Access to High Performance Computing Resources at Department of Energy National Labs

DATE: July 21, 2023
SUBJECT: Request for Information (RFI)

Description

This is a Request for Information (RFI) issued by the U.S. Department of Energy (DOE) on behalf of the Advanced Materials and Manufacturing Technologies Office (AMMTO) and the Fossil Energy and Carbon Management Office (FECM). The intent of this RFI is to better understand the perceived value of high-performance computing (HPC) capabilities to manufacturers and the experiences of companies that have interacted with the High Performance Computing for Energy Innovation (HPC4EI) program.

Background

The mission of DOE is to ensure U.S. security and prosperity by addressing its energy, environmental, and nuclear challenges through transformative science and technology solutions.[1] To advance its mission, the priorities of the DOE are to combat the climate crisis, create clean energy union jobs, and promote energy justice. Over the last decade, national investments in advanced manufacturing and decarbonization have grown significantly. DOE is investing more than ever in a decarbonized and competitive industrial sector and a domestic clean energy manufacturing base.

AMMTO's mission is to inspire people and drive innovation to transform materials and manufacturing for America's energy future. AMMTO programs support research, development, and demonstration of next-generation materials and innovative manufacturing technologies to increase U.S. industrial competitiveness and to drive economy-wide decarbonization.

The mission of FECM is to minimize the environmental impacts of fossil fuels while working toward net-zero emissions. FECM's programs use research, development, demonstration, and deployment approaches to advance technologies to reduce carbon emissions and other environmental impacts of fossil fuel production and use, particularly the hardest-to-decarbonize applications in the electricity and industrial sectors. Priority areas of technology work include point-source carbon capture, hydrogen with carbon management, methane emissions reduction, critical mineral production, and carbon dioxide removal to address the accumulated CO2 emissions in the atmosphere.

---

[1] U.S. Department of Energy, Mission, 2022. https://www.energy.gov/mission

---

This is a Request for Information (RFI) only. DOE will not pay for information provided under this RFI and no project will be supported as a result of this RFI. This RFI is not accepting applications for financial assistance or financial incentives. DOE may or may not issue a Funding Opportunity Announcement (FOA) based on consideration of the input received from this RFI.

HPC is the application of highly sophisticated computers, capable of massive parallel processing, to aid in research, problem-solving, and innovation. This practice has changed the way scientists and engineers pursue technological innovation. Traditionally, theory and experimentation, commonly known as the "two pillars of science," were used to drive discovery and understanding. With the development and maturity of computer science, simulation emerged as the third pillar. Even with conventional computing resources, such as the desktop computer and computer clusters, simulations have allowed scientists to gain insights previously unattainable through theory and experimentation alone. The introduction of supercomputers has enabled modeling and simulation with higher granularity and greater accuracy and speed, opening the door to new areas of scientific discovery and innovation. HPC is especially useful for complex processes and applications, such as stockpile stewardship, climate modeling, material design, and manufacturing innovation.

Manufacturers have long relied on conventional computing resources to assist in the design of processes and products through modeling and simulation. However, those computing resources limited models to simplified representations of physical systems. High-resolution models, now achievable through HPC, shed light on complex phenomena governing manufacturing processes. These models leverage more precise data that can be used to accelerate manufacturing innovations that improve performance, increase energy efficiency, and reduce waste and emissions. For U.S. manufacturing enterprises that lack onsite computing resources and modeling and simulation expertise, the opportunity to leverage DOE HPC resources provides a much-needed competitive edge. However, HPC resources are available at only a few select facilities, access is limited, and the U.S. manufacturing sector has yet to establish a broad awareness of the benefits HPC can provide.

The DOE has undertaken an effort to increase awareness of, familiarity with, and access to HPC resources for U.S. manufacturers. This RFI, the planned HPC4EI Workshop, and additional initiatives are all efforts toward that end. The DOE anticipates using the responses to this RFI and the information collected during the upcoming workshop to inform improvements to its HPC4EI program.

Purpose

The purpose of this RFI is to solicit feedback from the public, including key stakeholders in the manufacturing sector, especially from small and medium-sized manufacturers (SMMs) based in the U.S., past participants in funded programs through the DOE HPC4EI initiative, including HPC4Mfg (Manufacturing) and HPC4Mtls (Materials), and companies that may have an interest in participating in future HPC4EI programs.

_____

This is solely a request for information and not a Funding Opportunity Announcement (FOA). AMMTO and FECM are not accepting applications. DOE will not publish the information collected through this RFI. DOE may use the information provided through this RFI to develop funding opportunities, challenges, or prize competitions.

Disclaimer and Important Notes

This RFI is not a Funding Opportunity Announcement (FOA); therefore, DOE is not accepting applications at this time. DOE may issue a FOA in the future based on or related to the content and responses to this RFI; however, DOE may also elect not to issue a FOA. There is no guarantee that a FOA will be issued as a result of this RFI. Responding to this RFI does not provide any advantage or disadvantage to potential applicants if DOE chooses to issue a FOA regarding the subject matter. Final details, including the anticipated award size, quantity, and timing of funded awards, will be subject to Congressional appropriations and direction.

Any information obtained as a result of this RFI is intended to be used by the Government on a non-attribution basis for planning and strategy development; this RFI does not constitute a formal solicitation for proposals or abstracts. Your response to this notice will be treated as information only. DOE will review and consider all responses in its formulation of program strategies for the identified materials of interest that are the subject of this request. DOE will not provide reimbursement for costs incurred in responding to this RFI. Respondents are advised that DOE is under no obligation to acknowledge receipt of the information received or provide feedback to respondents with respect to any information submitted under this RFI. Responses to this RFI do not bind DOE to any further actions related to this topic.

Confidential Business Information

Pursuant to 10 CFR 1004.11, any person submitting information that he or she believes to be confidential and exempt by law from public disclosure should submit via email, postal mail, or hand delivery two well-marked copies: one copy of the document marked "confidential" including all the information believed to be confidential, and one copy of the document marked "non-confidential" with the information believed to be confidential deleted. Submit these documents via email or on a CD, if feasible. DOE will make its own determination about the confidential status of the information and treat it according to its determination.

Evaluation and Administration by Federal and Non-Federal Personnel

Federal employees are subject to the non-disclosure requirements of a criminal statute, the Trade Secrets Act, 18 USC 1905. The Government may seek the advice of qualified non-Federal personnel. The Government may also use non-Federal personnel to conduct routine, nondiscretionary administrative activities. The respondents, by submitting their response,

---

This is a Request for Information (RFI) only. DOE will not pay for information provided under this RFI and no project will be supported as a result of this RFI. This RFI is not accepting applications for financial assistance or financial incentives. DOE may or may not issue a Funding Opportunity Announcement (FOA) based on consideration of the input received from this RFI.

3

consent to DOE providing their response to non-Federal parties. Non-Federal parties given access to responses must be subject to an appropriate obligation of confidentiality prior to being given the access. Submissions may be reviewed by support contractors and private consultants.

Request for Information Categories and Questions

Please focus on the aspects that are most pertinent to you or your field and answer as few or as many of the questions below as you would like.

Category A: Respondent Type

1. What industry are you in?
2. Are you considered an 8(a) business?
3. Are you a Minority-Owned Small Business (MOSB)?
4. Are you a Woman-Owned Small Business?
5. How would you describe your application space and place in the supply chain ecosystem within that industry?
6. How would you describe your organization's modeling and simulation activities and/or needs?
7. What kind of computing resources does your organization utilize (e.g., cloud, desktop, dedicated cluster) to meet its modeling and simulation needs?
   a. To what extent has your company leveraged HPC resources in the past?

Category B: Value of HPC to Industry

8. If your company has not utilized advanced modeling, simulation, or used HPC, can you explain the obstacle(s) that have prevented your organization from exploring? Possible reasons could include, but are not limited to, lack of awareness or familiarity with these capabilities, not knowing how to access these capabilities, using these capabilities not a high enough priority or too expensive, etc.
9. If your company has used HPC for advanced modeling and simulation, what motivated you? Possible reasons could include, but are not limited to, identification of a difficult-to-solve problem that is key to business success, strong in-house knowledge on computation and modeling, having peers who have used HPC, compelling public information on the HPC program, etc.
10. How would you describe the value of HPC, to your industry in general and to your company specifically?
11. What ways can HPC contribute to AMMTO's mission?
12. What applications does your organization see as useful for general computational/modeling methods, and how does HPC differ?

_____

This is a Request for Information (RFI) only. DOE will not pay for information provided under this RFI and no project will be supported as a result of this RFI. This RFI is not accepting applications for financial assistance or financial incentives. DOE may or may not issue a Funding Opportunity Announcement (FOA) based on consideration of the input received from this RFI.

13. What use cases for HPC would be most useful for your company (modeling, machine learning, code building, other?) What types of problems (e.g. complex fluid flow, materials modeling, process parameter optimization) are you interested in modeling or investigating using HPC?
14. What use cases do you see for HPC in the context of smart manufacturing?
15. If you utilized HPC resources, does your company have any in-house expertise of computing, modeling, code building, etc.?
16. If you have used HPC, how did you determine whether the use of HPC was successful and to what degree?
17. What could encourage an increase in impactful HPC utilization in the manufacturing sector and by SMMs in particular? Would any particular programs, incentives, or policies help?
18. What capabilities would be helpful for your company, if you already do advanced modeling and simulation? What additional benefit would HPC offer?

Category C: Experience with HPC4EI program

19. If you were aware of the HPC4EI program prior to this RFI, how were you first made aware of the HPC4EI program?
    a. If you were aware of but have not engaged with the HPC4EI program, can you please provide specific reasons, if any, why you have not?
20. If you have applied for an HPC4EI award, please describe your experience with the HPC4EI application process.
    a. Describe any challenges or barriers you faced in completing the HPC4EI program application.
    b. Provide any suggestions you may have on improving the HPC4EI application process.
    c. If submitted an application that was not selected, please describe the feedback provided from the HPC4EI program on the unsuccessful application.
    d. Would you consider re-applying to HPC4EI for another project? What reasons motivate your choice?
21. HPC4EI projects typically take from 9-12 months to go from the initial Notice of Intent (NOI) to project start. Does the timeline for project award impact your organization's consideration for participating in the program and, if so, to what extent?
22. If you have participated in one or more HPC4EI project(s),
    a. What impacts have the HPC4EI projects had on your company?
    b. What challenges did your company face over the course of the project? Possible challenge areas include, but are not limited to, difficulties and/or delays in negotiating the project award, difficulties in getting compute time reserved or scheduled, difficulties in identifying or bringing on staff with the necessary expertise, unexpected challenges in model development, lack of useful results, etc.

_____

This is a Request for Information (RFI) only. DOE will not pay for information provided under this RFI and no project will be supported as a result of this RFI. This RFI is not accepting applications for financial assistance or financial incentives. DOE may or may not issue a Funding Opportunity Announcement (FOA) based on consideration of the input received from this RFI.

23. Have you applied for a phase 2 project?
    a. If so please describe the motivations for your decision to do so.
    b. If not please describe why you chose not to.
    c. What changes would your organization recommend to phase 2 projects in order to increase participation?
24. What changes would your organization recommend to increase overall participation in the HPC4EI program?
25. What recommendations do you have regarding how the program can best share helpful information gained and lessons learned from projects to the broader manufacturing community? What, if any, guidelines would you provide for deciding what information can be shared and how to share it?
26. What recommendations do you have regarding how the program can better engage with minority and women owned businesses?
27. What proposals do you have regarding how the program can increase engagement with diverse colleges and universities, including HBCUs and MSIs?
28. After participation in the HPC4EI program, is your organization still using results from the program?
29. In the past, the HPC4EI program has facilitated projects with a distinct teaming structures (one manufacturer, one lab). Would there be value in large, collaborative projects that involve multiple companies in similar/complimentary spaces? Or in projects that require regional collaboration? Please describe the value you see.
30. What other opportunities do you see to scale the impact of the program?
31. What is the most important business metric you think HPC could help your company/organization with?

Request for Information Response Guidelines

Comments must be received by 11:59 p.m. Eastern time on <mark>Friday, August 25, 2023</mark>. Submissions received after that date may not be considered.

Please identify your answers by responding to a specific category and corresponding question. Respondents may answer as many or as few questions as they wish.

Comments must be submitted by emailing <mark>hpc4ei-rfi@llnl.gov</mark> in the following formats: Word or PDF. Please submit comments only and include your name, organization's name (if any), and cite ''HPC4EI RFI Response'' in all correspondence. Comments containing references, studies, research, and other empirical data that are not widely published should include copies of the referenced materials.

_____

This is a Request for Information (RFI) only. DOE will not pay for information provided under this RFI and no project will be supported as a result of this RFI. This RFI is not accepting applications for financial assistance or financial incentives. DOE may or may not issue a Funding Opportunity Announcement (FOA) based on consideration of the input received from this RFI.

All comments responding to this document will be a matter of public record. Relevant comments will generally be available on the HPC4Mfg website.

AMMTO will not accept comments accompanied by a request that part or all of the material be treated confidentially because of its business proprietary nature or for any other reason. Therefore, do not submit confidential business information or otherwise sensitive, protected, or personal information, such as account numbers, Social Security numbers, or names of other individuals. For the RFI, AMMTO will hold informational webinars explaining how the public can submit comments. Details about these informational webinars, including dates and registration deadlines, will be announced at https://hpc4energyinnovation.llnl.gov/.

Contact

For questions about this RFI contact: Aaron Fisher, Head of Numerical Analysis and Simulations Group, Acting Director of the HPC for Energy Innovation Program, Lawrence Livermore National Laboratory email hpc4ei-rfi@llnl.gov. Please direct media inquiries to the DOE EERE communications team at ammto@ee.doe.gov.

EERE will not respond to individual submissions or publish publicly a compendium of responses. A response to this RFI will not be viewed as a binding commitment to develop or pursue the project or ideas discussed.

Respondents are requested to provide the following information at the start of their response to this RFI:
- Company / institution name;
- Company / institution contact;
- Contact's address, phone number, and e-mail address.

_____