Final Technical Report
DE-NA0002375

PSAAP-II Historical Report

The UQ-Predictive Multidisciplinary Simulation Center for High Efficiency Electric Power Generation with Carbon Capture

April 1, 2014 through December 31, 2020

Carbon Capture Multidisciplinary Simulation Center
The University of Utah

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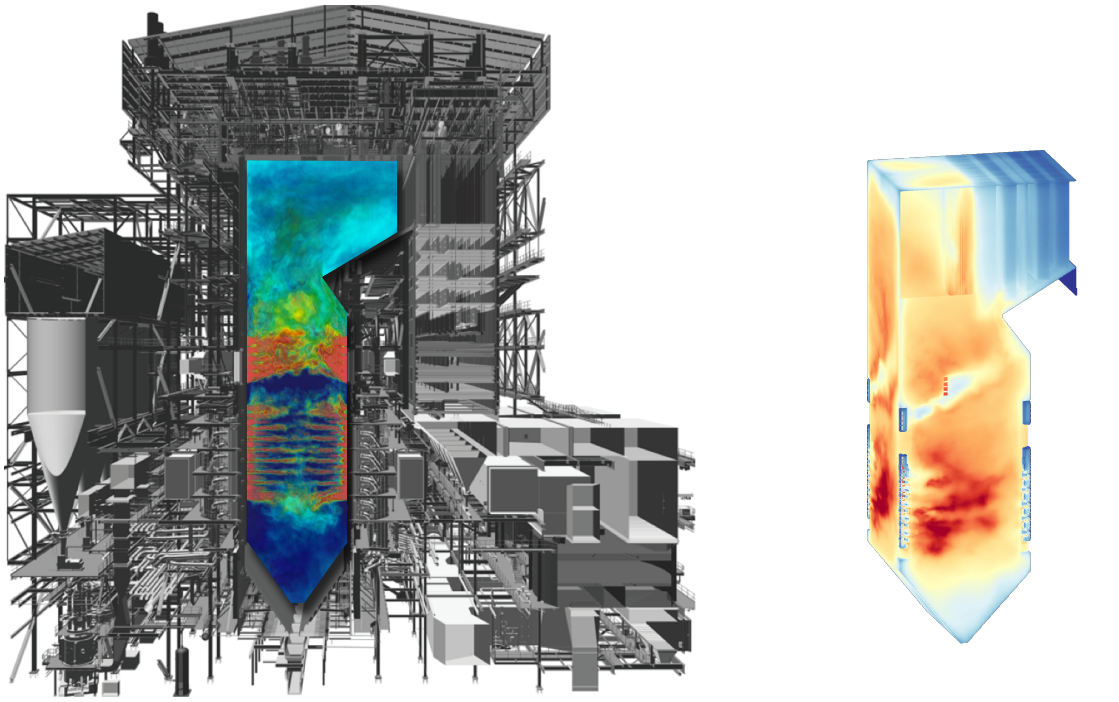
Carbon Capture Multidisciplinary Simulation Center
Institute for Clean and Secure Energy–The University of Utah

1 Abstract / Executive Summary

The University of Utah Multidisciplinary Simulation Center was established in April of 2014 by the United States Department of Energy, National Nuclear Security Administration (NNSA) for the purpose of developing and demonstrating the use of formal uncertainty quantification (UQ) methodologies in conjunction with scalable and portable high performance computing (HPC) strategies for solving large practical problems. Faculty, staff and students from the University of California, Berkeley, and Brigham Young University participated with those from the University of Utah in The Carbon Capture Multidisciplinary Simulation Center (CCMSC). The application selected by the Center was the demonstration of positive societal impact of HPC with UQ for the deployment of low-cost, low-carbon energy solutions for power generation. To accomplish this mission, we developed a multi-physics, large-eddy simulation (LES) code (Arches/Uintah) to run at scale on world-class computational resources made available to us by NNSA. To guide our application we partnered with two industrial collaborators, General Electric (GE Power) and Ontario Power Generation (OPG). Seventy-eight engineers and scientist worked together in three teams to complete the Center mission: the computer science team, the computational physics team, and the UQ team.

Our CCMSC industrial partners and their applications provided purpose and focus to the methodologies developed in the Center. With GE Power, our objective was to demonstrate the advantages of HPC with hierarchical UQ in design decisions by predicting the heat flux profile to a validated level of uncertainty for a full-scale, pulverized coal, thermal power generation boiler. We completed our capstone project in partnership with OPG, where we deployed all the methodologies of the Center to demonstrate dynamic, online artificial intelligence (AI) for operating a biomass-fired power generation boiler. The Atikokan Digital Twin starts with a large suite of our validated, multi-physics, LES simulations run on HPC resources. We selected these simulations from a design of experiments covering the full potential operational space for the power boiler. We then abstracted this suite of Arches/Uintah simulations into surrogate models for all quantities of interest (QOI). The digital twin AI uses our science-based Bayesian machine learning (ML) methods to combine these surrogate models with online power-plant measurements to produce real-time (3-5 minute updates) operational set points for continuous optimization of the biomass boiler in the presence of uncertainty.

A demonstration of the digital twin is accessed at https://chpc.utah.edu/~DigitalTwin.



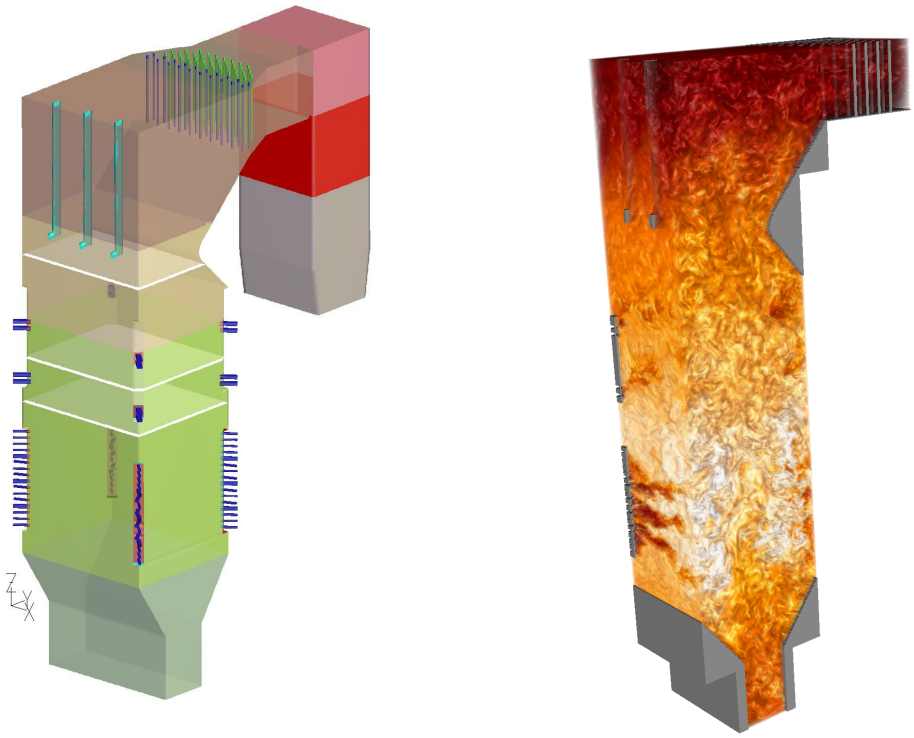
(a) boiler infrastructure **(b)** heat flux to boiler surfaces

Fig. 1. The 1200MW GE Power ultra-supercritical boiler: (a) the geometrical scale of the boiler showing the computed temperature profile, and (b) the heat flux distribution, the QOI for the CCMSC overarching problem.

2 Description of Overarching Problem

We created CCMSC to demonstrate positive societal impact of extreme computing by accelerating deployment of low-cost, low-carbon energy solution for power generation from pulverized solid fuels. The Center has been driven by the mission of predicting the heat flux profiles for the design of new technologies for full-scale, pulverized solid-fuel, thermal power generation boilers to a proven level of uncertainty using LES on the largest computational resources available to us (see Fig. 1). Our overarching problem then, our intended use of the simulation, has been to predict fireside performance of coal and biomass boilers to within a quantified uncertainty level of 5%.

The boiler design studies were conducted in conjunction with GE Power and included oxy-combustion, supercritical and ultra-supercritical boilers that employ exotic and expensive metal alloys to allow much higher steam temperatures than traditional boilers. These elevated steam temperatures increase the efficiency of the boiler significantly, thus "capturing" carbon by reducing the carbon footprint by an amount commensurate with the increase in efficiency. We also studied fuel switching from coal to biomass for reducing carbon footprints. In the capstone project performed in partnership with OPG (see section 3, we



(a) schematic of geometry

(b) gas temperature field

Fig. 2. The GE Power BSF: (a) A schematic showing blue inlet pipes for coal and air, and geometric components for the heat transfer surfaces around and in the boiler. The different colors depict different material thermal properties for each component. For scale, this boiler is four stories tall. (b) A volume-rendered image of the gas temperature field. The color depicts temperatures ranging from 800K-1800K. This image shows the scale of the turbulent eddies resolved by the Arches/Uintah LES code.

explored optimize operations in the presence of uncertainty for this carbon-negative solid fuel.

While the design boilers produced power ranging from 350-1200MW, our industrial partner (GE Power) provided data for a small-scale (15MW) boiler simulation facility (BSF) as shown in Fig. 2. More data were available for the BSF than for the full-scale system. The objective was to use these data, along with laboratory- and bench-scale experiments on specific components of the physics, to produce uncertainty that could be extrapolated to full scale. This UQ extrapolation problem became one of the Center's major missions and accomplishments: the development of an overarching methodology to extrapolate uncertainty. The problem was to ensure that we were interpolating physics while extrapolating scale, so that we could have confidence in our validation and uncertainty quantification (V/UQ) at scale.

The Center developed an hierarchical V/UQ methodology to guide decisions about research project selection, continuation and termination. Section 4.3 discusses the evolution of the CCMSC hierarchy. The objective was to identify sources of error and remove the largest sources as the program evolved. We constructed and changed the hierarchy in order to identify model form uncertainty and ritually improve the parts of the multi-physics model that contributed most to the uncertainty in our QOI. As the uncertainty diminished, the year-to-year changes in the hierarchy diminished.

Figure 3 shows the uncertainty in the overarching QOI, the heat flux profile, for the capstone project, the biomass boiler. These uncertainty distributions show that we were able to achieve our overarching goal of achieving nominally 5% uncertainty or less in the heat flux distribution for a full-scale industrial power boiler.

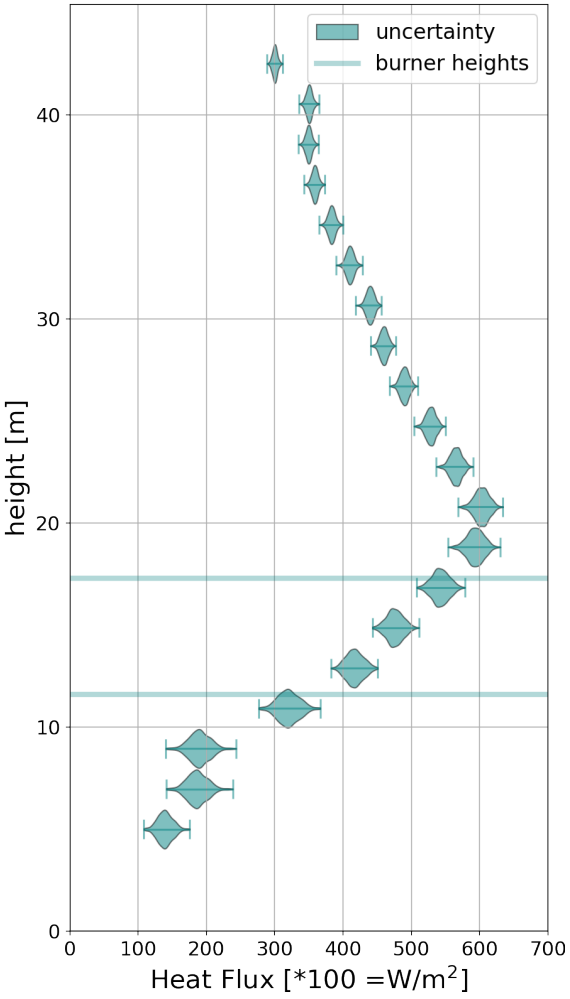


Fig. 3. For the capstone biomass boiler project, the uncertainty distributions are shown as violin plots for the average heat flux incident on the boiler walls in 20 horizontal bands around the boiler.

Accomplishing this overarching mission required advances in our three core disciplines: computer science, computational physics and V/UQ. To help visualize this overarching problem (see Fig. 1 and 2), we present images generated with the visualization tools developed by the computer science team. To reach our objectives, the computer science and computational physics teams developed the Arches/Uintah multi-phase combustion application code[1] and built it on the Uintah computational framework (UCF) [2, 3] to run efficiently on HPC platforms. Uintah's adoption of MPI+Kokkos and Hypre adds run-time parameters that allow users to optimize performance. We have shown strong and weak scaling for Uintah to 256k cores with 16k GPUs on a range of production machines from Titan through Mira. The V/UQ process employed at the Center, developed by the V/UQ team, has evolved as a hybrid of Bayesian and Bound-to-Bound methodologies for reducing the model bias in both the simulation models and the instrument models used to produce the experimental measurements. The accomplishments in these three disciplines are described in section 4.

Over the life of the Center, 78 faculty, staff and students participated in completing the Center objectives. The faculty and staff participants are shown in Fig. 4. The student participants, together with their laboratory internships and their post-CCMSC employers, are listed in section 5.

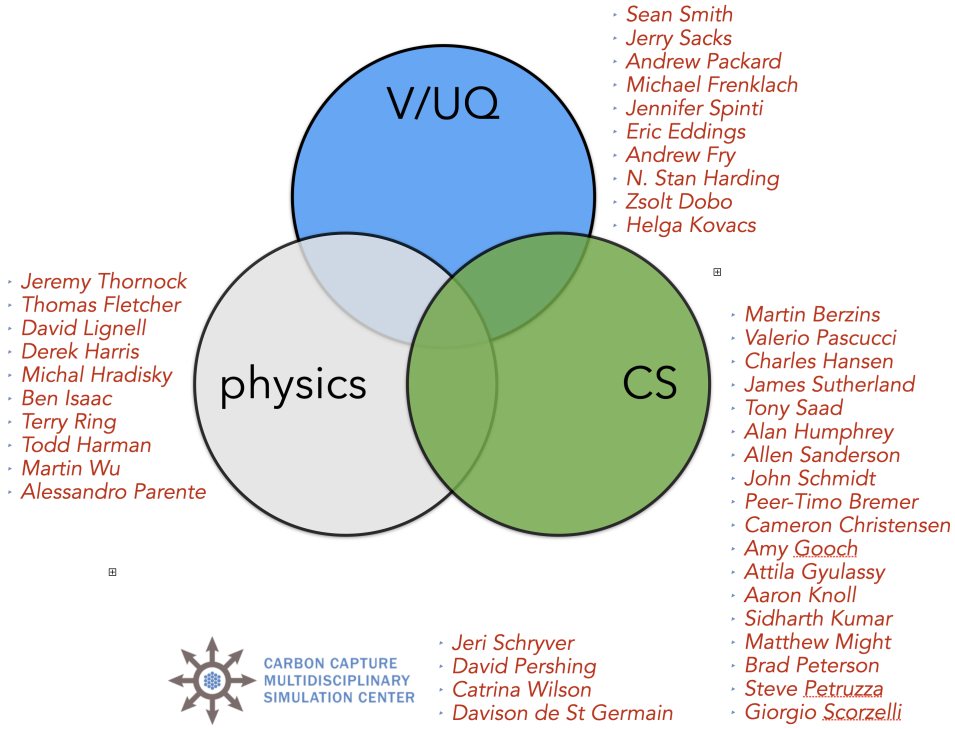


Fig. 4. CCMSC faculty and staff participants.

3 Capstone Project

In our capstone project, completed in partnership with OPG, we deployed all the methodologies of the Center to demonstrate dynamic, online AI for operating a biomass-fired power generation boiler. Since the inception of the Center, coal has fallen further out of favor as a thermal fuel for power generation. With the global search for carbon-neutral electric power generation, many countries, including the USA, are turning to biomass, a carbon-negative fuel, as an alternative to fossil fuel sources. Wood pellets have become the biomass feedstock of choice for their fuel handling and feeding advantages. An added benefit is that for existing coal-fired power plants that are older than 35 years or are fully paid for, "even with [biomass] pellet fuel 2.9 times more expensive per million BTU than coal, a converted coal plant generating power with pellets creates electricity at a rate that is less than one-third of a cent more expensive per kilowatt-hour than natural gas [4]." OPG, the first and only jurisdiction in North America to eliminate coal by converting to wood

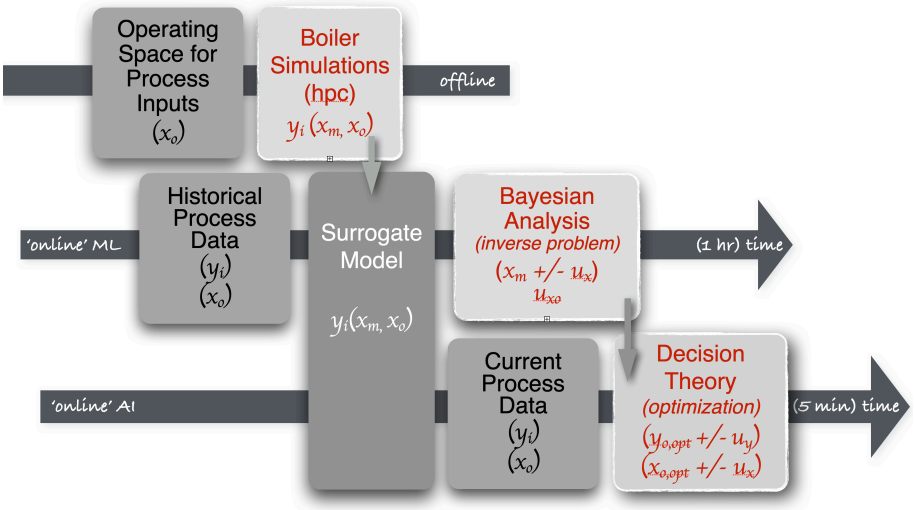


Fig. 5. Schematic of the Atikokan Digital Twin information flow.

pellets, agreed to join CCMSC to provide experience, data, and a platform (the Atikokan Power Station) for the demonstration of our capstone project.

The 200MW Atikokan tower boiler, fired with white biomass pellets, is located in Atikokan, Ontario, Canada and is owned by OPG. The plant, originally fired with lignite coal, was converted to fire 100% biomass (2012-2014) and became fully operational with biomass in September 2014. Because the boiler produces electricity on demand, it is not operating at full production throughout the day. While the cycle of operation varies from 40-200MW, generally only two of five mills are in operation with a resulting power generation range of 40-100MW. Each mill provides fuel to one level of burners; there are five levels in all with three burners per level. We focused our digital twin on the lower power generation range resulting from operation with only two mills (e.g. two burner levels) at a time.

The Atikokan Digital Twin starts with a large suite of our validated, multi-physics, LES simulations selected from a design of experiments covering the full potential operational space for the power boiler and run on HPC resources. We then abstract this suite of Arches/Uintah simulations into surrogate models for all QOIs. The digital twin AI uses our science-based Bayesian ML methods to combine these surrogate models with power-plant measurements to produce real-time (3-5 minute updates) operational set points for continuous optimization of the biomass boiler in the presence of uncertainty. This process is represented schematically in Fig. 5.

3.1 HPC Simulations

We performed simulations of the boiler in 420 specific operating states determined by a design of experiments. OPG provided geometry specifications (e.g. size and location of the tube banks, type and location of the burners), heat transfer characteristics (e.g. tube wall thermal conductivity, tube wall temperature) and operating condition data (e.g. biomass

flow rate, air flow rates, air temperatures, three measurements of oxygen at the boiler outlet, net power, gas temperature prior to the convective zone, several water temperatures). Additionally, OPG provided a biomass fuel sample from which we obtained physical (e.g. particle size distribution, particle true density) and chemical (e.g. proximate analysis, heating value, ash composition) properties that were needed in the simulations.

We used the Arches/Uintah LES code[1] for the simulations. Arches/Uintah has been used in several gas and coal-fired systems [5–10] and in several V/UQ studies [11, 12]. The various submodels used in the simulations are listed in Table 1. Throughout the Center history, we have developed models to simulate a range of solid fuel types. As can be seen in Fig. 6, wood is a continuation of heating value and composition properties of various types of solid carbonaceous fuels. We collected laboratory data on the performance of the wood pellets used at Atikokan and tested our models on this new fuel type. The extrapolation of these models to include wood happened without incident and is another demonstration of the strength of the hierarchical model development strategy. We tested and debugged a base simulation with these models until it was stable and at steady state.

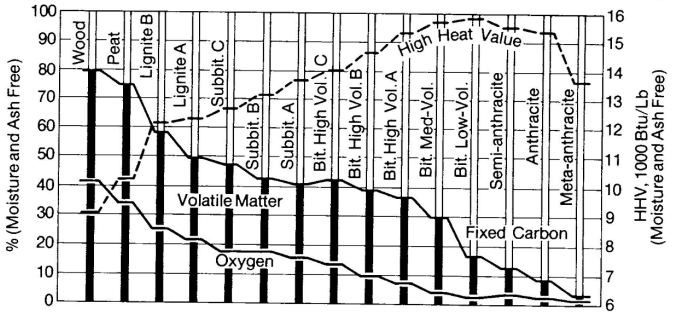


Fig. 6. Higher Heating Value (HHV), volatile matter, fixed carbon and oxygen content of a range of solid carbonaceous fuels.

To reduce the time for function evaluations (e.g. simulation output) in the digital twin from days to fractions of a second, we used surrogate models that were created from data extracted from the suite of 420 simulations. To determine this suite, we first considered the six operating knobs for each two-mill (e.g. two-burner-level) pair. Our computational resources required that we limit the degrees of freedom to four: total biomass flow rate (assume equal split between levels), total secondary air flow rate (assume equal split between levels), tramp air split (percent of secondary air fed through burners not firing biomass), and percent flue gas recycle (FGR) back into the boiler. We eliminated the biomass and secondary air splits between levels. Based on OPG data, we determined the operating range for each of these four parameters and performed an optimized design (42 samples) in this four-dimensional space. Figure 7 shows the 42 points in the design. Each of the symbols represents a simulation that we performed for a given pair of burner levels (e.g. levels 1&4 or levels 2&5). We performed 42 simulations for each of 10 level pairs for a total of 420 simulations. This design was constructed to satisfy stoichiometric constraints and to provide space-filling coverage. The number of points was increased iteratively in three stages: initially 20 points, a second set of 20, and the final two (shown in blue). Since the simulations require significant computational resources, the results of the UQ analysis in each iteration influenced the selection of points in subsequent iterations. For example, the the results of the first two iterations influenced expanding the bounds for the third iteration.

Table 1. Arches submodels used in Atikokan simulations

Physics	Description of the model Reference	
Fluid mechanics	LES with a dynamic Smagorinsky model.	[7, 9, 13]
Multi-phase flow	Direct quadrature method of moments with 4 environments. Transporting weights, particle velocities, raw coal, char mass, particle enthalpy, maximum particle temperature.	[7, 9, 14, 15]
Radiation	Discrete ordinates with S8 (80 directions).	[16]
Spectral properties of CO_2/H_2O mixtures	Model with 4 bands.	[17]
Gas-phase reactions	Equilibrium tabulated as a function of heat loss and 2 mixture fractions. Transport equations for mixture fraction define elemental composition, enthalpy yields a heat loss.	[11, 18]
Wall heat transfer	1D steady state model. Three regime model enables deposits to transition among dry, dry and wet, or wet based on incident heat flux and temperature.	
Emissivity model	Computes emissivity of deposits based on spectral properties of ash oxides. Includes sintering effects.	[19]
Ash deposition model	Calculates probability of particle deposition based on particle viscosity and maximum particle temperature.	[10]
Particle drag	Computes drag for each of 4 environment sizes based on gas-particle velocity difference.	
Devolatilization	Yield and rate model which includes a high temperature yield modification.	[20]
Char oxidation	Pore and surface reactions, including O_2 oxidation, CO_2 and H_2O gasification. Particle shrinks as surface reactions proceed. Devolatilization of products inhibits heterogeneous reactions.	[21, 22]

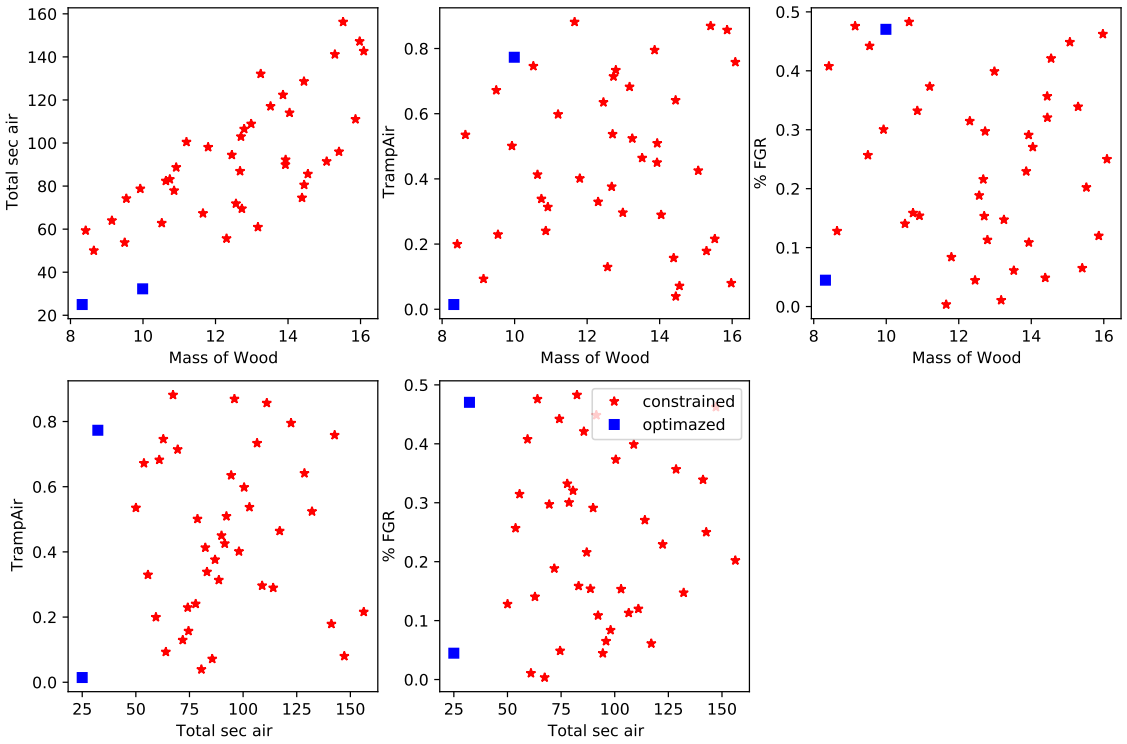


Fig. 7. Design points for the Atikokan simulations projected to various two-dimensional parameter spaces. Design satisfies the constraints discussed in sec. 3.3 and optimization was performed for space-filling and low-discrepancy. Existing 40 (red stars) points from the first two iterations are distinguished from the additional 2 (blue squares) points for the third and final iteration.

Most of the 420 simulations were run on Quartz at Lawrence Livermore National Laboratory (LLNL); approximately 20 simulations were run on HPC resources at the University of Utah. Each simulation required 1164 processors for 5-7 days to reach steady state. In addition, we had to run all cases for additional time due to model modifications and to generate sufficient images for movie-making. Because of the sheer volume of simulations, we developed tools to automate the job submission and data management processes. We also requested and received a large allocation (Tier-3) on LLNL scratch space. At the end of 2021, we had 455 TB of data and more than 41 million files.

The set of simulation output data required for the digital twin grew over time to include 60 variables grouped into three general categories:

- Variables measured at the plant: O_2 outlet concentration, gas temperature at the top of the boiler and at the outlet, net power, flame scanner signal strength (15 total, one per burner)

- Variables needed for constraint and optimization of the digital twin based on feedback from OPG personnel: CO concentration at the top of the boiler and at the outlet),

NO_x outlet concentration, maximum surface temperatures of tube banks in boiler and in convective pass

- Other variables of interest: wall heat flux profile (20 total), mass deposition on walls, total flue gas flow rate.

We developed an instrument model for each type of data that we extracted. For example, we computed the gas temperature at the top of the boiler by averaging the temperatures along a line of sight through the computational domain. We computed the outlet species concentrations by averaging across the outlet plane. We extracted the flame scanner data as the radiative intensity arriving from the orthogonal direction at a location just above the burner inlet. All data were averaged over the last 4 s of simulation time with the exception of the levels 1&2 cases, which were averaged over a residence time (from 8-28 s depending on the case).

We also generated a series of three-dimensional images for visualization purposes that span a range of variables and visualization types: slice (horizontal and vertical), surface (on all surfaces within the boiler), and volume (volume-rendered image of entire domain or with two cutting planes through the domain). This "Simulation Visualizer" is part of the digital twin and is accessed at https://chpc.utah.edu/~DigitalTwin. The user may query any two-level set/case combination, select the visualization type, and then choose a variable to visualize from the drop-down menu. The chosen variable can be viewed as a still or as an animated gif.

3.2 V/UQ (ML)

The primary advantages of our digital twin is its ability 1) to predict key process behavior with uncertainty even when the operating conditions are extrapolated beyond a region of previous operations, and 2) to achieve continuous optimization of plant operating parameters to meet a specified objective function. The accomplishment of the first advantage is described here in section 3.2. The second advantage is discussed in the following section 3.3.

Our validation methodology uses Bayesian ML to quantify the uncertainty in our boiler simulations. This validation process ties the physics-based HPC models (Arches/Uintah) together with experimental observations. The experimental data is of two types: the targeted validation experiments (TVE) which were used in the six years of the Center to achieve heat flux predictivity within 5%, and the online process data used to inform the boiler-specific, multi-physics model parameters. We used both of these experimental data types for model-form validation. First, we performed validation offline, using the TVEs, for each submodel identified by the top-down sensitivity/screening over the history of the Center. Second, for the integrated multi-physics model, we perform validation continuously and dynamically in the online digital twin. This overall dataflow was shown schematically in Fig. 5 ('online' ML).

A unique feature of our digital twin is that it is continuously learning simultaneously from experimental data as well as from the hierarchically validated, science-based, HPC

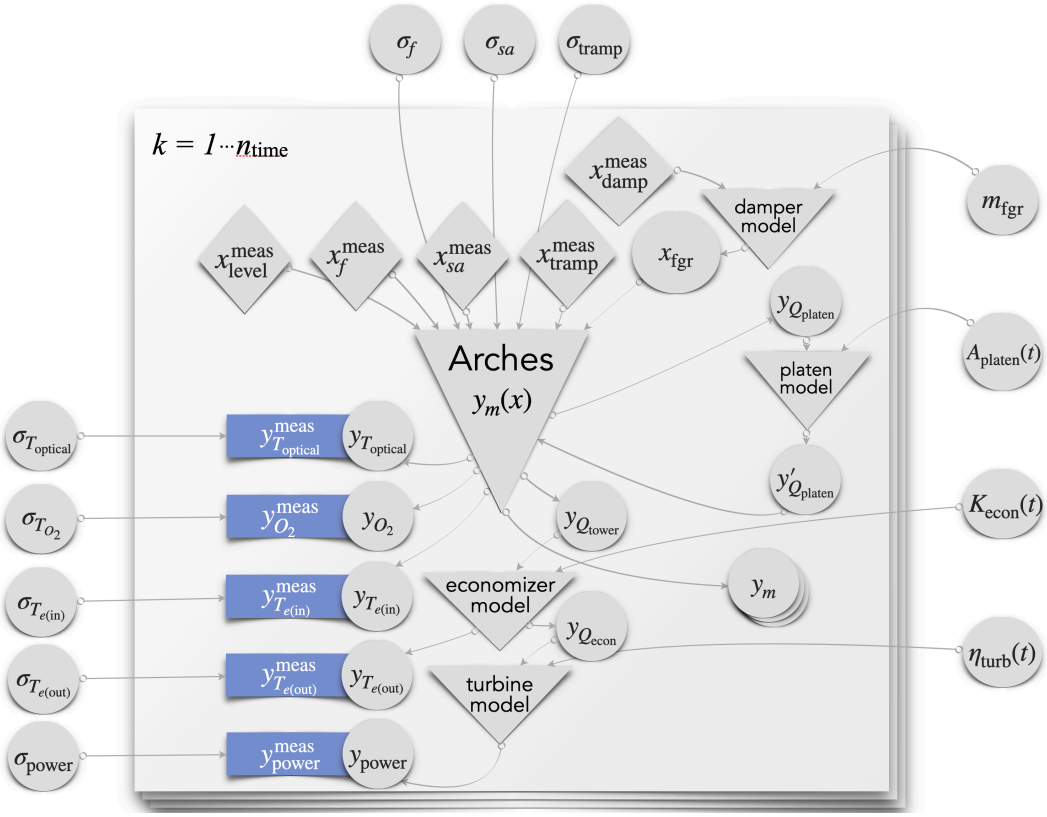


Fig. 8. The Bayes Diagram for the Atikokan Digital Twin.

Arches/Uintah model. While interest in ML is experiencing a period of impressive growth, its most common use is to incorporate large amounts of experimental data and provide empirical prediction. Within the simulation-science community, the common approach has been to use simulation data to train a surrogate model. Our UQ ML methodology combines these two approaches using a Bayesian analysis to perform model-form validation and to generate posterior predictives (QOIs with quantified uncertainty).

This Bayesian V/UQ, represented in the Bayes' diagram in Fig. 8, produces both the learned model parameters with their uncertainty and the posterior predictives of all QOIs from all surrogate models. The Bayesian analysis of the twin and the resulting inference can be performed with any set of data taken from the OPG Atikokan power plant. In the power plant implementation of the digital twin, we would perform this analysis online. For the capstone project, we performed it offline for one set of plant data then applied it to any set of operating conditions to produce posterior predictives. This "Offline Integration" tool is accessed at https://chpc.utah.edu/~DigitalTwin. The user may query the ML with a series of sliders for any set of operating conditions within the operating space of the design of experiments described in section 3.1.

3.3 Optimization (AI)

One of the key lessons we learned from interactions with our industry partners is that uncertainty itself has little value to decision makers unless the tools to make decisions, to optimize in the presence of uncertainty, are coupled with the uncertainty analysis itself. This is the objective of our digital twin: to perform calculations in real-time using the surrogate model and the posterior from the Bayesian inverse problem, to make predictions with uncertainty, and to incorporate formal decision theory to provide optimized decisions which account for the uncertainty. As shown in Fig. 5, the LES calculations are performed offline beforehand, the Bayesian inverse problem is solved online at a timescale commensurate with the changing dynamics of the plant (in this case on the order of hours), and the optimization is performed online in near real-time (in this case on the order of minutes). This section describes the decision theory used in the real-time optimization.

The optimization is performed with the use of a cost function. The cost function translates the physics QOI (power, NO_x concentration, deposit thickness, etc.) to a value to the decision maker (cost). This cost function is defined in collaboration with the decision maker and includes the constraints on the decision. However, the cost function alone is not the final function that is maximized. As E.T. Jaynes said: "An essential thing which is still missing ...is the rule by which it converts its final probability assignment into a definite course of action" [23]. This utility function incorporates the risk aversion propensity of the decision maker. We used the iso-elastic utility function.

For the capstone digital twin, this process is summarized as defining a cost function for a given risk aversion that will:

- generate a given power output y_p (i.e. 64MW)
- maximize boiler tower efficiency
- find the input operating parameters $(x_{level}, x_f, x_{sa}, x_{tramp}, x_{fgr})$
  - x_{level}: firing level pair,
  - x_f: total biomass fuel feed rate,
  - x_{sa}: total secondary air feed rate,
  - x_{tramp}: total tramp air split,
  - x_{fgr}: flue gas recirculation damper position,
- subject to the output constraints:
  - power produced within 5MW of y_p,
  - 6 flame scanners readings $>70\%$ for all burners firing biomass,
  - mole fraction O_2 at the outlet $>1.5\%$,
  - mole fraction CO at the outlet <200ppm,

– all tube metal temps < high-high alarm requirements of OPG,

– no natural gas.

This AI methodology is demonstrated for our capstone project in the ”Online Optimization” tool, which is also accessed at https://chpc.utah.edu/~DigitalTwin. This boiler is required to change load on a five minute dispatch. The data show all of the two-level firing modes dispatched for the Atikokan boiler in the month of December 2019. The user may query the AI with a series of sliders for any time in that month. The results show the actual conditions and the optimum operating conditions recommended by the digital twin for each five minute dispatch.

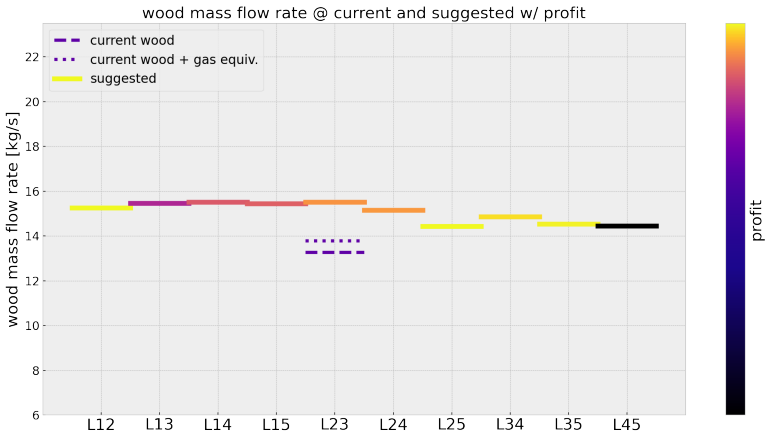


Fig. 9. Atikokan Digital Twin wood mass flow rate operating conditions for Dec 3, 2019 at 17:40.

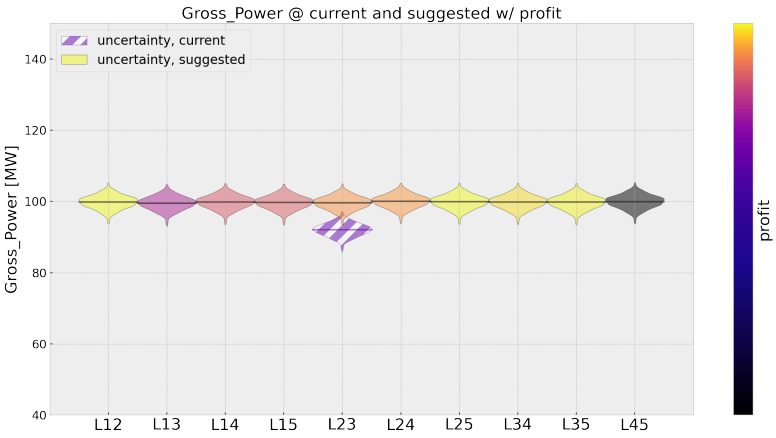


Fig. 10. Atikokan Digital Twin gross power generated for Dec 3, 2019 at 17:40.

For example, on December 3, 2019 at 17:40, the Atikokan boiler was dispatched to produce 100MW. Figure 9 shows the actual biomass wood firing rate at the power plant (natural gas was also fired), the equivalent firing rate of wood plus natural gas, and the optimum wood firing rates for each of the ten possible operating level pairs as identified by the digital twin. The power plant chose to fire biomass on levels 2&3. The color represents the utility or profit in operating at a given set of conditions with the overall optimum achieved by firing on levels 2&5. The optimum wood firing rate differs depending on the firing levels chosen.

Given the wood firing rates shown in Fig. 9, the power generated is shown in Fig. 10. The violin plot shows the uncertainty distribution in this QOI based on the uncertainties learned from the Bayesian inverse problem. The required dispatched 100MW is achieved with all optimum level pair firing rates. However, the actual firing rate (shown with the colored hatched symbol) does not achieve the desired power within the uncertainty of all measurements and models.

The Atikokan boiler tower efficiency is shown in Fig. 11 for the optimum operating conditions for each level pair and for the current operating conditions. This is the objective function for the optimization: to maximize this efficiency subject to the constraints. While the overall maximum efficiency is achieved by firing on levels 4&5, under no operating conditions can all the constraints be met as shown by the profit for this level pair. Specifically, the six flame scanners are not predicted to read above 70% under any operating conditions. The overall optimum that meets all constraints within what is known about the uncertainty can be achieved by firing on any of levels 1&2, 2&5, 3&4 or 3&5.

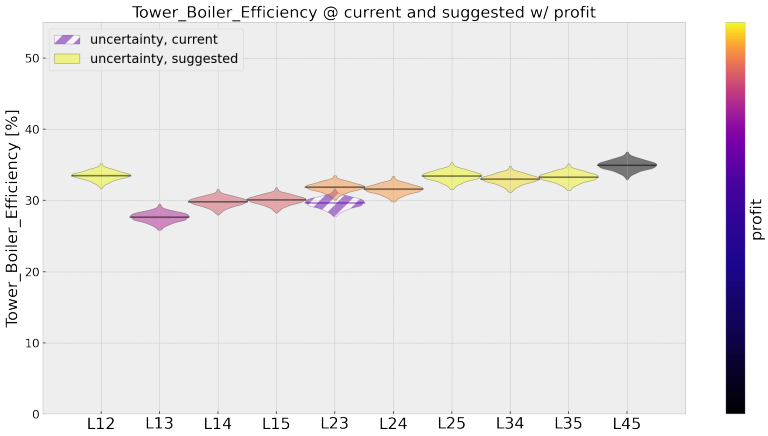


Fig. 11. Atikokan Digital Twin boiler tower efficiency for Dec 3, 2019 at 17:40.

One of the key achievements of the Center was to not only quantify the overall uncertainty in each QOI, but to produce a methodology that identified the source of these uncertainties. For example, consider the flue gas temperature at the outlet of the Atikokan boiler shown in Fig. 12 for the optimum operating conditions for each level pair and for the current operating conditions. For this QOI, there are continuous measurements made at the plant. Using this additional data and our errors-in-variables approach in the Bayesian analysis, we can identify sources of uncertainty due to simulation scenario parameters (discussed further in section **??**).

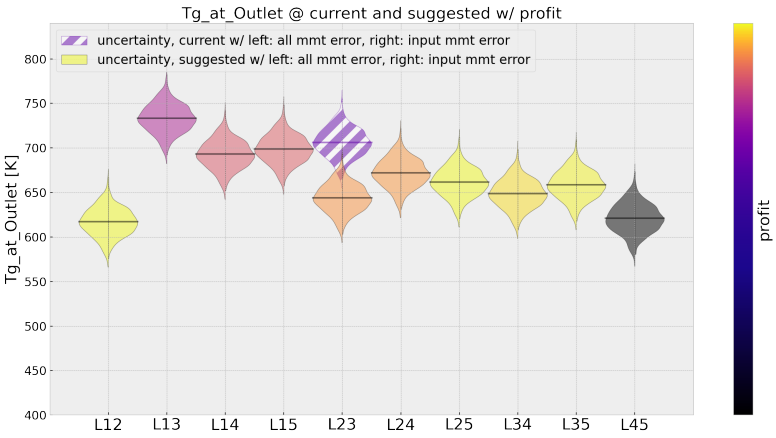


Fig. 12. Atikokan Digital Twin flue gas outlet temperature for Dec 3, 2019 at 17:40.

The distribution on the left side of each violin plot in Fig. 12 shows the temperature uncertainty at the outlet produced from all sources, while the distribution on the right side of each violin plot shows uncertainty in the outlet temperature produced only from scenario parameters. From this analysis we learn that the accuracy of the prediction of the outlet temperature is controlled more by the inaccuracies in the measured scenario parameters than anything else in the simulation. Thus, improving model form will not further improve the accuracy of the predicted outlet temperature.

Figure 13 further illustrates the information gained by the errors-in-variables analysis. This figure shows the predictions of and uncertainties in the flue gas temperature inside the boiler at a flow restriction above all burners called the "nose;" at this location, the flue gas enters the section containing all the convective tubes.

Here the flue gas is hot and temperature measurements are hard to acquire. The plant uses an optical instrument to continuously measure the average temperature. The distributions on the left side of the violin plots in Fig. 13 show the measurement uncertainty in the optical instrument, whereas the distributions on the right of each violin plot show the uncertainty arising from uncertain scenario parameters. Thus, the measurement error in the observed "nose" temperature dominates the uncertainty. The uncertainty in feed conditions that dominated the outlet temperature uncertainty has little effect on the "nose" temperature uncertainty.

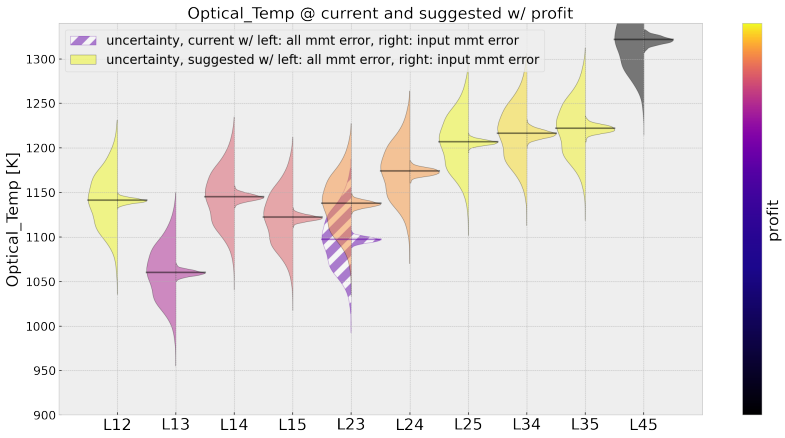


Fig. 13. Atikokan Digital Twin flue gas optical "nose" temperature for Dec 3, 2019 at 17:40.

The heat flux distribution for the Atikokan Digital Twin, the CCMSC ultimate QOI, is seen in Fig. 3 .

4 Key Accomplishments

Over its seven-year lifetime, the achievements of the Center have been accomplished by 78 individuals grouped into three research teams: the computer science, the computational physics and V/UQ. Significant achievements from these three groups include:

- Improvement in our UQ process for extrapolating uncertainty from the pilot-scale data to the full-scale prediction by identifying scenario parameter uncertainty and by propagating both model-parameter and model-form uncertainty into the prediction.
- Reduction of the model form bias in our overarching GE Power simulation from 30% to 5% by identifying the source of the largest bias, the ash deposition model, and then reducing that bias by improving the deposition model. These model improvements included models for particle sintering in the deposit and for the effect of sintering on surface emissivity.
- Demonstration of an online digital twin for OPG's Atikokan biomass boiler.
- Running 400 simulations of the Atikokan boiler on the Quartz machine at LLNL using the Arches/Uintah LES code. There were 10 combinations of burners and a

42-point design of experiments for each combination to cover the four-dimensional space of the four input parameters that we varied. Each simulation required 1164 processors for 5-7 days to reach steady state. We ran the remaining 20 simulations on local HPC resources.

- Demonstration that the Asynchronous Many Task (AMT) runtime system (Uintah) makes it possible to run complex, multi-phase, multi-physics applications such as the Atikokan boiler using Arches/Uintah at the largest processor counts available to us.
- Demonstration of strong and weak scaling of the most computationally challenging task, thermal radiation via ray tracing, and of performance portability by using the Kokkos system via a machine independent loop layer in Uintah.
- Development of the PIDX data I/O library from a proof of concept prototype to a fully integrated and supported file format within Uintah.
- Incorporation of in situ visualization in to the Uintah framework using VisIt's in situ interface, libsim, by expanding Uintah's runtime infrastructure in the form of a more centralized collection of performance data, simulation parameters, debugging mechanisms, and runtime controls and by presenting this collection to users via a simulation dashboard. This dashboard allows users to do interactive parameter exploration, visual debugging, and computational steering.
- Creation of a coupled simulation-machine layout, making it possible to identify computational bottlenecks that would otherwise be difficult to diagnose.

An elaboration of key accomplishments by team follows.

4.1 Computer Science

4.1.1 Uintah Computational Framework Our key accomplishments are described in the publications listed at the end of this report and summarized here.

We determined how to run efficiently with Uintah as-is on Intel's first generation Xeon Phi, Knights Corner, using Uintah's most complex standalone problem, a simulation of radiative heat transfer using reverse Monte-Carlo ray tracing (RMCRT). Through detailed studies, we also demonstrated how to manage thread placement and identified node-level, many-core domain decomposition challenges [24].

We performed the first study to support task scheduling and execution on GPUs within an AMT framework. We demonstrated how the Uintah AMT runtime can be adapted, making it possible for complex multi-physics applications with radiation to scale on current petascale and emerging exascale architectures. For Uintah, which uses a directed acyclic graph to represent the computation and associated data dependencies, we achieved these aims through: 1) using an AMT runtime; 2) adapting and leveraging Uintah's adaptive mesh refinement support to dramatically reduce computation, communication volume, and

nodal memory footprint for radiation calculations; and 3) automating the all-to-all communication at the runtime level through a task graph dependency analysis phase designed to efficiently manage data dependencies inherent in globally coupled problems. We modified the Uintah infrastructure to support these algorithms at large scale and achieved excellent weak and strong scaling for RMCRT up to 262,144 CPU cores and 16,384 GPUs, through a unique and novel application of Uintah's AMR support, specifically the aggressive coarsening of the global radiation mesh as problem size increases. We achieved efficient, automated halo management within an AMT runtime for globally coupled problems. Lastly, we demonstrated these ideas on an industrial-size production boiler problem, running on the largest petascale architectures available.

We implemented semi-coarsening algorithms for a "black box" Kokkos-based multigrid solver designed for problems discretized on structured meshes [25].

We ran with Kokkos::OpenMP at the node-level using a simple standalone problem. We performed detailed studies identifying what levels of performance Kokkos might offer Uintah and demonstrating node-level performance improvements up to 2.4x when refactoring for portability.

Next, we ran with Kokkos::OpenMP at both the node-level and at scale using RMCRT. We ported multiple RMCRT algorithms to Kokkos, implementing a MPI+Kokkos::OpenMP task scheduler to allow for parallel execution of individual tasks to address many-core domain decomposition challenges. We demonstrated good strong scaling of the resulting task scheduler to 65,536 threads across 256 Knights Landing processors on TACC's Stampede 2 and node-level performance improvements up to 3.0x when refactoring for portability.

We then ran with Kokkos:: OpenMP and Kokkos::CUDA at the loop-level using the most complex Arches/Uintah loop, which models the char oxidation of coal particles, and at scale using RMCRT. To do this, we ported the Arches/Uintah infrastructure and its most complex loop to Kokkos. We demonstrated node-level performance improvements up to 2.7x when refactoring for portability and up to 2.6x when more efficiently using a node via newly enabled parallel execution of individual tasks. We demonstrated good strong scaling of the MPI+Kokkos::OpenMP task scheduler to 442,368 threads across 1,728 Knights Landing processors on TACC's Stampede 2. Most importantly, we shared an extensive collection of good practices and lessons learned through our Kokkos porting efforts with the HPC community.

The evolution of the UCF required code modernization efforts with updates to the memory subsystem, MPI communication layers, and GPU data warehouse. Our resulting efforts yielded a reduction of code by moving to the C++11 standard library. In addition, we have distributed and managed the UCF through a Github branch, maintaining a portable version of Uintah that consists of tens of thousands of lines of changes across hundreds of files to enable use of OpenMP and CUDA via Kokkos in Uintah's infrastructure, standalone example problems, and Arches simulation component.

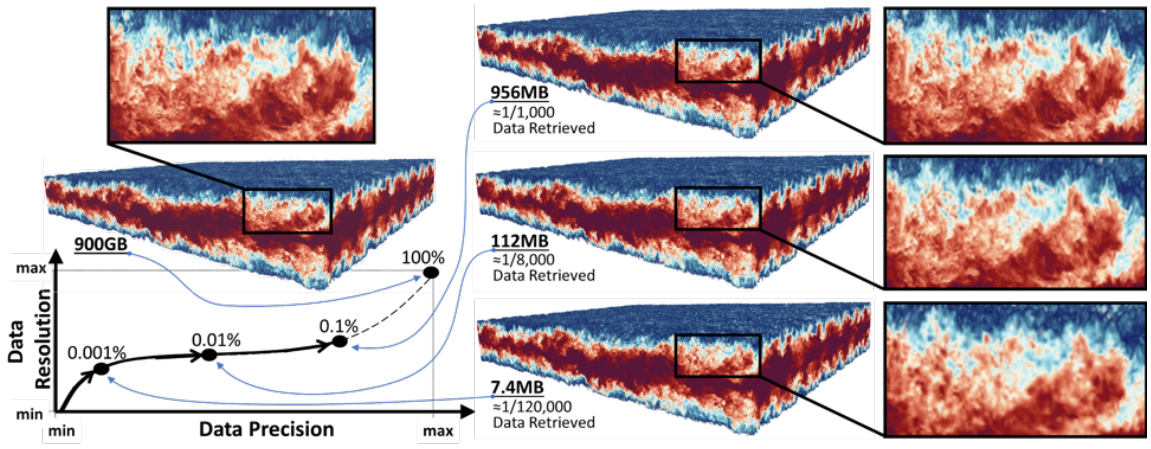


Fig. 14. Compression of 900 GB DNS dataset from turbulent mixing simulation (top-left) in a streamable format.

4.1.2 Data Management Over the history of the center, we have been working on scalable I/O strategies. One of our major contributions has been the development of a new data model that subsumes a number of traditional approaches by providing hierarchical data layouts that also include precision and resolution. Figure 14 shows one of our most recent results - a very high quality approximation is retrieved using only 1/1,000 of the 1 TB dataset. This new data model extends the current IDX used in the PIDX and OpenViSUS libraries and allows many progressive decodings that modulate incremental improvements in precision and/or resolution. The diagram at the bottom-left of Fig. 14 shows the 2D precision-resolution space where a progressive decoding can be traced as a curve (monotonic both in X and Y) starting from the origin (empty data set) and ending in the top-right corner (full resolution/precision data). The test dataset in Fig. 14 has a spatial resolution of 10240x7680x1536 and a numerical precision of float64. A coarse approximation (bottom-right) of resolution 640x480x96 and low precision is obtained by reading only 7.4 MB from the top of the hierarchy in the data layout. A medium approximation (middle-right) with improved resolution (1280x960x192) and precision is obtained by continuing to read up to 112 MB. A high-quality approximation (top-right) of further improved resolution (2560x1920x384) and precision is obtained with 956 MB of data decoded.

Our adaptive approach is able to improve write and read performance for imbalanced I/O workloads. Figures 15 and 16 provide empirical evidence of the effectiveness of our adaptive approach using a number of performance metrics.

With respect to interactive rendering, we have developed new strategies for low memory rendering of large scale particle data through the P-k-d tree; developed novel AMR data reconstruction strategies for volume and isosurface rendering which are now available to users through the OSPRay software framework; and explored how new GPU hardware can be leveraged to accelerate rendering of unstructured volumes. In the space of distributed

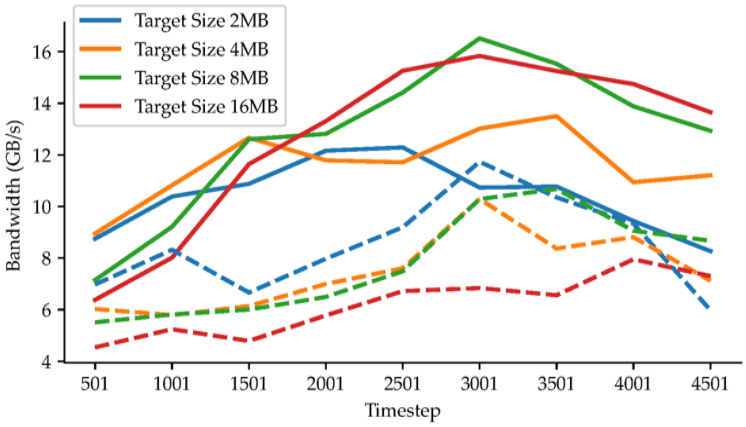
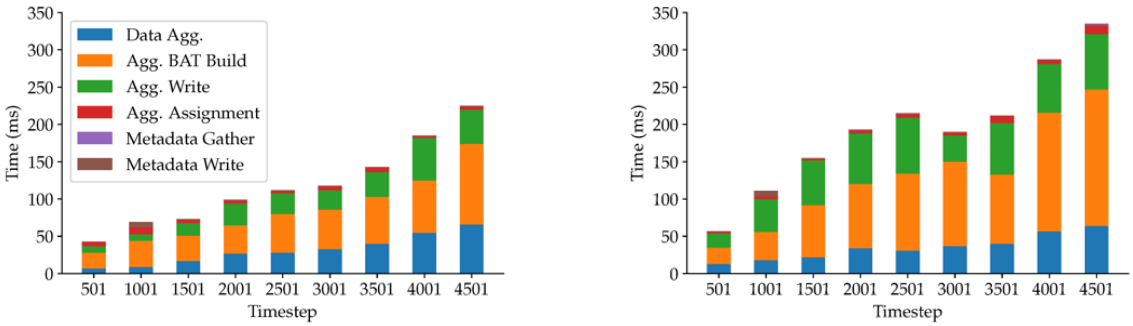


Fig. 15. Adaptive (solid) vs. fixed (dashed) I/O write performance on the Boiler Injection time series on 1536 ranks. Our adaptive approach is able to improve write and read performance for imbalanced I/O workloads.

rendering, we have done work in support of the VisIt system, which can now leverage OSPRay for scalable, high-quality distributed rendering and PIDX for fast I/O. We have also made advancements in fundamental distributed rendering and compositing algorithms, achieving scaling and absolute performance over IceT. These algorithms are easily accessible to users through OSPRay's MPI module, and we have demonstrated their effective use for in situ applications.

We have explored lightweight strategies for decoupled, asynchronous, in situ visualization and analysis. In contrast to larger libraries (e.g., Catalyst, LibSim), we have focused on small libraries which are easy to integrate and have minimal impact on the simulation. The simulation impact is further reduced by enabling asynchronous, in transit visualization, where the client can be run on a separate set of nodes to avoid slowing down the simulation process. With our approach, we have demonstrated integrations in Uintah, LAMMPS and DNS, and have evaluated impact on the simulation and client performance for rendering tasks using OSPRay. Although our focus has been on lightweight libraries and integrations, they can also be used as the base data transport layer for more full-featured systems such as SENSEI.

4.1.3 Radiation Integration One of the greatest challenges for CCMSC has been the cost of solving for the radiative heat flux divergence for thermal radiation transport. Initially, over one third of the computational cost of a simulation was consumed in the radiation solver alone. Our Center pursued both a sweeping algorithm for discrete ordinates and an RMCRT method to solve this problem. Sweeping discrete ordinates (SDO) is 5 to 50 times faster, depending on problem scale and optical properties, than using the linear solver. With the adoption of Kokkos and an inner-loop rewrite, we saw a 30x speed-up with RMCRT via an integrated effort from the computational physics and computer science groups. We accomplished an 8x speed-up via uti-



(a) Adaptive IO **(b)** Fixed IO

Fig. 16. Breakdowns of I/O on the Boiler Injection, 8MB target size. The improved load balance achieved by our approach reduces the time spent in the major components of the pipeline, improving write performance.

lization of the Kokkos scheduler and the reduction of memory reads and a 4x speed-up by reformulating the ray-tracing algorithm. Even with this dramatic improvement of efficiency, SDO still appears to out-perform RMCRT for heavy patch loading. However, for small patches, RMCRT may outperform discrete-ordinates radiation due to its impressive strong scaling ability. In the end, SDO was the most efficient method by orders of magnitude given the same accuracy constraints. This sweeping method resolved the issue to such a level that the radiation costs are now low enough that the pressure projection and other physics solvers dominate the cost of an Arches/Uintah computation.

With the development of SDO, we reduced radiation compute costs enough to explore spectral radiative effects. We added solver support for spectral radiation transport into Arches/Uintah. The radiation solver works in tandem with a new radiative properties model for five grey gases in Arches. This model works across all modes of operation within the code, with and without particles as well as with and without scattering physics. We have ported SDO to a Kokkos implementation, promising even more computational efficiency when Kokkos support is available for the entire framework.

The RMCRT approach for radiation modeling originally comes from the heat transfer and oncology communities, but it had never been modified or adapted for use at large scale. Our extensive work in implementing RMCRT is summarized here.

The RMCRT model requires all-to-all communication of the radiative properties, which is the single biggest drawback of the algorithm. We reduced the cost of the RMCRT all-to-all communication phase and the nodal memory footprint by using an adaptive mesh refinement (AMR) approach to achieve scaling. The AMR fine mesh is used only locally, and a coarse mesh is used elsewhere for the RMCRT ray-marching algorithm. Although the AMR methods used in this work are not new, the application of these methods to radiative heat transfer algorithms and their scalability is novel. We also investigated the impact of varying the number of rays per cell and the distance a ray would travel before moving to a coarser grid on a different level (halo distance). We implemented four additional tech-

niques for reducing the communications costs: 1) casting the communicated variables as floats instead of doubles, 2) utilizing Uintah's AMR infrastructure to communicate a coarse representation of the radiative properties, 3) temporal scheduling by constructing multiple taskgraphs with each taskgraph containing a different set of tasks and communication dependencies, and 4) spatial scheduling of the tasks that allows the developer to execute tasks on a subset of the domain. These temporal and spatial scheduling contributions have made Uintah the only AMT runtime offering auto MPI message generation and scalable task graphs when considering problems with global data dependencies.

We addressed complexity involved with Uintah task graphs at scale for RMCRT with task graph compilation and automated MPI message generation with global halos. We also introduced novel nonblocking, thread-scalable data structures for managing asynchronous MPI communication requests, replacing previously problematic Mutex-protected vectors of MPI communication records.

We developed RMCRT for the CPU and GPU, testing the framework and algorithm with simplistic scenarios. However, once we started running realistic production calculations, we encountered memory leaks/fragmentation issues in addition to excessive and expensive communication on non-radiation calculation timesteps, so we focused on cleaning these up.

We performed a strong scalability study on ALCF:Titan using the MPI/threaded scheduler and the AMR capabilities of the RMCRT algorithm for solving the radiative transfer equation. Our results showed good strong scaling characteristics up to 262K cores on three problem sizes (128^3, 256^3 and 512^3 on highest resolved level) on a grid consisting of two levels with a refinement ratio of two. Using the INCITE award on Titan (71M SUs), we performed a suite of verification tests for both the CPU and GPU versions of RMCRT on 8K, 16K, 32K, and 128K cores. We compared the QOIs (divergence of heat flux and wall heat flux) against simulations that used the discrete ordinates radiation model; the qualitative agreement of the QOIs was very good. Overall, the results from the INCITE runs demonstrated that RMCRT is a viable and competitive radiation model.

We also extracted the RMCRT virtual radiometer capability from the core RMCRT code and re-implemented it for use directly in the Arches component in conjunction with the discrete ordinates radiation solver. The virtual radiometer mimics a physical radiometer instrument. The computational cost of the radiometer code is a small fraction of the overall cost. We generalized the code so any number of radiometers can be specified. Each radiometer can be located anywhere in the domain and has unique properties (orientation, solid angle and number of rays).

4.2 Computational Physics

4.2.1 LES Integration The creation of the LES Integration Group (LESI) is an example of a key lesson learned in the execution of our multi-disciplinary project. Individuals at the interface of the three major disciplines of the Center (computer science, computational physics, V/UQ) were essential to the integration needed for success-

ful accomplishment of the Center's multi-disciplinary goals. LESI orchestrated the move to exascale coding paradigms within the application code, Arches/Uintah, while ensuring software quality through regression testing and both code and solution verification. LESI also served to bridge the computer science and computational physics within the Center. Physics model development occurred directly within LESI or in tight collaboration with model developers. Finally, LESI helped to ensure successful completion of large numbers of full-scale simulations on internal and external computational resources for the V/UQ effort.

Adopting an exascale approach within the Center was a highly collaborative effort between the LESI and computer science teams. LESI adopted a few principles in moving exascale code constructs to the Arches/Uintah physics code: 1) minimize disruption to the production UQ effort, 2) introduce more flexible code design within Arches, 3) provide capability for new physics to adopt new code constructs for immediate use in production runs on CPU-only and future heterogeneous architectures, and 4) provide a generic interface for the two approaches originally under consideration (Kokkos and DSL). This effort led to the development of an intermediate layer which served to buffer the physics development from the evolving exascale effort in the framework. The software layer was tailor-made for the Arches component and leveraged knowledge of the LES algorithm to simplify the layer. An unintended but positive outcome was that the software layer served as an intermediate framework for the computer science and LESI teams to communicate and to transfer design ideas because of the centralization of touch-points between the physics component and the framework. Another benefit was that the layer reduced lines of code within the physics models by encapsulating UCF boilerplate required for framework task scheduling and variable access. The layer also provides flexibility in how Arches physics tasks are packaged and scheduled through the UCF. This flexibility, in theory, may allow us to combine lightweight physics tasks that do not require ghost-cell exchange, potentially amortizing data movement costs in the cases of GPU portability.

After some exploration of the DSL and Sandia's Kokkos project, we adopted Kokkos as the performance portability approach. We have overcome several hurdles but several more still exist to demonstrate full portability for the target boiler problem. These challenges reside within the framework and physics efforts. The benefit of the approach, however, has been demonstrated on single-physics problems and some combined-physics problems.

At the inception of CCMSC, the Arches/Uintah physics component maintained one of the first deployments of solid fuel (coal) combustion in an LES paradigm. The extent of the physical modeling for the Center's primary goal was insufficient, however, for the required UQ bounds on key QOIs. Hence, over the lifetime of the Center, our team made several key physics contributions to coal modeling, from the fundamental particle scale through to the integrated, large-scale simulation. The following list highlights some of the key developments:

- Improvement to radiation modeling by exploring two radiation models, RMCRT and radiation sweeps

- Improvements to coal particle reaction modeling, devolatilization and char oxidation oxidation, from the detailed single-particle perspective to the integrated LES scale
- Improvements to the direct quadrature method of moments (DQMOM) implementation
- Development of a novel solid fuel NO_x model
- Development of a conjugate heat transfer model, including ash particle deposition
- Soot modeling
- Inclusion of particle size effects such as swelling and shrinking
- Expansion of the suite of turbulence models options within Arches.

These and other improvements to the multi-physics capability in Arches/Uintah have led to the improved predictability of Arches/Uintah for solid-fuel systems at a massive scale. However, with the addition of more tightly coupled physics, we needed to engineer a stable and robust algorithm in the LES context. The flow field within a solid-fuel-fired boiler is a highly turbulent system of multi-phase combustion reactions and intense radiative heat transfer. While many QOIs are time-averaged, non-linear, short-time-scale information impacts fundamental outcomes of the boiler operation. By using the LES code as the computational fluid-dynamics framework developed by CCMSC, we have been able to compute as many of these temporal and spatial scales as is both possible on an HPC machine and necessary for the prediction as measured by formal V/UQ.

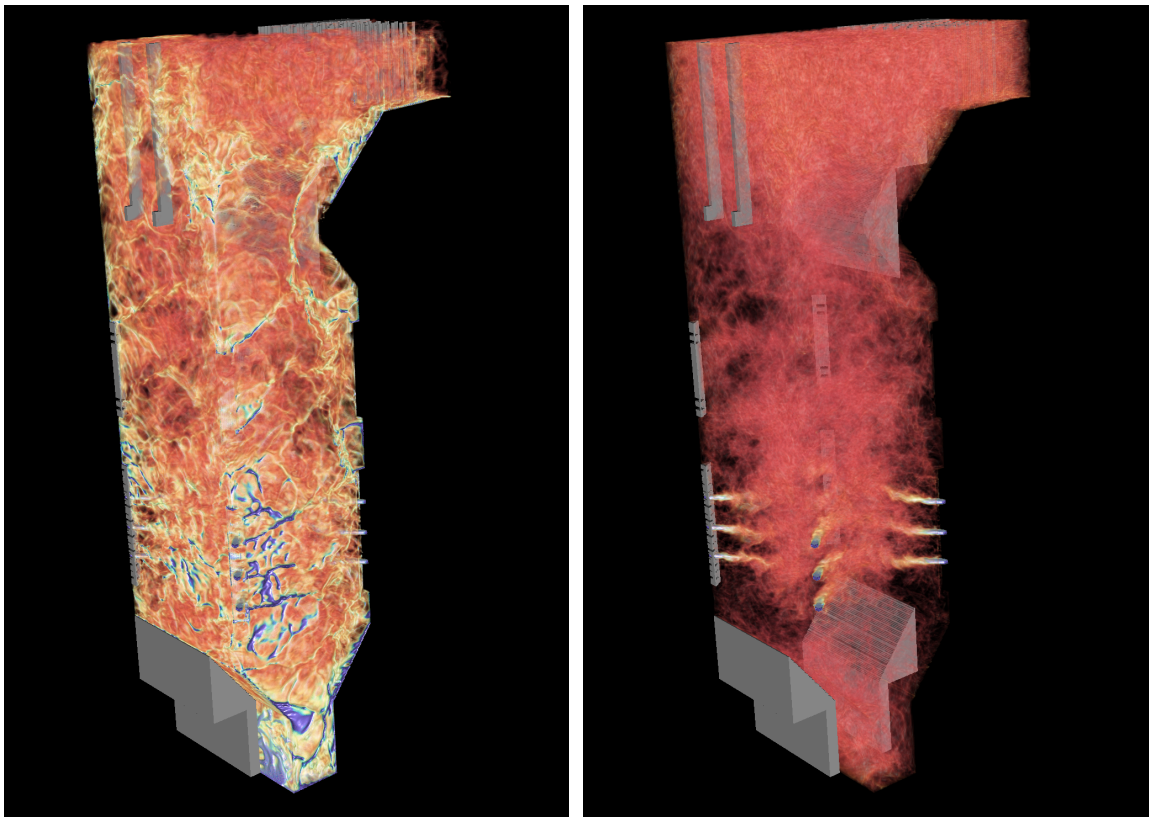
The turbulence in the solid-fuel boiler is characterized by the turbulent length scales (wavenumber), k (1/length scale), and the turbulent kinetic energy spectra, $EU(k)$. Resolving all turbulent scales in the boiler is intractable, even at exascale, given the size and complication of the target application. In LES modeling, a low-pass filter is applied to the governing equations, resulting in a portion of the energy spectrum that is resolved and a portion that requires modeling approximations to account for the eventual dissipation of energy at the smallest scales. In general, we have been able to capture a significant portion of the energy-containing eddies directly ($>80\%$). The frequency location where the hand-off occurs between grid-resolved and subgrid-modeled is the cut-off frequency. With the significant HPC resources available for this project, we added more resolution to a fixed problem, decreasing both the filter width and the dependence on the subgrid model. We created an approach which leverages resolved LES information for large length- or long time-scale phenomena. Our technique, which we call "rate clipping," involves a relaxation to equilibrium conditions at the unresolved scales below the cut-off frequency; that is, we clip the rate to equilibrium for time scales not resolved on the mesh. Each modeled physical phenomena has a unique relaxation. We exploited this technique in the Center for all multi-physics, subgrid modeling occurring in the solid-fuel boiler simulations. With this approach, we can use Arches/Uintah to address problems of interest at time scales ranging from 1e-6 to 1e4 seconds. Our approach is tightly integrated into the numerical algorithm

and has proven to be robust and reliable. Indeed, the final algorithm resolved many stability and efficiency issues seen in Year 1 of the Center. This key accomplishment allows for computational scaling as the HPC resources scale, greatly aiding in the accuracy of LES models. LESI led efforts to assess simulation quality and to test assumptions regarding the equilibrium assumptions.

For example, Arches/Uintah makes use of. DQMOM [14, 15, 26]. DQMOM solves the moment equations on an Eulerian mesh and avoids the potential number-of-particles-squared scaling of computational work that can be required for particle-particle interactions in a Lagrangian particle tracking method. DQMOM calculates the particle position, diameter, and composition, which in turn is used by the radiation modeling effort. The particle-dynamics submodels, including drag, devolatilization, char oxidation, and moisture evaporation, all appear as source terms in the DQMOM equations. Pulverized-fuel combustion in the boiler naturally has a wide range of length and time scales. LES modeling of this system at the scales of interest allows direct representation of several of these time scales - or at least resolution of a significant portion of these scales - which in turn allows the reduction of modeling dependency. This concept has been applied to the particle reactions (devolatilization, char oxidation, NO_x and CO formation) over the lifetime of this project.

4.2.2 Particle Physics The particle size distribution of pulverized fuel in our overarching problem exhibits a spectrum of physical behavior. The smallest particles behave as tracers for all of the resolved scales. Therefore, the drag of particles in this unresolved regime should be modeled in the subgrid-scale flux. In the extreme of zero Stokes number, the subgrid-scale flux is often modeled using gradient diffusion. Increasingly larger particles are in a regime such that they are ballistic with regard to all the unresolved scales – their trajectories are essentially unaffected by the presence or absence of the unresolved scales. For this reason, particles in the resolved regime should be modeled using the drag directly, as done in direct numerical simulations. As the scale of the computational effort increases, the Nyquist cut-off moves to smaller lengths, resulting in particles of smaller size moving from one regime to another. This regime change, when described by an appropriate change in modeling approach, results in more accurate and higher fidelity computations. The advantage of an HPC LES simulation is that with increasing computational power, more of the particle drag effects are resolved directly rather than being modeled.

This distribution of Stokes numbers as a function of particle size and eddy size results in a segregation of particles in the pulverized fuel boiler. Extreme computing with LES can capture this effect. Figure 17 shows volume-rendered images of the particle number density for two different particle sizes at the same timestep in the corner-fired GE Power boiler. The larger particles (blue color) concentrate along edges of eddies of much different size than the smaller particles, which, while still concentrating along edges of coherent structures, are much more uniformly dispersed than the larger particles. For the computations of the capstone project, we were able to resolve all of the particle drag effects for all relevant particles (all particles $>$ 10 microns in diameter) in the system.



(a) 90 micron particles **(b)** 30 micron particles

Fig. 17. Volume-rendered images of the particle number density field for two different particle sizes from the full particle size distribution in the GE Power BSF. These images show the particle size segregation in the turbulent field of the boiler. For this HPC LES simulation, we are resolving all of the particle drag effects for all relevant particles ($>$ 10 microns in diameter) in the system.

4.2.3 Multi-Phase Combustion Chemistry Models We have developed an open-source, solid-fuel database in the PrIMe cyberinfrastructure, archiving 1100 data records for devolatilization, char oxidation, and nitrogen release. Experiments span across 269 types of solid fuels including fossil, chars, biomass and blends. Using a cloud-based infrastructure, which supports crowdsourcing, Sandia National Laboratory (Livermore) contributed additional data records, including coal oxidation experiments from their Combustion Research Facility.

We proposed several forms of the char oxidation model to better agree with validation data. We performed the V/UQ for these models using the tools and methods of Bound-to-Bound Data Collaboration (B2BDC). We encountered two major difficulties when applying our standard validation strategies: 1) challenges in fitting surrogate models to the computer code, and 2) significant ambiguity in the reported data and experimental setup. To over-

come the first challenge, we developed a new strategy for constructing piecewise quadratic surrogate models with a more intelligent subdivision rule based on B2BDC's consistency measure. This new strategy demonstrated a significant reduction in the number of domain partitions required to accurately represent the char oxidation model. To address the second challenge, we conducted separate analyses based on two different assumptions about the data: 1) the particle diameter was initialized at the mean sieved bin size and 2) there was an ensemble of particle diameters based on a distribution (fit from the data). Our piecewise strategy demonstrated that the first analysis led to inconsistency; i.e., disagreement with the data. In contrast, the second analysis led to a consistent dataset with quantified uncertainties. We concluded that the model was tentatively valid as the second analysis made better use of the available data. Critically, however, this result calls for new experiments focusing on the characterization of the initial particle sizes.

Total volatiles yield is a principal QOI in large-scale coal combustion simulations. Complex and accurate pyrolysis models are too computationally expensive, so we developed and tested simpler model forms that would accurately describe total volatiles and tar yields as a function of residence time, temperature, and heating rate. We chose a two-step global model with series-type distributed activation energy based on simplicity and accuracy. Our next step was to provide simple ways to better describe the chemistry of the volatiles versus the char. The elemental composition of volatiles is higher in hydrogen and oxygen than the resulting char. We gathered elemental composition data for coal char and the corresponding tar from the literature and correlated it as a function of coal type, heating rate, and final temperature. Use of these elemental correlations in simulations can improve the predicted concentrations of O_2 and CO_2 in a boiler. We are working to correlate the heating value of the tar and char produced from pyrolysis in order to improve the energy distribution during coal pyrolysis and char conversion in large-scale simulations.

With respect to char conversion, our original goal was to investigate char conversion in oxy-fired environments. We curve-fit the best available data with a comprehensive char conversion model that included intrinsic reaction, pore diffusion, annealing, and changes in particle diameter and density. Our analysis showed that the particle temperature data were biased, with not enough sensitivity to particles that had burned out. We performed a sensitivity analysis to determine which processes were most important to the rate of char conversion. Other than the intrinsic kinetic rates, we found thermal annealing, which decreases the reaction rate as a function of residence time and temperature, to be the most important factor. We developed an improved, generalized thermal annealing model based on a much larger dataset than was available in previous modeling efforts. Our improved model is one way to train simpler global models of char conversion for use in large-scale simulations.

In coal and biomass systems, soot forms mainly from tar species. We developed a generalized soot model for both coal and biomass based on a previously-developed empirical soot model. The model depends on the accurate prediction of tar yield and molecular weight distribution during pyrolysis. We found gasification of soot to be important in oxy-fuel environments due to the high concentration of CO_2. We used the generalized model

to develop a reduced-order model of soot formation and conversion that is more compatible with large-scale simulations. We developed an open-source soot library that treats soot from gas, coal, and biomass combustion, including a number of chemical mechanisms and soot size distribution models.

4.2.4 Deposition Models Wall [27] showed that the total, or hemispherical, emissivity decreases with the temperature up to the point where particle agglomeration influences the scattering behavior of the formed structure. After that point, the emissivity increases with higher temperatures. We proposed a sintering model to represent particle agglomeration that could be coupled with the emissivity model and provide a better understanding of the effects of thermal radiation inside the boiler [28]. The proposed model is based on the works of Pokluda [29], which works for viscous sintering; we added the capability to work with systems of many particles. We applied this model to the sintering of the synthetic slags prepared by Boow and Goard [30]. Their work outlines the most relevant behavior of slag emissivity in presence of particle sintering.

The viscosity of slags is a critical quantity that influences the sintering behavior of particles and ultimately impacts the thermal radiation in the boiler. In the model we developed, we estimate the slag's viscosity using complex equilibrium models [31] for the solid-liquid equilibria of the oxides that are contained in various coals/biomass used in the CCMSC hierarchy. We then modify the Urbain viscosity model [32] by estimating model parameters from the computed equilibria for the oxides. These parameters, part of several UQ cycles over the six years of the Center, have an important role in the description of the wall heat transfer.

We created an ash emissivity model based on the works of Goodwin [33] and Ebert [34] that relies on the computation of the spectral emissivity of deposited ash which, in turn, requires knowledge of the optical properties of the deposits. The algorithm uses different correlations at specific wavelengths to compute the complex index of refraction based on a large dataset of measurements. The index of refraction is used to compute absorption, scattering and extinction properties for the particles via Mie Theory calculations [35] for single scatters.

We also created a thermal conductivity model to account for the morphology of the structures left by the ashes when they deposit on the walls. These structures form pores which affect the rate and efficiency of the heat transfer through the wall. Our model is based on the work of Hadley[36] and takes porosity of the structure as a model parameter.

4.3 Hierarchical Validation and Uncertainty Quantification

4.3.1 The CCMSC V/UQ Methodology The philosophy behind our Center's V/UQ methodology is founded in the context of epistemological skepticism and the scientific method at large. That is to say that all human attempts to understand truth are abstractions which can only approximate reality. These abstractions (*models & theory*) can only be informed through empiricism (*experiments & observation*) as illustrated in Fig. 18), and by their nature they cannot be proven to be

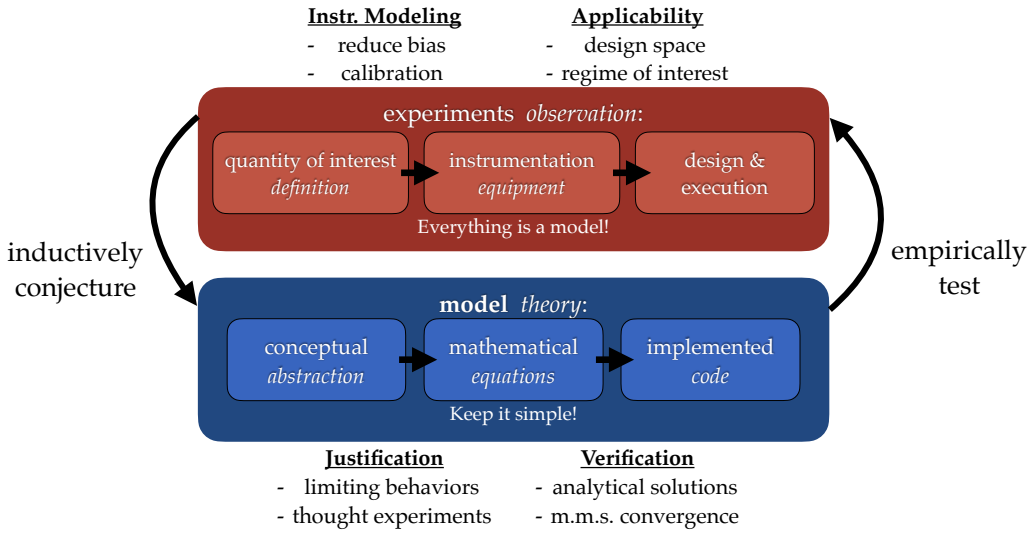


Fig. 18. Graphical diagram of the critical elements of the scientific method as incorporated in our Center's V/UQ methodology.

exactly correct. Our V/UQ approach provides tools to learn about reality in spite of our inherent limitations. First, we quantitatively compare an experimentally observed value, y_e, to a theoretically modeled value, y_m, which are both attempting to represent the same reality, y_R.

$$y_R = y_e + b_e \tag{1}$$

$$y_R = y_m + b_m \tag{2}$$

$$\Rightarrow \quad y_e - y_m = b_m - b_e = b. \tag{3}$$

Here, the b_e and b_m represent the bias in the experiment and model respectively. While making a single observation cannot reveal the associated experimental bias, comparison with theory can reveal the combined bias, $b \equiv b_m - b_e$. Repeated measurements only reveal that there is uncertainty in the bias for each individual observation. Furthermore, this comparison is complicated when calculation of the model requires knowledge of uncertain model parameters, x_m.

In our methodology, uncertainty is represented using probability theory — while we may not know the Platonic reality, the potential that each value might be true is identified by a probability distribution function. Wider distributions represent more uncertainty and narrower distributions represent less. In the context of probability theory, Bayes' law provides a rigorous mechanism for learning from experimental observation (see Fig. 19). In addition to the foundations of univariate and multivariate probability theory, we incorporate stochastic processes, Gaussian-process inference, machine learning (comparing artificial-

neural networks to Gaussian-process regression), surrogate modeling, artificial intelligence (through decision theory and maximization of expected utility) and Markov-chain Monte Carlo sampling.

Often[1] the physical model y_m is a function of both uncertain scenario (z) and model (x_m) parameters; that is, $y_m = f(z; x_m)$. The model parameters distinguish themselves from the scenario parameters by not being directly manipulated in the experiment. Additional uncertainty in y_m requires modeling latent physical phenomena which may occur uniquely for each measurement, and these effects are grouped into the parameter σ_y. The model and measurement parameters are collectively called x; that is, $x = (x_m, \sigma_y)$. Common application of Bayes' law assumes that there are no errors in the scenario parameters, z. We address these types of errors, termed 'errors-in-variables,' at the end of this section.

We[2] can see the value of this approach (physical modeling of the process of interest with Bayesian learning using calibration data) by contrasting it with two common engineering approaches: (1) using physical modeling of the process with standard error propagation to determine measurement uncertainty, and (2) using a purely empirical, least-squares regression to learn from the calibration data. First, the standard engineering practice is to estimate QOI uncertainties using error propagation through the forward problem alone. Consider that as a model is made more sophisticated, more parameters are introduced, and each carries its own uncertainty. The result is that, for the forward problem, the uncertainty in the QOI increases

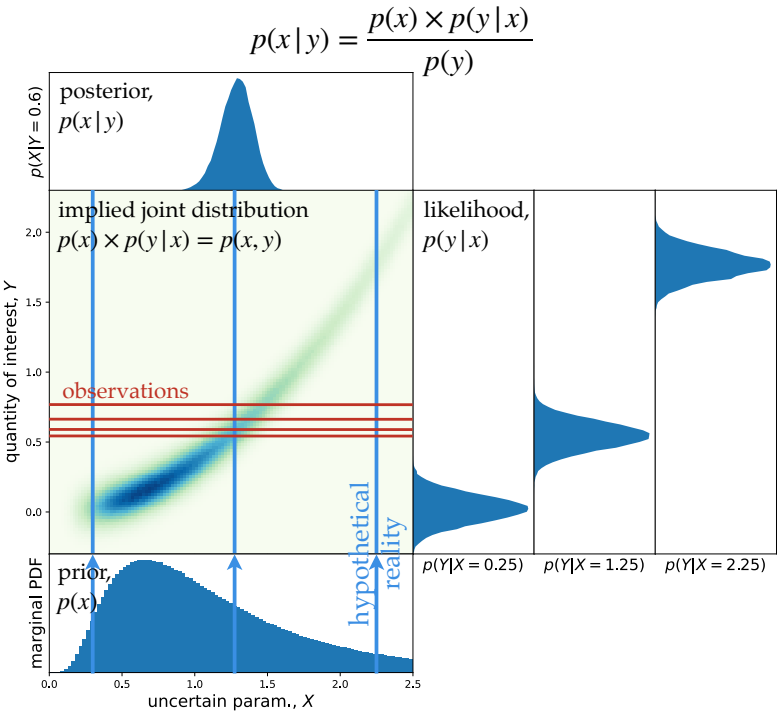


Fig. 19. A depiction of the information flow from prior to posterior knowledge through the likelihood with Bayes' law: the prior (what is known about the uncertain parameter x **before** learning from the observations), likelihood (what might be observed, y, in the hypothetical reality that a given x is true, e.g. 0.25, 1.25, 2.25), observed data (the concrete experimental results, y) and the resulting posterior (what is known about the uncertain parameter x **after** learning from the observations).

[1]The information in this paragraph has been adapted from our paper [37]
[2]ibid.

as the uncertainty in the model form decreases. Conversely, when the inverse problem is performed using Bayes' theorem, the uncertainty in the model form and thus in the QOI decreases as the model form improves – as it should. The better the instrument model, the less the uncertainty in the QOI prediction. We emphasize that the simple propagation of error does not allow one to learn from the calibration experiments, while least squares (and more generally Bayesian methods) do. Second, the empirical, curve-fitted calibration (e.g. using Taylor's series) may produce similar results to our Bayesian methodology for the measured QOI if the selected basis functions are flexible enough. However, without the physical underpinnings, all uses of the instrument in application (measurement) scenarios that differ from the calibration scenario are suspect. In contrast, the physics-based model allows the users of the instrument to understand its applicability and limitations for measurements in conditions other than in the calibration scenario. That is to say, empirical models cannot be trusted to extrapolate while physically based models may be extrapolated within their domain of applicability.

Model Form Uncertainty: Neither[3] of these two common engineering approaches addresses model-form uncertainty, nor does either propagate that uncertainty to the predicted quantities. While Bayesian calibration of a particular model form does propagate the uncertainty to the measurement, the calibration alone cannot eliminate model-form errors. This limitation is illustrated by recognizing that the scientific method employs only two approaches as it attempts to identify the Platonic reality, y_R: observation and theory. Each of these approaches has inherent error and uncertainty – b_e for the experimental bias (potentially varying from replicate to replicate), and b_m for the model bias (or model-form error). Momentarily putting aside any uncertainty in either the model or scenario parameters, the comparison of these two is performed through the defect (Eq. 3). With a single instrument, the model-form error cannot be uniquely identified from the experimental bias; we can only measure the difference between these two, b. Increasing model-form complexity to reduce model-form bias cannot be justified once the analysis has reached the limit where the experimental bias overshadows the model-form bias. Since the calibration experiment itself cannot explicitly identify the model form, it is necessary for the engineer to apply existing scientific knowledge, to make inductive leaps, and to apply appropriate approximations to provide the form. All the calibration can do is "reduce the uncertainty in the inputs in a manner consistent with the measured data" [38]. As E.T. Jaynes said, "In physics, we learn quickly that the world is too complicated for us to analyze it all at once... Nobody knows if there is some natural end to this process, or whether it will go on indefinitely... We shall feel that progress is being made if we are able to construct ideal mathematical models which reproduce a few of its features" [23]. We are satisfied when we reach a level of complexity in the model form that meets our needs for the level of uncertainty in the desired QOI.

There are two Bayesian approaches that seek to identify and/or reduce the model-form bias to levels consistent with the overall uncertainty:

(1) Starting with a simple model form, identify the uncertainty in the QOI. Increase the model complexity and repeat the Bayesian V/UQ with the parameters appropriate to

[3] ibid.

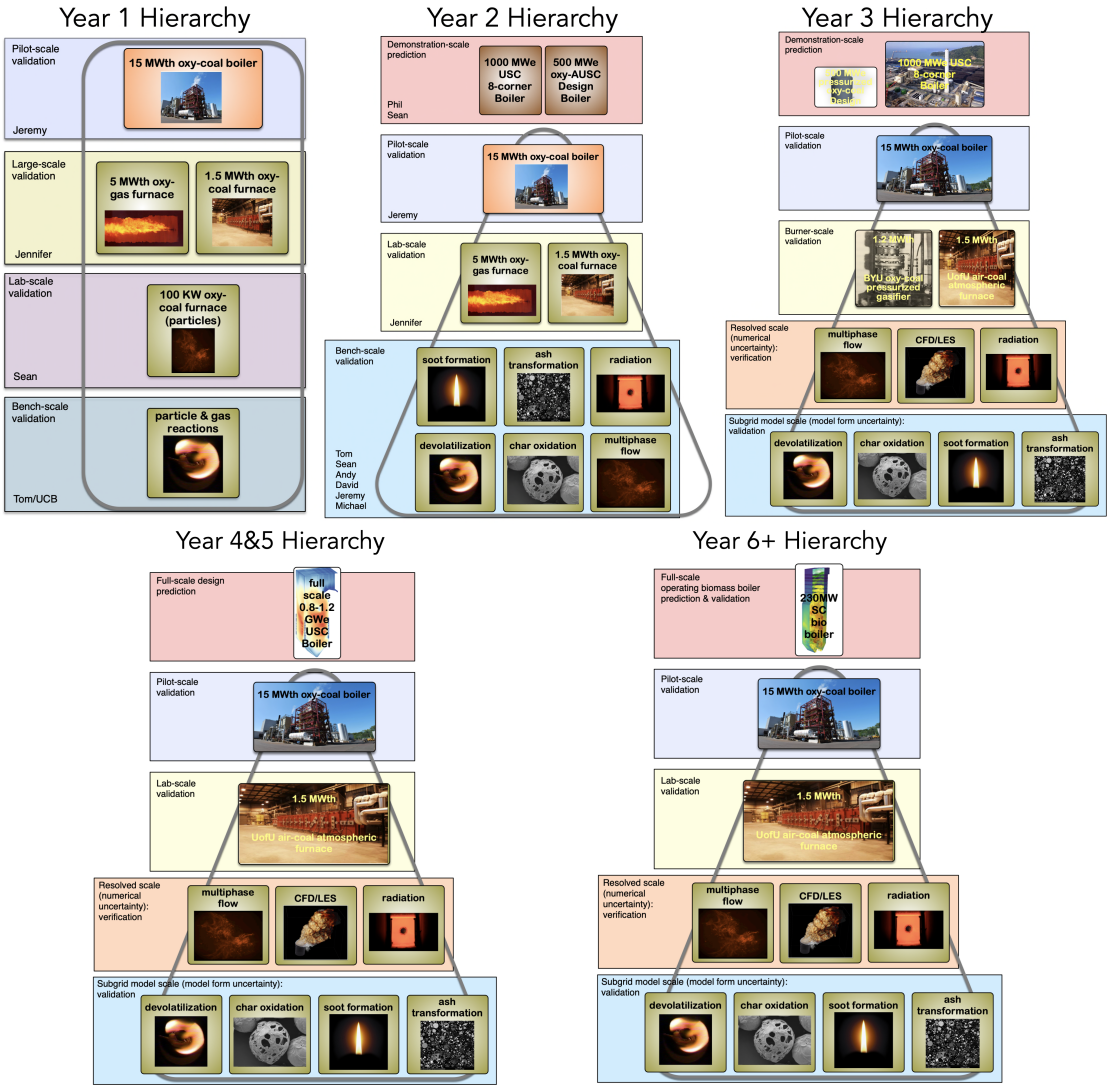


Fig. 20. Evolution of Center hierarchy in years 1 through 7.

the new model. Terminate this process when sufficiently diminishing returns are achieved. We follow this procedure for minimizing model-form uncertainty in the Bayesian analysis in our methodology. The model we present is the terminus of an iterative process. This Bayesian approach exhibits the following limiting behavior: if the model form is poor or it requires too many parameters (over fitting), then the propagation to the predicted quantities will correctly express larger uncertainty.

(2) Given sufficient experimental data of the correct type, identify a general functional form for the bias error in a given model form. This approach has been documented by Bayarri *et al*. [39].

A realistic perspective of the uncertainty provides the opportunity to retain simplicity in the physical modeling – of course it would wasteful to add features to the model which

involve code that is difficult to maintain and requires significant computational resources when the additional predictive accuracy it offers is negligible compared to the uncertainty. On the other hand, when the modeler desires to improve the fidelity of the physical modeling, the analysis of the uncertainty can indicate where the best opportunities exist. This is done through the impact factor, which is the product of sensitivity and uncertainty. As additional modeling is added, it may be natural to subdivide the physical phenomena being modeled. This leads to a hierarchical abstraction. Our hierarchy and the evolution of its abstraction over the period of the center is provided in Fig. 20. The objective of the hierarchy is to identify the requisite level of modeling for the overarching QOI and ensuring that we were encircling the application space so as to interpolate physics while extrapolating scale. This hierarchically driven problem solving gave us confidence in our V/UQ at scale.

Errors-in-Variables: Another aspect of indirect measurement is the error in the more directly-measured quantities. In the most common inverse calibration problems, e.g. ordinary linear regression, the scenario parameters, z, are specified as part of a design of experiments, and the associated errors in z are considered negligible. For linear regression, this neglect is not egregious because any errors in z propagate linearly into the QOI and the user most often evaluates uncertainty with an R-squared value. However, non-linearities often present in physics-based models necessitate a distinction between the errors in z and the errors in y (the QOI) as part of the analysis when they are not negligible. In Bayesian analysis, this complication is managed as errors-in-variables [40, 41], where measurement errors in the independent variables (the scenario parameters z) are accounted for by including them in the uncertain parameter set for the calibration.

In execution, each calibration measurement (at each scenario condition) contributes a unique error value to each scenario value, z, in the design of experiments. If each of these errors were included in the Bayesian analysis, the number of parameters in the distribution would become intractable – even exceeding the number of unique measurement values. This is the difficulty of including errors-in-variables. To address this problem, we used a *local linearization* of the non-linear physical model to analytically marginalize these proliferating variables as nuisance parameters. While a global linearization would negate the value of the non-linear modeling, a unique linearization at the point of each measurement value is sufficiently accurate as long as the measurement error is small relative to the global behavior of the model.

B2BDC: In the development of the theory, Bayes' law provides for the full shape of the posterior distribution. However, in practice, a reduced description of that posterior such as the confidence interval bounds are easily sufficient for subsequent analysis. To this end, we developed the B2BDC framework. The key feature is to directly calculate the bounds on the uncertainty given the constraint that the model must maintain consistency with all observed data.

The vector consistency measure (VCM) is a recent addition to the B2BDC framework that we developed during the course of this Center. This new tool aims at resolving inconsistency, i.e., disagreements between models and experimental observations. The VCM can be considered an extension of a previous tool, the scalar consistency measure (SCM).

Our works have demonstrated that the VCM approach is advantageous over B2BDC's sensitivity-based usage of the SCM when addressing inconsistency. This is particularly true when dealing with massively inconsistent datasets, i.e., datasets with numerous contributors to the inconsistency. In addition, we have established a new B2BDC workflow for model validation utilizing vector consistency. This workflow currently forms the foundation for how we are validating char oxidation models and model form uncertainty.

We have also incorporated model discrepancy into the B2BDC framework in order to resolve dataset inconsistency and perform prediction [42]. The addition of this discrepancy term is well motivated when the inconsistency is believed to be due to an inadequate model rather than incorrectly specified experimental bounds. In our framework, the discrepancy is formulated as a linear combination of basis functions depending only on the scenario parameters. This structure leads to an extended feasible set in the space defined by the uncertain model parameters and discrepancy coefficients.

We have continued our work in investigating similarities between techniques such as Bayesian history matching and B2BDC. In particular, we adopt the formalism of history matching's "waves" to iteratively assemble datasets in B2BDC. This strategy prioritizes accurate representation of QOIs in that only QOIs that can be accurately fit with B2BDC surrogates (quadratic/polynomial and rational quadratic models) are included during each iteration. As the iterations progress, QOIs are fit over the current stage's feasible set. Those that have accurate surrogate models are then incorporated into the dataset (with the corresponding experimental data) as model-data constraints, thus reducing the feasible region for the next iteration. We also included minimum volume ellipsoids as a way of incorporating sample-based feasibility criteria into B2BDC.

4.3.2 Development of Instrument Models Both[4] simulation and experimental data collection are modeling activities. All experimental data are uncertain and all data collection involves models [43]. The models we employ in experimental data collection, instrument models, range from purely empirical to purely theoretical, keeping in mind that physically based theory is itself only an abstraction of all previous empiricism. As an example of a simple empirical model, we measure temperature by recording a voltage signal from a thermocouple and then converting that voltage to a temperature via a polynomial calibration specific to the material. A more complex instrument model is required to measure radiative intensity and/or radiant heat flux in high-temperature (1200–2200 K) environments such as furnaces, boilers, and fires.

One of the lessons learned in the life of the Center is the need to apply the same methodology used for quantifying the uncertainty in the model to the uncertainty in the instruments used for the experimental measurements. This is schematically illustrated in Figure 21. This concept is integrated into our overall strategy as discussed in Section 4.3.1 and schematically represented in Figure 18.

As one example[5], we applied this methodology to the measurement of radiative inten-

[4] ibid.
[5] ibid.

sity in a 1.5 MW furnace (the QOI to be indirectly measured). The QOI refers to both y_m and y_e where y_m is the calculated (modeled) value, and y_e is the observed (experimental) value measured in the calibration experiment. We define the 'instrument model' as the physics-based model that calculates y_m as a function of scenario parameters, z, and uncertain model parameters, x_m; that is, $y_m = f(z;x_m)$. We developed an instrument model for a narrow-angle radiometer, coupled this instrument model with our Bayesian analysis tools to perform a calibration of the instrument, and then used the results of the analysis to compute quantifiable uncertainties for radiative intensity measurements made in the furnace. By identifying the uncertainty for each radiative-intensity measurement, we were able to extract the underlying signature of the temporal variations within the furnace.

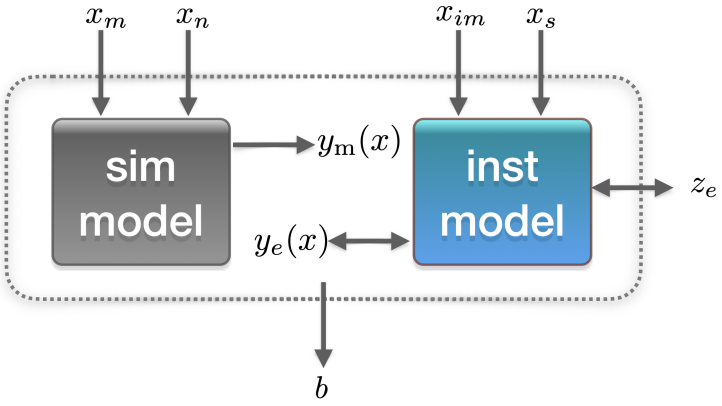


Fig. 21. Using V/UQ methodology to learn about bias (b) between simulation model outputs $y_m(x)$ and instrument model outputs $y_e(x)$, in the presence of uncertainty in simulation model parameters x_m, instrument model parameters x_{im}, numerical parameters x_n, scenario parameters x_s, and experimentally measured quantities z_e.

With Bayesian statistics[6], probability represents our current state of knowledge; each model parameter and the data inputs to the model are represented by a probability distribution. We update our state of knowledge regarding the computer model based on the data that we collect in some type of experiment. In the case of experimental-data uncertainty analysis, the model is the instrument model and the data used for updating the model are the observed calibration data. We emphasize the importance of a physics-based instrument model and recognize that the instrument model may be different between the calibration and the actual measurement because they are different scenarios. Cabrera *et al.* [44] allude to the importance of a physics-based instrument model when suggesting the need to revisit their one-dimensional, heat-conduction modeling assumptions to see if they still apply at higher heat fluxes and longer times.

When collecting experimental data[7], we measured the QOI in a calibration experiment and in a new scenario experiment (a 1.5MW furnace). In the calibration step, we used calibration experimental data within our V/UQ framework to refine instrument model parameters. In the new scenario experiment, we used the instrument model with its refined parameters to predict the distribution of the QOI. In our abstraction, the prediction we make with the instrument model is the "measurement," It uses as inputs what was actually

[6] ibid.
[7] ibid.

recorded during the scenario experiment and returns the QOI with an uncertainty distribution. This measurement can then be used for calibration/validation of a computer model of the scenario experiment.

We performed other experimental measurements related to the QOI (incident heat flux) for the lab-scale brick (1.5MW furnace) of the validation hierarchy (see Fig. 20). These measurements and their instrument models were designed to be used for the V/UQ analysis of the L1500. These measurements are grouped into the three broad categories as described below:

Optical heat flux measurements (infrared heat flux, thermal diffusivity, radiative intensity): We used an infrared camera to record incident heat flux in the infrared wavelength band through one of the optical access ports in the furnace. We used the same camera and a novel technique to measure the thermal diffusivity of the interior deposits in the furnace after it was cooled and the burner was removed. This technique involved heating a small area of deposit with a small precision torch and analyzing how quickly the heat diffused through the deposit using high-speed infrared video. We also used a narrow-angle radiometer to measure radiative intensity in the 1.5MW furnace and in a full-scale 500MW industrial power plant near Castle Dale, Utah. We pioneered a new technique for calibrating the radiometers that enabled a significant reduction in the uncertainty of the radiative-intensity measurements.

Heat absorption measurements (panel and coil heat absorption, multi-depth thermocouple heat flux measurements): We modified the first two sections of the furnace to accommodate flat heat flux panels. Due to their vertical, flat design, the panels could be cleaned during operation (soot blown) or removed for sampling of the surface deposits. We equipped the redesigned panels with two sets of multi-depth thermocouples as a method of measuring incident heat flux. We also performed extensive calibrations of the water flow meters.

Emissivity measurements (room temperature, high temperature, Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS)): As noted in Section 4.2.4, the emissivity of the ash deposits is a critical parameter in determining heat transfer within a furnace. We collected deposits after multiple campaigns in the 1.5MW furnace and assisted in measuring the reflectance (directly related to emittance) at room temperature with an FTIR for 400 samples. However, deposit emissivity varies greatly with temperature, so we decided that emissivity measurements at higher temperatures closer to actual operating conditions were needed. One of our team members, a graduate student, visited Ruhr University in Bochum, Germany and used their equipment to measure the deposit emittance at temperatures from 500-1000 °C. The sample deposits tested were taken from the near-burner region of the 1.5MW furnace. We also took reflectance data using DRIFTS measurements from room temperature up to 700 °C.

4.3.3 Boiler Simulation Facility (BSF) As part of the validation activities of the Center, we used data and simulations from the GE Power BSF as a significant brick in our hierarchy. Within the hierarchy, the BSF sat just below the full-scale system (see Fig 20). Through a V/UQ analysis of the BSF experimental and simulation data, we obtained meaningful model parameters for the full-scale systems at the top of the hierarchy. These BSF validation activities were among our key accomplishments in the Center.

We ran many sensitivity cycles to determine model parameter sensitivities that could affect the behavior of the models under particular circumstances. Table 2 presents a summary of the parameters we analyzed during the program with their respective values.

Table 2. Sensitivity analysis.

Model/Parameters		Priority	Range	Nominal	Comments
Devolatilization	v_{HiT}	2	0.1 - 0.9	0.54	high temperature volatile yield.
	T_{μ}	4	1300 - 1600	1500	K, temperature parameter from the volatile yield model.
	T_{hardB}	4	1000 - 2000	1500	K, critical temperature for breaking carbon bonds,
Char Oxidation	A_{CO_2}	4	506 - 2195	1053.3	$g/cm^2 atmO_2$, pre-exponential factor CO_2 reaction.
	E_{CO_2}	4	17984 - 78196	48090	$cal/gmol$ Activation energy, CO_2 reaction.
	A_{O_2}	4	14 - 163	47.5	$g/cm^2 atmO_2$ pre-exponential factor O_2 reaction.
	E_{O_2}	4	13574 - 27361	20468	$cal/gmol$ Activation energy, O_2 reaction.
	A_{H_2O}	2	3000 - 10000	7614	$g/cm^2 atmO_2$ pre-exponential factor H_2O reaction
	E_{H_2O}	2	40000 - 70000	60000	$cal/gmol$ Activation energy, H_2O reaction.
Wall models	A_{visc}	5	-38 - -31	-34.1	Pre-exponential factor particle viscosity model. In natural log space.
	K_{wall}	5	2.9 - 3.6	3.45	W/Km, effective thermal conductivity.
	ts_{dep}	5	1 - 10	4.5	Days, time scale of ash deposition.
	T_{slag}	5	1400 - 1600	1525	Kelvin, melting temperature of ash.
	ε_{enamel}	3	0.1 - 0.7	0.6	Porosity of the inner layers of deposits.
	δ_{enamel}	5	0.5 - 1.5	1.0	mm. Thickness of the inner deposit layer.
	y_{dep}	2	unspecified	–	Composition (mass fraction) of the deposits.
	ρ_{dep}	2	500 - 3000	2000	kg/m^3. Density of the ash deposits.
Radiation	N_{θ}, N_{ϕ}	2	s4 - s16	s8	Angular discretization of the space
	F_s	2	1 - 100	20	Radiation solve frequency: number of iterations before solving DO
	C_{abs}	4	0.5 - 2	1.0	Absorption coefficient gas and particles
Soot	y_{tar}	1	0.1 - 0.3	0.2	Mass fraction of tar yield.

What follows after a cycle of sensitivity analysis is a cycle of uncertainty quantification for model parameters. We ran at least six cycles of this nature during the life of the program. all of them. In order to quantify the multi-dimensional distribution of the model parameter values, we used Bayesian analysis. In the early stages of the program, we made simplifying

assumptions related to the surrogate representation of the simulations. We used linear surrogate models as an interpolating tool to represent the simulation space. As a result, we could account for a greater number of parameters in the analysis. Figure 22 shows the uncertainty ranges for a group of parameters.

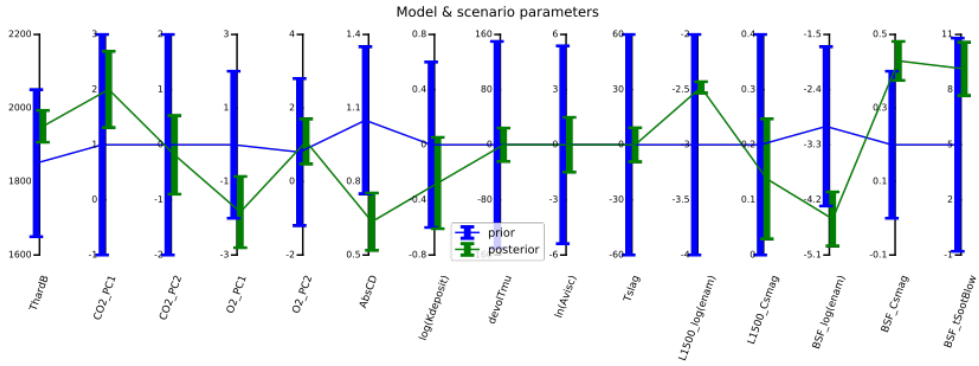


Fig. 22. Parallel plots for uncertain model parameters in the BSF.

In the latter phases of the program, we used more sophisticated mathematical analyses to represent the multi-dimensional distributions. For instance, we used Markov-chain Monte Carlo ensemble samplers like the emcee library [45] to sample the multi-dimensional distributions.

5 Laboratory Interactions

5.1 Internship and Student Lab Visit Record

Our center outreach includes many student internships and lab visits by our professional staff to all three of the collaborating federal labs. The support of lab personnel has been exceptional. As you will read in the next section, many of our students and staff are now contributing to research as members of a national laboratory.

- Kamron Brinkerhoff, Los Alamos National Laboratory, 2020
- Cameron Christensen, Lawrence Livermore National Laboratory, 2014
- Oscar Diaz-Ibarra, Sandia National Laboratory, 2016
- Teri Draper, Sandia National Laboratory, 2016
- Pascal Grossett, Los Alamos National Laboratory, 2014
- Daniel Gunderson, Lawrence Livermore National Laboratory, 2018

- Arun Hegde, Sandia National Laboratory, 2018
- Duong Thai Hoang, Lawrence Livermore National Laboratory, 2017
- Troy Holland, Los Alamos National Laboratory, 2016
- John Holmen, Sandia National Laboratory, 2016
- Ben Isaac, Los Alamos National Laboratory, 2017
- Alex Josephson, Los Alamos National Laboratory, 2017
- Mokbel Karam, Lawrence Livermore National Laboratory, 2018
- Mark Kim, Lawrence Livermore National Laboratory, 2015
- Pavol Klacansky, Lawrence Livermore National Laboratory, 2016
- Aaditya Landge, Lawrence Livermore National Laboratory, 2014
- Joshua McConnell, Sandia National Laboratory, 2016
- James Oreluk, Sandia National Laboratory, 2018
- J. Camillo Parra-Alvarez, Los Alamos National Laboratory, 2017
- Andrew Richards, Sandia National Laboratory, 2017
- Damodar Saharabudhe, Sandia National Laboratory, 2018
- Kaitlyn Scheib, Los Alamos National Laboratory, 2018
- William Usher, Lawrence Livermore National Laboratory, 2015 and Los Alamos National Laboratory, 2018
- Minmin Zhou, Lawrence Livermore National Laboratory, 2017

5.2 Post-Degree Employment

To the best of our knowledge, the following former students have employment at the entities noted. Former students who did not complete internships were paid from non-federal funds while contributing to the CCMSC research.

- Alexander Abboud, Idaho National Laboratory
- Michael D. Brown, Hi-Rez Studios
- Cameron Christensen, software engineer, University of Utah

- Oscar Diaz-Ibarra, Lawrence Livermore National Laboratory
- Christopher Earl, Lawrence Livermore National Laboratory
- Babak Goshayeshi, Merck Company
- Pascal Grosset, Los Alamos National Laboratory
- Daniel Gundersen, Big West Oil Refinery
- Arun Hegde, Sandia National Laboratory
- Troy Holland, Los Alamos National Laboratory
- Benjamin Isaac, Lawrence Livermore National Laboratory
- Alex Josephson, Los Alamos National Laboratory
- Mark Kim, Oak Ridge National Laboratory
- Aaron Knoll, Intel
- Siddharth Kumar, asst. professor, Computer Science, University of Alabama, Birmingham
- Aaditya Landge, Twitter
- Michael Matheny, Amazon
- Joshua McConnell, Sandia National Laboratory-Albuquerque
- James Oreluk, Sandia National Laboratory-Berkeley
- John Camilo Parra-Alvarez, National Renewable Energy Laboratory
- Steve Petruzza, asst. professor, Computer Science, Utah State University
- Siddartha Ravichandran, Expedia Group
- Andrew Richards, Los Alamos National Laboratory
- Kaitlyn Scheib, Lahainaluna High School
- Ben Schroeder, Sandia National Laboratory-Berkeley
- William Usher, Intel-Advanced Rendering and Visualization Group
- MinMin Zhou, Reaction Engineering International
- **Qi Wu, University of California/Davis

6 Educational Impact

We have sought to advance predictive science and computer science leading to exascale computing as an academic discipline at the University of Utah, the University of California at Berkeley and Brigham Young University. We have promoted interdisciplinary collaborations among engineering and computer science faculty and students of both disciplines. We provided the engineering students with tools to relate parallelism, code verification, solution verification, validation using experimental data, uncertainty in experimental results, accuracy of validations and uncertainty quantification.

The V/UQ faculty of the University of Utah and the University of California-Berkeley designed a course that was first offered in fall 2015. The course, "Predictivity with Verification, Validation and Uncertainty Quantification" is designed for graduate students at the three CCMSC universities: Brigham Young University, University of California-Berkeley and University of Utah. The course is taught in-person and remotely. Members of the full NNSA community were invited to participate. Class student projects have encompassed Center deliverables, including a range of instrument models, and projects by students outside the Center who have analyzed their own models and data. This course has been taught remotely during the pandemic. It will continue to be taught annually at The University of Utah to advanced graduate students from across engineering and science disciplines.

We held a Deep Dive Uintah Workshop in July 2014 that focused on implementing a compressible CFD algorithm (miniAero) within the Uintah runtime system. A follow on "Mini-Apps" workshop was held in Salt Lake City in November 2014. The Mini-Apps workshop focused on implementing miniAero) within the Uintah runtime system (TODD's writeup). The Mini-Apps workshop was designed to expose all of the details related to developing a new component in Uintah. Nine staff members of Sandia National Laboratory (SNL) participated; Janine Bennett, Hemanth Kolla, Keita Teranishi, Greg Sjaardema, Matt Bettencourt, Ken Franko, Steve Bova, Paul Lin and Gary Templet. The workshop provided an introduction to Uintah's patch-based domain decomposition along with the "rules" for writing a task. There was also a discussion on what the framework provides to component developers including geometry objects for domain initialization and boundary conditions. Details on requesting data from neighboring patches was discussed along with the available patch iterators. The original miniAero algorithm was broken down into tasks and the data dependencies between the tasks defined, forming an initial software design from which to iterate. Two coding teams were then formed that implemented software for a generalized simulation initialization specification, boundary conditions and the miniAero algorithmic tasks. At the end of the workshop, the 1D Riemann shock tube problem executed within Uintah's new miniAero component and performed all specified tasks, but it produced incorrect answers. Uintah and Sandia teams continued post-workshop development, adding a higher order spatial discretization scheme and a Runge Kutta RK4 algorithm for time integration. The Uintah team performed a strong and weak scaling study using the Riemann 3D shock tube problem as an initial condition. Three problem sizes were tested with (256^3 (16.7M), 512^3 (134.2M), and 1024^3 (1.07B)) cells respectively. Good strong and weak

scaling characteristics were demonstrated using 131K ALCF:Titan CPU cores. Given that the component had not been run at large scale previously, this is significant.

Other outreach efforts are:

- Over the course of the award, we maintained a public website that included program information, publications and updates.
- Qualifying students completed internships at national laboratories, and many have accepted positions with various national laboratories.
- We hosted annual review meetings with representatives of our Tri-lab Sponsor Team and Alliance Strategy Team that we opened to all students and professionals on our teams. These interactive meetings provided timely insights and feedback that was incorporated into research directions.
- Particle Physics Deep-Dive, (co-hosted with University of Florida) It was broadcast across all centers and to the national labs with broad participation.
- Members of CCMSC attended key meetings each year where developments of our research were presented and discussed in the broader computing and engineering communities: Combustion Institute, Clearwater Clean Energy Conference, WEST Workshops, PSAAP IPDPS Meetings, American Flame Research Committee, KOKKOS Technical Meeting, IEEE VIS Conferences, and SIAM CSE Conference among others.

The following students will continue working towards completion of their degrees in 2021.

- Kamron Brinkerhoff, Ph.D candidate, Brigham Young University (adviser: D. Lignell)
- Teri Draper, Ph.D. candidate, University of Utah (adviser: E. Eddings)
- Jebin Elias, Ph.D. candidate, University of Utah (adviser: J. Spinti)
- Duong T. Hoang, Ph.D. candidate, University of Utah (adviser: V. Pascucci)
- John Holmen, Ph.D. candidate, University of Utah (adviser: M. Berzins)
- Mokbel Karam, Ph.D. candidate, University of Utah (adviser: T. Saad)
- Wenyu Li, Ph.D. candidate, University of California-Berkeley (adviser: M. Frenklach)
- Damodar Sahasrabudhe, Ph.D. candidate, University of Utah (adviser: M. Berzins)
- Pavol Klacansky, Ph.D. candidate, University of Utah (adviser: V. Pascucci)

7 Adoption of Center Results

CCMSC has participated with and contributed to the NNSA defense laboratories in two software projects: 1) the Kokkos software project led by SNL (Albuquerque) and 2) the Hypre software project based at LLNL. As detailed in section 4.1.1, the Uintah and Kokkos teams have collaborate since 2015. Indeed, Uintah is one of the Kokkos structured-mesh-use cases. The Uintah team has used its GPU expertise to improve the performance of Kokkos on GPUs and contributed to its code base. The team has also shared an extensive collection of good practices and lessons learned through their Kokkos porting efforts with the HPC community. A University of Utah student helped with Kokkos code development during a 2018 internship along with two other students who developed code in Utah. Similarly, we have used the Hypre software in Uintah to solve large linear systems with great success since 2012. Recently we have greatly improved the performance of the OpenMP version of Hypre.

Our Center has had close interactions with Jim Ahren's group at LANL, the groups of Martin Schulz, Peer-Timo Bremer, Eric Brugger and Greg Burton at LLNL, as well as the groups of David Rogers, Jacqueline Chen, Chris Shaddix, and Stefan Domino at SNL. Each one of these staff members had strong collaborations with faculty and students at the University of Utah. Several laboratory staff (Alan Kerstein, Rod Schmidt, Jacqueline Chen) held adjunct appointments at the University of Utah during the lifetime of the Center and regularly served on PhD advisory committees.

A former member of CCMSC, Jeremy Thornock, is now working at LLNL and employing aspects of our V/UQ methodology in his current projects.

8 List of Publications

1. M. Zhou, J.C. Parra-Alvarez, Y. Wu, S.T. Smith, P.J. Smith, "Large-Eddy Simulation of Coal Combustion in 15MW Pilot Scale Boiler-Simulation Facility," manuscript accepted with AIChE Journal, Jan. 2021. DOI.

2. J. Spinti, S.T. Smith, P.J. Smith, N.S. Harding, K. Scheib and T.S. Draper, "Using Bayesian Analysis to Quantify Uncertainty in Radiometer Measurements," ASME Journal of Verification, Validation and Uncertainty Quantification. December 2020. DOI.

3. J. McConnell and J.C. Sutherland, "Assessment of Various Tar and Soot Treatment Methods and a priori Analysis of the Steady Laminar Flamelet Model for Use in Coal Combustion Simulation," Fuel 265:116775. April 2020. DOI.

4. A. Hegde, "Consistency Analysis in Bound-to-Bound Data Collaboration," Sandia National Laboratories, Livermore, CA, February 2020.

5. A. Hegde, "Consistency Analysis in Bound-to-Bound Data Collaboration," Lawrence Livermore National Laboratory, Livermore, CA, January 2020.

6. B. Peterson, A. Humphrey, D. Sunderland, J.C. Sutherland, T. Saad, H. Dasari and M. Berzins, "Automatic Halo Management for the Uintah GPU-Heterogeneous Asynchronous Many-Task Runtime," International Journal of Parallel Programming, 47(5-6):1086-1116. December 2019.

7. J.K. Holmen, B. Peterson and M. Berzins, "An Approach for Indirectly Adopting a Performance Portability Layer in Large Legacy Codes," IEEE/ACM International Workshop on Performance, Portability and Productivity in HPC. Denver, CO, November 2019. DOI.

8. A. Sanderson, A. Humphrey, J. Schmidt, R. Sisneros and M. Papka, "In Situ Visualization of Performance Metrics in Multiple Domains," Workshop on Programming and Performance Visualization Tools, (ProTools19). Denver, CO, November 2019.

9. O.H. Díaz-Ibarra, J. C. Parra-Álvarez, S. Harding, L. Marshall, S. Smith, J. Thornock, M. Hradisky, J. Spinti and P. Smith, "Development of a Digital Twin for a Biomass Boiler: Preliminary Results," Western States Section of the Combustion Institute Fall Technical Meeting. Albuquerque, NM, October 2019.

10. J. C. Parra-Álvarez, O.H. Díaz-Ibarra, S. Smith, M. Zhou, B. Isaac and P. Smith, "Modeling the Effect of Ash Build-up in Fire-side Furnace on Radiation Heat Transfer," Western States Section of the Combustion Institute Fall Technical Meeting. Albuquerque, NM, October 2019.

11. A.P. Richards, C. Johnson and T. Fletcher, "Correlations of Elemental Compositions of Primary Coal, Tar and Char," Energy Fuels, 33(10):9520-9537. October 2019. DOI.

12. A. Humphrey and M. Berzins, "An Evaluation of an Asynchronous Task Based Dataflow Approach for Uintah," IEEE 43rd Annual Computer Software and Applications Conference (COMPSAC), 2:652-657. July 2019. DOI.

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Coal and Pure Coal in a 1.5 MW Pilot-scale Furnace," 44th International Technical Conference on Clean Energy. Clearwater, FL, June 2019.

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34. M. Frenklach, "Bound-to-Bound-Data-Collaboration: Prediction on the Feasible Set," SAMSI MUMS Program Opening Workshop. Duke University, Durham, NC, August 2018.

35. M. Karam, F.M. Najjar, J. Ming, J.C. Sutherland and T. Saad, "Applying Machine Learning to Sedovvon-Neumann-Taylor (SNT) Blast Wave," Summer Internship Seminar, Lawrence Livermore National Labaoratory, August 2018.

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81. A. Humphrey, "The Uintah Runtime System," Workshop on Exascale Software Technologies (WEST). Stanford University, Palo Alto, CA, February 2017.

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