

Frederick National Laboratory for Cancer Research



Accelerating Therapeutics for Opportunities in Medicine (ATOM) - Update

Eric Stahlberg, PhD

Frederick National Laboratory Advisory Committee

October 29, 2018

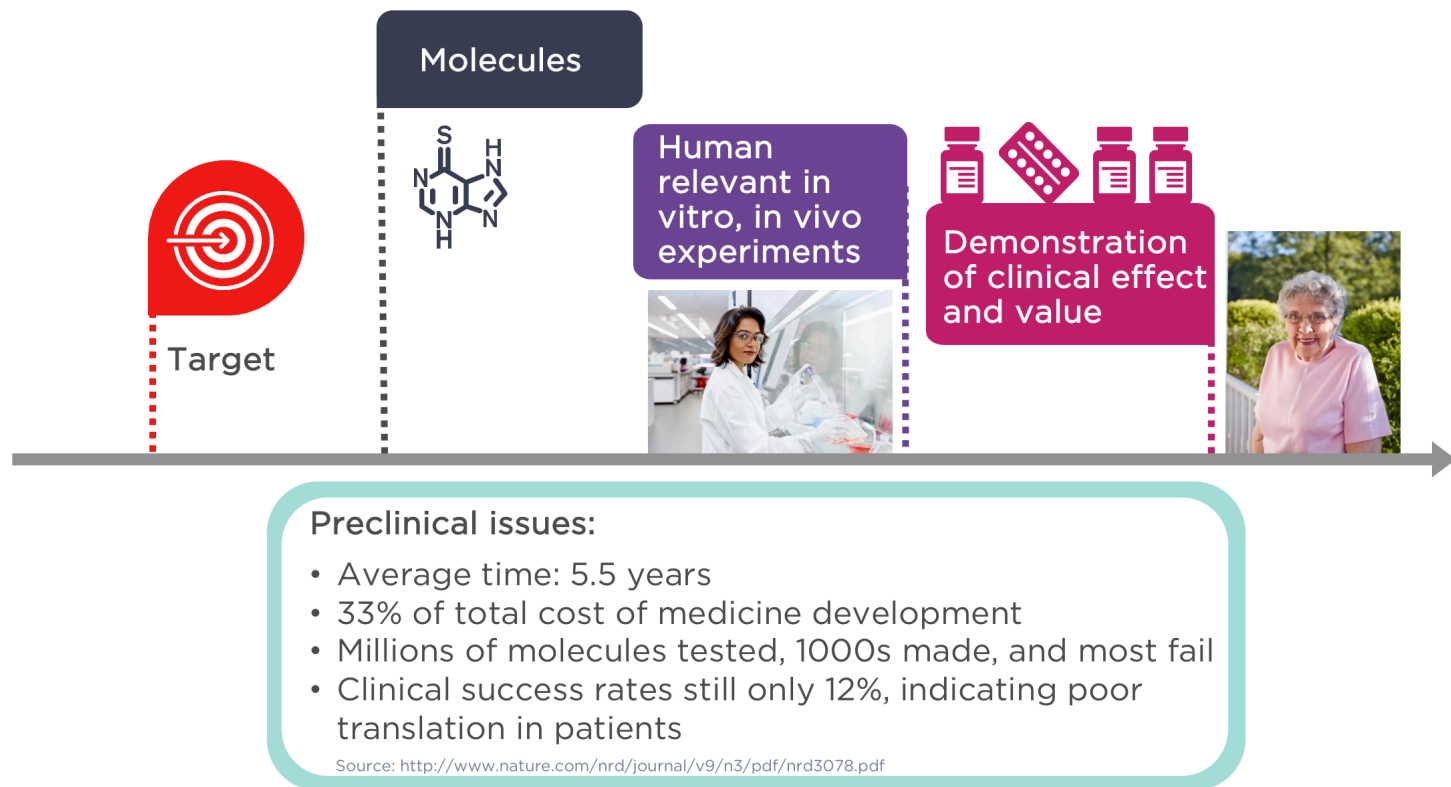
The Frederick National Laboratory is a Federally Funded Research and Development Center operated by Leidos Biomedical Research, Inc., for the National Cancer Institute
DEPARTMENT OF HEALTH AND HUMAN SERVICES • National Institutes of Health • National Cancer Institute

ATOM

An open, public-private consortium, launched with a CRADA, creating a national-scale pre-competitive resource to accelerate cancer drug development

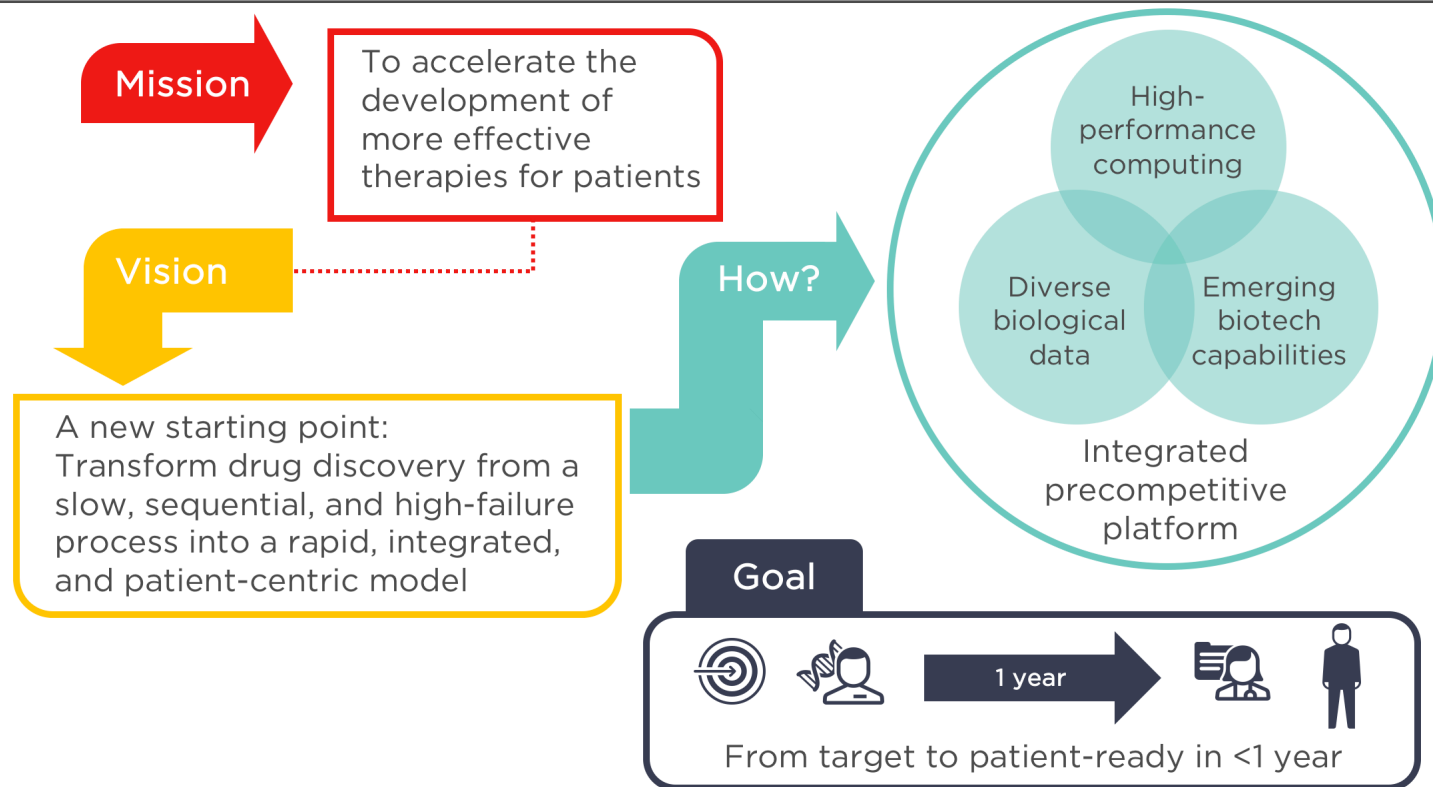
Drug Discovery: Long, Costly & High Failure

Seeking a better way to get medicines to patients



Accelerating Therapeutics for Opportunities in Medicine

About ATOM



ATOM

ATOM Integrated Platform – an Emerging Resource

From slow, sequential, & high-failure to rapid, integrated, and patient-centric

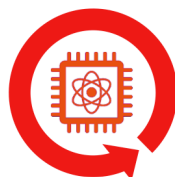
Computational
prediction at
the protein,
cell, tumor,
tissue, organ
and organism
level



Rapid empirical
testing is
focused on
validating and
optimizing
computational
predictions



In silico and
complex in
vitro models
reduce
reliance on
non-human
models

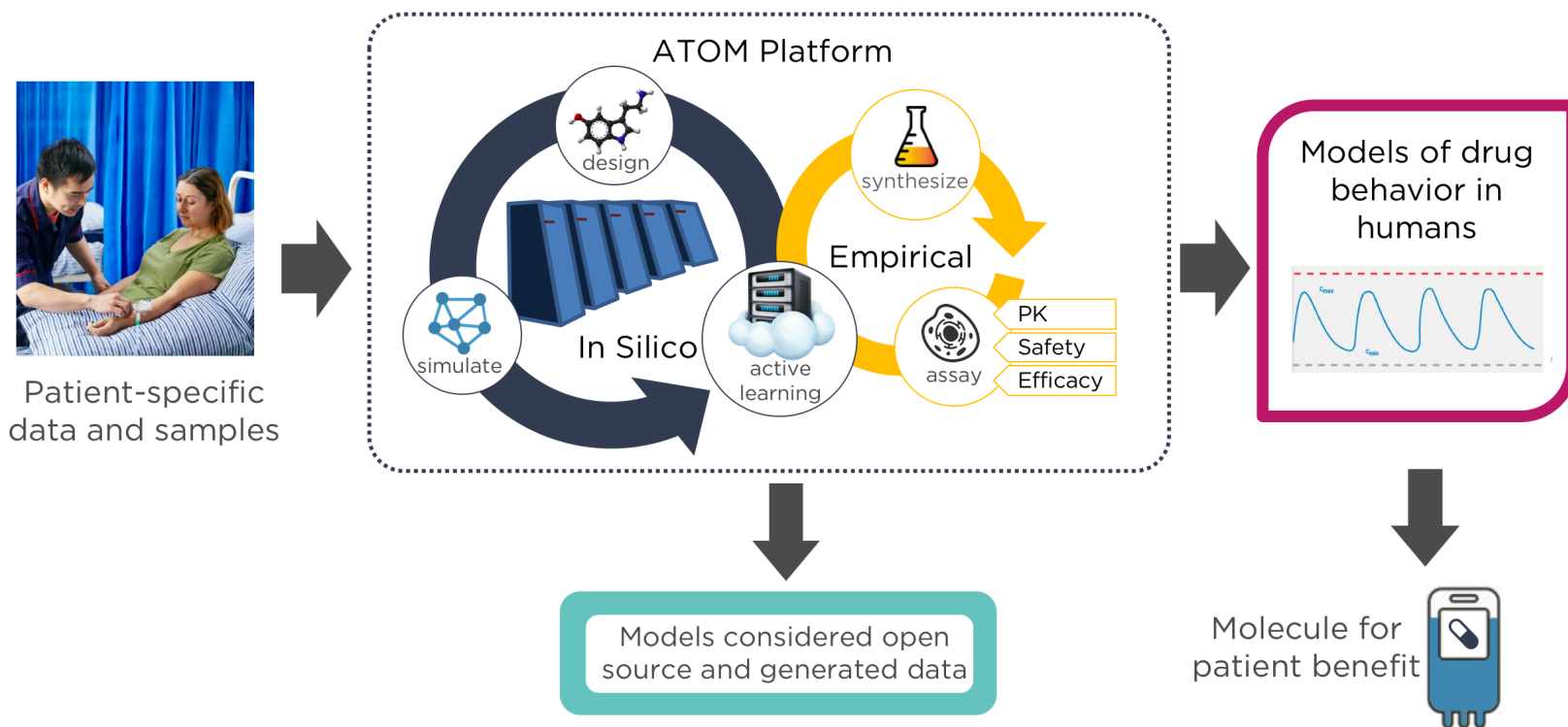


Regulatory
requirements
supported by
in vitro data
and in silico
predictions



Accelerated Drug Discovery Concept

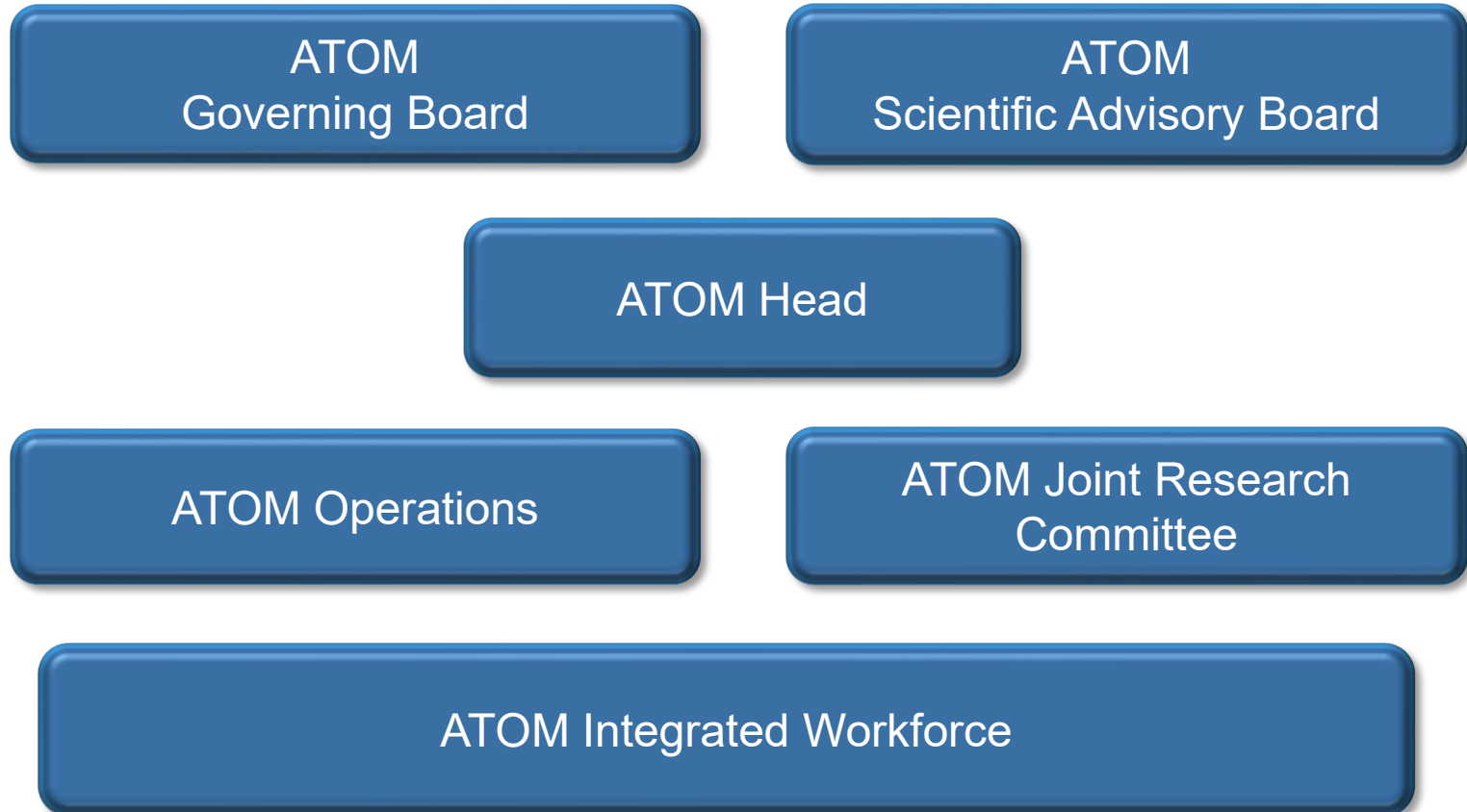
Vision of ATOM workflow in practice



ATOM

ATOM Organization

ATOM Organizational Structure



ATOM Leadership

ATOM Governance

Review of membership and votes

Joint Research Committee



Jim
Brase
CTO | Co-Lead
LLNL



Stacie
Calad-Thomson
COO | Co-Lead
GSK



Tom
Rush
CSO | Co-Lead
GSK



Michelle
Arkin
UCSF



Dwight Nissley
FNLCR

- 5 JRC/ co-lead members
- 4 votes on GB
(1 per organization)
- 1-3 GB members per
organization

Governing Board



John
Baldoni
GSK



John MacWilliams
LLNL



Alan
Ashworth
UCSF



Ethan
Dmitrovsky
FNLCR



Patricia Falcone
LLNL



Jason
Paragas
LLNL



Barry
Selick
UCSF



Eric
Stahlberg
FNLCR

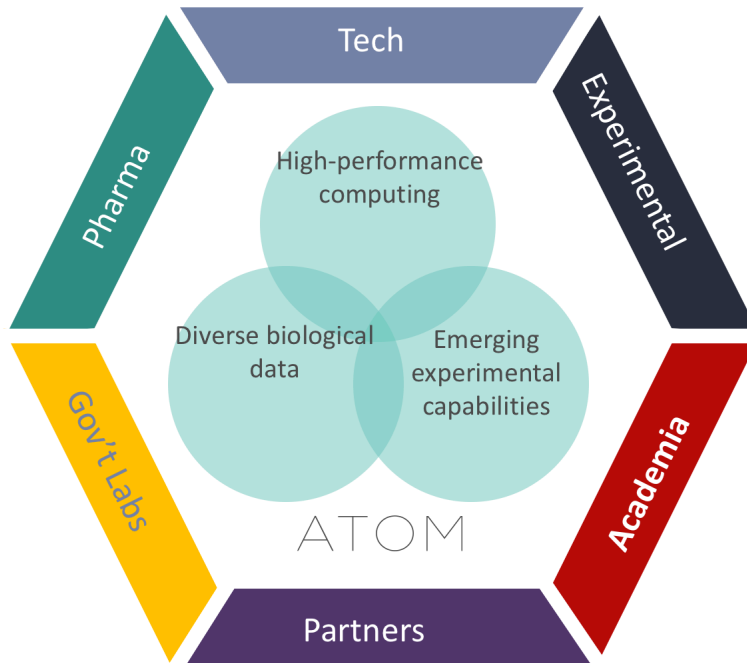
ATOM

ATOM Consortium Development Update

Engagement Summary

Growing the ATOM ecosystem

Partners build precompetitive drug discovery platform & form ecosystem



Business Development Metrics

- 2 types of partners – members & collaborators
- 149+ organizations across sectors
- 300+ external meetings with potential partners
- 150+ ATOM internal discussions
- 31 executed CDAs

(numbers based upon available information)

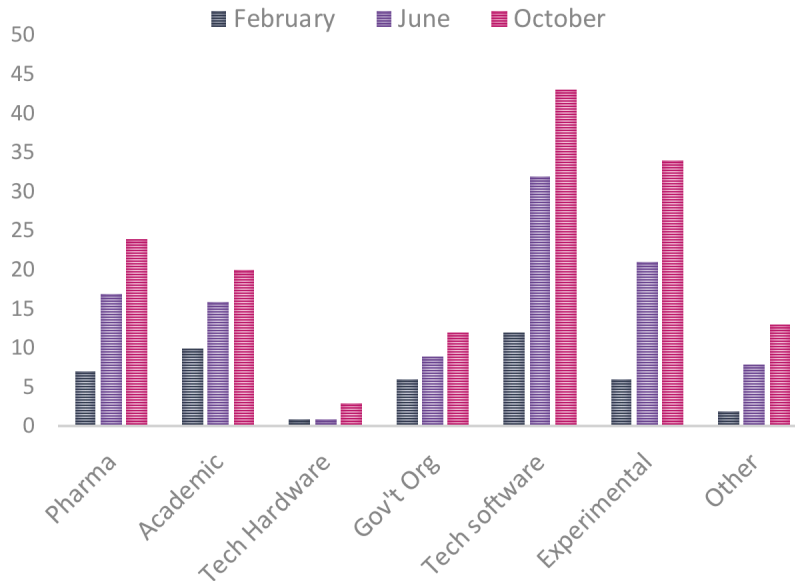
ATOM

Building an open ecosystem

Growing partnerships & community across sectors

Partner Pipeline Growth versus Sector

Cumulative No. of
Organizations



Met with 149 organizations across Sectors

Year 1-2 Strategy

Openness to all potential partners and prioritize BD efforts in sectors that foster early successes for membership growth

- Priority 1 – On-board Pharma members to build unique data lake, provide expertise & resources, and immediately use platform components
- Priority 2 – Grow software/modelling & experimental collaborators (public & private) to accelerate early R&D success

ATOM Participant Progression

Organizations under CDA in BD pipeline

Member



Collaborator

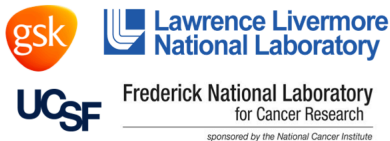
Sector	Vision & Technical Alignment	Consortium Contributions / SOW	Term Sheet	Contract In Preparation	Contract Executed
Pharma	Pharma 2	Pharma 1			
Hardware Tech		Hardware 1			
Gov't Org		DOE Lab 3	DOE Lab 2	DOE Lab 1	
Academia		University 1			
Software	Software 2	Software 1		Numerate + 2 more	DeepChem Advisor/B. Rhamsundar
Experimental	Exper. 2	Exper. 1			

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The ATOM ecosystem is growing

Partners build precompetitive drug discovery platform & form ecosystem

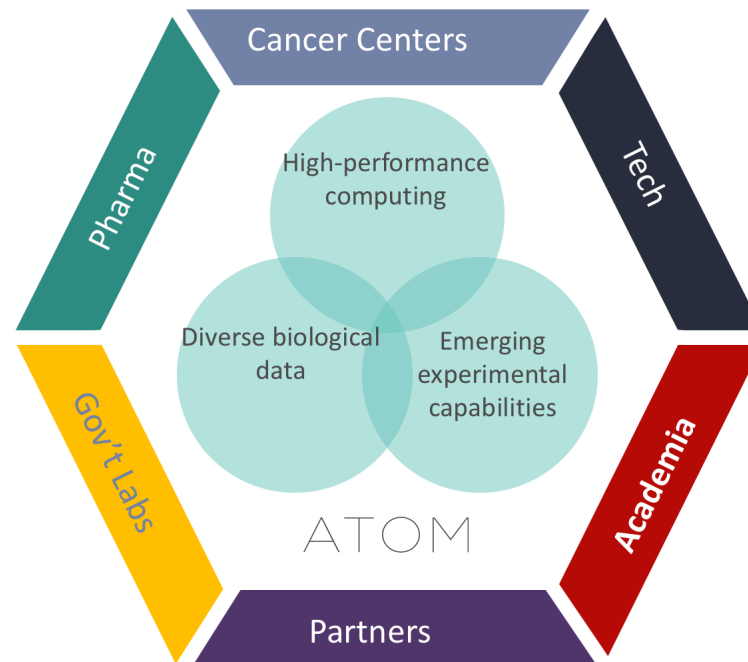
Founding Members:



Potential Members:

4 in discussion towards membership

1 pharma pilot project at SOW



Collaborators:

Numerate + 3 others in contract negotiation

Advisors:

2 on board & more to come
Michael Ringel, PhD, JD, ATOM
Advisory Board Chair
Bharath Ramsundar, PhD, ATOM
Technical Advisor

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ATOM Community Engagement

Selected ATOM presentations at 2018 conferences

34 conferences/meetings attended – Effectively growing ATOM partnership pipeline and greater community



ATOM Website Presence

Website - ATOMSCIENCE.ORG

HOME ABOUT US WHAT WE DO LEADERSHIP MEMBERSHIP CONTACT JOBS NEWS



HISTORY

In June 2016, GSK, the Department of Energy, and the National Cancer Institute announced their intent to create the ATOM partnership as one of the Cancer Moonshot task forces, with funding support under the 21st Century Cures Act.

The ATOM consortium was officially established in October 2017.

ATOM founding members are GSK, Lawrence Livermore National Laboratory, Frederick National Laboratory for Cancer Research, and the University of California, San Francisco.

Website Statistics

- 8.0k Visitors
- 13.4k Pageviews
- 51 new contacts including 2 pharmaceutical companies

ATOM Website Presence

Frederick
National
Laboratory
for Cancer Research

The screenshot shows the website frederick.cancer.gov. The header includes navigation links for Apple, Yahoo!, YouTube, Wikipedia, News, Popular, and Google. The main navigation bar features links for **SCIENCE & TECHNOLOGY**, **WORK WITH US**, **CAREERS**, **NEWS**, and **ABOUT**. A search bar is also present. The **SCIENCE & TECHNOLOGY** section is active, showing a breadcrumb trail: Home >> Science & Technology >> Overview. The **Overview** page features a large graphic of the word **ATOM** in white letters on a black background. To the left of this graphic is a sidebar with links: **ATOM**, **FNL's Contribution**, **Contact Us**, **News**, and **Upcoming Events**. Below the graphic, text states: "The Frederick National Laboratory is a founding member of the [Accelerating Therapeutics for Opportunities in Medicine \(ATOM\)](#) Consortium, a public-private partnership with the mission of transforming drug discovery by accelerating the development of more effective therapies for patients." Further down, it mentions: "The ATOM Consortium was officially established in October 2017. Founding members are [GSK](#), [Lawrence Livermore National Laboratory](#),

Join ATOM

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Contact info@atomscience.org
[@ATOM_consortium](#) [#ATOMscience](#)

Transform drug discovery, accelerate R&D,
and integrate data, AI, and supercomputing
to benefit patients

ATOM

Consortium Members: [NIH](#) [GSK](#) [Lawrence Livermore National Laboratory](#) [UCSF](#) [UCR](#)

sequential, and high-failure undertaking into a rapid, integrated, and patient-centric model.

Join ATOM

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FNLCR: Engagement point for the cancer research community

ATOM Community Development

ATOM Communications & Outreach

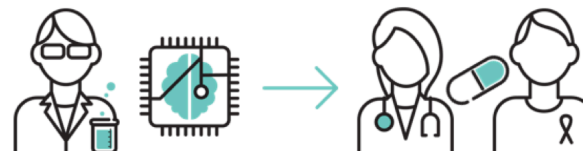
Growing membership and enlarging the community which shares ATOM's vision

Strategic use of:

- Website
- Social Media
- Press releases
- Conferences, Workshops & Events
- Outreach

Join ATOM

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Contact info@atomscale.org
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Transform drug discovery, accelerate R&D,
and integrate data, AI, and supercomputing
to benefit patients

ATOM

Consortium
Members:

Frederick
National
Laboratory
for Cancer Research



ATOM

ATOM Engagement is an Integrated Effort

ATOM Communications Team

FNLCR, GSK, LLNL, UCSF, DOE, NCI



Izumi
Hinkson, NCI



Frank
Blanchard, FNLCR



Mary Ann
Rhyne, GSK



Max
Cole, FNLCR



Nina
Ghanem, NCI



Michael
Cooke, DOE



Chris
Miller, DOE



Andrea
Peterson, DOE



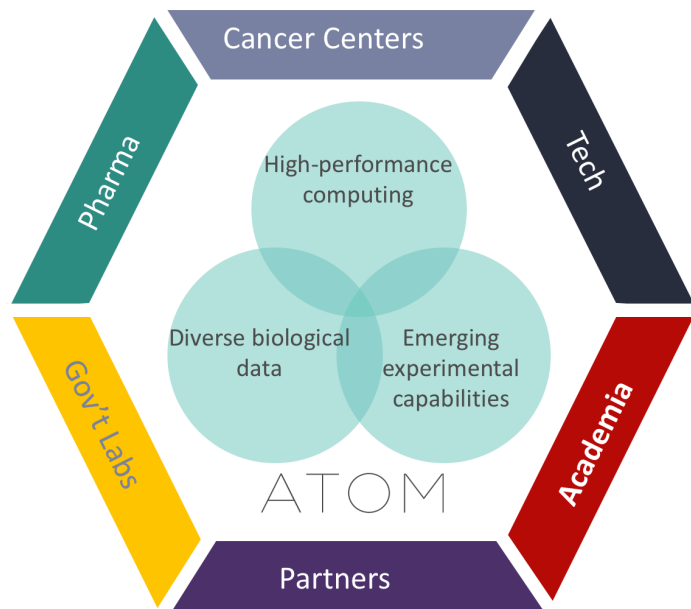
Jeremy
Thomas, LLNL



Laura
Kurtzman, UCSF

Technical Progress

ATOM Technical Progress Snapshot



Accelerating Therapeutics
for Opportunities in Medicine

Data and Modeling groundwork:

- Ingested private and public datasets into compound library
- Identified diversity & data gaps
- Computed sophisticated descriptor sets of chemical features for ATOM library (>2M compounds)
- Developed automated framework for creating models and tracking model output (model zoo)

PK and Safety data-driven modeling:

- Built 35 baseline models for PK parameters and 84 common liability assays with multiple featurization methods
- Benchmarked ATOM DeepChem models and showed improved performance over classical machine learning models
- Generated additional safety data sets to fill data gaps

Novel hybrid model development:

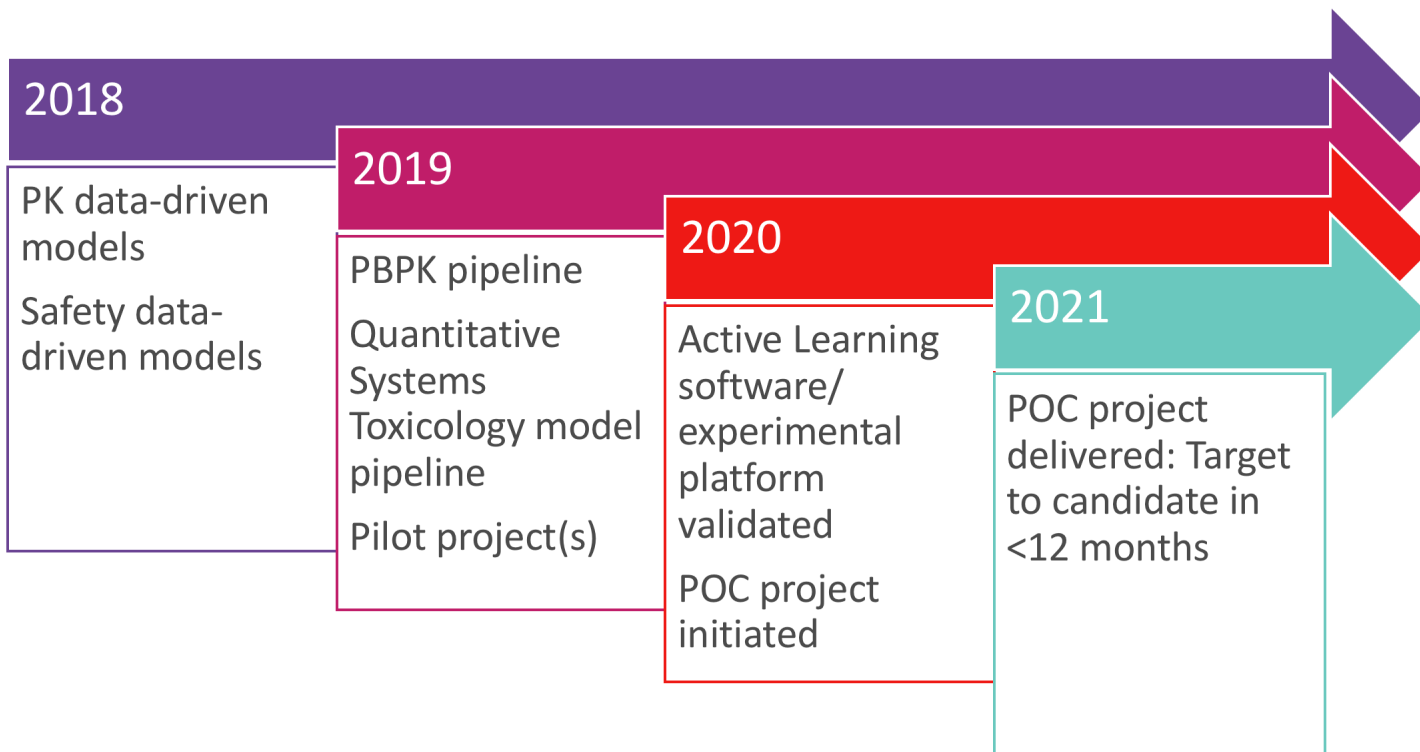
- Demonstrated that hybrid models promise improved performance over typical molecule descriptor approaches

Active Learning Integrated Loop

- Proof of concept multi-parameter simulations of active learning process.

Looking Ahead

High-level ATOM deliverables



Questions and Discussion

info@atomscience.org

www.atomscience.org