COVID19 SUPERCOMPUTING CONSORTIUM OVERVIEW

Discussion for Supercomputing Response.org

NVIDIA

29 April 2020

AGENDA

PROGRAM OVERVIEW

OBSERVATIONS

A DEEPER LOOK

CONCLOUSION

COVID19 CONSORTIUM SUMMARY

- Primary Sites
  - ORNL, LLNL, NERSC, TACC, SDSC, NCSA, PSC, NASA AMES, AWS, MSFT
- 37 Projects with new entries daily
- 50% Apply AI/ML or HPC*AI/ML
- Most PIs are US based
  - Nepal 1, Porto 1, India 1
- NV is offering technical support to each team
  - Outreach completed with 80% to date

PI	Project
Bryan M Wong, UC Riverside	Harnessing Large-Scale Quantum-Based DFTB Calculations for a More Accurate Assessment of COVID-19 Inhibitors and Their Binding Dynamics
Olexandr Isayev, Carnegie Mellon University	Assisting SARS-CoV-2 computational drug discovery efforts with artificial intelligence (AI) and AI-accelerated quantum mechanics
Arvind Ramanathan, Argonne National Laboratory (Part of Rick Stevens Ask)	Artificial intelligence driven integrative biology for accelerating therapeutic discovery against SARS-CoV-2
Guowei Wei, Michigan State University	AI-based repositioning of existing drugs for COVID-19
Viktor Stolc, NASA Ames Research Center	Whole genome analysis using the NASA Ames supercomputer to define risk groups for severe pulmonary disease associated with COVID-19 and other illnesses
Gerardo Cisneros, University of North Texas	Using MD and QM/MM to improve drug candidates for nCoV-19 targets
Mahmoud Moradi, University of Arkansas	Conformational free energy landscapes of SARS coronavirus spike glycoproteins
Jeremy Smith, University of Tennessee, Knoxville	Rapid antiviral drug discovery for SARS-CoV-2: AutoDock and MD Sim
Aaron Morris, PostEra	PostEra: COVID MoonShot
Thomas Cheatham, University of Utah	Ensemble-based simulation and analysis workflow for design of novel peptidic inhibitors of COVID-19 main protease
Stratos Davlos, Innoplexus	COVID-19 novel molecule generation with reinforced learning
Ahmet Yildiz, University of California, Berkeley	Exploring binding and fusion mechanism of SARS-CoV-2 spike glycoprotein using molecular dynamics simulations
Wei Li, Children's National Medical Centre	Target Identification for Broad Antiviral Therapy using Functional Genetic Screening Datasets
Debsindhu Bhowmik, Oak Ridge National Laboratory	Discovering molecular targets of the human coronavirus with HPC and AI
Yang Zhang, University of Michigan	Request computing resource for de novo protein therapeutics design simulations to treat the COVID-19 disease

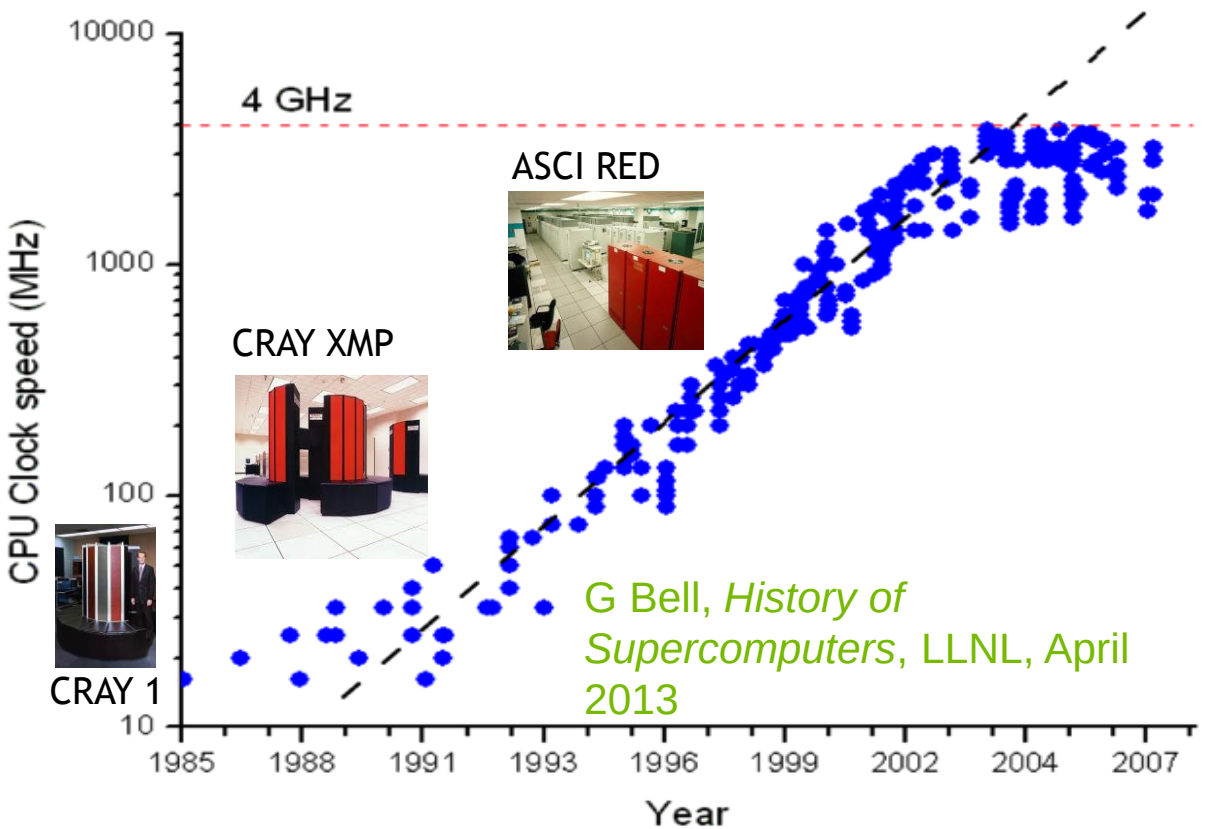
PI	Project
Bo Liang, Emory University	Characterization and structures of the SARS-CoV-2 polymerase and its complex with RNA or potential inhibitors
Chia-en Chang, University of California, Riverside	iterative information from computational and experimental investigation can efficiently discover new lead compounds and assist drug design targeting papainlike protease of SARS-CoV-2.
Zach Shahn, IBM	Allocation of Scarce Resources During the COVID-19 Pandemic
Pete Riley, Predictive Science Inc	Forecasting COVID-19 transmission in the USA using DICE (Dynamics of Interacting Communty Epidemics)
Padilla-Sanchez, Victor, Catholic University of America	SARS-CoV-2 structural analysis and insights on antibody engineering in silico
Dustin Machi, U of Virginia	HPC Support for COVID-19 Response
Mark Flynn, LANL	Incidence of SARS-CoV-2 in SRA metagenomic samples
Kevin Esvelt, MIT	Designing virus-specific sACE2 mimics for competitive inhibition of SARS-CoV-2
Oscar Bastidas, U of Minnesota	Modeling the Dynamic Behavior of Surface Spike Glycoprotein of COVID19 Coronavirus and Designing Biomimetic Therapeutic Compounds
Ou, Shujun Iowa Sate	The evolutionary history of SARS-CoV-2
Rath, Soumya National Institute of Technology Warangal	Dependence of Structure and Dynamics of SARS-CoV-2 on Temperature and Humidity in the Atmosphere
Michael Feig, Michigan State	High Accuracy Modeling of SARS-CoV-2 Membrane Proteins via Machine Learning and Physics-Based Refinement
Stephan Irle, ORNL	Quantum Mechanics-based Refinement of SARS-CoV-2 Inhibitors from Classical Docking
Numan Oezguen, Baylor College of Medicine	Dynamics of SARS-CoV2 spike protein RBD and core S2 domains
Cesar de la Fuente, UPenn	Effects of genetic variants of human ACE2 protein on SARS-CoV-2 spike protein binding

PI	Project
David Wright, Kuano.ai (start-up?). Inspire	Drug-repurposing for Covid-19 with 3D-aware machine learning
Gomez-Bombarelli, Rafael	COVID-19: RNA-seq analysis to identify potential biomarkers indicative of disease severity
Beheshti, Afshin, NASA	Physical Models of COVID-19 Related Proteins
Ken Dill, SUNY Stony Brook,	A Dynamic Structural Model of the SARS-CoV-2 Main Protease to Guide Drug Design and Repurposing
Jennifer Klein, UW-LaCrosse	Dissecting inhibitor impacts on viral RNA polymerase and fidelity control of RNA synthesis in SARS-CoV-2
Jin Yu, UC-Irvine	A drug discovery project against the main protease of COVID-19
Maria Ramos, University of Porto	Computer Simulation of COVID-19 Spread in Nepal
Bishesh Khanal, Nepal Applied Mathematics and Informatics Institute for Research	Drug-repurposing for Covid-19 with 3D-aware machine learning

THE EVOLUTION OF HPC SYSTEMS

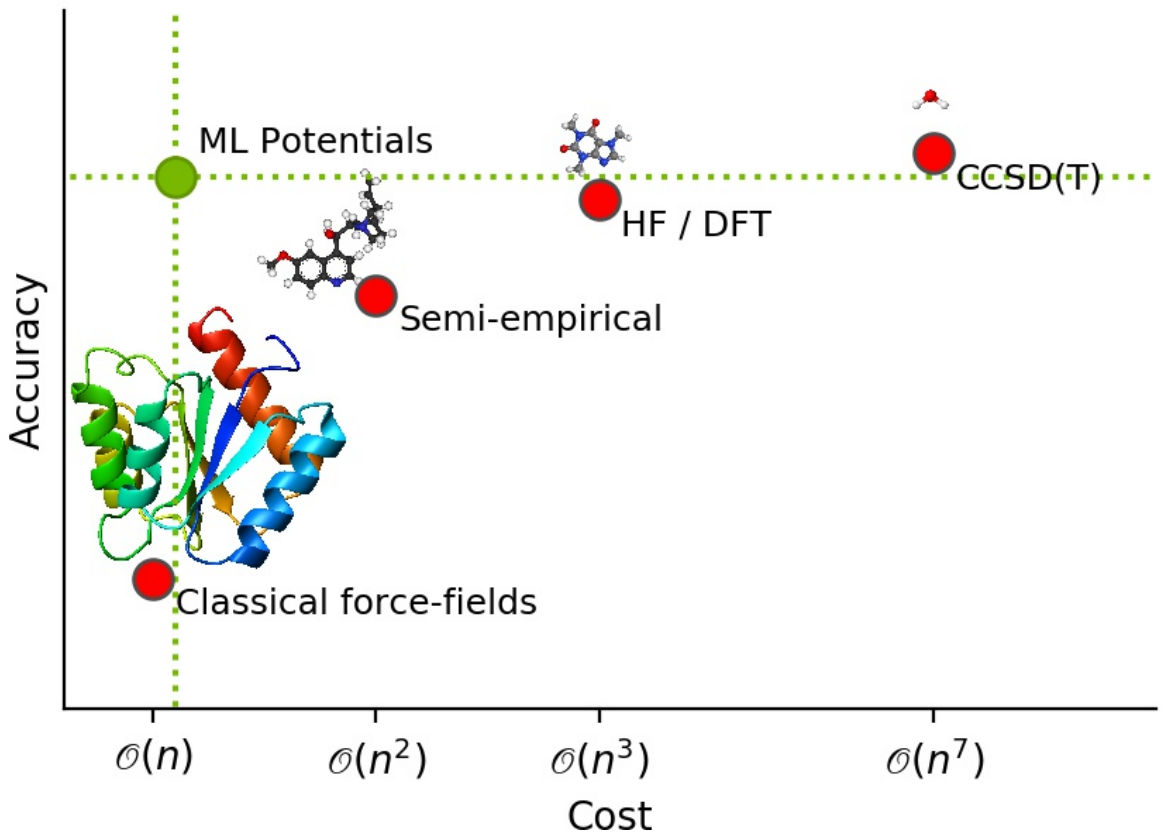
We Want to GO Here

We Are Here



G Bell, *History of Supercomputers*, LLNL, April 2013

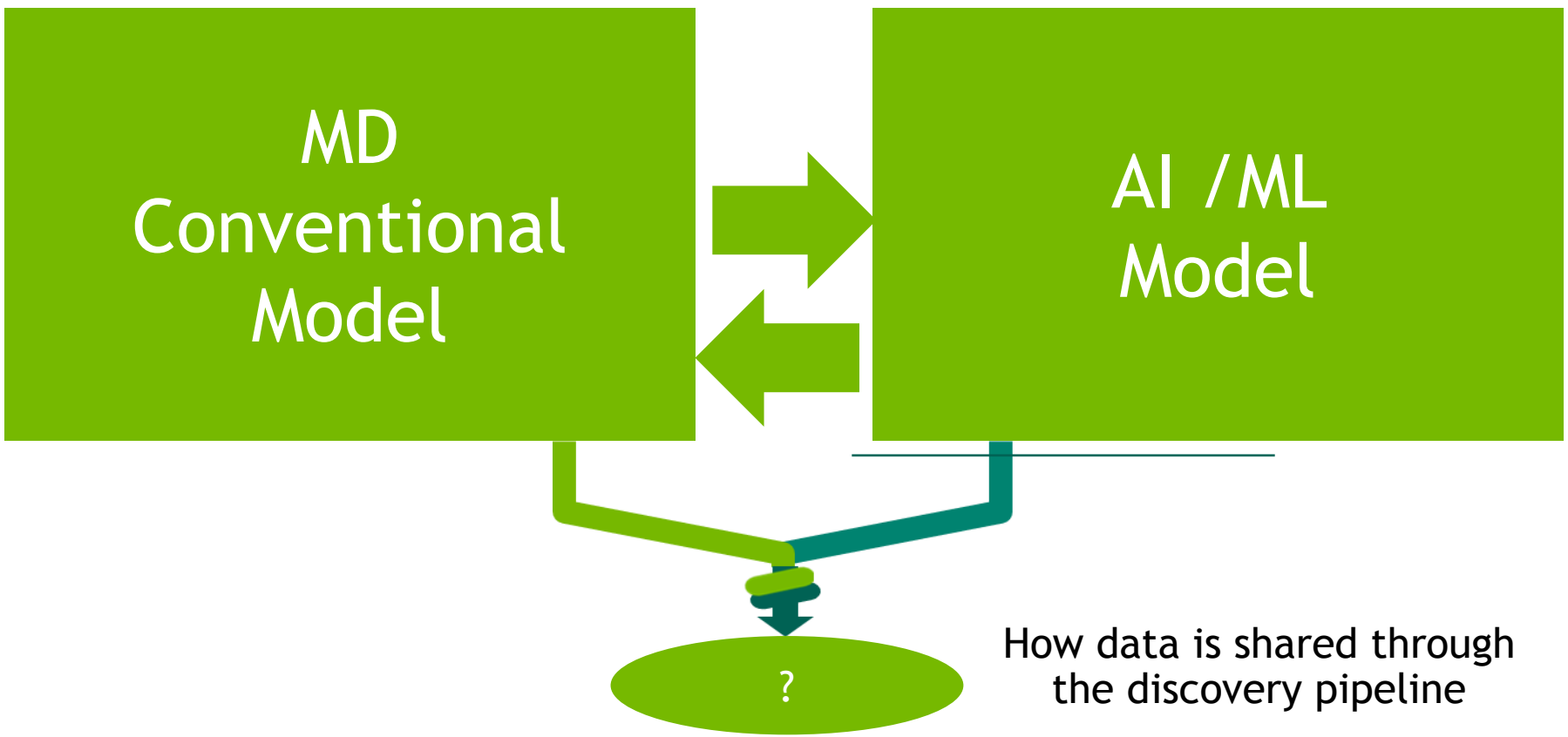
ACCURACY- COMPUTE COST TRADE-OFF



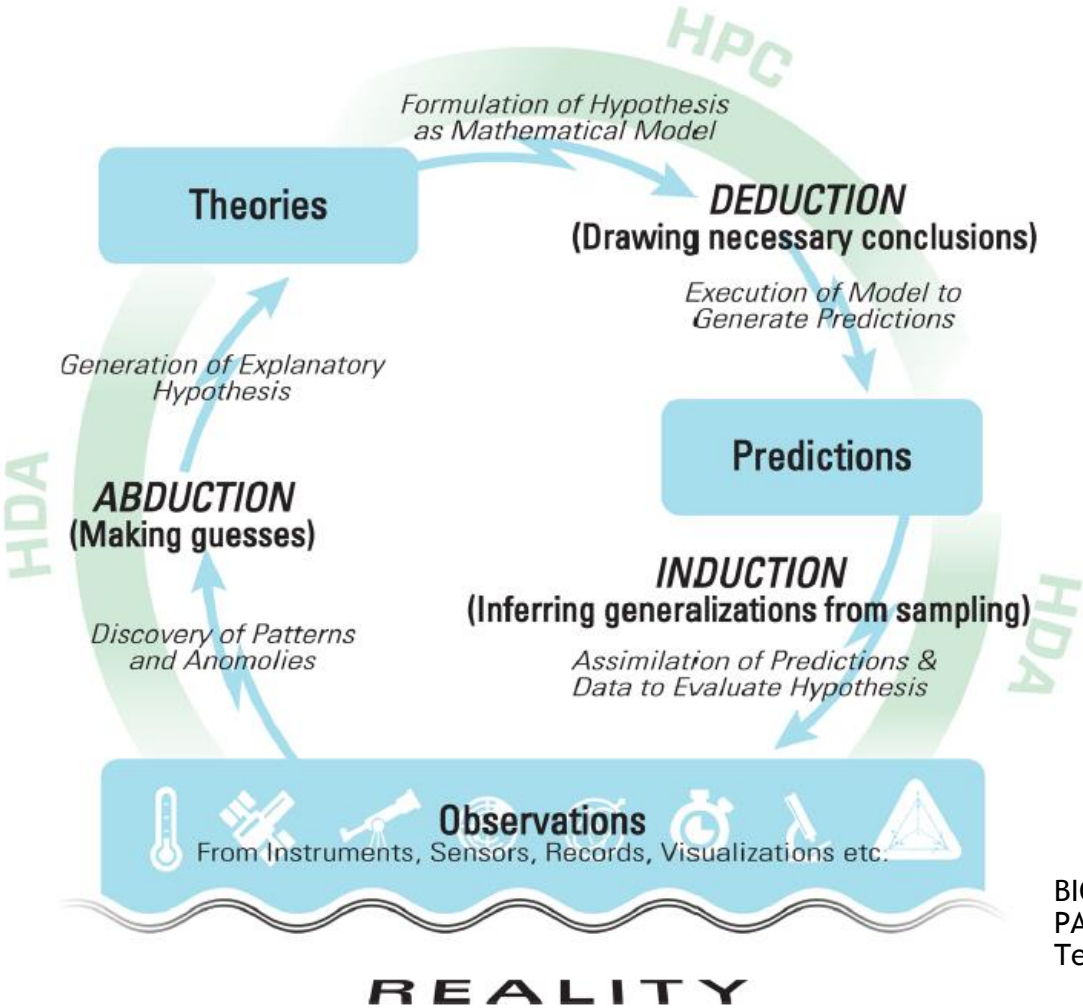
DEEPER DISCUSSION

PI	Site	Description	Key Points
Converrged			
Jeremy Smith ORNL	SUMMIT	In silico to In Vitro Autodock, Gromacs	Combine (restrained T-REMD) simulations with virtual high-throughput screening in an ensemble docking campaign to identify well-characterized drugs
Arvind Ramanathan ANL	SUMMIT	AI Steering with AMBER and Autodock	Adaptive conformational sampling using molecular dynamics (MD) simulations, and building all-atom models for the entire viral envelope
Olexandr Isayev CMU, UFLA	Bridges	TorchANI steering AMBER with RDKit and Openeye	Creating a library of screened candidates using AI and MD and docking
Debsindhu Bhowmik (ORNL)	SUMMIT	Adaptive Drug Discovery VAE + NAMD + scikit	Application of molecular phylogenetics combining MD and AI simulation and combinatoric search
Large Scale Conventional MD Models			
Chia-en Chang UC Riverside	COMET	Optimized long time scale AMBER	500,000 Atoms for usec simulation time
Rommie Amaro	Frontera	Large Scale MD with NAMD	Currently 2Mn Atoms usec scale. Goal is 200Mn Atoms usec

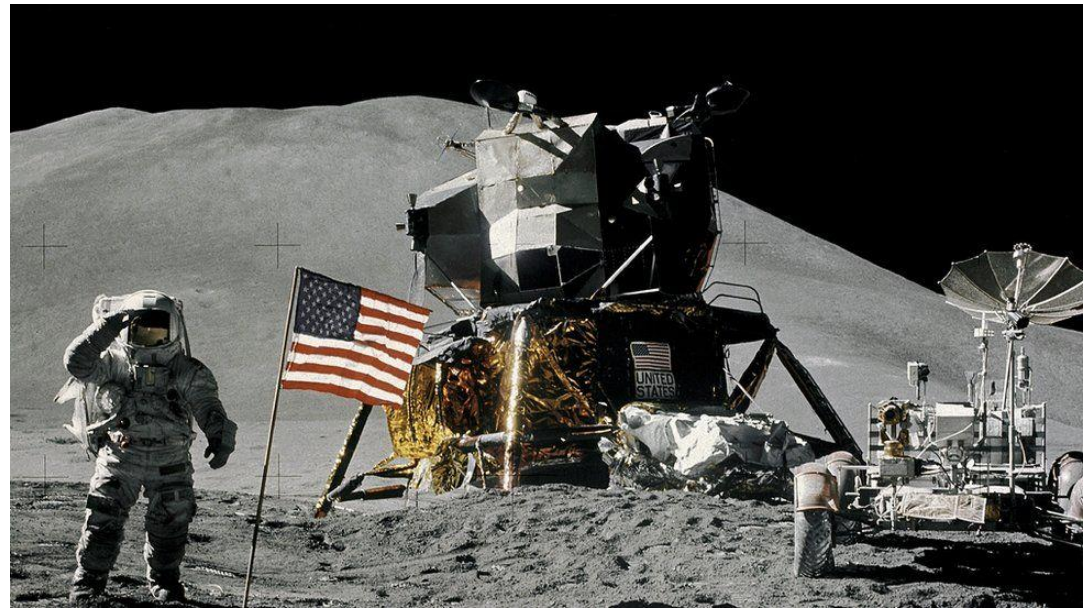
COMMON APPROACH



CONVERGED HPC*AI SYSTEM



BIG DATA AND EXTREME-SCALE COMPUTING:
PATHWAYS TO CONVERGENCE
Tech Report No. ICL-UT-17-08


UNITED
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