HPC4EnergyInnovation Program:
Collaborations 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 Department of Energy's (DOE) National Laboratories. HPC4EI is the umbrella initiative for the HPC4Manufacturing (HPC4Mfg) and HPC4Materials (HPC4Mtls) Programs which are the sponsors of this solicitation. Through support from DOE's Office of Energy Efficiency and Renewable Energy (EERE) Advanced Materials and Manufacturing Technologies Office (AMMTO), Industrial Efficiency and Decarbonization Office (IEDO), and the 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.

DOE's 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 severe 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 raw 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.

The solicitation will encourage applicants to partner with a diverse range of universities and community colleges; including Historically Black Colleges and Universities (HBCUs) and Minority Serving Institutes (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.

AMMTO and IEDO supports and encourages the advancement of Diversity, Equity, Inclusion, and Accessibility (DEIA) in HPC National Laboratory applicants. The adoption of a diverse workforce and an equitable and inclusive workplace culture that values and celebrates a diversity of people, ideas, practices, cultures, and educational backgrounds is aligned with AMMTO and IEDO's mission. Such qualities are essential for establishing the creative and innovative work environments necessary for the success of the National Laboratories and continued delivery on DOE's vital missions.

Selected projects will be awarded up to $400,000 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 to previously awarded, successful projects in these areas will be considered. Follow-on 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 follow-on 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; of this, at least half must be in cash to support the National Laboratory work.

Background

DOE maintains world-class HPC expertise and facilities, currently hosting several of the top 20 most powerful computers in the world as ranked by TOP500 in November 2022. 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 high potential for U.S. industry to utilize the power of HPC. The HPC4EI Program is intended to provide HPC expertise and resources to industry to lower the risk of HPC adoption and broaden its use to support transformational and early-stage technology development. The HPC4EI Program hopes to provide this HPC expertise by supporting targeted collaborations between industry and DOE's National Laboratories.

Successful applicants will work collaboratively with staff from one or more of the DOE National Laboratories to conduct project activities across the various HPC areas of expertise, including development and optimization of modeling and simulation codes, porting and scaling of applications, application of data analytics, 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

DOE's Advanced Materials and Manufacturing Technologies Office (AMMTO) within the Office of Energy Efficiency and Renewable Energy (EERE) is the primary sponsor of the HPC4Mfg Program. Other Technology Offices within EERE and DOE's Office of Fossil Energy and Carbon Management may also sponsor select projects in this portfolio. AMMTO partners with private and public stakeholders to increase the competitiveness of the U.S. manufacturing and clean energy sectors and drive economy-wide decarbonization through process innovations, research and development, and technical assistance and workforce training. AMMTO supports cost-shared research, development, and activities in support of crosscutting next-generation materials and processes that accelerate the development and scale-up of technologies that support the transition to a clean energy economy and significantly improve energy efficiency and reduce emissions, industrial waste, and the life- cycle energy consumption of manufactured products.

The primary goals of the HPC4Mfg Program are to 1) improve manufacturing performance to lower the cost and improve the functionality of clean energy technologies, 2) improve the efficiency and productivity of U.S. manufacturing, and 3) reduce carbon emissions across the industrial sector. The program solicits proposals that require HPC modeling and simulation to overcome impactful manufacturing process challenges resulting in improved performance, reduced lifecycle energy consumption, greenhouse gas emissions, and/or increased productivity. Proposals should provide a realistic assessment of the carbon emissions reduction, energy impact, the improvement in U.S. manufacturing competitiveness, and the increase in U.S. manufacturing jobs that a successful outcome of the project could have across the industrial sector.

Of particular interest to AMMTO are:

- Introduction of new materials or advanced manufacturing processes, as well as improvements in existing ones, that support the transition to the clean energy economy and/or that result in significant lifecycle carbon emissions reduction and energy savings. Examples include:

    a. Improvements in materials performance and efficiency (e.g. conductive-enhanced materials, novel composites, functionally-gradient materials, advanced coatings, high-entropy alloys, etc.);

    b. Improvements in modeling prediction and closed-loop control for smart manufacturing systems; and

    c. Improvements in the performance and scale of advanced manufacturing processes (e.g. additive manufacturing, electrospray deposition, field assisted manufacturing, and alternatives to conventional processing methods).

- Improvements in the resiliency or circularity of material supply chains (e.g. advanced separations and material processing). Examples include:

a. Improvements in recyclability or material recovery from systems or components at their end of life, or from waste products generated along the supply chain;

b. Improvements of material quality or purity from materials recovery that facilitate requalification or remanufacturing processes that have lower energy or carbon footprints than mining and refinement of equivalent materials;

c. Improvements in separation and processing for critical materials (e.g., rare earth elements) especially from domestically available and/or unconventional sources; and

d. Development of materials that reduce reliance on Critical Materials without sacrificing performance.

- Improvements in semiconductor technologies that will result in operational energy efficiency improvements, supporting achieving the goals of Energy Efficiency Scaling for 2 Decades (EES2). Examples include:

  a. Improvements of advanced materials crucial to more energy efficient semiconductor devices and systems; and

  b. Process improvements in semiconductor manufacturing that lower the embodied energy of or otherwise result in more energy efficient semiconductor systems (e.g. improving yield).

- Improvements in manufacturing processes that result in reduced embodied carbon, improved efficiency, or significantly lower cost for energy conversion and storage technologies. Examples include:

  a. Improvements in lithium-ion battery material, component, or cell manufacturing processes, including conventional roll-to-roll processes and complementary or alternative processes;

  b. Improvements in design and process optimization for battery component manufacturing and system assembly that improve capacity, operational lifetime, or reduce embodied energy/carbon; and

  c. Improvements in flow battery material, component, or system manufacturing.

- Improvements in the operational performance or efficiency of energy conversion and storage technologies. Examples include:

  a. Improvements in material or component designs to improve the overall efficiency or waste heat recovery for thermal energy storage systems.

- Improvements in system energy density or cost

  a. Improvement in thermal management of energy storage systems.

IEDO

The Industrial Efficiency and Decarbonization Office (IEDO) builds on the legacy of the Advanced Manufacturing Office (AMO) to lead U.S. efforts to reduce emissions from the industrial sector. 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.

Of particular interest to IEDO are:

- Improvements to industrial process heating applications that achieve drastic efficiency improvements or emissions reductions. Examples include:

    a. Electrified core unit operations of industrial processes.
    b. Alternative fuels, feedstocks, and energy sources to provide process heat.
    c. Processes that significantly reduce or eliminate the heat needed for industrial processes.
    d. Advancements in technologies that enable industrial flexibility such as thermal energy storage systems.
    e. Effective capture, storage, and/or utilization of waste heat for use in industrial processes.

- Emissions reductions and/or efficiency improvements in core unit operations of energy- and emissions-intensive industries such as chemicals, iron & steel, cement, food & beverage, and forest products.

- Improvements in energy efficiency and/or emissions reductions of water treatment.

Area 2: HPC4Mtls

The Carbon Dioxide Removal (CDR) and Conversion Program funded by DOE's Office of Fossil Energy and Carbon Management (FECM) is the participating sponsor for this call of the High Performance Computing for Materials program.

CDR refers to approaches that remove carbon dioxide (CO2) from the atmosphere and durably stores the CO2 in geological, terrestrial, or ocean reservoirs, or in the form of long-lived products. This suite of technologies encompasses a wide array of approaches, including direct air capture coupled to permanent geologic storage, soil carbon sequestration, biomass carbon removal and storage (BiCRS), enhanced mineralization, marine CDR, and afforestation/reforestation. Paired with simultaneous deployment of mitigation measures and other carbon management practices, CDR is a tool to address emissions from the hardest to decarbonize sectors—like agriculture and transportation—and to eventually remove legacy CO2 emissions from the atmosphere. CDR does not refer to point source carbon capture from industrial facilities and power plants.

The world faces an urgent need to stop the increase of atmospheric greenhouse gas (GHG) levels. Given limited progress on rapidly cutting global GHG emissions—or mitigation—over the past several decades, CDR is now recognized as a critical component for achieving the ambitious climate goals of a net zero GHG economy by 2050. To achieve these goals, FECM's Carbon Dioxide Removal and Conversion Program is helping to advance diverse CDR approaches to facilitate gigatonne-scale removal by mid-century, and is actively making investments in technologies with commercialization potentials, including direct air capture.

Related to direct air capture, the following topic areas are of particular interest:

- Improving the understanding of the materials design and systems integration considerations on capturing CO2 directly from the air, especially for novel regeneration pathways that reduce overall energy requirements for releasing captured CO2;
- Use of computational databases and machine learning for development of novel CO2 binding materials and/or support structures for effectively capturing CO2 from the air with long term stability;
- Elucidation of the chemical degradation mechanisms of sorbents and solvents used in direct air capture applications under several realistic deployment conditions; and
- Investigation of systems integration considerations such as process control, utility balancing, and/or multi-unit vs. modular design on overall economics and energy requirements.

Related to BiCRS, the following topic areas are of particular interest:

- Elucidating the effects of biomass feedstock properties in BiCRS applications, with consideration of environmental impacts and assessment of carbon removal durability;
- Exploration of biomass feedstock and composition impact (e.g., moisture level, elemental composition, density, high heating value etc.) on downstream processes (e.g., conversion reactor configuration, CO2 capture system etc.) and overall economics and energy requirements;
- Analysis of the impact of CO2 capture technology selection on the environmental impact of bioenergy with carbon capture and storage (BECCS) processes;
- Exploration of the CO2 capture requirements to achieve net-negativity in BECCS processes;
- Investigation of the permanence of the removed CO2 and/or quantification of reversal risks; and
- Development of monitoring, reporting and verification (MRV) tools (e.g., sampling algorithms, databases, models etc.) for the cost-effective, accurate and transparent quantification of carbon content in biomass feedstocks and storage/utilization products to reduce uncertainty.

Related to enhanced mineralization, the following topic areas are of particular interest:

- Advancing the understanding of mineral reactivity in enhanced rock weathering applications, with consideration of environmental impacts and assessment of carbon

removal permanence;
- In-depth characterization of mineral reactivities during enhanced weathering under different deployment conditions (e.g., temperature, rainfall, particle size, application rate, plant-mineral interactions, pre-treatment steps etc.);
- Evaluation of tradeoffs between process co-benefits and environmental harms in the deployment of enhanced weathering technologies;
- Modeling of heavy metal leaching impacts on ecosystems, with assessment of critical element recovery/extraction for additional revenue generation;
- Investigation of the fate and durability of the removed CO2 and/or quantification of reversal risks; and
- Development of MRV tools (e.g., sampling algorithms, databases, models etc.) for the cost-effective, accurate and transparent quantification of carbon drawdown rates associated with enhanced weathering processes to reduce uncertainty.

Related to marine CDR, the following topic areas are of particular interest:

- Improving the understanding of the materials design and systems integration considerations on removing CO2 directly from the ocean;
- In-depth characterization and evaluation of aquatic environmental impacts in response to deployment of marine CDR technologies;
- Establishing tools for identifying optimal marine CDR reactor design and deployment locations, with consideration of process operating requirements, permitting needs, CO2 transport and storage mechanisms and potential co-product generation and integration into existing supply chains and markets;
- Investigation of the permanence of the removed CO2 and/or quantification of reversal risks; and
- Development of MRV tools (e.g., sampling algorithms, databases, models etc.) for the cost-effective, accurate and transparent quantification of carbon drawdown rates associated with marine CDR processes to reduce uncertainty.

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 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 follow-on) 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 follow-on 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**

Follow-on 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 two-page concept paper and seven-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 www.hpc4energyinnovation.org. Event dates are subject to change.

Event	Dates (2023-2024)
Call for Proposal	July 21, 2023
Concept Paper Due	August 17, 2023
Request for Full Proposal	October 2023
Full Proposal Due	November 2023
Finalists Notified	January 2024

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 (www.hpc4energyinnovation.org) and the electronic proposal system (https://proposalshpc4.inl.gov). This template should be used to prepare your submission. The concept paper should not exceed two (2) single-spaced pages using 12-point Times New Roman font, 1" 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: (not included in page limit)** *Include proposal tracking number, the project title,and company name.*
- **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 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:** *Estimate how this specific HPC effort will result in national-scale, long-term energy savings 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 improvements, carbon reductions, performance increases, cost savings, and/or time reductions.*

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.*

For follow-on projects, the concept paper should not exceed three (3) single-spaced pages using 12-point Times New Roman font, 1" 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, please articulate the differences.*

- **Appendix A: References (not included in page count)** *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
- 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 seven (7) single-spaced pages using 12-point Times New Roman font, 1” margins, and formatted in a PDF file. Follow-on project proposals should not exceed nine (9) single-spaced pages using 12-point Times New Roman font, 1” 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 following 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.*

- **Follow-on Projects Only - Results from the Prior Funded Project (two pages 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, please articulate the differences.*

- **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.*

- **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(ies) 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.*

- **Impact:** *Estimate how this specific HPC effort will result in national-scale, long-term energy savings 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. Explain how this specific HPC work contributes to a transformational change in the energy sector and enduring economic impact. Describe the alternative actions if this effort is not funded including reliance on experimental technologies or other courses of action. Describe how this effort will specifically impact your company/entity. Include metrics for energy improvements, carbon reduction, performance increases, cost savings, and/or time reductions.*

- **Energy Savings Estimates:** *Proposals must include numerical estimates for annual energy savings, carbon savings, and justifications for these estimates. Energy and carbon savings should be on an annual basis, assuming successful implementation of the technology being enabled by the HPC effort. Estimates for market penetration used for the savings should be realistic and conservative.*

- **Implementation and Adoption:** *Describe how this work will be incorporated into companyand industry-wide operations. Describe the follow-on activities to extend this effort to solve the broader problem being addressed.*

- **Other Impacts:** *Describe other impacts this work will have on manufacturing and HPC communities. Describe 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.*

Appendixes

Appendix A: **References (not included in page count)**

Appendix B: **Project Summary of Tasks and Schedule** (not included in page count): *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 (not included in page count) *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. 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.*

Appendix D: Computational Resources (not included in page count) *Describe the computational approach, the performance of the codes, and the resources requested (platform and number of core hours). Provide information about whether the code can run efficiently on a GPU platform or requires a CPU platform. If the estimated computational resource requirement is over 10 million CPU core-hours or 1 million node hours on a GPU platform, describe how these resources will be obtained.*

Appendix E: Pictures for Publication (not included in page count) *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 (not included in page count) *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 (not included in page limit) *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 (not included in page limit) *Include resumes of project team to industry parnter PI(s), national laboratory PI(s), and/or university or non-profit organization.*

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 five 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 large 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, as well as 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 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 a clearly stated plan for broad deployment of project artifacts or knowledge gained?
    - 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 HPC4EnergyInnovation 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 containsprovisions relating to proprietary information and intellectual property. Because of the need for accelerated placement and execution of the projects, 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.