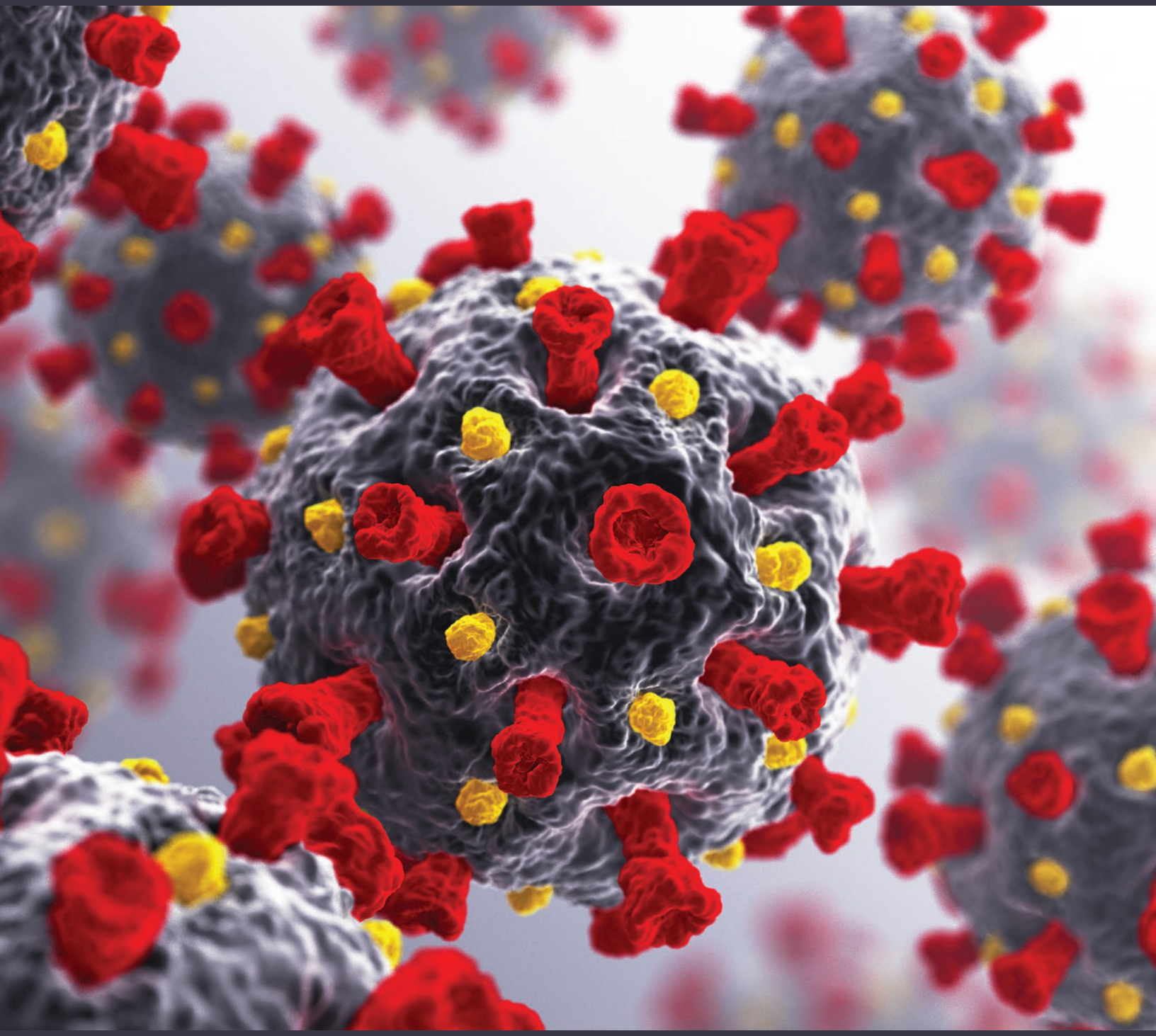
U.S. Department of Energy

National Virtual Biotechnology Laboratory

Report on Rapid R&D Solutions to the COVID-19 Crisis



U.S. DEPARTMENT OF ENERGY | Office of Science

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Report on Rapid R&D Solutions to the COVID-19 Crisis

DOE Office of Science

Executive Oversight: Harriet Kung, Harriet.Kung@science.doe.gov
Michelle Buchanan, Michelle Buchanan@science.doe.gov
Ashley Predith, Ashley.Predith@science.doe.gov

Co-Directors

Stephen Streiffer, Argonne National Laboratory
Marianne Walck, Idaho National Laboratory

Project Leads

Materials and Manufacturing of Critical Supplies: Lonnie Love, Oak Ridge National Laboratory
Molecular Design for COVID-19 Therapeutics: Martha Head, Oak Ridge National Laboratory
COVID-19 Testing: Patrick Fitch, Los Alamos National Laboratory
Epidemiological Modeling: Budhendra Bhaduri, Oak Ridge National Laboratory
Viral Fate and Transport: Katrina Waters, Pacific Northwest National Laboratory

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Correction: On page 3, Dr. Peter Tsai was mistakenly identified as the inventor of the N95 mask. In fact, Dr. Tsai was one of several inventors of different types of filter material used in N95 respirators.

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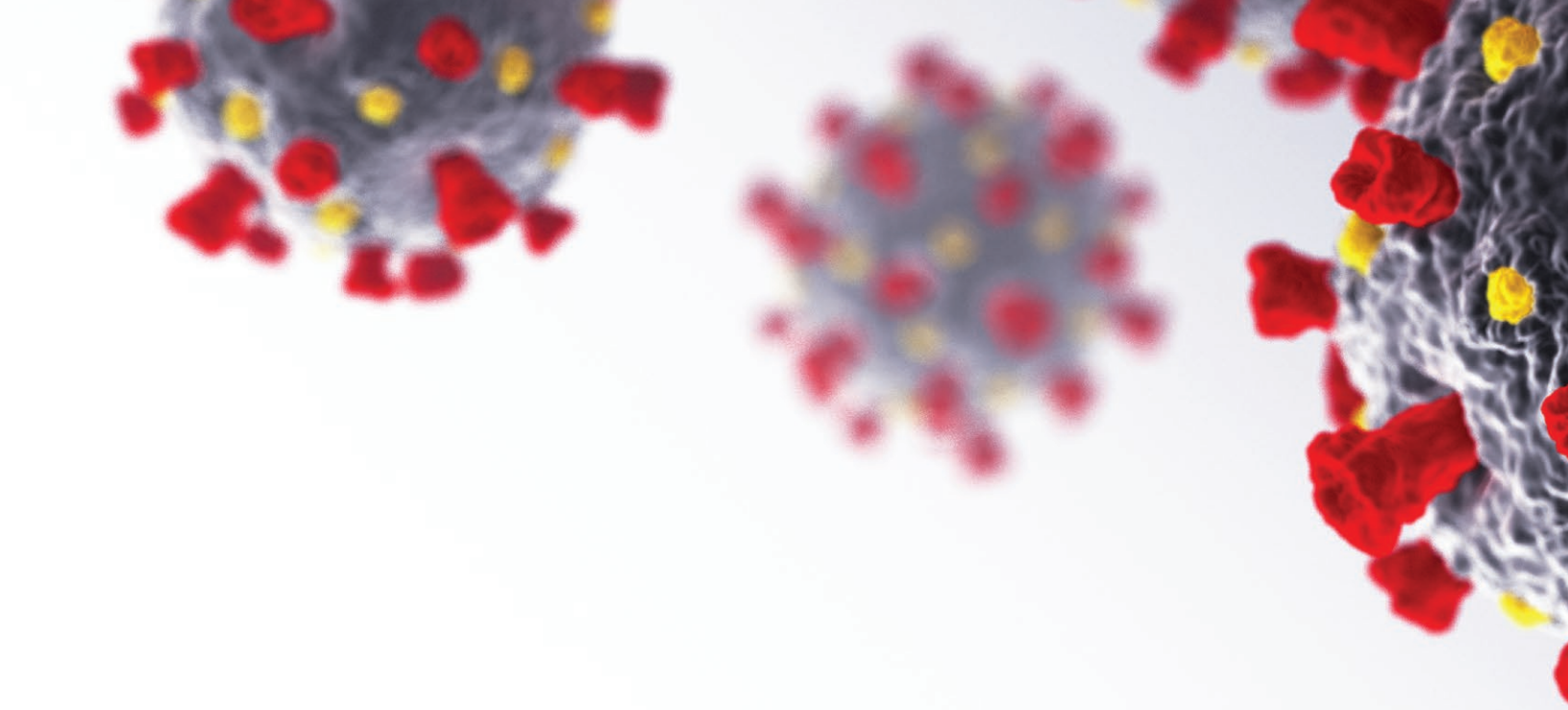

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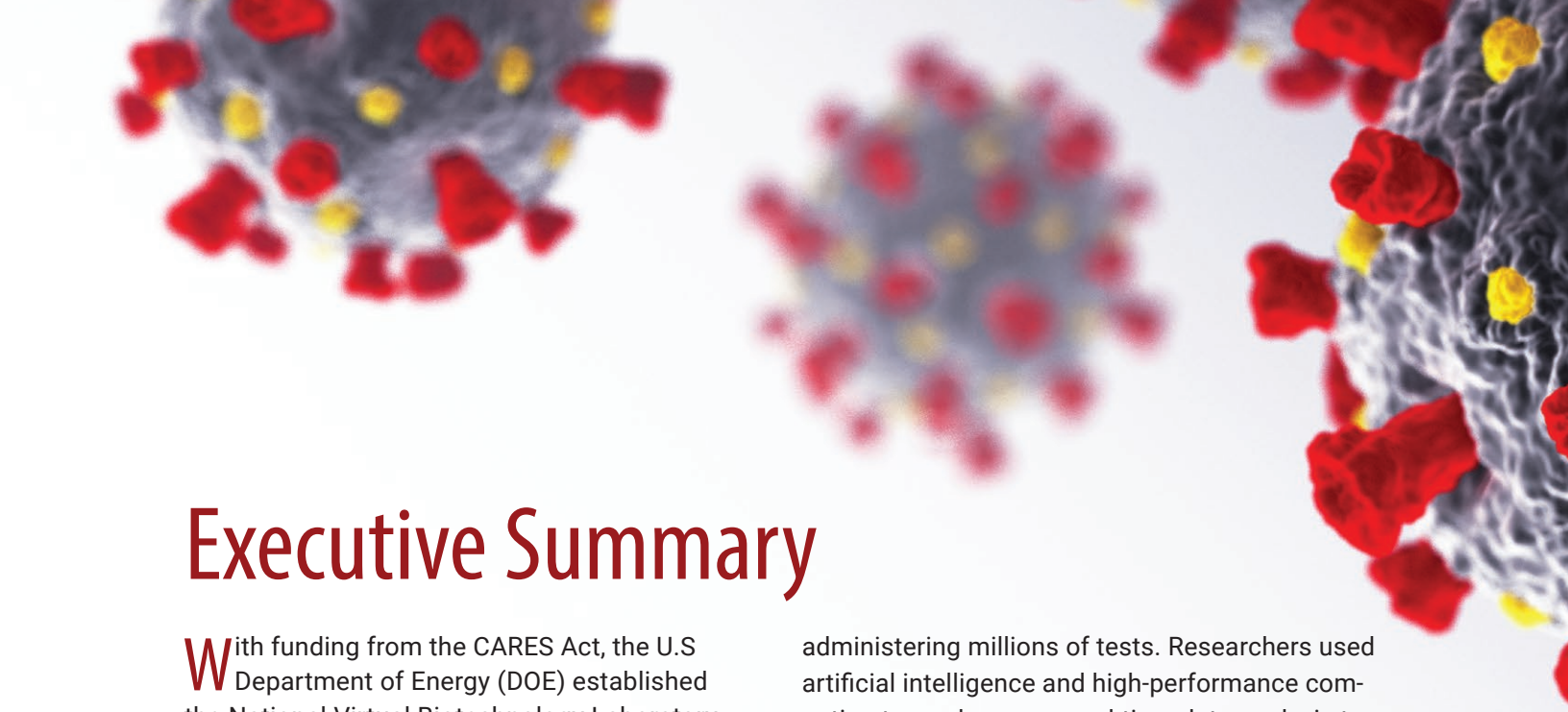


Executive Summary

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. NVBL brought together the broad scientific and technical expertise and resources of DOE's 17 national laboratories to help tackle medical supply shortages, discover potential drugs to fight the virus, develop and validate 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 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 U.S. 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 data analysis to forecast disease transmission, stress on public health infrastructure, and economic impact, which supported 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.

NVBL's accomplishments demonstrate not only the powerful resource represented by DOE's national laboratories working together to meet national needs, but also the effectiveness of the integrated NVBL framework for rapidly responding to emergencies with research and development (R&D) solutions. As the fight against COVID continues, sustained efforts are needed to confront this pandemic as well as future threats. Examples include:

- Establishing "supply chains on demand" to meet emergency production needs by leveraging the materials and manufacturing expertise of DOE national laboratories and developing advances in electronics, sensing, robotics, and automation capabilities.
- Improving the speed and robustness of drug discovery by integrating experimental platforms with DOE's computational and experimental user facilities, which provide unique resources to support the discovery of high-potential therapeutic agents.

- Protecting public, environmental, and animal health by developing new testing protocols and instrumentation adaptable to diverse sample types (both physiological and environmental) to quickly detect a wide range of pathogens and monitor other biorisks.
- Supporting near-real-time data needs of decision-makers at the local, regional, state, and national levels by advancing data curation, analysis, and modeling using artificial intelligence and new data science tools for managing and evaluating large diverse datasets.
- Harnessing DOE's expertise in environmental modeling to design rooms and air handling for offices, classrooms, restaurants, and other structures to minimize biorisk transmissions.

Going forward, NVBL is poised to apply the unique capabilities and expertise of the national laboratory complex to future national and international emergencies, both natural and engineered. Through this framework, the Office of Science will continue to be an integral component of agency-wide efforts to prepare for and respond to biorisks and other crises.

CHAPTER 1

NVBL Contributions to the COVID-19 Response: An Introduction

In March 2020, DOE quickly marshaled the unique expertise and resources of its national laboratories to provide R&D solutions to critical challenges posed by the global pandemic. With funding from the CARES Act, DOE established the National Virtual Biotechnology Laboratory, a consortium of 17 DOE national laboratories, each with core scientific and technical capabilities for confronting the COVID-19 crisis. These capabilities include world-leading user facilities, such as light and neutron sources, nanoscale science research centers, sequencing and biocharacterization facilities, and high-performance computing facilities, all broadly available to the research community.

As part of the NVBL framework, DOE rapidly assembled five project teams to (1) address supply chain bottlenecks by harnessing extensive additive manufacturing capabilities, (2) identify new targets for medical therapeutics, (3) develop innovations in testing capabilities, (4) provide epidemiological and logistical support, and (5) understand viral fate and transport in the environment. Each research team was charged with defining high-impact projects that could be completed in a 6-month sprint while coordinating their developments with academia, other government agencies, and the private sector.

Within months, NVBL teams produced innovations in materials and advanced manufacturing that mitigated shortages in test kits and 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. Teams of biochemistry experts developed new diagnostic targets and sample collection approaches while supporting national guidelines used in millions of tests. NVBL researchers used state-of-the-art methods in artificial intelligence (AI) and high-performance computing to produce near-real-time data analysis to forecast disease transmission, stress on public health infrastructure, and economic impact, supporting decision-makers at the local, state, and national levels. They 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 its national laboratories. NVBL serves as an outstanding model for developing and sustaining capabilities to prepare for and respond to future national needs or emergencies.

The chapters that follow outline key accomplishments of NVBL's five project teams—Materials and Manufacturing of Critical Supplies, Molecular Design for COVID-19 Therapeutics, COVID-19 Testing, Epidemiological Modeling, and Viral Fate and Transport—and identify critical R&D areas essential for future biorisk preparedness.

CHAPTER 2

Materials and Manufacturing of Critical Supplies

Objectives and Approach

From the outset of the COVID-19 pandemic, medical supply chain shortages became serious bottlenecks for frontline responders. To mitigate these shortages, 16 DOE national laboratories partnered to bring deep expertise in materials science, advanced manufacturing, and characterization capabilities to catalyze the manufacture and production scale-up of critical supplies. The NVBL Manufacturing team's efforts resulted in production of more than 10 million test kits per week (partnering with Coca-Cola and Thermo Fisher Scientific), over 3 million masks and N95 respirators per day (partnering with Cummins Filtration and DemeTech), and 250,000 nasal swabs per day by additive manufacturing. The team's accomplishments also led to the commercialization of a BioMedInnovations ventilator (which received FDA Emergency Use Authorization) and creation of two factories with over 1,000 new jobs.

To address specific supply chain bottlenecks, the Manufacturing team formed three subgroups: Personal Protection Equipment (e.g., N95 masks and face shields), Consumables (e.g., test tubes and swabs for test kits), and Ventilators. Each subgroup drew upon extensive expertise in materials science, materials characterization, manufacturing, and computation at the national laboratories to identify new approaches for producing and validating the performance of manufactured items. These activities heavily leveraged DOE user facilities, such as light and neutron sources, nanoscale science research centers, and high-performance computing facilities. In many cases, the subgroups found that the most critical component required for expanding manufacturing was the tooling required to establish a production line. With conventional tooling approaches, establishing production lines can take months. However, with advanced manufacturing methods, molds and other components

Fig. 1. New N95 respirator (left) produced at DemeTech factory (right). [Courtesy DemeTech]

can be produced in hours, enabling production lines to launch in a matter of weeks. In all cases, the subgroups established strategic industry partnerships for deploying developed capabilities.

Outcomes and Impact

Personal Protective Equipment

One of the first areas PPE researchers addressed was to relieve the critical shortages of N95 masks used by medical professionals. To help meet demand, the Carbon Fiber Technology Facility at Oak Ridge National Laboratory was converted to produce the filter media used in N95 masks. The PPE subgroup also teamed with Dr. Peter Tsai (University of Tennessee), inventor of a nonwoven filtration fabric used in N95 masks, to generate an open-source design for the charging system needed for N95 mass production. N95 filter media uses the charge placed on the fabric to capture small virus particles more effectively than the standard surgical mask. To assure their effectiveness, the produced materials were extensively tested at DOE's light sources and nanoscale science research centers.

Additionally, the subgroup partnered with Cummins Filtration (Nashville, Tenn.) to convert an oil filter production line to one for N95 filter media, enabling production of material for over 3 million masks per day. The subgroup also partnered with DemeTech (Miami Lakes, Fla.) to convert N95 material to medical masks and N95 respirators, which received certification from the National Institute of Occupational Safety and Health in September 2020 (see Fig. 1, this page). As a result, DemeTech established a new production facility that created 600 new manufacturing jobs, and the masks are commercially available.

The PPE subgroup also partnered with DeRoyal Industries (Powell, Tenn.) to develop new capabilities for high-throughput production of face shields. The partners used extensive capabilities in metal additive manufacturing to rapidly produce metal injection molds using 3D printing (see Fig. 2a, p. 4). These molds enabled production of 40,000 new face shields per day, per machine (see Fig. 2b and c, p. 4).

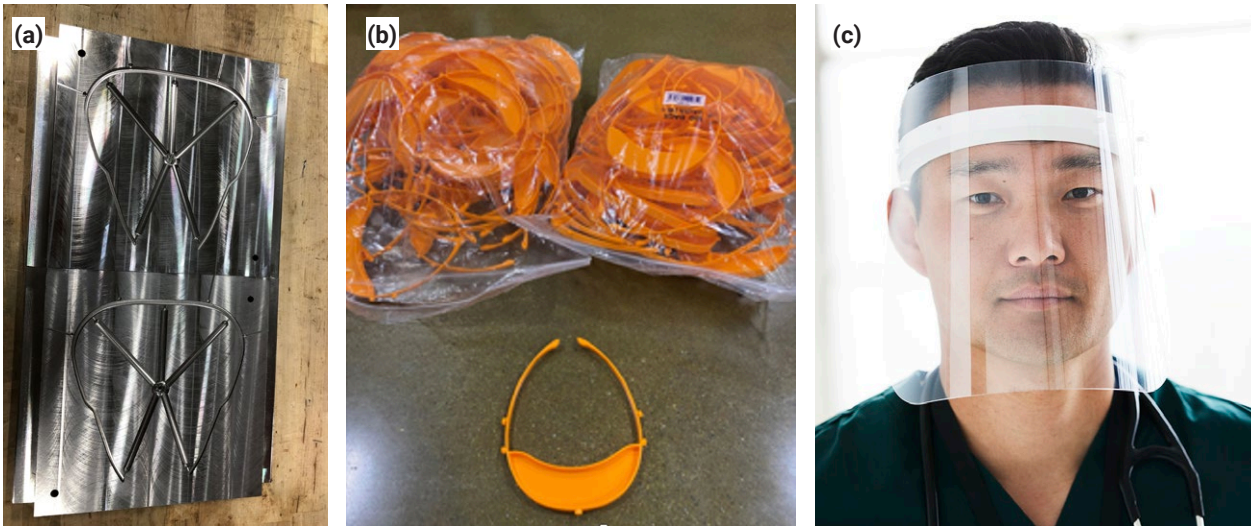


Fig. 2. The Manufacturing team partnered with DeRoyal Industries on **(a)** 3D-printed tooling for **(b)** injection molds used to produce **(c)** face shields. [Courtesy Oak Ridge National Laboratory (a, b) and Getty Images (c)]

Consumables for Test Kits

The Consumables subgroup partnered with the U.S. Department of Health and Human Services (HHS) to rapidly scale up production of consumables for test kits. These consumables included multi-well sample trays and nasal swabs (see Fig. 3, this page), along with sample collection tubes.

A critical shortage of test tubes used to collect nasal swabs emerged early in the pandemic. Working with The Coca-Cola Company, the Consumables subgroup identified bottle preforms (capped tubes that are blown with hot air into familiar drink bottles) as an excellent surrogate for these sample tubes. To evaluate the viability of using these preforms as collection tubes, the subgroup partnered with Coca-Cola (which produces 2 billion preforms per week), HHS, and five different testing companies. From this collaboration, Longhorn Therapeutics, a testing company based in Bethesda, Md., began taking delivery of 2 million preforms in April 2020.

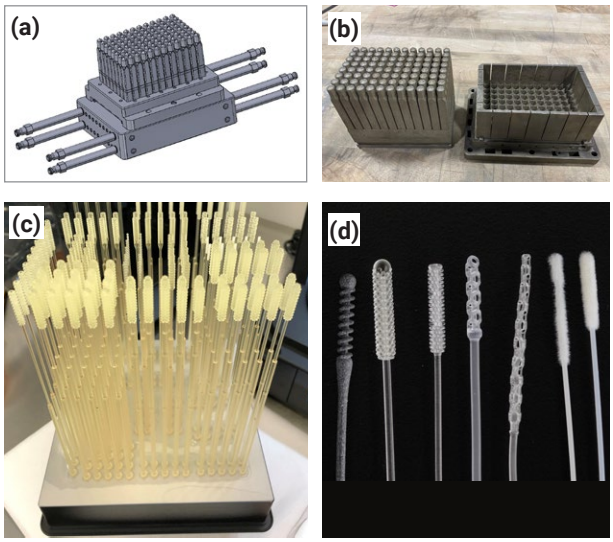


Fig. 3. Mold design for **(a)** 96-well sample plate. **(b)** 3D-printed mold used to form sample plates. **(c)** 3D-printed swabs and **(d)** closeup of a printed swab tip. [Courtesy Oak Ridge National Laboratory (a, b), and Lawrence Livermore National Laboratory (c, d)]

In parallel, the subgroup designed and rapidly prototyped a mechanism to 3D print the tooling needed to mass produce the original sample collection tube by injection mold processes, working with Thermo Fisher Scientific. In August 2020, Thermo Fisher opened a factory in Lenexa, Kan., creating more than 300 domestic medical manufacturing jobs (see Fig. 4, p. 5). In early 2021, this

Fig. 4. Thermo Fisher Scientific facility in Lenexa, Kan., that manufactures COVID-19 sample collection products. [Courtesy Thermo Fisher Scientific]

factory produced about 8 million test kits per week, with plans to scale to over 20 million per week.

Ventilators

During the early phases of the pandemic, national needs required the immediate production of an additional 400,000 to 600,000 ventilators. To meet this challenge, the Ventilator subgroup focused on materials and manufacturing processes that would assist industry in rapidly accelerating the manufacture of domestically producible FDA-approved ventilator technologies. The subgroup developed a new low-cost ventilator with BioMedInnovations, LLC (Denver, N.C.) that was commercialized and approved by the FDA. This ventilator required no existing ventilator supply chain components and thus circumvented anticipated shortages for traditional components (see Fig. 5, this page).

The subgroup also performed high-fidelity modeling of human lungs to better understand ventilator control and accelerate mucus removal from the lungs. Finally, collaborating with Percussionaire (Sandpoint, Idaho), the subgroup explored transformative ventilation methods and developed prototype systems for next-generation Intrapulmonary Percussive Ventilation. One of these prototype developments includes a variant that replaces air with an oxygenated liquid perfluorocarbon in a process that the collaboration named Intrapulmonary Percussive Liquid Ventilation.

Fig. 5. Production-level ventilator developed with BioMedInnovations, LLC. [Courtesy BioMedInnovations, LLC]

CHAPTER 3

Molecular Design for COVID-19 Therapeutics

Objectives and Approach

Since the pandemic's onset, only a few medicines have received U.S. FDA Emergency Use Authorization (EUA) for directly treating COVID-19. To accelerate discovery of potential treatments and identify small molecules and antibodies that interact with key viral targets, the Molecular Design team leveraged DOE national laboratory capabilities and analytical resources in high-performance computing, AI, structural biology, and chemistry. Even with the rapid discovery and development of several vaccines (which recently received FDA approval or EUA)[1], ongoing therapeutics development remains an important component of an integrated pandemic response as well as strategies to prepare for future viral challenges. To that end, the Molecular Design team continues to apply DOE capabilities to accelerate discovery of medical therapeutics targeting the virus responsible for the current pandemic—severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Their work has and continues to complement other public and private-sector activities.

The team has focused on identifying small molecules and antibodies that inhibit all parts of the viral life cycle. This work capitalized on an integrated computational and experimental platform established at the national laboratories and supported over time by DOE, the National Institutes of Health (NIH), DoD, Defense Advanced Research Projects Agency (DARPA), and other funding sources. The design platform's starting point includes structures of viral proteins, multiple antibody templates developed for earlier coronaviruses, and databases of chemical structures of small molecules for experimental confirmation. These inputs feed into a computational approach that combines

[1] DOE's light sources were accessed as part of the development process for all three COVID-19 vaccines authorized or approved for use in the United States: Pfizer-BioNTech, Moderna, and Johnson & Johnson's Janssen.

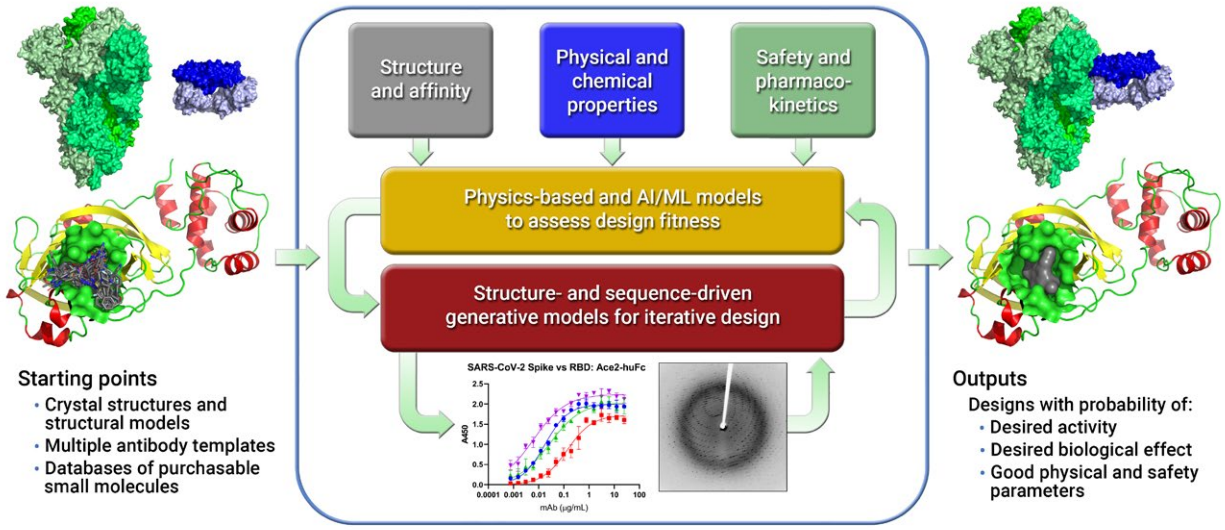


Fig. 6. Integrated computational and experimental platform for designing COVID-19 therapeutics. [Courtesy Oak Ridge National Laboratory]

simulation and AI methods, along with structure- and sequence-driven models, to iteratively design, make, and test new molecules. Data from experimental assays and structural characterization are then fed back into the computational methods for multiple design rounds. Platform outputs include identification of small molecules and antibodies with confirmed inhibition of a viral protein and predicted probability for good physical and safety parameters (see Fig. 6, this page). All project data will be made public, and team members are partnering with public and private organizations to further advance these discoveries along the pathway to clinical impact.

Outcomes and Impact

Antibody Discovery

The starting points for antibody design involved three antibodies known to bind to the spike protein of SARS-CoV-1 (the virus that caused the 2003 SARS outbreak) but *not* to the spike protein of SARS-CoV-2. The Molecular Design team's goal was to modify these existing antibody scaffolds to create new antibodies that effectively bind to and neutralize SARS-CoV-2. The team used AI methods to sample more than 10^{40} possible antibody variations, from which about 300 designed antibodies were generated and experimentally screened. Using this combined computational and experimental approach, the team identified experimentally confirmed hits for all three antibody scaffolds. All hits bind to the SARS-CoV-2 spike protein and block it from binding to the human ACE2 receptor. Additionally, some of these hits can block a pseudovirus (a harmless virus modified to include the SARS-CoV-2 spike on its surface) from entering human cells, demonstrating that these antibodies have the potential to block the first step in the infection process.

Inhibitors of Viral Cysteine Proteases

Two viral proteases, 3 chymotrypsin-like protease (3CLpro) and papain-like protease (PLpro), are essential for SARS-CoV-2 replication and thus are important targets for pharmaceutical drug design and discovery. Both belong to the cysteine protease family, a structural family not amenable to traditional docking-based modeling pipelines, which use computational approaches to characterize and

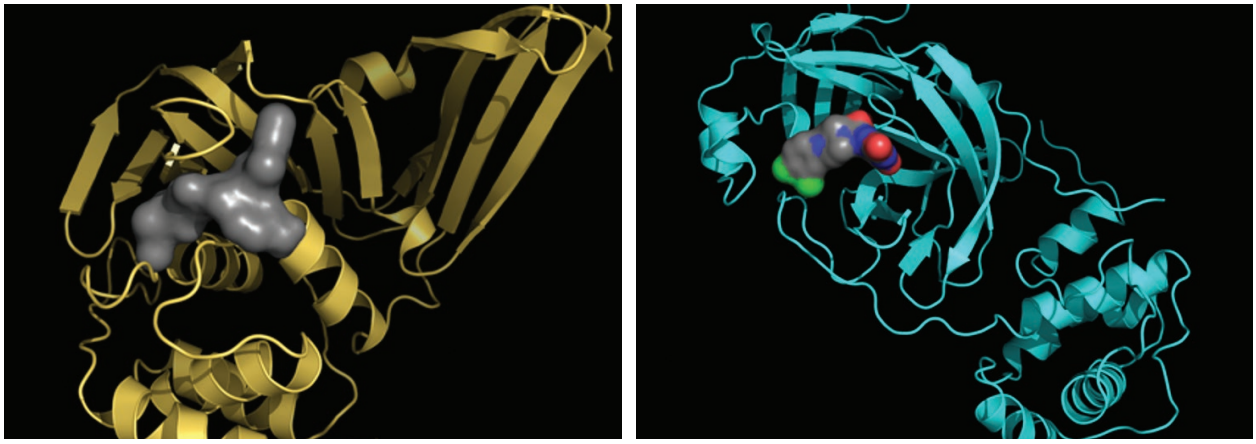


Fig. 7. The Molecular Design team identified two small-molecule inhibitors for the viral proteases PLpro and 3CLpro. Shown here are the PLpro inhibitor (gray, left) and 3CLpro inhibitor (multicolor, right). [Courtesy Oak Ridge National Laboratory]

predict the atomic-level interactions of small molecules in a target protein's binding site. To identify small molecules that can inhibit the activity of these proteases, the Molecular Design team therefore needed to create an integrated, multipronged, comprehensive workflow that combined docking, molecular dynamics, and quantum mechanical simulation approaches. They used this workflow to identify, design, and optimize small-molecule protease inhibitors for both 3CLpro and PLpro that have been experimentally confirmed (see Fig. 7, this page).

The identified PLpro inhibitor binds to the PLpro protein and then reacts to form a chemical bond with its cysteine residue, which is vital for enzyme activity. In addition to the experiments confirming that the designed molecule is a potent PLpro inhibitor, further experiments have characterized the chemical reaction with cysteine and used structural biology and X-ray crystallography to reveal atomic-level details of the interaction between PLpro and the inhibitor. Moreover, partners at the University of Tennessee Health Sciences Center Regional Biocontainment Laboratory have experimentally confirmed that the designed molecule inhibits viral infection in a cell-based assay.

The 3CLpro inhibitor, identified using computational docking studies, binds to the 3CLpro protein but does not form a chemical bond with its cysteine. An X-ray crystal structure revealed important atomic-level details of how the molecule interacts with the protein. Based on this structural information, the team used the computational workflow to design molecules with improved properties. A set of about 50 closely related molecules have been ordered for experimental testing, and the team is synthesizing and experimentally validating additional new molecules.

Computational Antiviral Screening

Using the power of DOE's Leadership Computing Facilities for computational docking calculations and AI methods, the Molecular Design team computationally screened tens of millions of small molecules against more than 100 binding sites of the SARS-CoV-2 viral proteins. They also docked larger databases (on the order of 50 to 100 million molecules) against a subset of these binding sites. From these computational screens, the team acquired more than 2,000 small molecules for experimental validation in an antiviral screen. Of these molecules, 56 show some inhibition of viral infection in a cell-based assay. The team is using an independent antiviral screen to confirm the 56 hits and conducting ongoing experiments to understand which parts of the viral life cycle each confirmed hit is inhibiting.

CHAPTER 4

COVID-19 Testing

Objectives and Approach

The beginning of the COVID-19 pandemic prompted numerous challenges to providing analytical tests for clinical and environmental virus detection and characterization. To address these challenges, NVBL formed the COVID-19 Testing team, composed of experts in genomics, biotechnology, biochemistry, nanoscience, and synthetic biology from 10 DOE national laboratories. The Testing team identified priority R&D gaps by gathering input from end-users and decision-makers and collecting first-hand experiences from several DOE national laboratories initiating in-house testing capabilities. Based on this information, the team developed an R&D roadmap to address the need to increase the availability of validated, effective, and reliable COVID-19 tests.

Key elements of the R&D roadmap were to reduce dependencies on reagents and materials for the limited approved tests by (1) identifying new diagnostic targets; (2) demonstrating new chemistries and instruments; (3) providing experimental data to support federal guideline decisions; and (4) experimentally validating new approaches for virus collection, storage, and detection. Drawing on team expertise and DOE resources, including the DOE Joint Genome Institute, the team worked to enable access to alternative testing methods and reagents to meet near-term needs while preparing for future outbreaks with new approaches and technologies. These approaches included using RNA sequence data to identify new strains and employing computer validation to rapidly evaluate diagnostic efficacy. Moreover, the team's efforts provided critical data that supported national guideline decisions used in administering millions of tests.

Outcomes and Impact

Identifying New Diagnostic Targets

The key to designing molecular detection assays for SARS-CoV-2 is identifying regions in its RNA genome that distinguish it from all other

Fig. 8. The nucleic acid testing process involves five phases, outlined above. [Courtesy Los Alamos National Laboratory]

viruses. The Testing team designed 78 DNA signatures from conserved regions of 41,540 SARS-CoV-2 genomes. These signatures are 60-mer in length with less than 20% probability of mapping to other viral genomes. They were incorporated into the Lawrence Livermore Microbial Detection Array (LLMDA) for detecting SARS-CoV-2 and other co-infecting pathogens and showed excellent sensitivity. The signatures can also be used in other multiplexed assays to rapidly detect SARS-CoV-2.

Using LLMDA, a technology that can detect more than 12,000 microbial species in a single test, the Testing team analyzed archived nasal pharyngeal, nose, and throat swabs to determine co-infections that could contribute to disease severity. Of all tested swabs, 91% of the COVID-19 positive samples were also positive for *Streptococcus pneumonia* compared to 18% of COVID-19 negative samples. *Streptococcus pyogenes* was detected in 82% of the COVID-19 positive samples and 25% of the COVID-19 negative samples. Additional studies are underway to correlate other COVID-19 co-infections.

The Testing team developed several analysis tools to maintain awareness of the evolution of the SARS-CoV-2 RNA genome as it relates to nucleic acid–based assays. For example, a platform for COVID-19 genome analytics (covid19.edgebioinformatics.org) offers an automatic *in silico*, or simulated, evaluation of diagnostic assays used around the world. In December 2020, this web application provided comparisons for 17 assays using 44,224 SARS-CoV-2 genomes.

Nucleic acids, such as RNA in SARS-CoV-2, are one target for diagnostic tests and are used in reverse transcription polymerase chain reaction (RT-PCR) tests. Virus proteins provide complementary targets for identification and can often be used in less expensive and simpler-to-use test formats, such as lateral flow assays. These strip tests, similar to home pregnancy test kits, require an antibody that recognizes a viral protein target. The Testing team developed an affinity reagent pipeline to screen libraries for highly specific antibodies that recognize key domains of the SARS-CoV-2 spike protein.

Providing Data Underpinning National Guidelines

In an effort launched by the Diagnostics sub-group of the White House Coronavirus Task Force, the Testing team collaborated with DoD, CDC, and FDA to provide experimental data in support of national guidelines throughout all phases of the nucleic acid testing process (see Fig. 8, this page). The team's contributions included:

- Identifying and characterizing potential contamination in commercial kits.
- Evaluating sample pooling approaches to assess those with the potential to reduce per-test costs by a factor of 10.

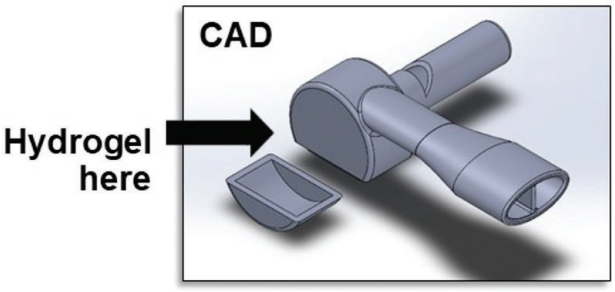


Fig. 9. The COVID Whistle Breath Collector traps breath in a removable hydrogel insert for ease of testing. [Courtesy Oak Ridge National Laboratory]

- Assessing multiple viral transport media and protocols to assure test accuracy, even after less-than-desirable shipping or storage.
- Evaluating virus inactivation and extraction for test efficacy and protection of frontline health care workers.

Using Novel Approaches for Virus Collection and Detection

To simplify breath collection and virus extraction, the Testing team developed a simple COVID Whistle Breath Collector with a hydrogel insert (see Fig. 9, this page). After breath is collected with the whistle, the hydrogel containing the sample can be removed for testing. The additively manufactured whistle can be readily modified to optimize collection parameters. In addition, a phone or web application can provide users with audio cues and help monitor patient variation. A university clinical partner is evaluating whistle prototypes.

Fig. 10. Reveal-CoV uses Reverse Transcription Loop-mediated isothermal AMPlification (RT-LAMP) to rapidly detect SARS-CoV-2. An initial inactivation step is performed at 95°C followed by amplification of the target sequence at 65°C and visual detection of color change. Total time from sample to answer is less than 1 hour. [Courtesy Lawrence Livermore National Laboratory]

The Testing team also developed the Reveal-CoV, a small, rapid nucleic acid test instrument for detecting SARS-CoV-2 (see Fig. 10, this page). The assay replaces the two step RT-PCR amplification process with a one-step amplification process called Reverse Transcription Loop-mediated isothermal AMPlification (RT-LAMP). This one-step process enables the Reveal-CoV test to provide more timely and sensitive nucleic acid detection: sample heat inactivation and lysis are performed in 5 minutes, followed by approximately 30 minutes to detect a red-to-yellow color change for a SARS-CoV-2 positive sample.

CHAPTER 5

Epidemiological Modeling

Objectives and Approach

To assist decision-makers in understanding COVID-19 spread and impact across the nation, NVBL's Epidemiological Modeling team brought together experts in spatial demography and human dynamics research; agent-based modeling systems; and transportation, infrastructure, economic, and risk modeling. Comprising researchers from six national laboratories, the team coupled its extensive expertise with DOE's powerful supercomputers and data capabilities. Building on prior work with CDC, NIH, DoD, and the Federal Emergency Management Agency (FEMA), they created a data platform that forecasts (1) disease transmission, (2) stress on public health infrastructure, and (3) U.S. economic outlook. The following accomplishments illustrate team-developed capabilities that provided unrivaled understanding of COVID-19 impacts.

- Officials in Chicago, New York City, Illinois, New Mexico, and Tennessee, among others, used the team's data and modeling efforts to illustrate county-level trends and forecasts, pinpoint locations (such as bars and restaurants) significant to transmissions, and identify the importance of contact tracing.
- The Chicago Transit Authority and New York Metropolitan Transit Authority used the team's transportation modeling to forecast ridership under various economic reopening scenarios.
- Decision-makers at DOE, the National Nuclear Security Administration, and FEMA used results from the team's data platform, and the team shared its findings from economic impact modeling with the U.S. Bureau of Economic Analysis.
- The CDC's modeling group used the team's ensemble dashboard to visualize output data from forecast models. In addition, the CDC

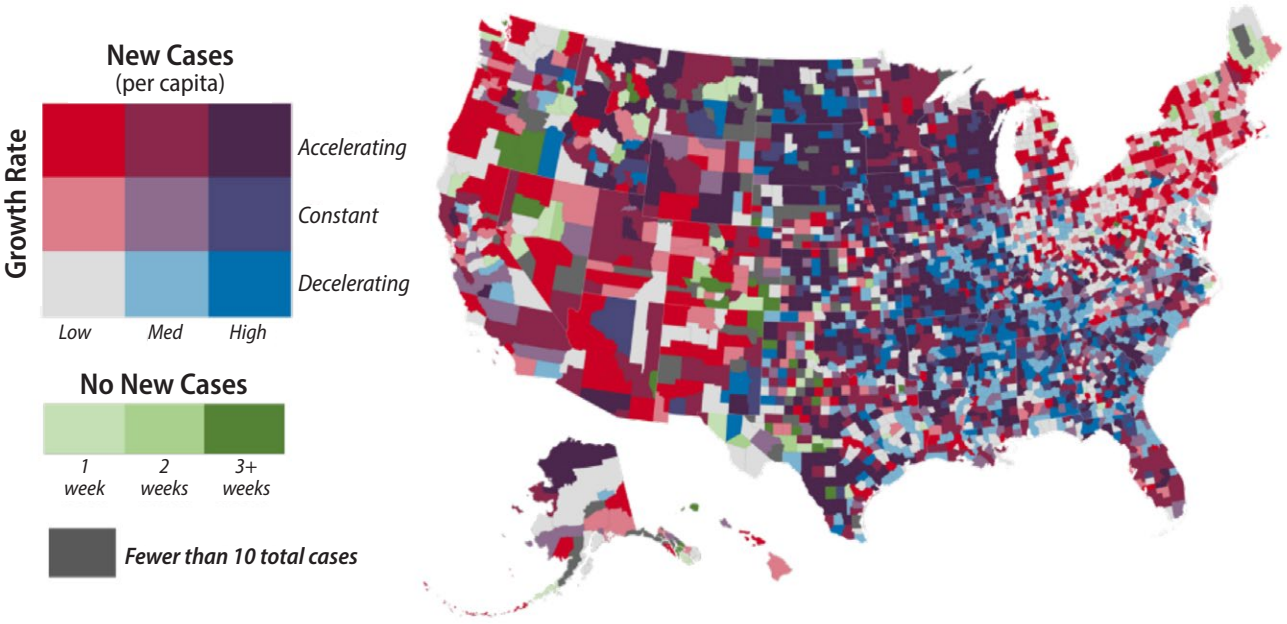


Fig. 11. Bivariate choropleth map showing the changes in COVID-19 velocity and acceleration rates at the U.S. county level from one week in September 2020 to the next (as opposed to total number of cases). [Courtesy Oak Ridge National Laboratory]

Minority and Rural Health groups benefitted from the team's efforts to (1) identify communities most vulnerable to K-12 school reopening disruptions (including specific geographic locations); (2) determine states with high vs. low COVID burden; and (3) compare urban vs. rural COVID mobility and burden.

Outcomes and Impact

Near-Real-Time Situational Awareness

One strategy for describing the state of a public health crisis involves using a pair of easily understood values to map the conditions in a more complex region, such as a state or country, based on collective measurements from its constituent regions (e.g., counties). Using this data science approach, the Epidemiological Modeling team developed a bivariate choropleth map to simultaneously show two variables—COVID-19 velocity and acceleration rates—at the U.S. county level.

For every county, the map's 2D color legend indicates the rate at which the number of new COVID-19 cases increases over a week (velocity) and how this rate changes over that same period (acceleration). This approach to mapping velocity and acceleration provided a unique perspective on transmission dynamics and daily criticality of the COVID-19 pandemic (see Fig. 11, this page).

National Data Resource for Pandemic Modeling

The unprecedented nature of the COVID-19 pandemic has highlighted the need for a data infrastructure that supports disease-tracing models with robust calibration and validation. To address this challenge, the team developed a data collection and curation platform to collect and curate disease data (600,000 data records per week for 12 weeks) on the many attributes influencing response outcomes. Compared to most public sites, the resulting NVBL platform includes far

more attributes and has created the foundation for a unique national data resource to support future epidemiological and pandemic modeling.

Predictive Models of COVID-19 Dynamics

For short-term forecasts, the team developed data-driven statistical models that predict new case counts at state, county, and metropolis scales, enabling short-term planning for contact tracing staff and testing capacity needs. For long-term forecasts, the team advanced existing epidemiological modeling capabilities with platforms known as EpiGrid, EpiCast, and CityCOVID.

EpiGrid is a model of disease progression that predicts geographic spread based on classifying populations as susceptible, exposed, infectious, or recovered. It produces results at 5-km resolution that cover the entire United States. EpiCast and CityCOVID are agent-based models that simulate the actions and interactions of autonomous characters, or "agents," following rule-based behaviors to assess their individual effects on the collective behavior of the entire system. EpiCast, originally designed to simulate community-level influenza transmission across the country, predicts COVID outcomes at the census-tract level. CityCOVID modeled hourly activities of ~3 million people across 1.2 million locations for the greater Chicago metropolitan area (see Fig. 12, this page).

Together these models perform scenario-based analysis and mitigation planning and provide local, regional, and state-level decision-makers with information on intervention effects before they are implemented. Such information includes (1) experiments to understand stay-at-home and reopening order effects and timing; (2) comparison of the impacts of bar and school reopenings on COVID spread; and (3) effects of increased holiday gatherings and interactions on COVID spread. Additionally, these models enable simulations of various vaccination protocols to forecast effects on COVID spread.

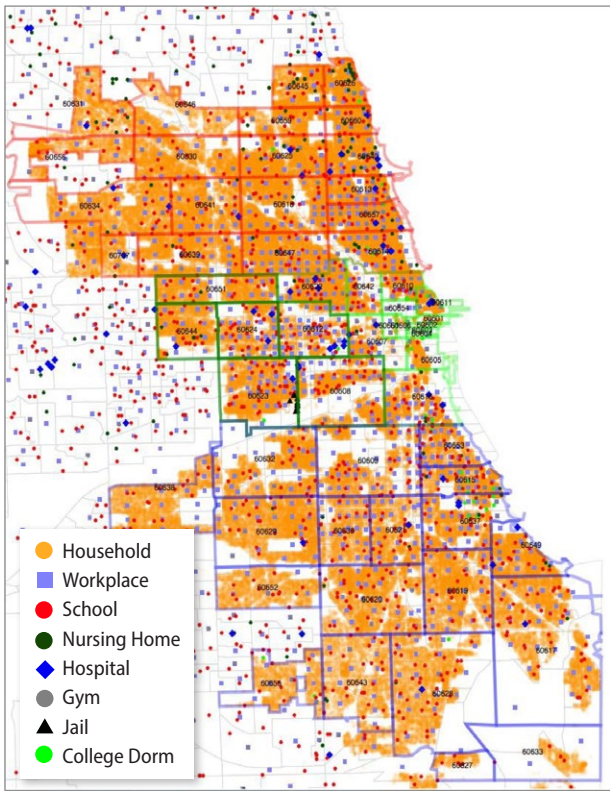


Fig. 12. The CityCOVID model simulates how the virus moves through populations. It generates mobility patterns based on the actions and interactions of individual people (agents). The above simulation forecasts hourly activities of 2.7 million people across 1.2 million locations in the greater Chicago metropolitan area. [Courtesy Argonne National Laboratory]

Resource, Economic, and Vaccination Modeling

Using output from epidemiological models, the team calculated demand for practitioner types as well as committed and consumable resources for each U.S. county in multiple scenarios. They also applied models to forecast COVID-19 economic impact under multiple scenarios for virus progression and to estimate the cumulative economic impacts of shutdowns and potential recovery strategies. In addition, the team developed a new epidemiological modeling approach to quantify contact tracing, testing, and vaccination strategies in resource-constrained environments and to help

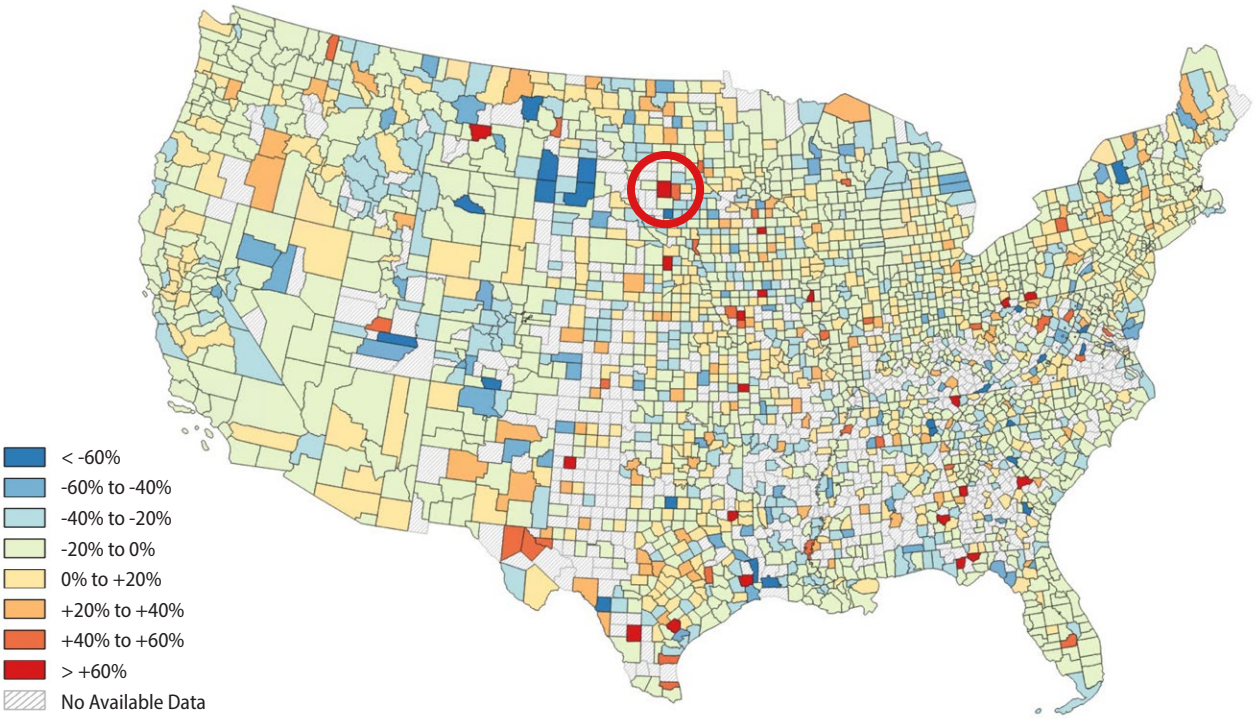


Fig. 13. Cellular phone–based movement data provided assessment of social gatherings and explained consequent changes in COVID cases. For example, this data helped explain and validate a sixfold increase in COVID cases in Sturgis, S.D. (inside the red circle) following an August 2020 motorcycle rally. [Courtesy Oak Ridge National Laboratory]

identify optimal vaccination strategies for states and large metropolitan areas.

Mobility Modeling

Team members developed approaches to assess mobility behavior changes, for personal and freight movements, in response to SARS-CoV-2 and variants across the United States. Analysis of commercial vehicle and cellular phone–derived mobility data revealed travel patterns for commercial activity by type and across industries, including bars and restaurants as well as passenger, fleet, and heavy-duty vehicles (see Fig. 13, this page). Three different agent-based transportation modeling and simulation systems—POLARIS, BEAM, and CommuterSim—provided scenario-based transportation analysis. Scenarios were developed and assessed for the greater Chicago and New York City areas, with emphasis on public transit impact. The models provided ridership forecasts for various degrees of economic reopening with aversion to shared mobility such as public transit.

COVID-19 Data and Visualization Platform

The Epidemiological Modeling team developed a comprehensive data access and visualization platform that can process multimodal and multisource data, enabling informed decision-making and monitoring of potential recovery efforts. In addition to showing current infection spread, the platform also captures the impact of human dynamics on disease spread and location and the availability of critical infrastructure. The platform can support epidemiological and pandemic modeling and simulations driven by high-performance computing, and it is extensible, allowing third-party integration and services to use the curated data and analytics in near-real time.

CHAPTER 6

Viral Fate and Transport

Objectives and Approach

SARS-CoV-2 is thought to be passed principally between people through inhalation of expelled droplets and aerosolized particles, but transmission through contact with contaminated surfaces remains a concern under certain circumstances. Data suggest aerosolized SARS-CoV-2 can persist in enclosed environments (especially in poorly ventilated spaces) for several hours, and the virus can persist on some surfaces for days. A lack of understanding of SARS-CoV-2 transport and fate and associated particles in the environment, including air, water, and surfaces, limits the ability to devise strategies to reduce virus uptake and prevent infection. Controlling community and workplace spread requires understanding the factors regulating SARS-CoV-2 viability, transmission, and transport as well as virus prevalence in the environment.

To better understand these factors, the Viral Fate and Transport team mobilized researchers across 11 DOE national laboratories and combined unique experimental facilities with physics-based, data-driven modeling and simulation to study SARS-CoV-2 transmission, transport, and fate. The resulting information has provided key insights required to understand factors involved in emergence, circulation, and resurgence of pathogenic microbes and to support pandemic response. The team focused on understanding and ultimately predicting SARS-CoV-2 viability in varied environments, with the goal of rapidly informing strategies that guide the nation's return to normal activities. Primary team objectives included (1) prioritizing administrative and engineering controls that reduce the risk of SARS-CoV-2 transmission within an enclosed environment, (2) identifying the chemical and physical properties that influence SARS-CoV-2 binding to common surfaces, and (3) understanding the contribution of environmental reservoirs and conditions to SARS-CoV-2 transmission and resurgence.

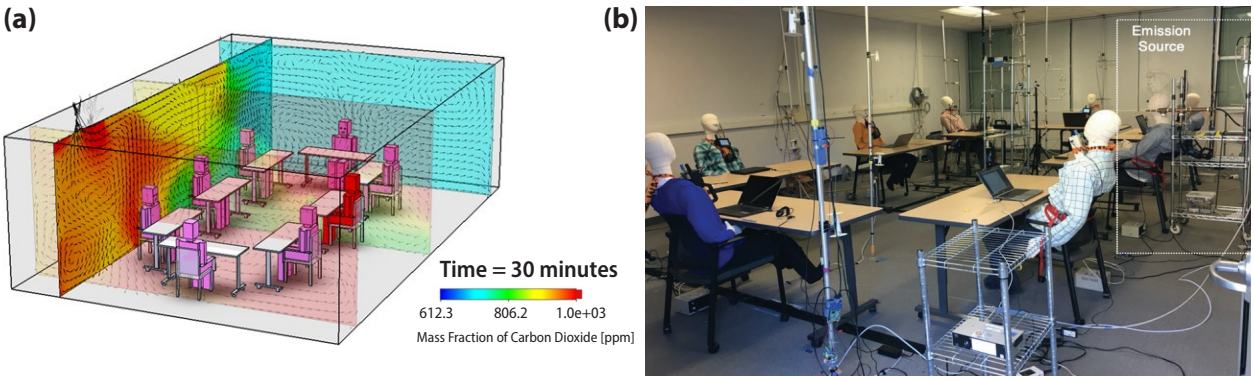


Fig. 14. (a) Computational fluid dynamic simulation of the airflow and distribution of expelled respiratory particles within a classroom or office configuration. **(b)** Experimental setup to measure particle distribution in a classroom or office configuration. [Courtesy Sandia National Laboratories (a) and Lawrence Berkeley National Laboratory (b)]

Outcomes and Impact

Airborne Viral Transport and Fate Indoors

Leveraging highly instrumented, configurable facilities and computational capabilities available at DOE national laboratories, the Viral Fate and Transport team uncovered robust and quantitative information about how behavioral, environmental, and operational conditions affect airborne transmission risk. For example, the team used computational fluid dynamic models to learn about airborne virus transport and how to reduce risk of indoor transmission in spaces like classrooms and conference rooms. Simulations are based on experimental results obtained using carbon dioxide gas and different particle sizes released in a manner mimicking respiratory gas and fluid emissions into the air (see Fig. 14, this page).

Surface Chemistry and Material Science Solutions

The Viral Fate and Transport team designed new antiviral materials with low potential toxicity to humans. One class of materials is based on composites of a transition metal oxide (component A) combined with a copper-based virucidal agent (component B) that can adsorb SARS-CoV-2, trapping it in a thin film on the material's surface and thereby deactivating it. When tested individually, the A and B components demonstrate little to no virucidal properties, but their combination, A x B, produces strong antiviral activity against SARS-CoV-2 (see Fig. 15, this page). This research examined binding of surrogate virus systems, as well as the SARS-CoV-2 spike protein, to nonbiological surfaces. Supporting this research, the team also conducted direct imaging of virus-surface interactions using a range of imaging techniques available at DOE scientific user facilities.

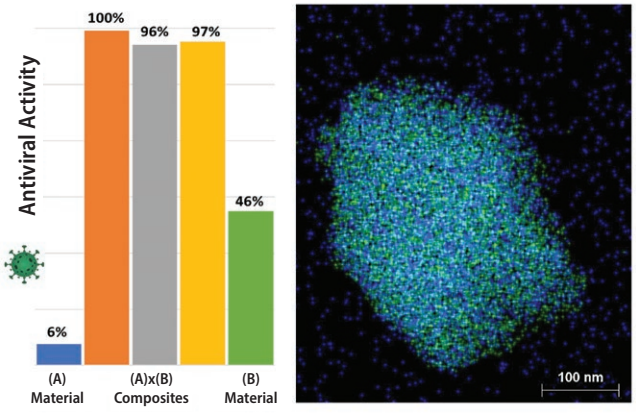
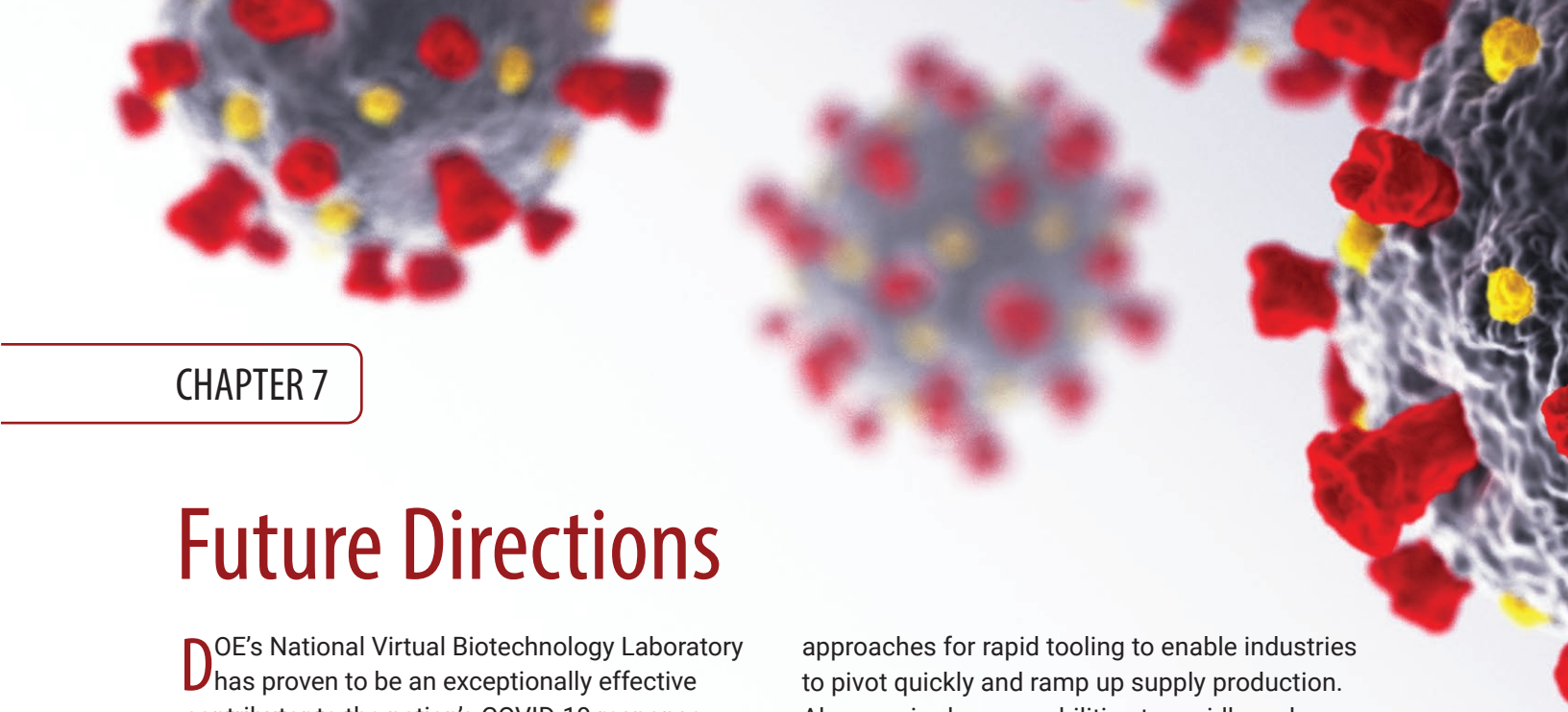


Fig. 15. Antiviral activities of studied material systems vs. pure constituents (A) and (B) are shown in the graph. The image at right, taken using energy-dispersive X-ray spectroscopy (STEM-EDS), illustrates distribution of the materials (A, green) and (B, blue) on the surface of the developed composite antiviral materials (A)x(B). [Courtesy Ames Laboratory and Iowa State University]

Viral Transport and Emergence from Environmental Reservoirs

The Viral Fate and Transport Team analyzed datasets to produce validated models for SARS-CoV-2 fate and transport in wastewater and groundwater. Scenarios of particular interest were sewer water or septic tank seepage into groundwater and associated subsurface transport, potential exposure routes, and risks to the population. The team also determined the effects of climate conditions on viral environmental transport and compared viral DNA sequences from wastewater and groundwater sites to analyze SARS-CoV-2 fate and infectivity associated with genomic change. The primary result from both groundwater and wastewater modeling is development of 1D and 3D models using literature data for other viruses. Important transport-related model parameters are advection, diffusion, colloid facilitated processes, adsorption/desorption, and inactivation. Scenarios run with these parameters show that in unconsolidated subsurface environments, 200 m from origin, viral concentrations are 10% of the concentration found at the source.



CHAPTER 7

Future Directions

DOE's National Virtual Biotechnology Laboratory has proven to be an exceptionally effective contributor to the nation's COVID-19 response. NVBL accomplishments demonstrate not only the game-changing resource represented by DOE's 17 national laboratories working together to meet national needs, but also the framework's effectiveness in rapidly responding to emergencies with R&D solutions. Because the COVID-19 fight is far from over, a continuing, sustained effort is needed to meet pandemic challenges, as well as future natural or manmade biorisks. The NVBL framework can effectively integrate the project areas described in this document, as well as define new projects to support scalable biosurveillance and prediction capabilities. The following sections outline major R&D areas essential to preparing for future national threats and challenges.

Materials and Manufacturing of Critical Supplies

DOE's extensive expertise and capabilities in materials and manufacturing are critical to the discovery of new materials important in fighting infectious agents. New fabric that combines improved filtering and antimicrobial or antiviral agents is necessary for reducing the volume of face masks or other essential PPE. Moreover, new materials are needed to improve the ability to sterilize and reuse consumables. The supply chain shortages experienced early in the COVID-19 pandemic revealed the need for advanced manufacturing approaches for rapid tooling to enable industries to pivot quickly and ramp up supply production. Also required are capabilities to rapidly and resiliently establish supply chains to meet emergency needs (i.e., "supply chains on demand"). The COVID crisis also demonstrated major bottlenecks in assembly processes. Although parts could be mass produced during the pandemic, assembly lagged, illustrating the need for new electronics, sensing, robotics, and automation capabilities to facilitate rapid assembly.

Molecular Design for Medical Therapeutics

NVBL made major advances in not only understanding the structure and function of biological threats, but also in supporting the development of molecular therapeutics for COVID-19 and other biorisks. Underpinning these achievements are the unparalleled capabilities of DOE's high-performance Leadership Computing Facilities, combined with structural biology studies at its light, neutron, and nanoscale science research center user facilities. However, the job is not finished. New computational approaches are needed to improve the rapid screening of millions of test molecules against virus and bacterial targets to quickly converge on high-potential therapeutic agents. Integrating these computational tools with experimental platforms available at DOE user facilities would vastly improve the robustness of effective drug selection.

Pathogen Testing

Future protection of public, environmental, and animal health through rapid detection and monitoring of viral and bacterial agents requires fast, patient-friendly, and cost-effective testing protocols along with new types of instrumentation. Such testing approaches are needed to address the evolution of the SARS-CoV-2 virus (or other viruses or bacteria) and provide early warning of future pandemics. These new tests should be adaptable to a range of sample types—both physiological (nasal, saliva, blood, urine, and feces) and environmental (air, surfaces, and wastewater or groundwater). Advanced testing approaches that use multiple pathogen and host-response signatures to detect a wide array of pathogens are needed to, for example, understand the role of co-infections in patient outcomes.

Epidemiological Modeling

The COVID-19 pandemic underscored the challenge of managing huge amounts of data to support decisions at the local, regional, state, and national levels. Advances are needed to integrate data from new physiological and environmental tests with myriad other types of monitored data. Also, a new framework is needed for data curation, analysis, and modeling that will respond to the near-real-time requirements of decision-makers during public health emergencies. Such a framework could foster epidemic surveillance through development of a critically needed national public health data and reporting standard. Further, new data science and advanced AI approaches to biosurveillance and data fusion are needed to evaluate diverse mobility and demographic datasets. These approaches could be used to generate not only "early warning" alerts, but also impactful model-derived assessments of outbreak potential. DOE's scalable data and high-performance computing capabilities would enable the synthesis of dynamic, accurate, and multimodal operations frameworks to parameterize epidemiological models on human mobility and interactions. Such an approach would (1) greatly improve both the accuracy and granularity of predictive epidemiological models; (2) reduce uncertainties associated with prior approaches to contact network simulation; and (3) establish a modeling approach to rapidly quantify contact tracing, testing, and vaccination strategies in resource-constrained environments. These frameworks would also serve as essential tools to help identify optimal vaccination strategies for states and large metropolitan areas.

Viral Fate and Transport

Designing engineered solutions that mitigate disease spread requires enhanced understanding of how infecting agents are transported in the environment, both indoors and outdoors in air and water sources. DOE's expertise in building technologies and computational modeling can provide the knowledge needed to effectively design rooms and air handling for offices, classrooms, restaurants, and other structures to minimize biohazard transmission. In addition, DOE's vast experience in understanding contaminant transport in the environment can reveal how viruses and bacteria are spread in these settings.

Conclusion

Through the integrated NVBL framework, DOE has demonstrated the power of bringing together the unique expertise and capabilities of its national laboratories to meet the challenges of an international pandemic. Since March 2020, NVBL advancements in manufacturing, therapeutics, testing, modeling, and viral fate and transport have illuminated the importance of essential, effective R&D in bioemergency preparedness and response. Going forward, NVBL can serve as a critical component of DOE's integrated response to future biorisks and other emergencies, both natural and engineered.

Appendix A

Publications and Research Output

The following list represents publications as of December 2021 and does not include manuscripts in preparation or review.

Chapter 2: Materials and Manufacturing of Critical Supplies

Publications

DeAngelis, H. E.; Grillet, A. M.; Nemer, M. B.; Wasiolek, M. A.; Hanson, D. J.; Omana, M. A.; Sanchez, A. L.; Vehar, D. W.; Thelen, P. M. Gamma Radiation Sterilization of N95 Respirators Leads to Decreased Respirator Performance. *PLoS One* **2021**, *16* (4), e0248859. DOI: 10.1371/journal.pone.0248859

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Patents

Zhang, Y.; Powers, D. J.; Pupek, K. Z.; Hryn, J. N.; Krumdick, G. K.; Chaudhuri, S. Nanofiber Filter Medium for Reusable Facemask and Filtering Facepiece Respirator. ANL IN-20-055.

Chapter 3: Molecular Design for COVID-19 Therapeutics

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Chapter 4: COVID-19 Testing

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Patents and Invention Disclosures

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Joint invention disclosure submitted for COVID Whistle.

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Appendix B

Research Team

Materials and Manufacturing of Critical Supplies

Samantha Adikari
Los Alamos National Laboratory

Daniel Akerib
SLAC National Accelerator Laboratory

Andrew Ames
SLAC National Accelerator Laboratory

Marie Arrowsmith
Sandia National Laboratories

Shaine Athey
Lawrence Livermore National Laboratory

Celeste Atkins
Oak Ridge National Laboratory

William Bachman
Sandia National Laboratories

Teresa Barnes
National Renewable Energy Laboratory

Abby Barnes
Oak Ridge National Laboratory

Todd Barrick
Sandia National Laboratories

Katherine Barrick
Sandia National Laboratories

Andy Beasley
Idaho National Laboratory

Clint Bedick
National Energy Technology Laboratory

Bryan Bellaire
Ames Laboratory

Donald Benza
Savannah River National Laboratory

John Bernardin
Los Alamos National Laboratory

Emma Betters
Oak Ridge National Laboratory

Randy Bewley
Idaho National Laboratory

Beth Boardman
Los Alamos National Laboratory

John Bobbitt
Savannah River National Laboratory

David Bock
Brookhaven National Laboratory

Yannick Bomble
National Renewable Energy Laboratory

Martin Breidenback
SLAC National Accelerator Laboratory

Michael Bressack
SLAC National Accelerator Laboratory

Pieter Breur
SLAC National Accelerator Laboratory

Kevin Byerly
National Energy Technology Laboratory

Rafael Campos
SLAC National Accelerator Laboratory

James Carney
Sandia National Laboratories

Alberta Carpenter
National Renewable Energy Laboratory

Eric Charles
SLAC National Accelerator Laboratory

Santanu Chaudhuri
Argonne National Laboratory

Victor Chavez
Sandia National Laboratories

Phillip Chesser
Oak Ridge National Laboratory

Wah Chiu
SLAC National Accelerator Laboratory

Josef Christ
Pacific Northwest National Laboratory

Steven Chu
SLAC National Accelerator Laboratory

Peter Ciesielski
National Renewable Energy Laboratory

Kyle Cluff
Los Alamos National Laboratory

Bruce Cohen
Lawrence Berkeley National Laboratory

Adam Cook
Sandia National Laboratories

Cody Corbin
Sandia National Laboratories

Andres Cortez
Los Alamos National Laboratory

Corson Cramer
Oak Ridge National Laboratory

Jun Cui
Ames Laboratory

Yi Cui
SLAC National Accelerator Laboratory

Jeremy Danielson
Los Alamos National Laboratory

Nitin Daphalapurkar
Los Alamos National Laboratory

Panos Datskos
National Renewable Energy Laboratory

Jack Dean
Lawrence Livermore National Laboratory

Vincent DeAndrade
Argonne National Laboratory

Haedi Deangelis
Sandia National Laboratories

Ryan Dehoff
Oak Ridge National Laboratory

Patrick Dempsey
Lawrence Livermore National Laboratory

Alexander Dudchenko
SLAC National Accelerator Laboratory

Eric Duoss
Lawrence Livermore National Laboratory

Steve Eglash
SLAC National Accelerator Laboratory

Jeffrey Elam
Argonne National Laboratory

Amy Elliott
Oak Ridge National Laboratory

Ken Enstrom
Lawrence Livermore National Laboratory

Rebecca Erikson
Pacific Northwest National Laboratory

Tom Feldhausen
Oak Ridge National Laboratory

Michelle Fenn
Pacific Northwest National Laboratory

Don Ferguson
National Energy Technology Laboratory

Patrick Finnegan
Sandia National Laboratories

Matthew Folsom
Savannah River National Laboratory

Dennis Freeman
Lawrence Livermore National Laboratory

William Fuger
Idaho National Laboratory

Nathan Fuller
Sandia National Laboratories

Jon Fulton
National Energy Technology Laboratory

David Gaga
SLAC National Accelerator Laboratory

Kumkum Ganguly
Los Alamos National Laboratory

Randall Gentry
National Energy Technology Laboratory

Kevin Gervais
Pacific Northwest National Laboratory

Jeremy Gleick
Lawrence Livermore National Laboratory

Andrew Glen
Sandia National Laboratories

John Greenhall
Los Alamos National Laboratory

Lisa Gribble
Sandia National Laboratories

Anne Grillet
Sandia National Laboratories

Lorenzo Gutierrez
Sandia National Laboratories

Steven Guzorek
Lawrence Livermore National Laboratory

Ryan Haggerty
Sandia National Laboratories

Michael Ham
Los Alamos National Laboratory

Razi Haque
Lawrence Livermore National Laboratory

Jennifer Harris
Los Alamos National Laboratory

Marcus Hays
Argonne National Laboratory

Ryan Herbst
SLAC National Accelerator Laboratory

Chris Hershey
Oak Ridge National Laboratory

Michael Himmel
National Renewable Energy Laboratory

Andrew Honeycutt
Oak Ridge National Laboratory

Nick Horvath
Oak Ridge National Laboratory

Peter Hosemann
Lawrence Berkeley National Laboratory

Peter Hsieh
National Energy Technology Laboratory

Christina Ignarra
SLAC National Accelerator Laboratory

Ralph James
Savannah River National Laboratory

Todd Jankowski
Los Alamos National Laboratory

Dale Jenne
National Renewable Energy Laboratory

Jing Jin
SLAC National Accelerator Laboratory

Joel Johnson
Idaho National Laboratory

Robert Johnston
Sandia National Laboratories

Mike Kirka
Oak Ridge National Laboratory

Matthew Koetting
Kansas City National Security Campus

Jeffrey Koplow
Sandia National Laboratories

Jack Kotovsky
Lawrence Livermore National Laboratory

Gary Krugger
Los Alamos National Laboratory

Gregory Krumdick
Argonne National Laboratory

Wendy Kuhne
Savannah River National Laboratory

Ian Ladner
Lawrence Livermore National Laboratory

Justin Lajoie
Ames Laboratory

Candace Langan
Savannah River National Laboratory

Greg Larsen
Oak Ridge National Laboratory

Matthew Lee
Los Alamos National Laboratory

Thomas Lewis
Idaho National Laboratory

John Lindahl
Oak Ridge National Laboratory

Peter Lloyd
Oak Ridge National Laboratory

Thomas Lograsso
Ames Laboratory

Lonnie Love
Oak Ridge National Laboratory

Steffen Luitz
SLAC National Accelerator Laboratory

Leah Lujan
Los Alamos National Laboratory

Therese Lujan
Los Alamos National Laboratory

Monear Makvandi
Sandia National Laboratories

Dan Manha
Lawrence Livermore National Laboratory

Ruben Manzanares
Los Alamos National Laboratory

Alex Marchi
Los Alamos National Laboratory

Amy Marschilok
Brookhaven National Laboratory

Adam Martinez
Los Alamos National Laboratory

Mathew Mate
SLAC National Accelerator Laboratory

Chris Matranga
National Energy Technology Laboratory

Michael Maxwell
Savannah River National Laboratory

Sean McGaughey
Pacific Northwest National Laboratory

Eric Miller
SLAC National Accelerator Laboratory

Doug Modlin
Lawrence Livermore National Laboratory

Marwan Mohamed
Los Alamos National Laboratory

Arvind Mohan
Los Alamos National Laboratory

Brian Mong
SLAC National Accelerator Laboratory

Patrick Moo
Idaho National Laboratory

Murray Moore
Los Alamos National Laboratory

Robert Morgan
Los Alamos National Laboratory

Monica Moya
Lawrence Livermore National Laboratory

Elvin Munoz
Pacific Northwest National Laboratory

Du Nguyen
Lawrence Livermore National Laboratory

Greg Norton
Lawrence Livermore National Laboratory

David Nuttall
Oak Ridge National Laboratory

Andrzej Nycz
Oak Ridge National Laboratory

Austin Nye
Lawrence Livermore National Laboratory

Robert O'Brien
Idaho National Laboratory

Michael Omana
Sandia National Laboratories

Scott Paap
Sandia National Laboratories

Cristian Pantea
Los Alamos National Laboratory

Parans Paranthaman
Oak Ridge National Laboratory

Phil Paul
Lawrence Livermore National Laboratory

Jeremy Payton
Los Alamos National Laboratory

Martin Perraglio
Los Alamos National Laboratory

Matt Pharr
Lawrence Livermore National Laboratory

Brian Post
Oak Ridge National Laboratory

Krzysztof Pupek
Argonne National Laboratory

Samantha Reese
National Renewable Energy Laboratory

Steve Richardson
National Energy Technology Laboratory

Bryce Ricken
Sandia National Laboratories

Jacob Riglin
Los Alamos National Laboratory

Jason Roadman
National Renewable Energy Laboratory

Larry Rodriguez
Los Alamos National Laboratory

Mohammad Roni
Idaho National Laboratory

Alex Roschli
Oak Ridge National Laboratory

Alexander Rose
Los Alamos National Laboratory

Michael Sabo
Sandia National Laboratories

Bradley Salzbrenner
Sandia National Laboratories

Andres Sanchez
Sandia National Laboratories

Daniel Schabacker
Argonne National Laboratory

Andrew Schmalzer
Los Alamos National Laboratory

Patrick Scholl
Lawrence Livermore National Laboratory

Eric Shaner
Sandia National Laboratories

Maxim Shusteff
Lawrence Livermore National Laboratory

Randall Schunk
Sandia National Laboratories

Tom Shutt
SLAC National Accelerator Laboratory

Graham Simmons
SLAC National Accelerator Laboratory

Michael Sinclair
Sandia National Laboratories

Julie Slaughter
Ames Laboratory

Denver Smith
Los Alamos National Laboratory

Scott Smith
Oak Ridge National Laboratory

Brittnee Smith
Pacific Northwest National Laboratory

David Soscia
Lawrence Livermore National Laboratory

Christopher Spadaccini
Lawrence Livermore National Laboratory

Dusan Spernjak
Los Alamos National Laboratory

Aaron Sperry
Lawrence Livermore National Laboratory

Mike Steinzig
Los Alamos National Laboratory

Christopher Takacs
SLAC National Accelerator Laboratory

Deepti Tanjore
Lawrence Berkeley National Laboratory

Bryce Tappan
Los Alamos National Laboratory

Antionette Taylor
Los Alamos National Laboratory

Paul Thelen
Sandia National Laboratories

Merlin Theodore
Oak Ridge National Laboratory

Angela Tooker
Lawrence Livermore National Laboratory

Katherine Tremba
Sandia National Laboratories

Michael Triplett
Lawrence Livermore National Laboratory

Jacob Trueblood
Lawrence Livermore National Laboratory

Charles Turick
Savannah River National Laboratory

Jeffrey Urban
Lawrence Berkeley National Laboratory

Victor Vargas
Lawrence Livermore National Laboratory

Vanessa Vargas
Sandia National Laboratories

Joshua Vaughan
Oak Ridge National Laboratory

Eliel Villa-Aleman
Savannah River National Laboratory

Lei Wang
Brookhaven National Laboratory

Peter Wang
Oak Ridge National Laboratory

Scott Weaver
SLAC National Accelerator Laboratory

Nina Weisse-Bernstein
Los Alamos National Laboratory

Dora Wiemann
Sandia National Laboratories

Brian Wihl
Lawrence Livermore National Laboratory

Zachary Wilson
Sandia National Laboratories

Edward Winrow
Sandia National Laboratories

Matthias Wittgen
SLAC National Accelerator Laboratory

Shan Yan
Brookhaven National Laboratory

Allison Yorita
Lawrence Livermore National Laboratory

Qinghui Yuan
Argonne National Laboratory

Yuepeng Zhang
Argonne National Laboratory

Molecular Design for COVID-19 Therapeutics

Paul Adams
Lawrence Berkeley National Laboratory

Nanda Aduri
SLAC National Accelerator Laboratory

Chase Akins
Argonne National Laboratory

Jonathan Allen
Lawrence Livermore National Laboratory

Marc Alvarez
Los Alamos National Laboratory

Lindsey Anderson
Pacific Northwest National Laboratory

Babak Andi
Brookhaven National Laboratory

Gyorgy Babnigg
Argonne National Laboratory

Yadu Babuji
Argonne National Laboratory

Alexander Batyuk
SLAC National Accelerator Laboratory

Kellon Belfon
Stony Brook University

Debsindhu Bhowmik
Oak Ridge National Laboratory

Benjamin Blaiszik
Argonne National Laboratory

Swen Boehm
Oak Ridge National Laboratory

Peter Bonnesen
Oak Ridge National Laboratory

Jim Brase
Lawrence Livermore National Laboratory

Tom Brettin
Argonne National Laboratory

James Brown
Lawrence Berkeley National Laboratory

Garry Buchko
Pacific Northwest National Laboratory

Seth Carbon
Lawrence Berkeley National Laboratory

Kyle Chard
University of Chicago

Ryan Chard
Argonne National Laboratory

Andrew Chen
Lawrence Berkeley National Laboratory

Julian Chen
Los Alamos National Laboratory

Samuel Chen
Brookhaven National Laboratory

Wah Chiu
SLAC National Accelerator Laboratory

Nicholas Choma
Lawrence Berkeley National Laboratory

Austin Clyde
Argonne National Laboratory

Leighton Coates
Oak Ridge National Laboratory

Matthew (Matt) Coleman
Lawrence Livermore National Laboratory

Connor Cooper
Oak Ridge National Laboratory

Abbigayle (Abby) Cuomo
Stony Brook University

Andy DeGiovanni
Lawrence Berkeley National Laboratory

Thomas Desautels
Lawrence Livermore National Laboratory

Emily Dietrich
Argonne National Laboratory

Peng Ding
Argonne National Laboratory

Mitchel Doktycz
Oak Ridge National Laboratory

Xiaotian Duan
University of Chicago

Chris Ellis
Oak Ridge National Laboratory

Aidan Epstein
Lawrence Livermore National Laboratory

Daniel Faissol
Lawrence Livermore National Laboratory

Lucy Fallon
Stony Brook University

Yichong Fan
Oak Ridge National Laboratory

Song Feng
Pacific Northwest National Laboratory

William Fischer
Los Alamos National Laboratory

Nicholas (Nick) Fischer
Lawrence Livermore National Laboratory

Ian Foster
Argonne National Laboratory

Magdalena (Magda) Franco
Lawrence Livermore National Laboratory

Stephanie Galanie
Oak Ridge National Laboratory

Carlos Gamboa
Brookhaven National Laboratory

Umamaheswari Ganapathy
Brookhaven National Laboratory

Cornelius Gati
SLAC National Accelerator Laboratory

Sandrasegaram Gnanakaran
Los Alamos National Laboratory

Jose Guerra
Stony Brook University

Mikhail Hameedi
SLAC National Accelerator Laboratory

Brooke Harmon
Sandia National Laboratories

Nomi Harris
Lawrence Berkeley National Laboratory

Darin Hauner
Pacific Northwest National Laboratory

Stewart He
Lawrence Livermore National Laboratory

Martha (Marti) Head
Oak Ridge National Laboratory

Dean Hidas
Brookhaven National Laboratory

Elijah Hoffman
Lawrence Berkeley National Laboratory

Kunlun Hong
Oak Ridge National Laboratory

Zhi Hong
University of Chicago

Naoki Horikoshi
SLAC National Accelerator Laboratory

Kim Hoshin
Pacific Northwest National Laboratory

Mark Hunter
SLAC National Accelerator Laboratory

Stephan Irle
Oak Ridge National Laboratory

Srinivas Iyer
Los Alamos National Laboratory

Daniel Jacobson
Oak Ridge National Laboratory

Rhema James
Pacific Northwest National Laboratory

Songhao Jiang
Argonne National Laboratory

Marcin Joachimiak
Lawrence Berkeley National Laboratory

Jessica Johnson
Argonne National Laboratory

Rajendra Joshi
Pacific Northwest National Laboratory

Ai Kagawa
Brookhaven National Laboratory

Richard Keith
Lawrence Berkeley National Laboratory

Michael Kent
Sandia National Laboratories

Vilmos Kertesz
Oak Ridge National Laboratory

Kerstin Kleese van Dam
Brookhaven National Laboratory

Daniel Kneller
Oak Ridge National Laboratory

Bette Korber
Los Alamos National Laboratory

Andrii Kovalevskyi
Oak Ridge National Laboratory

Kristen (Kris) Kulp
Lawrence Livermore National Laboratory

Neeraj Kumar
Pacific Northwest National Laboratory

Audrey Labbé
Oak Ridge National Laboratory

Joshua Ladau
Lawrence Berkeley National Laboratory

Edmond Lau
Lawrence Livermore National Laboratory

Joseph Laureanti
Pacific Northwest National Laboratory

Wellington Leite
Oak Ridge National Laboratory

Zhouzhao Li
University of Chicago

Felice Lightstone
Lawrence Livermore National Laboratory

Xuefeng Liu
Argonne National Laboratory

Heng Ma
Argonne National Laboratory

Carla Mann
Argonne National Laboratory

Irimpan Mathews
SLAC National Accelerator Laboratory

Stefan Maxwell
Sandia National Laboratories

Sean McCorkle
Brookhaven National Laboratory

Jason McDermott
Pacific Northwest National Laboratory

Kevin McLoughlin
Lawrence Livermore National Laboratory

Sean McSweeney
Brookhaven National Laboratory

Ryszard Michalczyk
Los Alamos National Laboratory

Chris Mungall
Lawrence Berkeley National Laboratory

Daniel Murphy-Olson
Argonne National Laboratory

Oscar Negrete
Sandia National Laboratories

Peter Nugent
Lawrence Berkeley National Laboratory

Carlos Olivares-Reboredo
University of Chicago

Hugh O'Neill
Oak Ridge National Laboratory

Swati Pant
Oak Ridge National Laboratory

Jerry Parks
Oak Ridge National Laboratory

Alexander Partin
Argonne National Laboratory

Jose Pereira
Lawrence Berkeley National Laboratory

Gwndalyn Phillips
Oak Ridge National Laboratory

Sai Venkatesh Pingali
Oak Ridge National Laboratory

Martin Purschke
Brookhaven National Laboratory

Emily Purvine
Pacific Northwest National Laboratory

Shuo Qian
Oak Ridge National Laboratory

Xiaohui Qu
Brookhaven National Laboratory

Lauren Raguette
Stony Brook University

Maksim Rakitin
Brookhaven National Laboratory

Arvind Ramanathan
Argonne National Laboratory

Simone Raugei
Pacific Northwest National Laboratory

Justin Reese
Lawrence Berkeley National Laboratory

Yihui Ren
Brookhaven National Laboratory

Andria Rodrigues
Lawrence Berkeley National Laboratory

Nickolaus Saint
Argonne National Laboratory

Kenneth Sale
Sandia National Laboratories

Brian Sanders
Oak Ridge National Laboratory

Anthony Savushkin
Argonne National Laboratory

Jurgen Schmidt
Los Alamos National Laboratory

Joe Schoeniger
Sandia National Laboratories

Ashka Sha
University of Chicago

Carlos Simmerling
Stony Brook University

Suhas Somnath
Oak Ridge National Laboratory

Chris Stanley
Oak Ridge National Laboratory

Darya (Dasha) Stepanenko
Stony Brook University

Rick Stevens
Argonne National Laboratory

Jacob Sumner
Oak Ridge National Laboratory

Li Tan
Brookhaven National Laboratory

Oleg Tchoubar
Brookhaven National Laboratory

Marisa Torres
Lawrence Livermore National Laboratory

Anda Trifan
Argonne National Laboratory

Deepak Unni
Lawrence Berkeley National Laboratory

Hubertus van Dam
Brookhaven National Laboratory

Van Vuong
Oak Ridge National Laboratory

Rick Wagner
University of California San Diego

Soichi Wakatsuki
SLAC National Accelerator Laboratory

Yuzhang Wang
Stony Brook University

Logan Ward
Argonne National Laboratory

Katrina Waters
Pacific Northwest National Laboratory

Amber Webb
Oak Ridge National Laboratory

Bobbie-Jo Webb-Robertson
Pacific Northwest National Laboratory

Kevin Weiss
Oak Ridge National Laboratory

Kelly Willams
Sandia National Laboratories

Sergio Wong
Lawrence Livermore National Laboratory

Yulun Wu
Lawrence Berkeley National Laboratory

Yue Yang
Lawrence Livermore National Laboratory

Hyunseung Yoo
Argonne National Laboratory

Qiu Zhang
Oak Ridge National Laboratory

Mowei Zhou
Pacific Northwest National Laboratory

Fangqiang Zhu
Lawrence Livermore National Laboratory

Ying Zhu
Pacific Northwest National Laboratory

COVID-19 Testing

Rebecca Abergel
Lawrence Berkeley National Laboratory

Paul Adams
Lawrence Berkeley National Laboratory

Dion Antonopoulos
Argonne National Laboratory

Gyorgy Babnigg
Argonne National Laboratory

Scott Baker
Pacific Northwest National Laboratory

Daniel Bedinger
Carterra

Monica Borucki
Lawrence Livermore National Laboratory

Steven B. Bradfute
University of New Mexico

Thomas Bunt
Lawrence Livermore National Laboratory

Chris Daum
Lawrence Livermore National Laboratory

Patrick Fitch
Los Alamos National Laboratory

Vince Gerbasi
Pacific Northwest National Laboratory

Paul Gilna
Oak Ridge National Laboratory

David Graham
Oak Ridge National Laboratory

Michael Guarnieri
National Renewable Energy Laboratory

Sally Hall
Lawrence Livermore National Laboratory

Nathan Hillson
Lawrence Berkeley National Laboratory

Elizabeth Hong-Geller
Los Alamos National Laboratory

Greg Hura
Lawrence Berkeley National Laboratory

Crystal Jaing
Lawrence Livermore National Laboratory

Ramesh Jha
Los Alamos National Laboratory

Andrzej Joachimiak
Argonne National Laboratory

Bishoy Kamel
Lawrence Berkeley National Laboratory

Jeff Kimbrel
Lawrence Livermore National Laboratory

Antonietta M. Lillo
Los Alamos National Laboratory

Betty Mangadu
Sandia National Laboratories

Robert Meagher
Sandia National Laboratories

Joseph Moon
Lawrence Livermore National Laboratory

Nigel Mouncey
Lawrence Berkeley National Laboratory/DOE Joint Genome Institute

Michael Morrison
Lawrence Livermore National Laboratory

Nisha Mulakken
Lawrence Livermore National Laboratory

Hau Nguyen
Los Alamos National Laboratory

Marit Nilsen-Hamilton
Ames Laboratory

Kristin Omberg
Pacific Northwest National Laboratory

Hugh O'Neal
Oak Ridge National Laboratory

Jerry Parks
Oak Ridge National Laboratory

Lili Pasa-Tolic
Pacific Northwest National Laboratory

Christa Pennacchio
Lawrence Berkeley National Laboratory

Dave Rakestraw
Lawrence Livermore National Laboratory

Scott Retterer
Oak Ridge National Laboratory

Marc Salit
SLAC National Accelerator Laboratory

Blake Simmons
Lawrence Berkeley National Laboratory

Anup Singh
Sandia National Laboratories, now Lawrence Livermore National Laboratory

Jess Sustarich
Sandia National Laboratories

James Thissen
Lawrence Livermore National Laboratory

Nileena Velappan
Los Alamos National Laboratory

Geoff Waldo
Los Alamos National Laboratory

Kelly Williams
Sandia National Laboratories

Jesse Wilson
Pacific Northwest National Laboratory

Chunyan Ye
University of New Mexico

Malin Young
Pacific Northwest National Laboratory

Yuko Yoshinaga
Lawrence Berkeley National Laboratory

Mowei Zhou
Pacific Northwest National Laboratory

Epidemiological Modeling

Erin Acquesta
Sandia National Laboratories

James Ahrens
Los Alamos National Laboratory

Joshua Auld
Argonne National Laboratory

Paula Austin
Sandia National Laboratories

Ryan Aydelott
Argonne National Laboratory

Andrew Bartlow
Los Alamos National Laboratory

Joshua Bergerson
Argonne National Laboratory

Anne Berres
Oak Ridge National Laboratory

Walter Beyeler
Sandia National Laboratories

Budhendra Bhaduri
Oak Ridge National Laboratory

Alec Biehl
Oak Ridge National Laboratory

Patrick Blonigan
Sandia National Laboratories

Brennan Borlaug
National Renewable Energy Laboratory

Christa Brelsford
Oak Ridge National Laboratory

Benjamin Brodsky
Sandia National Laboratories

Lauren Castro
Los Alamos National Laboratory

Youngsoo Chang
Argonne National Laboratory

Supriya Chinthavali
Oak Ridge National Laboratory

Blair Christian
Oak Ridge National Laboratory

Timothy Cleland
Los Alamos National Laboratory

Nicholson Collier
Argonne National Laboratory

Scott Collis
Sandia National Laboratories

Jessica Conrad
Los Alamos National Laboratory

Elton Cranfill
Oak Ridge National Laboratory

Leticia Cuellar-Hengartner
Los Alamos National Laboratory

Chad Davis
Sandia National Laboratories

Lori Dauelsberg
Los Alamos National Laboratory

Rich Davies
Oak Ridge National Laboratory

Haedi DeAngelis
Sandia National Laboratories

Sean DeRosa
Sandia National Laboratories

Sara Del Valle
Los Alamos National Laboratory

Bradley Dickerson
Sandia National Laboratories

Andrew Duvall
National Renewable Energy Laboratory

Samantha Erwin
Oak Ridge National Laboratory

Mary Ewers
Los Alamos National Laboratory

Jeanne Fair
Los Alamos National Laboratory

Geoffrey Fairchild
Los Alamos National Laboratory

John Farrell
National Renewable Energy Laboratory

Kyle Feffer
Argonne National Laboratory

Paul Fenimore
Los Alamos National Laboratory

Melissa Finley
Sandia National Laboratories

Patrick Finley
Sandia National Laboratories

Joseph Fish
National Renewable Energy Laboratory

Michael Ford
Sandia National Laboratories

Christopher Frazier
Sandia National Laboratories

Venu Garikapati
National Renewable Energy Laboratory

Jared Gearhart
Sandia National Laboratories

Timothy German
Los Alamos National Laboratory

Dax Gerts
Los Alamos National Laboratory

Phwey "Danny" Gil
Argonne National Laboratory

Morgan Gorris
Los Alamos National Laboratory

Josh Grant
Oak Ridge National Laboratory

Ann Hammer
Sandia National Laboratories

Desmond Harmon
Sandia National Laboratories

Nicolas Hengartner
Los Alamos National Laboratory

Michael Hilliard
Oak Ridge National Laboratory

William Hlavacek
Los Alamos National Laboratory

Rossitza Homan
Sandia National Laboratories

John Hummel
Argonne National Laboratory

Aundre Huynh
Sandia National Laboratories

Ho-Ling Hwang
Oak Ridge National Laboratory

Brian Ingram
Argonne National Laboratory

Dean Jones
Sandia National Laboratories

Jessica Jones
Sandia National Laboratories

Kyungsoo Jeong
National Renewable Energy Laboratory

Chaitanya Kaligotla
Argonne National Laboratory

Jason Kaufman
Oak Ridge National Laboratory

Thomas Kirchstetter
Lawrence Berkeley National Laboratory

Katherine Klise
Sandia National Laboratories

Daniel Krofcheck
Sandia National Laboratories

Haitam Laarabi
Lawrence Berkeley National Laboratory

Diane Lauderdale
Argonne National Laboratory

Rene Leclaire
Los Alamos National Laboratory

David LePoire
Argonne National Laboratory

Drew Levin
Sandia National Laboratories

Lawrence Paul Lewis
Argonne National Laboratory

Yen Ting Lin
Los Alamos National Laboratory

Charles Macal
Argonne National Laboratory

Margaret MacDonell
Sandia National Laboratories

Monear Makvandi
Sandia National Laboratories

Carrie Manore
Los Alamos National Laboratory

Carianne Martinez
Sandia National Laboratories

Ignacio Martinez-Moyano
Argonne National Laboratory

Taylor McKenzie
Sandia National Laboratories

Benjamin McMahon
Los Alamos National Laboratory

Isaac Michaud
Los Alamos National Laboratory

Mike Mills
Lawrence Berkeley National Laboratory

Jacob Miner
Los Alamos National Laboratory

Jessica Moehl
Oak Ridge National Laboratory

Matthew Moniot
National Renewable Energy Laboratory

Judith Mourant
Los Alamos National Laboratory

Aaron Myers
Oak Ridge National Laboratory

Zach Needell
Lawrence Berkeley National Laboratory

David Osthus
Los Alamos National Laboratory

Jonathan Ozik
Argonne National Laboratory

Byung Park
Oak Ridge National Laboratory

Nidhi Parkh
Los Alamos National Laboratory

Alina Peluso
Oak Ridge National Laboratory

Jordan Perr-Sauer
National Renewable Energy Laboratory

Sinem Perk
Argonne National Laboratory

Frederic Petit
Argonne National Laboratory

Jesse Piburn
Oak Ridge National Laboratory

Teresa Portone
Sandia National Laboratories

Julia Potter
Sandia National Laboratories

Rosalyn Rael
Los Alamos National Laboratory

Phillip Rauscher
Argonne National Laboratory

Srinath Ravulaparthy
Lawrence Berkeley National Laboratory

Jaideep Ray
Sandia National Laboratories

Nicholas Reinicke
National Renewable Energy Laboratory

Sara Rimer
Argonne National Laboratory

Mark "Danny" Rintoul
Sandia National Laboratories

Amy Rose
Oak Ridge National Laboratory

William Rosenberger
Los Alamos National Laboratory

Aymeric Rousseau
Argonne National Laboratory

Angelika Saeger
Los Alamos National Laboratory

Cosmin Safta
Sandia National Laboratories

Erik Schmidt
Oak Ridge National Laboratory

Scott Schlueter
Argonne National Laboratory

Courtney Shelley
Los Alamos National Laboratory

Anup Singh
Sandia National Laboratories

Nagendra Singh
Oak Ridge National Laboratory

Braeton Smith
Argonne National Laboratory

Asael Sorensen
Sandia National Laboratories

Alex Sorokine
Oak Ridge National Laboratory

Tina Sowers
Oak Ridge National Laboratory

Kevin Sparks
Oak Ridge National Laboratory

Pamela Spetz
Argonne National Laboratory

Anna Spurlock
Lawrence Berkeley National Laboratory

Abby Stevens
Argonne National Laboratory

Robert Stewart
Oak Ridge National Laboratory

Bingrong Sun
National Renewable Energy Laboratory

Laura Swiler
Sandia National Laboratories

Varisara Tansakul
Oak Ridge National Laboratory

Robert Taylor
Sandia National Laboratories

Kirsten Taylor-McCabe
Los Alamos National Laboratory

Gautam Thakur
Oak Ridge National Laboratory

Katherine Tremba
Sandia National Laboratories

Lawrence Trost
Sandia National Laboratories

Majbah Uddin
Oak Ridge National Laboratory

Vanessa Vargas
Sandia National Laboratories

Omer Verbas
Argonne National Laboratory

Sarah Voter
Los Alamos National Laboratory

Amanda Wagner
Argonne National Laboratory

Laurie Wallis
Sandia National Laboratories

Cheng Wang
Argonne National Laboratory

Ross Wang
Oak Ridge National Laboratory

Rashid Waraich
Lawrence Berkeley National Laboratory

Chrysm Watson
Los Alamos National Laboratory

Eric Webber
Oak Ridge National Laboratory

Tom Wenzel
Lawrence Berkeley National Laboratory

Celine West
Sandia National Laboratories

Matthew Whitehead
Oak Ridge National Laboratory

Kristen Wilding
Los Alamos National Laboratory

Alana Wilson
National Renewable Energy Laboratory

Murray Wolinsky
Los Alamos National Laboratory

Justin Wozniak
Argonne National Laboratory

Fei Xie
Oak Ridge National Laboratory

Haowen Xu
Oak Ridge National Laboratory

Stanley Young
National Renewable Energy Laboratory

Zijia Zhong
National Renewable Energy Laboratory

Viral Fate and Transport

Jesse Ahlquist
Lawrence Livermore National Laboratory

Allison Aiken
Los Alamos National Laboratory

Kevin Anderson
Pacific Northwest National Laboratory

Ramesh Balakrishnan
Argonne National Laboratory

Viktor Balema
Ames Laboratory

Bryan Bellaire
Iowa State University

Robin Brigmon
Savannah River National Laboratory

Michael J. Brown
Los Alamos National Laboratory

Carolyn Burns
Pacific Northwest National Laboratory

Jules Cacho
Argonne National Laboratory

Jack Cahill
Oak Ridge National Laboratory

Andrew Costinett
Pacific Northwest National Laboratory

Richard Daniel
Pacific Northwest National Laboratory

William Delp
Lawrence Berkeley National Laboratory

Armand Dichosa
Los Alamos National Laboratory

Michael Dillon
Lawrence Livermore National Laboratory

Liz Dobitz
SLAC National Accelerator Laboratory

Stefan Paul Domino
Sandia National Laboratories

Mavendra Dubey
Los Alamos National Laboratory

Som Dutta
Utah State University

Anne Marie Erler
Lawrence Livermore National Laboratory

Yan Feng
Argonne National Laboratory

Laura Fierce
Brookhaven National Laboratory, now Pacific Northwest National Laboratory

Paul Fischer
University of Illinois at Urbana-Champaign

Julia Flaherty
Pacific Northwest National Laboratory

Erika Fong
Lawrence Livermore National Laboratory

Laura Forde
Lawrence Livermore National Laboratory

Matthias Frank
Lawrence Livermore National Laboratory

Brian Fricke
Oak Ridge National Laboratory

Brad Fritz
Pacific Northwest National Laboratory

Jamie George
Pacific Northwest National Laboratory

Andrew Glen
Sandia National Laboratories

Kyle Gorkowski
Los Alamos National Laboratory

Larry Hamm
Savannah River National Laboratory

Ihor Hlova
Ames Laboratory

Clifford Ho
Sandia National Laboratories

Dan James
Pacific Northwest National Laboratory

Staci Kane
Lawrence Livermore National Laboratory

Thomas Kirchstetter
Lawrence Berkeley National Laboratory

Rao Kotamarthi
Argonne National Laboratory

Gourihar Kulkarni
Pacific Northwest National Laboratory

Brady Lee
Savannah River National Laboratory

Patricia Lee
Savannah River National Laboratory

Robert Lutes
Pacific Northwest National Laboratory

Naila Mahdi
Argonne National Laboratory

Simo Makiharju
University of California, Berkeley

Bob McGraw
Brookhaven National Laboratory

Richard Mills
Argonne National Laboratory

Kashif Nawaz
Oak Ridge National Laboratory

Oscar Negrete
Sandia National Laboratories

Cristina Negri
Argonne National Laboratory

Ralph Nichols
Savannah River National Laboratory

Aleks Obabko
Argonne National Laboratory

Brian O'Callahan
Pacific Northwest National Laboratory

Ronald Ott
Oak Ridge National Laboratory

Aaron Packman
Northwestern University

Jovan Pantelic
University of California, Berkeley

Ali Passian
Oak Ridge National Laboratory

Leonard Pease
Pacific Northwest National Laboratory

Kruttika-Suhas Phadke
Iowa State University

Chelsea Preble
University of California, Berkeley

Tanya Prozorov
Ames Laboratory

Odeta Qafoku
Pacific Northwest National Laboratory

John Quinn
Argonne National Laboratory

Edwin Saavedra
Northwestern University

Anne Sakdinawat
SLAC National Accelerator Laboratory

Timothy Salsbury
Pacific Northwest National Laboratory

Andres Lorenzo Sanchez
Sandia National Laboratories

Callen Schwefler
Lawrence Livermore National Laboratory

Brett Singer
Lawrence Berkeley National Laboratory

Rajesh Singh
Pacific Northwest National Laboratory

Michael Sohn
Lawrence Berkeley National Laboratory

Eric Thacher
University of California, Berkeley

Bill Thompson
SLAC National Accelerator Laboratory

Ronald Underhill
Pacific Northwest National Laboratory

Evan Variano
University of California, Berkeley

Brian Viner
Savannah River National Laboratory

Alex Vlachokostas
Pacific Northwest National Laboratory

Nora Wang
Pacific Northwest National Laboratory, now American Council for an Energy-Efficient Economy

Katrina Waters
Pacific Northwest National Laboratory

David Werth
Savannah River National Laboratory

Elizabeth Wheeler
Lawrence Livermore National Laboratory

Annmarie Wood-Zika
Lawrence Livermore National Laboratory

Eugene Yan
Argonne National Laboratory

Haoran Zhao
Lawrence Berkeley National Laboratory

Appendix C

Acronyms and Abbreviations

1D, 2D, 3D	one-, two-, three-dimensional
3CLpro	3 chymotrypsin-like protease
ACE2	angiotensin-converting enzyme 2
AI	artificial intelligence
CARES Act	Coronavirus Aid, Relief, and Economic Security Act
CDC	Centers for Disease Control and Prevention
COVID-19	Coronavirus disease 2019
DARPA	Defense Advanced Research Projects Agency
DoD	U.S. Department of Defense
DOE	U.S. Department of Energy
EUA	Emergency Use Authorization
FDA	U.S. Food and Drug Administration
FEMA	Federal Emergency Management Agency
HHS	U.S. Department of Health and Human Services
LLMDA	Lawrence Livermore Microbial Detection Array
ML	machine learning
NIH	National Institutes of Health
NVBL	National Virtual Biotechnology Laboratory
PLpro	papain-like protease
PPE	personal protective equipment
QC	quality control
R&D	research and development
RT-LAMP	Reverse Transcription Loop-mediated isothermal AMPlification
RT-PCR	reverse transcription polymerase chain reaction
SARS-CoV-2	severe acute respiratory syndrome coronavirus 2
STEM-EDS	scanning transmission electron microscopy–energy-dispersive X-ray spectroscopy