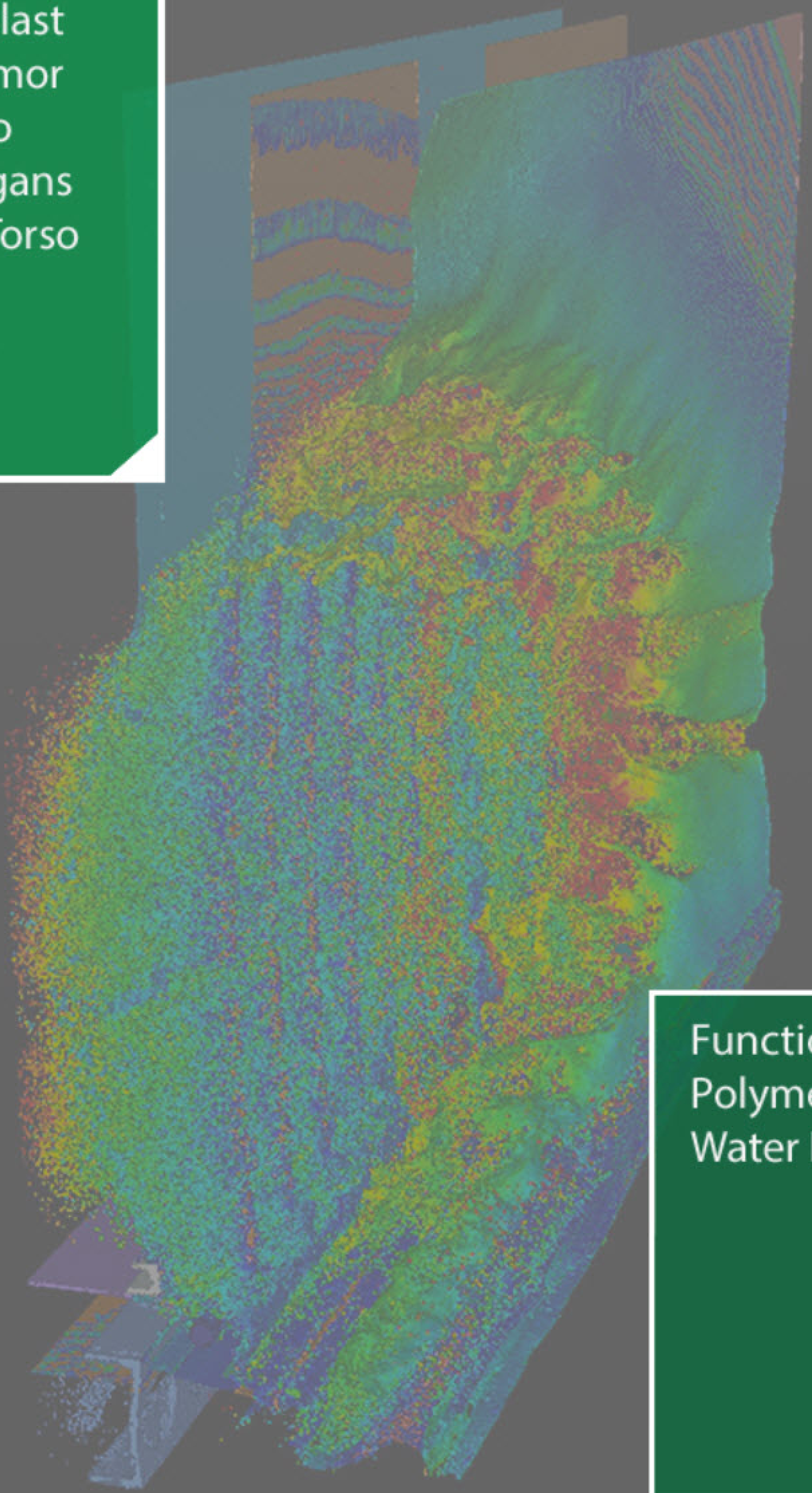
Sandia National Laboratories



Simulation of Blast and Behind-Armor Blunt Trauma to Life-Critical Organs in the Human Torso

Modeling of Arctic Storms with a Variable High-Resolution General Circulation Model

Rapid Development of an Ice Sheet Climate Application Using the Components-Based Approach

Characterizing quantum devices using model selection

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Kokkos Programming Model and Library

Functional Polymers for Water Desalination

Sandia National Laboratories

Kokkos Programming Model and Library

Carter Edwards (PI), Christian Trott, Daniel Sunderland, Mark Hoemmen, Simon Hammond

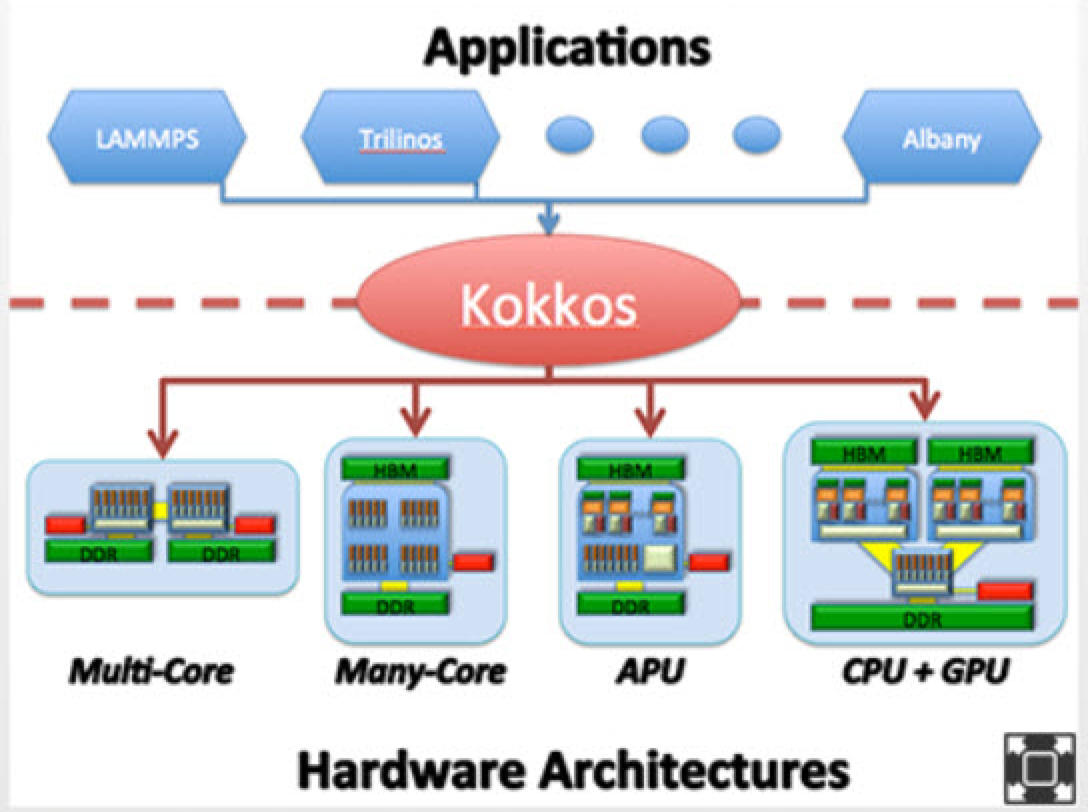
Sandia's Center for Computing Research (CCR) solves the performance portability barrier for high performance computing (HPC) across heterogeneous many-core architectures by developing and deploying the Kokkos programming model and library.

High performance computing is in the midst of a many-core revolution driven by rapidly evolving microchips with diverse and heterogeneous architectures, increasing concurrency (thread count), and decreasing memory per thread. Our HPC applications face a major challenge to effectively use these microchips with a single code base that is performance portable across these evolving architectures.

Kokkos was developed to enable on-chip concurrency and manage architecture-dependent constraints on memory access patterns. The goal is to maximize the amount of application code that is portable across diverse architectures and still obtain the same (or nearly) performance as a variant of that code written specifically for that architecture. The Kokkos team has ongoing R&D co-design collaborations with Sandia's and vendors' microchip and system engineers to rapidly incorporate evolving computer architecture features into Kokkos. The team is also providing leadership for DOE laboratories' participation on the ISO/C++ language standard committee to subsuming Kokkos features into a future standard.

The Center for Computing Research Advanced Architecture Test Bed program has been critical to the success of Kokkos. This program fields leading industry vendors' first-of-a-kind prototype computing architectures for early application porting and performance analysis across DOE's Sandia National Laboratories, Lawrence Livermore National Laboratory, and Los Alamos National Laboratory tri-lab complex. Test beds included hardware and software environment prototypes for the forthcoming Advanced Simulation and Computing (ASC) Trinity and Sierra platforms.

Application and domain library projects are adopting Kokkos to enable performance portability through the ongoing HPC many-core revolution. Within the DOE laboratories, these include Trilinos, Sierra Mechanics, Zoltan, LAMMPS, Albany, ASCR MultiphysicsMHD, FASTMath SciDAC, Empress, SHIFT, and others. Outside of DOE, the US Army Research Laboratory, Swiss Supercomputing Center, Helmholtz-Zentrum Dresden-Rossendorf German research laboratory, University of Utah, and King Abdullah University of Science and Technology have expressed interest in adopting Kokkos for new projects.



For more details about the Kokkos programming model, visit the Poster presentation in Level 4-Lobby
C++ Abstraction Layers – Performance, Portability and Productivity
PREVIEW HERE

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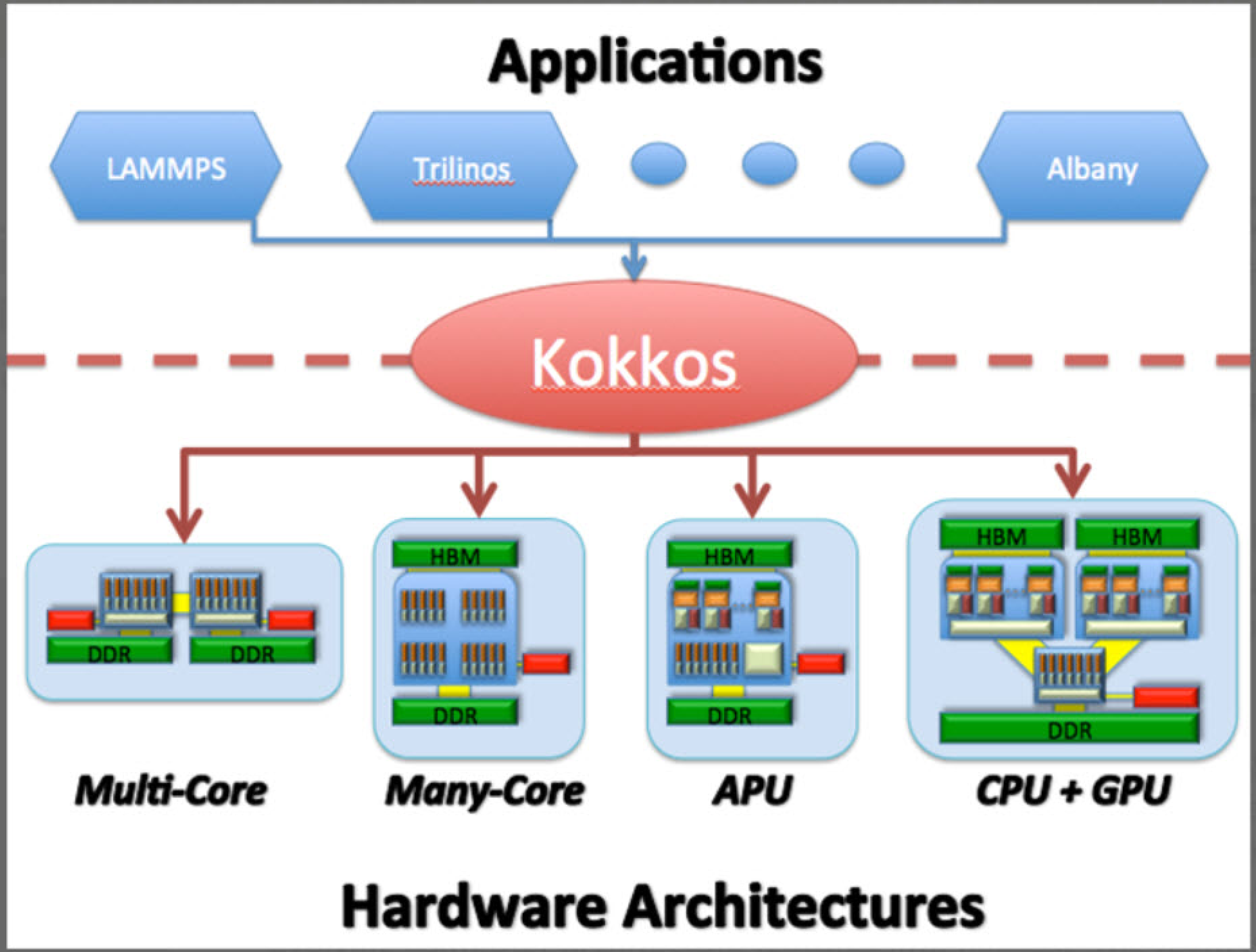

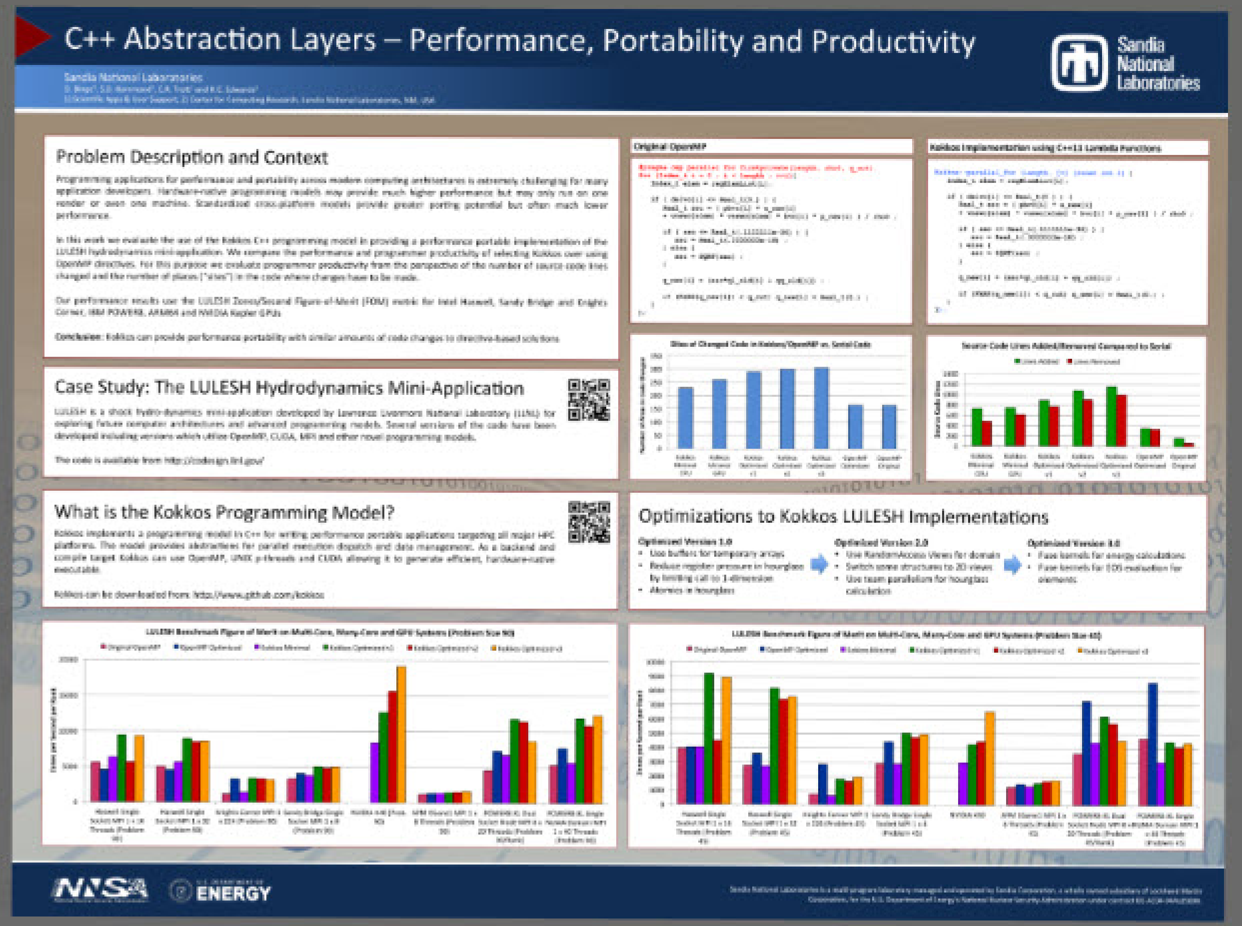

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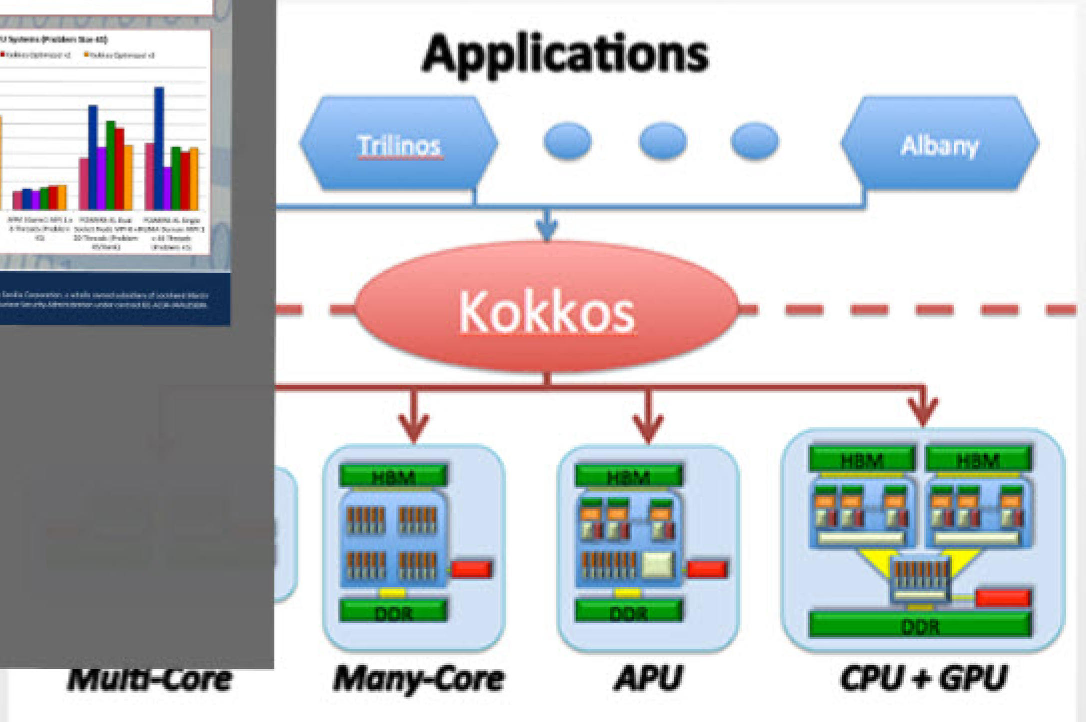

Hardware Architectures

CONTACT: H. Carter Edwards (hcedwar@sandia.gov)
CONTRIBUTORS: Carter Edwards (PI), Christian Trott, Daniel Sunderland, Mark Hoemmen, Simon Hammond
FUNDING AGENCY: DOE (NNSA/ASC)

FUNDING ACKNOWLEDGEMENT: Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
DOCUMENT NUMBERS: SAND2015-8505R (Unclassified Unlimited Release)
(Kokkos poster preview SAND2015-6734 D)

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The Center for Computing Research Advanced Architecture Test Bed program ha… program fields leading industry vendors' first-of-a-kind prototype computing arc… performance analysis across DOE's Sandia National Laboratories, Lawrence Liver… National Laboratory tri-lab complex. Test beds included hardware and software … Advanced Simulation and Computing (ASC) Trinity and Sierra platforms.

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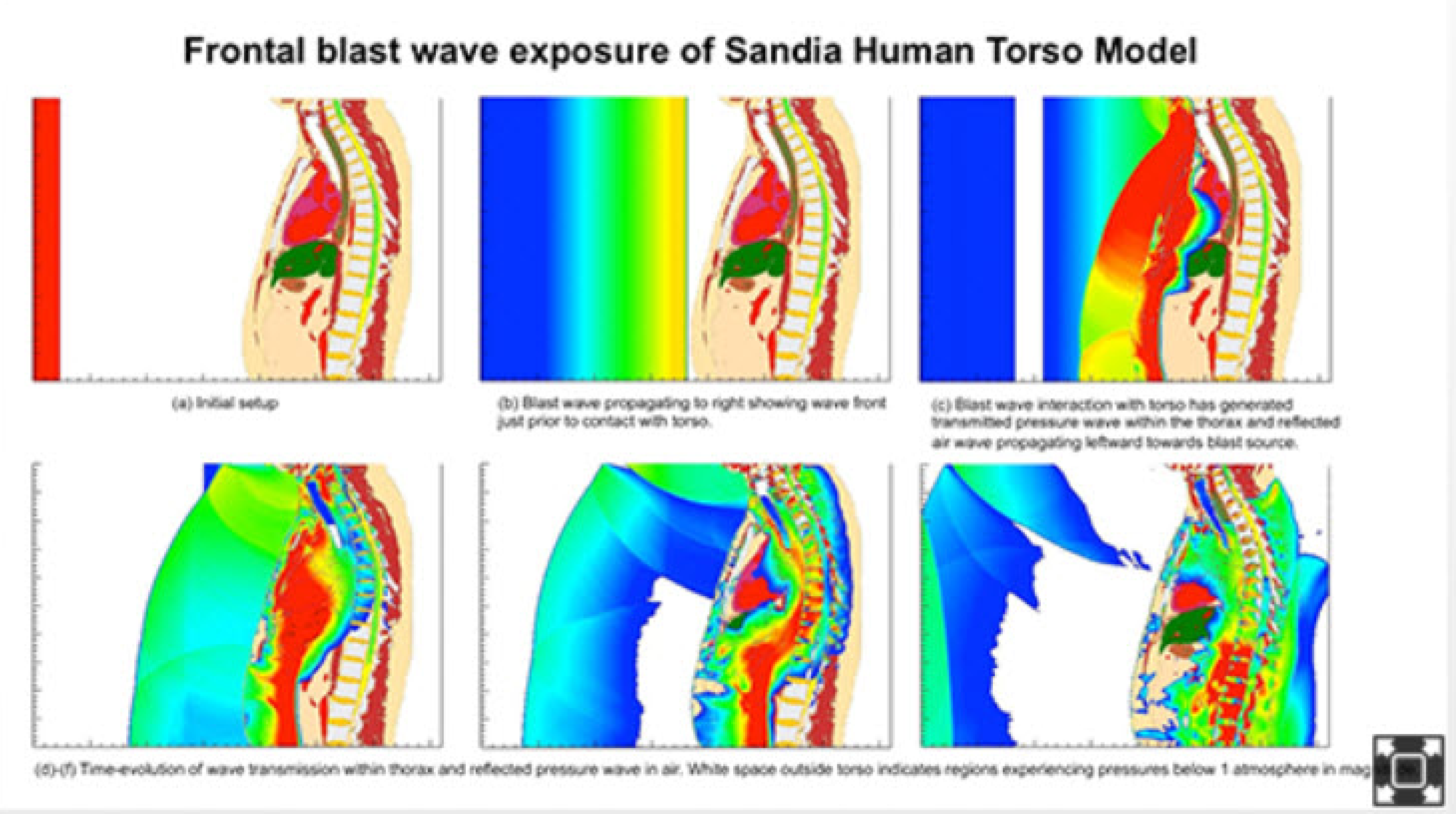
Sandia National Laboratories

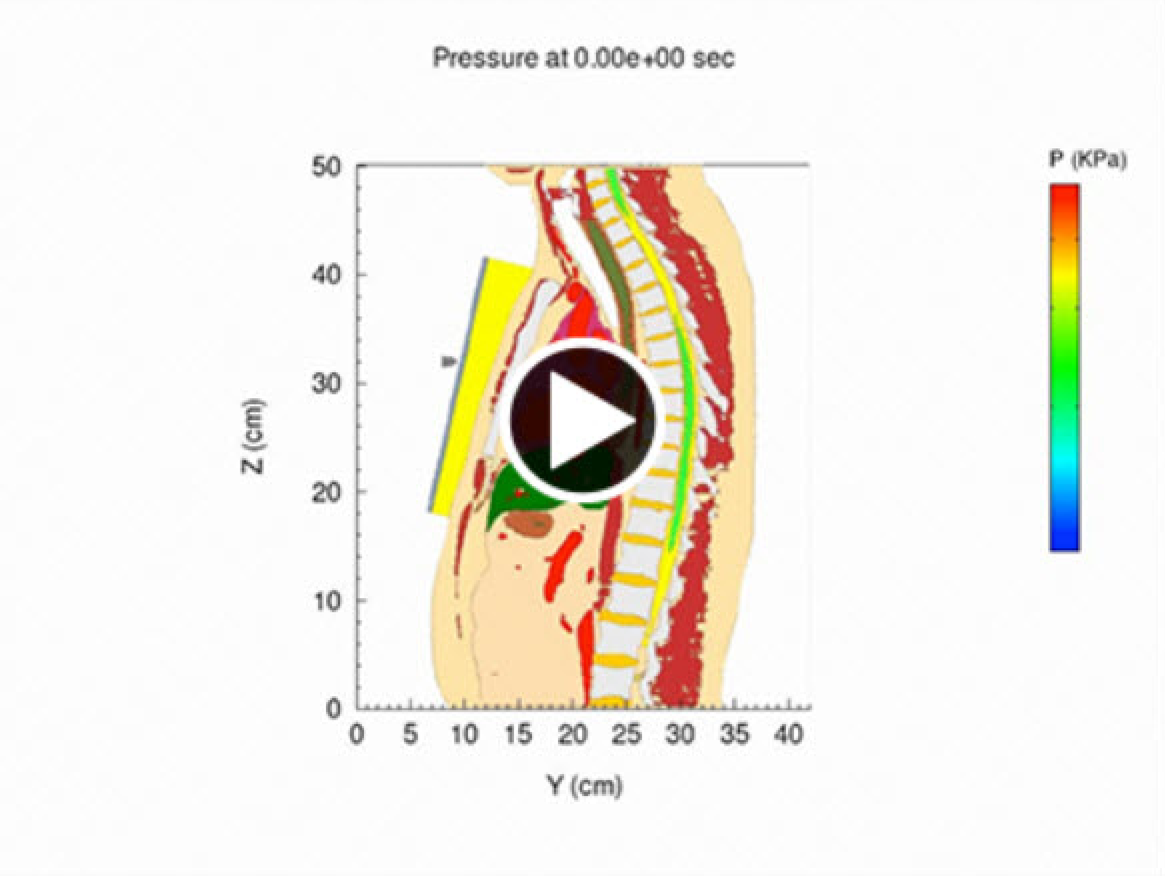
Simulation of Blast and Behind-Armor Blunt Trauma to Life-Critical Organs in the Human Torso

Paul A. Taylor (PI), Candice F. Cooper

This work is focused on providing the means to understand the mechanics of wound injury to the U.S. warfighter and developing a new approach with which to assess new personal armor designs for their protection.

Researchers at Sandia National Laboratories have developed a high-fidelity virtual model of the human torso to investigate the details of life-threatening injury to the respiratory and cardiovascular systems as a result of blast exposure and behind-armor blunt trauma. This model is an extension of the Sandia virtual head-neck model developed previously to investigate the connection between blast exposure and traumatic brain injury. The Sandia human torso model possesses anatomically correct distributions of bone, cartilage, intervertebral disks, vasculature, blood, airways, lungs, heart, liver, stomach, kidneys, spleen, spinal cord, muscle, and fat/skin. The torso model is used with the Sandia wave physics code CTH to simulate blast loading and ballistic projectile impact to the torso, without and with protective armor, to investigate the details of injury to life-critical organs such as the lungs, airways, heart, blood vessels, and liver as a result of the intrathoracic pressure waves that are generated from a blast or impact. The intent of this work is to demonstrate the advantages of applying a modeling and simulation approach to the investigation of wound injury dynamics and to assess protective body armor for the U.S. warfighter under conditions of blast and ballistic projectile impact. A typical torso injury scenario simulation requires anywhere from 448 to 960 cpu-cores, running the calculation for 30 to 60 cpu-hours, and generating over 500 Gb of raw data that is post-processed at a later time for injury investigation and/or protective armor assessment.





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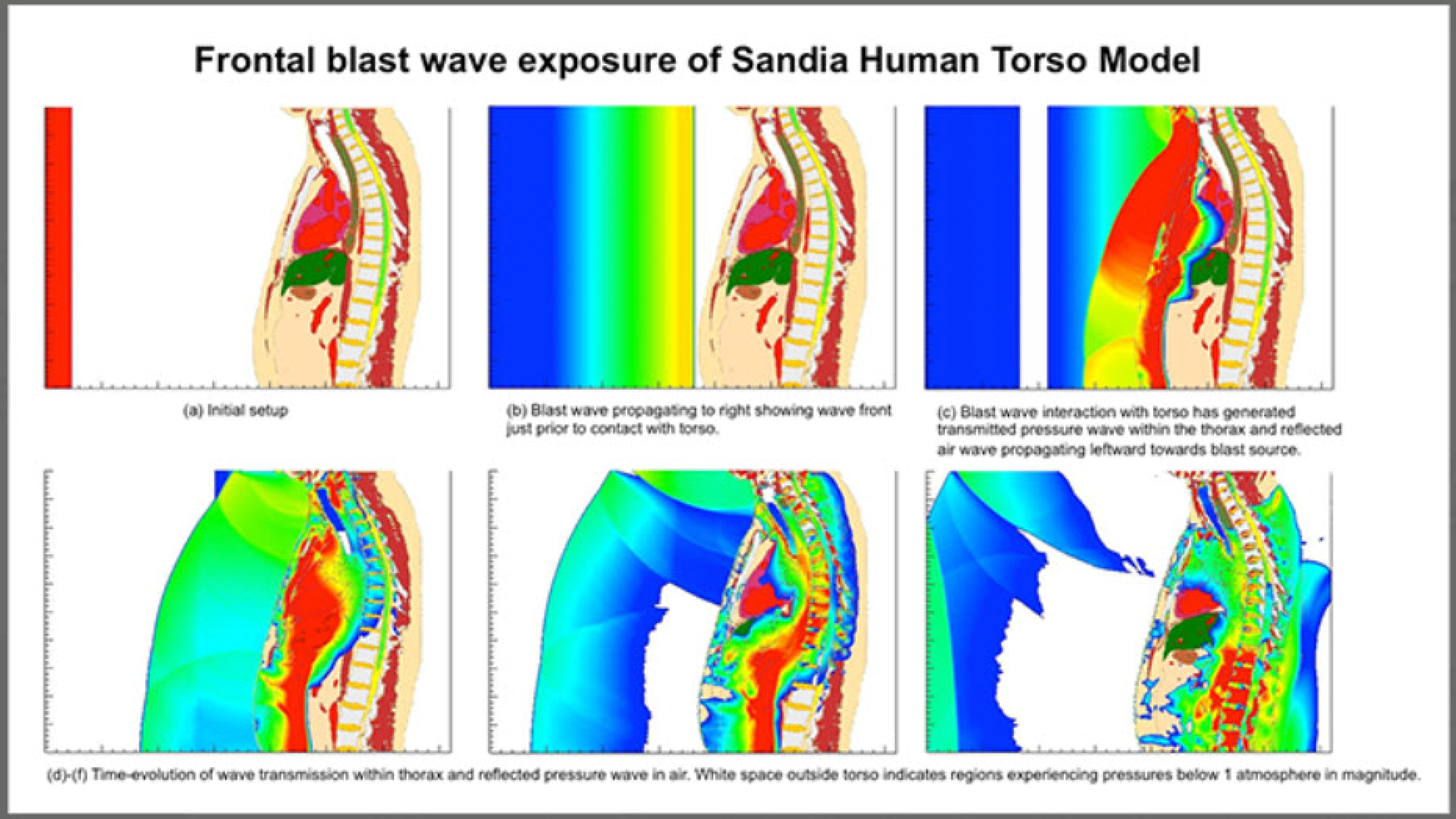

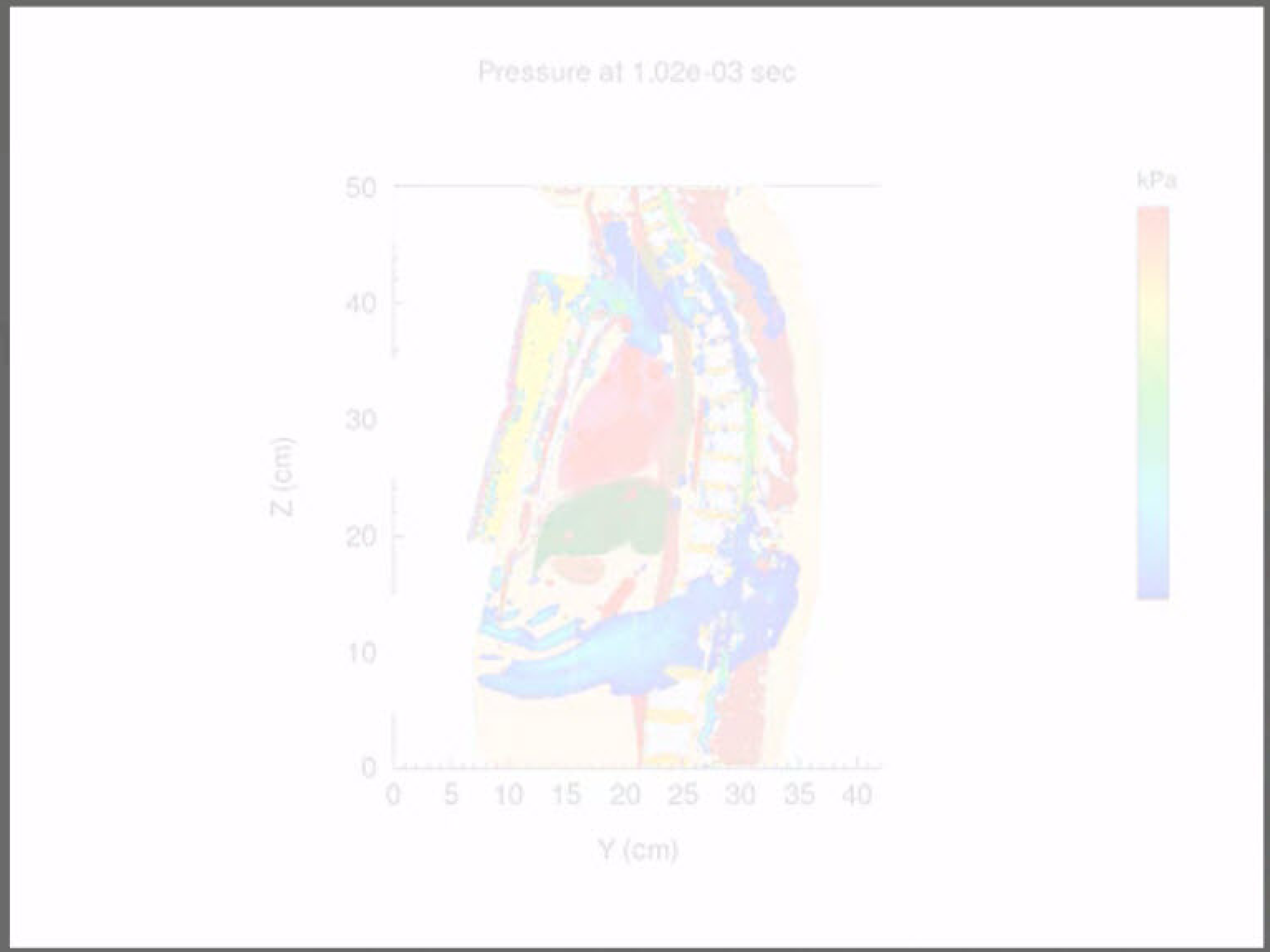

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armor assessment.

PROCESSING HOURS: 1,051,120
CONTACT: Paul A. Taylor (pataylor@sandia.gov)
CONTRIBUTORS: Paul A. Taylor, Candice F. Cooper
PROGRAM: Defense Systems & Assessments
FUNDING AGENCY: DOE (LDRD)
FUNDING ACKNOWLEDGEMENT: Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
DOCUMENT NUMBER: SAND2015-8505 R (Unclassified Unlimited Release)

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Sandia National Laboratories

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Functional Polymers for Water Desalination

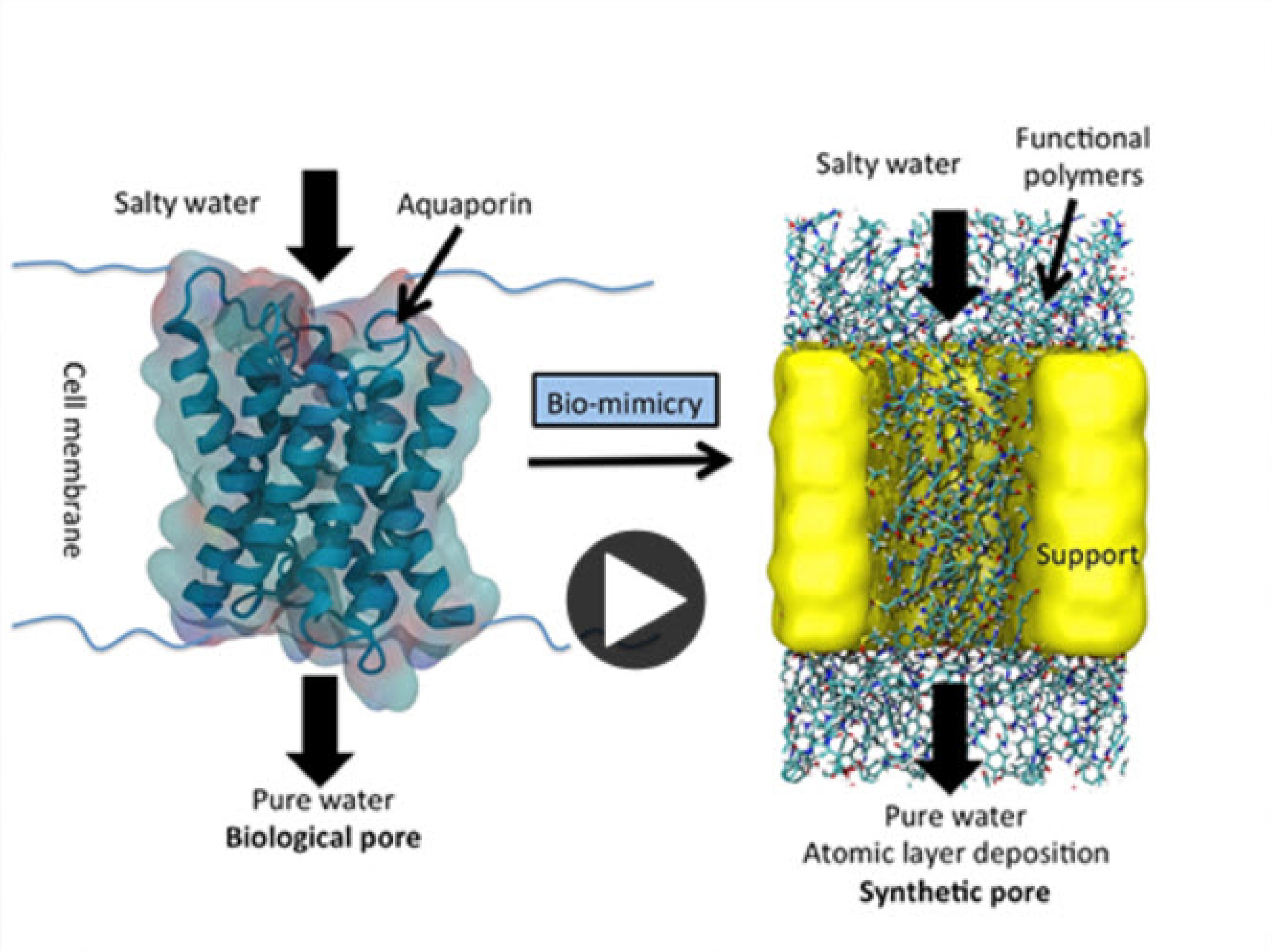
Susan Rempe (PI), Mangesh Chaudhari, David Rogers, Jeff Brinker, Ying-Bing Jiang, Shaorong Yang

We are excited to extend our research in the coming years to develop ion-selective channels for diverse applications such as electrodialysis, battery electrolytes, and separating toxic metals from water.

Water, energy, and food are interconnected and present a technological challenge that is hard to over-estimate. Dating back to 2003, an article in Nature magazine stated that, "More than 1 billion people in the world lack access to clean water, and things are getting worse. Over the next two decades, the average supply of water per person will drop by a third," (Aldous, 2003). More recently, a brighter future could rely on advanced water desalination techniques that use less energy to produce clean water at lower cost. An example is Perth, Australia where half of its water comes from the Indian Ocean on the basis of wind-powered reverse osmosis (Newman, 2014).

Currently, polymers form the active component of reverse osmosis membranes used to separate water from salty solutions. Compared with cellular membranes, synthetic membranes lag behind in terms of water selectivity and permeation rate. To address this problem, researchers from Sandia and the University of New Mexico (UNM) partnered to develop synthetic membranes that mimic nature, called Biomimetic Membranes.

Membrane design and fabrication involved both theoretical and experimental efforts. To understand the relationship between molecular structure and selective water permeation, Dr. Susan Rempe and co-workers from Sandia applied molecular simulation techniques to two systems: 1) aquaporin Z, a water-selective channel protein in cellular membranes; and 2) synthetic nano-pores 'decorated' with functional polymers to mimic the biological channel behavior. Colleagues at UNM used an advanced atomic layer deposition (ALD) technique to fabricate synthetic membranes. To estimate the work needed to move water and ions through the permeation pathways, the simulation specialists computed free energy profiles. Both the synthetic and biological channels show lower free energy barriers for water compared with competing ions like sodium (Na+) and chloride (Cl-). A systematic arrangement of functional polymers, achieved using ALD, improved water permeation rates by at least five-fold when compared with commercial membranes. An assessment of local coordination structure of water and ions along the permeation pathway in biological and synthetic membranes provides clues to the observed differences in behavior.



The researchers performed simulations using the high performance Red Mesa cluster at Sandia. The Gromacs molecular dynamics simulation package was used to compute the ion and water free energy profiles. Electronic structure calculations were also performed to obtain more details about the ion hydration structures and free energies.

The first implementation of the water-selective membranes won an R&D 100 award. Licensing and commercialization are being pursued.

FUNDING & CREDITS

Desalination

inker, Ying-Bing Jiang, Shaorong Yang

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PROCESSING HOURS: 1,915,031
PLATFORM: Red Mesa
CONTACT: Susan Rempe (slrempe@sandia.gov)
CONTRIBUTORS:
Computation: Mangesh Chaudhari, David Rogers, Susan Rempe
Experimentalists: Jeff Brinker, Ying-Bing Jiang (UNM), Shaorong Yang (UNM)
FUNDING AGENCY: DOE (Energy & Climate LDRD), AFOSR
FUNDING ACKNOWLEDGEMENT: Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
DOCUMENT NUMBER: SAND2015-8505 R (Unclassified Unlimited Release)

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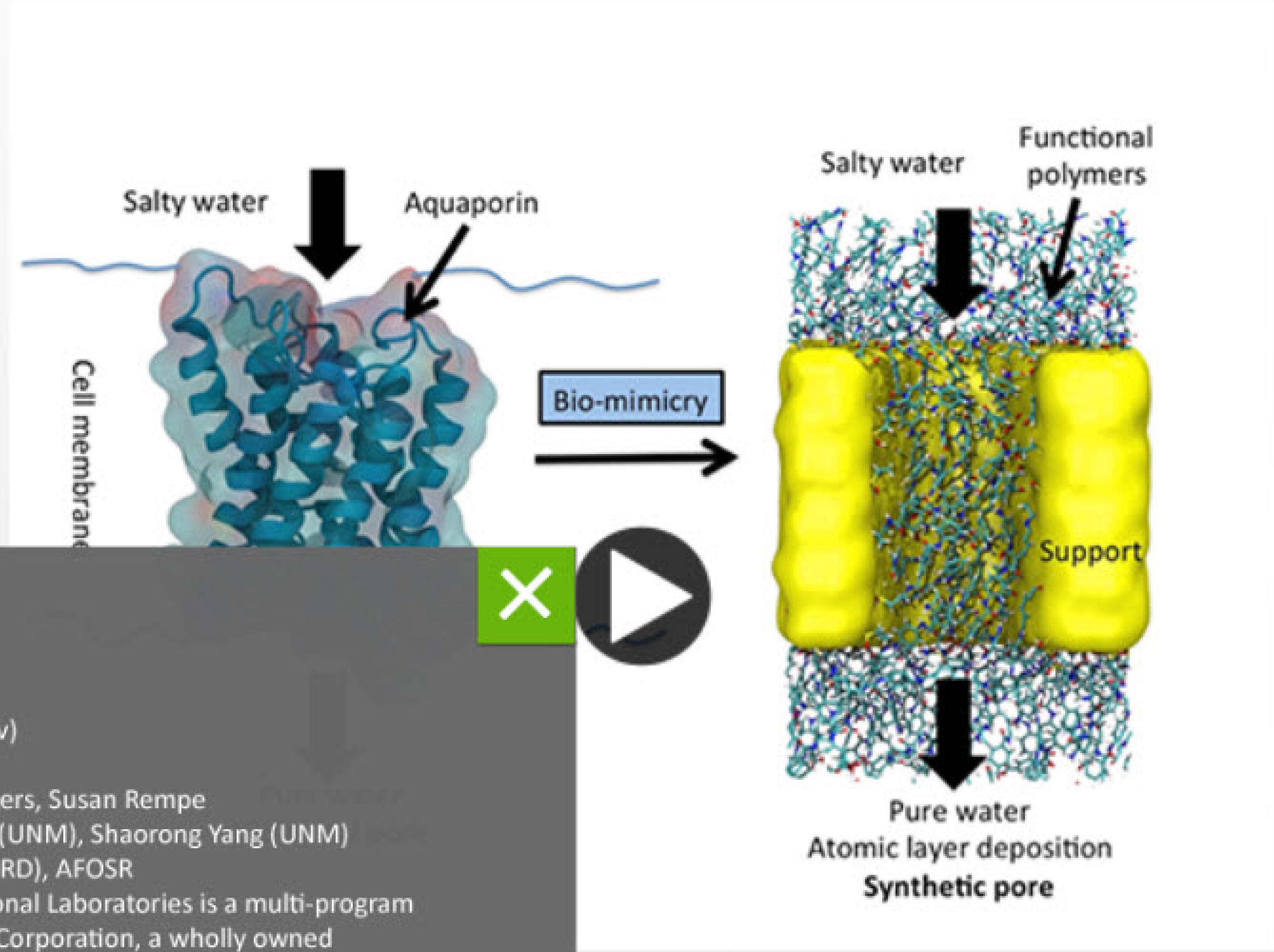

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The first implementation of the water-selective membranes won an R&D 100 award. Licensing and commercialization are being pursued.

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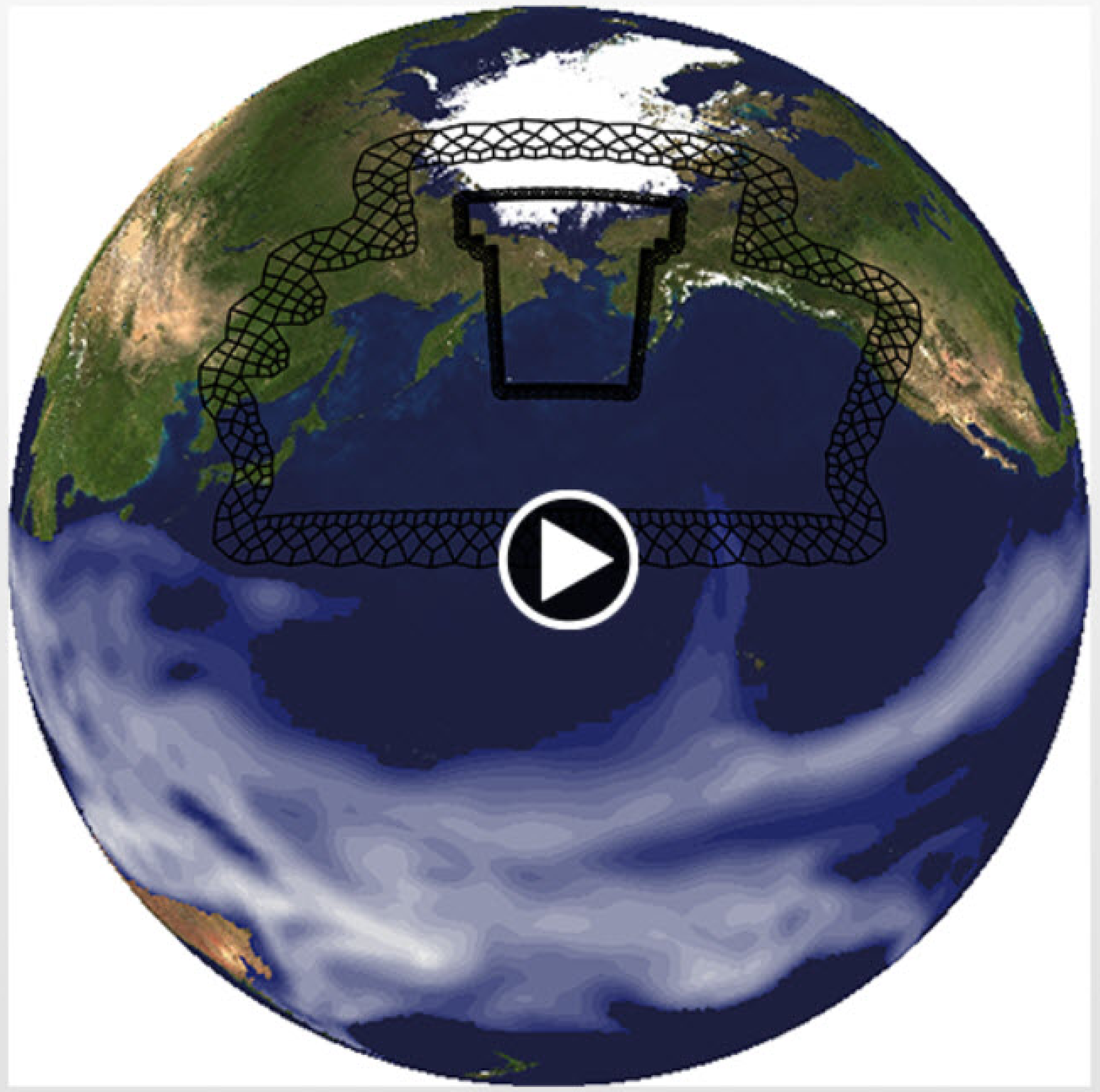
Modeling of Arctic Storms with a Variable High-Resolution General Circulation Model

Mark A. Taylor (PI), Erika L. Roesler, Peter Bosler

Our team is composed of atmospheric scientists with backgrounds in physics, math, and computer science. We are driven by the need to develop the best climate model for predicting the future climate of this country.

This figure shows the northern Pacific Ocean basin. The colored contours represent the total amount of water in the atmosphere at a given time and location as simulated by the atmospheric model. The lighter, whiter color indicates the presence of a higher water concentration, which also indicates where precipitation is likely to occur. The model was run in a variable resolution configuration using the spectral element atmospheric dynamical core. Areas of higher-resolution in atmospheric models develop more realistic storms. This grid will be used to study Arctic storms, polar lows, and the energetics of storms hitting the Alaskan coast. The resolution in the smallest area outlined over the Bering Sea has an effective resolution of about 13 kilometers (1/8-degree). The area outlined in the northern Pacific Ocean basin stretching from the west's Sea of Okhotsk to the east's Gulf of Alaska has an effective resolution of about 27 kilometers (1/4-dgree). For the remainder of the globe, the effective resolution is about 110 kilometers (1-degree).



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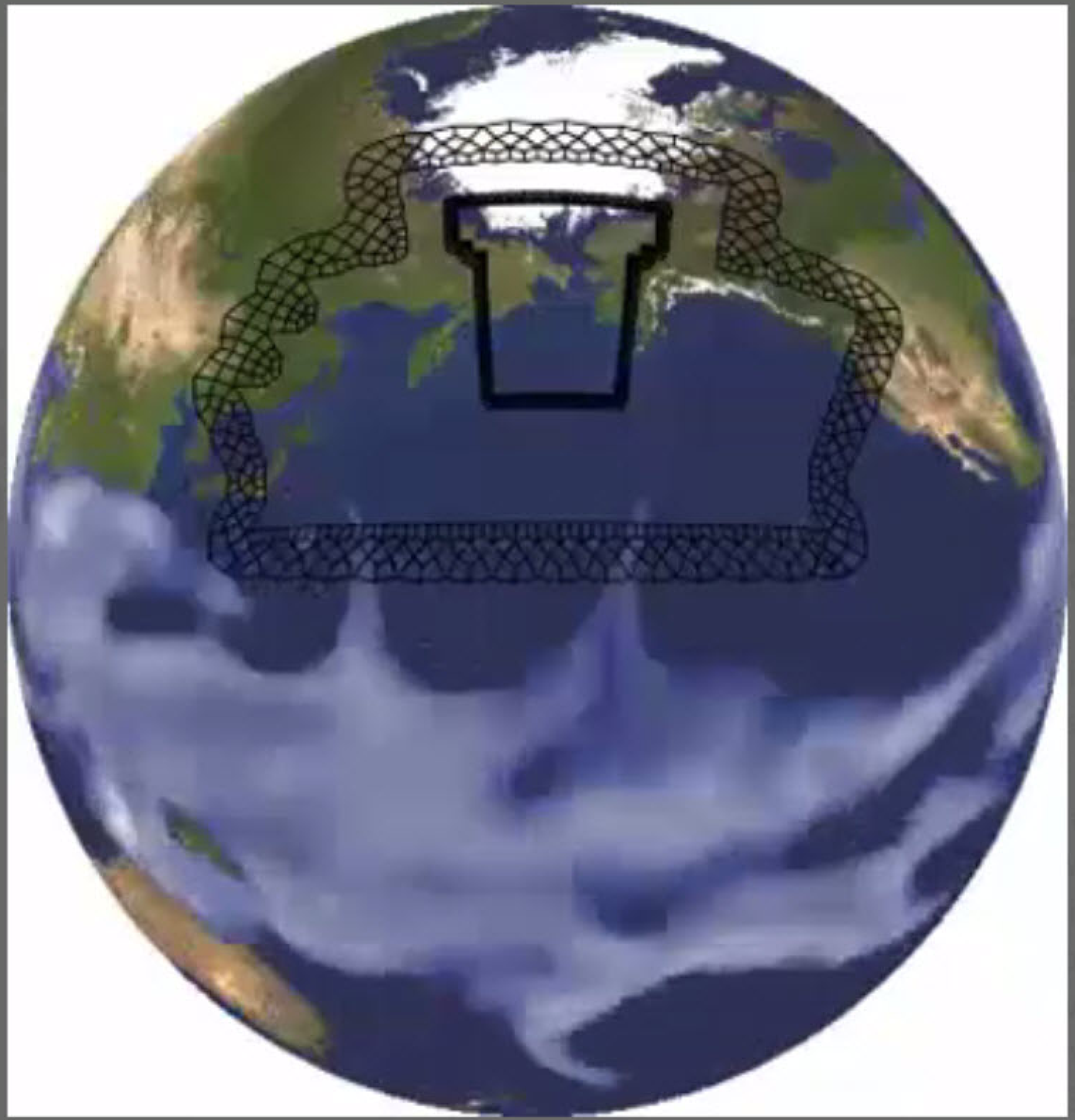


The Department of Energy's (DOE) Biological and Environmental Research project, "Water Cycle and Climate Extremes Modeling" is improving our understanding and modeling of regional details of the Earth's water cycle. Large uncertainties exist in the ability of today's climate models to simulate regional water cycle extremes such as storms, droughts and floods. Increased model resolution is a key tool for improved modeling of extremes. However, global high-resolution simulations are computationally expensive and usually performed at leadership computing facilities. Work at Sandia has led to dramatic improvements in scalability of DOE's atmosphere component model, making these high-resolution simulations possible, and at the same time also supporting a variable resolution capability where high resolution is used over fixed locations on the globe. This new capability allows scientists to gain insight into high-resolution model behavior over a smaller domain at a fraction of the computational cost.

Our team is using variable resolution to investigate storms in the Arctic. Strong storms in the Arctic are believed to further break-up sea ice. The sea ice extent affects storm tracks, and accurate predictions of the sea ice extent is desired by many agencies.

Currently, it is unknown if or how powerful storms will change in the future climate. To help answer this question, our team developed a variable resolution region in the Arctic to compare the number of storms and their properties in the low, high, and variable resolution simulations, using Red Sky and Sky Bridge for the simulations, data processing, and analysis. We developed a new storm-detection tool used to identify and track storms. As the resolution of the model is increased, it can capture small-scale storms that are not possible to resolve at low resolution, establishing our new variable resolution capability is an effective tool that will allow the climate modeling community achieve a better understanding of Arctic storms.

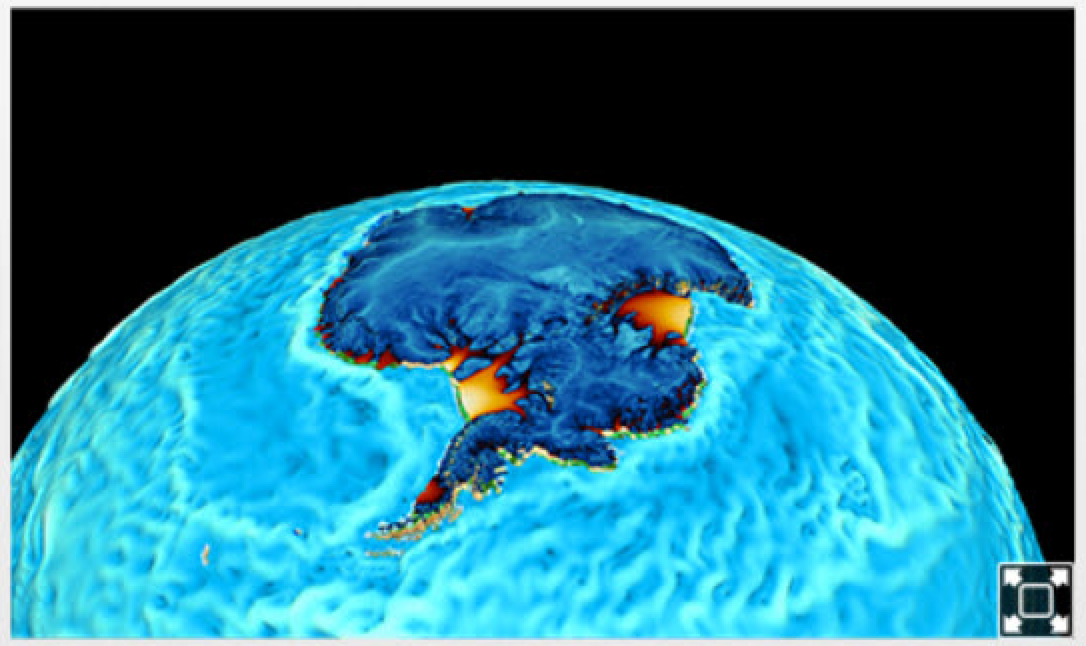
PROCESSING HOURS: 1,615,722
PLATFORMS: Red Sky, Sky Bridge
CONTACT: Mark A. Taylor (mataylo@sandia.gov)
CONTRIBUTORS: Mark A. Taylor, Erika L. Roesler, Peter Bosler
FUNDING AGENCY: DOE (LDRD, EC)
FUNDING ACKNOWLEDGEMENT: Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
DOCUMENT NUMBER: SAND2015-8505 R (Unclassified Unlimited Release)

Sandia National Laboratories

Rapid Development of an Ice Sheet Climate Application Using the Components-Based Approach

Andrew Salinger (PI), Irina Tezaur, Mauro Perego, Raymond Tuminaro, Stephen Price (LANL)

As computational scientists with expertise in math and algorithms, it is challenging to get deep enough into a new science application area to make an impact. This team has made a sustained effort in learning about ice sheets and building relationships with climate scientists, and has been rewarded seeing our code on the critical path of DOEs climate science program.



In the third year of a five-year jointly funded project, Sandia's Albany/FELIX simulation code for ice sheet dynamics is being developed to be run in two modes: (1) as a stand-alone model for scientific investigations, and (2) as part of the land-ice component of coupled climate simulations in the Department of Energy's (DOE's) earth system model. The land-ice component simulates changes to the Greenland and Antarctic ice sheets, including their contributions to global sea-level rise. Using high performance computing (HPC), Sandia has recently completed a controlled mesh convergence study to compute the rate at which the Greenland ice sheet is flowing. The study demonstrated that the HPC code is capable of working accurately, efficiently, and reliably on larger scales (over 1 billion unknowns). The study also identified, for the first time, the minimum number of vertical levels needed in the mesh to maintain accuracy.

The rapid development of this impressive simulation capability was enabled by our components-based approach to computational science. Under our "Agile Components" strategy, small teams of experts develop independent math libraries, which are designed to be interoperable through software interfaces, and maintained and deployed for subsequent application by following software engineering best practices. The Albany code benefited from dozens of previously developed capabilities, and in turn, has improved the foundational code base for other applications.

Funded by the DOE Office of Science Scientific Discovery through Advanced Computing program (SciDAC), this project is a collaborative effort between the Climate (BER) and Applied Math (ASCR) programs. Partnering with Los Alamos National Laboratory, Sandia National Laboratories analysts have recently integrated the Albany/FELIX code into LANL's MPAS-LI code, the land ice component of DOE's Accelerated Climate Model for Energy (ACME) earth system model. In ACME, the Albany code will be coupled with the atmospheric, ocean, land, and sea ice components, and used in climate projections in support of DOEs energy and security missions. Demonstrating the capability for interagency computing, this work primarily uses the computing systems as National Energy Research Scientific Computing Center (Hopper) and Oakridge Leadership Computing Facility (Titan)).

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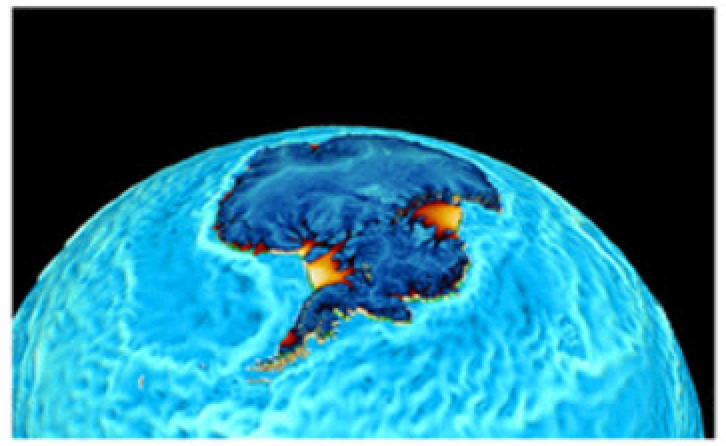

Figure 1: Visualization of the computed surface velocity of the Antarctic Ice Sheet, which clearly shows the fast-moving ice shelfs (red-orange colors). For visualization, the vertical dimension of the ice sheet is stretched and the figure is superimposed on an ocean model simulation result, foreshadowing our ongoing work in integrating the ice sheet model into global earth system models. (Graphic by P. Wolfram [LANL]).

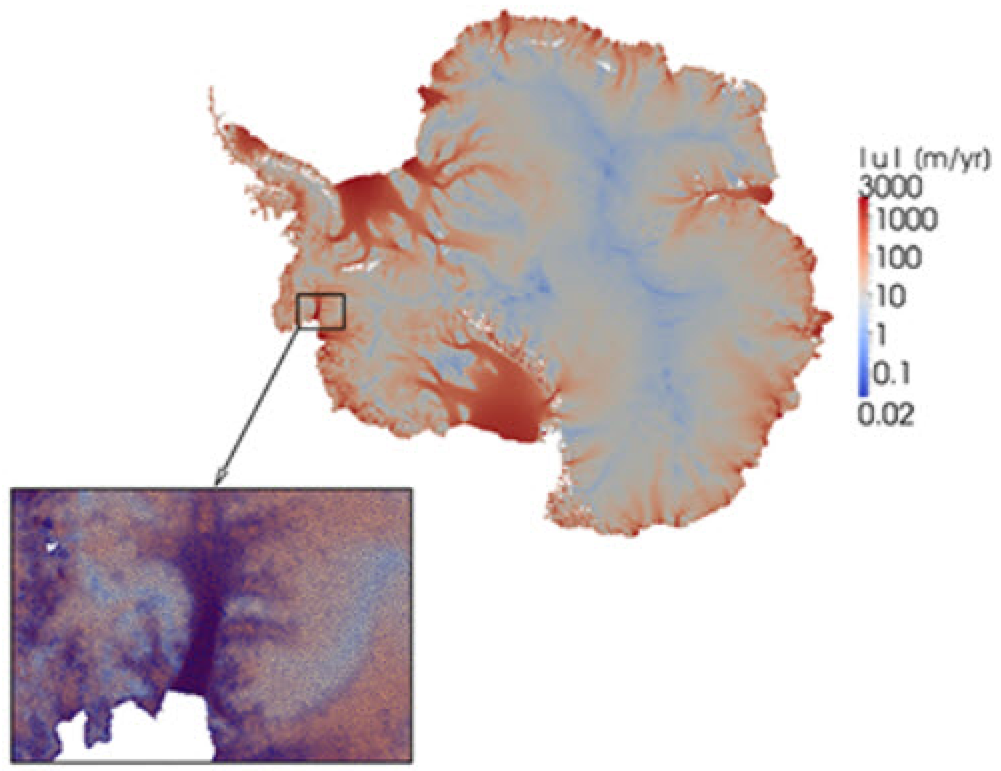

Figure 2: Computed surface velocities for both the Greenland and Antarctic Ice Sheets. The insets show how our unstructured-grid approach allows for enhanced resolution in the critical locations of fast-moving ice streams at greatly reduced computational costs over uniform grid approaches.

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...ymond Tuminaro, Stephen Price (LANL)

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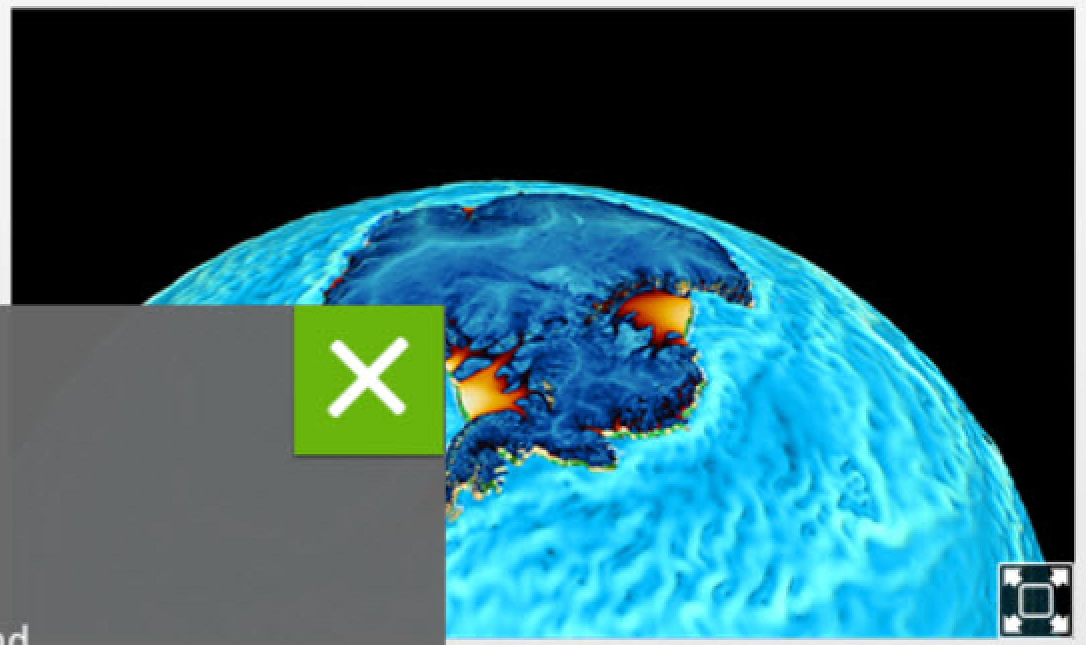

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PROCESSING HOURS: 1,000,000
PLATFORMS: Hopper (NERSC), Titan (OLCF)
CONTACT: Andrew Salinger (agsalin@sandia.gov)
CONTRIBUTORS: Andrew Salinger, Irina Tezaur, Mauro Perego, Raymond Tuminaro, Stephen Price (LANL)
FUNDING AGENCY: DOE (ASCR, BER, SciDAC)

FUNDING ACKNOWLEDGEMENT: Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
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Sandia National Laboratories

Characterizing quantum devices using model selection

Robin Blume-Kohout (PI), Travis Scholten

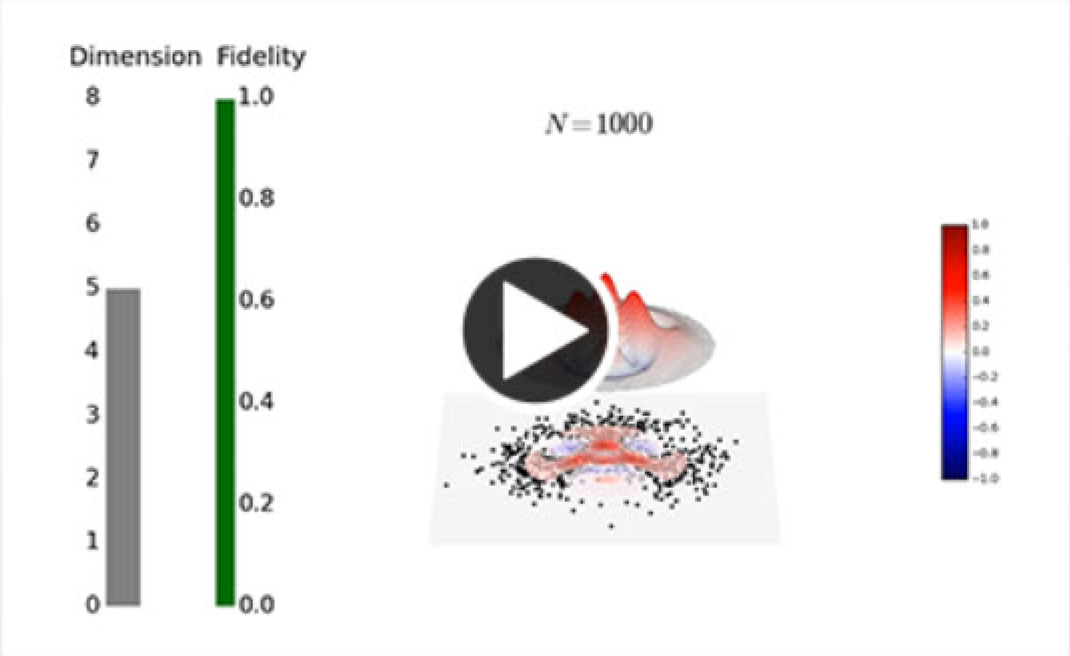
Monte Carlo simulations on Red Sky allowed us to explore the enormous space of test cases for our algorithm, and thus to figure out how model selection could enhance quantum tomography.

Quantum information processors are a new kind of computing device with the potential to solve certain problems very quickly. The quantum bits, or "qubits," that enable such processors are being developed at Sandia and around the world. In support of this effort, Sandia's Center for Computing Research is designing methods and algorithms to characterize and debug the behavior of experimental qubits, such as trapped ions and electron spins in silicon.

This is a challenge, because qubits are hard to characterize for exactly the same reason that they are powerful. Their behavior (and misbehavior) is far richer and more complicated than that of classical bits! The most reliable models of quantum errors have infinitely many parameters, and we never have enough data to fit all of them. Until now, researchers simply threw out most of these parameters resulting in a crude approximation that makes the problem tractable, but isn't reliable or accurate enough for Sandia's experimental work.

Our new techniques use statistical model selection to identify "significant" error parameters on the fly, applying a data-driven information criterion to choose a Hilbert space that describes the data well without overfitting. To find a reliable criterion, we needed to evaluate many candidates on an enormous corpus of test cases–for which we relied on Red Sky's ability to run parallel Monte Carlo simulations. Our computations demonstrate how classic model selection methods have to be modified for quantum devices. These results will enable new techniques that identify the effective dimension of as-built qubits on the fly, and then use this information to reliably pin down error behaviors and produce successively better and more useful qubits.

This project highlights the close and productive relationship between Sandia and the University of New Mexico, where Travis Scholten is working towards a Ph.D. in physics. Both the intellectual environment of UNM and the high-powered supercomputing available at Sandia were critical ingredients in achieving our research goals.



The black dots represent 1,000 numerically generated data points. The contour map created from the model illustrates that the estimate of the quantum state fits the data well. The estimate has a high degree of accuracy, as indicated by the fact the fidelity with the true state is close to 1.

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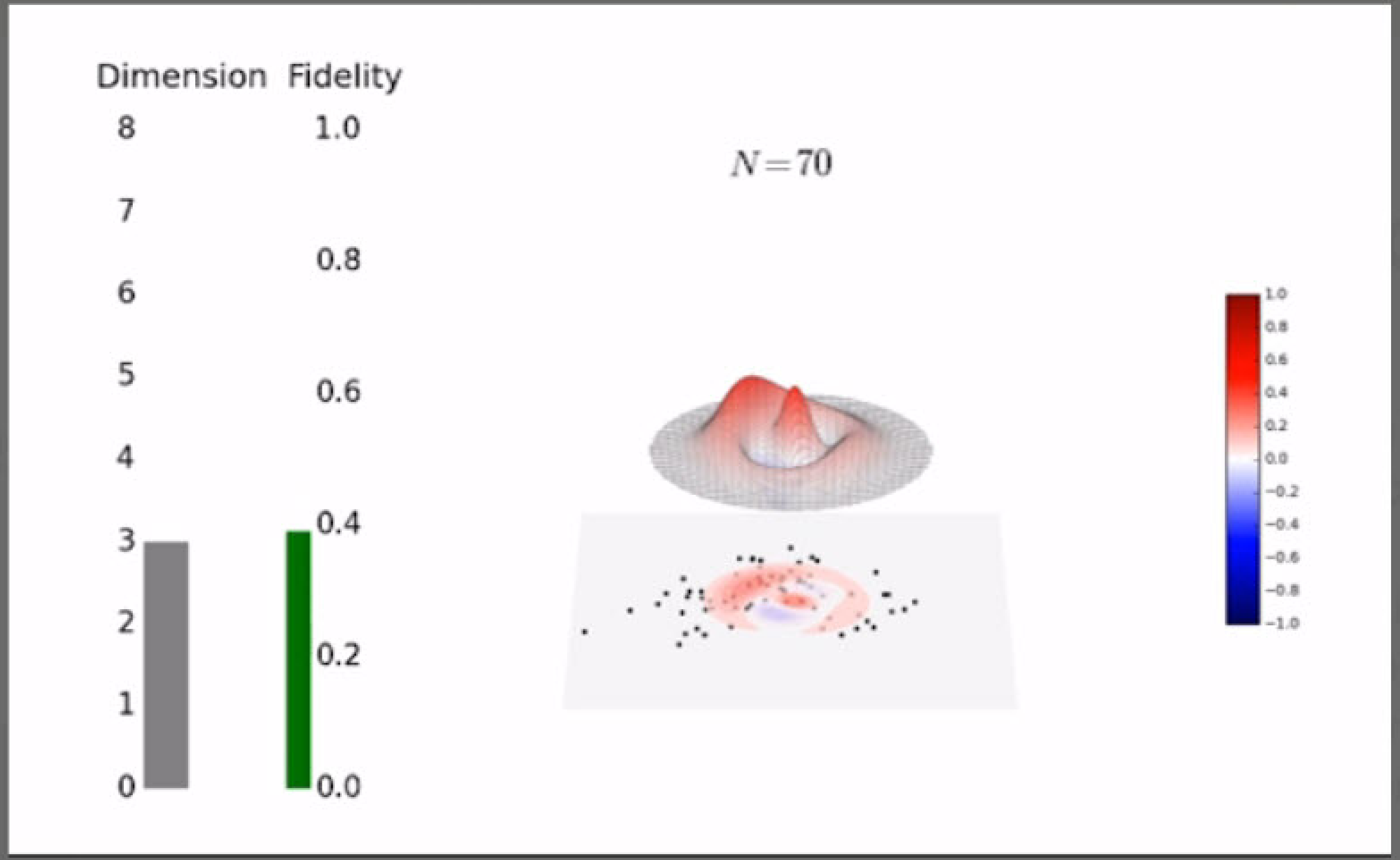

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…ces using model selection

…the enormous space of test cases for our algorithm, and thus to …omography.

…ing device with the potential to solve certain problems very …cessors are being developed at Sandia and around the world. In …ch is designing methods and algorithms to characterize and debug …nd electron spin in silicon.

…ard to characterize for exactly the same reason … That … and more complicated than that of classical … parameters, and we never have enough data to … parameters resulting in a crude approximation that … reliable or accurate enough for Sandia's experimental work.

PROCESSING HOURS: 659,107
PLATFORM: Red Sky
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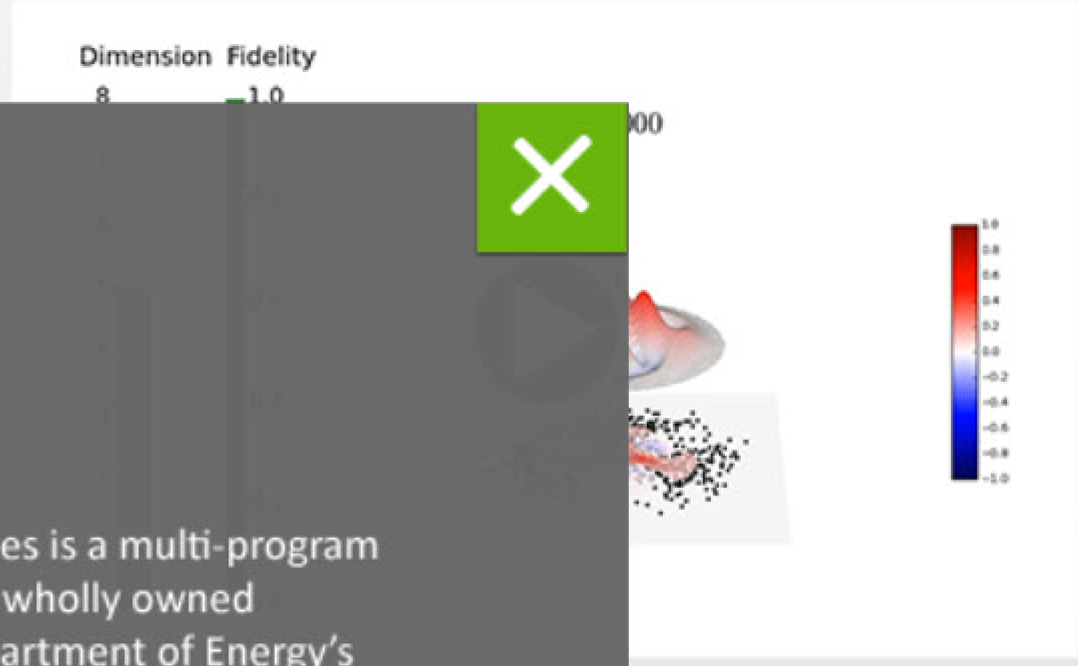

…merically generated data …rom the model illustrates …state fits the data well. …accuracy, as indicated by …tate is close to 1.

Our new techniques use statistical model selection to identify "significant" error par… information criterion to choose a Hilbert space that describes the data well without overfitting. To find a suitable criterion, we needed to evaluate many candidates on an enormous corpus of test cases—for which we relied on Red Sky's ability to run parallel Monte Carlo simulations. Our computations demonstrate how classic model selection methods have to be modified for quantum devices. These results will enable new techniques that identify the effective dimension of as-built qubits on the fly, and then use this information to reliably pin down error behaviors and produce successively better and more useful qubits.

This project highlights the close and productive relationship between Sandia and the University of New Mexico, where Travis Scholten is working towards a Ph.D. in physics. Both the intellectual environment of UNM and the high-powered supercomputing available at Sandia were critical ingredients in achieving our research goals.