

The HPC Innovation Award and Winners

Examples of Previous Winners



Ohio Supercomputer Center
An OH-TECH Consortium Member



Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Continuous Casting Consortium



Cornell University
Center for Advanced Computing



MARY BIRD PERKINS
CANCER CENTER



Queen Mary
University of London



The Trophy for Winners



HPC Award Program Goals

- **#1 Help to expand the use of HPC by showing real ROI examples:**
 1. Expand the “Missing Middle” – SMBs, SMSs, etc. by providing examples of what can be done with HPC
 2. Show mainstream and leading edge HPC success stories
- **#2 Create a large database of success stories across many industries/verticals/disciplines**
 - To help justify investments and show non-users ideas on how to adopt HPC in their environment
 - Create many examples for funding bodies and politicians to use and better understand the value of HPC → to help grow public interest in expanding HPC investments
 - For OEMs to demonstrate success stories using their products

Users Submit the Value of the Accomplishment

- **Users are required to submit the value achieved with their HPC system, using 3 broad categories, following a very specific set of guidelines:**
 - a) Dollar value of the HPC usage
 - e.g., made \$\$\$ in new revenues, saved \$\$\$ in costs, made \$\$\$ in profits, etc.
 - b) Scientific or engineering accomplishment
 - e.g., discovered how xyz really works, developed a new drug that does xyz, etc.
 - c) Value to society as a whole
 - e.g., ended nuclear testing, made something safer, provided protection against xyz, etc.

... and the investment in HPC that was required

The Judgment Process – Clear, Fair And Transparent

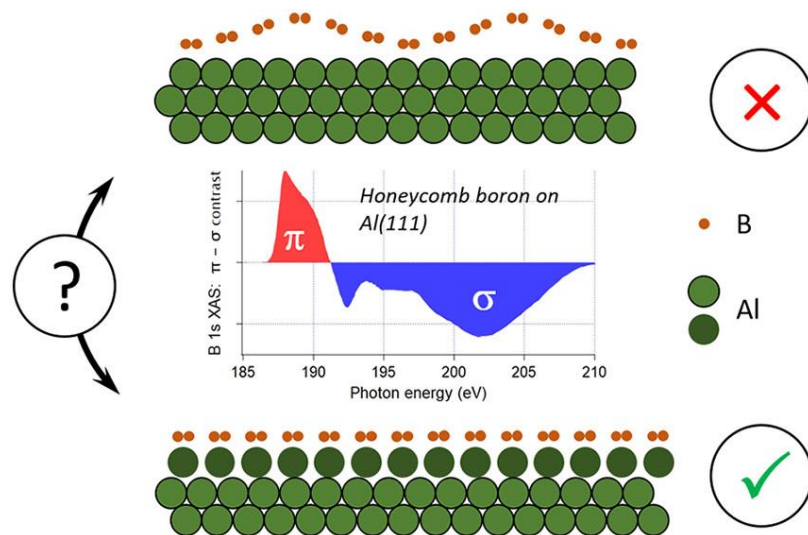
- **The ranking of the accomplishments are done by only HPC USERS, following very specific rules**
- **A three-step process is used:**
 1. First the submission has to be complete with a clear “value” shown
 - Some submissions were good, but needed a little more information
 2. Secondly, the HPC User Forum Steering Committee evaluates if the submission presents a realistic assessment of the value/returns
 3. Then, in cases where the value isn’t clear or a deeper technical depth is required, the final evaluation is by experts in the specific area/discipline

SC22 Winners: HPC User Innovation Awards

HPC-driven design of innovative functional materials for catalysis, energy conversion, and storage

Andrey Lyalin, Hokkaido University ICReDD

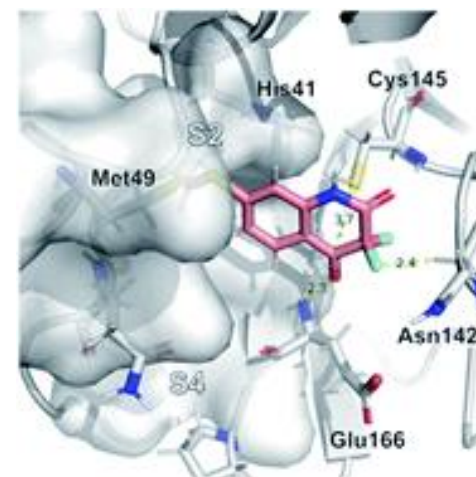
- Successfully predicted a variety of unique materials for catalysis, energy conversion, and storage applications which were then experimentally confirmed
- Developed novel computational methods in quantum chemistry, materials informatics, and machine learning that can be used to discover further materials for energy and environmental applications



Fast-track computationally-driven discovery of new SARS-CoV-2 Main Protease (Mpro) inhibitors: from HPC to experimental drug candidates

Jean-Philip Piquemal, Sorbonne Université and Qubit Pharmaceuticals

- **Synthesized 2 new families of compounds in less than 3 months that were experimentally validated**
- **Produced a high-resolution molecular dynamics simulation of the SARS-CoV2 Main protease protein**
 - Modeled interaction with water
 - Unraveled potential druggable sites
 - Identified potential drug candidates
 - Predicted absolute free energies of binding with potential active molecules
- **Opens routes for further drug discovery and design**



**SORBONNE
UNIVERSITÉ**



Qubit
pharmaceuticals

An automated agent-based simulation method for the prediction of intensive care unit (ICU) occupancy due to COVID-19

Ralf Schneider, High Performance Computing Center Stuttgart

- **Weekly production of 4-week forecasts of ICU occupancy in Germany due to COVID-19**
 - This is the first time that a federal HPC-center in Germany delivers such a service in production
 - This proved for the first time that HPC for Global System Science can support decision makers in critical situations and can make a difference for society.
- **Forecasts are simulated by a model initially developed by the Federal Institute for Population Research**



High-Performance Computing Center Stuttgart

AI-based emulator of Computational Fluid Dynamic simulations for urban wind flow and gas dispersion

Francisco Ramirez Javega, Bettair Cities SL



- **Air pollution is the single largest environmental health risk in Europe and a major cause of premature death and disease, but most urban air quality problems are hyper-local (e.g., land use, traffic)**
- **Ran CFD simulations of wind flow and dispersion patterns on a large data set and trained a DNN to simulate the results at a fraction of the time and cost**
 - This research empowers local communities, municipalities, and regional governments with accessible, actionable information about local emissions in real-time
- **This work has been funded within the FF4EuroHPC European project, Experiment 1012: Improving Bettair Air Quality Maps**
- **Part of the project was performed by a team from the Barcelona Supercomputing center using ALYA**

LS-DYNA Scaling with the direct implicit solver

Todd Simons, Rolls-Royce



- **Provided a grand challenge problem with 200 million degrees of freedom, a large thermo-mechanical model of a gas turbine engine.**
- **Collaborated with the developers of LS-DYNA to make improvements with their implicit solver so that it would run at scale (on 16,384 cores), reducing time to solution from over 1,000 hours to 10 hours**
 - Able to incorporate high fidelity modelling in the design cycle rather than being used as a post-design analysis
 - Able to influence design with high fidelity digital twins that can provide better designs and improve fuel efficiency of gas turbine engines
- **This project utilized resources at Oak Ridge National Lab through a US DOE proposal**

Thank you!

For questions:
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