



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Department of Energy and National Cancer Institute Partnership

Overview

September 17, 2018

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Office of Science, U.S. Department of Energy**

National Cancer Institute (NCI)

Federal Government's principal agency for cancer research and training (est 1937)

Part of the National Institutes of Health (NIH)

Largest of 27 institutes, directed by political appointee

Supports intramural and extramural researchers

Frederick National Laboratory (FNL or FNLRC)

NCI's National Laboratory (Federally Funded Research and Development Center)

Precision Oncology – Precision Medicine for Cancer

Tailoring treatment and prevention to an individual's characteristics: genetics, environment, and lifestyle

Call to Partnership

All of government approach to challenge problems

- **National Strategic Computing Initiative (July 2015)**
 - Calls upon DOE, a “lead agency” to partner with “deployment agencies” (includes NIH) to maximize impact of HPC for the United States
- **Precision Medicine Initiative (Jan 2015)**
 - NIH key agency in this R&D initiative to improve health and treatment of disease by taking into account individual differences in people’s genes, environment and lifestyle
- **21st Century Cures Act (Legislation, December 2016)**
 - Cancer Moonshot: NCI key agency, supports all of government approach to accelerate cancer treatment and prevention



DOE and NCI Partnership

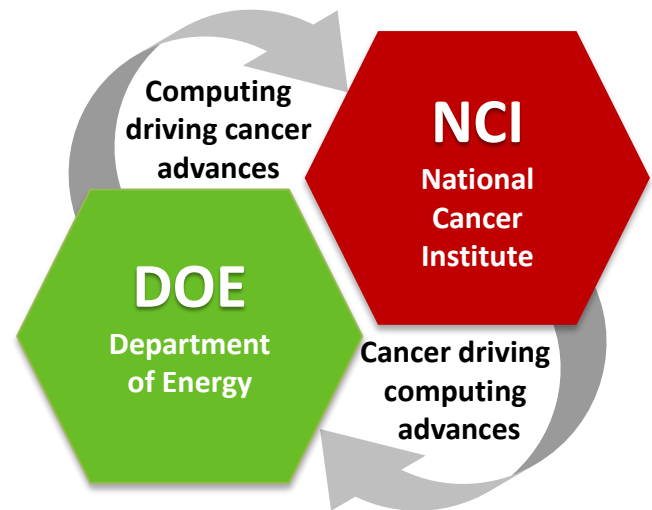
Accelerate both agency's missions by partnering computing and precision oncology

NCI Precision Oncology Mission - *Inject HPC and AI at scale into NCI challenges*

- **Mission:** Accelerate design and testing of effective, tailored treatments for cancer
- **Need:** Critical need for increase computational capability to meet mission objectives

DOE Exascale Mission – *Exascale and AI computing innovation inspired by fresh challenges and complex data*

- **Mission:** Sustain and enhance US technological and economic leadership in HPC research development and deployment
- **Need:** Multidisciplinary efforts needed to develop next generation advanced computing platforms for science and engineering



NCI Precision Oncology Challenge

Embedded in NCI precision oncology goal is data and physics problems that are exciting and push DOE thinking

Precision Medicine can only come about with understanding from data and new physics

Large, complex data: Data ranges from experimental to doctor's notes from across the country

Multi-scale problem : Scale of science encompasses molecular to population scale and time-scales of ms to a lifetime

Unknown physical models: Components of challenge space we do not yet have underlying physical models for

Exciting challenge for computation- Push intersection of big data, model and simulation, and machine learning

Current Activities

Joint Design of Advanced Computing for Cancer (JDACS4C)

(Frederick National Laboratory, NCI, ANL, ORNL, LLNL, LANL)

- **Three science pilots** developing deep learning at scale
- **CANDLE** (CANcer Distributed Learning Environment) An Exascale Computing Project (ECP) to develop Machine Learning framework for Cancer.
- **Uncertainty Quantification for Deep Learning**

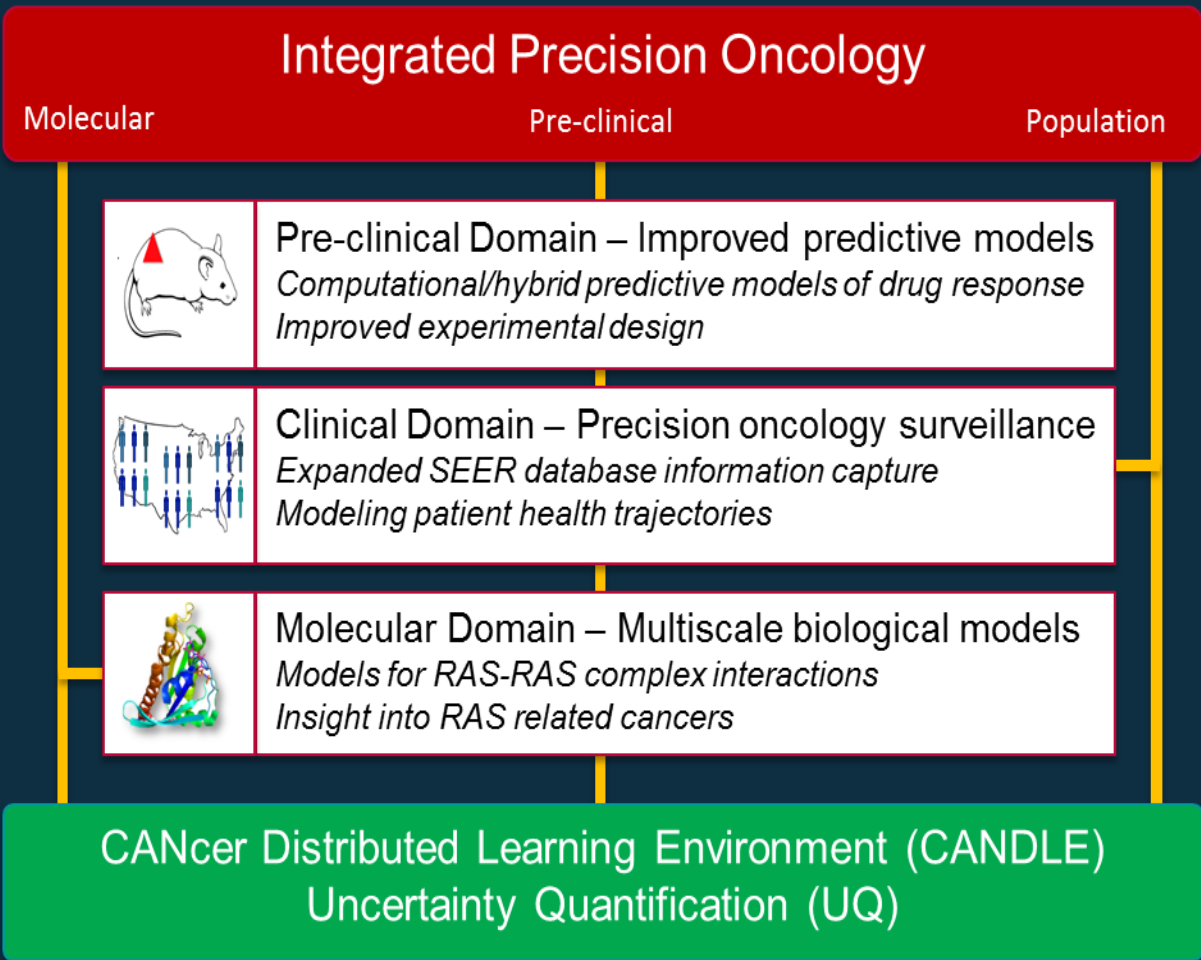
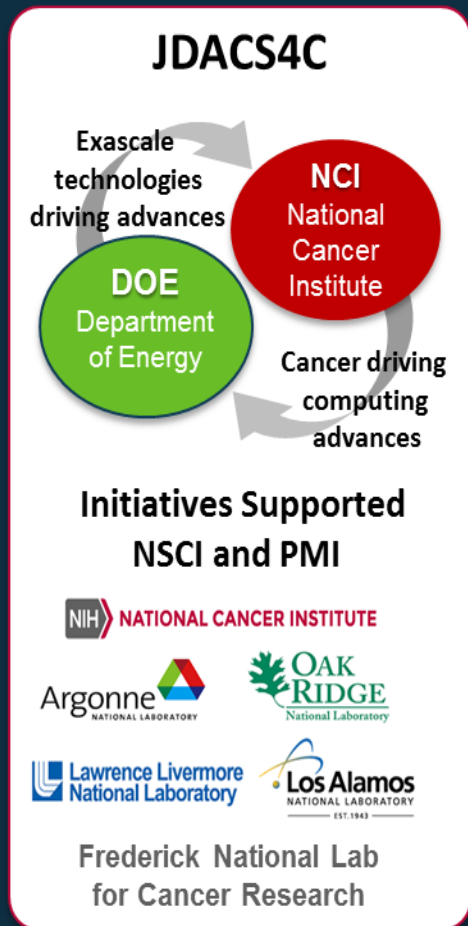
Accelerating Therapeutics for Opportunities in Medicine



(GlaxoSmithKline, FNL, UCSF, and LLNL)

- Reduce the time from bio-target to first in human testing from 6 years to 1
- Advance predictive models partnering DOE HPC expertise, NCI cancer research knowledge, and pharma large-scale data on failed drug compounds

JDACS4C – (more from our next speakers)



Management Teams

Governance Review Committee

- Provides high-level federal oversight and guidance
- Meets 3-4 times per year since Fall 2016
- Leadership from NCI and DOE (NNSA, NNSA-ASC and SC, SC-ASCR)

Management Team

- Provides program management of partnership activities
- Federal Program Management Team (NCI, DOE)
- Laboratory Program Management Leads (LLNL, FNL)

Communications Committee

- DOE and NCI federal and lab participation to ensure co-ordinated messaging

IP and Data Policy Committee

- Federal and lab team to streamline and implement data and IP policies and requirements from both agencies

DOE federal engagement includes:

Office of Science (ASCR, HEP, OSTI), NNSA (ASC)

Advisory Working Group

“Frederick National Laboratory Advisory Committee NCI-DOE Collaborations Ad-hoc Working Group”

- Provide input on the DOE-NCI partnership to help agencies meet goals
- External experts that serve and advise the Frederick National Laboratory Advisory Committee (FNLAC)
 - Similar to standing subcommittee of ASCAC
- Members include reps from ASCAC (Martin Berzins), FNLAC, and the NCI and DOE research communities
- Delayed start - first two meetings in year 2 of the pilot projects March and July of 2018

Partnership Impacts

- We are seeing exciting developments in machine learning at scale (more from next speakers)
- We are having impact with vendors
 - Advancing cancer in the space of hardware vendors (established and startups)
 - Collaborating on modeling capabilities with companies focused on targeted cancer treatment
- The broader NCI community is growing in engagement
 - CANDLE hackathons with NCI community are full,
 - DOE-NCI-SEER (state cancer registries) hackathons
 - State cancer registries and academic partners are starting to pro-actively engage Pilot 3 (a JDACS4C pilot)
- SC-16,17 and 18 Workshop on Computing for Cancer



Broader Observations

DOE brings more than HPC – bring DOE experience and thinking

- Leaning into “impossible” problems
- Stewardship in tackling Big Science
- Large, multidisciplinary teams



Interagency partnerships can strengthen collaboration within DOE laboratories

DOE scientists are excited to be working in this new challenge space – brings their best thinking

Next

- **Martin Berzins (ASCAC and Working Group member)**
 - Overview and perspective on JDACS4C
- **Fred Streit (LLNL pilot lead in JDACS4C)**
 - Update from JDACS4C Pilot 2 (molecular scale pilot)