radiatively heated particles; reusable, open benchmarks that strengthen technology transfer across academia, national labs, and industry; and workforce development through openly available training materials and contributor pathways.

1. **Pointer to Existing Open-Source Product:** The product repository is publicly available (see References Cited).

2. **Current Status:** FAME employs a finite volume method (FVM) development model integrated with a convolution hierarchical deep-learning neural network (C-HiDeNN) for thermal-fluid simulations, with testing focused on validation against experimental benchmarks like NIST AM datasets. Dissemination occurs through GitHub hosting, comprehensive documentation via ReadTheDocs (including installation guides using Anaconda and conda environments), and academic publications. The user base is currently limited to a small number of academic researchers (evidenced by initial downloads and feedback from early adopters in AM studies), with no formal releases yet published, indicating an early-stage but robust prototype. The contributor base consists primarily of the core development team (2-3 individuals based on commit history), with open invitations for pull requests to encourage expansion.

3. **Problem Addressed and Novelty:** FAME addresses the challenge of accurately predicting melt pool dynamics, cooling rates, and defect formation in laser powder bed fusion (LPBF) AM processes, where process variabilities (e.g., laser power, scan speed) and high computational costs hinder part qualification and certification in critical sectors like aerospace and energy. Its novelty lies in a physics-guided heat source model calibrated via higher-order proper generalized decomposition (HOPGD) and ML techniques, simplifying complex thermal-fluid interactions (e.g., Marangoni flow, vaporization, keyhole formation) into efficient cylindrical representations while coupling with modern ML libraries for surrogate modeling and optimization—superior to proprietary tools or heuristic models that often overlook volumetric energy density correlations. Substantiating evidence includes validation against the NIST AM Bench 2022 Challenge, achieving $< 5\%$ relative error in melt pool dimensions and $< 20\%$ in cooling rates/time above melting for IN718 builds, demonstrating 30-50% improvements in prediction accuracy over scaling law-based alternatives, as shown in blind experimental comparisons [1].

4. **Team Qualifications:** The team is well-qualified to lead this OSE transition, with Principal Investigator Dr. Abdullah A. Amin bringing over 5 years of expertise in physics-based modeling for LPBF AM, including development of FAME and related publications on heat source calibration for defect prediction. As a researcher in the Mechanical and Aerospace Engineering Department at the University of Dayton, Dr. Amin has presented on AM process modeling and validated tools against NIST standards. Co-Principal Investigator Dr. Andrew J. Schrader, Assistant Professor and Director of the Dayton Thermal Applications (DaTA) Laboratory at the University of Dayton, contributes deep domain knowledge in thermal sciences and energy systems, with research on concentrated solar-thermal applications, sCO_2 systems, and innovative energy technologies. His synergistic activities include mentoring

students in computational thermo-fluids and collaborating on open-source initiatives, ensuring the team's ability to formalize governance, engage communities, and sustain the OSE.

Technical Components of the Proposed OSE

The proposed OSE builds on FAME as the core open-source product while integrating complementary tools—DEM+ for high-speed radiative heat transfer and a GPU-based DEM solver—to create a unified, particle-centric ecosystem for thermo-fluid simulations in additive manufacturing (AM) and thermal energy storage (TES) systems. This integration leverages shared particle simulation capabilities to enable fast, user-friendly design and analysis, fostering collaboration among developers in manufacturing, energy, and computational science communities. Below, we detail each component and the planned integration strategy.

FAME: ML-Augmented CFD for Additive Manufacturing

FAME is an open-source, machine learning (ML)-augmented finite-volume-based thermal computational fluid dynamics (CFD) solver tailored for LPBF AM processes [1]. It addresses key challenges in predicting melt pool dynamics, cooling rates, and defect formation under varying process parameters (e.g., laser power, scan speed, spot diameter). The core innovation is a physics-guided heat source model calibrated via higher-order proper generalized decomposition (HOPGD) and ML techniques, simplifying complex thermal-fluid interactions like Marangoni flow, vaporization, and keyhole formation into efficient cylindrical representations.

FAME integrates data-augmented modeling with ray-tracing-based radiative heat transfer to capture beam-powder interactions and phase change dynamics, enabling accurate predictions of defect formation and microstructure evolution. Designed for heterogeneous CPU/GPU architectures, it supports scalable simulations and couples physics-based solvers with ML libraries (e.g., PyTorch) for surrogate modeling, real-time optimization, and intelligent process control. Validation against NIST AM Bench 2022 experiments shows ¡5% relative error in melt pool dimensions and ¡20% in cooling rates for IN718 builds, outperforming heuristic models by 30-50%.

In the OSE, FAME serves as the AM-specific module, providing extensible APIs for particle melting/sintering simulations. Its ML capabilities allow neural network-informed predictions, reducing computational costs for high-fidelity thermo-fluid analysis in manufacturing workflows.

DEM+: High-Speed Radiative Heat Transfer for Particle Systems

DEM+ is a novel, open-source radiative modeling toolset developed to extend particle-based simulations (e.g., discrete element method, DEM) to concentrated solar power (CSP) and TES environments [2]. Optimized for desktop workstations rather than high-performance computing (HPC) systems, it addresses the need for accessible, efficient radiative heat transfer modeling in granular media up to 800°C.

Key features include multiple radiative models: an accelerated Monte-Carlo Ray Tracing (MCRT) for high accuracy (application-agnostic but computationally intensive), a database of distance-based approximations for speed (computationally light but application-limited), and a weighted blending approach achieving >90% reduction in computation time with equivalent accuracy to MCRT. DEM+ was validated using ceramic sintered bauxite proppants, with experimental facilities measuring radiative and flow properties at elevated temperatures.

In TES applications, DEM+ optimizes particle heating in dilute curtains or dense packs, supporting equipment design for next-generation CSP facilities. For the OSE, DEM+ provides the radiative heat transfer module, enabling particle warming simulations that feed into downstream processes like melting in AM.

GPU-Based DEM Solver and Ecosystem Integration

The GPU-based DEM solver is an asynchronous, high-performance particle dynamics tool embedded via dynamic-linked libraries (DLLs), supporting polyhedral meshes for complex geometries [3]. It improves stability and performance by eliminating network communication needs, streamlining particle-cell searches, and leveraging GPU acceleration for 16x speed boosts over CPU-based solvers. Validated against fluidized bed experiments, it handles millions of particles with flexible meshing, crucial for industrial-scale simulations. As a dynamic library, it can be coupled with any CFD solver, such as FAME, and transported to other solvers that future developers may prefer for DEM and particle simulations.

The solver's object-oriented design facilitates extensions like heat and mass transfer modules, aligning with FAME's needs for particle-scale simulations in AM, where detailed thermo-fluid interactions (e.g., melting, sintering) require granular-level resolution.

This solver acts as the unifying "backbone" for the OSE, providing fast DEM particle simulations that integrate FAME's ML-CFD for AM melting/sintering and DEM+'s radiative heat transfer for particle heating. Connections will be achieved through modular APIs and shared libraries: e.g., DEM+ outputs radiative-heated particle states to the GPU-DEM core, which then passes dynamic particle data to FAME for thermo-fluid analysis. Initial scoping in Phase I will explore DLL-based direct coupling and open standards like OpenFOAM-compatible interfaces for cross-platform compatibility.

The resulting ecosystem enables seamless workflows: particles heated via DEM+ radiative models, simulated dynamically via GPU-DEM, and analyzed for melting/sintering via FAME's ML-CFD. Together, DEM+, GPU-based DEM, and FAME open the door for particle-resolved simulations of novel phenomena, such as sintering of particles like sand in TES or hybrid AM-TES applications. This invites developers from AM, TES, and particle simulation communities to contribute extensions (e.g., via GitHub forks), with outreach to groups like ASME and AIAA fostering adoption. Figure 1 illustrates the integration flowchart.
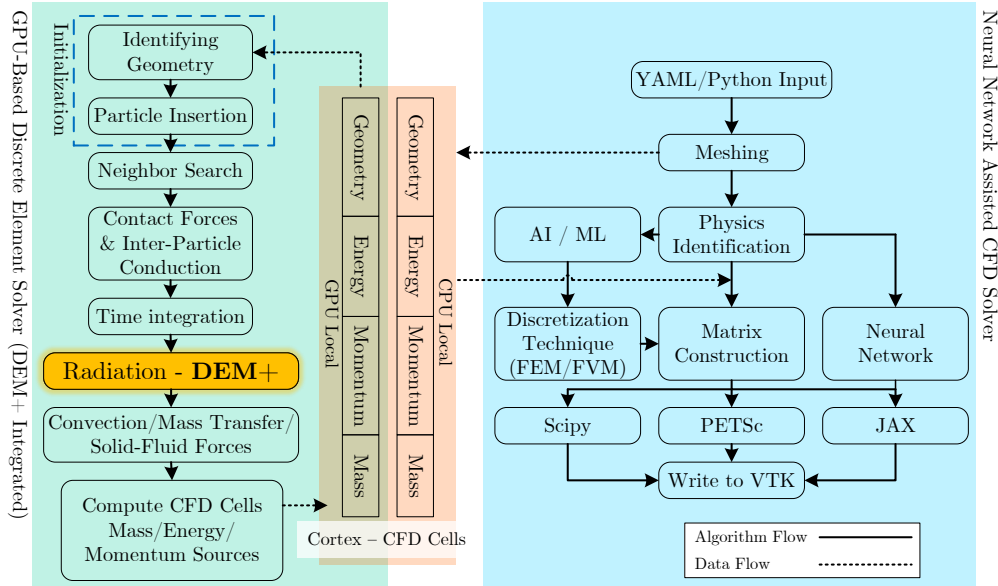
Figure 1: DEM+ provides radiative heating to GPU-DEM particles, which feed into FAME for ML-CFD analysis in the OSE.

Broader Impacts

This OSE will reduce the time and cost of qualifying AM parts and designing TES/CSP systems by enabling open, reproducible, particle-resolved thermo-fluid simulations. Public training materials (tutorials, example cases, and conformance tests) will accelerate workforce readiness in computational manufacturing and energy. Open benchmarks and validation workflows will improve scientific reproducibility and technology transfer across academia, national labs, and industry. Results and training will be disseminated through peer-reviewed publications, conference tutorials, and an openly accessible documentation portal.

Risk Analysis/Security Plan

Supply-chain security. Adopt *OpenSSF Best Practices*, generate SBOMs (SPDX), enforce provenance (baseline *SLSA*), sign releases, and maintain a coordinated vulnerability disclosure process with tracked CVEs [4, 5, 6].

This project identifies several key risks associated with transitioning FAME into an OSE, particularly those related to open-source products involving computational simulations and ML components. Primary risks include security vulnerabilities in the codebase that could lead to inaccurate thermal-fluid predictions, potentially compromising safety in AM processes (e.g., defect formation leading to structural failures in manufactured parts) or sCO_2 energy systems (e.g., inefficient heat transfer models). Data privacy concerns arise from handling experimental datasets, such as NIST AM benchmarks, which may contain sensitive material properties or proprietary process parameters. Ethical risks in AI/ML outputs include biases in the physics-guided heat source models, resulting in skewed surrogate predictions that disproportionately affect underrepresented applications in sustainable manufacturing. Additional risks encompass contributor attrition in the current small team, supply chain vulnerabilities from dependencies (e.g., PyTorch or NumPy libraries prone to unpatched exploits), and safety issues if collaboratively released artifacts enable misuse in high-stakes environments like aerospace certification.

To mitigate these, the project will follow CISA/NSA guidance on securing software supply chains, emphasizing secure-by-design principles such as integrating security early in development, conducting regular vulnerability management through automated scanning, and implementing identity and access controls to prevent unauthorized modifications [7]. OpenSSF best practices will be adopted, including SLSA frameworks for ensuring supply chain integrity (e.g., verifiable builds and artifact provenance), security scorecards to assess project health, and standardized vulnerability disclosure policies [8]. Specific strategies include establishing patching protocols (e.g., addressing known vulnerabilities within 30 days using tools like Dependabot), anonymizing datasets to comply with standards like GDPR or NIST privacy frameworks, and maintaining chain of custody via Git version control with signed commits. For ML-specific risks, bias audits will be incorporated to evaluate model fairness across diverse AM process parameters.

Phase I activities will explore mechanisms to ensure quality, secure modification, integration, and release of content. This includes conducting third-party security audits of the FAME codebase to identify baseline vulnerabilities, performing privacy impact assessments on sample datasets, and hosting workshops with experts to evaluate tools for identity and access management (e.g., GitHub's OAuth for contributor authentication). Exploration will also cover secure development methodologies, such as mandatory code reviews for pull requests and policies for patching dependencies, to build a robust foundation for collaborative OSE growth while addressing safety and privacy risks in released artifacts.

Scoping Activities for Phase I

- **I-Corps for POSE training:** 3–5 team members (including one external OSE mentor) will complete the mandatory training (41 hours over 7 weeks) and conduct at least 60 discovery interviews (per NSF guidance), with a target of 100+ interviews; salary time is budgeted.
- **Discovery interviews:** Conduct 100+ structured interviews across AM OEMs, TES/CSP integrators, powder vendors, national labs, and OSS maintainers to validate value propositions and governance expectations.
- **Timeline & roles:** Month 1–2 scoping; Month 3–4 public API
  textitdraft and review; Month 5–6
  textitfeasibility exercises using existing code and minimal adapters; Month 7 public roadmap.

Phase I scoping activities will focus on actionable planning to evaluate FAME's readiness for transition into a sustainable OSE, assess the viability of its emerging user base in AM and sCO_2 research communities, and identify a distributed developer community for ongoing maintenance and innovation. These activities are designed to be completed within the 1-year award period and \$300K budget, leveraging virtual tools, surveys, and targeted consultations to minimize costs while maximizing insights. Outputs will include a detailed roadmap for Phase II, such as drafted governance documents, community engagement strategies, and a prioritized list of ecosystem gaps. Activities will be coordinated by the PI team, with input from an external mentor experienced in open-source CFD ecosystems, and will incorporate feedback loops through quarterly progress reviews.

Specific scoping activities for Phase I include:

- **Ecosystem Discovery:** To evaluate the technological landscape, the team will conduct a comprehensive literature review and competitor analysis, surveying similar open-source CFD and ML tools (e.g., OpenFOAM for thermal-fluid simulations and PyTorch for ML integration). This will justify the need for FAME's innovation by highlighting gaps in physics-guided models for LPBF AM and sCO_2 systems, such as limited support for real-time optimization in proprietary alternatives. The OSE approach will be validated as ideal for distributed innovation, enabling asynchronous contributions unlike closed systems that restrict extensibility. Methods to identify potential users and developers include online surveys distributed to 50-100 stakeholders in AM/energy sectors (e.g., via professional networks like ASME and AIAA mailing lists) and analysis of GitHub metrics (e.g., forks, stars, and related repositories) to map interest from academia and industry.

- **Organization and Governance:** Activities will benchmark organizational models against established foundations (e.g., Apache Software Foundation for community-led governance or Linux Foundation for industry consortia) through case study reviews and consultations with 3-5 experts. Licensing options will be evaluated (e.g., MIT for permissiveness vs. GPL for copyleft protections) to ensure compatibility with ML dependencies like PyTorch. CI/CD infrastructure needs will be assessed, such as integrating GitHub Actions for automated testing on heterogeneous CPU/GPU setups to support asynchronous, distributed development. Processes for quality, security, privacy, and ethical concerns will be drafted, including guidelines for validating new ML models against NIST benchmarks. Sustainability methods will explore funding models (e.g., grants, donations via Open Collective) and metrics for long-term success, such as contributor retention rates >50%, user support response times <48 hours, and onboarding completion rates measured via tutorial analytics.

- **Risk Analysis/Security:** Building on the dedicated risk plan, scoping tasks will include a third-party security audit of FAME's codebase using tools like SonarQube

to baseline vulnerabilities, and privacy impact assessments on sample AM datasets to identify anonymization needs. Workshops (2 virtual sessions with 20-30 participants) will explore secure development practices, such as adopting OpenSSF scorecards for dependency management. Mechanisms for quality assurance (e.g., automated unit tests for thermal predictions), secure content integration (e.g., enforced code reviews via GitHub pull requests), identity and access management (e.g., OAuth for contributor authentication), and chain of custody (e.g., Git signed commits for provenance tracking) will be evaluated, with a focus on ML-specific risks like model bias through fairness audits.

- **Community Building:** To engage potential users and intellectual content developers, activities will identify required capabilities (e.g., proficiency in Python, CFD/ML for contributors; domain knowledge in AM/sCO_2 for users) via targeted surveys and interviews. Mechanisms include hosting 2-3 virtual workshops (e.g., introductory sessions on FAME's heat source modeling with 50+ participants from universities and labs) and a themed hackathon focused on extending FAME for sCO_2 applications. Online forums (e.g., GitHub Discussions) and research coordination networks (e.g., via Slack channels) will facilitate engagement. Inclusivity will be emphasized through scholarships for underrepresented participants (e.g., from HBCUs or women in STEM groups) and accessible materials, aiming to grow the contributor base from 2-3 to 10+ by project's end.

Community Outreach Plan

Developer-first engagement. We will target technical contributors and early adopters through: (i) quarterly deep-dive webinars (architecture, coupling APIs, CI pipelines); (ii) hands-on tutorials (AM-Bench reproduction; DEM+ radiation benchmarks; FAME↔GPU-DEM minimal coupling); (iii) interoperability hackdays focused on adapter conformance; and (iv) office-hours for prospective maintainers.

Channels and partners. Outreach will emphasize technical venues: ASME/AIAA CFD tracks, SIAM CSE, ICCFD, and domain meetings (AM Bench, RAPID+TCT). We will coordinate with U.S. national labs (e.g., NIST for AM benchmarks; ORNL, LLNL, Sandia for AM/TES modeling) and relevant NASA ISRU/regolith efforts as a potential use case for particle sintering on the Moon (see [9, 10]).

Contributor journey. Clear contribution guides, labeled "good first issues," mentorship to reviewer/maintainer roles, and a public RFC process for API changes. We will publish reference implementations of conformance tests and maintain a backlog of adapter tasks aligned to the roadmap.

Discovery and conversion. Month 1–2: stakeholder mapping and surveys ($\geq$100 outreach targets); Month 3–4: tutorials & API RFC; Month 5–6: interoperability hackday; Month 7–12: maintainer cohort formation and pilot feasibility exercises.

Success metrics. Monthly active contributors; time-to-first-PR; number of external maintainers; # adapters passing conformance tests; AM/TES benchmarks reproduced; industrial/national-lab pilots initiated.

Evaluation Plan

Metrics: monthly active users/contributors; Time-to-first-PR; number of external maintainers; CI pass rate; SBOM coverage; SLSA level; number of AM/TES benchmarks reproduced; number of industrial pilots; training completions; governance participation

The evaluation plan for this Phase I project will employ actionable, quantitative, and qualitative

metrics to assess progress toward scoping a sustainable OSE for FAME, focusing on product readiness, user base viability, and developer community potential. Drawing from metrics and indicators discussed in the Linux Foundation's report on open source for sustainability [11, 12, 13], including CHAOSS frameworks for community health and , the plan integrates traditional tracking with novel approaches like AI-driven sentiment analysis on community feedback to provide dynamic insights. Evaluation will inform adaptive adjustments, ensuring alignment with NSF goals, and culminate in a Phase II readiness report. An external mentor will provide independent reviews, while the PI team conducts internal assessments.

Key metrics include: number of new contributors engaged (target: 10+ from baseline of 2-3, measured via GitHub commits and pull requests); user adoption growth (target: 50% increase in downloads/stars, from current low baseline); completion of governance artifacts (e.g., 1 draft framework, 2-3 policy documents); community engagement levels (e.g., 100+ survey responses, 50+ event participants); and ecosystem health scores (e.g., CHAOSS-derived activity index >0.5, incorporating openness via license compatibility and scalability via modular extensions). Innovative metrics will track g., 30% from underrepresented groups, using self-reported demographics) and innovation impact (e.g., number of novel use cases proposed, assessed via hackathon outputs).

Assessment methods will combine repository analytics (e.g., GitHub Insights for contribution trends), pre/post-event surveys (e.g., Net Promoter Score for satisfaction), and automated tools like natural language processing for sentiment analysis on forum discussions and feedback forms to gauge inclusivity and ethical concerns. Quarterly reviews (Months 3, 6, 9, 12) will involve stakeholder meetings to analyze data, adjust activities (e.g., pivot outreach if engagement lags), and document lessons learned, ensuring transparent, data-driven progress toward OSE viability.

Budget Overview (Phase I)

POSE Phase I funds will support scoping and planning (not product development). We anticipate the following budget emphases (final details in the budget & justification):

- **Personnel:** one postdoctoral researcher (lead: DEM solver repository maintenance and coupling specification) at ∼$100,000 total (salary+fringe); one M.S. graduate student; partial support for PI/Co-PIs.
- **Training:** time for the mandatory *I-Corps for POSE* training (3–5 team members), including discovery interviews.
- **Travel:** I-Corps activities; technical workshops; targeted conference tutorials (e.g., RAPID+TCT, ASME IMECE) aligned to outreach.
- **Workshops/Events:** virtual tutorials and interoperability hackdays (participant support, materials).
- **Materials & Supplies/Services:** CI compute, documentation hosting, and code-signing services.

Note: No equipment is requested in Phase I, in accordance with the POSE-I solicitation.

Prior NSF Support

The PI's have no prior NSF support.

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