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Research domain(s), discipline(s)/sub-discipline(s)

Mechanical & Aerospace Engineering; Computational materials science and molecular simulations; mechano-chemistry

Title of Response

Further enhancing computational molecular science and cyber related development

Abstract

While computational simulation and characterization becomes a simulation-based research pillar along with theory and experimentation for nanoscience research, the current funding strength is far below basic support for key personnel.

Question 1 (maximum 400 words) – Data-Intensive Research Question(s) and Challenge(s). Describe current or emerging data-intensive/data-driven S&E research challenge(s), providing context in terms of recent research activities and standing questions in the field. NSF is particularly interested in cross-disciplinary challenges that will drive requirements for cross-disciplinary and disciplinary-agnostic data-related CI.

Low funding strength, largely from single program limits the productivity, while the project itself encompasses multi-program interests. For example, CMMI, CHE, DMR, and CBET.

Question 2 (maximum 600 words) – Data-Oriented CI Needed to Address the Research Question(s) and Challenge(s). Considering the end-to-end scientific data-to-discovery (workflow) challenges, describe any limitations or absence of existing data-related CI capabilities and services, and/or specific technical and capacity advancements needed in data-related and other CI (e.g., advanced computing, data services, software infrastructure, applications, networking, cybersecurity) that must be addressed to accomplish the research question(s) and challenge(s) identified in Question 1. If possible, please also consider the required end-to-end structural, functional and performance characteristics for such CI services and capabilities. For instance, how can they respond to high levels of data heterogeneity, data integration and interoperability? To what degree can/should they be cross-disciplinary and domain-agnostic? What is required to promote ease of data discovery, publishing and access and delivery?

Affordable compute cluster for PI to quickly test algorithm and ideas outside large national compute centers to which PIs frequently encounter long waiting time for job running is needed.

Question 3 (maximum 300 words) – Other considerations. Please discuss any other relevant aspects, such as organization, processes, learning and workforce development, access and sustainability, that need to be addressed; or any other issues more generally that NSF should consider.

Work force training, particularly at postdoc level needs high pay for these key personnel.

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