

High Performance Computing for Manufacturing:

Using Supercomputers to Improve
Energy Efficiency and Performance

May 2021



PROCESS OPTIMIZATION



PRODUCT PERFORMANCE



MATERIALS DISCOVERY



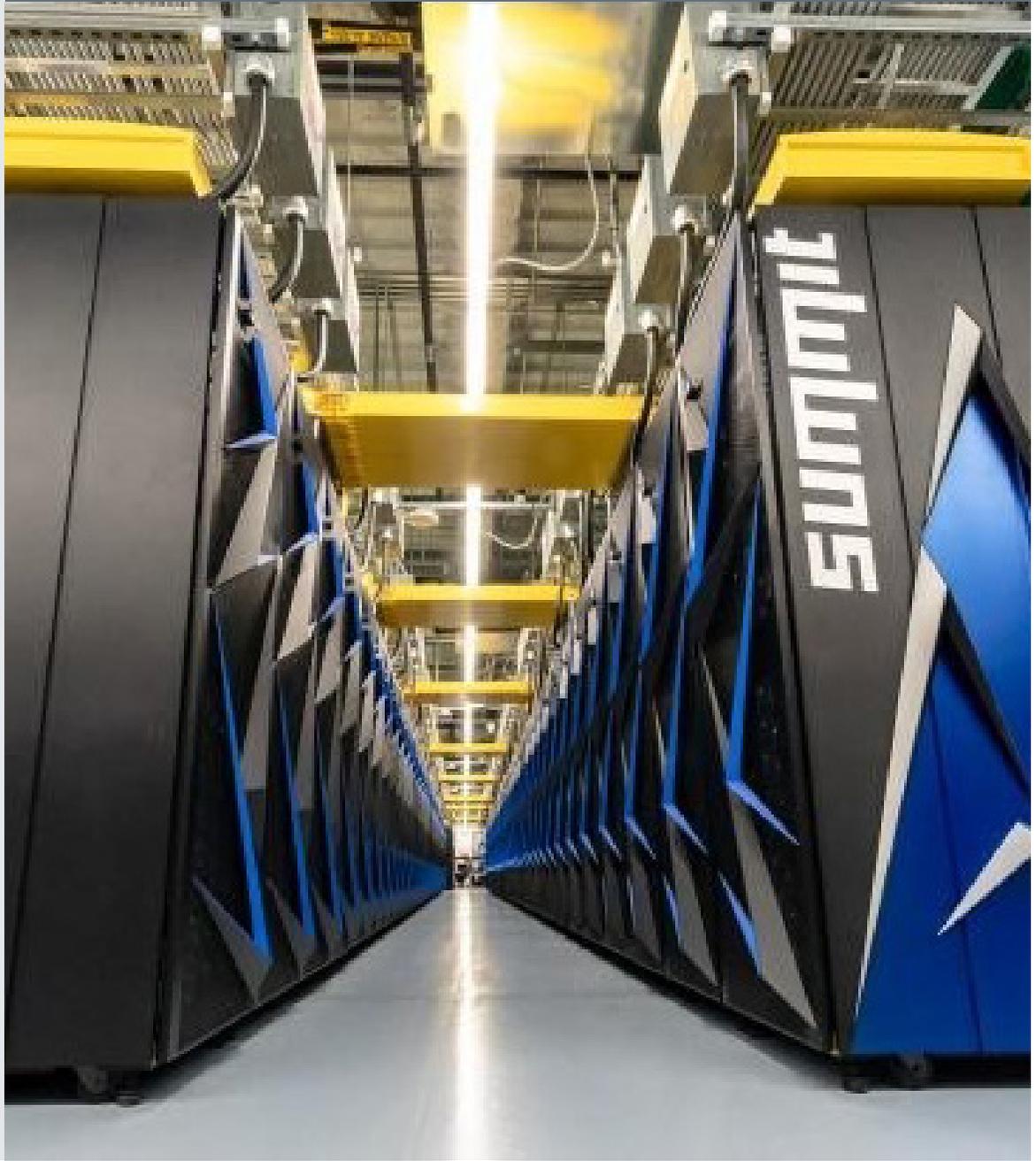
NOVEL DESIGN



PERFORMANCE PREDICTION



**ACCELERATED
MARKET ENTRY**



High performance computing offers an extraordinary opportunity for the United States to design products faster, minimize the time to create and test prototypes, streamline production processes, lower the cost of innovation, and develop high-value innovations that would otherwise be impossible.

**Modeling, Simulation and Analysis, and High Performance Computing:
Force Multiplier for American Innovation**
Council on Competitiveness

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About AMO

EERE's Advanced Manufacturing Office (AMO) partners with industry, academia, states, and National Laboratories to catalyze R&D and the adoption of advanced manufacturing technologies and practices. AMO works to increase material and energy efficiency in manufacturing to improve energy productivity, drive economic growth, and shrink the sector's carbon footprint.

AMO's High Performance Computing for Manufacturing Program (HPC4Mfg) awards federal funding for public/private R&D projects aimed at solving key manufacturing challenges. Under the program, each selected industry partner gains access to the DOE National Labs' supercomputers and expertise. These collaborative projects help these industries become more competitive, boost productivity, and support American manufacturing jobs.

The HPC4Mfg Program is a part of the High Performance Computing for Energy Innovation (HPC4EI) initiative. In addition to manufacturing, the initiative includes subprograms for materials and mobility.

HPC Overview: The Next Frontier in Manufacturing Innovation

Supercomputers help companies solve complex manufacturing challenges—and deliver new ways to innovate, improve performance, and cut costs.

High performance computing can help solve some of the toughest technical challenges in manufacturing. Manufacturers have relied on computers for modeling during process and product development and in-plant troubleshooting for decades. Recent increases in computer processing power have enabled dramatically faster and more accurate modeling, simulation, and data analysis.

Supercomputers are the apex of computing capability; they are the fastest, most sophisticated computers available for many applications. They can run large models that create more realistic ‘virtual’ physical systems. As a result, complex behavior in a system can be studied in great detail. Applying this advanced technology to research, problem-solving, and innovation is, for purposes of this document, called high performance computing (HPC).

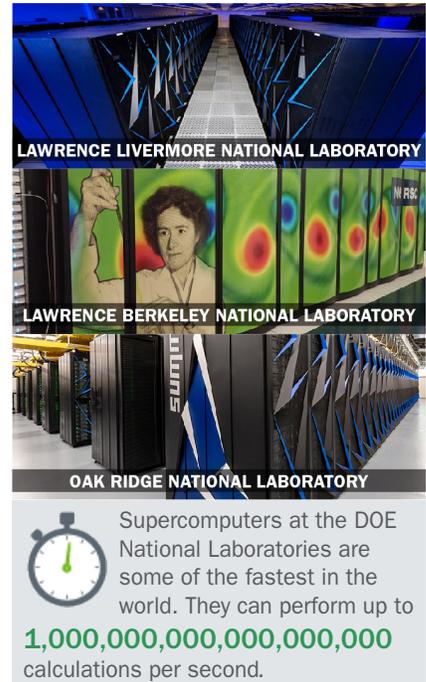
In manufacturing, HPC is used to:

- Simulate the operation of highly complex processes and advanced technologies
- Accurately predict the effects from changing design configurations
- Rapidly analyze huge data sets
- Gain a deeper understanding of the underlying physical behavior to inform decision-making.

HPC offers enormous potential for future innovation. HPC helps researchers understand complex interactions and identify the best ways to improve performance, increase energy efficiency, and cut emissions. HPC offers solutions for previously intractable problems. It helps manufacturers:

- Design and test products faster
- Predict failures and improve quality
- Streamline production processes
- Lower energy and material use and costs
- Accelerate innovation and sector progress toward zero-carbon emissions.

Supercomputers—with ultra-fast speeds and massively parallel processing—can run models that deliver highly detailed and realistic simulations.



What are supercomputers?

Supercomputers are among the fastest, largest, most powerful computer systems available. They are used to simulate behavior in complex physical systems.

What is high performance computing?

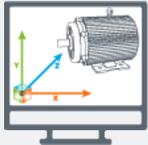
HPC is the use of supercomputers, sophisticated models, and large data sets to study and solve complex scientific and technological challenges.

Supercomputers can significantly improve products and processes by running far more accurate models much faster

Through DOE's HPC4Mfg Program, National Laboratory scientists—working with manufacturing companies—develop sophisticated computer simulations to solve complex challenges in industrial processes and technologies. The use of the nation's most powerful supercomputers and high-fidelity models increases the speed, accuracy, and scope of model predictions. HPC can accelerate innovation, improve performance, and cut costs in diverse applications.



Ultra-fast computations: HPC systems perform quadrillions of calculations per second. Results are delivered in hours or days (instead of weeks or months with smaller computers).



More detailed models: Large, highly complex physics models can be constructed to more accurately represent a physical system. In the model, mathematical equations describe the physical phenomena in the system—including billions of interactions over a span of time.



Large number of simulations: Thousands of design iterations can be run to predict the outcomes of proposed changes and optimize critical factors. The relative importance of variables and physical effects can be distinguished. Data from process sensors and controls, product samples, and experiments can be compared to the model outputs to validate model accuracy.



Idea Testing: Manufacturers can test and fine-tune new ideas virtually—before building the first prototype or making process changes. Computer simulations reduce the need for physical trial-and-error experiments, prototypes, and testing cycles—saving time and money.



Big data analytics: Advanced analytics can turn immense quantities of scientific and raw plant data into a more detailed understanding of physical behavior as well as useful simulation tools for in-plant use. Artificial intelligence (including machine learning and neural networks) can yield new, unforeseen insights and solutions.



Adjustable scale of analysis: Models can analyze phenomena at different length scales anywhere in a process or technology. Information from the micro- and macro-scales can be combined. Data also can be combined across time scales.



Better-informed decisions: Company decision-makers can have greater confidence in the results of technical analysis and their ensuing investment plans.

Throughout manufacturing, research and development (R&D) has improved energy efficiency and productivity over time. The more easily achievable progress has been made; the so-called ‘low hanging fruit’ have been picked. Problems and opportunities for improved productivity and performance remain, yet next-generation innovations tend to be more complex and carry higher risk. More sophisticated research approaches are needed to identify opportunities. Detailed analysis with HPC can discern cost-effective ways to improve productivity, increase sustainability, and save energy.

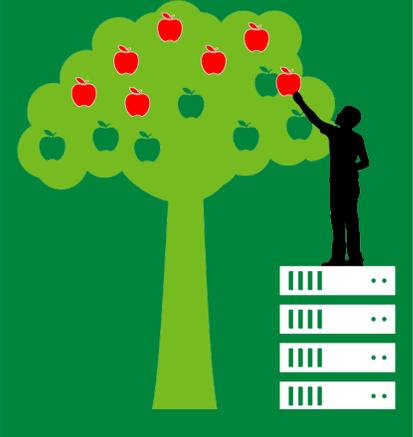
Manufacturing systems are complex due to numerous interacting physical phenomena and variables. These factors influence performance to different degrees, and even small changes can have ripple effects throughout an entire system. A greater understanding of these interactions helps manufacturers leverage the phenomena for productive uses.

Modeling, simulation, and analysis with HPC helps manufacturers predict the behavior of physical phenomena in a select area of a complex system. Once a numerical model is built and validated, variables can be changed to predict the effects and answer specific questions about system performance. Products can be optimized before building the first prototypes or risking disruptions to plant operations. Modeling and simulation are especially useful in harsh manufacturing environments, where current sensors cannot survive. Machine learning (ML) and other artificial intelligence (AI) approaches—that are beyond the capability of typical data-processing software—can extract useful information from very large or complex data sets and reveal new ways to improve performance and efficiency.

Manufacturing is extremely diverse, with many different and complex processes and products. HPC is a cross-cutting technology that can be used in problem solving in a wide range of applications. Supercomputers help evolve legacy industries (like iron and steel) and more recent manufacturing sectors (like additive manufacturing). Multi-component advanced technologies as well as consumer products are improved with HPC.

HPC helps companies reach the ‘high-hanging fruit.’

HPC can be used to identify cost-effective energy savings opportunities that are still obtainable in manufacturing.



Examples: physical phenomena in manufacturing

- Turbulent flow of a liquid or gas
- Transmission of heat, electricity, or sound from one point to another
- Tension on the surface of a liquid
- Light reflected from or transmitted through a material
- Surfaces in contact creating friction and wear
- Condensation forming on exposed components
- Fine solid particles suspended in air or another gas.

Diverse industries and applications can make significant gains using supercomputer analysis

U.S. manufacturers bring difficult technical challenges to the DOE National Laboratories through the HPC4Mfg Program. Technical advancements have been achieved by HPC modeling, simulation, and analysis in the following applications:

 <p>Steel blast furnace optimized to reduce coke use and CO₂ emissions</p>	 <p>Lead furnace for converting reclaimed components into elemental lead</p>
 <p>Natural gas reactor design improvements</p>	 <p>Paper making with a more efficient microfiber configuration and drying process</p>
 <p>Catalysts that are more reactive and lower cost</p>	 <p>Coatings that are more resistant to heat and corrosion</p>
 <p>Turbine components that last longer in higher temperature operations (2,700°F)</p>	 <p>Data center processors with integrated magnetic inductors for DC-DC power converters</p>
 <p>Truck engines with synthetic fuel fluid-jet controls designed for ultra-efficiency</p>	 <p>Supercritical CO₂ (liquid phase) for more efficient power production</p>
 <p>Aluminum-lithium mixtures produced to make lightweight and stronger materials</p>	 <p>Additive manufacturing with new feedstock materials and melting systems, leading to more durable fabricated parts</p>
 <p>Membrane design for more efficient chemical separations and water purification</p>	 <p>Batteries with solid-state electrodes that are not a fire hazard</p>
 <p>Plastics with tailored properties to enable composting and energy savings</p>	 <p>Semiconductor deposition process modeling to improve interconnects in next-generation devices</p>
 <p>Emissive film designs that are low-cost and scalable to dramatically reduce energy use in diverse cooling applications</p>	 <p>Heat exchanger design for improved low-temperature waste heat recovery</p>
 <p>Welding modeling tools to minimize dimensional distortion and weld-induced residual stress</p>	 <p>Carbon fiber manufacturing optimization to reduce the energy intensity of the plasma treatment process</p>
 <p>Aluminum sheet metal processing strategies were analyzed with artificial intelligence to deliver desired performance</p>	 <p>Fiber spinning optimization to minimize energy consumption</p>

Manufacturers can access world-class supercomputers and expertise at the DOE National Laboratories. DOE's High Performance Computing for Manufacturing (HPC4Mfg) Program offers U.S. manufacturers access to the Labs' exceptional computing power and expertise. Leveraging these resources is a differentiator that gives U.S. manufacturers a competitive edge. Through the Program, our Nation's supercomputers are helping manufacturers achieve significant energy and cost savings, improve product performance, expand their markets, and grow the economy.

HPC4 MANUFACTURING

Manufacturers partner with the DOE National Laboratories through the HPC4Mfg Program.

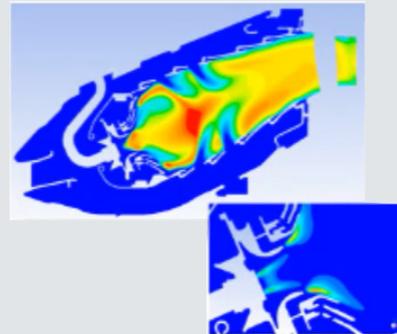
HPC can deliver significant new benefits to companies and consumers.

Economic and energy advantages accrue to U.S. industry, while delivering consumer benefits—such as new and higher-performing products with lower lifecycle energy use. By applying HPC, American manufacturers have the opportunity to capitalize on better predictive capabilities for competitive advantage.



High performance jet engine design

Project Goal: Use high-resolution turbulence models to design a new jet engine that significantly improves aerodynamic performance, durability, and fuel efficiency.



GE partnered with Lawrence Livermore National Laboratory (LLNL) and Oak Ridge National Laboratory (ORNL).
Photo from GE. Computational results images from LLNL and ORNL.

HPC contribution:

- Large jet engine study included the combustor and high pressure turbine components.
- Performed Large Eddy Simulations (LES) to understand the interaction of multiple physical phenomena impacting performance across three size scales to guide design optimizations.

Energy Impact Potential

- A 2% reduction in fuel consumption can save almost 1 billion gallons of fuel annually

VITRO GLASS

Machine learning can emulate scientific modeling and be incorporated into real-time process controls.

Engineers at Vitro Glass, in partnership with HPC experts at Lawrence Livermore National Laboratory (LLNL), created a machine-learning (ML) algorithm that allows the company to adjust furnace operations in real time.

Plate glass, commonly used in windows and doors, is produced in furnaces that melt raw materials, strip gases and impurities, and homogenize the glass. Small variations in this process can lead to temperature disruptions that affect the production efficiency and lower the quality of the final product.

Glass engineers have traditionally used complex computational fluid dynamics (CFD) models in the plant to observe these disruptions and devise strategies to return to normal production. Figuring out how to correct the process can take up to two weeks, during which

time the furnace cannot produce a viable product.

Engineers at Vitro Glass worked with researchers at LLNL to use HPC to reduce the time required to correct a furnace's operational parameters in the event of a process disruption. They developed a machine-learning tool that is much less computationally intensive than the original CFD model and can be used as a real-time furnace control system. This tool can run optimizations on a desktop computer at the plant in minutes rather than weeks. LLNL's supercomputer ran the simulations needed to generate the tool.

To build the tool, Vitro Glass identified a range of parameter settings of interest for its glass furnace. Then, LLNL researchers ran hundreds of CFD simulations to produce detailed predictions of

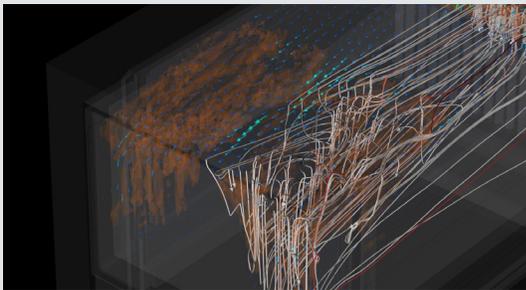
furnace operating conditions at these settings. The data from these detailed CFD simulations, combined with ML techniques, allowed researchers to train a neural network on how the system operations respond when an operator adjusts process parameters or when sensor readings change.

This tool can prevent roughly two weeks of lost production per furnace every year. The prediction tool can also significantly reduce the amount of substandard glass that must be discarded, increasing glass-manufacturing productivity by 2%. If implemented broadly, these improvements could save the U.S. glass industry approximately 2.5 TBtu of energy per year—nearly 4% of the energy used to produce flat glass.



Process modeling for glass melt furnace optimization

Project Goal: Leverage advanced visualization and analysis software coupled with machine learning techniques to develop a real-time process control system capable of running on a desktop computer at the plant.



Visualization of molten glass flows generated by computer simulations. *Computational results image from LLNL.*



Raw materials entering a float-glass furnace tank for production of architectural glass. *Photo from Vitro Glass.*

Vitro Glass partnered with the Lawrence Livermore National Laboratory.

HPC contribution:

- Use complex, high-fidelity computational fluid dynamics modeling to train machine learning code to extract the most relevant process parameters.

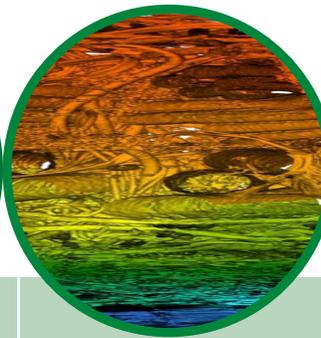
Energy Impact Potential

- 2.5 TBtu per year of energy if adopted industry wide — nearly 4% of the energy used to produce flat glass
- 130,000 metric tons of CO₂ emissions



Optimize manufacturing in ways not previously possible.

HPC helps industrial experts understand the impacts of interactions and how performance can be improved. Significant advantages can be gained in diverse applications, as shown in these examples.

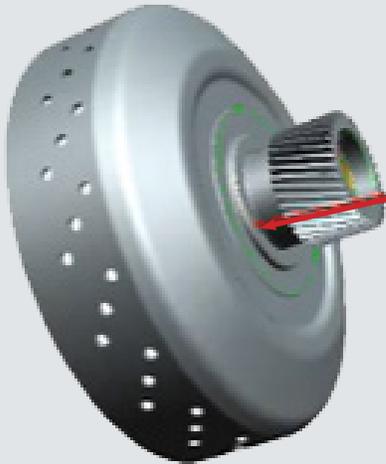


	Spray Painting & Coating	Paper Pressing & Drying	Steel for Lightweighting
Opportunity/ Problem	Paints and coatings could be sprayed on at a faster rate if the way droplets form and disperse could be highly controlled.	Wet paper reabsorbs some moisture when the pressure applied by rollers is released prior to drying.	Variations in steel (temperature, microscale structure, etc.) as it is rolled into thin strips affects its strength during end use.
HPC Challenge for Lab Experts	Develop an algorithm that models the fluid properties of droplets as they leave the sprayer under high pressure to form a fine mist.	Build a detailed, microscale model of the way water flows through paper during and after the pressing process. Validate using plant data and experiments.	Run multiple simulations of a computational fluid dynamics model to generate data. Feed that data into a machine learning tool that will help to develop a faster model for use at the plant.
Solution for Manufacturer	Use algorithms to engineer new paints and coatings that form a uniform mist and adhere evenly at much higher flow rates.	Use information from modeling to design more efficient processes and equipment.	Optimize a near-real-time model to accurately predict and control how steel is rolled and coiled.
Results	<ul style="list-style-type: none"> Reduces energy used for air-driven turbines. Applies coatings evenly to cut waste. Decreases paint booth size to reduce need for humidity and temperature controls. 	<ul style="list-style-type: none"> Significantly reduces energy for drying. Increases production speed and saves more energy. 	<ul style="list-style-type: none"> Reduces electrical and thermal energy for rolling. Improves steel quality and reduces rework. Reduces energy use in transportation applications.
Partner	PPG Industries, Inc.	Alliance for Pulp & Paper Technology Innovation	AK Steel



Laser welded dissimilar steel joints

Project Goal: Optimize weld design to eliminate weld cracking. Accelerate the use of laser welding technology to join components made with high-alloy, low-carbon steel and tool steel.



Full penetrating lap welds for transmission sun gear assembly
Weld width: 1.6mm; Weld depth: 6mm



Weld Crack

Weld improvements in transmission system compared to weld crack.
GM collaborated with Oak Ridge National Laboratory. *Photos from GM.*

HPC contribution:

- Captured the large thermal gradient in the weld zone in much greater detail (mesh size about 50 μm).
- Demonstrated material property changes at fast cooling rates in small time increments (5 milliseconds).
- Enhanced code reduces computational time from weeks to hours in ongoing research to scale up production and use of advanced high-strength steels in diverse areas of auto manufacturing.



Advanced high-strength steels can contribute to energy savings and emissions reduction

Energy Impact Potential

- 300 lbs. weight reduction equates to 4.5% fuel economy increase
- 164 million gallons of fuel saved per year if used nationwide

In-Depth: HPC Use in Manufacturing

Supercomputers can run more detailed models faster to more accurately simulate complex industrial problems.

1. WHEN IS IT APPROPRIATE TO USE SUPERCOMPUTERS INSTEAD OF CONVENTIONAL COMPUTERS?

Companies use supercomputers because their current computers and models are incapable of providing the computational speed, specificity, and certainty necessary for solving the complex technical challenges they face.

Analyzing increasingly complex problems requires progressively more computing power. In manufacturing, computer simulations now often complement traditional engineering techniques to solve complex problems. The steady increase in computational capability and model resolution (level of detail considered) has progressively enabled more accurate representations of physical systems for problem solving.

Companies routinely use desktop computers with computer-aided design (CAD) software to develop 3D models of a product and its components during the design phase. Often, this CAD software has a basic physics modeling capability that can predict performance at a limited level of detail. Other commercially available software packages offer more detailed modeling capabilities and can run on a desktop computer to study the simultaneous interactions of multiple physical phenomena, such as heat, stress, and chemical changes. Larger, more sophisticated multi-physics models, which can consider the impacts of interactions on performance at a level of detail that is up to hundreds of thousands of times greater, require larger computing platforms—like supercomputers and specialized software to run on them.

HPC makes it possible to study complex problems that cannot be addressed with other computers. HPC helps manufacturers when complex calculations are needed to find solutions. Conventional computers would take too long and lack the processing power to accurately represent a complex manufacturing system or predict results in enough detail. Some multi-physics models are coded explicitly for use on supercomputers; these models leverage computational capabilities that are not available currently on other types of computers.

Supercomputing compared to other types of computing used in manufacturing



Desktop and laptop computers are too slow. Personal computers can run many types of physics models but do not have the processing power required to solve more difficult problems in a practical amount of time. For example, it could take months to run one simulation of a complex problem.



Cloud computing cannot meet data exchange speed requirements. While dispersed cloud computing collectively has sufficient processing power to analyze highly complex problems, it does not deliver the fast networking speeds among processors required to solve large-scale problems in a practical timeframe.

If an extremely large number of calculations need to be computed to solve a problem, a supercomputer may be required. The threshold for deciding whether to use a supercomputer for a manufacturing problem is based on the number of calculations required to generate a solution with sufficient accuracy and precision within a reasonable period of time. The most difficult technical problems typically require a high level of detail, complex equations (and corresponding computer code), and many model simulation runs; therefore, these problems require more computer processing power to complete the calculations.

In manufacturing, HPC is reserved for high-impact projects with potentially high returns. Supercomputers are expensive and require specialized expertise to operate—they are not ‘plug and play’ devices. Because of the expense, HPC is reserved for projects with significant potential impacts and energy savings. Some manufacturing problems cannot be solved cost-effectively, even with HPC.

Most day-to-day manufacturing operations do not require supercomputers. Plant operations can be impacted by natural variability in feedstocks, ambient conditions, vibrations, unforeseen dynamic processes, automatic and manual adjustments, and many other factors. Sensors and controls are used in the plant to monitor system performance, provide feedback, and bring the system back under control if it goes off specifications. Recalibrating and optimizing a continuous manufacturing process can take hours, days, or weeks. Supercomputers are too expensive and complex for use in controlling dynamic manufacturing operations. However, they can be used to develop fast, accurate, in-line “reduced-order” models that can operate on personal computers at the plant.

Reduced-order models (ROMs) simplify the computational complexity while maintaining a detailed understanding of the behavior and effects. A ROM generated using ML, for example, can integrate the results of multi-physics models and sensor data. As a result, in-plant models enhanced with HPC can optimize a plant’s control systems in real-time (or near real-time). This can significantly decrease waste and downtime, as well as prevent added energy use from restarting processes.

Manufacturing systems can be so complex that the whole system is not modeled. Detailed HPC-scale models of entire manufacturing systems are rare, if they exist at all; they would take a long time to develop and run (perhaps years). For this reason, HPC is normally used only for important problem areas within a manufacturing application. Even this requires a significant investment in specialized software, the development of custom algorithms, and dedicated engineering talent. In addition, algorithms developed for other computers need to be reformatted into steps that can be calculated in parallel on a supercomputer.

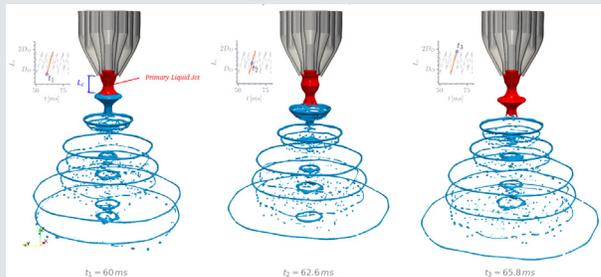
Threshold for using a supercomputer to solve a complex problem

- Size of the problem space, which is divided into myriad tiny zones
- Number of zones in the physical space to consider in simulations
- Number of physical phenomena interacting (and associated number variables) per zone
- Complexity of the phenomena and their interactions, which require more complex equations and calculations for each zone
- Number of simulations required to solve the problem.

EASTMAN

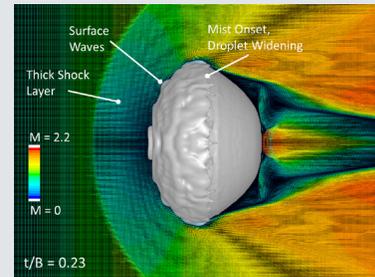
Optimizing slurry atomizers for large-scale energy production

Water cracking is an industrial process used to produce hydrogen gas for diverse applications. Complex injectors atomize the fuel slurry and feed it into the large-scale cracker for energy production. An advanced numerical interface tracking method has been developed to simulate the complex fuel atomization process. Eastman is using the methodology to gain insight into the spray physics and optimize the nozzle design to significantly improve the efficiency of the energy production process.



The interface between the fuel slurry and gas is shown at three different times. The primary jet is shown in red, and the atomized droplets are shown in blue.

Computational results images from Argonne National Laboratory.



Vector plot colored by Mach number of a normal shock wave moving from left to right in air just having passed over a single droplet of water.

Energy Impact Potential

- 2% energy savings—\$10 million reduction in fuel costs



AY

CRAY

CRAY

CRAY

Geo



2. WHY IS HPC USED IN MANUFACTURING?

Companies use HPC when more sophisticated computer simulated analysis is needed for research or problem solving. Manufacturing systems can be optimized in ways that were not previously possible—creating a new space for innovation and discovery.

A supercomputer’s enhanced processing capabilities deliver more information for better decisions. Compared to other computers, supercomputers today can provide a much more detailed understanding of complex physical systems and run a much larger number of simulated model iterations in far less time. This increases the accuracy of model predictions, reduces uncertainty and error, and enables product and process optimization.

Traditional ‘trial and error’ physical experiments can be too expensive, slow, risky, or infeasible. Historically, advancements in manufacturing have relied on repetitive trial-and-error development and experimentation. These research methods can be expensive and have inherent limitations. Understanding what is actually occurring in a system can be elusive. ‘Computational experiments’ on a supercomputer can explore complex manufacturing systems that are difficult to simulate using physical experiments and typical computers. They can consider complex physical interactions happening in real-world manufacturing environments.

HPC can reduce the need for sequential prototype development and other time-consuming trial-and-error experimentation—thereby lowering the overall costs of process and product innovation. At any point in the modeled space, a user can take simulated measurements of variables, including in locations with extremely high temperatures, corrosive chemicals, and rapidly changing conditions. Correcting design mistakes early in the process can increase safety. The underlying causes of behavior in a physical system that defied analysis in the past can be illuminated and understood.

An HPC analysis can provide the blueprint for improvement. HPC analysis can generate more robust design plans for processes, technologies, and consumer products—as well as increase confidence in investment decisions. HPC can shorten the transition from research to breakthroughs and market-ready products and accelerate the scale up of production from a small experimental system to a large, high-volume process. Ultimately, this research leads to more efficient and innovative manufacturing systems and products.

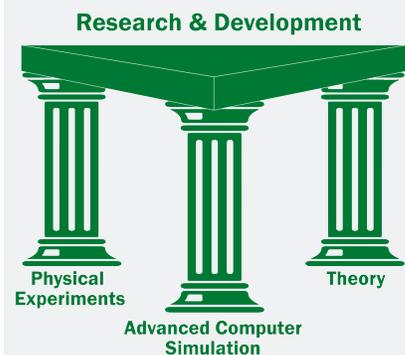
Companies are learning that the computational results simulated by HPC can have the same validity as physical experiments. Ultra-fast, HPC-driven simulations enable new pathways for discovery and engineering, especially when combined with AI and ML. HPC can now more accurately predict the behavior of complex systems, so it can be used as a “third pillar” for innovation. A cultural change is underway in companies as engineers and business leaders gain confidence in HPC simulations.

Ultra-fast supercomputers deliver **more:**

- Detailed understanding
- Simulations faster
- Accurate predictions

Leading-edge computing simulations provide new insights

HPC is changing the way manufacturers pursue science and technology development.



'Virtual' R&D with HPC provides new, advanced manufacturing capabilities that deliver benefits to both manufacturers and consumers

Computational experiments performed on a supercomputer can displace some traditional manufacturing research steps, enable investigative analysis that previously was not possible, and open up a new space for innovation.

- **Explore manufacturing systems that are too complex, dangerous, large, tiny, fleeting, or inaccessible for physical experimental methods.** Simulations can overcome the difficulties of experimental observation and reveal underlying mechanisms that cannot be accessed, viewed, or tested economically or at all.
 - Conditions can be assessed at any point in a modeled system, such as in harsh environments where sensors could not survive.
 - Scientific and technological questions can be answered to gain new insights.
 - Evolutionary details of chemical reactions can be explored; otherwise, they occur too quickly to be studied.
- **Reduce the need for physical experiments, testing, and prototyping.** Computer simulations offer a faster and more efficient way to iterate and optimize the design of processes and devices. They can be used with confidence to replace the need for costly physical 'trial-and-error' development steps. Testing cycles can be accelerated or, in some cases, eliminated.
 - Designs can be tested safely and errors can be corrected before building the first prototype.
 - Product 'use cases' can be run to predict wear and tear over time.
 - Failure of metal, plastic, and ceramic parts can be predicted and used to schedule preventive maintenance.
- **Optimize performance of new technologies and lower resource use.** New designs can be explored that push the limits of known technologies. Energy and material use (including critical materials) can be minimized. Diverse configurations can be investigated to evaluate tradeoffs and select the best design. HPC is opening a whole new space for discovery and applied research.
 - More robust control systems for plant operations can recalibrate and optimize performance in real time.
 - Lifecycle energy consumption of technologies can be decreased and compared.
 - Proposed process changes can be evaluated to reduce the risks and shorten the time to adoption.
 - Material and energy inputs, waste, and the number of rejected parts can be reduced.

3. HOW DO SUPERCOMPUTERS SOLVE COMPLEX PHYSICS PROBLEMS?

To solve a complex challenge, a supercomputer runs a sophisticated model that is capable of representing a manufacturing system at a high level of detail. To compute a solution, simple computational steps are broken up and distributed among thousands of processors. More than a quadrillion calculations are executed every second by the processors, which are grouped on the nodes. Interim answers are stored on nodes until needed by other nodes for their calculations. Parallel processing of these computational steps and the coordinated exchange of interim data—all at ultra-fast speeds—enable more detailed and accurate simulations and predictions.

Supercomputers contain tens of thousands of processors, thousands of nodes, and extremely fast network interconnections to expedite communication.

Nodes contain the processors that perform computations. The number of nodes and processors is often used to characterize and compare supercomputers. Characteristics of a supercomputer include a large number of the following:

- **Processors** are the data processing units that read and execute compute instructions from the multi-physics model and carry out the computational steps. Each processor works on an individual compute step of a specific task while other processors simultaneously work on other steps. Each processor typically handles different types of computational tasks. Supercomputers have tens of thousands of processors operating simultaneously.
- **Nodes** are fundamental units of a supercomputer. Each node consists of multiple processors connected together as well as on-node memory. Nodes receive and send information to other nodes within the network. For example, they serve as redistribution points for hundreds of compute operations needed to solve a set of equations.
- **High-speed interconnections** are used to connect all of the nodes together in a network. They enable ultra-fast coordination and data exchange between nodes so they can efficiently collaborate on different steps of the same computational task at the same time.

HPC in manufacturing applications entails the use of supercomputers and multi-physics models

Supercomputers

- Ultra-fast processing speeds
- Many processors to perform calculation steps
- Parallel processing of data
- Nodes to redistribute interim calculation results
- High-speed interconnections and other peripheral supports.



Extremely detailed multi-physics models

- Mathematical equations to represent multiple important physical phenomena
- Coupled calculations with each phenomenon to represent interactions at each point in the modeled system
- Sophisticated computational approaches to mathematical problem solving
- Simulations of dynamic, complex behavior over a time span and at various scales (resolutions).

Software models translate physics equations into a long series of simple computational steps.

Supercomputers are the hardware used to run detailed models. The model provides detailed instructions for computing a massive number of calculations. Instructions for executing the steps in parallel on a supercomputer must be established by the model.



Instructions for the calculations to solve physics equations are broken down into simple steps. Technical problems in a manufacturing application are solved by computing a long series of mathematical tasks broken down into steps.

- **The processors are the calculators for these steps.** A software program sends mathematical instructions to each processor so they can be executed. The processors do small computational steps and the results are shared with processors on other nodes. The mathematical operations that these processors do are the same as what can be performed with a four function calculator (+, -, *, /). Often, processors are dedicated to performing a specific function such as add, subtract, multiply, or divide. In parallel processing, diverse processors do many different things simultaneously. Supercomputers are the fastest ‘calculators’ available.
- **Each step is a ‘compute cycle’ to carry out instructions.** A processor receives an instruction from the model, executes a computational step, and saves results back to the memory on its node. Up to a quadrillion calculation cycles can be executed every second on a supercomputer.
- **Data is exchanged after the completion of a step.** Tasks run in parallel typically need to exchange data. The processors run calculation steps and store interim results (data useful for other calculations) locally on the nodes where they are computed. The data generated is stored until needed by other nodes as inputs for their subsequent calculations. Solutions to interdependent sub-problems require frequent exchanges of partial results between dispersed nodes. Supercomputers have extremely fast networking hardware to facilitate these exchanges. As a result, supercomputers can work on hundreds of thousands of interconnected math problems at the same time.
- **Completion of the tasks/steps leads to a solution to a problem.** Calculations are coordinated by the nodes and simultaneously computed on thousands of processors. Each step contributes to completing a mathematical task. To complete a task, results from steps calculated on diverse processors are recombined. The supercomputing software provides an overall control/coordination mechanism to bring the results together and compute an overall solution.

Meshing

To show the complex interactions among diverse physical phenomena (and variables), physics equations use a process known as meshing. Meshing breaks the problem space into small 3D portions called zones.

For each zone, a typical model may incorporate five to ten equations that mathematically describe separate physical phenomena. Each equation may include one to six variables to simulate a phenomenon’s behavior and interactions.

The behavior in each zone can impact neighboring zones. Model iterations enhance understanding of how a system behaves under a defined set of conditions and may lead to better control of physical phenomena to improve system performance.

The instructions for solving physics equations are translated into code.

Every equation in the model has to be translated into computer code such as C++ or other high-level language. This code provides instructions for solving complex problems with simple calculations. In addition, software called a compiler is used to translate the computer code into machine language (binary 0 and 1 bits) before the computer can execute the calculations..

Parallel processing provides the ‘special sauce’ of a supercomputer: multiple processors working together to perform quadrillions of calculations every second.

Ultra-fast speeds are achieved by breaking problems into pieces and running them in parallel on thousands of processors. Mathematical problems are separated into pieces, and the supercomputer coordinates and calculates the problems simultaneously on numerous processors. This parallel processing enables supercomputers to concurrently execute up to a quadrillion calculation steps every second across a network of thousands of computer processors. This level of computing power is needed to simulate behavior in complex systems.

Nodes provide an important infrastructure element that enables parallel processing. In addition to nodes, high-speed interconnect hardware and data input/output capability are required to deliver the rapid networking connections needed. Massively parallel processing of computations requires the rapid retrieval of stored data and compute instructions. Supercomputers also need large storage capacity; high-resolution and/or large-scale problems require a large amount of storage.

What is ‘parallel’ processing?

‘Massively parallel processing’ is the use of a huge number of computer processors to simultaneously perform coordinated computations (i.e., in parallel).

Supercomputers can run more detailed simulations in less time because the steps to complete tasks are broken up and distributed among thousands of processors.

Large, complex multi-physics models can provide instructions to run hundreds of thousands of computational tasks at once.

Mathematical descriptions of the physics are translated into computer code

Describe → Translate → Calculate

Mathematical equations are used to describe physical phenomena.

This understanding is encoded into bit patterns that are used in calculations.



**Physics Equations
(predictions of behavior)**



**Computer Code
(instructions)**



For manufacturing problems, parallel processing enables thousands of processors to efficiently collaborate on solving interlinked physics equations.

Complicated math equations describe the complex interactions among multiple physical phenomena that occur concurrently in a manufacturing system. Steps to solve the equations are computed simultaneously; data is generated and nearly instantaneously exchanged to compute the effects of the interactions on behavior in the system.

The speed of the calculations is measured in Floating Point Operations Per Second (FLOPS).

Floating point numbers are the standard for how numbers with a decimal point are stored and processed in computers. A computer that runs calculation steps at a rate of 10 FLOPS computes 10 of these operations per second. Desktop computers run at a rate of billions of FLOPS. Supercomputers run at a rate of quadrillions of FLOPS—millions of times faster than a desktop computer.

A supercomputer's powerful processing capabilities permit many more iterations of a multi-physics model in less time—significantly improving the model's accuracy and predictions.

Supercomputers have high-throughput processing capabilities, so they can run hundreds or thousands of simulated iterations in hours or days.

Other computers would take weeks, months, or years to process the same amount of data. Plus, these simulations show more detail and finer increments of change.

The difficulty of the technical problem typically determines the number of simulation runs needed to optimize a system design. Likewise, the scale of the problem and complexity of the equations (and corresponding computer code and number of calculations) determine how much time the computer will need to complete the calculations.

With atomistic modeling advancements, the behavior of atoms can now be analyzed to predict properties and performance during a production process or the use of a technology over a range of time scales. With adequate computing platforms, phenomena can be studied at both tiny and large scales—and this analysis can be mathematically interlinked in the same multi-physics model.

Supercomputers can run model iterations much faster

Supercomputers can do in one day what it would take an average personal computer 20 years to achieve.

Supercomputers enable users to:

- Cut down the time it takes to conduct experiments
- Explore dozens of ideas quickly
- Iterate quickly to accelerate research progress.

Engineers study how to prevent and predict material failure by understanding phenomena across size scales

0.5 nm **m**

Material defects originate with the behavior of atoms and molecules. For example, uneven cooling rates can create a patchwork pattern at the nanoscale.

Mass material behavior over time can cause cracks to occur during use.

Glass Fiber Manufacturing

Optimizing the extrusion process to prevent glass fiber breakage, downtime, waste, and energy loss

To make glass fiber, molten glass is pulled through pin holes in nozzle tips—4,000 fibers at a time per station. The diameter of the fiber typically ranges from 3.5 to 20 μm , depending on the application. During this extrusion process, if even one fiber breaks, the entire production process of the station must be shut down and manually restarted, which takes over an hour. Breakage is a long-standing problem across the fiber industry.

Understanding the mechanisms of fiber breakage can help engineers modify the process and increase yields. However, at 1600 K (over 2,400 °F) sensors and conventional measuring devices cannot survive. HPC can help understand the causes.

During the complex transition from molten glass to individual solidified fibers, diverse physical phenomena and variables are controlled. The design of the manufacturing process leverages the phenomena and impacts performance. The key factors include the following:

- Interface materials (what the glass comes in contact with) at each station
 - Furnace that melts the input materials and the reservoir of molten glass located above the nozzles
 - 4,000 bushings—the material that lines the tips of the nozzle openings; an electric current passes through each bushing to create radiant heat while the molten glass pours through pin holes
 - Spool winder for the solidified glass fiber
- Glass temperature must be carefully controlled throughout the entire process
 - Radiant heat transfer rates from the glass to the air control the phase transformation from liquid, to multi-phase, to solid
 - Air flow variations and humidity affect glass cooling rates and heat distributions
- Glass composition (includes impurities and bubbles) impacts glass viscosity and

the velocity at which it flows through the bushings.

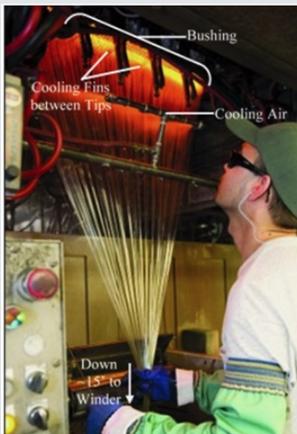
- Glass fiber is ‘pulled’ from the nozzles at a specific drawing rate and angle to minimize variation and stabilize the glass until it is spooled on the winder.
 - As the pulled fiber narrows and solidifies, the geometry (size/radius, shape, thickness, and surface area of the ‘cone’ of glass) and the stress (pressure and tension on the glass) must be controlled.
 - The fill level of the reservoir and the distance between the reservoir and winder impact the pulling process.

Imagine tracking one drop of molten glass—and following what happens at the microscopic and macroscopic level—as it transforms to a delicate room-temperature fiber of glass. Accurately simulating a process at this level of detail can help optimize production and save energy and materials. That’s the promise of advanced large-scale modeling with supercomputers.



Modeling the glass fiber pull process to show the causes of breakage

Project Goal: Develop a model of heat flow and fluid motion as molten glass flows from a reservoir, is drawn through a nozzle, and solidifies into a glass fiber.



Nippon Electric Glass (formerly PPG Industries, Inc.) partnered with Lawrence Livermore National Laboratory. *Photo from Nippon Electric Glass.*

HPC contribution:

- Proprietary, commercial, and lab-developed physics code were combined in a large computational fluid dynamics model and run on a supercomputer. For the first time, non-uniformities in the temperature distribution and glass flow from the furnace were revealed and linked to the behavior of individual fibers.
- Preliminary plans for a more detailed model were developed—coupled with plans for physical experiments using high-speed photography to validate model results—to better understand diverse aspects of the fiber drawing process.

Preventing glass fiber breakage can improve the efficiency of producing fiberglass and other fiber applications.

Energy savings potential industry wide:

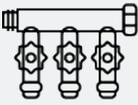
- 1.7 trillion Btus
- \$8.5 million

Increasing fiber yield by 1% could lead to an additional \$1 million in saleable product per year:

- Reduce production downtime
- Reduce material waste

Interactions among physical phenomena: examples from manufacturing applications

Multi-physics simulations help manufacturers examine the effects of interrelated phenomena in any combination, providing a more accurate prediction of behavior than examining each effect separately. The following examples describe the relationship between phenomena to illustrate how an analysis of interactions can improve understanding and performance.

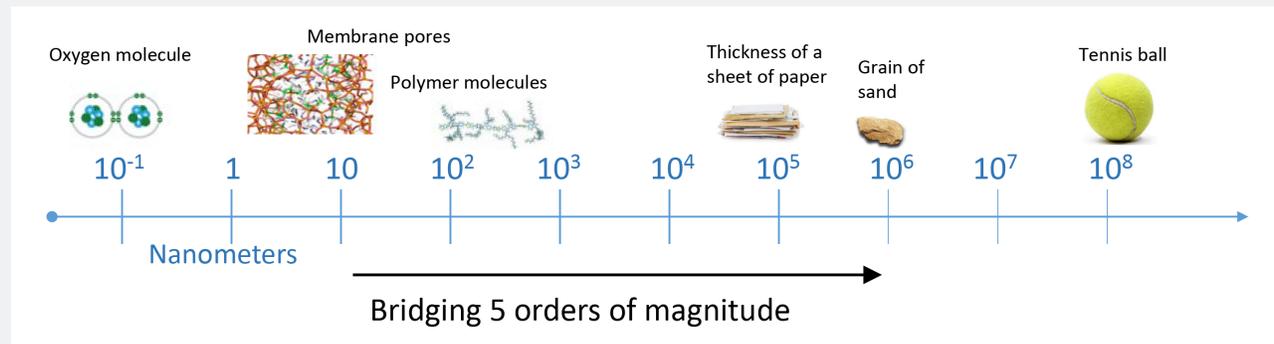
Application in industrial process or equipment	Interacting phenomena	Manufacturers' need for detailed understanding of physical behavior
 Electronics manufacturing	Electrical Current Flows + Temperature	Define conductor and insulator specifications to effectively manage heat dissipation in electrical equipment
 Piping networks for high temperature fluids	Temperature + Pressure	Determine induced stresses and displacements on piping structure from the thermal load and fluid flow to inform pipe system design and selection of materials
 Motors	Electromagnetic Fields + Temperature + Mechanical forces	Pinpoint stress points in motor components from heat and vibrations so new designs can be optimized for reliability and efficiency
 Novel compounds in chemicals production	Chemical Reactions + Flow + Temperature	Predict heat and mass flows in transport reaction processes to determine energy and material requirements in a new system
 Paper drying	Flow + Pressure + Mechanical Forces	Predict flow changes at various pressures to better inform paper pressing configuration
 3D printing metal	Electromagnetic Fields + Temperature	Determine relationship between optical laser power and applied heat for uniform temperature gradient in metal powders
 Crystal growth	Chemical Reactions + Temperature + Flow	Predict heat and mass flows in chemical reaction processes to optimize defect-free growth of crystals
 Water purification	Pressure + Flow + Conductivity	Identify charge interactions of water, ionic species, and membrane materials with respect to flow and pressure to increase efficiency in water purification
 Protein separation	Conductivity + Surface Energy + Flow	Evaluate how conductivity and surface energy modalities on proteins affect protein binding efficacy and location
 Spray drying (atomization)	Flow + Temperature	Predict mass, heat, and momentum flow in transport problems to determine design requirements for dryers
 Material failure	Temperature + Pressure + Structural Mechanics	Determine the thresholds for maintaining structural integrity under extreme pressure and temperature conditions

Supercomputers can bridge length scales and include a high level of detail

The behavior of physical phenomena can have different impacts at very small scales (e.g., nanoscale) as compared to large scales (e.g., macroscale). Supercomputers can be used to conduct analyses that simultaneously consider behavior at different size scales. This type of analysis can be used to solve manufacturing problems. Supercomputers can model behavior in a system at tens of thousands to hundreds of thousands times greater resolution (level of detail) compared to other computers. Thus, supercomputers are capable of bridging scales four or five orders of magnitude greater than models run on ordinary computers.

Bridging scales example:

Understanding nanoscale physics—such as fluid behavior moving across membrane pores—involves modeling interactions that occur at about 100 nm or less in length. To study the impact of these interactions at the macroscale (visible to the naked eye), the interactions must be scaled by at least four orders of magnitude, or 10,000 times greater, to about 1,000,000 nm—which is about the size of a grain of sand. This amount of scaling requires modeling and calculating an enormous number of nano-sized interactions.



Interactions and effects of physical phenomena often take place across a range of measurement scales.

Scales are used to measure a relative size, quantity, or quality of something, and characterize degrees of differences. Comparisons across scales help scientists organize and understand information and investigate phenomena.

Scales of different lengths can be considered in models at the same time (bridging scales). For example, material behavior that is observed and measured at the nanometer scale can affect performance at the meter scale.

Temporal scales are the period over which events occur. For example, chemical reactions can be measured in a timespan from milliseconds (one thousandth of a second) to years.

Spatial scales are the extent of an area (or region) over which something happens. Different areas of a problem can be studied at different levels of detail. For example, the performance of a computer chip can be analyzed with a spatial scale of a square picometer, nanometer, or millimeter.

How are multi-physics models different?

Multi-physics models provide deeper insight into the behavior of complex manufacturing systems. Multi-physics models mathematically describe the interactions among the most important physical phenomena in the problem space of the system studied. In addition to simulating the behavior of each physical phenomena individually, these models computationally describe the intricate interactions between phenomena. This is called ‘coupling.’

What types of data are used in multi-physics models?

Most of the data used in multi-physics modeling are generated by the model itself—specifically, data are generated by solving physics equations, and those data help solve subsequent equations. Physics data from other sources, such as experimental or sensor data, are used to establish initial and boundary conditions and to verify and validate performance and predictions.

- **Model-generated data:** A multi-physics model mathematically characterizes the interactions and impacts of physical phenomena in a system, and it provides approaches for solving the equations. Physics data are generated by computing these equations. These data include the properties, quantities, and qualities of each phenomena. This is the main type of computer-generated data used in multi-physics models of manufacturing systems.
- **Research data:** Scientists and engineers have amassed large amounts of experimental physics data from decades, sometimes centuries, of published scientific and engineering research on physical phenomena.

What are multi-physics models?

Multi-physics models mathematically describe the interplay of diverse physical phenomena and variables in a system. They can simulate the complex interactions and isolate the relative effects of each variable.

Once a model is generated, changes can be made to predict the effect on performance.

‘Multiple’ physical effects can be studied and compared at different size scales.

Simulating the interactions among phenomena requires solving complex mathematical equations.

- **Company data:** Manufacturing companies collect data from their products, technologies, and operations (including sensor data). More recently, this may include proprietary data received from mechanical and electronic devices connected through the internet. Company datasets are often used to verify the results of physics models.
- **AI and numerically generated data:** Data can be generated from computer-driven numerical analysis. AI and ML approaches can be used to identify patterns in the data for potential use in multi-physics models. This data can also be used in other ways to accelerate research and improve performance in diverse manufacturing systems.

Physics data used in multi-physics modeling of manufacturing systems

Main source:

- Computer-generated physics data generated by calculating physics equations that characterize the system; these equations describe mathematical relations defined by theories and laws of physics

Other sources:

- Experimental physics data measured through research at a laboratory, plant, or on operating equipment
- Performance data measured in plant operations/equipment
- Sensor data from a production process or product
- Control system data from a production process
- Product-use data from sensors embedded in products
- Numerically generated data from AI and numerical analysis of large data sets (without plant or product operations data)
- Numerical results from modeling on a different computing platform
- Data to re-test plant models on a supercomputer (after applying HPC results in the plant and collecting new data).

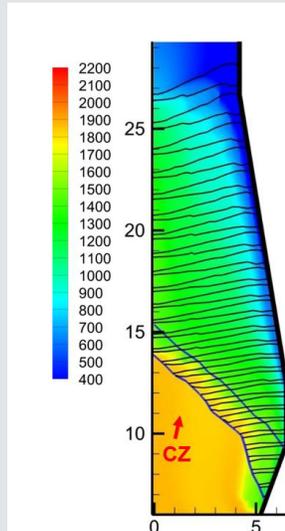


Blast furnace optimization for smelting

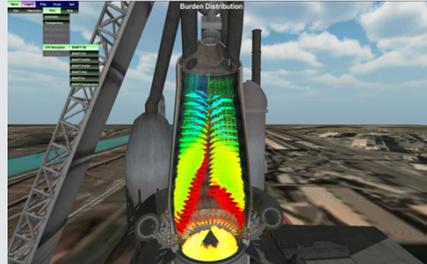
Project Goal: Develop model to simulate new blast furnace operating conditions that increase natural gas use (and reduce coke use)—significantly reducing furnace energy use, carbon emissions, and process costs.



Stelco and the Steel Manufacturing Simulation and Visualization Consortium (SMSVC) partnered with Lawrence Livermore National Laboratory.
Photo from Stelco.



Temperature profile with new optimal fuel mix.



Computational results image from Lawrence Livermore National Laboratory.

HPC contribution:

- Upgraded existing blast furnace models to run on HPC clusters.
- Simulated complex reactive flows of coke and iron ore particles to identify optimal furnace conditions and set points with higher natural gas injection rates.
- Discovered optimal furnace conditions that save 25 kg/thm of coke while maintaining stable operating temperatures.

Energy Impact Potential

- 1.4 trillion Btus/yr in a blast furnace producing 6500 thm/day

DOE's HPC4Mfg Program

Manufacturers bring complex problems to the DOE National Laboratories.

Manufacturers can access HPC at the DOE National Laboratories—and leverage world-class resources for competitive gain. The DOE HPC4Mfg Program offers U.S. manufacturers access to the nation's most powerful supercomputers, advanced software models, and specialized expertise. The Program helps manufacturers to

- Address tough problems that they are unable to solve on their own
- Push the boundaries of knowledge to advance technology innovation
- Discern new information that otherwise would be impossible to calculate.

The steps often taken during an HPC4Mfg project are described below. Companies identify important technical challenges that large-scale HPC can uniquely address. Experts at the Labs help conduct the HPC research project, and a company-designated lead collaborates to steer the project toward feasible, customized solutions. After modeling manufacturing challenges on supercomputers offsite, solutions are brought back to the company, where they are likely to influence investments and make an impact.

At the National Labs, government resources that are not available elsewhere can be applied to U.S. manufacturing challenges:

- Supercomputers that are among the world's largest, fastest, and most sophisticated.
- Computational scientists that possess the expertise needed to maximize the use of supercomputers.

HPC provides a previously unavailable R&D capability to solve complex problems in manufacturing.

Examples of HPC activities conducted at the DOE National Laboratories for manufacturers

- Explore the complex interactions among physical phenomena in the system
- Include more interdependent variables at higher resolutions (smaller size scales) in 1D, 2D, and 3D models
- Speed up modeling simulation time so more data can be considered to reduce uncertainty
- Develop new physics algorithms that capture scientific knowledge of physical phenomena
- Scale up new understanding to improve plant operations
- Test theories and innovative design ideas
- Determine the experiments needed to validate model results
- Use models to validate experimental results
- Conduct experiments to validate model simulations
- Compare proposed improvements to existing performance
- Use simulation data to set up machine learning reduced-order models for faster computation on smaller computers
- Use machine learning in plant process controls.

HPC4Mfg Program helps manufacturers improve and optimize a system in a way that leads to product benefits while lowering costs, energy and material use, and emissions. Through the HPC4Mfg Program, manufacturers have access to new R&D modeling techniques and numerical methods. This advanced research capability enables manufacturers to reduce energy and material use during manufacturing—and design and manufacture better, higher-value products that are more energy efficient during end use. Furthermore, HPC is a strategic way to reduce costs. A wide range of benefits are possible once the knowledge gained from research is implemented in the plant or incorporated into existing/new products and technologies.

HPC is new for most companies. Early adopters are leading the way. Many companies have limited (or no) experience estimating the return on investment (ROI) on difficult computational efforts, so they are often reluctant to fund HPC research projects. A computational leader in a company typically takes on the challenge of selling the benefits of HPC-enabled analysis to management. Once companies learn the value of better, faster product and process innovation, they are more willing to pursue an HPC project.

The capability to analyze highly complex problems was not widely available before. Advancements in computer simulation of physical phenomena, coupled with big data analytics, have launched a digital revolution in manufacturing R&D. HPC use is now considered by many manufacturers as essential to competitiveness. Companies not leveraging these new capabilities are learning they could be undercut by more sophisticated rivals.

Technical and economic benefits from HPC in manufacturing

Types of Benefits	Examples
Energy	<ul style="list-style-type: none"> • Lower lifecycle energy demand • Increased energy efficiency and performance
Materials	<ul style="list-style-type: none"> • Reduced material demand • Longer lasting materials • Lighter-weight materials • Reduced use of critical materials in short supply • Increased recyclability
Emissions	<ul style="list-style-type: none"> • Lower air pollutants • Reduced toxic emissions
Waste	<ul style="list-style-type: none"> • Fewer rejected parts • Less unused materials and byproducts
Costs	<ul style="list-style-type: none"> • Lower production costs • Reduced technology operating costs • Lower input costs of material and energy • Increased reliability / Reduced unexpected downtime • Better scheduling of preventive maintenance
Competitiveness	<ul style="list-style-type: none"> • Innovative designs that differentiate the manufacturer • New products that meet customer needs • New patents

Through the Program, DOE is promoting the uptake of advanced computing by manufacturers of all sizes. The HPC4Mfg Program is broadening the use of HPC to support transformational and early-stage technology development. Participating companies are learning that solving problems with HPC can lead to large savings in diverse applications. Results of this program are helping companies justify future investments in advanced computational analysis. Over time, U.S. manufacturers will increasingly turn to HPC modeling and simulation as trusted design tools. Maintaining an edge in the global economy will require the design and development of next-generation technologies and processes—and this innovation will require high-fidelity software and advanced computational technologies like HPC.

Applying to the HPC4Mfg Program

Companies can access the Labs through a competitive solicitation process. Applications are solicited twice each year. The R&D topics in the DOE solicitations directly align with AMO goals. Proposed projects should address technical challenges to save energy in process optimization, advanced product design, or performance prediction. Specific topic areas may vary. U.S. manufacturing sectors and companies of all sizes are eligible to apply.

A preliminary technical approach to HPC problem solving is established during a two-stage proposal development process:

- Stage 1: Concept paper. Companies submit two-page concept papers describing a project idea.
- Stage 2: Proposal. A technical review committee selects projects, and companies are invited to submit six-page proposals. National Lab experts with relevant experience are matched with each selected project idea to help companies develop proposals.

Manufacturers do not need in-house computational experts nor familiarity with a laboratory or its personnel. The proposals must describe why HPC is uniquely needed to address the challenge, include a feasible technical plan, and identify the needed computational resources at the Lab(s). These demonstration projects must significantly improve energy efficiency, have broad national impact, and advance the state-of-the-art for the industry sector. The industry partner applies to the program and contributes 20% in-kind resources to the project. DOE provides funding to the Labs for the use of the supercomputers and the time of Lab experts. Duration of a project is one to two years. For additional information, visit the HPC4EI website.

Partnering with the Labs is easier than ever before. Working with a National Laboratory means collaborating on proprietary research with a trusted research partner, not a competitor. To streamline and expedite the development of partnership agreements, companies and Labs are asked to sign the ‘model’ short form Cooperative Research and Development Agreement (CRADA). In addition, a streamlined agreement with the Lab can be established to protect a company’s trade secrets and intellectual property (IP). With these business-friendly terms, companies can leverage decades of investments in software platforms, codes, and expertise.

The HPC4Mfg Program, which is part of the High Performance Computing for Energy Innovation (HPC4EI) Initiative, is funded by the Office of Energy Efficiency and Renewable Energy’s Advanced Manufacturing Office (AMO). In addition to manufacturing, the Initiative includes subprograms that focus on materials and mobility.

All DOE National Laboratories can participate in the HPC4Mfg Program

The U.S. government makes huge investments in supercomputers to stay on the leading edge of computational science and technology development for national security missions. The DOE National Laboratories have unparalleled HPC assets developed over many decades. America's leadership in large-scale HPC is sustained through continued investment in research that advances the scientific frontiers of computational innovation. Supercomputers at the Labs are some of the best in the world. They are typically a decade ahead of most commercial/industrially owned capabilities, and the level of investment is often ten or more times that of systems built in the private sector. Lab researchers strive to develop next-generation computational systems and methods to deliver greater accuracy and predictive capacity. The Labs have a wide range of detailed physics models as well as state-of-the-art methods for multi-scale, multi-physics analysis.

The Labs tackle multidisciplinary problems with long time horizons, often integrating fundamental discovery research, technology development, and demonstration projects. While the Labs are dedicated primarily to national security missions and critical governmental functions, they provide cutting-edge resources for the entire American research community. These resources include scientific expertise, facilities and equipment, and science and technology capabilities. The Labs serve an important role in helping the private sector move innovation into the marketplace and strengthen U.S. competitiveness.

Manufacturing companies can collaborate with any Lab associated with the HPC4Mfg Program, including:

- Argonne National Laboratory (ANL)
- Lawrence Berkeley National Laboratory (LBNL)
- Lawrence Livermore National Laboratory (LLNL)
- Los Alamos National Laboratory (LANL)
- National Energy Technology Laboratory (NETL)
- National Renewable Energy Laboratory (NREL)
- Oak Ridge National Laboratory (ORNL)
- Pacific Northwest National Laboratory (PNNL)
- Sandia National Laboratories (SNL)

Learn more about the computing resources at each Lab at hpc4energyinnovation.llnl.gov/computing_resources.html

U.S. Companies Access World-class Supercomputers and Expertise at the DOE National Laboratories

Steps in an HPC4Mfg project workflow

Each manufacturing challenge is unique and requires a customized solution. The modeling approach depends on the problem. Projects seek to discern a greater understanding and ways to gain control over physical phenomena. Company experts in simulation and/or product design can collaborate with Lab experts and use the predictive power of HPC. The typical steps taken during an HPC4Mfg project are outlined below:

Companies identify project objectives: analyze difficult problems, test innovative design ideas, or set ambitious goals. After concept papers submitted in response to a DOE solicitation are accepted, companies prepare proposals with assistance from a Lab expert.

National Laboratory scientists conduct the analysis using supercomputers. At the project kickoff, companies bring their challenges to the Lab(s). A computational expert, scientist, or engineer from the company—with specific knowledge of their processes and products—collaborates with one or more Lab experts to conduct the steps in the HPC analysis.

Frame the problem. Translate the manufacturing challenges into scientific problem statements that can be analyzed with multi-physics modeling. Determine the relevant scales for the events and variables to be considered. Consider physical constraints and performance requirements. Port code from other industry models, if applicable, and re-write for parallel processing. Analyze the data provided by the company to validate model results (e.g., from sensors, product samples, experimental research). Identify any physical experiments that may be needed.

Prepare the multi-physics model. Identify the physics and scientific equations that must be solved. Divide the problem space into a grid. Select the software.

Choose the analytical methods. Determine the computational techniques for solving the numerical equations. Develop new modeling and analytical methods if needed. Conduct computational analysis to determine the best approach.

Run model simulations. Run model iterations until the analysis converges on new product or process configurations and useful answers. Prioritize these computationally intensive simulations.

Validate the model with real data. Compare the simulation results to the data collected. Determine if the relevant phenomena are captured correctly.

Fine tune the model. Adjust the model to better simulate what is transpiring physically.

Run iterations to optimize new configurations. Change the physical parameters of the process or product modeled until the targeted outcomes are achieved. Test the impact of proposed changes computationally. Consider using the simulation runs to train a neural network and build a reduced-order model for in-plant use.

Create graphics to explain the results. Interpret the data. Describe how performance could be improved. Estimate the benefits. Transform calculations into visualizations that are easier to understand.

Companies take the results back to decision-makers. Results from the off-site computational analysis are provided to design engineers, plant operators, and business managers. Data is used to inform technical decisions, plan new investments, and conduct follow-on modeling and techno-economic analysis. Energy and material savings are realized after improvements are implemented.

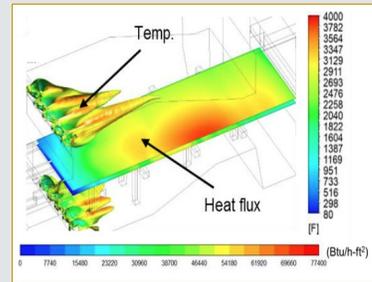


Optimize reheating furnace efficiency in steel manufacturing

Project Goal: Analyze complex physical phenomena to improve heating uniformity and decrease energy consumption in hot rolling steel slabs.



Semi-finished steel is reheated using a dynamically controlled process before entering the hot rolling operations. Reheating uses 70-80% of total energy used in rolling mills.



ArcelorMittal partnered with Argonne National Laboratory and Steel Manufacturing Simulation and Visualization Consortium (SMSVC) at Purdue University Northwest.

Photo from ArcelorMittal.

Computational results image from Argonne National Laboratory and the Steel Manufacturing Simulation and Visualization Consortium (SMSVC) at Purdue University Northwest.

HPC contribution:

- Computational fluid dynamics (CFD) method was used in a large-scale study to optimize furnace operations. Flame characteristics vary with the degree of oxygen enrichment, input flow rates, and burner positions in heating zones.
- Predicted optimal temperature and heat flux distribution on the slab with a new fuel and oxidizer mixes.

Energy Impact Potential

- **16 trillion Btu of fuel annually**

Companies Transforming Manufacturing with HPC: Examples from Diverse Industries

The HPC4Mfg Program expands its impact by supporting diverse industries and tackling technological challenges.

Manufacturers from large, medium, and small companies bring their toughest challenges to the HPC4Mfg Program. A wide range of technical challenges have been studied with HPC at the DOE National Laboratories. Descriptions of the R&D projects funded by the Advanced Manufacturing Office (AMO) since the Program’s inception are listed below—and examples of specific HPC4Mfg projects are summarized throughout this document. These projects have produced a range of technical, financial, and societal benefits. For an individual company, the value and gains from HPC are often held close for competitive advantage. Each manufacturer typically has unique, proprietary production processes, though some commonalities exist within an industry. The HPC4Mfg Program has contributed to technological innovation and energy savings in a wide range of industries and specific companies.

A wide range of industry challenges have been studied with HPC at the DOE National Laboratories.

SPRING 2020

Ford Motor Company partnered with ORNL to improve part-scale modeling of laser powder bed fusion to improve car part quality and reduce scrap rate in a project titled “Extend an Innovative HPC-Compatible Multiple Temporal-spatial Resolution Concurrent Finite Element Modeling Approach to Guide Laser Powder Bed Fusion Additive Manufacturing.”

Raytheon Technologies Research Center (RTRC) collaborated with ORNL to develop multi-physics and machine learning optimization algorithms to upscale MAP technology to an industrial level in a project titled “Multiphysics Models and Machine-learning Algorithms for Energy Efficient Carbon Fiber Production Using Microwave-assisted Plasma (MAP).”

Futamura Group collaborated with NREL to accelerate development of next-generation recyclable cellulose-based packaging materials in a project titled “In Silico Design of Next Generation Cellulose-Derived Packaging Materials.”

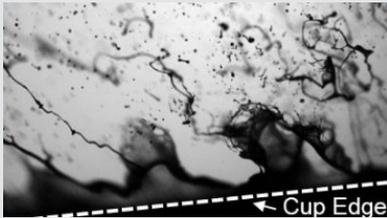
Raytheon Technologies Research Center (RTRC) collaborated with ORNL to optimize microwave-enhanced manufacturing of ceramic matrix composites in a project titled “Modeling Driven Manufacturing Process Intensification.”

Machina Labs collaborated with LLNL to perform informed aluminum sheet metal processing for bending and reducing springback for aerospace and automotive applications in a project titled “Advanced Machine Learning for Real-time Performance-informed Thermo-mechanical Processing of Sheet Metal Parts.”

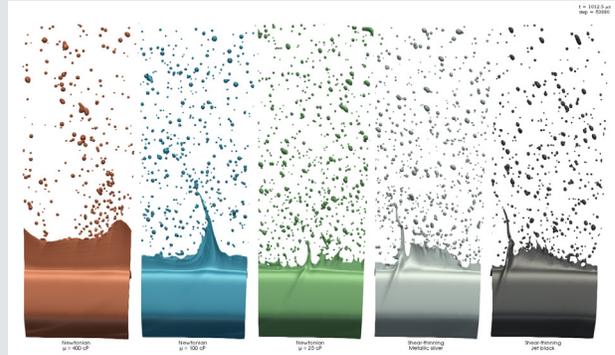


New algorithms to reduce energy costs of painting cars

Project Goal: Model the fluid properties of paint droplets applied under pressure with a high-speed rotary bell atomizer to identify ways to significantly reduce energy consumption and material waste.



In rotary bell atomization, paint flows to a cup rotating at 30,000-70,000 rpm and is driven by centrifugal forces to form thin sheets and tendrils at the cup edge, where it then atomizes into droplets. *Photos from PPG.*



High-resolution peta-scale modeling of liquid atomization comparing different liquid rheologies. *Paint dispersion simulations from LBNL.*

PPG worked with Lawrence Berkeley National Laboratory. HPC contribution:

- State-of-the-art mathematics and numerical methods to model rotary bell atomization at industrially relevant conditions, including advanced implicit mesh discontinuous Galerkin methods, hybrid level set methods, and tailored adaptive mesh refinement algorithms.
- Unveiled different kinds of atomization behavior depending on fluid rheology, including non-Newtonian flow.
- Varied process conditions such as rotation speed, fluid injection rates, shaping air currents, and cup geometry to gain statistical insight about droplet trajectories, angular momentum, and size distributions to guide new design.
- Results can be extended to other kinds of multi-physics fluid problems.

Industrial spray painting

Energy Impact Potential

- 70% of energy consumed during automobile assembly is associated with painting operations
- 20% faster spray application could save 7 trillion Btus per year in the U.S. automobile industry alone

Rolls-Royce Corporation collaborated with ORNL and LLNL to use HPC to study heat transfer coefficients between the quench oil and solid-state components in the quench heat-treatment processes for gas turbine parts in a project titled “Nucleate Boiling of Quench Oils Used in the Heat Treatment of Critical Aerospace Components.”

General Electric and GE Research partnered with ORNL to improve ceramic matrix composites for aviation by using advanced computational fluid dynamics and modern data analytics on HPC to rapidly develop a high-fidelity CVI kinetics model in a project titled “Data-driven Kinetics Modeling of Chemical Vapor Infiltration for Ceramic Matrix Composites Manufacturing.”

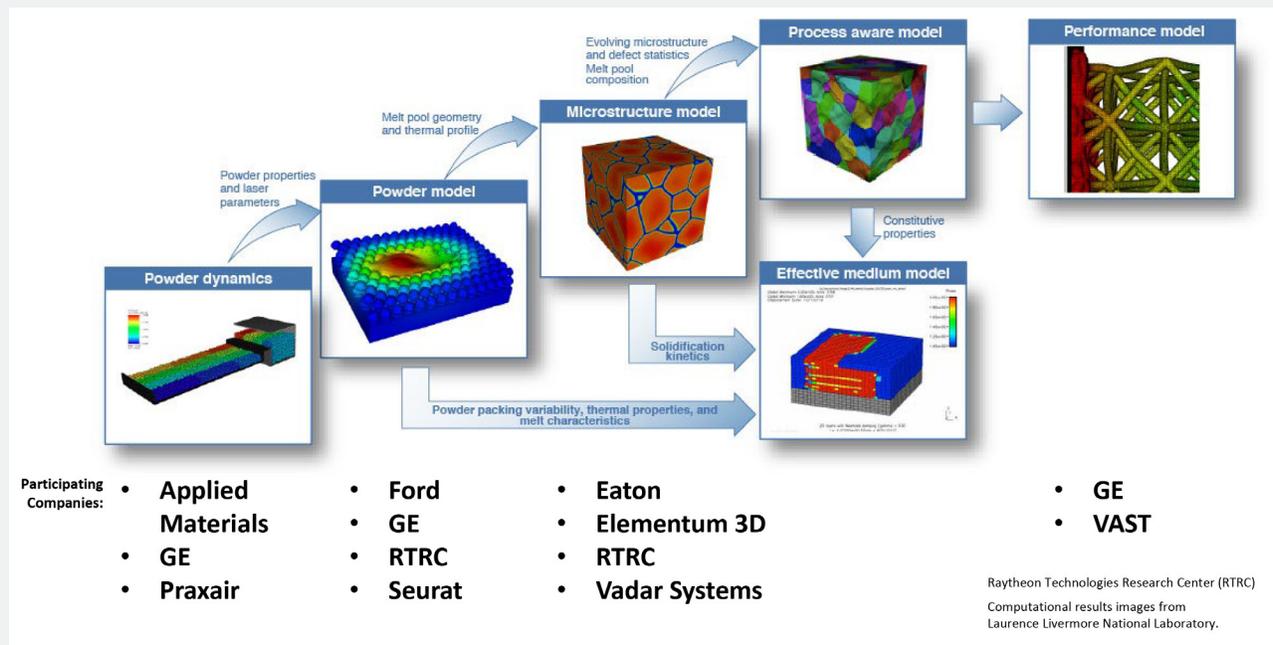
The Procter & Gamble Company collaborated with SNL to identify process parameters to efficiently and effectively utilize raw materials and reduce energy consumption in the dewatering/drying of random foam and structured papers in a project titled “Highly-Scalable Multi-Physics Simulation for an Efficient Absorbent Structure.”

Toyota Motor Engineering & Manufacturing North America partnered with LLNL to improve understanding of the relationship between properties in specific solid electrolytes in a project titled “Multiscale Simulations of Novel Lithium Electrolytes for Improved Processability and Performance of Solid-state Batteries.”

VAST Power Systems, Inc. continued their partnership with ANL and LLNL in a project titled “Ultra-Clean Transient Turbine Combustor,” which seeks to increase the number of simulations to improve the efficiency of VAST’s combustors for rapid transients in energy production.

Additive Manufacturing

Diverse companies improved key additive manufacturing production steps with HPC. Improvements to each company’s 3D printing platforms reduced material use, defects, and surface roughness—and improved the overall durability of parts.





Procter and Gamble

Designing paper products that require less energy to manufacture

With the naked eye, a roll of paper towels doesn't seem too complicated. But look closely and you'll see it's made up of layers of fibers—with thousands of intricate structures and contact points. These fluffy fibers are squeezed together before they are printed in patterns, and the resulting texture, absorption, and softness are key to the paper's performance.

Procter and Gamble regularly uses modeling and simulation to develop its products. However, representing the way paper fibers should contact each other to maximize performance is complicated and expensive. It can be a major bottleneck in product design—requiring time and energy.

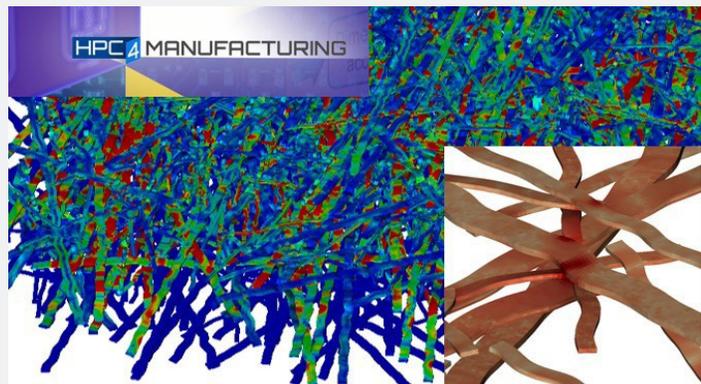
To speed up the product development process, Procter and Gamble partnered with LLNL to develop a large, multi-scale model of paper products that simulates thousands of fibers with a resolution to the micron scale. Modeling this complex system required a National Lab-scale supercomputer with thousands of cores. The project goal was to reduce paper pulp in products by 20 percent, which could result in significant cost and energy savings in one of the most energy-intensive industries, under a project titled: “Highly-Scalable Multi-Scale FEA Simulation for Efficient Paper Fiber Structure.”

LLNL developed a parallel computing program called p-fiber, which can quickly prepare the fiber geometry and meshing input data needed to simulate thousands of fibers. A meshing tool called Cubit, created at Sandia National Laboratories, was used to generate the mesh for each individual fiber. P-fiber prepares the input data for ParaDyn, the parallel-computing version of DYNA3D, a code for modeling and predicting thermomechanical behavior.

In the model, each individual paper fiber was represented by as many as 3,000 “bricks” or finite elements. The model generated up to 20 million finite elements and modeled 15,000 paper fibers. Using parallel processing on a supercomputer, LLNL was able to run design simulations up to 225 times faster than meshing the fibers sequentially on P&G's computer. Model iterations were used to calculate the stress and strain on the paper during simulated use and determine how much force is needed to tear the paper.

This project earned an HPC Innovation Excellence Award in 2017 from Hyperion Research for the outstanding application of HPC computing for business and scientific achievements. It was aimed at speeding up product development and reducing energy use and costs during paper product manufacturing.

Finite element model of a paper product down to the detail of each independent fiber, and with the contact pressure (blue) between the fibers or the effective stress (red) calculated by the massively parallel explicit finite element code Paradyne. Computational results image from Lawrence Livermore National Laboratory.



WINTER 2020

CHZ Technologies, LLC partnered with NREL to use HPC to deepen understanding of material transport, heat transfer, phase-change, and chemistry in the Thermolyzer™ technology that converts waste hydrocarbon materials into fuel gas and saleable byproducts in a project titled “Simulation of Complex Reacting Media in Multidimensional Reaction Chamber.”

Raytheon Technologies Research Center (RTRC) partnered with ORNL to use HPC-based phase-field simulations along with experimental validation to design novel titanium (Ti) alloy compositions for additive manufacturing to potentially replace currently used wrought Ti alloys in a project titled “Development of HPC-Based Phase Field Simulation Tool for Modification of Alloy Morphology to Enhance Material Properties During Additive Manufacturing Process.”

Materials Sciences LLC partnered with LLNL to combine recent advances in topology optimization-based design, HPC, and additive manufacturing technology to develop high pressure and temperature heat exchangers in a project titled “HPC-Enabled Optimization of High Temperature Heat Exchangers.”

ESI North America, Inc. partnered with PNNL to use HPC resources to develop a data driven approach to link features of the material and manufacturing processes to the mechanical properties of thermoplastic composite parts in a project titled “Development of Efficient Process for Manufacturing of Thermoplastic Composites with Tailored Properties.”

FALL 2019

OxEon Energy, LLC partnered with LLNL to reduce the number of reactor tubes in Fischer Tropsch reactors to lower cost and improve performance in a project titled “Topology Optimization of Fischer Tropsch Reactor Design for Synthetic Fuel Production.”

Flawless Photonics partnered with LLNL to simulate both the heated glass flow and nucleation and growth of crystal nuclei to find the drawing conditions that suppress the growth of light-scattering crystalline defects in ZBLAN in a project titled “Modeling and Simulation of the Manufacture of a Superior Fiber Optic Glass.”

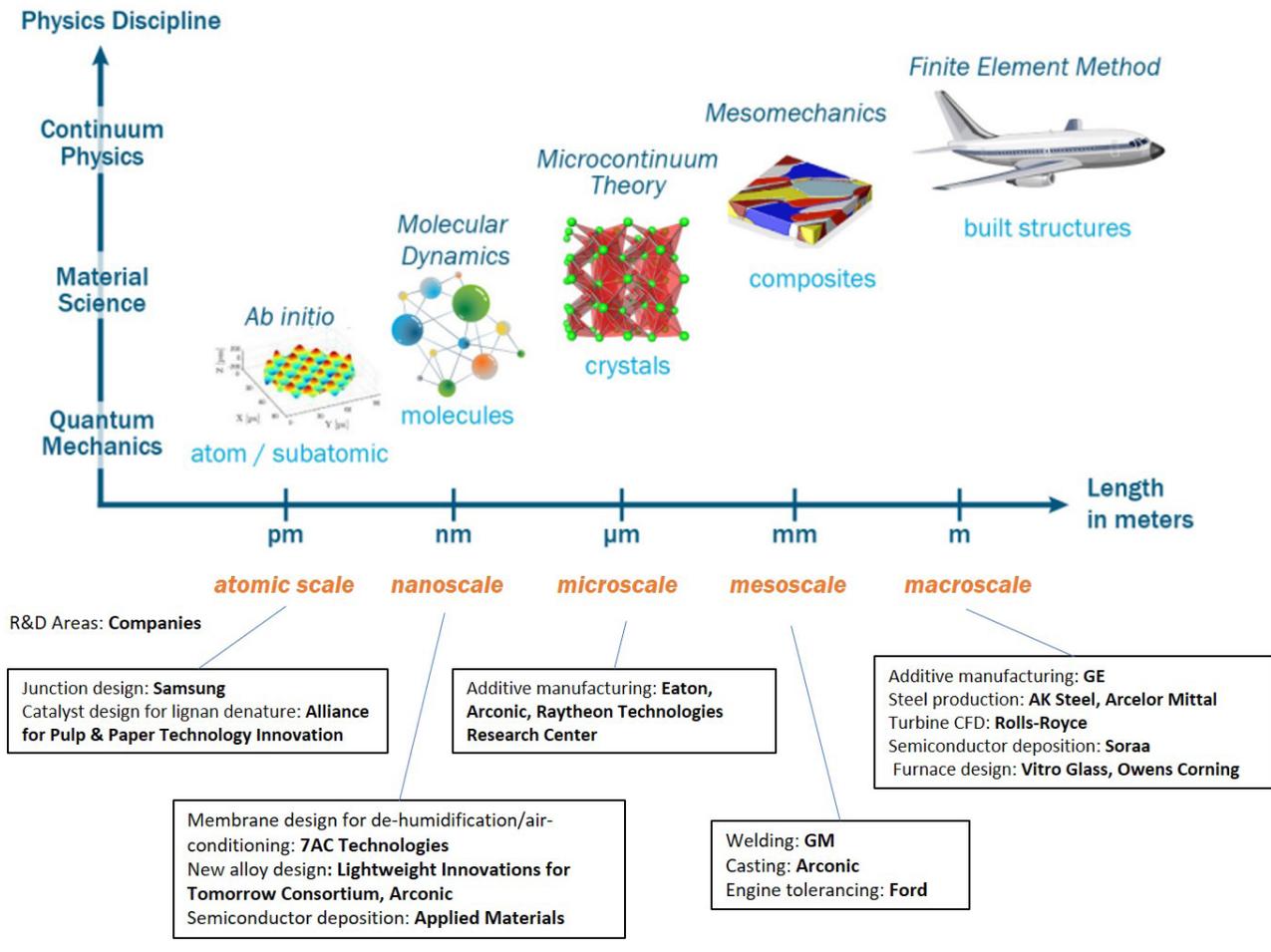
3M Company continued a partnership with SNL for a follow-on project to enhance non-equilibrium thermal radiation computation capability in a multi-physics framework of a passive cooling installation on a project titled “Passive Cooling Film Optimization.”

NLMK USA partnered with ORNL to use computational fluid dynamics methodology to optimize scrap melting in electric arc furnaces in a project titled “Optimization of Scrap Melting Using an Electric Arc in Steel Manufacturing.”

PPG Industries partnered with LBNL to use HPC in the modeling of the paint drying process to enable energy savings through co-curing in a project titled “Modeling Coating Flow and Dynamics During Drying.”

Physics model types used to analyze phenomena at different length scales

HPC is used to simulate the conditions impacting manufacturing at different size scales



- **Ab Initio** modeling framework rely on basic and established natural laws (first principles) in their calculations. These pico-scale models examine the parts of an atom, such as the position of the nucleus, photon flux, quantum efficiency, electron densities, energies, and other quantum chemistry phenomena. This level of analysis is used to better understand physical and chemical interactions that impact manufactured products. Factors modeled at this scale are ignored in larger scale models.
- **Molecular dynamics** analyzes physical movements and interactions of atoms and molecules. In manufacturing processes, simulations at this resolution study interactions of different chemical species at the molecular level.
- **Microcontinuum theory** is used to model materials (solids and fluids) as a continuous body in microscopic space that can deform and interact with mechanical forces and electromagnetic fields during short time increments. This modeling resolution is used to study lattice deformations and displacements in crystal structures.
- **Mesomechanics** models the discrete mechanics of microstructural constituents in heterogenous (or multi-phase) materials or systems. This technique is used to model individual components of composites and complex structures.
- **Finite element method** is a method that divides large structures into small “elements” to approximate solutions for field or transport equations used in engineering analysis. This technique is applicable for modeling a wide range of structure sizes, from jet engines to small processing equipment for manufacturing.

Challenges companies bring to the Labs require simulations at different length scales

Raytheon Technologies Research Center partnered with ANL to predict flow and heat transfer characteristics of cooling air in gas turbine hot section combustion liners in order to increase operating efficiency and reduce fuel consumption in a project titled “Pseudo-Spectral Method for Conjugate Heat Transfer Prediction of Impinging Flows Over Rough Surfaces.” This project was selected by both the HPC4Mfg and HPC4Mtls programs and was co-funded by AMO in the DOE Energy Efficiency and Renewable Energy Office as well as by the Office of Fossil Energy.

ArcelorMittal USA collaborated with ORNL to reduce the yield loss caused by inclusions forming in the refining ladle process in a project titled “Reduced Order Modeling and Performance Prediction for Steel Refining Ladle Processing via HPC.”

ArcelorMittal collaborated with LLNL and ANL to develop next generation lightweight advanced high strength steels with the help of HPC and artificial intelligence to positively impact the U.S. energy landscape during both production and use in a project titled “Ab-initio Guided Design and Materials Informatics for Accelerated Product Development of Next Generation Advanced High Strength Steels (AHSS).”

Guardian Glass, LLC collaborated with LLNL to reduce energy consumption in glass making by using computational fluid dynamics (CFD) simulations and machine learning in a project titled “Rapid CFD Using Machine Learning Algorithms.”

SPRING 2019

Raytheon Technologies Research Center partnered with ANL to develop innovative and affordable machine learning-enabled high-fidelity flow-physics models to be used in the design cycle of a gas turbine engine in a project titled “Deep Learning-Augmented Flow Solver to Improve the Design of Gas-Turbine Engines.”

General Motors LLC (GM) partnered with ORNL to develop a residual stress model for laser-welded dissimilar joints (HSLA/CE steel) for car light-weighting in a project titled “Simulation Tools for Characterizing Stress Distribution in Laser Welded Dissimilar Joints.”

RTRC in collaboration with SNL conducted research to develop a first-principles based simulation framework for predicting deposition of dirt, sand, volcanic ash, and other particulates on aero-engine components operating in polluted urban environments in a project titled “Fully Resolved DNS Simulation of Particulate Deposition for Aeroengine Combustor Applications.”

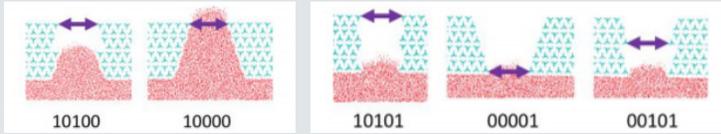
Praxair, Inc. partnered with ORNL to develop a multi-physics 3D CFD model of an Oxygen Transport Membrane (OTM) reactor module in a project titled “High Performance Computing for Improvement of Syngas Production Efficiency with OTM Technology.”

Dow Chemical Company partnered with NREL to model how molecular flow in molten plastic during manufacturing impacts material properties in a project titled “Non-equilibrium Molecular Simulations of Polymers under Flow: Saving Energy through Process Optimization.”



Membrane modeling for a more robust air conditioner

Project Goal: Simulate interactions at the membrane/liquid/air interface to determine optimal membrane properties enabling development of smaller, more durable, and less expensive membrane air conditioning systems.

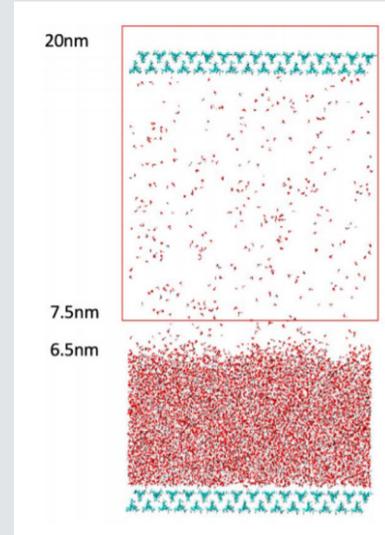


Membrane pores with different cross-sectional areas but identical slit lengths were studied for pore breakthrough strength.

7AC partnered with the National Renewable Energy Laboratory. Computational results images from NREL.

HPC contribution:

- Developed molecular dynamics simulations for transient evaporation and condensation to better understand transport phenomena at membrane surface
- Evaluated various cross-sectional nano-sized pore shapes to show that a single pore shape does not have an advantage over another but rather depends on the pore area, in preventing pore breakthrough.



Transient simulation of liquid/gas interface in water transport

Owens Corning & Saint Gobain Ceramics & Plastics and DBA

SEFPRO collaborated with LLNL to optimize the operating conditions in the glass manufacturing process in a project titled “Spectral Radiative Modeling of Glass Furnaces.”

Raytheon Technologies Research Center collaborated with LANL on developing a multiscale model to predict the mechanical behavior of additively manufactured components, particularly for creep applications in a project titled “Integrated Predictive Tools for Property Prediction in Additive Manufacturing.”

FALL 2018

Ferric, Inc. partnered with LBNL to develop analytical tools that combine traditional electromagnetic finite-element analysis with micromagnetic simulation in a project titled “Combined Micromagnetic and Finite-element Simulation of Integrated Magnetic Inductors for Improved DC-DC Voltage Regulator Energy Efficiency and Manufacturing Yield.”

Gopher partnered with Gas Technology Institute (GTI) and ORNL to develop a high-fidelity computational fluid dynamics model of a directly fired reverberatory style secondary lead furnace in a project titled “High-Performance Computing to Increase Productivity of Secondary Lead Furnaces.”

Applied Materials partnered with LLNL for a Phase II project to continue development of predictive modeling capabilities for the advanced film deposition technique, High Power Impulse Magnetron Sputtering (HiPIMS), in a project titled “Modeling HiPIMS plasma sources at reactor scale for reactive Physical Vapor Deposition (PVD) processes used in fabrication of high efficiency LEDs and solid-state non-volatile energy efficient storage class memory devices.”

Eastman partnered with ANL to optimize the non-Newtonian slurry atomizers for large-scale energy production facilities in a project titled “Simulation-driven optimization of non-Newtonian slurry atomizers for large-scale energy production.”

Praxair Surface Technologies, Inc. partnered with Ames Laboratory to enhance the efficiency/precision and quality of metal powder production for additive manufacture processes in a project titled “CFD Simulations of Metal Powder Production by Gas Atomization.”

SUMMER 2018 – Focus on steelmaking and aluminum production processes

United States Steel Corporation (USS) partnered with LLNL in developing the expansion of the thermomechanical profile across a hot strip mill simulation model that provides predictions of through-thickness temperature, deformation behavior, and associated microstructure in a project titled “Hot Strip Mill Simulation Model.”

AK Steel Corporation partnered with LLNL to improve real-time modeling of hot strip milling in a project titled “Application of HPC for Hot Rolling of Next Generation Steels.”

“Kinetic simulation has provided us with the insight of plasma behavior. This allows us to see the evolution of sputtered material distribution within the magnetron chamber, leading to possible optimizations by adjusting the geometry of the device.”

– Ihor Holod, Scientist, LLNL

Machine learning with HPC can accelerate innovation

Machine learning coupled with HPC simulations can greatly speed up optimization efforts to improve product quality, increase process efficiencies, and reduce waste. Supercomputers can run massively parallel virtual experiments for faster time-to-solution.

Experimental data can be added to a reduced-order model built on simulation data to evaluate a greater number of variables and improve product quality

Machine learning with HPC speeds up the development of new products / processes



Arconic

Reducing residual stress for aluminum casting

Direct chill casting produces 70% of all aluminum ingots. During the casting solidification process, a significant amount of ingots crack and are reworked. Arconic partnered with LLNL and ORNL to better understand aluminum ingot casting physics to reduce the scrap rate. Researchers used commercially available software and HPC to conduct virtual experiments to fill gaps in the understanding of the physics involved. Model simulations of the casting process enabled an extensive study of process parameters in a reasonable amount of time. A machine learning (ML) algorithm was trained with simulation data. Pilot production data was added to the ML algorithm to map the optimal configuration of process variables to reduce rejection rates and production costs.



Cast aluminum ingots will crack if the process conditions are not optimal. Photo from Arconic Aluminum.

Product optimization through simulations improves performance and reduces costs

Machine learning with HPC enables faster, cheaper design iterations



VAST Power Systems

Turbine combustor design optimization

VAST Power Systems, in collaboration with LLNL and ANL, investigated how to reduce the startup time of gas turbine combustors as well as the fuel demand during startup. A combustion model was used to simulate gas turbine combustion for various design and operation parameters. Model data was fed into a machine learning neural net to optimize design and operation parameters to increase fuel efficiency and decrease emissions. VAST is conducting research to increase the fuel efficiency of a turbine by 24%; increase the net power output of a generator by 60% (the total power generated and amount of useful output per unit of energy input); and keep emissions below California mandates without the use of catalysts or ammonia during startup.



Experimental combustion rig is used to determine emissions under various conditions. Photo from VAST Power Systems.

Process control optimization can take place in real-time (or near real-time)

Machine learning with HPC can deliver a paradigm shift in process control systems.



AK Steel

AK Steel

Hot roll process optimization

Hot rolling is a process in which steel is heated to become malleable, shaped into the desired configuration, and cooled at room temperature. During the cooling process, the steel shrinks non-uniformly, making it difficult to predict material properties. Hot roll process optimization is critical for the steel industry to reduce variation and non-conforming products, thereby saving time, money, and energy. AK Steel, in collaboration with LLNL, created a model to predict the properties of steel coils after hot rolling to improve product consistency and quality. Researchers leveraged HPC capabilities to run simulations and construct a fast-running machine learning reduced-order model to create a near real-time modeling capability that is inserted into the process control loop in actual production.



Hot rolling process is used to produce sheet steel. Photo from AK Steel.

ArcelorMittal USA, LLC partnered with LLNL to enable production of defect-free steel slabs with minimal trial and error in a project titled “Energy Efficient Manufacturing of Steel Slabs with the Application of High Performance Computing and Machine Learning.”

Alcoa USA Corporation collaborated with ORNL to advance the performance of Alcoa’s new advanced smelting cell in a project titled “Optimization of Alumina and Aluminum Fluoride Feeding in Advanced Aluminum Smelting Cells Using Large Eddy Simulation.”

WINTER 2018

Alliance for Pulp & Paper Technology Innovation (APPTI) partnered with NREL and ORNL to improve pulp yield during the kraft pulping process in a project titled “Molecular Modeling to Increase Kraft Pulp Yield.”

Dow Chemical Company partnered with SNL to reduce the thermal conductivity of insulating foam polyurethane products while using less polymer in its products in a project titled “Predictive Modeling of Polyurethane Foam Processes to Optimize Thermal Performance and Reduce Waste.”

Seurat Technologies partnered with LLNL to optimize their innovative laser powder bed fusion additive manufacturing printer in a project titled “Fluid and Particle Dynamics in Metal Area Printing.”

SFP Works, LLC partnered with ORNL to understand phase transformations that occur during the flash processing of steels in a project titled “High Performance Computing to Quantify the Evolution of Microscopic Concentration Gradients During Flash Processing.”

3M partnered with SNL to enhance the design of emissive films on building windows for cooling in a project titled “Passive Cooling Film Optimization.” Project will be co-funded by AMO and the Building Technologies Office.

VAST Power Systems, Inc. partnered with LLNL and ANL to increase the efficiency and reduce start-up times of gas turbine combustors in a project titled “Ultra-Clean Transient Turbine Combustor.” Project will be co-funded by AMO and the Office of Fossil Energy.

Arconic Inc. partnered with ORNL to model rolling processes to observe the evolution of porosity in a project titled “Computational Modeling of Industrial Rolling Processes Incorporating Microstructure Evolution to Minimize Rework Energy Losses.”

GE Global Research Center partnered with LANL to improve the Truchas code for single crystal casting in a project titled “Highly Parallel Modeling Tool to Drive Casting Development for Aerospace and Industry Gas Turbines (IGT) Industries.”

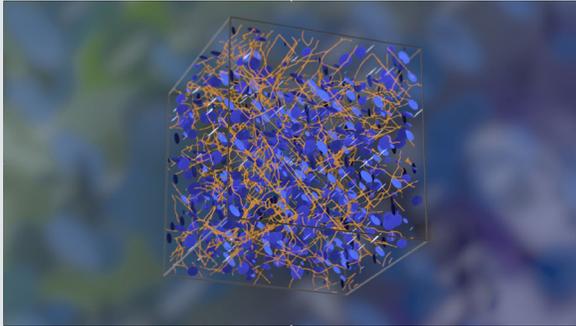
3M partnered with ANL to optimize its fiber spinning manufacturing process in a project titled “Next Generation Nonwovens Manufacturing based on Model-driven Simulation Machine Learning Approach.”

Raytheon Technologies Research Center (RTRC) partnered with ORNL to understand microstructure evolution during heat treatment of additively manufactured parts in a project titled “Predictive Tools for Customizing Heat Treatment of Additively Manufactured Aerospace Components.”



Developing lightweighting materials for aircraft engines

Project Goal: Accelerating aluminum-lithium (Al-Li) alloy materials development through predictive material modeling, manufacturing simulations, and product performance analysis in turbine service conditions to significantly reduce fuel consumption in aircraft.



Lithium (gold) is added to aluminum (purple) to strengthen the resulting alloy. The model predicted alloy strength as a function of the percentage of lithium in the alloy. *Computational results image from LLNL.*

LIFT partnered with Lawrence Livermore National Laboratory.

HPC contribution:

- Evaluate stress/strain behavior of aluminum and Al-Li alloy for different lithium content, shapes, and volumes
- Model validation of dislocation mobility, a property of alloys under stress.

Energy Impact Potential

- Over 13 million gallons (\$26 million) in jet fuel can be saved per year industry-wide by using Al-Li alloys

Steel Manufacturing Simulation and Visualization Consortium (SMSVC) and ArcelorMittal USA partnered with ANL to improve the efficiency of the reheat furnace process in steel manufacturing in a project titled “Application of High-Performance Computing to Optimize Reheat Furnace Efficiency in Steel Manufacturing.”

Transient Plasma Systems Inc. partnered with ANL to develop more efficient dilute-burn engines in a project titled “Modeling of Non-equilibrium Plasma for Automotive Applications.” This project was co-funded by AMO and the Vehicle Technologies Office.

SPRING 2017

PPG Industries, Inc. partnered with LBNL to continue the modeling of an electrostatic rotary bell atomizer used to paint automobiles in a follow-on project titled “Optimizing Rotary Bell Atomization.”

Vitro Flat Glass LLC partnered with LLNL to develop real-time glass furnace control using a neural net-based reduced order model of a CFD simulation of molten glass flow in a follow-on project titled “Advanced Machine Learning for Glass Furnace Model Enhancement.”

Caterpillar Inc. partnered with ANL to increase efficiency and reduce emissions by optimizing heat transfer in diesel engines through simulations of piston and spray geometry in a project titled “Heavy-duty Diesel Engine Combustion Optimization for Reduced Emissions, Reduced Heat Transfer, and Improved Fuel Economy.” This project was co-funded by AMO and the Vehicle Technologies Office.

Eaton Corporation partnered with ORNL to develop waste heat recovery technology that can be applied to industrial manufacturing processes and vehicle operations in a project titled “High Performance Computing to Enable Next-Generation Low-Temperature Waste Heat Recovery.”

General Motors LLC partnered with LLNL to reduce cycle time in composite manufacturing in a project titled “Computational Modeling of High Pressure Resin Transfer Molding (HP-RTM) for Automotive Structural Carbon Fiber (CF) Composites.” This project was co-funded by AMO and the Vehicle Technologies Office.

Arconic Inc. partnered with LLNL and ORNL to develop an advanced understanding of the non-equilibrium metallic phases established during metal additive manufacturing (AM) processes in a project titled “Multiscale Modeling of Microstructure Evolution During Rapid Solidification for Additive Manufacturing.” This project was co-funded by the Office of Fossil Energy as an HPC4Materials for Severe Environments seedling project and by the Advanced Manufacturing Office as part of the HPC4Mfg portfolio.

Vader Systems, LLC partnered with SNL to understand the physics needed to apply transition MagnetoJet (MJ) 3D printing technology to higher melting point metals and higher ejection rates in a project titled “Computational Modeling of MHD Liquid Metal 3D Printing.”

FALL 2016

Ford Motor Company partnered with ANL to study the effect of dimensional tolerances on the cylinder-to-cylinder variation in engine performance in a project titled “CFD Study of Impact of Part-to-Part Variations on Spark-Ignition Engine Charge Formation.”

Arconic, Inc. partnered with ORNL to develop high-melting-point, lightweight alloys in a project titled “High Performance Computing for Phase Predictions for Multi-Component Alloy Systems.”

GE Global Research partnered with ORNL to reduce process development time and accelerate process certification of additively manufactured parts in a project titled “Powder Spreading Process Maps for Metal Additive Manufacturing.”

United Technologies Research Corporation partnered with LLNL to reduce defects in additively manufactured parts in a project titled “High Fidelity Physics-based Model Driven Process Parameter Selection for LPBF Additive Manufactured Metallic Aerospace Components.”

General Electric Research Corporation partnered with ORNL to reduce manufacturing costs in a project titled “Surface Roughness Effects from Additive Manufacturing in High Efficiency Gas Turbine Combustion Systems.”

Applied Materials, Inc. partnered with LLNL to improve powder bed formation in additively manufacturing processes in a project titled “Simulating Properties of Metal Powder Beds Used for Additive Manufacturing of Parts in Semiconductor, Solar and Display Equipment.”

Samsung Semiconductor, Inc. (USA) partnered with LBNL to optimize the performance of semiconductor device interconnects in a project titled “Making semiconductor devices cool through HPC ab initio simulations.”

Arconic, Inc. partnered with LLNL and ORNL to develop new lightweight alloys in a project titled “Computational Modeling of Multi-Strand Aluminum DC Vertical Casting Processes Incorporating Cast Structure and Thermal Treatment Effects Contributing to Rework Energy Losses.”

7AC Technologies partnered with NREL to improve air conditioning technologies in a project titled “Modeling water vapor transport at liquid/membrane interfaces for applications in liquid desiccant air conditioners.”

The Timken Company partnered with ORNL to improve reliability and lifetime of wind turbines in a project titled “Crystal Plasticity Finite Element Model to Study the Effect of Microstructural Constituents on White Etch Area formation in Bearing Steels.”

SPRING 2016

Shiloh Industries partnered with ORNL to study phase change cooling of tooling to speed up casting processes in a project titled “Development of a Transformational Micro-Cooling Technology for High-Pressure Die Casting using High-Performance Computing.”

Rolls-Royce Corporation partnered with ORNL to improve silicon carbide composites in a project titled “Level-set Modeling Simulations of Chemical Vapor Infiltration for Ceramic Matrix Composites Manufacturing.”

Alliance for Pulp & Paper Technology Innovation (APPTI) partnered with ORNL to design better catalysts for lignin breakdown in a project titled “Catalytic Pulping of Wood.”

GE Global Research Center partnered with LLNL to study how to mitigate defects caused by direct metal laser melting in a project titled “Minimization of Spatter during Direct Metal Laser Melting (DMLM) Additive Manufacturing Process using ALE3D Coupled with Experiments.”

PPG partnered with LBNL to decrease the time needed to paint automobiles in a project titled “Modeling Paint Behavior During Rotary Bell Atomization.”

Actasys, Inc. partnered with ORNL to decrease the fuel consumption of trucks by actively modifying the flow around the trucks in a project titled “High Performance Computational Modeling of Synthetic Jet Actuators for Increased Freight Efficiency in the Transportation Industry.”

Carbon, Inc. partnered with LBNL to increase the speed of polymer additively manufactured components in a project titled “Multi-physics Modeling of Continuous Liquid Interface Production (CLIP) for Additive Manufacturing.”

American Chemical Society Green Chemistry Institute partnered with LBNL to systematically explore lower energy mechanisms of chemical separation using adsorbents and membranes in a project titled “Accelerating Industrial Application of Energy-Efficient Alternative Separations.”

Alzeta Corporation partnered with LBNL to destroy effluents from semiconductor processing that could potentially harm the ozone layer in a project titled “Improving Gas Reactor Design With Complex Non-Standard Reaction Mechanisms in a Reactive Flow Model.”

Sepion Technologies partnered with LBNL to make new membranes to increase the lifetime of Li-S batteries in a project titled “Improving the Manufacturability, Performance, and Durability of Microporous Polymer Membrane Separators for Li-S Batteries using First Principles Computer Simulations.”

Applied Materials, Inc. partnered with LLNL to enable the manufacture of higher quality, more efficient LEDs for lighting in a project titled “Modeling High Impulse Magnetron Sputtering (HiPIMS) plasma sources for reactive Physical Vapor Deposition (PVD) processes used in fabrication of high efficiency LEDs.”

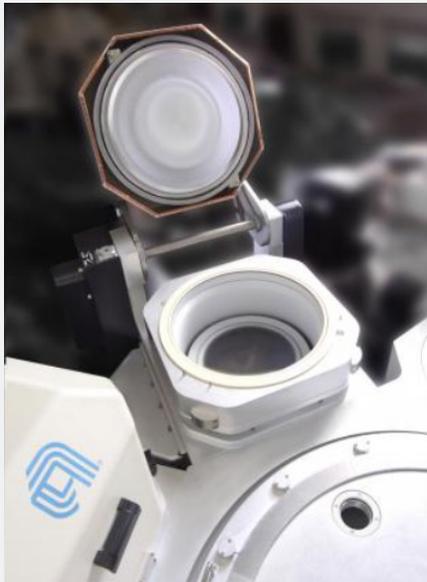
General Motors LLC and EPRI partnered with ORNL to improve welding techniques for automobile manufacturing and power plant builds in a project titled “High Performance Computing Tools to Advance Materials Joining Technology.”

Harper International Corp. partnered with ORNL to reduce the cost of carbon fibers in a project titled “Development and Validation of Simulation Capability for the High Capacity Production of Carbon Fiber.”

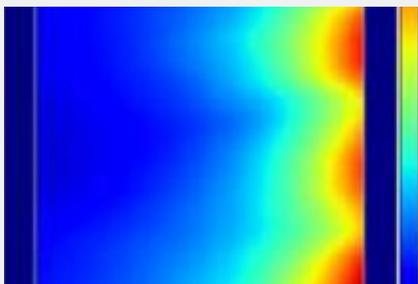
Thin films of materials for energy-efficient electronics, renewable energy supplies, and more durable coatings

Thin films, less than a nanometer to a few microns thick, are needed to make diverse technologies such as energy-efficient memory devices for data centers, semiconductor devices, and LEDs. In some deposition methods, materials in gas form (under high pressure) are injected into a chamber, and the vaporized materials are then condensed into a film on a surface using a highly controlled process. In other methods, charged particles collide with targets formed from the desired deposition material. Atoms of the material are knocked free and land on the substrate surface, creating a thin film. Advanced film deposition techniques can reduce manufacturing costs and make higher-performing products.

 **Applied Materials, Inc.** and LLNL developed computationally intensive model simulations to address a range of requirements for a new full-scale reactor design to make advanced thin films. The deposition technique called High Power Impulse Magnetron Sputtering (HiPIMS) was modeled at several time scales to accurately predict realistic particle densities and magnetic fields. This technique relies on a leading-edge magnetron, which is a vacuum tube that controls the flow of electrons by an applied magnetic field to generate power at microwave frequencies.

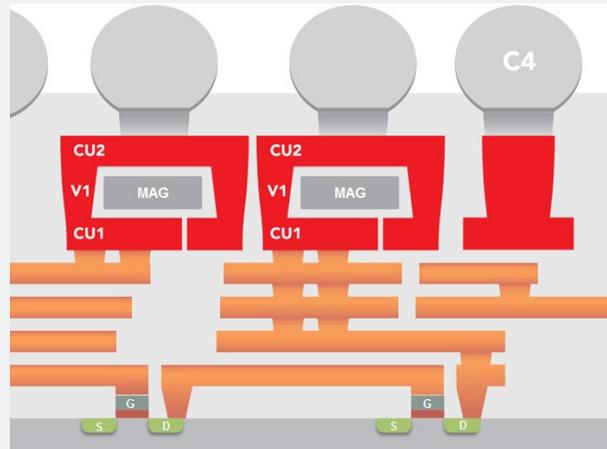


A single wafer process chamber used by Applied Materials to perform physical vapor deposition on any type of wafer, including the sapphire substrates used in this HPC project. *Photo from Applied Materials.*



Cross sectional magnetic field of the magnetron in the high-power impulse magnetron sputtering system. *Computational results image from LLNL.*

 **Ferric, Inc.** and LBNL developed models to optimize the performance of a thin-film ferromagnetic inductor technology that operates in conjunction with an integrated circuit. Integrated voltage regulators (IVRs) are a novel DC-DC power converter technology to improve semiconductor energy efficiency and reduce size relative to traditional solutions. Accurate modeling is paramount for achieving high conversion efficiency (η) in these products, which will reduce energy consumption in the data center processors. Thin-film magnetics simulation is computationally expensive and is a primary obstacle to reducing design-cycle time and further optimizing converter products.



A cross-sectional view of a CMOS chip, Ferric's thin film magnetic inductor technology, shown in gray within the red box, is integrated into the back-end-of-line processing. *Illustration from Ferric, Inc.*

FALL 2015

Raytheon Technologies Research Center partnered with ORNL and LLNL to develop and deploy simulation tools that predict the material microstructure during the additive manufacturing process to ensure that critical aircraft parts meet design specifications for strength and fatigue resistance, in a project titled “Integrated Predictive Tools for Customizing Microstructure and Material Properties of Additively Manufactured Aerospace Components.”

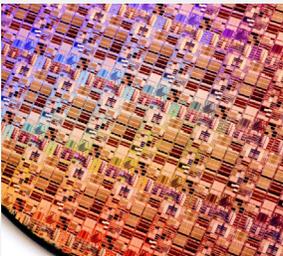
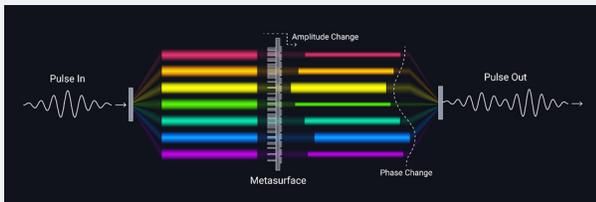
Procter & Gamble partnered with LLNL to reduce paper pulp in products by 20 percent, which could result in significant cost and energy savings in one of the most energy-intensive industries. The project is titled “Highly Scalable Multi-Scale FEA Simulation for Efficient Paper Fiber Structure.”

General Electric (GE) partnered with ORNL to assist in the local control of melt pool and microstructure in additively manufactured parts. The project is titled “Process Map for Tailoring Microstructure in Laser Powder Bed Fusion Manufacturing (LPBFAM) Process.”

GE, in a separate project, partnered with ORNL and LLNL to improve the efficiency and component life of aircraft engines through design optimization, in a project titled “Massively Parallel Multi-Physics Multi-Scale Large Eddy Simulations of a Fully Integrated Aircraft Engine Combustor and High Pressure Vane.”

Ohio Supercomputer Center (OSC) AweSim program and the Edison Welding Institute (EWI) partnered with ORNL to deploy a cloud-based advanced welding simulation tool for broad industry use. The project is titled “Weld Predictor App.”

Applications for Thin Films

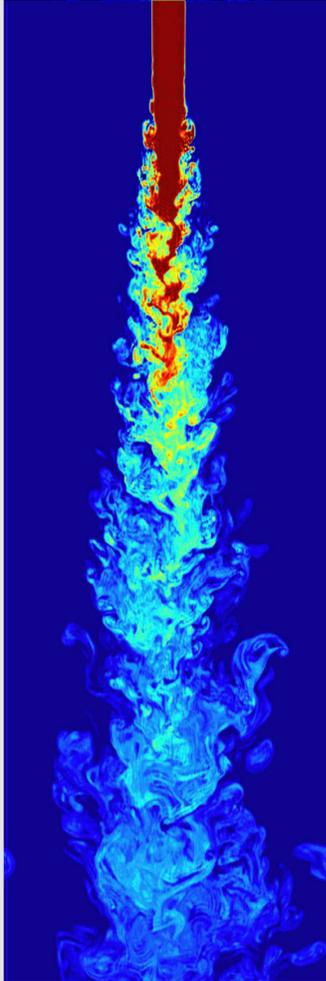




ZoomEssence

Liquid flavors are swirled into powder form using high-speed physics instead of high heat.

Computational fluid dynamic (CFD) models were used to explore radically new, air flow designs for spray drying to optimize the process and improve energy efficiency.

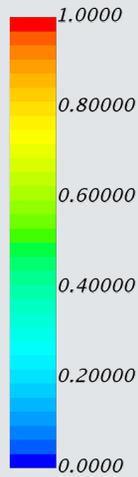


Dried food powders

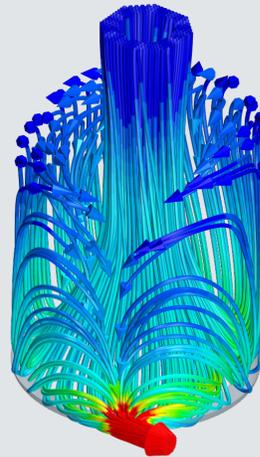


Mean of Turbulent Kinetic Energy (J/kg)

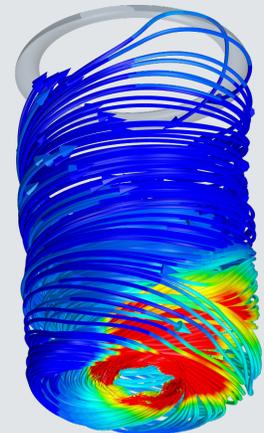
Mean TKE (J/kg)



Design A



Design B



Two inlet design configurations were analyzed with a CFD model to improve the spray drying process. Computational results images from Lawrence Livermore National Laboratory.

PPG Industries, Inc. partnered with LLNL to model thermo-mechanical stresses involved in forming and solidifying glass fibers to understand fracture-failure mechanisms to significantly reduce waste in a project titled “Numerical Simulation of Fiber Glass Drawing Process via a Multiple-Tip Bushing.”

PPG of Pennsylvania (a separate project) partnered with LLNL to develop a reduced computational fluid dynamics (CFD) model of a glass furnace to make informed line adjustments in near real-time, under the title: “Development of Reduced Glass Furnace Model to Optimize Process Operation.”

Lightweight Innovations for Tomorrow (LIFT) Consortium in Michigan partnered with LLNL to develop, implement, and validate a defect physics-based model to predict mechanical properties of Al-Li forged alloy in a project titled “Integrated Computational Materials Engineering Tools for Optimizing Strength of Forged Al-Li Turbine Blades for Aircraft Engines.”

ZoomEssence, Inc. partnered with LLNL to optimize the design of a new drying method using HPC simulations of dryer physics in a project titled “High Performance Computing Analysis for Energy Reduction of Industry Spray Drying Technology.”

SEEDLINGS 2015

HPC4Mfg seedlings established the program infrastructure with a focus on challenges in a broad range of energy-intensive industries.

Alliance for Pulp & Paper Technology Innovation (APPTI), a paper-making consortium, partnered with LLNL and LBNL to reduce energy in paper-making, saving up to 80 trillion Btu per year.

Purdue Calumet and LLNL advanced steel blast furnace modeling to reduce coke usage in steelmaking, which could save up to \$80 million per year.

Soraa partnered with LLNL to scale up their new GaN process to yield cheaper LED lighting and new power electronics.

Eaton and LLNL developed methods to predict the microstructure in additively manufactured metal parts to aid in qualification.

Carbontec Energy Corporation and Purdue Northwest partnered with LLNL on research to enable the scale up of the E-Nugget production process, which replaces coal with bio-mass in pig iron production.



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Participating Manufacturers:



Manufacturers can bring complex manufacturing problems to the National Labs.

The DOE High Performance Computing for Manufacturing Program (HPC4Mfg) promotes collaboration between U.S. manufacturers and the DOE National Labs.

- Applications are solicited twice each year.
- Companies submit two-page concept papers describing a project idea.
- National Lab experts help companies develop full proposals (six pages) for selected projects.

The Advanced Manufacturing Office (AMO)—within DOE’s Office of Energy Efficiency and Renewable Energy—leads the HPC4Mfg Program. Manufacturers use advanced modeling, simulation, and analysis to achieve significant energy and cost savings, expand their markets, and grow the economy.

All DOE National Laboratories can participate.



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To learn about the program and sign up to receive solicitation announcements, please visit:

hpc4mfg.llnl.gov/

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