High-Performance Computing for Energy Innovation Program: Collaboration for U.S. Manufacturers

The High-Performance Computing for Energy Innovation (HPC4EI) program is seeking qualified industry partners to participate in high-impact collaborative projects with the U.S. Department of Energy's (DOE) national laboratories.

The HPC4EI program works with a variety of DOE offices to bring national lab computing expertise to industry. The program is highly aligned with DOE's priorities on true technological breakthroughs including Artificial Intelligence (AI) and High-Performance Computing (HPC[1]). This solicitation is for topics of interest for DOE's Advanced Materials and Manufacturing Technologies Office (AMMTO) and the Industrial Technologies Office (ITO). Selected industry partners will receive access to (HPC) facilities and world-class science and engineering staff at DOE's national laboratories.

The HPC4EI program supports collaborative projects that address complex manufacturing and materials challenges relevant to the U.S. energy sector. The program is designed to reduce production costs, improve efficiency and performance, strengthen domestic supply chains, and enhance U.S. industrial competitiveness in global markets. These objectives are achieved by pairing industry-defined challenges with national laboratory supercomputing capabilities and technical expertise.

Eligibility for participation in the HPC4EI program is limited to U.S.-based manufacturers and organizations that directly support these manufacturers.

Selected Phase I projects will receive awards of up to $400,000 per project to support high-performance computing cycles and technical work performed by the national laboratory staff. Industry partners are required to provide an in-kind cost share of at least 20% of the total project funding. All cost share contributions must come from non-federal funding sources.

Follow-on Phase II projects may be proposed by teams with previously awarded and successfully completed Phase I projects under this program. Phase II projects are intended to transition validation HPC applications toward implementation in industrial settings, enabling broader operational deployment and national impact.

Selected Phase II projects will receive similar funding amounts and are subject to the same cost-share requirements like Phase I. At least half of the 20% cost-share contribution must be a cash contribution used to support national laboratory work.

[1] Sec. Wright Memorandum on Unleashing the Golden Era of American Energy Dominance, February 5, 2005. Wright Department of Energy Memorandum.pdf

The HPC4EI program is managed by Lawrence Livermore National Laboratory (LLNL) for the U.S. Department of Energy's Office of Critical Minerals and Energy Innovation, Hydrocarbons and Geothermal Energy Office, and Office of Science. Prepared by LLNL under Contract DE-AC52-07NA27344. HPC4EI-2026SP-RN-SOL LLNL-MI-2016829
April 21, 2026

Background

The U.S. Department of Energy (DOE) operates and maintains world-class high-performance computing (HPC) facilities and expertise, currently hosting several of the top 20 most powerful computers globally as ranked by TOP500 (November 2025)[2]. From detailed subatomic- and molecular-scale phenomena to massive, system-level models, these resources enable research at scales and levels of fidelity that are not achievable through experimental methods alone. Scientific insights gained from these computational studies have drastically impacted research and technology across industrial and technological domains. Examples include additive manufacturing, aerospace systems, oil production and recovery, drug development, materials discovery and design, genomics, and exploration of fundamental particles that represent building blocks of our universe. From industry to academia, the growing demand for advanced computational modeling and simulation continues to drive innovation and development for future high-performance computing architectures.

U.S. industries and manufacturers have a significant opportunity to expand their use of high-performance computing (HPC) to address complex technical challenges and accelerate technology development. The HPC4EI program lowers barriers to adoption by providing HPC resources and technical expertise to industries, enabling broader and more effective use of advanced computational methods. Through targeted collaborations between industry and one or more of DOE's national laboratories, HPC4EI program seeks to empower businesses to leverage HPC effectively.

Successful applicants will work collaboratively with national laboratory staff to execute project activities across relevant HPC areas of expertise. These areas may include development and optimization of modeling and simulation codes, porting and scaling of applications, application of data analytics and machine learning, as well as applied research and development of tools or workflows.

To maximize impact across the U.S. industrial community, project teams are expected to share non-proprietary results at program sponsored workshops and at regional or national technical conferences. Publication of results is also encouraged, consistent with the protection of proprietary and export-controlled information.

Area 1: Office of Critical Minerals and Energy Innovation's (CMEI) Advanced Materials and Manufacturing Technologies Office (AMMTO)

The Advanced Materials and Manufacturing Technologies Office (AMMTO) works to strengthen America's manufacturing and industrial base, ensuring it remains globally competitive and central to the nation's energy security. AMMTO drives innovation in advanced materials, manufacturing technologies, and workforce development to support reliable, affordable, and secure energy systems and supply chains. By providing research, development, and demonstration AMMTO helps accelerate the transition from laboratory breakthroughs to commercial deployment while building the skilled workforce needed for long-term U.S. leadership in advanced manufacturing.

[2] TOP500 list of the world's most powerful supercomputers, SC25 Conference, November 2025. Home - | TOP500

Proposals should demonstrate credible pathways to advancing American manufacturing competitiveness, improving supply chain security, enhancing energy system reliability, and creating high-quality domestic jobs.

Of particular interest to AMMTO are:

1. **Development of advanced materials to improve the performance, durability, and cost-effectiveness of energy systems and technologies**

AMMTO seeks to accelerate the discovery, development, qualification, and deployment of advanced materials by addressing cross-cutting barriers that slow adoption, increase costs, or limit performance in energy applications. Of particular interest are modeling and simulation approaches that increase the manufacturing readiness of advanced materials for affordable, reliable, and secure energy technologies, including fossil fuels, advanced nuclear, geothermal, and grid infrastructure. Proposals should focus on innovative approaches that address cross-cutting barriers and result in reducing time-to-market, enabling manufacturability at scale, and improving system-level performance. Examples of barriers and topics to be addressed include, but are not limited to:

a. **Qualification and certification barriers**
Data-driven and model-based approaches to reduce the prohibitive time and cost of qualifying advanced materials for critical applications and shorten the pathways to industrial adoption. This includes digital twin-based certification systems, accelerated validation and verification (V&V) frameworks, predictive lifetime performance models, interoperable digital standards, and predictive models for structural and functional materials performance.

b. **Scaling and manufacturability challenges**
Simulation and design-for-manufacturability tools that reduce cost and risk in scaling up advanced materials, such as composites for reactors and turbines or high-performance alloys for harsh environments. Proposals may include pilot-scale validation of scalable processing routes or integration of manufacturability assessments into early-stage materials discovery.

c. Critical materials and critical minerals for energy manufacturing
Modeling and simulation-enabled approaches that accelerate the development, substitution, efficient use, and recovery of critical materials/minerals essential to U.S. energy systems and manufacturing. Of particular interest are computational methods that reduce technical, cost, and supply chain risks associated with materials such as rare earth elements, battery materials, among other critical materials/minerals identified on DOE's list[3].

d. **System performance in demanding environments of critical energy systems**
Material innovations integrated into system designs to meet urgent performance

[3] Notice of Final Determination on 2023 DOE Critical Materials List, August 2023. Federal Register :: Notice of Final Determination on 2023 DOE Critical Materials List

requirements under extreme operating conditions (e.g., high temperature, radiation, corrosion, high stress). Focus areas include multifunctional materials with combined structural, thermal, and electrical performance; high-conductivity materials for transmission and motors; and advanced thermal management solutions for power electronics, semiconductors, and computing systems.

e. **Leveraging smart manufacturing and digitally-enabled technologies across the advanced materials lifecycle**
   Integration of advanced digital tools to accelerate the entire materials lifecycle from discovery and property prediction to process optimization, qualification, and system integration. Of particular interest are artificial intelligence/machine learning- (AI/ML) driven materials informatics, end-to-end digital thread platforms, and smart manufacturing approaches that enable faster development, improved reproducibility, and reduced cost of advanced materials deployment.

f. **Supply chain and cost barriers**
   Modeling of material systems that enable cost-effective domestic production and reduce reliance on vulnerable foreign supply chains. Examples include rare-earth-free magnetic materials, substitutes for critical minerals, closed-loop recycling methods for composites and polymers, and cost-optimized alloy or composite systems for grid and energy infrastructure.

2. Development of manufacturing processes to strengthen U.S. industrial competitiveness and energy security

AMMTO seeks to advance innovative manufacturing processes that enhance the cost competitiveness, quality, time-to-market, and reliability of domestic production for critical energy applications. Proposals should address cross-cutting challenges that limit throughput, increase cost, or slow time-to-market for components and systems vital to the nation's energy infrastructure and supply chain security. Examples include, but are not limited to:

a. Cost and throughput barriers
   Modeling of production processes that improve dimensional accuracy, increase throughput, and lower costs while reducing material waste and energy consumption. Of particular interest are advanced reactors, turbine systems, grid-scale storage, and mobility components where reduced cycle times and higher yields directly improve competitiveness.

b. Time-to-market and qualification barriers
   Simulation of advanced manufacturing methods (e.g., additive manufacturing, convergent and hybrid processes) with in situ monitoring, real-time feedback, and digital twin–based validation to accelerate qualification of critical components and reduce lead times from prototype to deployment.

c. Quality challenges
   Modeling of high-throughput machining, finishing, and forming technologies that deliver greater precision and reliability at scale, enabling consistent production of large-scale and complex components for nuclear, turbine, and geothermal applications.

d. **Integration of advanced digital tools into manufacturing processes**
Use of AI/ML, integrated computational materials engineering (ICME), and smart manufacturing platforms to optimize process control, improve reproducibility, and drive asset optimization across the production cycle.

e. **Supply chain security**
Modeling of modular, continuous, or distributed manufacturing approaches (e.g., advanced casting, forging, forming, or joining) that improve domestic supply chain security by enabling scalable, flexible, and geographically distributed production of critical energy system components.

Area 2: Office of Critical Minerals and Energy Innovation's Industrial Technologies Office

ITO works to strengthen America's industrial sector and advance global competitiveness of U.S. industry by funding research, development, and demonstration (RD&D) of secure and cost-effective industrial technologies. ITO funds both sector-specific technology solutions—with a focus on helping the most energy-intensive industries overcome barriers and benefit from the latest in technology innovation and strategic analysis—and cross-cutting technologies that can be applied across the industrial sector. ITO also works to accelerate the commercialization of new technologies by addressing adoption barriers to technology deployment, including through tailored technical assistance programs to help manufacturers save money and streamline operations.

U.S. industry is foundational to the nation's economic growth and prosperity, where every $1.00 of manufacturing investment creates $2.64 of total benefit to the U.S. economy.[4] Industrial innovation has improved the lives of millions and has enabled modern society as we know it. Today, the U.S. industrial sector creates more than 21 million stable, well-paying American jobs, and is a critical driver of national productivity, contributing $4.8 trillion to the U.S. economy.[5,6] HPC can play a key role in accelerating the innovation that is core to the competitiveness of American industry. Previous efforts in HPC4EI have used artificial intelligence to identify and mitigate inclusions in molten steel, developed models to increase the efficiency of drying processes in papermaking, and created machine learning tools that improve process control for plate glass manufacturing, among other successes.[7]

This topic aims to advance DOE's priorities for the industrial sector:

- Strengthen the global competitiveness of the U.S. industrial sector by reducing costs, improving product value, and generating American jobs.
- Enable energy abundance and industrial growth by reducing the energy intensity of industrial processes and facilities.

[4] National Association of Manufacturers, "Facts About manufacturing," accessed June 2025, https://nam.org/mfgdata/facts-about-manufacturing-expanded/.
[5] U.S. Bureau of Labor Statistics, "Industries at a Glance: Goods-Producing Industries," accessed January 2025, www.bls.gov/iag/tgs/iag06.htm.
[6] U.S. Bureau of Economic Analysis, "Interactive Data Application: Interactive Access to Industry Economic Accounts Data," accessed January 2025, apps.bea.gov/iTable/?reqid=150&step=2&isuri=1&categories=gdpxind.
[7] HPC4EnergyInnovation, "Success Stories," https://hpc4energyinnovation.llnl.gov/success-stories.

- Improve the reliability and security of American energy infrastructure by increasing the flexibility and responsiveness of industrial sector demand.
- Secure American supply chains through technical innovation to onshore industrial excellence and ensure domestic availability of critical products.

ITO seeks to advance highly innovative and impactful technologies through HPC4EI. The potential industry-wide impacts of projects will be a major consideration in the evaluation of proposals. Proposals with limited impacts (e.g., not translatable beyond the applicant organization or a specialty product) are unlikely to be successful. Therefore, **applications under this topic <u>must</u> include quantitative analysis of energy and cost impacts.** Additional metrics should be included as needed to demonstrate the full impact and business case for the technology.

Of particular interest to ITO are development, optimization, scale-up, and integration of:

- Technologies that significantly improve productivity optimization in energy-intensive industries for manufacturing competitiveness. Industries of interest include:

  a. *Chemicals and Fuels*, including the exploration of (1) process innovations, (2) novel reactor and separation technologies, (3) the development of low-cost, high-performance, robust catalyst structures, and (4) advanced materials development and scale-up for chemical manufacturing.
  b. *Iron and Steelmaking, Aluminum, and Other Metals,* including innovative processes for primary metals production, methods to optimize productivity, methods to de-copperize steel, and practical methods to approach the thermodynamic minimum in metals production. Chemical processing of novel mineral sources for multiple value streams, and ore beneficiation process innovations, are also of interest. Smart Manufacturing applications in both existing commercial processes and in novel innovative processes are of interest.
  c. *Food and Beverage Products,* including sector-specific processing that optimize productivity by (1) efficient recovery and cost-effective reuse of waste energy (in both latent and sensible form) and (2) establishing alternative process routes and emerging technologies to extend products' shelf life and minimize waste.
  d. *Cement and Concrete, Asphalt, and Glass*, including process innovations, alternative source materials, novel material compositions, and innovative solutions to reduce waste along the value chain. <u>Not of interest</u>: Advancements centered around Ordinary Portland cement (OPC) type I/II.
  e. *Forest Products,* including novel dewatering or drying technologies and improved pulping and chemical recovery processes.

- Equipment and processes that improve industrial process heating, including reducing cost, improving efficiency, or enhancing product quality. Areas of interest include:

  a. *Electrified or hybrid heating approaches*, including technologies such as induction, electric arc/plasma, electromagnetic, and resistive heating.
  b. *Heat upgrading technologies*, including models informing development of vapor compression-based technologies as well as thermally driven, solid state, and other non-vapor compression solutions.

c. *Utilization of on-site fuels* (e.g., natural gas, hydrogen, biofuels) and integration of emerging on-site heat sources (e.g., geothermal, small modular nuclear reactors, combined heat and power, thermal energy storage).
d. *Heat exchangers for harsh industrial conditions* (e.g., temperatures over 800 C, corrosive environments) with reduced cost, reduced maintenance, improved performance, and/or smaller footprint.
e. *Efficient fuel-flexible combustion system designs*, including digital twins for real-time optimization of combustion processes with improved performance and accurate prediction of pollutant formation from multiple fuels as well as multiphase combustion behavior.

- Non-thermal processes for cost-competitive separations and treatments. Areas of interest include:

a. *Membrane separations*, including development of novel membrane separations and improvements to incumbent membrane separations. Of particular interest is development and scale-up of molecularly thin membranes.
b. *Other technologies that significantly reduce or eliminate the heat needed for industrial processes*, such as non-thermal drying and electrochemical processes.
c. *Improvements to other energy-intensive non-thermal equipment and processes* (e.g., comminution).

- Industrial technologies that can ensure grid reliability in the face of industrial demand growth. Areas of interest include:

a. *Technologies that enable flexible industrial energy use* (e.g., processes that can ramp up/down without disrupting operations) and industrial grid edge capabilities (e.g., providing demand response and other grid services).
b. *Thermal energy storage technologies*, including sensible, latent, and thermochemical systems for either hot or cold storage.
c. Technologies that can reduce the electrical demand of data center operations, such as onsite combined cooling and power systems, novel or retrofittable cooling systems (e.g. liquid-cooled servers, chillers, cooling towers), and waste heat recovery and integration systems. <u>Not of interest</u>: innovations in algorithms or IT hardware, such as microelectronics.

- Technologies at the water-energy nexus that enable production of fit-for-purpose water. Areas of interest include:

a. Equipment, control systems, processes, and treatment trains to improve efficiency of water and wastewater treatment, including for industrial and agricultural wastewaters.
b. Technologies that reduce the direct water consumption of data centers, such as on-site water recycling or treatment for zero-water or low-water operations.

- Opportunities across the areas of interest above to leverage emerging artificial intelligence and machine learning methods. Of particular interest is the use of AI to accelerate R&D and optimize processes within these domains.

For this topic, the following types of applications are specifically not of interest:
- Applications focused on electricity generation systems or components, except electricity generation from waste heat.
- Applications focused on CO_2 capture and/or storage.

Eligibility

Eligibility is limited to U.S. manufacturers, defined as entities that are incorporated (or otherwise formed) under the laws of a particular state or territory of the United States, and that manufacture products in the United States or that manufacture, distribute, or otherwise deploy software and/or hardware systems as described above or that develop and/or manufacture new or modified materials in the United States. Project work must be executed in the United States.

U.S. universities, institutes, and other non-profit organizations are also eligible to participate as collaborators. Funding for university and/or non-profit participants may be provided by the national laboratory or the industrial partner. If the funding for a university or non-profit participant is to be provided by DOE through the DOE laboratory partner, funding requests must be less than half of the total DOE funds. Funding provided to a university and/or non-profit by the industrial partner can be considered a component of the industrial partner's in- kind funding contribution.

An entity may only submit one Concept Paper and one Full Proposal (Full Application) per Area. If an entity submits more than one Concept Paper in an area, the review committee will select no more than one proposal from this entity to advance to the Full Proposal (Full Application) stage. This limitation does not prohibit an applicant from collaborating on other applications (e.g., as a potential subrecipient or partner) so long as the entity is only listed as the applicant on one Full Application per area for this solicitation. In organizations with more than 5,000 employees, an "entity" can be considered to be a major business unit within the company, for example, an Aerospace Division as distinct from a Central Research Division.

Funding Requirements

The DOE monetary contribution for each project will not exceed $400,000. For new initial (not Phase II) projects, an industry partner must provide a participant contribution of at least 20% of the total project funding to support industry expertise to the project. Total project funding is defined as the DOE contribution plus the contributions (in-kind and cash) from the industry partner. Cash contributions are funds supplied by the industry partner to collaborators external to the company. The participant contribution can take the form of monetary funds in or "in-kind" contributions and must come from non-federal sources unless otherwise allowed by law. For Phase II projects, defined as a project that is using the results of a previously funded project within the HPC4EI portfolio, the industry contribution is 20% of the total project funding of which at least half of this amount is a cash contribution. Sample budgets are shown below. DOE funding will be provided to the national laboratory (or laboratories) in support of their work under the HPC4EI program.

Sample Budget

Project (New project, total project funding of $500K)

TASK	DOE Funds	Industry Partner Cash Contribution	Industry Partner In-kind
Total Project Funding = $500K	**$400K**		**$100K**

Phase II Project (uses results from a previously funded project, total project funding of $500K)

TASK	DOE Funds	Industry Partner Cash Contribution	Industry Partner In-kind
Total Project Funding = $500K	**$400K**	**$50K**	**$50K**

Note: THIS IS NOT A PROCUREMENT REQUEST.

Solicitation Process and Timeline

This solicitation comprises a two-stage process consisting of the submission and evaluation of a **2-page Concept Paper** and **7-page Full Proposal** submitted by the industrial principal investigator (PI). These will be evaluated by a technical review committee on the technical challenge to overcome; how this advances the state of the art for the industrial sector; how HPC can uniquely contribute to the solution of the technical challenge; and the company specific and broad national impact that a successful project can have. A notional project plan should be included.

Successful concept papers will be paired with a national laboratory partner for the development of the full proposal. Full proposals will be reviewed by a technical committee against the criteria given below. The portfolio of proposals recommended by the committee will be submitted to DOE senior managers for final selection, subject to the availability of funding. All DOE funding decisions shall be final.

Upon approval of funding selections by DOE, the HPC4EI program will issue a written response to each applicant in the form of an email. Applicants selected for funding will subsequently engage in a formal agreement with the partnered laboratory before work may begin.

Private sector applicants will engage in a DOE Short Form Cooperative Research and Development Agreement (CRADA) for the successful proposal. Once both parties approve the Short Form CRADA, project execution may begin. Failure to engage promptly in CRADA negotiations can result in rejection or cancelation of the project.

The portfolio of projects will be posted on the HPC4EI website. The HPC4EI program reserves the right to select all, a portion, or none of the submissions.

If a concept paper or full proposal is technically strong, but is not selected for funding, the program management team may share them with other DOE program offices for consideration for possible funding through those offices.

Timeline

Current solicitation schedule dates will be posted on the HPC4EI website. Event dates are subject to change.

Event	**Dates (2026)**
Call for Proposal	April 28, 2026
Concept Paper Due	May 27, 2026
Request for Full Proposal	July 2026
Full Proposal Due	August 2026
Finalists Notified	October 2026

Concept Paper Guidelines

Interested parties will submit a concept paper describing the project objectives by the due date provided above. The concept paper will be evaluated against the documented criteria. Successful concept papers will be invited to submit a full proposal.

The concept paper template can be downloaded from the HPC4EI website and the electronic proposal system. This template should be used to prepare your submission. The concept paper should not exceed 2 single-spaced pages using 12-point Times New Roman font, 1-inch margins, and formatted in a PDF file. The concept paper **must include** the following components under the corresponding headings below. A concept paper that does not meet the guidelines may be rejected for review. The following is a description of the concept paper template.

- **Title Page:** *Include proposal tracking number, the project title, and company name. The title page is not included in the page limit.*

- **Abstract:** *Provide a* ***non-proprietary, publishable*** *summary,* ***150 words or less****, of the problem being addressed, why the problem is important to the energy future of the United States, a plan to address the problem, and the impact the solution will have.*

- **Background:** *Explain the technical challenge to be addressed; the state of the art in this area, and how this work advances the state of the art; how solving this problem will meet the goals of the HPC4EI program as defined by the list of topics of interest; the relevant expertise of the industry partners; what national laboratory expertise is needed; and why national laboratory HPC resources are required and how they will be used.*

- **Project Plan and Objectives:** *Describe the technical scope of work to be performed and how this project fits into an overall solution strategy for the challenges being addressed. Describe how the results of the project will be validated, including availability of data. If possible, identify specific simulation codes to be used in this effort. Summarize how your project plan will address the key proposal review criteria: advances the state of the art in the industrial sector, technical feasibility, relevance to high-performance computing.*

- **Impacts:** *Describe how this specific HPC effort will lead to national impact, encompassing one or more of the following: 1) national-scale, long-term energy and cost reductions across the industry; 2) the performance improvements that are expected over existing technologies; 3) improvements in the ability of industry to accelerate the adoption of emerging technologies; 4) transformational change in the industrial sector and enduring economic impact; 5) improvements to product quality or reliability; 6) improvements to U.S. security such as onshoring of critical technologies and supply chains; 7) improvements to cybersecurity of manufacturing operations. Provide clear, evidence-based benefits, including energy and cost savings, productivity improvements, and/or other quantitative benefits, that will have a broad (national-scale) industrial impact through development and/or improvement of manufacturing technologies,* *improved global market competitiveness, impact on employment and manufacturing in the United States, and/or improved affordability, reliability, or security of the U.S. energy and manufacturing supply chains. Describe additional impacts this work will have on manufacturing and HPC communities. Include plans for any publications, improvements to open-source software, public databases that will be released or improved, and training provided for students or postdocs, etc.*

For Phase II projects, the concept paper should not exceed 3 single-spaced pages using 12-point Times New Roman font, 1-inch margins, PDF file format, and should include all the components described above. In addition, the following component is required:

- **Results from the prior funded project (one page maximum with figures)** *Review the results and knowledge gained from the prior funded project. Explain how these results will be used to address the objectives of this proposal. If you believe that the current proposal is distinctly different from the previous project and should not be considered as a follow-on project, articulate the differences.*

The following appendices are also required and are **not included in the page count**:

- **Appendix A: Quantitative Analysis** *Applicants must provide a quantitative analysis of: energy savings, cost savings, improvement in product quality, improvement in product durability, improvement in product reuse and recyclability, improvement in operational flexibility,* ***and/or*** *reduction in waste during manufacturing,* ***as applicable to the project****. Note that applicants responding to* ***Area 2*** *must at least include quantitative analysis of energy and cost impacts*.

- **Appendix B: Changes from Previous Submissions (Reapplications)** *For proposals that have been re-submitted from a previous solicitation, briefly describe how you have incorporated changes based on reviewer comments from the previous submission.*

- **Appendix C: References** *Relevant references are considered to be citations of publications or conference proceedings. Additional information such as company descriptions, graphics or other descriptions are not considered appropriate for this section and will not be reviewed by the reviewers.*

Completed **concept papers**, derived from the provided template, **must be submitted to the electronic proposal system at https://proposalshpc4.inl.gov by 5:00 p.m. PT on the deadline indicated on the submission website.** Submission includes completion of electronic applicant form and upload of concept paper in PDF file format. Concept papers will be evaluated against the criteria listed in the Evaluation Criteria Section.

Full Proposal Guidelines

Successful concept paper submissions will be notified and paired with a PI from one, or a combination, of the following laboratories:

- Ames Laboratory
- Argonne National Laboratory
- Brookhaven National Laboratory
- Idaho National Laboratory
- Los Alamos National Laboratory
- Lawrence Berkeley National Laboratory
- Lawrence Livermore National Laboratory
- National Energy Technology Laboratory
- National Laboratory of the Rockies
- Oak Ridge National Laboratory
- Pacific Northwest National Laboratory
- Sandia National Laboratories
- Other DOE Laboratories

Partners will then collaborate on the development of a full proposal. Full proposals will be evaluated against the criteria described in the Evaluation Criteria Section.

The full proposal template can be downloaded from the HPC4EI website and the electronic application system. This template should be used to prepare your submission. Proposals should not exceed 8 single-spaced pages using 12-point Times New Roman font, 1-inch margins, and formatted in a PDF file. Follow-on project proposals should not exceed 10 single-spaced pages using 12-point Times New Roman font, 1-inch margins, in PDF file format, and should include all the components with additional Results from Prior Funded Project section. The full proposal **must include** the components under the corresponding headings below. Proposals that do not meet the guidelines may be rejected for review.

- **Title Page (not included in page limit):** *Include the proposal tracking number, the project title, company name, and national laboratory PI contact information.*

- **Abstract (150 words or less):** *Provide a* ***non-proprietary, publishable,*** *summary of the problem being addressed, why the problem is important to the energy future of the United States, a plan to address the problem, and the impact of the solution. If selected for the HPC4EI program, this abstract will appear on award announcements sent to the press and posted on the program website.*

- **Background:** *Describe the technical challenge to be addressed; the state of the art in this area and how this work advances the state of the art; how solving this problem will meet the goals of the HPC4EI program as defined by the list of topics of interest; the relevant expertise of the industry partners; what national laboratory expertise is needed; and why national laboratory HPC resources are required and how they will be used.*

Indicate if the proposed project will accelerate transformational technological advances in areas that industry by itself is not likely to undertake because of technical and financial uncertainty.

- **Phase II Project Proposals Only - Results from the Prior Funded Project (two additional pages maximum with figures):** *Review the results and knowledge gained from the Phase I project. Explain how these results will be used to address the objectives of this proposal. If you believe that the current proposal is distinctly different from the previous project and should not be considered as a Phase II project, articulate the differences which must be substantial.*

- **Project Plan and Objectives:** *Describe the technical scope of work to be performed and how this scope will fit into the broader solution for the challenges being addressed, including, for example, relevant experimental work. Outline a set of tasks to be performed by each participant. Include description of work activities performed by the industry partner, national laboratory partner, and/or university or non-profit. Describe how the results of the project will be validated, including availability of data. If possible, identify simulation codes to be used in this effort and any modifications to the software that are needed to solve the proposed problem. Summarize how your project plan will address the following key proposal review criteria: advances the state of the art in the industrial sector, technical feasibility, and relevance to high-performance computing.*

- **Tasks, Milestones, Deliverables, and Schedules:** *Include goals, timelines, and due dates throughout the life of the project. Not every milestone needs to have a deliverable. Include deliverables from all partners, not just the national laboratory partner(s). Indicate responsible party (parties) for each deliverable. Include deliverables from one partner to another, as well as those to the DOE program sponsors.*

- **Validation and Verification Plan:** *Summarize how the model will be validated and the simulations verified. Include information about the experimental data that will be used for verification, its nature and source.*

- **Impacts:** *Describe how this specific HPC effort will lead to national impact, encompassing one or more of the following: 1) national-scale, long-term energy and cost reductions across the industry; 2) the performance improvements that are expected over existing technologies; 3) improvements in the ability of industry to accelerate the adoption of emerging technologies; 4) transformational change in the industrial sector and enduring economic impact; 5) improvements to product quality or reliability; 6) improvements to U.S. security such as onshoring of critical technologies and supply chains; 7) improvements to cybersecurity of manufacturing operations. Provide clear, evidence-based benefits, including energy and cost savings, productivity improvements, and/or other quantitative benefits, that will have a broad (national-scale) industrial impact through development and/or improvement of manufacturing technologies, improved global market competitiveness, impact on employment and manufacturing in the United States, and/or improved affordability, reliability, or security of the U.S. energy and* *manufacturing supply chains. Describe additional impacts this work will have on manufacturing and HPC communities. Include plans for any publications, improvements to open-source software, public databases that will be released or improved, and training provided for students or postdocs, etc.*

- **Implementation and Adoption:** *Describe the steps the industry partner will take to incorporate this work into their business. Describe the post-project activities to extend this effort to solve the broader problem being addressed, and how those efforts will be funded.*

The following appendices are also required and are **not included in the page count**:

Appendix A: **References** *Include a list of any relevant references.*

Appendix B: **Project Summary of Tasks and Schedule** *Provide a summary of the tasks and subtasks in a table format that includes the milestones, deliverables, and schedule. Include a schedule summary in Gantt chart format.*

Appendix C: Project Budget *Summarize project costs including amount and source of participant contribution in the table provided. Indicate in-kind and/or cash contribution for industry funding. Include a description of how this funding will make a large difference relative to existing funding from other sources, including the private sector, and why the government should fund this work. Funding for university and/or non-profit participants may be provided by the national laboratory or the industrial partner. If the funding for a university or non-profit participant is to be provided by DOE through the DOE laboratory partner, funding requests must be less than half of the total DOE funds. Industry partner cash contributions are made to either the laboratory or a university or non-profit. Total DOE funds must not exceed $400K. DOE funding to the university must not exceed 50% of the total DOE funds. Total industry contributions (including in-kind and cash) must be at least 20% of the total project funding. Industry contributions for Phase I projects may be 100% in-kind contributions, whereas Phase II projects require at least 50% of the industry contribution to be in cash. Total project funding must not exceed $500K.*

Appendix D: Computational Resources *In paragraph form, describe the computational approach, the performance of the codes, and the resources requested (platform and number of core hours). Platforms are listed on the [HPC4EI Computing Resource web page;] indicate a preference and why that system is preferred. Provide information about whether the code can run efficiently on a GPU platform or requires a CPU platform. Also describe how the results are to be disseminated to the end users. If you plan to use a GPU based machine, indicate the machine name and provide your compute time in node hours; otherwise provide your compute time in core hours. For* ***requests over 10 million core-hours on a CPU resource or equivalent on a GPU resource****, describe how you plan to gain access to this level of resources, and tell us who your contact is at the computing facility where you will be accessing those resources.*

Appendix E: Pictures for Publication *Include one or two non-proprietary pictures/images with a short caption and photo credit that can be used in a press release and posted on the website* *should this project be funded. If project is selected, high resolution image(s) will be requested by HPC4EI administrator.*

Appendix F: Discussion of How This Work Benefits the Laboratory *Briefly discuss new or enhanced capabilities that will be gained by the partnering laboratory or explain how this will help to maintain existing laboratory capabilities.*

Appendix G: Biographies *Include one paragraph* ***non-proprietary*** *biography for the industrial PI(s) and partnering laboratory PI(s). These may be posted on the HPC4EI website should this project be funded.*

Appendix H: Resumes *Provide resumes of project team to include industry partner PI(s), national laboratory PI(s), and/or university or non-profit organization.*

Appendix I: Improvements from Previous Full Proposal Submission *For proposals invited to re-submit a full proposal from a previous solicitation, briefly describe changes made based on the review comments from the previous submission.*

Completed **proposals**, derived from the provided template, **must be submitted to the electronic proposal system at https://proposalshpc4.inl.gov by 5:00 p.m. PT on the deadline indicated on the submission website.** Submission includes completion of electronic applicant form and upload of full proposal in PDF file format. This date will be approximately four weeks after concept paper notifications have been issued.

Evaluation Process

Both concept papers and full proposals will be evaluated by a Technical Merit Review Committee consisting of experts in the application of HPC modeling, simulation, and data analysis drawn from participating DOE national laboratories, and members of the DOE program offices with knowledge of the U.S. industry. Subject Matter Experts will be consulted to verify claims, including the description of current state of the art and estimate of project impact (e.g., cost and energy savings).

Concept papers will be evaluated primarily on the technical challenge and potential impact of using HPC to solve the industrial challenge. Concept papers should articulate, to the extent possible, the technical plan for performing the work. The committee recognizes that those industrial PIs who have not yet identified a national laboratory partner to work with may not have a complete picture of the technical solution techniques that are possible.

Full proposals will be evaluated against all the criteria listed below. Because the industrial partner will have an assigned laboratory partner to work with to develop the full proposal, the technical plan and feasibility will be expected to be well articulated. In addition, strong evidence of communication and planned collaborations between the national laboratory and industrial participants is expected in the full proposals.

Final funding decisions will be made by the sponsoring DOE office. DOE reserves the right to fund none, one, several or all the submitted proposals. All DOE funding decisions will be final.

Evaluation Criteria

- **Advances the State of the Art in the Industrial Sector: (Weight 20%)**
  - Does the proposed work take the industrial sector to a new level; provide a wholly new capability; or make an existing, energy-intensive technology obsolete in the industrial sector?
  - Does the proposed work take materials performance and behavior to a new level in a specific energy application environment; scale up the production of a new or modified material; provide a wholly new capability; or dramatically decrease the time required to certify or qualify a new or modified material?
  - Is the technical readiness level appropriate for a one-year project to produce meaningful results for the industrial sector?

- **Technical Feasibility: (Weight 20%)**
  - Does the proposal have a clearly stated technical approach including a description of the software to be used and any needed modifications?
  - Does the proposal match team expertise to the problem to be solved; have modeling expertise on both the national laboratory and industry sides; and process experts for the model validation if necessary?
  - Does the proposal clearly state roles and responsibilities for the participants and provide evidence of a strong collaboration between the industrial and national partners through joint milestones and deliverables?
  - Is the project plan clearly constructed with realistic time frames for each technical step?
  - Is there a solid verification and validation plan with validation data available?

- **Relevance to HPC: (Weight 20%)**
  - Does the proposed work fully utilize the unique expertise and capabilities at the DOE national laboratories to solve a problem that could not be solved in any other way?
  - Does it demonstrate the ability to use significant fractions of the machine to solve a truly large-scale problem and provide clear estimates of the compute cycles necessary for the work to be performed?

- **Impacts: (Weight 40%)**
  - Does the proposal respond to the specific topic areas listed and interests of the DOE sponsor office?
  - Does the proposal provide clear, evidence-based cost and energy savings that will a *have broad (national-scale) industrial impact* through development and/or improvement of efficient manufacturing technologies, and/or an impact on employment and manufacturing in the United States?
  - Affordability – How does the proposed project and knowledge it will generate help make costs more affordable for the American consumer?
  - Reliability – How does the proposed work and its goals help make production and distribution of energy or industrial supply chains more reliable?

- Security – How does the proposed project and its goals help to secure U.S. domestic supply chains against disruption (both adversarial and natural)?
- Competitiveness – How does the proposed work help the manufacturing company, industry, or nation produce goods efficiently, cost-effectively, and with high quality while maintaining or improving its position in the global or domestic marketplace?
- Does the proposal have a clearly stated plan for broad deployment of project artifacts or knowledge gained? Are specific numerical energy or other relevant metrics included with a solid justification for the impact estimates?
- Does the proposal provide clear, evidence-based improved materials performance, energy savings, cost savings or reduced time to market that will *have broad (national-scale) industrial impact, as well as an impact on employment* in the United States?
- Does the proposal have additional impacts for the community such as publications, improvements to open-source software, public databases that will be released or improved, and training provided for students or postdocs, etc.?

Point of Contact

During the period of the call for proposals, all questions relating to this announcement can be directed to the HPC4EI program at hpc4ei@llnl.gov.

Intellectual Property and Proprietary Data

The HPC4EI program respects the importance of industry's intellectual property and data security.

Industrial partner awardees are expected to enter into a DOE Model Short Form Cooperative Research and Development Agreement (CRADA) with the national laboratory or laboratories that will be performing the work. This CRADA contains provisions relating to proprietary information and intellectual property. Because of the need for accelerated placement and execution of the projects, the terms of the CRADA will not be subject to negotiation. To review the proposed terms that make up the DOE Model Short Form CRADA, please see the sample posted on the HPC4EI solicitation website. CRADA forms for different national laboratories will vary, but the terms are substantively similar.

A Non-Disclosure Agreement can be put into place during development and submission of the proposal to facilitate discussions while protecting the partner's proprietary information.

To the extent possible, it is preferred that proprietary information NOT be included in the submitted proposal. If company proprietary information is included in the proposal, the specific information should be marked as such. The HPC4EI program officials will utilize reasonable efforts to treat the information as business sensitive.

Failure of the industry partner to finalize the CRADA within one year following receipt of the notification letter to fund the project or other significant delays in finalizing the CRADA could result in rejection/discontinuation of the proposal/project.