Three DOE/FNLCR Collaborations

(JDACS4C, RAS pilot, ATOM)

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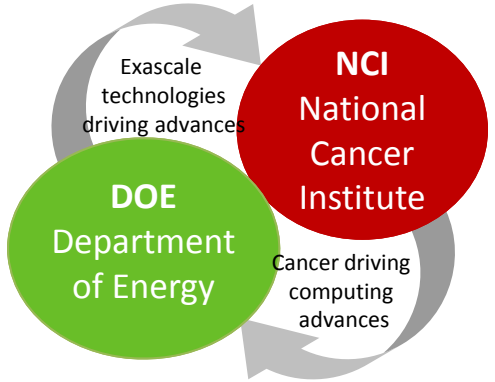
May 8th, 2017

1. *Background*
2. *JDASC4C*
3. *RAS Pilot*
4. *ATOM*

Thanks to many folks for slides, but especially Jerry Lee

Joint Design of Advanced Computing Solutions for Cancer

DOE-NCI partnership to advance exascale development through cancer research



Warren Kibbe (NCI) & Dimitri Kusnezov (DOE)

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National Strategic Computing Initiative (NSCI)

Executive Order, July 30, 2015

It is the policy of the United States to sustain and enhance its scientific, technological, and economic leadership position in HPC research, development, and deployment through a coordinated Federal strategy guided by four principles:

1) The United States must deploy and apply new HPC technologies broadly for economic competitiveness and scientific discovery.
2) The United States must foster **public-private collaboration**, relying on the respective strengths of government, industry, and academia to maximize the benefits of HPC.
3) The United States must adopt a "whole-of government" approach that draws upon the strengths of and seek cooperation among all Federal departments and agencies with significant expertise or equities in HPC in concert with industry.
4) The United States must develop a comprehensive technical and scientific approach to efficiently transition HPC research on hardware, system software, development tools, and applications into development and, ultimately, operations.

This order establishes the NSCI to implement this whole-of-government strategy, in collaboration with industry and academia, for HPC research, development, and deployment.

DOE is a Lead Agency for NSCI
NIH/NCI is a Broad Deployment Agency for NSCI

President Obama's Precision Medicine Initiative (PMI)

January 30, 2015

Objectives of the Precision Medicine Initiative:

1. **More and better treatments for cancer** *NCI will accelerate the design and testing of effective, tailored treatments for cancer by expanding genetically based clinical cancer trials, exploring fundamental aspects of cancer biology, and establishing a national "cancer knowledge network" that will generate and share new knowledge to fuel scientific discovery and guide treatment* decisions.
2. Creation of a voluntary national research cohort
3. Commitment to protecting privacy
4. Regulatory modernization
5. **Public-private partnerships** *The Obama Administration will forge strong partnerships with existing research cohorts, patient groups, and the private sector to develop the infrastructure that will be needed to expand cancer genomics, and to launch a voluntary million-person cohort. The Administration will call on academic medical centers, researchers, foundations, privacy experts, medical ethicists, and medical product innovators to lay the foundation for this effort, including developing new approaches to patient participation and empowerment. The Administration will carefully consider and develop an approach to precision medicine, including appropriate regulatory frameworks, that ensures consumers have access to their own health data – and to the applications and services that can safely and accurately analyze it – so that in addition to treating disease, we can empower individuals and families to invest in and manage their health.*

Vice President Biden's Cancer Initiative

January 2016

Scientific Objectives of the Vice President's Cancer Initiative Blue Ribbon Panel

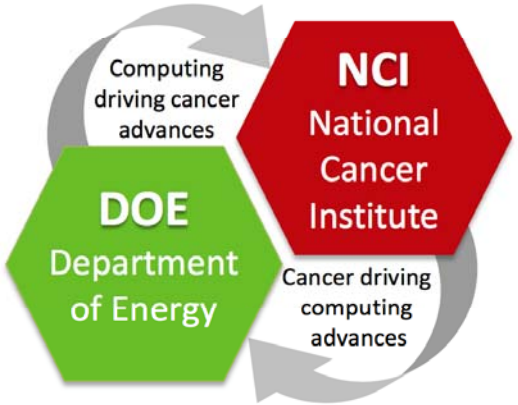
- Prevention and Cancer Vaccine Development
- Early Cancer Detection
- Cancer Immunotherapy and Combination Therapy
- Genomic Analysis of Tumor and Surrounding Cells
- Enhanced Data Sharing
- Oncology Center of Excellence
- Pediatric Cancer
- Exceptional Scientific Opportunities in Cancer Research

Joint Design of Advanced Computing Solutions for Cancer (JDACS4C)

DOE-NCI partnership to advance exascale development through cancer research

March 28, 2017

Presented to:
DOE-NCI Governance Review Committee



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This work has been supported in part by the Joint Design of Advanced Computing Solutions for Cancer (JDACS4C) program established by the U.S. Department of Energy (DOE) and the National Cancer Institute (NCI) of the National Institutes of Health. This work was performed under the auspices of the U.S. Department of Energy by Argonne National Laboratory under Contract DE-AC02-06-CH11357, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, Los Alamos National Laboratory under Contract DE-AC5206NA25396, and Oak Ridge National Laboratory under Contract DE-AC05-00OR22725. LLNL-MI-727782.

Recent governance review

Crosscut: Integrated Precision and Predictive Oncology

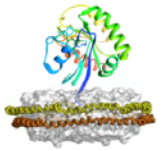
Pilot 1
Pre-clinical Model Development

Aim 1: Predictive Models of Drug Response (signatures)

Aim 2: Uncertainty Quantification and Improved Experimental Design

Aim 3: Develop Hybrid Predictive Models

Pilot 2
RAS Therapeutic Targets



Aim 1: Adaptive time and length scaling in dynamic multi-scale simulations

Aim 2: Validated model for Extended RAS/RAS-complex interactions

Aim 3: Development of machine learning for dynamic model validation

Pilot 3
Precision Oncology Surveillance

Aim 1: Information Capture Using NLP and Deep Learning Algorithms

Aim 2: Information Integration and Analysis for extreme scale heterogeneous data

Aim 3: Modeling for patient health trajectories

Crosscut: Uncertainty Quantification (UQ) and CANDLE exascale technologies

Milestones for 3-year pilots

Pilot 1: Framework for predictive models for preclinical screening. Initial integration of machine learning functionality into CORAL nodes

Pilot 2 Extended RAS-complex interaction model
Adaptive time and length scaling in dynamic multi-scale simulations
Development of machine learning for dynamic validation of models

Pilot 3 Modeling framework for predictive simulations of patient health trajectories.
Integration of big data analytics with data-driven modeling and simulation for CORAL architectures

NCI Precision Oncology – Extending the Frontiers

- Identify promising new treatment options through the use of advanced computation to rapidly develop, test and validate predictive pre-clinical models for precision oncology.

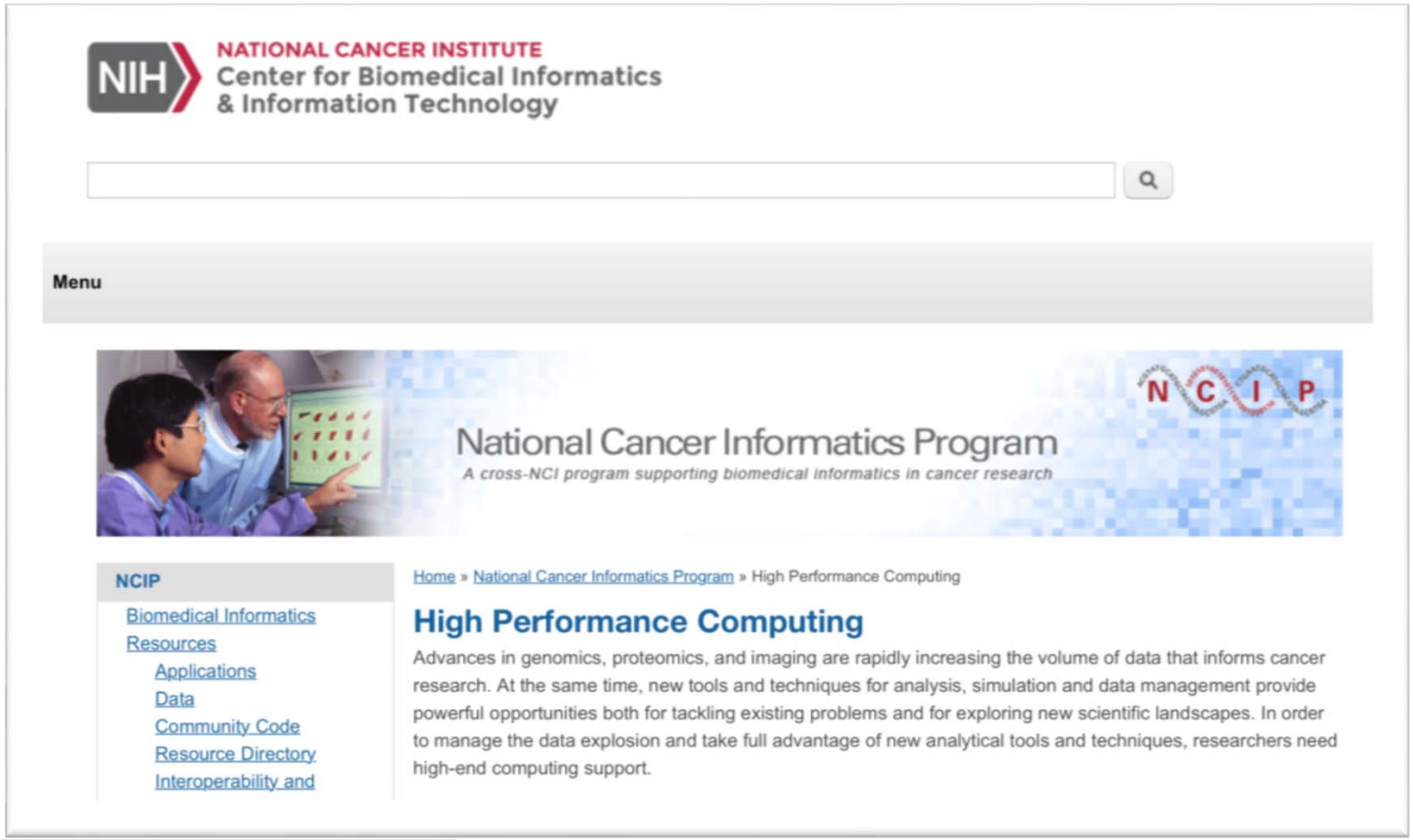
- Deepen understanding of cancer biology and identify new drugs through the integrated development and use of new simulations, predictive models and cutting-edge information spanning the range from molecular biophysical properties to patient outcomes.

- Transform cancer care by applying advanced computational capabilities to population-based cancer data to understand the impact of new diagnostics, treatments and patient factors in real world patients.

What these pilots offer:

- **Jointly supported efforts**
- **Jointly managed and planned**
- **Three 3-year pilots**
- **Four DOE Labs, one NCI Lab**
- **Builds on CORAL**
- **Pushes the frontiers in Oncology and Exascale simultaneously**
- **Supports all 4 policy goals of the NSCI and 4 of 5 objectives**
- **Supports 2 of 4 objectives of the PMI**
- **Aligned with the Beau Biden Cancer Moonshot**
- **Draws in private sector interests**

Web presence – https://hpc.cancer.gov



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Community Outreach

- 10th Meeting of the Frederick National Laboratory Advisory Committee (FNLAC) at the Shady Grove Campus, NCI – May 11, 2016
- Frontiers of Predictive Oncology and Computing, DC – July 12-14, 2016
- RAS Structures and Dynamics in Cellular Membranes Workshop (FNLCR-ATRF) – October 20, 2016
- Supercomputing 2016 (SC16) Plenary presentation (Salt Lake City, UT) – November 13-18, 2016
- International SISA Workshop (Tokyo, JAPAN) – January 18-20, 2017
- Precision Medicine World Congress (Santa Clara, CA) – January 23-25, 2017
- Pilot 1 Hack-a-thon at LANL – January 25-26, 2017
- Biophysical Society Meeting (New Orleans, LA) – February 11-15, 2017
- CANDLE Hack-a-thon at ANL – March 1-2, 2017
- Enterprise HPC 2017 (Ponte Vedra Beach, FL) – March 19-21, 2017
- NIH/NCI Session at AACR Annual meeting in Washington, DC – The NCI RAS Initiative at the Frederick National Laboratory for Cancer Research – April 2, 2017
- CANDLE Workshop for Cancer Researchers at NCI – April 18-19, 2017
- Featured in May 2017 issue of *Cancer Discovery* (AACR)
- NVIDIA GPU Technology Conference (GTC) in VA – May 8-10, 2017
- CANDLE Hack-a-ton at ANL – June 5-8, 2017
- ISC17 Precision Medicine Workshop – June 22, 2017
- Frontiers of Predictive Oncology and Computing II – October 2017
- SC17 Workshop Computational Approaches for Cancer – November 2017

Questions?

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