Greenspan_2019 ML-MSM Meeting - Abstract Submission Form

Title: NCI-DOE Collaborations: Extending Frontiers of Predictive Oncology and Exascale Computing

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The National Cancer Institute (NCI), coordinating the United States National Cancer Program, and the U.S. Department of Energy (DOE), a leader in world-class high performance computing (HPC) resources and expertise, established an inter-agency collaboration in June of 2016 through a 5-year memorandum of understanding to accelerate precision oncology research and shape the future for emerging exascale computing. The initial partnership program, *Joint Design of Advanced Computing Solutions for Cancer (JDACS4C)*, is driven and enabled by several government initiatives, including the Precision Medicine Initiative (PMI), the National Strategic Computing Initiative (NSCI), the Exascale Computing Leadership Act, and the Cancer Moonshot^{SM}. JDACS4C, which involves the NCI, Frederick National Laboratory for Cancer Research (FNLCR), and four of the DOE Laboratories (Argonne National Lab, Los Alamos National Lab, Lawrence Livermore National Lab, and Oak Ridge National Lab), explores three co-designed pilot efforts where exascale computing capabilities and computational approaches join precision oncology priorities. The high-level goals of these pilots push the frontiers of computing technologies in three specific areas, or levels, of cancer research: 1) Cellular-level: develop predictive models for screening tumor drug response to identify new treatments; 2) Molecular-level: further understand the basic biology of undruggable targets, such as the RAS protein; and 3) Population-level: gain critical insights on the drivers of population cancer outcomes.

Using co-design principles, each of the pilots in the JDACS4C collaboration is based on, and driven by, team science, which is the hallmark of the collaboration's success. The partnership is also developing new cross-cutting technologies including uncertainty quantification (UQ) methods to evaluate the level of confidence or certainty in AI model predictions and a scalable, open source deep learning environment (CANDLE). CANDLE is now deployed as a module on NIH Biowulf and is available to any NIH investigator with a Biowulf account. CANDLE code is also available via GitHub to any researchers able to set up their own instances of the environment.

To build upon the nascent predictive oncology community driven by JDACS4C, in March 2019 the NCI, in coordination with FNLCR and DOE, held a workshop entitled, *Envisioning Computational Innovations for Cancer Challenges (ECICC) Scoping Meeting*. Cancer, biomedical, bioinformatics, engineering, data and computational scientists at various career stages from government, academia, and industry were invited to participate in an collaborative, interactive event to identify and discuss cancer challenge areas that push the limits of current cancer research computational practices and compel development of innovative computational technologies. Going forward, both agencies are supporting the growth of this emerging community through follow-on events and an online forum as well as developing new collaboration ideas to simultaneously accelerate predictive oncology and development of advanced computing approaches.

The NCI-DOE Collaboration has demonstrated there are compelling opportunities to apply HPC and advanced computing to develop machine-learning (ML)-based predictive models and simulations in cancer research across molecular, cellular and population scales. These opportunities can successfully inform hypothesis generation and experimental design as well as lead to new biological insights.

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