Supercomputer Thwarts Flu

Detecting weak areas in our vaccine distribution infrastructure

Quick read
The Lab's rock-solid model improves national emergency response, protecting our homeland from rapidly spreading pathogens.

Using supercomputers to respond to a potential national health emergency, scientists have developed a simulation that makes stark predictions about an avian influenza pandemic. This model helps providers stockpile vaccines appropriately and prepare emergency response—vital actions for containing a rapidly spreading pathogen or bio threat.
The large-scale, stochastic simulation model examines the nationwide spread of a pandemic influenza virus strain, such as an evolved avian H5N1 virus, should it become transmissible human-to-human. The simulation rolls out a city- and census-tract-level picture of the spread of infection through a synthetic population of 281 million people over the course of 180 days and examines the impact of interventions, from antiviral therapy to school closures and travel restrictions, as the vaccine industry struggles to catch up with the evolving virus.
"Based on the present work, we believe that a large stockpile of avian influenza-based vaccine containing potential pandemic influenza antigens, coupled with the capacity to rapidly make a better-matched vaccine based on human strains, would be the best strategy to mitigate pandemic influenza," say the authors of a National Academy of Sciences publication, Timothy Germann, Kai Kadau, Ira Longini, and Catherine Macken.
"It's probably not going to be practical to contain a potential pandemic by merely trying to limit contact between people, but we find that these measures are useful in buying time to produce and distribute sufficient quantities of vaccine and antiviral drugs," said Germann of Los Alamos' Applied Physics Division.
"Based on our results, combinations of mitigation strategies, such as stockpiling vaccines or antiviral agents, along with social distancing measures could be particularly effective in slowing pandemic flu spread in the U.S.," added the University of Washington's Longini.
The results show that advance preparation of a modestly effective vaccine in large quantities appears to be preferable to waiting for the development of a well-matched vaccine that may not become available until a pandemic has already reached the United States.
"Because it is currently impossible to predict which of the diverging strains of avian H5N1 influenza virus are most likely to adapt to human transmission, studies of broadly cross-reactive avian-influenza based vaccines with even modest immunogenicity in humans are important," said Macken, an influenza researcher in the Los Alamos Theoretical Division.
Ideally, both vaccine strategies would be done in parallel: stockpile a vaccine to use while the more effective one is being developed.

How it all Computes

The computer simulation models a synthetic population that matches U.S. census demographics and worker mobility data by randomly assigning the simulated individuals to households, workplaces, schools, and the like. Department of Transportation travel data is used to model long-distance trips during the course of the simulation, realistically capturing the spread of the pandemic virus by airplane and other passenger travel across the United States.
"In the highly mobile U.S. population, travel restrictions alone will not be enough to stop the

spread; a mixture of many mitigation strategies is more likely to be effective than a few strictly enforced ones," said Kadau, also of Los Alamos' Theoretical Division.
The model of disease transmission involves probabilities that any two people in a community will meet on any given day in any one of a number of settings, such as home or workplace. Thus, simulated disease transmission is more likely for two people in the same household and less likely for two people who have less in common. "So we are only computing the probability of any person becoming infected on any given day, and a roll of the dice is needed to decide whether they are infected or not," said Germann.
Other elements of randomness modify the simulated disease course. A significant fraction of infected people (33 percent in the present model) never develop clinical symptoms, although they are themselves infectious. In addition, the durations of the incubation and infectious periods can vary and are randomly chosen from distribution functions for each individual, involving more throws of the virtual dice.
"Computer models serve as virtual laboratories where researchers can study how infectious diseases might spread and what intervention strategies may lessen the impact of a real outbreak," said Jeremy M. Berg, director of the National Institute of General Medical Sciences. "This new work exemplifies the power of such models and could aid policymakers and health officials as they plan for a possible future pandemic."
The pandemic simulation model has been implemented in the Laboratory's celebrated scalable parallel short-range molecular dynamics (SPaSM) large-scale simulation platform developed for the nuclear weapons program. It runs on the Los Alamos supercomputer known as Pink, a 1,024-node (2,048 processor) LinuxBIOS/BProc "Science Appliance" running Clustermatic 3, the largest single-system image Linux cluster in the world.
The project's research team includes scientists from Los Alamos National Laboratory, the University of Washington, Emory University, and the Fred Hutchinson Cancer Research Center in Seattle.
Images and Quicktime video of the computer simulation are available at http://www.lanl.gov/news/images/avianflu.shtml online.

Blue: Few or none of the population is showing symptoms.

Green: 50 per 1,000 cases.

Red: 100 or more cases per 1,000 people.

Pushing Frontiers

In the second half of 2008, Los Alamos National Laboratory made significant advances in its primary mission: safeguarding the U.S. nuclear deterrent and pushing the frontiers of science on multiple fronts.
The national stockpile stewardship program achieved a major milestone in September with the production of the first life-extended W76-1 ballistic missile warhead for Trident submarines. The achievement culminated more than a decade of work by scientists and engineers at Los Alamos and across the nuclear weapons complex-including two crucial experiments conducted by the Laboratory's Hydrodynamic Experiments Division.
Another highlight: Roadrunner reached a new performance record of 1.105 petaflops, keeping it atop the list of the world's fastest supercomputers. Built by IBM for the Lab, Roadrunner was the first computer the crack the petaflop barrier: one thousand TRILLION operations per second. Initial applications will range widely: studying in great detail the evolution of HIV... exploring deeply the formation—as well as deformation—of metallic nanowires...and-toward producing biofuels more efficiently-unraveling the processes by which bacteria break down cellulose.
Safety and environmental stewardship were again a major theme for our work in the latter half of 2008. In November, the last group of unvented high-activity drums left Los Alamos for the Waste Isolation Pilot Plant near Carlsbad. That shipment fulfilled a commitment to the Defense Nuclear Facilities Safety Board to prioritize disposal of the highest-activity transuranic wastes stored at the Lab.
Los Alamos also strengthened security, ensuring that nearly six dozen classified and unclassified computing systems are managed and operated securely. The Lab has now

complied with all 14 security actions mandated two years ago by the Department of Energy. And, through our program to recruit cognizant systems engineers, we met the crucial need for sufficient numbers of engineers to keep vital mechanical and electrical safety systems functioning properly in our nuclear facilities.

The latter half of 2008 proved once again why Los Alamos is the nation's premier institution for scientific research. Capping the list of accomplishments was a new technology called MagViz that could eventually provide increased security at major airports. Based on medical MRI technology, MagViz can identify contents of bottles and other containers, distinguishing potentially hazardous liquids from the harmless shampoos and perfumes a traveler might carry onboard a jet. MagViz was demonstrated successfully in December at Albuquerque's airport.

We continued a long tradition of supporting U.S. space exploration. A NASA mission, launched in October to probe the far edge of the solar system from a high Earth orbit, carried a Los Alamos device called the High Energy Neutral Atom Imager. Its goal: to detect atoms emitted from a region where the outermost reaches of our solar system meet the vast interstellar space-giving us a panoramic view of this gateway to the galaxy.

Closer to home, Los Alamos continues to explore solutions to the energy needs of tomorrow. For example, scientists at the Lab hope to use tiny semiconductors called quantum dots to convert sunlight to electricity more efficiently than is possible with current solar panels-and to create new, efficient solid-state lighting.

Equally electrifying, Los Alamos materials scientists are helping unravel the mysteries of superconductivity. During the latter half of the year, LANL researchers identified entirely new mechanisms for superconductivity that could form the basis for new superconducting materials.

Underscoring the wealth of scientific talent at the Lab, Bob Albers, Paul Johnson, and Kurt Sickafus were named Laboratory Fellows in December. These three Fellows represent diverse disciplines, including theoretical physics, energy science, and geophysics.

Los Alamos may be one of the world's great technology incubators, yet we also strive to help others develop new ideas and products. In January, the Lab selected four young local companies as the newest recipients of awards from the LANS Venture Acceleration Fund. LANS, which manages and operates the Lab, supports the fund through donations from its earnings.

The Lab and LANS also teamed last September with a venture capital firm and a local venture capital fund to spin off technology developed by Lab scientists, with an emphasis on creating companies in Northern New Mexico. The Lab could contribute up to one million dollars to the initiative over the first three years.

We also are pushing to build top-flight research facilities for the future. In July 2008, workers hoisted the final steel beam atop the skeleton of what will be the Radiological Laboratory Utility Office Building, part of the Lab's Chemistry and Metallurgy Research Replacement Project. Once completed, the CMRR nuclear facility will house several of the Lab's mission-critical projects, including analytical chemistry, materials characterization, and actinide research and development capabilities. They'll be relocated from their current location in the historic—yet antiquated—Chemical and Metallurgy Research building at Technical Area 3.

In December, Los Alamos welcomed hundreds of employees who transferred from KSL, the subcontractor whose work the Lab brought in-house. The move was geared to improve efficiency and reduce costs associated with site-support services, including maintenance, waste removal, and custodial work.

Throughout the Lab's history, Los Alamos has helped play a vital role in the surrounding communities, and in 2008, that tradition continued. Lab employees pledged a million dollars, and LANS matched one hundred percent: a record Los Alamos contribution to United Way of TWO MILLION dollars. Contributions from the Lab and LANS also helped fund dozens of nonprofit organizations and scholarship programs, including a LANS donation of $500,000 to a LANL Foundation scholarship named for former long-time New Mexico Senator Pete Domenici.

These accomplishments and many more added up to a strong year. Our customer, the National Nuclear Security Administration, reached the same conclusion in its very favorable assessment of the Lab's performance for fiscal year 2008. It's unmistakable: the extraordinary talent, commitment, and creativity that Los Alamos employees dedicate every day to national security science and the betterment of their communities.

About Our Capabilities, Facilities, and Staff

"Los Alamos National Laboratory plays an indispensable role in building America as a science and technology powerhouse, and our staff are an incredible resource to the nation and the world." Michael Anastasio, Dir.

Solving Complex R&D Problems with Special Blend of Staff, Capabilities and Facilities
Now in its seventh decade, LANL is one of the few laboratories that can bring great breadth of fundamental and discovery science, technology, and engineering rapidly together to create tangible solutions for national security needs.
Our staff, working with partners throughout science and industry, must be able to deliver today's solutions while maintaining the depth of capabilities to deliver the next generation of discoveries.
Los Alamos has demonstrated a cycle of innovation where we have developed world-leading capabilities and facilities in response to urgent, unique missions. Our new discoveries continue to responde to emerging missions.
Being able to integrate and apply our capabilities rapidly to new challenges will be a key advantage in an increasingly competitive landscape.

Our Science, Technology and Engineering Priorities
Science that Matters

Information science and technology enabling integrative and predictive science
Experimental science focused on materials for the future
Fundamental forensic science for nuclear, biological, and chemical threats

How We Work

Collaborate, partner and team to make decisive contributions to our sponsors
Outstanding operational excellence for safety, security, and efficient pursuit of ST&E for our missions

Transform Our Scientific Campus

Campus for 2020 (consistent with complex transformation)
Modern science facilities: LANSCE refurbishment, CMR replacement, Science Complex
Signature facilities