Precision Medicine Initiative, Cancer Moonshot, and National Strategic Computing Initiative recommendation: **increasing public-private partnerships**
Accelerating Therapeutics for Opportunities in Medicine (ATOM) overview

- MOA to establish public-private partnership with GSK, DOE, and NCI in January 2017
- Goal is to accelerate pre-clinical drug design/development through use of advanced computational and *in silico* technologies
  - Relevant research tools, models, data, etc. **pre-competitive** and ultimately **made open/shareable**, 
  - Create a network of parallel activities, and
  - Ultimately shorten time required to achieve eIND starting from known cancer-relevant target(s)
- Aligns with NCI/FNL interests in delivering open data, open tools, and new capabilities to the broader cancer research community as well as ultimately improving cancer patient treatment and outcomes
- NCI/FNL contributes expertise in cancer, computational chemistry/biology, high performance computing, and supports sharing/distribution of data and models
NCI, DOE, GSK partnership is basis for ATOM Consortium

- Intended Consortium Founding Members: GSK, LLNL, FNLCR, and UCSF
  - Member resources and expertise are well positioned to integrate, build multi-disciplinary workflows, and support team science
  - Intended Consortium model will allow expansion to make additional partnerships with qualified pharma, biotech, academic, government, and other organizations
Proposed timelines for ATOM Consortium

**Year 1**
- Establish place, recruit people, establish workflows, invite other partners to join, identify problems
- Expect establishment of Consortium in Spring 2017
- Plan for Consortium location near UCSF’s Mission Bay Campus
- FNL to provide specific research expertise onsite and remote
- NCI to provide subject matter expertise, program management onsite and remote

**Year 2**
- Refine processes, solve problems, gain expertise, build and test models

**Year 3**
- Start: Patient presents indication where there is an identified target on a pathway that is druggable
- End: File Investigational New Drug (IND) application with FDA

**Goal:** in <12 months, to deliver a patient-ready cancer therapy and associated IND filing for a validated target
ATOM workflow: hybrid computational/experimental process
FNL specific technical/research contributions

▪ Data management and computing infrastructure
  ▪ Developing and deploying methods for representing ATOM-developed computational models
  ▪ Proposing and establishing the infrastructure, policies, and procedures for the public release of models and data.

▪ Computational models R&D
  ▪ Gap analysis and plan to fill gaps for multi-scale, mechanistic, and data-driven models
  ▪ Building initial models and assessing the predictivity and uncertainty thereof. Identifying missing parameters and/or experimental data needed to optimize models.

▪ Active Learning R&D
  ▪ Developing initial framework for integrating mechanistic predictions, data-driven models, translational assays, and design and synthesis processes
Ideas for increased engagement across broader research communities

- NCI/FNL have focus on expanding involvement and impact to broader cancer research community
- ATOM has the potential to integrate and draw capabilities from across the NCI-DOE pilots (JDACS4C) and CANDLE
- Specific modes of engagement and impact include:
  - Open/shareable models, tools, data, other capabilities
  - Fellowship/training exchange program
  - SBIR contract topic
  - SMEs/consultants and compound libraries/data from NCI DCTD and CCR (intramural)
  - Supplements to existing grants in related areas
  - Outreach to establish additional partnerships
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