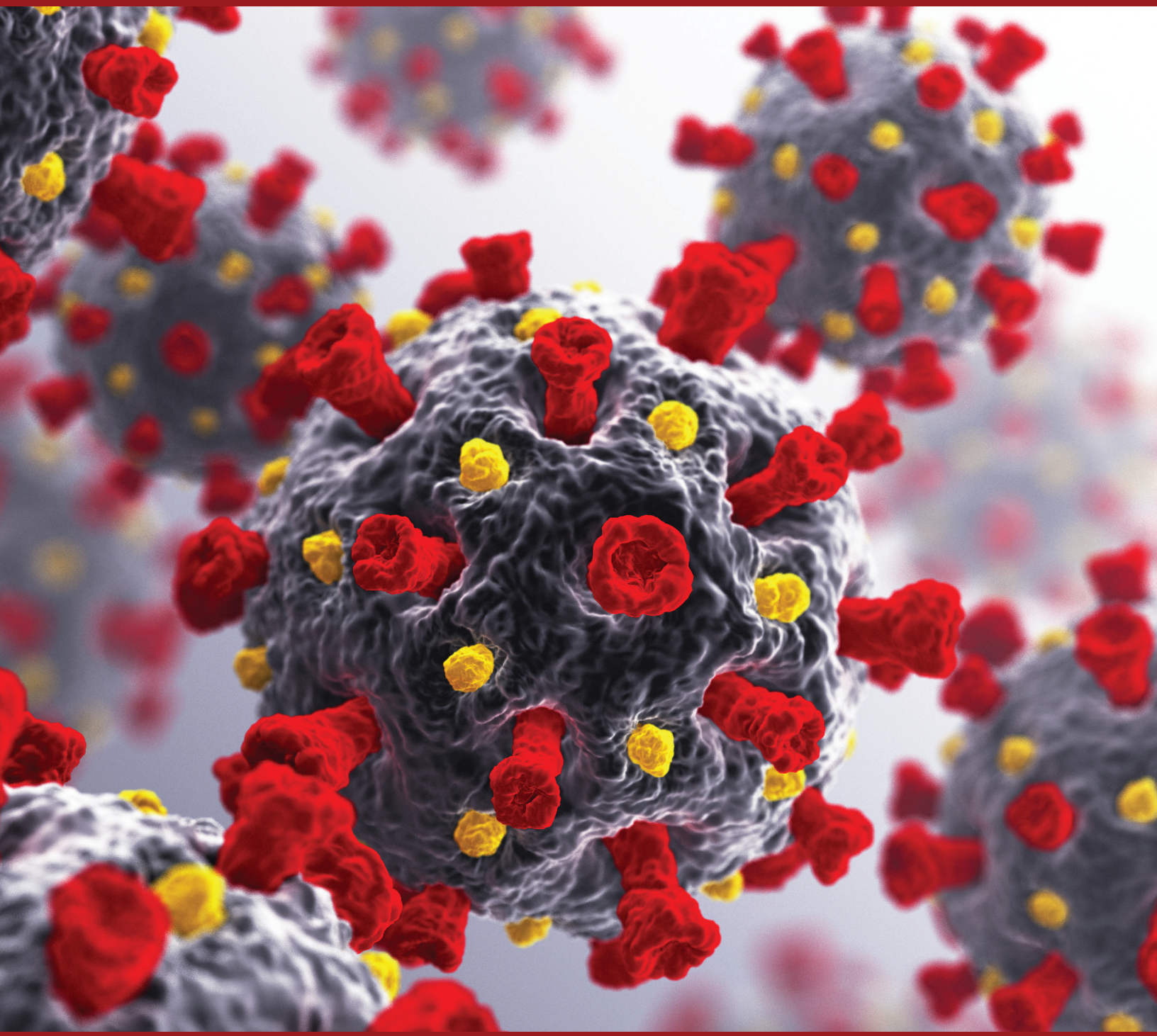
U.S. Department of Energy

National Virtual Biotechnology Laboratory

R&D for Rapid Response to the COVID-19 Crisis



U.S. DEPARTMENT OF ENERGY | Office of Science

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National Virtual Biotechnology Laboratory

A Game-Changing Framework for Responding to the Nation's Needs

With funding from the CARES Act, the U.S. Department of Energy (DOE) established the National Virtual Biotechnology Laboratory (NVBL) in March 2020 to address key challenges associated with the COVID-19 crisis. The NVBL brought together the broad scientific and technical expertise and resources of DOE's 17 national laboratories to address medical supply shortages, discover potential drugs to fight the virus, develop and verify COVID-19 testing methods, model disease spread and impact across the nation, and understand virus transport in buildings and the environment. National laboratory resources leveraged for this effort include a suite of world-leading user facilities broadly available to the research community, such as light and neutron sources, nanoscale science research centers, sequencing and biocharacterization facilities, and high-performance computing facilities.

Within just a few months, NVBL teams produced innovations in materials and advanced manufacturing that mitigated shortages in test kits and personal protective equipment (PPE), creating nearly 1,000 new jobs. They used DOE's high-performance computers and light and neutron sources to identify promising candidates for antibodies and antivirals that universities and drug companies are now evaluating. NVBL researchers also developed new diagnostic targets and sample collection approaches and supported U.S. Food and Drug Administration (FDA), Centers for Disease Control and Prevention (CDC), and Department of Defense (DoD) efforts to establish national guidelines used in administering millions of tests. Researchers used artificial intelligence and high-performance computing to produce near-real-time analysis of data to forecast disease transmission, stress on public health infrastructure, and economic impact, supporting decision-makers at the local, state, and national levels. NVBL teams also studied how to control indoor virus movement to minimize uptake and protect human health.

Through its NVBL framework, DOE has contributed significantly to the nation's COVID response, demonstrating in only a few months the critical impact of the national laboratories. The NVBL serves as an outstanding model for developing and sustaining capabilities to respond to future national needs or emergencies. Examples of NVBL COVID-19 accomplishments are outlined below, and more details are available at science.osti.gov/nvbl.

NVBL Accomplishments

Materials and Manufacturing for Critical Supplies

- Designed a system for mass producing N95 filter media, enabling Cummins Filtration (Nashville, Tenn.) to produce material for more than 3 million masks per day, and worked with DemeTech (Miami Lakes, Fla.) to convert the N95 material to masks and respirators, creating over 1,000 new manufacturing jobs.
- Worked with the U.S. Department of Health and Human Services and Coca-Cola (Atlanta, Ga.), which produces 2 billion bottle preforms per week, to evaluate the use of these preforms to alleviate shortages of test tubes used to collect nasal swab samples.

Materials and Manufacturing for Critical Supplies. NVBL teams developed a mechanism to 3D print the tooling needed to mass produce sample collection tubes for COVID-19 test kits. [Courtesy Thermo Fisher Scientific Inc.]

- Developed an approach to 3D print the tooling needed to produce over 8 million sample collection tubes weekly by Thermo Fisher Scientific, Inc. (Lenexa, Kan.), creating more than 300 jobs.
- Developed a new low-cost ventilator with BioMedInnovations (Denver, N.C.) that received FDA Emergency Use Authorization approval.

Molecular Design for Medical Therapeutics

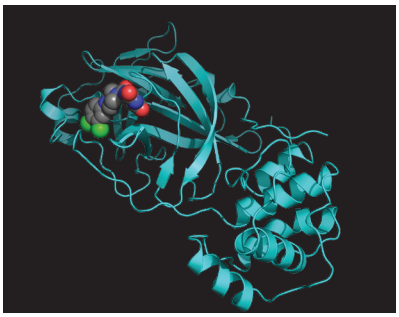
- Used artificial intelligence methods to computationally screen 10^{40} possible antibody variations, identifying the best hits that could be used as an antiviral against the Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) spike protein.
- Computationally screened tens of millions of small molecules against SARS-CoV-2 viral proteins and then experimentally evaluated top hits, greatly accelerating the search for antiviral therapeutics.

Development and Evaluation of COVID-19 Testing

- Collaborated with DoD, CDC, and FDA to provide experimental data in support of national testing guidelines, assessing potential contamination in commercial kits, evaluating sample pooling approaches, examining viral transport media and protocols, and evaluating virus inactivation and extraction methods to assure test efficacy and protect frontline health care workers.
- Developed analysis tools to assess global evolution of the SARS-CoV-2 RNA genome, as it relates to nucleic acid–based assays.
- Identified distinguishing signatures in the SARS-CoV-2 RNA genome that can be used to rapidly detect this pathogen and other co-infecting pathogens in multiplexed assays.
- Developed a small nucleic acid test instrument to rapidly detect SARS-CoV-2 with high sensitivity.

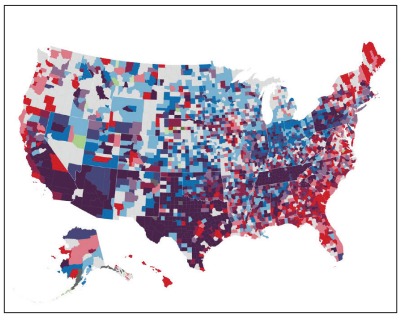
Epidemiological Modeling

- Created an approach to forecast COVID-19 case counts at state, county, and metropolis scales using data-driven statistical models, enabling short-term planning of contact tracing, staffing, and testing capacity needs.
- Created the ability to perform longer-term, scenario-based analysis and mitigation planning to support decision-makers with information on effects of interventions before they are implemented.



Molecular Design for Medical Therapeutics. Scientists used computational modeling and simulation approaches as well as molecular dynamics to design and optimize small molecules that are experimentally confirmed to inhibit viral proteins, such as the 3CLpro cysteine protease shown here. [Courtesy Oak Ridge National Laboratory]

Development and Evaluation of COVID-19 Testing. NVBL researchers provided experimental data that helped inform national guidelines used in millions of tests. [Courtesy Los Alamos National Laboratory]

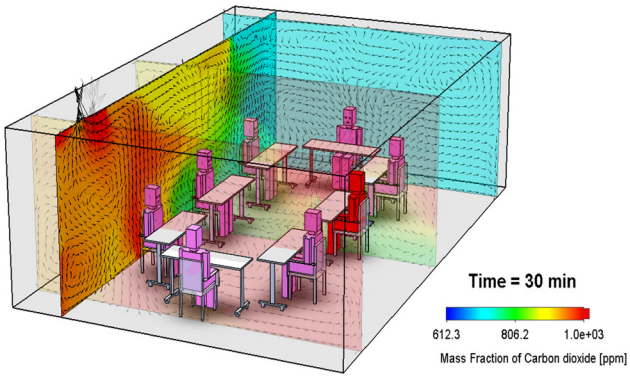


Epidemiological Modeling. Data scientists developed tools to forecast and visualize in near-real time COVID-19 transmission rates and dynamics at the county level. [Courtesy Oak Ridge National Laboratory]

- Produced a platform with comprehensive data access and visualization capabilities to process near-real-time, multi-modal, and multi-source data to support informed decision-making and monitor potential recovery efforts.
- Collected and curated disease data, creating a unique national data resource to support epidemiological and pandemic modeling, including assessment of the impact of human dynamics on infection spread and location and the availability of critical infrastructure.
- Developed an approach to assess mobility behavior changes in response to COVID-19 using cellular phone- and vehicle-derived data to reveal travel patterns for commercial activity by type and across industries, including bars and restaurants, as well as passenger, fleet, and heavy-duty vehicles.
- Established a novel epidemiological modeling approach to quantify contact tracing, testing, and vaccination strategies in resource-constrained environments and to help identify optimal vaccination strategies for states and large metropolitan areas.

Viral Fate and Transport

- Provided critical information about how behavioral, environmental, and operational conditions affect the risk of airborne virus transmission indoors, such as in classrooms, offices, and conference rooms, to mitigate viral spread in enclosed spaces.
- Designed new antiviral materials that can adsorb SARS-CoV-2 virus and deactivate the pathogen.
- Produced and validated models for SARS-CoV-2 fate and transport in wastewater and groundwater arising from seepage of sewer water or septic tanks into groundwater and the associated transport through the subsurface and potential exposure routes and risks to the population.



Viral Fate and Transport. NVBL researchers used computational fluid dynamics simulations to examine airborne transport of the virus indoors. Shown here is a simulation of the airflow and distribution of expelled respiratory aerosols within a classroom or office configuration. [Courtesy Sandia National Laboratories]

Summary

DOE's NVBL has proven to be an exceptionally effective contributor to the nation's COVID response, quickly marshaling unique national laboratory expertise and capabilities to meet the most critical needs. For example, the NVBL supported manufacturers to address key shortages in medical supply chains, creating nearly 1,000 new medical manufacturing jobs. Working closely with other federal agencies and state and regional decision-makers, the NVBL provided solutions across a range of COVID challenges. These accomplishments demonstrate the game-changing resource represented by DOE's 17 national laboratories working together within the integrated NVBL framework. Going forward, the NVBL can bring these resources to bear on future national and international needs and emergencies.