

# NVBL Overview

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**#NATLABSINTHEFIGHT**

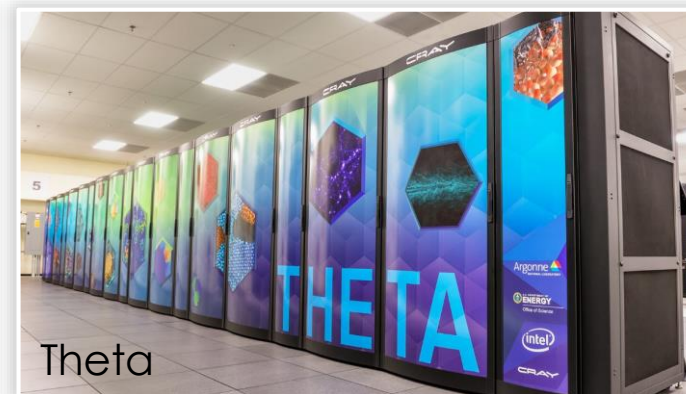
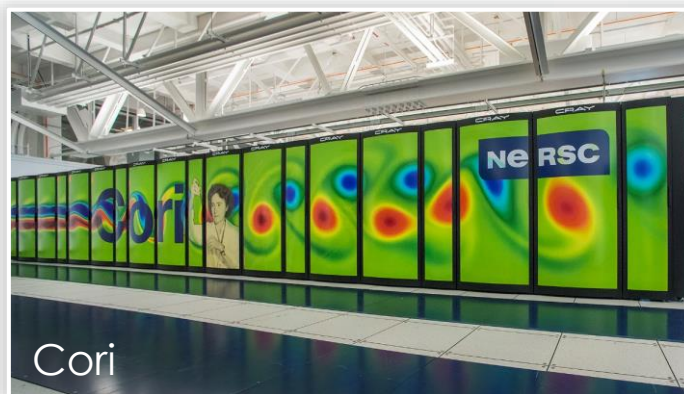
# High Performance and Leadership Computing Facilities

## Computational modeling and simulation

- Protein–small molecule docking for drug discovery
- Optimization of protein–antibody interactions
- Pandemic modeling to assist local, state, and federal officials
- Modeling fate and transport of virus in buildings and transportation venues

## COVID-19 HPC Consortium

- Government, industry, and academic members
- Providing access to the world's most powerful computers



# Light and Neutron Sources

High-throughput  
structures of proteins

Examination of  
enzyme reactions  
during virus  
replication

Virus–membrane  
interactions

Dynamic studies of  
drug and antibody  
interactions with  
proteins





# Nanoscale Science Research Centers

Small molecule synthesis for antiviral assays

Deuteration for structural studies

Electron microscopy for materials characterization

Scanning probes for examining surface contamination

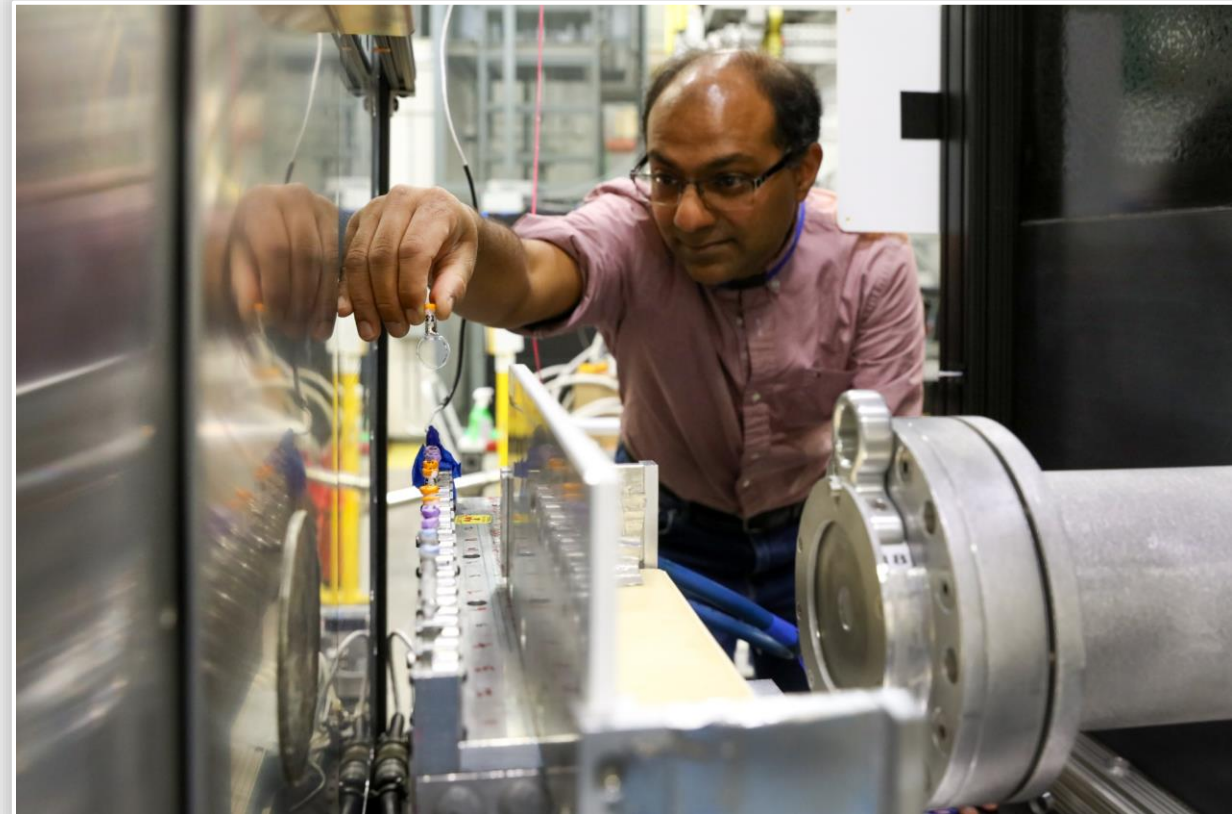
Polymer and materials synthesis



# DOE Laboratories have broad capabilities for addressing the COVID-19 crisis

Scientists and engineers with deep expertise relevant to:

- Development of analytical technologies and trace detection
- Design and discovery of antiviral drugs and vaccines
- Advanced manufacturing to address supply chain issues
- Predictive modeling for emergency response and epidemiology
- Molecular and structural biology



# National Virtual Biotechnology Laboratory

## Consortium of 17 DOE National laboratories

- Initiated in March 2020
  - Executive committee named and working group formed
  - Teams formed rapidly, integrating expertise in physical, biological and computational sciences
  - Concept papers developed and down-selected
- NVBL acts as single point of contact for COVID R&D activities
- Highly coordinated with other Federal Agencies

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## National Virtual Biotechnology Laboratory (NVBL)

The U.S. Department of Energy National Virtual Biotechnology Laboratory (NVBL) is a consortium of DOE National laboratories, each with core capabilities relevant to the threats posed by COVID-19. The NVBL is taking advantage of DOE user facilities, including light and neutron sources, nanoscale science centers, sequencing and bio-characterization facilities, and high performance computer facilities, to address key challenges in responding to the COVID-19 threat. Examples include developing innovations in testing capabilities, identifying new targets for medical therapeutics, providing epidemiological and logistical support, and addressing supply chain bottlenecks by harnessing extensive additive manufacturing capabilities. The NVBL collaborates extensively with researchers, both in academia and the private sector. In addition, the DOE user facilities are available to users in all sectors of the research community.

**DOE Lab Capabilities**

[This document](#) summarizes the capabilities of U.S. Department of Energy (DOE) laboratories that may be responsive to the threats posed by COVID-19, from near-term responses to longer-term research and development (R&D) opportunities.

**DOE National Virtual Biotechnology Laboratory Capabilities Summary**

<https://science.osti.gov/nvbl>



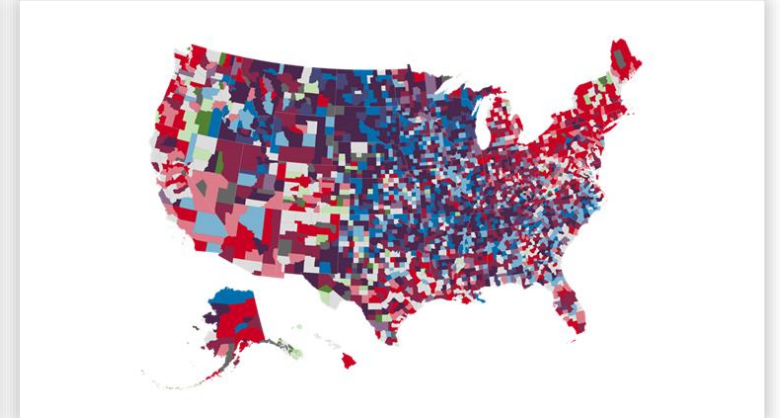
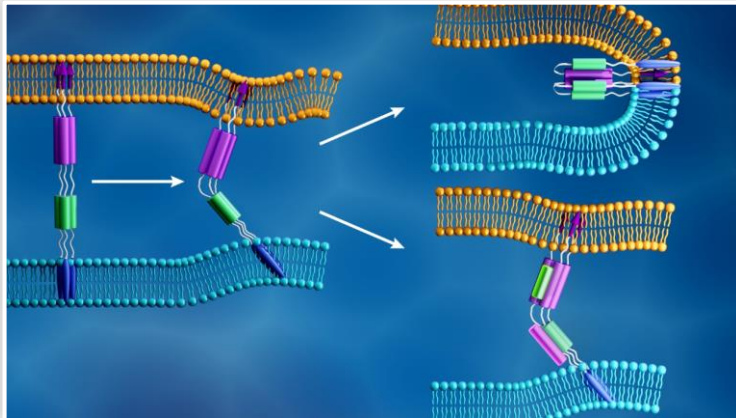
# NVBL is having lasting impact

Teams that quickly pivoted to integrate expertise and resources to address COVID-19 challenges

Capabilities applied to successfully tackle problems that would be difficult to solve in industry or academic labs

New capabilities developed that have broad applicability for addressing future national needs

Demonstrating the value of focusing capabilities of the national lab complex on national challenges



# National Virtual Biotechnology Laboratory

COVID-19 R&D for the nation



<https://science.osti.gov/nvbl>





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