

An Update on Cardinal: Toward full core pebble simulations

Nuclear Science and Engineering Division

May 31, 2020

About Argonne National Laboratory

Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC under contract DE-AC02-06CH11357. The laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Lemont, Illinois 60439. For information about Argonne and its pioneering science and technology programs, see www.anl.gov.

Availability of This Report:

This report is available, at no cost, at <http://www.osti.gov/bridge>. It is also available on paper to the U.S. Department of Energy and its contractors, for a processing fee, from:

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
phone (865) 576-8401
fax (865) 576-5728
reports@adonis.osti.gov

Disclaimer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor UChicago Argonne, LLC, nor any of their employees or officers, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of document authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof, Argonne National Laboratory, or UChicago Argonne, LLC.

An Update on Cardinal: Toward full core pebble simulations

Elia Merzari², Derek Gaston⁴, Ronald Rahaman¹, Patrick Shriwise³, and Haomin Yuan²

¹Mathematics and Computer Science Division, Argonne National Laboratory

²Nuclear Science and Engineering Division, Argonne National Laboratory

³Computational Science Division, Argonne National Laboratory

⁴Idaho National Laboratory

**Nuclear Science and Engineering Division
Argonne National Laboratory**

May 31, 2020

Contents

Executive Summary	ii
1 Introduction	1
2 Previous work in Cardinal	3
2.1 Design of Cardinal	3
2.2 Build system	3
2.3 Verification and validation	3
2.4 Previous coupled simulations	6
3 Extension to NekRS	6
3.1 NekRS	6
3.2 Updates to Cardinal	8
3.3 Verification	10
4 Major update to OpenMC Heat Source	11
4.1 Updating Temperature Values	14
5 Demonstration simulation	15
5.1 Numerical Setup	15
5.2 Results	15
5.3 Projection to full core	16
6 Conclusions and Future Work	17
Acknowledgments	19
References	19

Executive Summary

The new DOE-NE Center of Excellence for Thermal-fluids applications in Nuclear Energy inaugurated in April 2018 considers and researches novel new solution strategies for historically challenging flow issues that still plague the current fleet of deployed Light Water Reactor (LWR) nuclear reactors as well as predicting various fluid flow and fluid related issues with advanced reactor technologies. Our advanced thermal-fluids research and development approach synergistically combines three natural, though overlapping, length and time scales in a hierachal multi-scale approach to avoid the temptation and pitfalls of attempting to develop a single solve all algorithm for physical fluid flow problems that will span 10^9 in spatial and temporal scales.

To demonstrate the multi-scale philosophy of the center we focus on Fluoride Cooled High Temperature Reactors (FHRs), and in particular on the Berkley's PB-FHR Mark-I design. The Fluoride salt cooled High temperature Reactor (FHR) is a class of advanced nuclear reactors that combine the robust coated particle fuel form from high temperature gas cooled reactors, direct reactor auxiliary cooling system (DRACS) passive decay removal of liquid metal fast reactors, and the transparent, high volumetric heat capacitance liquid Fluoride salt working fluids - Flibe - from molten salt reactors. This combination of fuel and coolant enables FHRs to operate in a high-temperature low-pressure design space that has beneficial safety and economic implications. The PB-FHR reactor relies on a pebble bed approach and pebble bed reactors are in a sense the poster child for multiscale analysis.

The lower length-scale simulator for pebble reactor cores comprises three physics: neutronics (OpenMC), thermal-fluids (Nek5000/NekRS) and fuel performance (BISON). As part of center of excellence ongoing research efforts we have developed Cardinal, a new tool platform for lower length-scale simulation. Cardinal tightly couples all three physics and leverages advances in MOOSE such as the MultiApp system and the concept of MOOSE-wrapped Apps. The present report provides an update on the development of Cardinal with an extension of Cardinal to GPUs. We also perform a first-of-a-kind demonstration simulation on Summit representing a $10x$ capability increase in terms of pebble count for Cardinal.

1 Introduction

The DOE-NE Center of Excellence for Thermal-fluids applications in Nuclear Energy inaugurated in April 2018 considers and researches novel new solution strategies for historically challenging issues that still plague the current fleet of deployed Light Water Reactor (LWR) nuclear reactors as well as predicting various fluid flow and fluid related issues with advanced reactor technologies, which includes advanced Small Modular Reactor (SMR) concepts, micro-reactors, and Advanced Reactor Concepts (ARC), utilizing coolants such as liquid metal, chloride and fluoride salts, or gas, for accident-tolerant reactors. These new solution strategies and algorithms will then be implemented into a modern software design methodology, using best software quality practices, and then delivering validated NQA-1 level software to the nuclear power community.

Ultimately, this goal requires a facility where a strong collaborative environment can be established between computational scientists and scientists conducting fluid dynamic experiments. The center addresses a pressing need in advanced reactor development and commercialization. Advanced reactor fluid problems are currently high priority and lend themselves to advanced modeling and simulation due to the presence of complex flow and lack of empirical data. In fact, advanced modeling and simulation tools are poised to play an important role: providing deep insight, enhancing the experimental process and accelerating the regulatory process. The center supports a coherent approach, and establishes a true front door for engaging industry. The current approach makes it difficult for customers to engage - single-PI efforts, while individually excellent, have been somewhat disparate, and not coordinated. The CFD/Thermal-Hydraulic Center is truly a multi-lab approach analogous to that used in the very successful fuels M&S area of NEAMS.

NEAMS and Hub Thermal-Hydraulic/CFD tools are far enough along to warrant this approach. Our advanced thermal-fluids research and development approach synergistically combines three natural, though overlapping, length and time scales in a hierachal multi-scale approach to avoid the temptation and pitfalls of attempting to develop a single solve all algorithm for physical fluid flow problems that will span 10^9 in spatial and temporal scales. A more tractable approach is grouping physics with similar multi-scale requirements into a common algorithm, developing separate software applications to address the separate scales, and then coupling the applications where appropriate. This multi-scale modeling and simulation template has proven to be highly successful in the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program to simulate the evolution of nuclear materials under irradiation. These three overlapping thermal-hydraulic scales are defined across all reactor concepts as:

- **Lower Length Scale.** The Lower Length Scale will focus upon resolving the high-resolution physics associated with single and multi-phase, highly turbulent conjugate heat transfer (CHT) with highly resolved thermal boundary layers (heat flux).
- **Engineering Length scale.** The Engineering Length Scale will integrate coarse mesh approaches for homogenized multi-dimensional CHT, such as those found in gas-cooled pebble-bed reactors, or three-dimensional sub-channel capabilities tightly coupled to nuclear fuels performance.
- **System Scale.** System Scale analysis for nuclear reactors is composed of one-dimensional fluid flow pipe networks and zero-dimensional system components. These classes of algorithms and corresponding approaches are basically reduced order models (ROM) of the more complex scales and allow for more efficient calculations. These reduced order systems rely heavily on empirical correlations or models, as many of the flow features and phenomena are no longer resolved.

To demonstrate the multi-scale philosophy of the center we focus first on Flouride Cooled High Temperature Reactors (FHRs), and in particular on the berkley's PB-FHR design Mark-I design. The Fluoride salt cooled High temperature Reactor (FHR) is a class of advanced nuclear reactors that combine the robust coated particle fuel form from high temperature gas cooled reactors, direct reactor auxiliary cooling system (DRACS) passive decay removal of liquid metal fast reactors, and the transparent, high volumetric heat capacitance liquid fluoride salt working fluids - Flibe - from molten salt reactors. This combination of fuel and coolant enables FHRs to operate in a high-temperature low-pressure design space that has beneficial

safety and economic implications. In 2012, UC Berkeley was charged with developing a pre-conceptual design of a commercial prototype FHR - the Pebble Bed- Fluoride Salt Cooled High Temperature Reactor (PB-FHR) [?]. The Mark 1 design of the PB-FHR (Mk1 PB-FHR) is a 236 MWt Flibe cooled pebble bed nuclear heat source that drives an open-air Brayton combined-cycle power conversion system. The PB-FHR's pebble bed consists of a enriched uranium fuel core surrounded by an inert graphite pebble region that shields the outer solid graphite region, core barrel and reactor vessel. The fuel reaches an average burnup of 178000 MWt-d/MT. The Mk1 PB-FHR exhibits strong negative temperature reactivity feedback from the fuel, graphite moderator and the Flibe coolant but a small positive temperature reactivity feedback of the inner region and from the outer graphite pebble region. Pebble bed reactors are in a sense the poster child for the sort of analysis described above.

FHR pebble beds in particular are comprised of hundreds of thousands of pebbles, and a CFD-grade detailed description of the flowfield through these pebbles for an entire reactor core is not practical with current simulation technology. However, as this report will demonstrate we have a credible pathway toward a full core high-fidelity CFD capability in this geometry.

For practical, fast-running, design-related purposes porous media formulations are usually employed. However, simple porous media approximations are often incapable of capturing key details of the flow field such as the wall channeling effect due to the change in porosity in the proximity of the vessel walls. Advanced formulations for the “engineering scale” have the potential to address these issues but data from finer scale simulations is needed to build closure relationships. Pronghorn is the platform of the center of excellence for engineering scale thermal- fluids simulations. Finally, finer scale calculations are needed to establish local temperature peaking and fuel temperatures.

An overall multi-physics strategy for FHR simulation might look like in Figure 1. SAM, the system analysis tool for systems analysis of advanced reactors with coolants in the liquid phase, drives the simulation of the engineering scale tools (Pronghorn and Rattlesnake/Mammoth). The lower length-scale tools can be run concurrently to provide dynamic closures for the engineering scale or offline to produce correlations (which would be more likely). The lower length-scale simulator may comprise neutronics (e.g., OpenMC), thermal-fluids (Nek5000-NekRS) and fuel performance (BISON).

Cardinal is the tool developed in the center of excellence for lower length-scale simulation. This new platform tightly couples all three physics and leverages advances in MOOSE [?] such as the MultiApp system and the concept of MOOSE-wrapped Apps. Moreover it is designed from the ground-up to scale on massively parallel architectures and perform well on world-class super-computing architectures. Initial efforts in the development of the Cardinal were presented in a recent report [?].

In this report we provide a major update to the high fidelity modeling of FHR pebble beds. A particular effort of this year’s efforts have been to transition to a hybrid GPU-CPU model to leverage the potential of pre-exascale supercomputer architectures (i.e., Summit).

In particular, we:

- Summarize some of the previous work conducted with Cardinal (Section 2);
- Provide an extension of Cardinal to work on GPU-based system (Section 3), this part includes the creation of a new API to NekRS [?]; the new GPU port of Nek5000, and it includes verification of the coupling to MOOSE;
- Discuss the introduction of mesh-based tallies in OpenMC (Section 4) and the introduction of mesh-tally transfer with Cardinal;
- Discuss a set of demo simulations (Section 5) related to an FHR comprising 1568 pebbles (10x what previously done with Cardinal), providing a pathway toward full core simulations.

We emphasize the importance of the data generated with these high fidelity conjugate heat transfer simulations of pebble beds. They represent an important stepping stone for developing wall-channeling effects models for Pronghorn, and a resource for confirmatory analysis of reduced order models.

2 Previous work in Cardinal

MOOSE was originally developed for solving fully coupled systems of partial differential equations (PDEs) using fully implicit timestepping. To utilize MOOSE developers create small C++ objects which represent their partial differential equations, boundary conditions, initial conditions, etc. MOOSE will then coordinate PETSc and libMesh to perform a Newton solve over all of the physics to find the solution to the multiphysics problem. While this is still the primary way to use MOOSE, the library has also gained capability for loosely coupled solves, Picard iteration and even coupling to external applications (such as OpenMC and Nek5000). Discussion on the MultiApp features of MOOSE used in Cardinal are provided in [?]. When utilizing MOOSE to couple multiple disparate codes together a new MOOSE-based application was created [?] which compiles all of the codes into one executable. For the previous study that code was named Cardinal and combines BISON, OpenMC and Nek5000 to achieve high-fidelity simulation of FHR reactors.

2.1 Design of Cardinal

Cardinal utilizes the MOOSE MultiApp capability to place each of the applications to be coupled within a hierarchical tree-based structure as shown in 1. This structure was chosen based on how tightly coupled the physics are. BISON and Nek5000 form one branch due to the instantaneous feedback between the conjugate heat transfer and the pebble temperature. The Nek5000 solution provides the temperature boundary condition on the exterior of each pebble while BISON returns the heat flux at each point around the pebble to Nek5000. Another benefit of having BISON and Nek5000 on their own branch is the way it impacts timestepping. Within the MultiApp setup shown in Figure 1 the branch containing BISON and Nek5000 can take many small timesteps, and even iterate between BISON and Nek5000 within a timestep, without needing to re-solve OpenMC. This greatly increases the runtime speed of the application. OpenMC is then separate from the other two. It receives fuel/pebble temperatures from BISON and returns a heat source which is transferred down to BISON. OpenMC is currently solving for steady state neutronics and can therefore take larger timesteps compared to BISON and Nek5000 (which are both performing transient heat conduction and CFD solves respectively). The flexibility of the MOOSE MultiApp system allows for just such a setup. Discussions on the related APIs for each of the codes mentioned are contained in the previous report [?].

This structure has been updated in the present report to allow for NekRS to be used instead of Nek5000 allowing for execution of the fluid problem (by far the most expensive of the three) on GPUs.

2.2 Build system

All libraries get config info from PETSc for consistent compilation. After installing PETSc and libmesh, Cardinal can be built in one step.

The build system of Cardinal has largely been kept intact for the present work. We have however added a branch of the repository that compiles NekRS instead of Nek5000. The build system has also been updated to allow Cardinal to run on the ORNL supercomputer Summit.

2.3 Verification and validation

In order to verify the fluid flow model and the solution transfer we have devised two cases including a single pebble and a two pebble case. The Nek5000-MOOSE coupling was verified to yield the same results as stand-alone Nek5000 conjugate heat transfer results. We note that work in Cardinal was based on previous work conducted on Nek5000-MOOSE coupling [?]. The single pebble (Figure 3) and two pebble (Figure 4) cases were also used to verify the OpenMC and BISON coupling. For instance the neutronics results showed a clear bias between pebbles and a tilt induced by the temperature gradient.

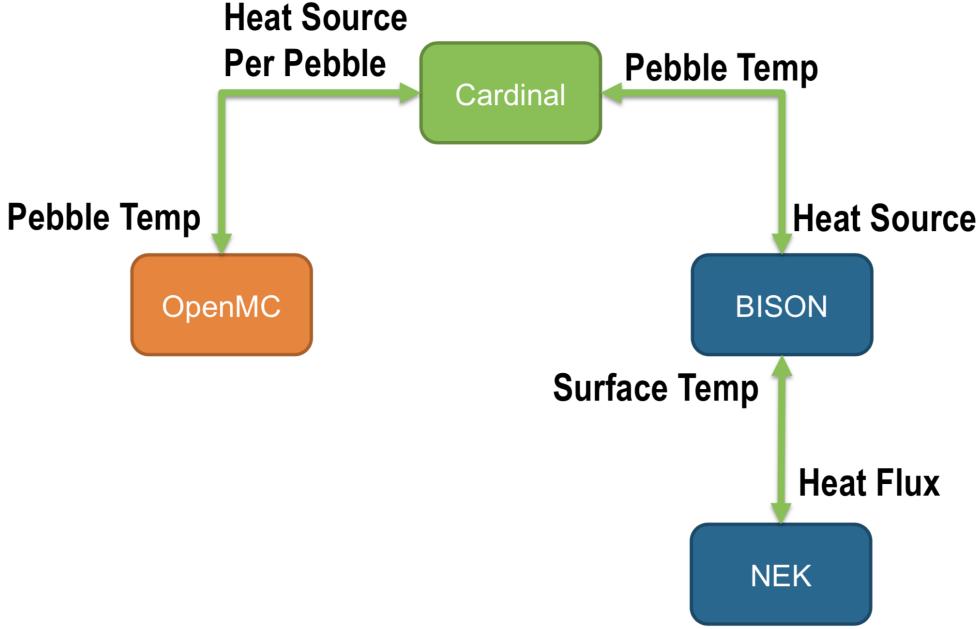


Figure 1: Diagram showing the design of Cardinal.

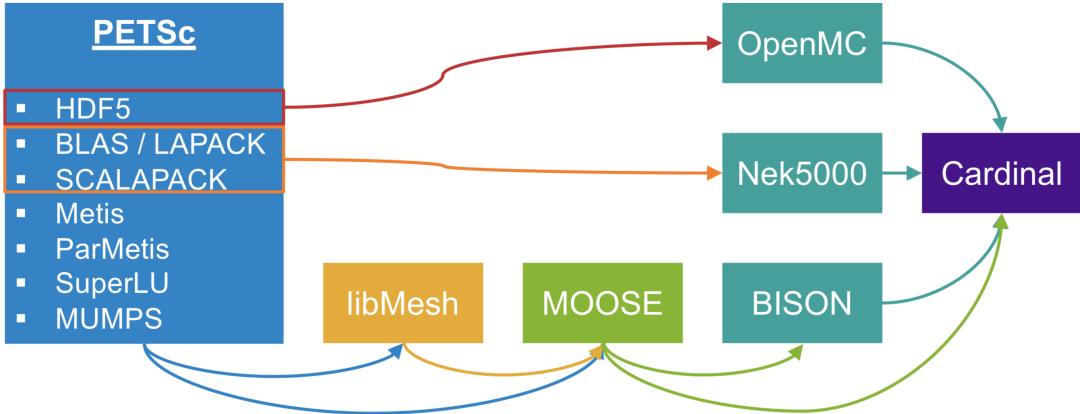


Figure 2: Diagram describing the build system of Cardinal.

Selected results from the single pebble case were also compared with results from experimental and computational studies carried out by using a similar geometry (Figure 3). A well quantified quantity for flow over a single-sphere is the averaged stream-wise velocity along the domain axial center line. Figure 4 compares our result with completed numerical results. The figure shows the profile generated from DNS data in [?] at $Re = 3,700$ and shows the downstream location ($z = D$) and magnitude of the maximum recirculation (i.e. negative streamwise) velocity for LES and DES data generated at $Re = 10,000$. One can see that for increasing Reynolds number, the magnitude of the recirculation velocity increases, while the downstream distance from the sphere where this maximum occurs, decreases. We do not quantify the

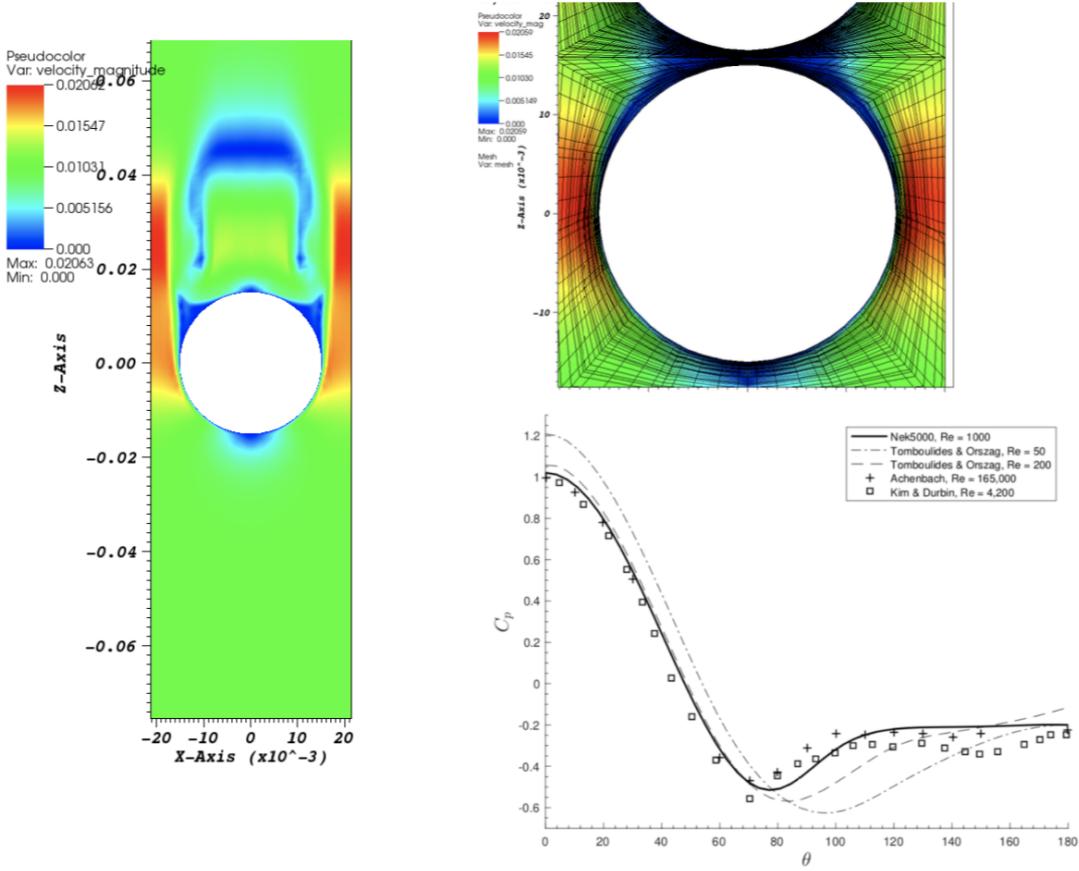


Figure 3: Verification test - Single pebble and comparison with experiment.

specific dependence of this trend on the Reynolds number here, but our result seems to be consistent with the literature.

Over the past several years NEAMS has dedicated several efforts to the modeling and simulation of the detailed flow in a pebble bed. For instance, Fick et al. [?] performed a complete Direct Numerical Simulation of pebble bed flow. Complete statistical data was obtained from this DNS study, with an investigation of low-frequency temporal instabilities. However, Fick's study [?] used a structured pebble bed, which limits its application. Nonetheless it was compared against other available DNS data and proved Nek5000 can deliver high quality simulation data for pebble beds. A more recent study was aimed at simulating the flow in a random pebble bed [?]. This random pebble bed geometry was obtained from an experiment conducted by Nguyen et .al [?]. However, only a small section of the whole domain from the experiment was studied. A picture of the experimental facility is shown in Figure 5, while a snapshot of the PIV field examined is shown in Figure 6.

To create a pure hexahedral mesh for a random pebble bed is very challenge if using traditional blocking method. However, with the tet-to-hex meshing method, we could create pure hexahedral mesh for this geometry. To reduce the total element number, chamfers are created at pebble-pebble interfaces. As discussed, the computational domain is only a small section of the whole experimental domain, therefore we applied periodic boundary conditions at the inlet/outlet to mimic the upstream/downstream. Figure 7 shows the

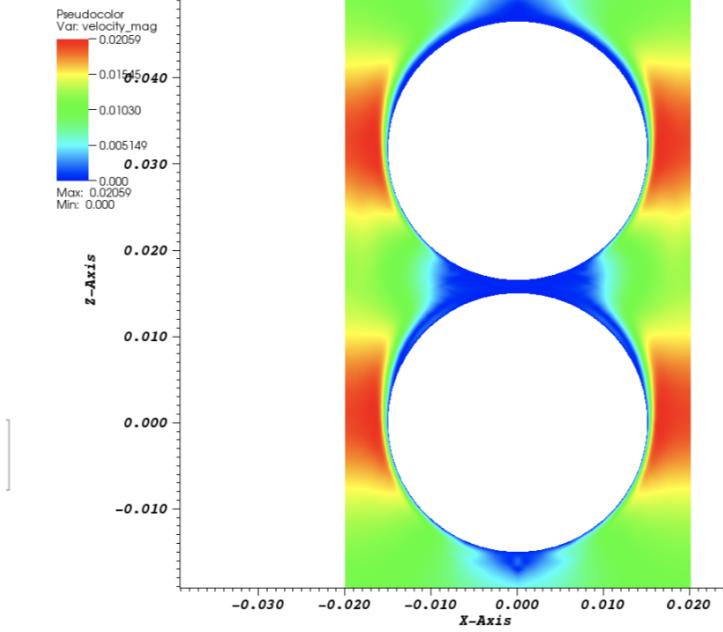


Figure 4: Verification test - Two pebbles.

instantaneous velocity field at cross sections of the random pebble bed, as well as the near wall mesh at the pebble surface. In Figure 8, the flow field is very complex due to the randomly distributed pebbles. Despite the complexity of the geometry the computational results compared favorably.

2.4 Previous coupled simulations

Using the Nek5000 model of the TAMU experiment as a basis, we have developed a multi-physics simulation of a bed comprising 146 pebbles. The numerical setup and results are discussed in more detail in [?]. We report here only some select results on the average temperature distribution and power distribution (Figure 9 and Figure 10).

3 Extension to NekRS

A good portion of the work on Cardinal this year has been the extension of Cardinal to the use of GPUs. The primary reason for this effort is to eventually exploit the potential of pre-exascale and exascale systems. All such systems in the United States will involve CPU-GPU hybrids. The simulation of a pebble bed reactor core using computational fluid dynamics resolving every pebble requires such computational power.

3.1 NekRS

NekRS is the novel GPU port of Nek5000, although it is also capable of running on CPUs. It represents a significant redesign of the code, with major differences. It is primarily based on C++, but it also links to Nek5000 as a library for pre-processing and post-processing. It has been built primarily under the auspices of the Exascale Computing Program. It is able to reach excellent weak scaling performance. For example,



Figure 5: TAMU experiment - Picture of the facility.

we discuss here weak-scaling studies performed on Summit (Oak Ridge National Laboratory), the fastest supercomputer in the world as of June 2020, using NekRS. Table 1 shows the solution times, parallel efficiency, and number of points per rank for the Summit results.

We observe in Table 1 near-perfect weak-scaling performance up to 2,048 nodes considering 8,000 elements/GPU at $N = 7$. The case considered is the DNS of Taylor-Green vortex flow with a triple periodic domain. We report results for 100 time-steps; at 2,048 nodes the runtime was 90 seconds. We note that the performance falls off for GPUs when decreasing the DOF per GPU. Therefore, strong-scaling studies are not particularly meaningful. Future large scale calculations will likely suffer from even longer runtimes. These performance results are in keeping with earlier performance analysis presented in [?, ?]. .

We compare also the performance of the GPU Nek5000 port with the CPU performance on Summit for 1,024 nodes. The CPU simulation was performed with 42 MPI ranks per node, and the GPU simulation was performed with 6 MPI ranks per node. Overall the GPU solver was 11.5 times faster than the standard

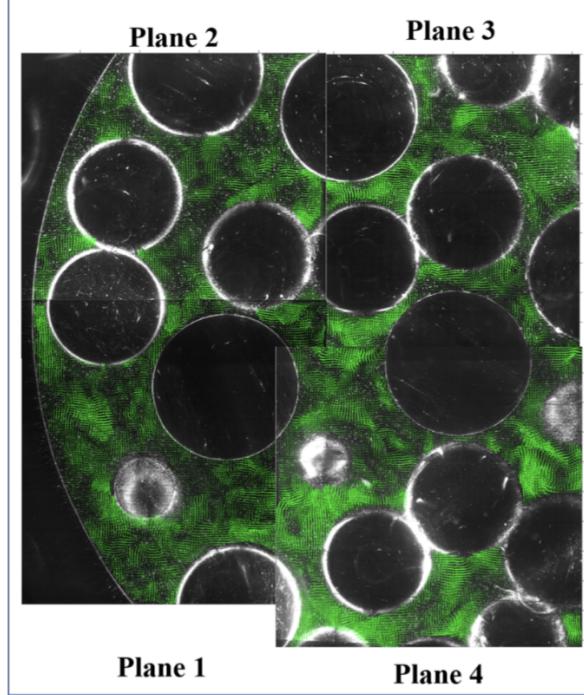


Figure 6: TAMU experiment - PIV snapshot.

Nek5000 CPU solver for the same number of nodes.

We note that NekRS shares a similar verification and validation basis with Nek5000.

3.2 Updates to Cardinal

The first step has been to create a NekRS branch. This branch has an updated build system that replaces Nek5000 with NekRS. The build system has been tested on various computing systems (Summit, Sawtooth, Workstations on MCS and Macbook laptops) and has been found to be robust.

The second step has been to create an API between NekRS and MOOSE. The interface mimics closely the one with Nek5000 and in fact relies on the same Fortran routines for consistency. However additional steps had to be introduced to rely on the very different code structure of NekRS. The updated interface has

# of Nodes on Summit	DoF (billion)	Efficiency on GPUs
128	3.1	1.0
512	12.6	0.92
1024	25.2	0.88
2048	50.3	0.88

Table 1: Weak-scaling on Summit. 8,000 elements per GPU, $N = 7$.

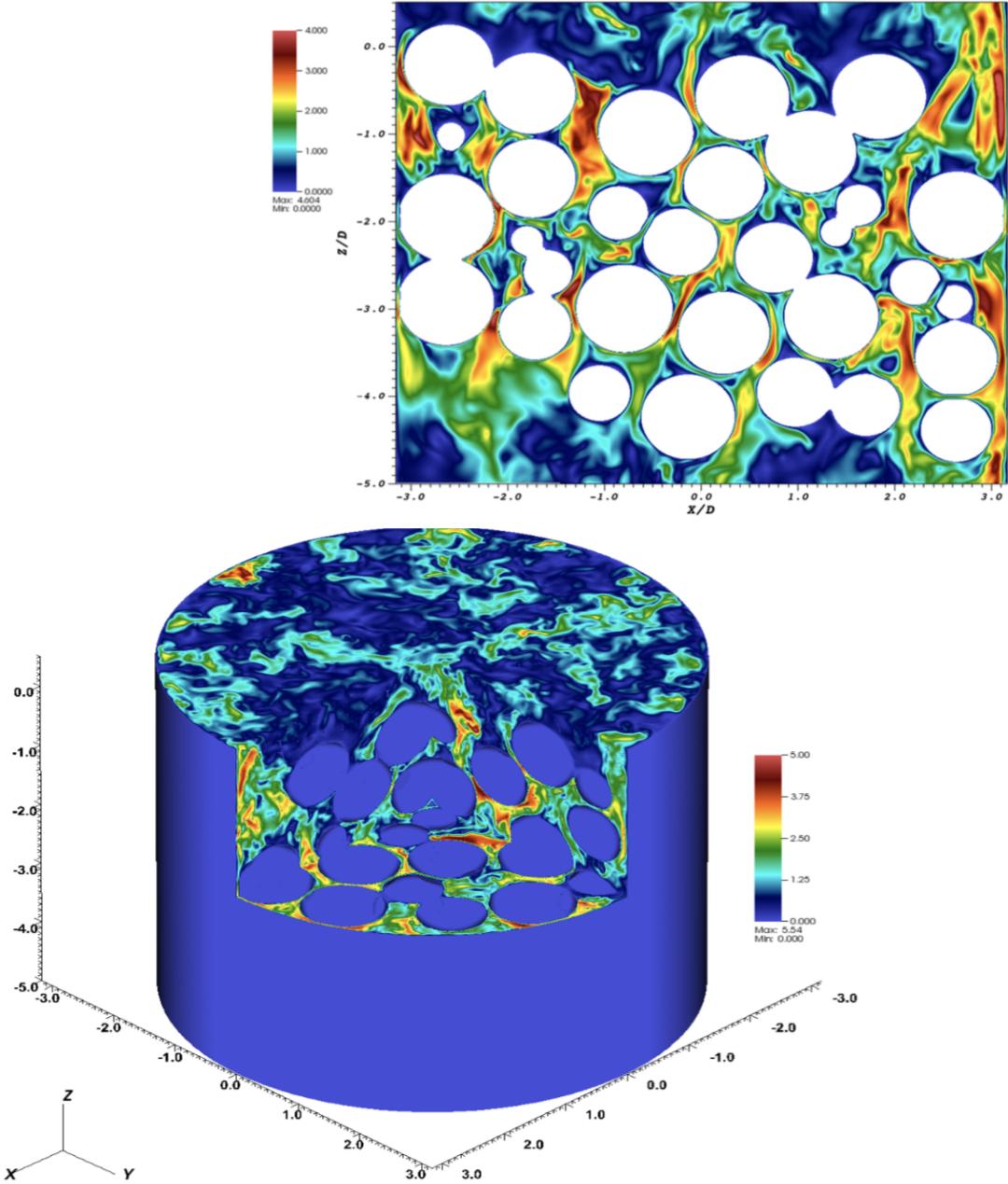


Figure 7: TAMU experiment - Simulation results.

been tested on the single pebble problem discussed in Section 2. The results of the verification are discussed in Section 3.3.

The Fortran routines find and list all mesh elements (quadrilateral surface elements) on the surface of the pebble mesh. The quadrilateral data can be linear (built on one quad for each NekRS quad) or quadratic (built on four quads for each NekRS quad). MOOSE then constructs the transfer mesh, which be distributed or serialized, based on the quadrilateral data. Data for temperature and heat flux are passed between NekRS

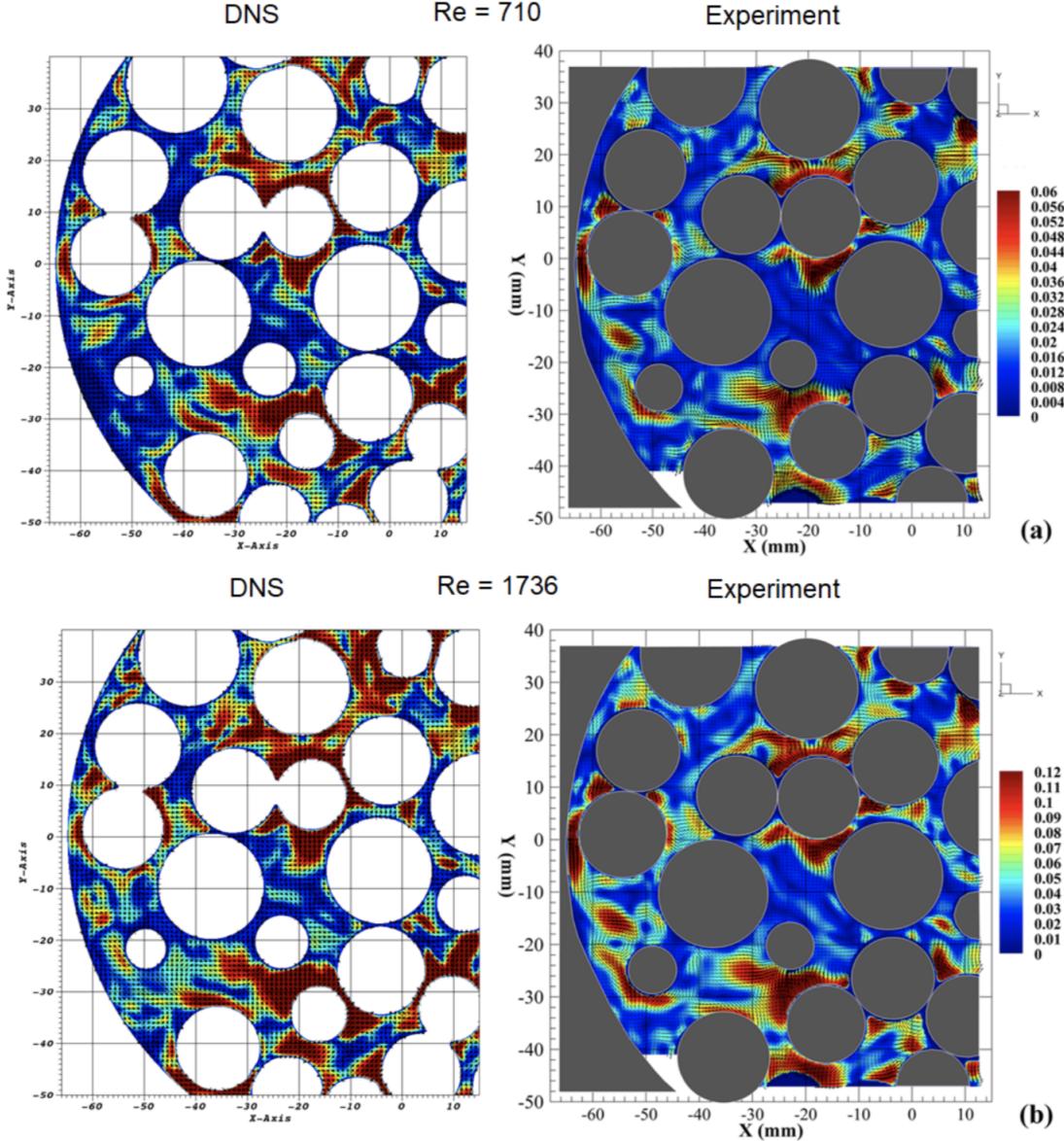


Figure 8: TAMU experiment - Comparison with experiment.

and MOOSE on the transfer mesh.

3.3 Verification

The results for the NekRS branch of Cardinal are discussed in the following. The case setup is identical to the one used for the verification of the MOOSE-Nek5000 coupling. Some results for the temperature distribution are shown in Figure 11.

Figure 12 presents a comparison between single pebble results in Cardinal versus results obtained in Nek5000 stand-alone with a conjugate heat transfer mesh. Temperature profiles are compared on a line at

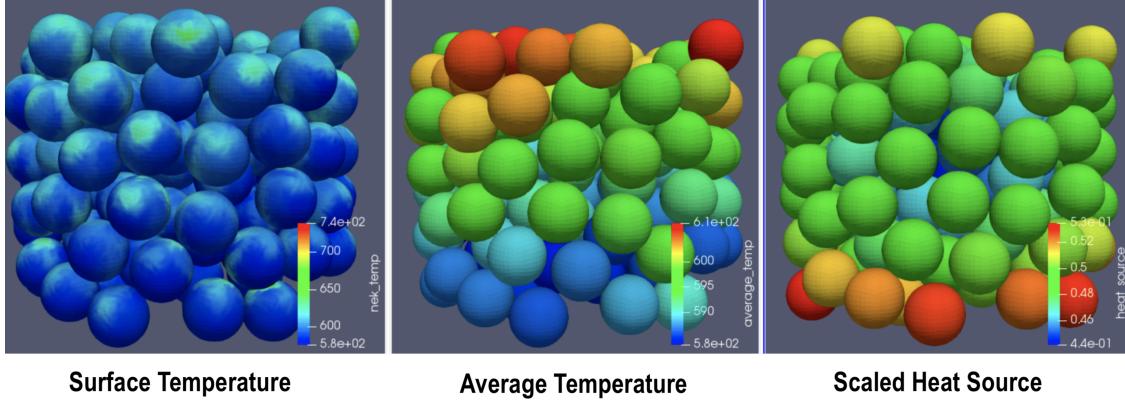


Figure 9: TAMU demo Results. From left to right: snapshots of temperature on surface, average temperature in solid and average heating

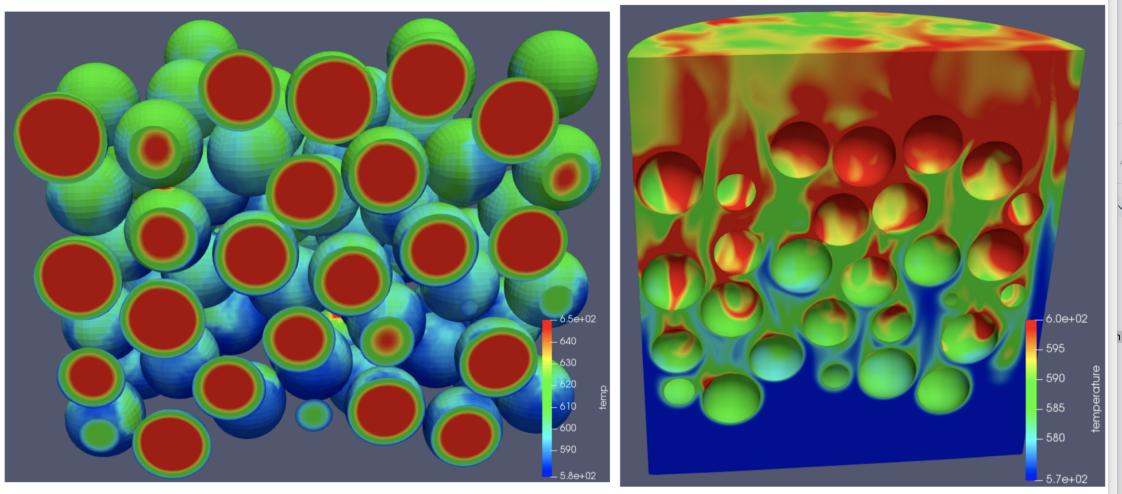


Figure 10: TAMU Demo Results. Right - temperature in the solid. Left - temperature details in the fluid.

$y = 0.016m$ and $x = 0m$ (we note that the domain is centered at the pebble center and the pebble diameter is $D = 0.03m$). We note that the results are nearly identical if a quadratic representation of the surface is employed.

4 Major update to OpenMC Heat Source

In addition to the changes in NekRS we introduced some major changes in the way Cardinal interfaces with OpenMC.

To capture heat generation in the OpenMC simulation, a tally scoring the amount of total recoverable fission energy per source particle is applied to the outer cell of each pebble in the bed. These tallies are created at runtime during the problem setup by using a list of pebble centers to locate the uppermost cell in the CSG geometry hierarchy containing that point.

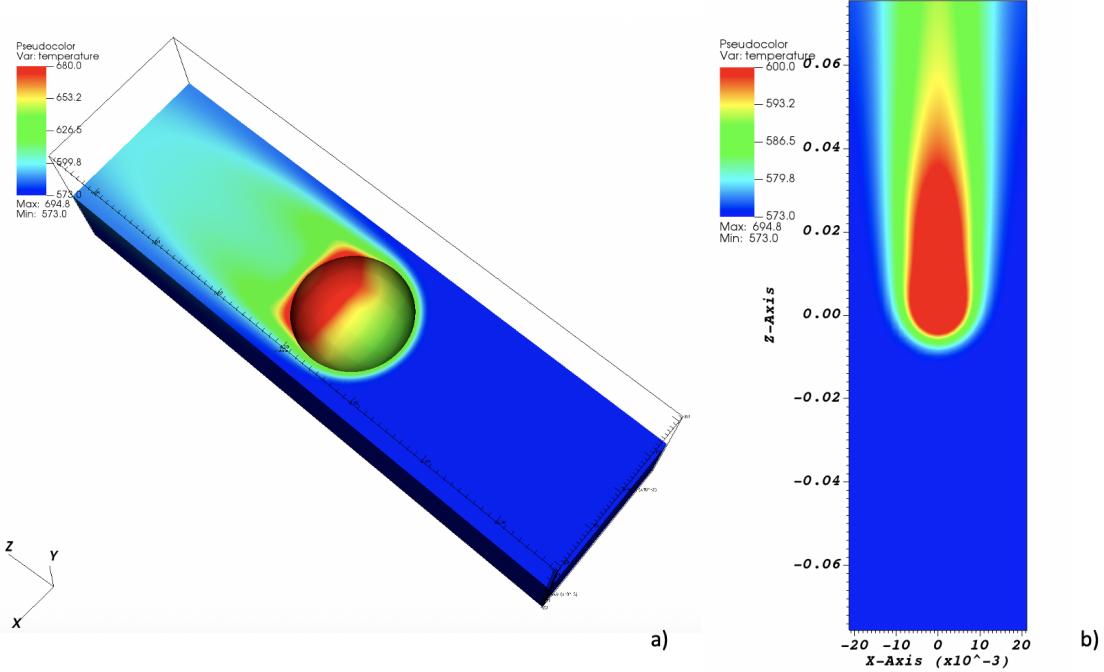


Figure 11: Verification test - Single pebble result. a) 3D temperature distribution in the whole domain. b) Cross section at $y = 0.016m$.

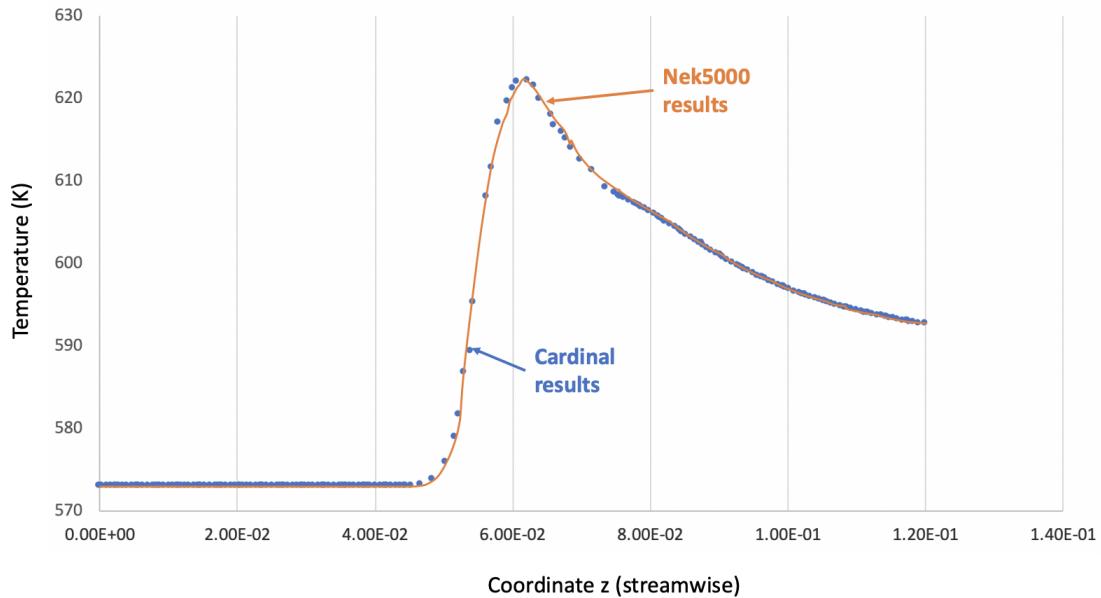


Figure 12: Verification test - Single pebble comparison with standalone Nek5000 results.

As summarized in [Equation 1](#), the energy deposition for each pebble, \hat{q}_i , is normalized by the total

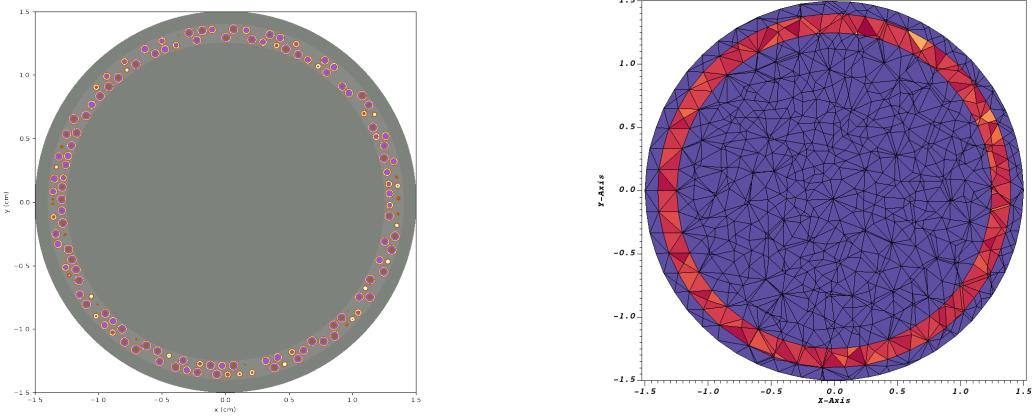


Figure 13: Qualitative view of a heating tally on an unstructured mesh. Left: Cut-away of the pebble geometry as represented in OpenMC. Right: Result of an applied heating tally where heating only occurs in the region of the pebble containing TRISO particles.

energy deposition in the bed and multiplied by the total thermal power of the reactor, Q to obtain a an average heat generation rate for each pebble, q_i . This value is then divided by the volume of each pebble, V_p , to obtain a volumetric heat generation rate, q''_i .

$$q''_i = \frac{Q q_i}{V_p \sum_i q_i} = \frac{[W][J/source]}{[cm^3][J/source]} = \frac{[W]}{[cm^3]} \quad (1)$$

This results in a single average heating value for the entire pebble. Before being transferred to the MOOSE mesh, these values are normalized by the total heat

For improved spatial resolution of heat generation in the pebble bed, unstructured mesh tallies have been implemented in OpenMC. Figure 13 provides an example of this capability applied to a single pebble. The unstructured mesh representation relies on a LibMesh mesh instance and currently conforms to the OpenMC model in which the mesh structure and tally data are separated. The separation of this information allows the unstructured mesh to be applied in a mesh filter without knowledge of the underlying mesh type. The mesh filter can then be used in one or more tallies in combination with other specified filters, scores, and nuclides to form a tally. Calls into the LibMesh library from OpenMC are agnostic to the type of elements being used, so meshes can be formed using any element type supported by LibMesh.

A mesh for each pebble is applied in the Cardinal problem to capture the heat generation distribution throughout the pebble bed. To avoid replicating a mesh representing all of the pebbles from either MOOSE or NEKRS, an option for adding translations to mesh filters was introduced in OpenMC. Placing the translation at this layer of the tally structure allows all tallies to rely on a single LibMesh mesh instance acting as a template for a single pebble as shown in Figure 14. This results in a very low memory footprint for the tally, even when extended to an entire pebble bed.

The translation values for each mesh filter are set using the list of pebble centers provided in the MOOSE input file. During problem initialization, these translations are used to adjust the location of element centers in the mesh template when transferring heat generation value to MOOSE. As the only additional input information required for the unstructured mesh tallies is the specification of a mesh template input file, the unstructured mesh tallies can be specified at runtime by setting the appropriate tally type parameter in the OpenMC MOOSE input file.

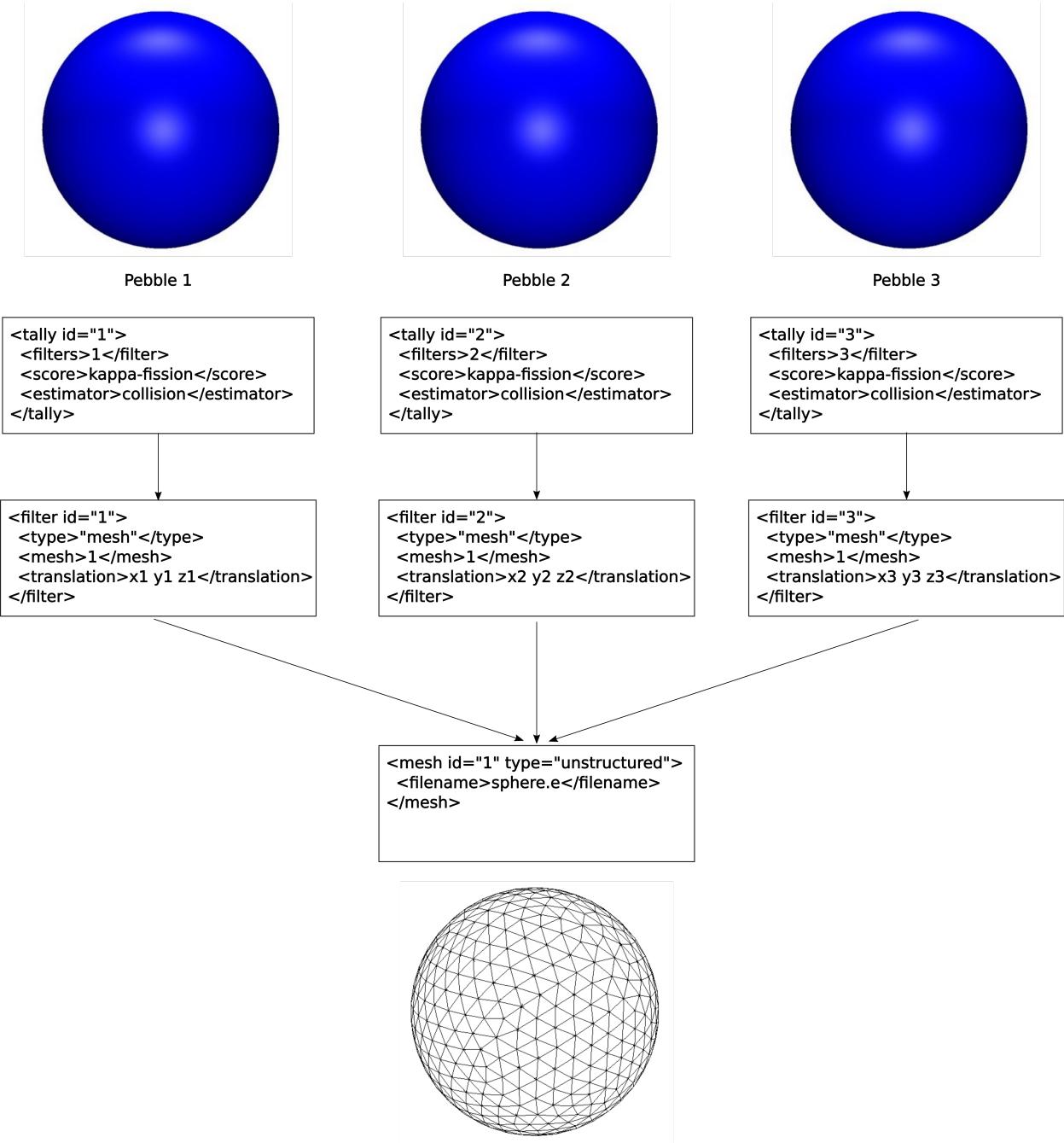


Figure 14: Organization of unstructured mesh tallies for heat generation in OpenMC.

4.1 Updating Temperature Values

Temperature values from MOOSE are updated in OpenMC using an average temperature value at the pebble center. To simplify the process of updating the temperature of all cells inside the pebble, an option has been added in OpenMC to propagate a temperature value into all cells filled by a material if the cell whose

property is being updated contains a universe or lattice.

5 Demonstration simulation

To demonstrate the new capability of Cardinal we demonstrate here the use of Cardinal on Summit to perform coupled multi-physics simulations of pebble beds.

5.1 Numerical Setup

The case presented here comprises 1568 pebbles. The pebble configuration has been obtained using a discrete element method (DEM) code. A major overhaul on the mesh generation for the fluid domain has been necessary to automatize as much as possible the process and reduce the number of elements per pebble. The new meshing tool is based on a Voronoi cell strategy. It has allowed to produce high quality hexahedral meshes, while reducing the mesh count to roughly 300-400 elements per pebble.

Examples for these meshes are provided in Figure 15 for the 1568 pebble configuration and in Figure 16 for a pebble configuration with over 3,000 pebbles. Both meshes have a similar density.

We note that 1568 pebbles is a significant size for a coupled calculation and representative for instance of the SANA experiments.

For this demonstrations, the sizes and composition of the TRISO particles were based on TRISO manufactured at INL, following the practice established in the previous report [?]. Though these particles were developed for the Advanced Gas Reactor (AGR) fuel, particles with the same specifications are used for FHR test reactors and computation benchmarks. The sizes and compositions of the pebbles were taken from the Mark-1 FHR reactor constructed at UC Berkeley.

For BISON, and the demonstration problem under consideration we consider only the conduction equation and as such it is a relatively straightforward setup. Properties are constant and adapted from available correlations. The mesh for a single sphere is generated and replicated at run time. The same mesh is used for the mesh tallies in OpenMC.

5.2 Results

The model described in the previous section has been run on 12 and 20 nodes of Summit, with 6 MPI ranks on each node, corresponding to the 6 GPU on each node. The OpenMC and BISON models are designed to run on CPU while the NekRS model runs on the GPU.

Stand-alone NekRS simulations have been run first up to 25 convective time units to develop turbulence - Figure 17 using a Large Eddy Simulation (LES) approach.

A restart file has then been generated and used to restart a transient simulation in Cardinal representing an heat-up of the pebbles. The time step has been fixed to $5(10^{-4})$ s in both BISON and NekRS. The temperature at time zero has been set to 300 C everywhere. Figure 18 presents the temperature at the surface of the pebbles in BISON at three points in time. The simulations took 2.5s per coupled time step on 20 nodes, requiring transfer between physics at each time step. However this could be greatly optimized by relaxing the requirement, as data transfer from GPU to CPU should be minimized as much as possible.

The results of OpenMC simulations coupled with the heat conduction module are shown in Figures 19 and 20 with the same time step parameters as the NekRS simulations described above. An eigenvalue simulation using 150 batches with 50 inactive batches was executed in each time step. 50,000 particles per batch were used to converge the pebble-averaged heat source from the OpenMC cell tally while the unstructured mesh heat source tally required 500,000 particles per batch to produce the heat source presented here. Production simulations may require a an even higher number of particles per batch to more tightly

DB: peb1568_n2t1bnb.nek5000
 Cycle: 7000 Time:22.9

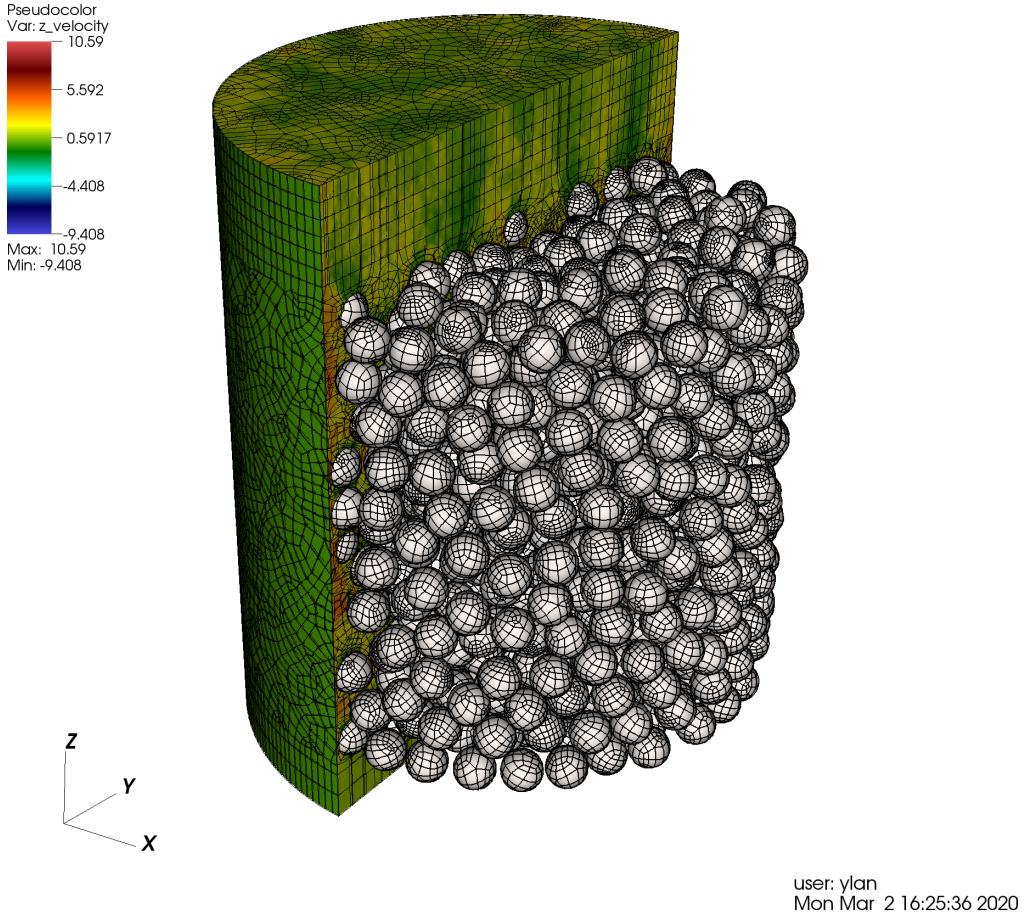


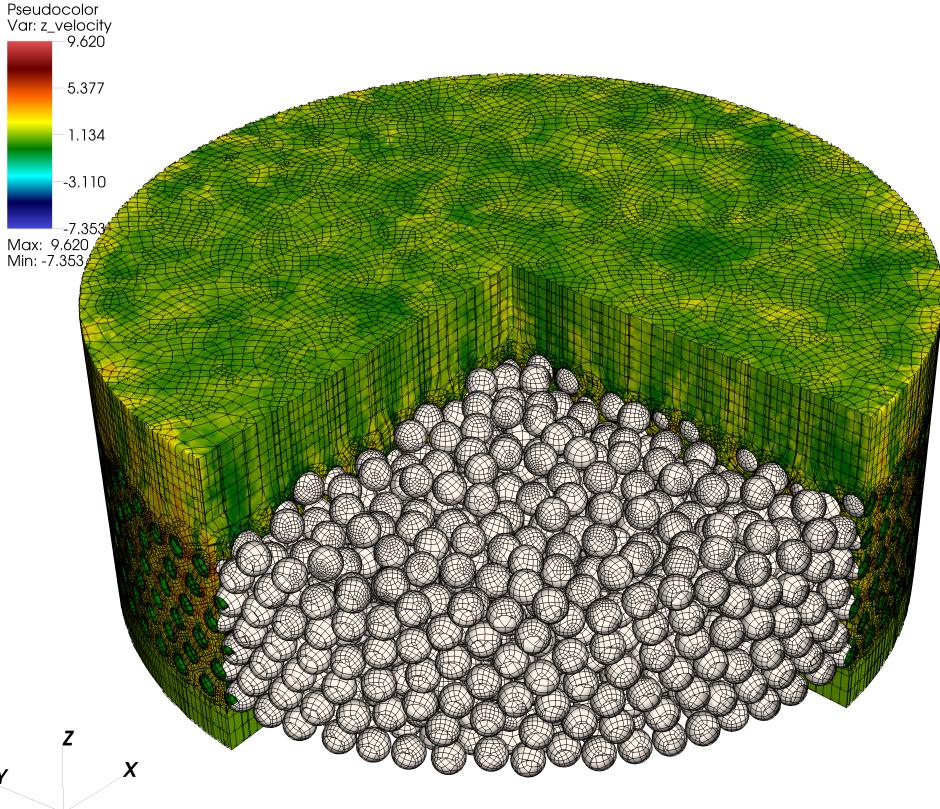
Figure 15: NekRS Mesh for 1568 pebble configuration

converge the heating distribution when using the unstructured mesh heat source due to the decreased number of samples per source particle in the tally bins. Figure 21 demonstrates the effect of the improved spatial resolution provided by the unstructured mesh heat source from OpenMC on the temperature distribution within a representative pebble. In the case of the pebble-averaged heat source the temperature profile is symmetric, reflecting the uniform heat source applied in that region, while an asymmetry can be seen in the profile generated from the unstructured mesh heat source indicating that the improved spatial resolution of the source has an impact on the temperature distribution in the solid and will in turn affect the resulting heat transfer to the fluid.

5.3 Projection to full core

20 nodes of Summit represents less than 1% of the computing power available on Summit. We estimate that 80% of the machine will be sufficient to perform full core calculation in FHRs corresponding to 300,000 pebbles.

DB: peb3344_n3.nek5000
 Cycle: 9000 Time:24.3



user: user
 Wed Jun 10 11:16:37 2020

Figure 16: NekRS Mesh for 3260 pebble configuration

6 Conclusions and Future Work

In this report we describe the extension of Cardinal to GPUs including a demonstration simulation on Summit. Cardinal provides a platform for running coupled OpenMC+(Nek5000/NekRS)+BISON. We demonstrated the application of Cardinal with a first-of-a-kind simulation on Summit, representing a $10\times$ pebble count increase compared to previous simulations. This exercise demonstrates that the Moose-Wrapped-App paradigm is working well even on a GPU platform like Summit.

We aim to conduct massively parallel simulations going up to 80% of Summit for full core simulations. The current results provide a clear pathway toward full core simulations. Future work on Cardinal will involve a more sophisticated thermal contact treatment between pebbles leveraging novel ideas using MOOSE constraints. Radiation heat transfer will also be added.

These simulations may involve asynchronous parallel execution between the physics. Finally a multiscale approach may be employed to simulate a select number of fuel particles directly.

DB: peb1568_n2t1bnb.nek5000
Cycle: 7000 Time:22.9

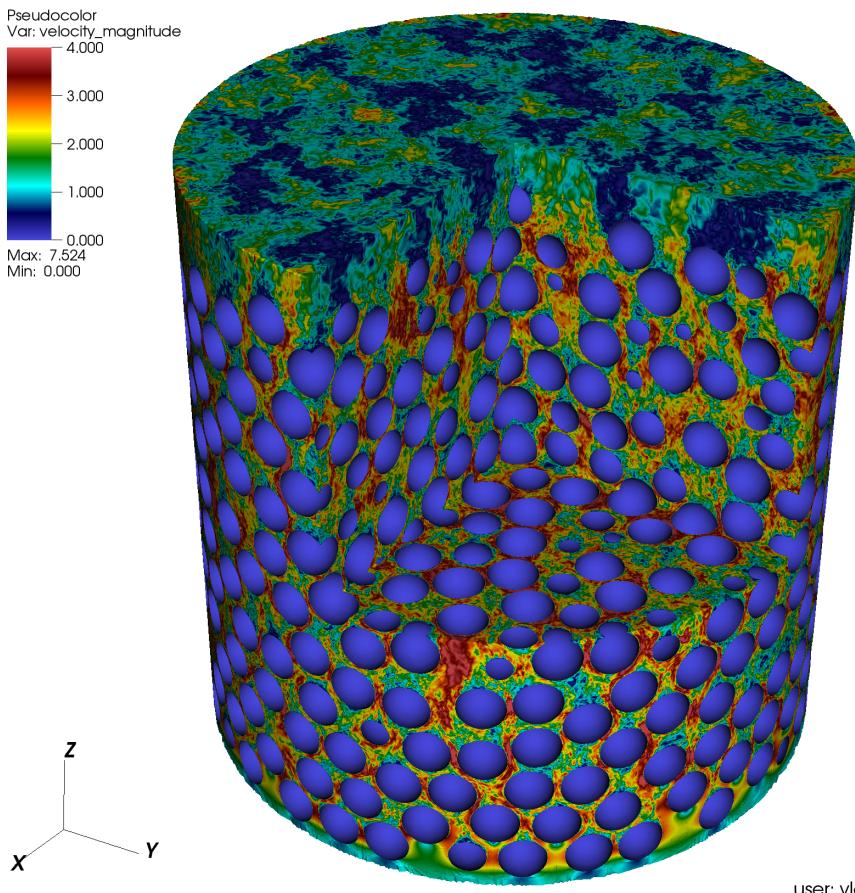


Figure 17: NekRS results for the velocity field.

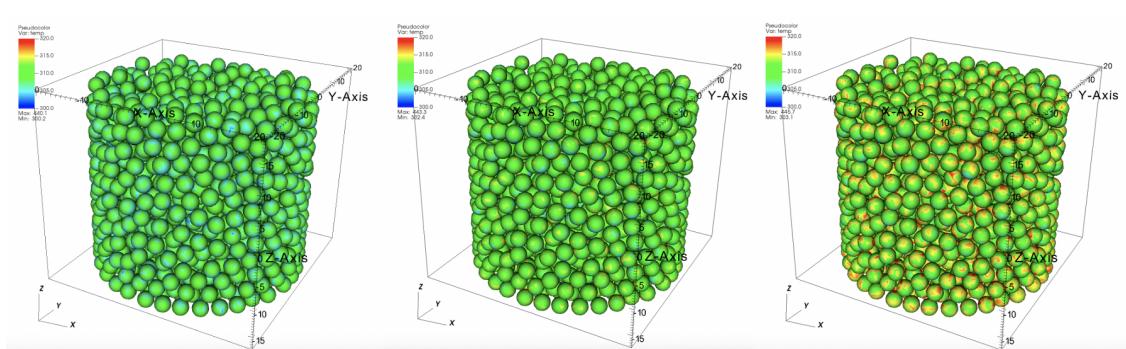


Figure 18: Temperature result for the pebble surface temperature at three points in time.

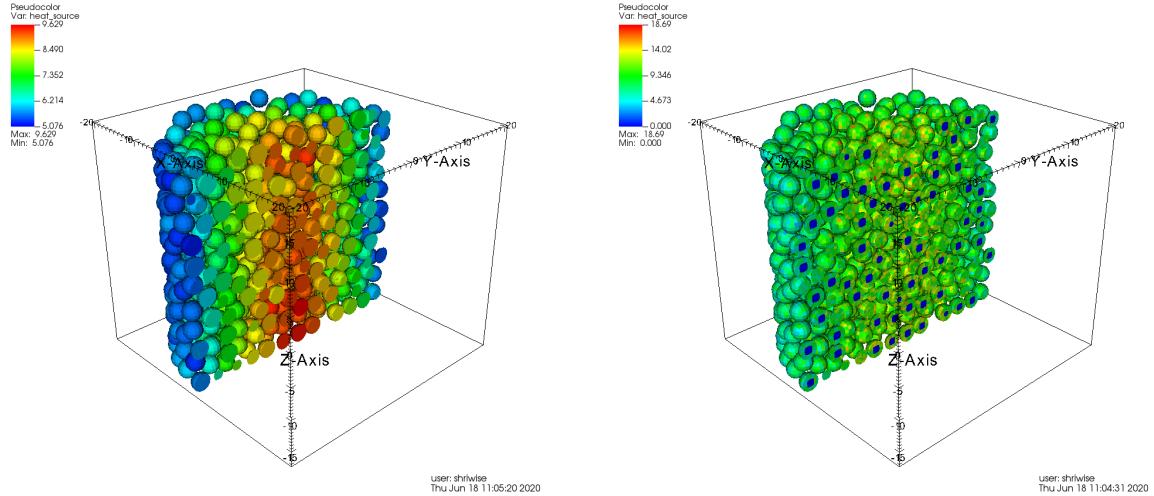


Figure 19: Left: Heat source using the original cell tallies to produces an average heat source per-pebble. Right: Heat source produced using an OpenMC unstructured mesh tally.

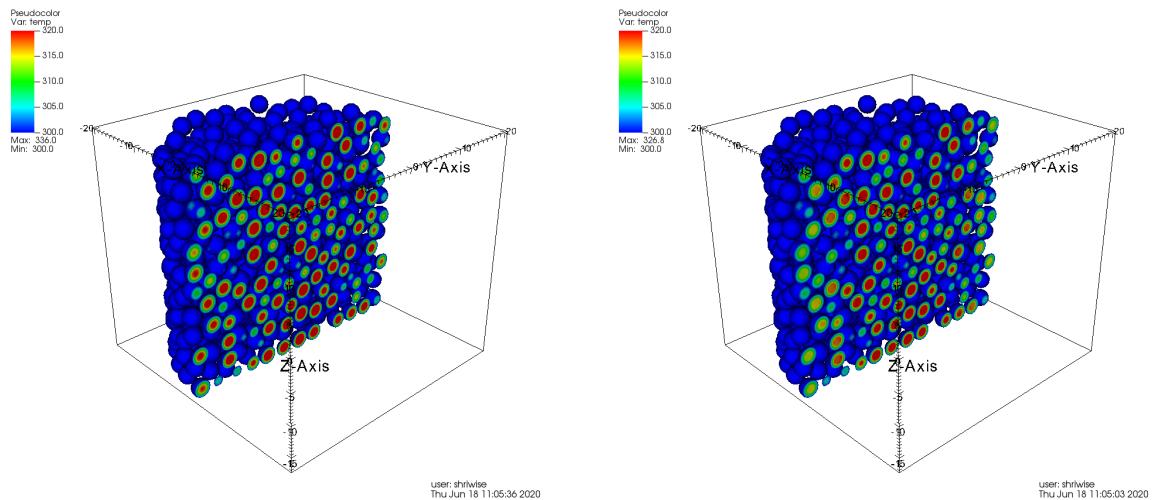


Figure 20: Left: Temperature in the solid resulting from the cell-based heating tally. Right: Temperature in the solid resulting from the unstructured mesh heating tally in OpenMC.

Acknowledgments

Argonne National Laboratory's work was supported by the U.S. Department of Energy, Office of Nuclear Energy, Nuclear Energy Advanced Modeling and Simulation (NEAMS), under contract DE-AC02-06CH11357.

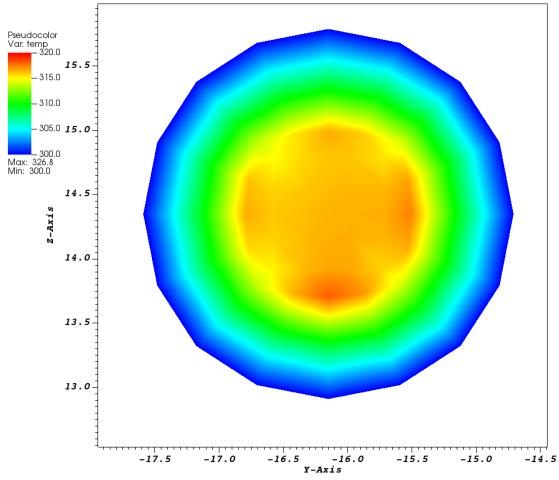
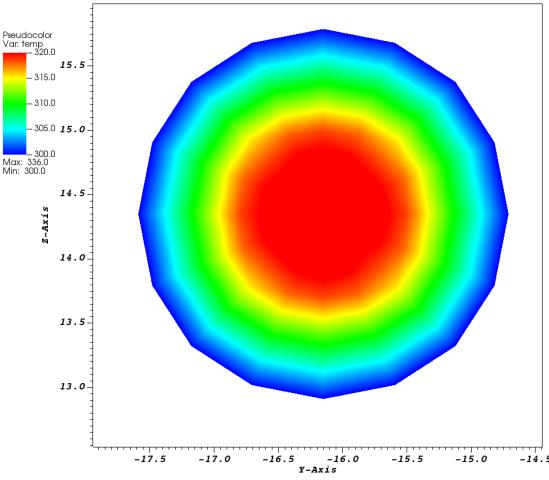


Figure 21: Temperature profiles of the same pebble in the 1568 pebble demo using the pebble-averaged heating (left) and the unstructured mesh heating (right).



Nuclear Science and Engineering Division
 Argonne National Laboratory
 9700 South Cass Avenue, Bldg. 240
 Lemont, IL 60439

www.anl.gov



Argonne National Laboratory is a U.S. Department of Energy
 laboratory managed by UChicago Argonne, LLC