

Abstract Submitted
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Enabling Computational Discovery and Design DARYL HESS, Division of Materials Research, National Science Foundation, USA — Advanced cyber-infrastructure(CI), increases in computing power, and increasing use of data volumes are revolutionizing how science is done, changing the nature of the questions we ask, and opening new frontiers. From discovering new phenomena and states of matter to the challenge of designing new materials and matter, the focus on problems with many complex interacting degrees of freedom through computational investigation often leads to large amounts of data that require analysis, preservation, curation, and sharing across the community. Data from many sources plays an increasingly important role as a driver of discovery. I will discuss opportunities in computational and data enabled science and in building the CI of the 21st century. Sustainable, maintained, and reliable shared software is an important component of a National CI framework that will empower computational scientists to engage the scientific frontiers and the pressing problems around us. The success of computational data enabled science requires innovation that leads to paradigms in attacking difficult problems. Education will play an important role in realizing the full potential of computation and data enabled science for discovery and design. Participation of the computational science community is an important ingredient to create a CI that will propel science forward; some self-assembly is required. NSF provides funding opportunities to help.

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