Computing and AI for Pandemic Response: Looking Forward

Advances in biological sciences, combined with the accelerating development of computing, data processing, and artificial intelligence (AI), are fueling a new wave of innovation that could have significant impact in sectors across the economy, from healthcare and agriculture to consumer goods and energy – *McKinsey Global Institute May 2020*

October 28, 2020

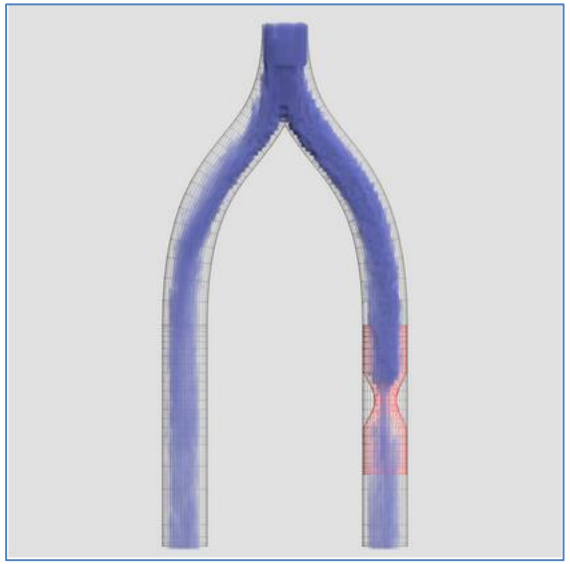
James M. Brase
Lawrence Livermore National Laboratory

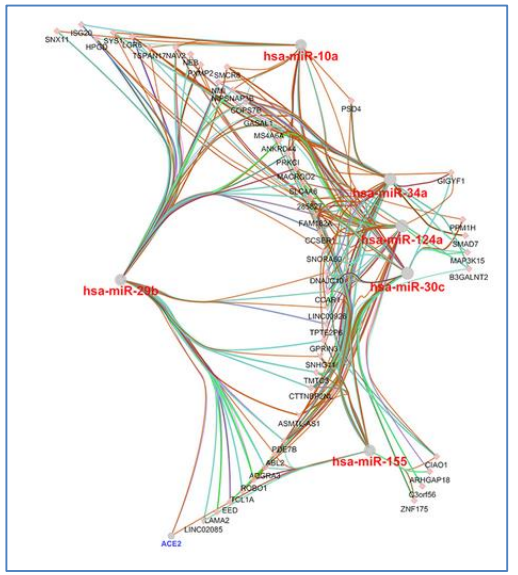
LLNL-PRES-760736
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

Computing has been an important tool for COVID-19 response

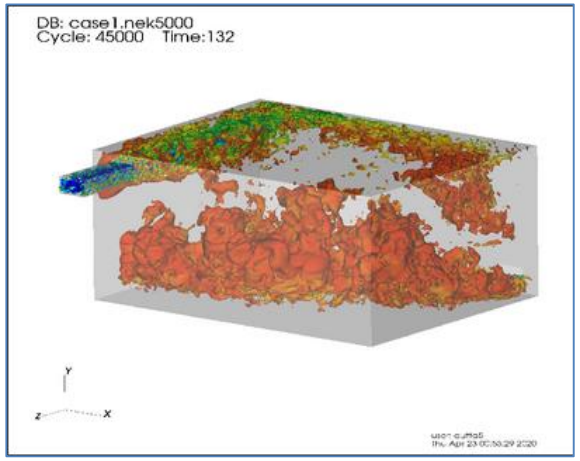
Simulation of ventilator splitting
- Amanda Randles
- Duke University
- Microsoft Azure

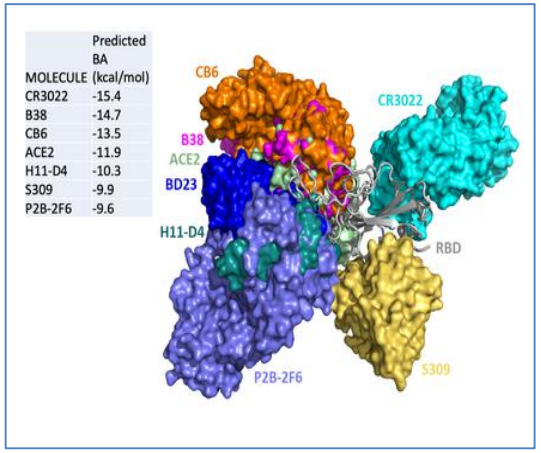




Patient response models from transcription data
- Afshin Beheshti
- NASA Ames
- NASA HEC

Modeling aerosol movement in a ventilated room
- Som Dutta
- Utah State University
- NCSA Blue Waters

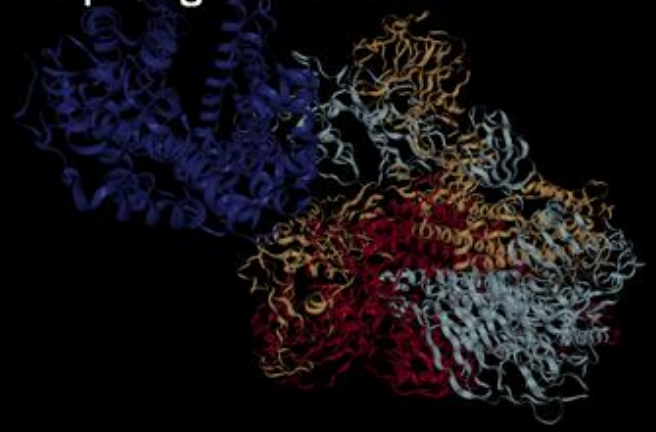




Screening approved drugs with AI-driven models
- Gouwei Wei
- Michigan State University
- DOE Summit

COVID-19 HPC Consortium | Who We Are | Collaborations | Projects | News & Press | Blog | Apply

The COVID-19 High Performance Computing Consortium



Bringing together the Federal government, industry, and academic leaders to provide access to the world's most powerful high-performance computing resources in support of COVID-19 research.

89
Projects

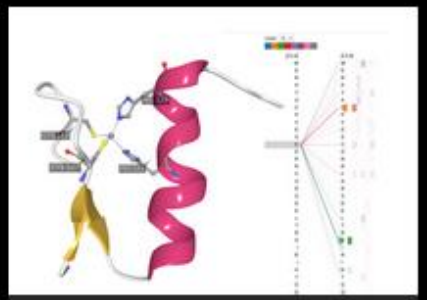
600
Petaflops

Active

Fighting COVID-19 will require extensive research in areas like bioinformatics, epidemiology, and molecular modeling to understand the threat we're facing and to develop strategies to address it.

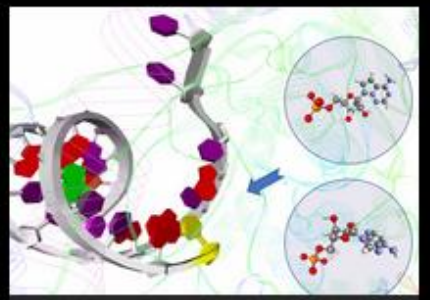
Here are some of our projects.

See all



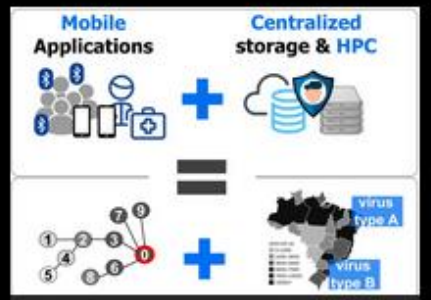
Accelerate SARS-CoV-2 research with transfer learning using pre-trained language modeling models

Basic science



The Competition of Antiviral Drugs with ATP to Inhibit the SARS-CoV-2 RNA-dependent RNA Polymerase: A Key t...

Therapeutics



Privacy-aware Contact Tracing with Knowledge Mining Mechanisms to Monitor and Understand the COVID-...

Patients

https://covid19-hpc-consortium.org/

Members

Industry

- IBM
- Amazon Web Services
- AMD
- BP
- D. E. Shaw Research
- Dell Technologies
- Google Cloud
- Hewlett Packard Enterprise
- Microsoft
- NVIDIA
- Intel

Academia

- Massachusetts Institute of Technology
- Rensselaer Polytechnic Institute
- University of Illinois
- University of Texas at Austin
- University of California - San Diego
- Carnegie Mellon University
- University of Pittsburgh
- Indiana University
- Massachusetts Green High Performance Computing Center (MGHPCC)
- University of Wisconsin-Madison
- Ohio Supercomputer Center
- UK Digital Research Infrastructure
- CSCS – Swiss National Supercomputing Centre
- SNIC PDC – Swedish National Infrastructure for Computing, Center for High Performance Computing

Department of Energy National Laboratories

- Argonne National Laboratory
- Lawrence Livermore National Laboratory
- Los Alamos National Laboratory
- Oak Ridge National Laboratory
- Lawrence Berkeley National Laboratory
- Sandia National Laboratories
- Idaho National Laboratory

Federal Agencies

- National Science Foundation
  - XSEDE
  - Pittsburgh Supercomputing Center (PSC)
  - Texas Advanced Computing Center (TACC)
  - San Diego Supercomputer Center (SDSC)
  - National Center for Supercomputing Applications (NCSA)
  - Indiana University Pervasive Technology Institute (IUPTI)
  - Open Science Grid (OSG)
  - National Center for Atmospheric Research (NCAR)
- NASA

International Government Agencies and National Laboratories

- Korea Institute of Science and Technology Information (KISTI)
- Ministry of Education, Culture, Sports, Science and Technology (MEXT)-JAPAN
  - RIKEN Center for Computational Science (R-CCS)

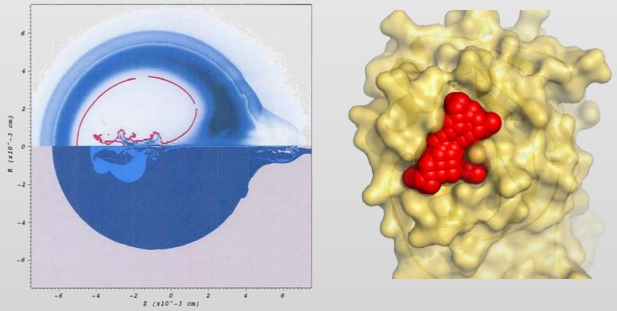
Collaborating Initiatives

Consortium collaborating initiatives represent efforts organized regionally around the world that are also working to accelerate research for fighting COVID-19. The Consortium is working with these initiatives and collaborating to share knowledge gained from our respective efforts.

- EU PRACE COVID-19 Initiative
- NCI Australia and Pawsey Supercomputing Centre

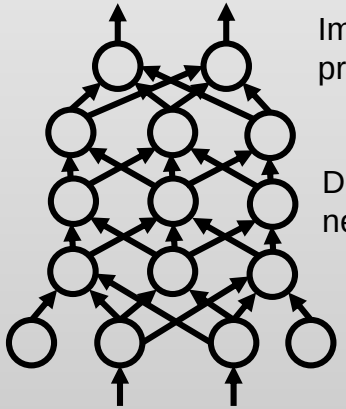
AI is being used to integrate increasingly complex simulations and growing but still limited data sets

Traditional pillar
high-performance computing



High-fidelity simulation
- Hydrodynamic
- Molecular dynamics

New pillar
Machine learning provides a framework for integrating simulation and experiment

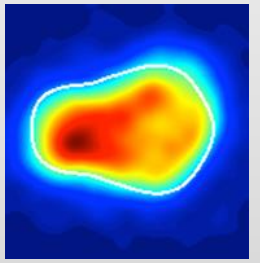


Improved prediction

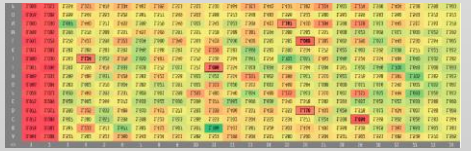
Deep neural network

Complete simulation and experiment data

Traditional pillar
Large-scale experiments



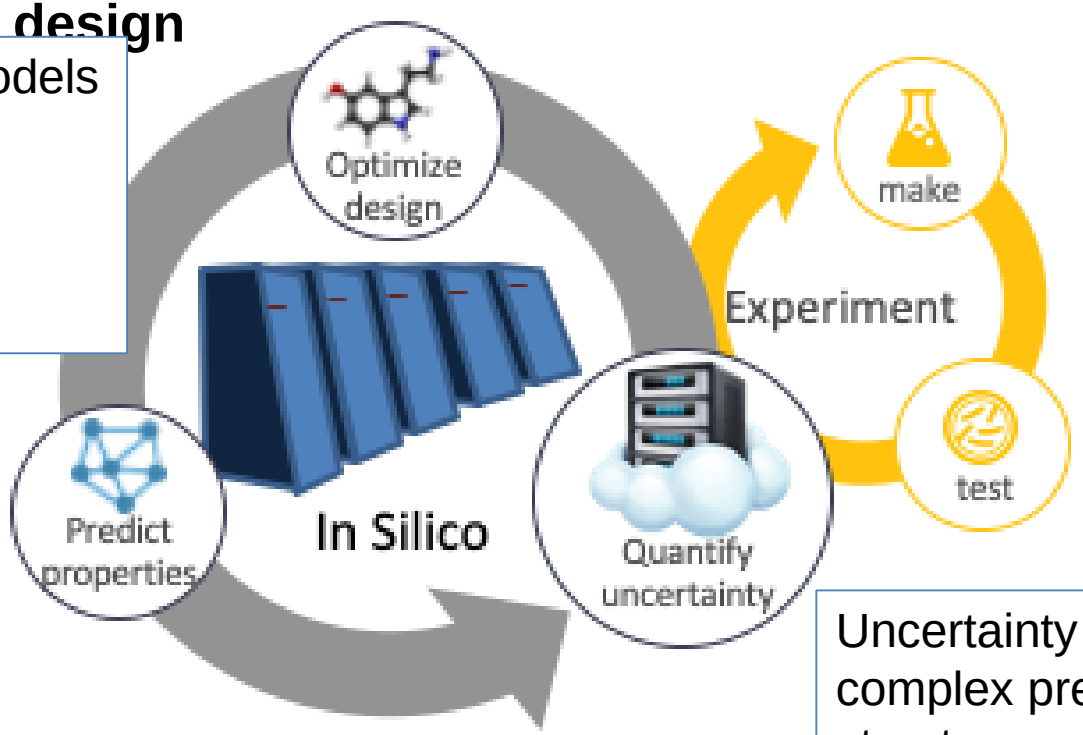
NIF X-ray image



High throughput binding assay

- **Improvement of prediction performance and uncertainty quantification**
- **New machine learning-driven approaches to design**
- **Amplification of our effective computational power**

AI-driven systems for therapeutic acceleration push on the frontiers of machine learning and predictive modeling



Large-scale generative models for design optimization
- Learned latent spaces
- Complex representations
- Joint optimization of multiple molecular properties

Integrating automated synthesis and assays with computational workflows

Improving prediction performance with limited data
- Domain of applicability
- Integrated mechanistic models
- Transfer from related targets
- Multiscale models for human properties

Uncertainty quantification for complex predictions – graphs, 3D structures, multiple assays

AI-driven CogSim tools can integrate community data to improve understanding of differences in disease spread among counties

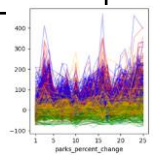
Community data

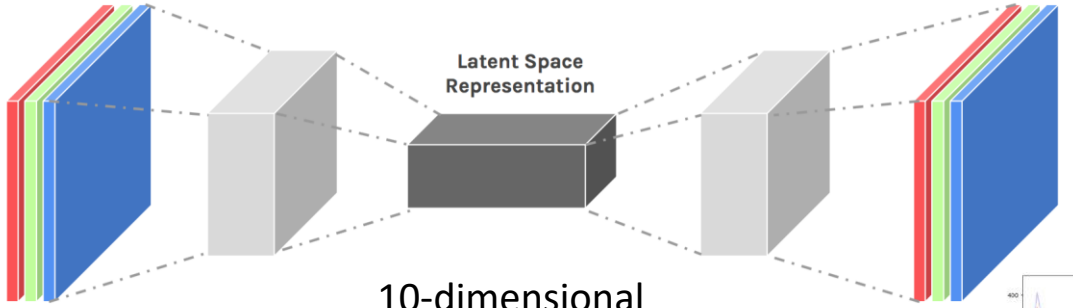
Confirmations

Deaths

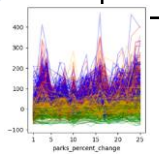
Mobility (parks, retail, ...)

2k-dimensional time histories





10-dimensional minimally correlated scalars



Community data

Confirmations

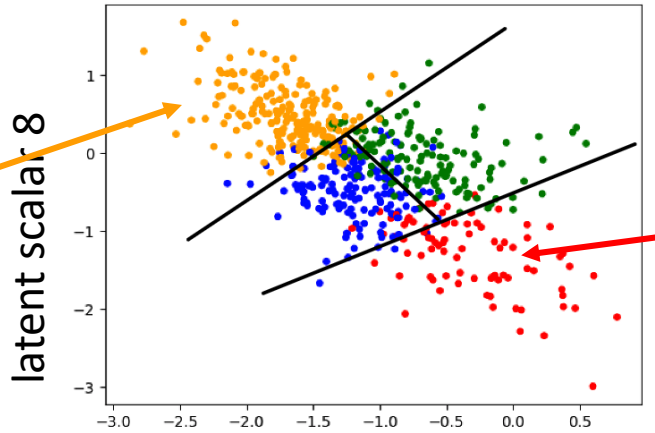
Deaths

Mobility (parks, retail, ...)

2k-dimensional time histories

Ft. Hood
Ft. Bragg
Ft. Campbell
Ft. Stewart
Ft. Carson*
Ft. Sill
Camp Lejeune

counties that react weakly to NPI



Ft. Carson*
Ft. Lewis*
Ft. Bliss
Camp Pendleton

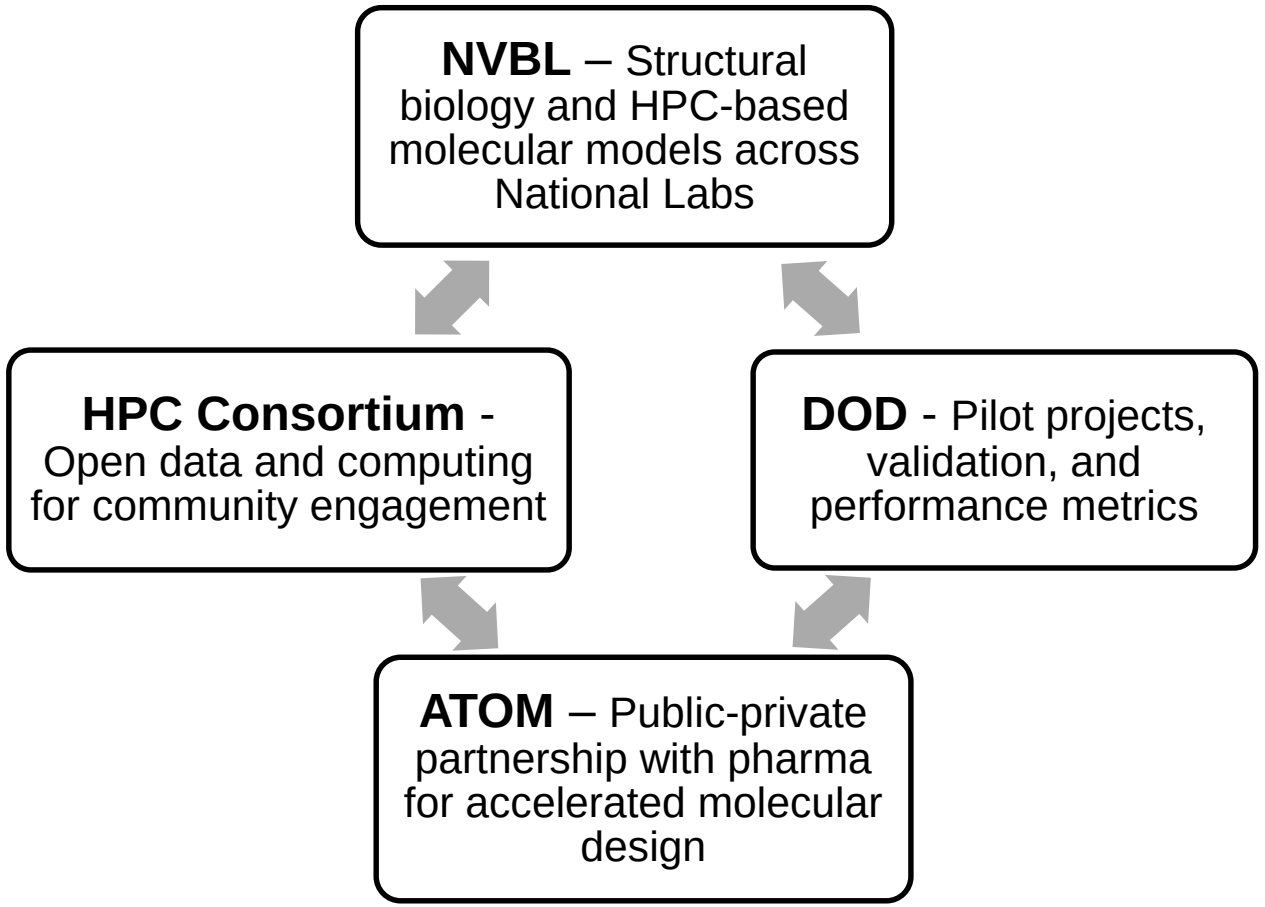
counties that react strongly to NPI

Ft. Carson*
Ft. Lewis*

Ft. Dix
Alameda/LLNL

What are the implications for key Army platforms?

The nation has an urgent need for new capabilities in accelerated therapeutic development



A new public-private partnership to ….

1. Pre-position large scale data resources on viral interactions
2. Establish and grow an open predictive modeling R&D community for viral therapeutics
3. Develop the molecular design platform and pre-position probe molecules for interacting with viral proteins
4. Exercise and validate the platform through a sustained program of drug discovery for the public good

Current DOE partnerships provide a strong starting point

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