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

The High-Performance Computing for Energy Innovation (HPC4EI) program seeks qualified industry partners to participate in short-term collaborative projects with the U.S. Department of Energy's (DOE) national laboratories. HPC4EI is the umbrella initiative for the High-Performance Computing for Manufacturing (HPC4Mfg) and High-Performance Computing for Materials (HPC4Mtls) programs, which are the sponsors of this solicitation. Through support from DOE's Advanced Materials and Manufacturing Technologies Office (AMMTO), Industrial Efficiency and Decarbonization Office (IEDO), and Office of Fossil Energy and Carbon Management (FECM), the selected industry partners will be granted access to high-performance computing (HPC) facilities and world-class scientists at DOE's national laboratories.

The HPC4Mfg program is interested in establishing collaborations that address key energy and decarbonization-related challenges for domestic manufacturers. The HPC4Mfg program is designed to improve manufacturing processes, address products lifecycle energy consumption, and increase the efficiency of energy conversion and storage technologies. The HPC4Mtls program is interested in collaborations that address key challenges in developing, modifying, and/or qualifying new or modified materials that perform well in harsh or complex environments through the application of HPC, modeling, simulation, and data analysis. These objectives are met by providing access to national laboratory supercomputing resources and expertise for high-performance computing projects. This program harnesses the processing power of national lab supercomputers to decarbonize U.S. industry and move us closer to an equitable, clean energy future that benefits all Americans.

Eligibility for the HPC4EI program is limited to entities that manufacture in the United States for commercial applications and the organizations that support these entities.

Applicants are encouraged to partner with a diverse range of universities and community colleges; including Historically Black Colleges and Universities (HBCUs) and Minority Serving Institutions (MSIs), and non-profit organizations, especially those located in disadvantaged and underserved communities, to ensure HPC national laboratory resources and technologies promote equitable access, use, and benefits.

DOE's AMMTO, IEDO, and FECM support and encourage the advancement of diversity, equity, inclusion, and accessibility (DEIA) in the context of HPC national laboratory applicant submissions.

Selected projects will be awarded up to $400,000 each to support compute cycles and work performed by the national laboratory. The industry partner must provide a participant contribution of at least 20% of the total project funding. The industry contribution must come from non-federal funding sources.

In addition, follow-on projects (also known as Phase II projects) to previously awarded, successful projects in these areas will be considered. Phase II projects should focus on the further implementation of the demonstrated HPC application in the industrial setting, taking it closer to operational use and broad national impact. Selected Phase II projects will be awarded up to $400,000 to support computing cycles and work performed by the national laboratory, university, and non-profit partners. The industry partner must provide a participant contribution of at least 20% of the total project funding, at least half of which must be in cash to support the national laboratory work.

Background

The U.S. Department of Energy (DOE) maintains world-class high-performance computing expertise and facilities, currently hosting several of the top 20 most powerful computers in the world as ranked by TOP500 in June 2024. From detailed subatomic-level simulations to massive cosmological studies, researchers use HPC to probe science and technology questions inaccessible by experimental methods. Scientific insights gained from these computational studies have drastically impacted research and technology across industrial sectors and scientific fields. Examples include additive manufacturing, aerospace, oil recovery, drug development, climate science, genomics, and exploration of fundamental particles that make up our universe. From industry to academia, the scientific need for advanced computing continues to drive innovation and development for future high-performance computers and their capabilities.

There is a significant opportunity for U.S. industries to harness the power of HPC. The HPC4EI program aims to offer HPC expertise and resources to help industries adopt this technology more easily and expand its application in supporting transformational and early-stage technology development. By facilitating targeted collaborations between industry and DOE's national laboratories, the HPC4EI program seeks to empower businesses to leverage HPC effectively.

Successful applicants will work collaboratively with staff from one or more of DOE's national laboratories to conduct project activities across the various HPC areas of expertise. These areas 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 methods.

To make the broadest impact across the industry, the project teams are expected to present their results at workshops associated with the program and at regional and national conferences. Publications are also encouraged.

Area 1: HPC4Mfg supported by AMMTO

The Advanced Materials & Manufacturing Technologies Office (AMMTO) supports a globally competitive U.S. manufacturing sector that accelerates the adoption of innovative materials and manufacturing technologies in support of a clean, decarbonized economy. AMMTO partners with private and public stakeholders to advance materials and manufacturing technologies for our clean energy future through process innovations, research and development, and workforce development. AMMTO supports cost-shared research, development, and other activities in crosscutting next-generation technologies and processes that hold high potential to enable the manufacture of next generation clean energy technologies.

AMMTO's primary goal in the HPC4Mfg program is to increase cost competitiveness and resilience of clean energy manufacturing supply chains, develop materials that improve the durability and performance of clean energy technologies, and develop processes that enhance quality. Proposals should provide a realistic assessment of improvements in U.S. manufacturing competitiveness, improvements in supply chain security, lifecycle carbon emissions reduction, and the increase in U.S. manufacturing jobs that a successful outcome of the project could have across the manufacturing sector.

Of particular interest to AMMTO are:

- Development of manufacturing processes to increase cost competitiveness and resiliency of domestic production of clean energy. Examples include but are not limited to:
    a. Modeling of manufacturing processes to help competitively manufacture large near net shape (or, ideally, true net shape) components domestically for energy applications (e.g., wind, hydro, nuclear, etc.).
    b. Modeling of manufacturing processes that improve throughput, increase product quality, reduce waste, and reduce costs of clean energy technologies such as solar panels, wind turbines, battery packs, and electric vehicle chargers.
    c. Modeling of high-throughput machining technologies that can operate at higher frequencies for reduced part production time and energy savings.
    d. Modeling of high shear rate and extrusion processing of metal, ceramic, semiconductor, and polymer materials and components that can outperform conventionally processed materials and that help advance renewable energy and energy efficiency efforts.
    e. Modeling of high-throughput continuous or quasi-continuous manufacturing processes (including, but not limited to, roll-to-roll processes) that are applied to clean energy/high-efficiency technologies such as batteries, fuel cells, photovoltaic modules, OLED and LED lighting, micro-/nano-electronics, wide bandgap power electronics, heat pump components, thermal insulation, etc.
- Development of materials to improve clean energy technology efficiency, durability, and cost-effectiveness. Examples include but are not limited to:
    a. Modeling of composite materials and/or composite-based component manufacturing for wind, hydrogen storage, and electric vehicles.
    b. Modeling of materials and/or components that operate in harsh environments applied to clean energy applications (e.g., hydro and pumped hydro, wind,

concentrated photovoltaic, solar thermal, battery storage, electric vehicles, electrified aircraft, and electrified marine vessels).

c. Modeling of the local atomic structure (short range order) of a chosen refractory multi-principal element alloy (MPEA) to help predict the alloy's solidification behavior and ultimately control the properties of the alloy.
d. Modeling to predict the tensile properties of high entropy alloys (HEA) to optimize the search for HEAs with desired tensile properties.
e. Modeling of electrical conductivity-enhanced materials and/or components made from such materials (e.g., transmission cables and wiring for electric motors) that are as cost effective and durable as Cu and Al but that have improved electrical conductivity over a wide ambient temperature range (i.e., from –40 C to 50 C).
f. Modeling of thermal transport phenomena in semiconductor devices such as logic chips and wide bandgap power devices as well as modeling of cooling technologies for micro-/nano-electronics and/or power electronics to optimize heat management and improve system efficiency.
g. Modeling of design and process optimization for battery component manufacturing and system assembly that improve capacity, operational lifetime, or reduce embodied energy/carbon.

- Development of manufacturing processes that enhance product quality, support process innovation, accelerate materials development, enhance materials circularity, and drive asset optimization. Examples include, but are not limited to:
    a. Modeling of smart manufacturing processes that allow for less material waste and better performing products; this could include additive manufacturing techniques (e.g., wire arc, powder, biopolymer), ideally coupled with in situ characterization and feedback that could help improve material quality and ensure that the desired material properties are achieved during the manufacturing process.
    b. Modeling of hybrid (i.e., convergent) manufacturing techniques that directly couple additive manufacturing and subtractive manufacturing (machining, grinding, polishing) so that net shape, rather than near net shape, parts can be fabricated with a single toolset.

Area 2: HPC4Mfg supported by IEDO

The Industrial Efficiency and Decarbonization Office (IEDO) provides funding, management, and the strategic direction necessary for a balanced national program of research, development, and demonstration (RD&D), as well as technical assistance and workforce development, to drive improvements in energy, materials, and production efficiency and to accelerate decarbonization across the industrial sector. IEDO and its programs are critical to putting the nation on a pathway to achieve net-zero carbon emissions by 2050.

The industrial sector is considered one of the most difficult to decarbonize due to the diversity and complexity of energy inputs, processes, and operations. Achieving net-zero emissions across the U.S. economy by 2050 will require an aggressive, multidimensional approach to eliminating industrial emissions. Based on analysis in DOE's Pathways to Commercial Liftoff Reports, while some technologies are ready to deploy today, it's estimated that addressing over 60% of emissions reductions needed in heavy industry currently costs more than $50 per metric ton CO_2, making those solutions unlikely to be deployed on an economic basis. Additional RD&D is essential to reduce these costs and to unlock new pathways to reduce emissions. HPC can play a key role in accelerating the advancements needed to realize these goals.

This topic aims to advance the strategies identified in DOE's Industrial Decarbonization Roadmap and support the goals of the Industrial Heat Shot. IEDO seeks to advance highly innovative and impactful technologies through HPC4Mfg. The potential greenhouse gas (GHG) impacts of projects will be a major consideration in the evaluation of proposals. Technologies with only marginal impacts on GHG emissions or energy use are unlikely to be of interest. Therefore, **applications under this topic must include quantitative analysis of energy and GHG emissions impacts.** Additional metrics may be included as appropriate.

Of particular interest to IEDO are:

- Development, optimization, and/or integration of equipment and processes that contribute to DOE's Industrial Heat Shot by significantly reducing emissions from industrial process heating. Areas of interest include:
    a. Electrified heating technologies, such as electric resistance, induction, electric arc/plasma, electromagnetic, and hybrid technologies. For example, application-specific optimization of energy-material interactions is a critical barrier to development of electromagnetic heating technologies.
    b. Industrial heat pumps, including models informing development of components and integrated systems that can deliver heat at or above 200°C. For example, compressor operation at high temperatures and pressures is limited by lubricant performance.
    c. Utilization of alternative fuels and energy sources, such as clean hydrogen, biofuels, and solar thermal. For example, hydrogen combustion characteristics are different from natural gas, requiring new optimization of components and overall combustion systems.
    d. Processes that significantly reduce or eliminate the heat needed for industrial processes, such as membrane separations, nonthermal drying, and electrochemical processes.
    e. Thermal energy storage technologies, including sensible, latent, and thermochemical systems.
- Advancements in technologies that significantly reduce emissions from energy- and emissions-intensive industries. Reductions in core process emissions as well as reductions in lifecycle emissions (e.g., improving material circularity or enabling use of alternative feedstocks) are both of interest. Industries of interest include:
    a. *Chemicals and Fuels*, including the exploration of novel low emission processes, the development of high efficiency catalytic structures, advanced membrane materials and scaleup of membrane manufacturing processes, and sustainable feedstocks like CO_2, biomass, waste plastics, and other sources.
    b. *Iron and Steelmaking, Aluminum, and Other Metals,* including electrification of primary processes, development of low-carbon production pathways, and reducing energy consumption in ironmaking and steelmaking. Mineral processing and ore beneficiation processes to reduce energy demand or utilize novel feedstock materials are also of interest. By-product material and heat recovery from high temperature processes are also of interest. Specifically of interest are

proposals leveraging HPC to develop process models and simulations that seek to accelerate the development, scaling, and commercialization of alternative ironmaking technologies that present a significant GHG reduction opportunity compared to BF or NG-DRI production. Not of interest: Direct reduction of iron ore using diatomic hydrogen in a shaft furnace.

c. *Food and Beverage Products,* including sector-specific processing that reduces energy consumption and carbon intensity 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 recycling along the value chain. Not of interest: 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.

- Advancements in technologies that enable flexible industrial energy use and industrial grid edge capabilities (i.e., interaction with the electric grid).
- Advancements in technologies that can reduce the energy, emissions, and water impact of data center operations. Thermal management technologies are of particular interest. Not of interest: chip-level innovations.
- Improvements in energy efficiency and/or emissions reductions for water and wastewater treatment, including for industrial and agricultural wastewaters.

For this topic, the following types of applications are specifically not of interest:

- Applications focused on electricity generation systems or components, including combined heat and power (CHP) and waste heat to power (WHP) technologies.
- Applications focused on CO_2 capture and/or storage.

Area 3: HPC4Mtls supported by FECM's Point Source Carbon Capture Program

FECM's Point Source Carbon Capture program works to accelerate the deployment of technologies that capture carbon dioxide (CO_2) emissions from industry and power generation sources over the next decade, with the goal of creating highly efficient, transformational carbon capture technologies. These technologies will be capable of operation under flexible duty cycles and foster creation of regional power generation that can achieve greater than 95% carbon capture with lower capture cost and greater operational efficiencies.

Proposals for the HPC4Mtls program should provide a realistic assessment of the proposed project's benefits to the domestic materials supply chain and/or fossil energy application (e.g. reduced energy consumption and/or greenhouse gas emissions for the industrial sector such as cement and steel producers, power plants, or clean hydrogen producers/users).

Topic areas of interest for FECM's Point Source Capture program are:

- Reactive Carbon Capture

a. Development of tools for identifying optimal deployment locations for reactive carbon capture approaches, with consideration of CO_2 sources (exhaust streams at electric generation facilities, industrial facilities or directly from the atmosphere), availability of required energy sources and co-reactants (e.g., carbon-free electricity, green hydrogen), process operating requirements, and integration of product(s) generated into existing supply chains and markets.
b. Development of modeling and optimization approaches to increase operational flexibility of reactive carbon capture systems to adapt to fluctuations in CO_2-containing gas streams and intermittent renewable energy supply.

- Emissions
    a. Development of dynamic process control models that can be integrated with online measurements, engineering controls and machine learning tools, to manage and mitigate non-CO_2 emissions from installing carbon capture on industrial and electricity generation sources.
        (i) Elucidation of the chemical degradation mechanisms of sorbents and solvents for point source capture for industrial applications.
        (ii) Use of computational databases and machine learning for development of novel CO_2 binding sorbent materials / membrane materials to achieve over 99% capture efficiency with low concentration CO_2 point source capture streams for NGCC applications.
        (iii) Use of computational databases and machine learning for development of novel reactive capture materials.
        (iv) Development of monitoring, reporting and verification tools (e.g., sampling algorithms, databases, models etc.) for non-CO_2 emissions from installing carbon capture systems on industrial and electricity generation sources.
        (v) Development of atmospheric chemistry models for non-CO_2 emissions from installation of carbon capture systems on industrial and electricity generation sources.
        (vi) Development of process models for modular design carbon capture systems to improve process flexibility.

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. The solicitation will encourage applicants to partner with a diverse range of universities, community colleges, and non-profit organizations, especially those located in disadvantaged communities, to ensure the equitable use and benefits of HPC national laboratory resources and technologies. 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). 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. Total project size cannot exceed $500,000. 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 developmentof 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 (2024-2025)**
Call for Proposal	November 14, 2024
Concept Paper Due	December 11, 2024
Request for Full Proposal	February 2025
Full Proposal Due	March 2025
Finalists Notified	May 2025

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 Romanfont, 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 UnitedStates, 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 current state of the art in the industrial sector; technical feasibility, relevance to high-performance computing.*
- **Impact:** *Describe how this specific HPC effort will result in national-scale, long-term energy, and emissions reductions across the industry; the performance improvements that are expected over existing technologies; and the ability of industry to accelerate the adoption of energy-efficient technologies. Describe how this specific HPC work contributes to a transformational change in the energy sector and enduring economic impact. Describe how this effort will result in changes in the way your company operates. Describe the alternative actions if this effort is not funded including reliance on experimental technologies or other courses of action. Include metrics for energy/carbon improvements, performance increases, cost savings, and/or time reductions. 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, industry staff, etc.

For Phase II projects, the concept paper should not exceed 3 single-spaced pages using12-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 beused 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, reduction in emissions (which can include greenhouse gases, particulates, and other pollutants), 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* ***Topic Area 2*** *must at least include quantitative analysis of energy and greenhouse gas (GHG) emissions 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. PDT 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

- Idaho National Laboratory
- Los Alamos National Laboratory
- Lawrence Berkeley National Laboratory
- Lawrence Livermore National Laboratory
- National Energy Technology Laboratory
- National Renewable Energy Laboratory
- 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 7 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 9 single-spacedpages 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 projecttitle, 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 thegoals 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 believethat 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 to the state of the art in the industrial section, 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 forverification, its nature and source.*

- **Impact:** *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 emissions 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 energy technologies; and 4) transformational change in the energy sector and enduring economic impact.*

- **Quantitative Analysis:** *Applicants must provide a quantitative analysis of: energy savings, reduction in emissions (which can include greenhouse gases, particulates, and other pollutants), 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* ***Topic Area 2*** *must at least include quantitative analysis of energy and greenhouse gas (GHG) emissions impacts*.

- **Implementation and Adoption:** *Describe how this work will be incorporated into the company and industry-wide operations. Describe the post project activities to extend this effort to solve the broader problem being addressed. If a new or modified material is developed, can the team provide preliminary techno-economic analysis by the close of the project?*

- **Other Impacts:** *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.*

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. PDT 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 and Criteria

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

manufacturing 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?

- **Impact, Including Life-Cycle Energy Impact: (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 energy savings and carbon emissions reductions that will a *have broad (national-scale) industrial impact* through development and/or improvement of energy-efficient manufacturing technologies, and/or an impact on employment and manufacturing in the United States?
  - 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, carbon 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 datasecurity.

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.