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Release on the Virtual Test Bed of a Coupled SAM-Pronghorn Model of the Molten Salt Reactor Experiment using the Domain Overlapping Approach

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INTRODUCTION

The nuclear industry is taking leaps in innovations with companies seeking a sustainable energy future through advanced nuclear reactors. The Department of Energy (DOE)'s Nuclear Energy Advanced Modeling and Simulation (NEAMS) program seeks to substantiate and bolster the deployment of advanced reactors through flexible multifidelity, multiphysics simulations of advanced nuclear reactors. Applications like SAM for one-dimensional systems thermalhydraulics, and Pronghorn for multidimensional coarse mesh thermal-hydraulics, are geared to support innovations in industry by facilitating design, optimization, and licensing of advanced nuclear reactors.

Coupling systems thermal-hydraulics and computational fluid dynamics codes can be difficult as the pressure coupling converges slowly; however, it is important to obtain the desired accuracy in each part of the primary loop. The authors of this model created an Overlapping-Domain Coupling (ODC) [1] approach to coupling SAM and Pronghorn. Leveraging this coupling technique, a Molten Salt Reactor Experiment (MSRE) model was developed and released to the NEAMS/National Reactor Innovation Center (NRIC) Virtual Test Bed (VTB). The MSRE was chosen to be modeled because of the wealth of experimental data available and because of the strong physics coupling between the core and primary circuit [2].

This paper contextualizes the history of the MSRE, describes the thermal hydraulics models used, and detail the implementation of multidimensional thermal-hydraulics and system codes based on the ODC method [3] for the MSRE model. Finally, this paper presents how other modelers could apply the SAM-Pronghorn ODC for other advanced reactor models.

DESCRIPTION OF THE MSRE

The MSRE at Oak Ridge National Laboratory (ORNL) (1965–1969) was the first liquid fuel reactor moderated with graphite; it famously used molten salts as both a fuel medium and coolant. The reactor ran for more than 13,000 hours at full power before its final shut down in 1969. ORNL reported that the graphite lining the reactor core showed little-to-no damage from heat, radiation, or chemical corrosion [4]. The general layout of the experiment is shown in Figure 1.

There are three main features of this experiment aside from the specifications shown in Table I. First is the core circulation system, where the molten salt fuel flows through rounded-rectangular channels in the vertical graphite moderator stringers. Next is the centrifugal pump that provided

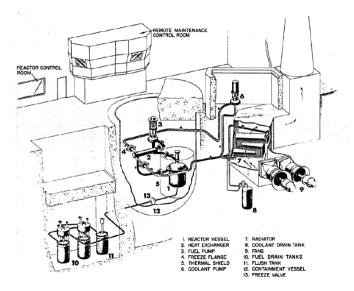


Fig. 1: Schematic design of MSRE loops [5].

TABLE I: MSRE Reactor Specifications [5]

Parameter	Value
Core Power $[MW_{th}]$	10
Core height [m]	1.63
Core diameter [m]	1.39
Fuel Salt	LiF-BeF ₂ -ZrF ₄ -UF ₄
Fuel salt molar mass	65.0%-29.1%-5.0%-0.9%
Fuel salt enrichment	33.0%
Channels in graphite moderator	3.05 cm x 1.016 cm
Channels' rounded corners radii	0.508 cm
Vertical graphite stringers	5.08 cm x 5.08 cm

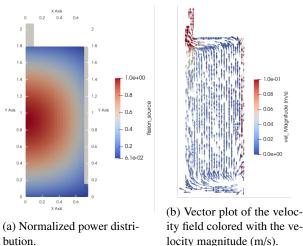
continuous circulation and facilitated heat transfer and the removal of fission products. Last is the two-loop heat exchanger system with a fuel loop circulation time in reactor of about 25 seconds. We note that the MSRE was a thermal reactor with a highly negative reactivity temperature coefficient.

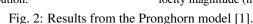
COMPUTATIONAL TOOLS

SAM and Pronghorn are advanced simulation tools that contribute to the development and safety analysis of nuclear systems. SAM is designed for a system-level thermalhydraulic analysis of plants in steady state and transient conditions. Pronghorn is a medium-fidelity, coarse mesh multidimensional thermal hydraulics code. While SAM offers a one-dimensional plant-wide view, Pronghorn offers a detailed multidimensional analysis of advanced reactor cores and integral loops. Coupling these tools is especially important where multiple inlets and outlets or strong flow dimensionality in the core complicate reductivist analyses.

THERMAL HYDRAULICS MODELS OF THE PRI-MARY LOOP

The Pronghorn model is a vertically axisymmetric model of the core. A porous media approximation is used to represent the core. The model utilizes a vertical porosity of 0.22283 in the core. The Griffin model [6] provides the normalized power distribution we use as the normalized power source, shown in Figure 2. As a result, the velocity in the core is much lower than that of the pipes due to the former having a much larger cross-sectional area. The normalized power source and the delayed neutron precursor sources were computed by the neutronics code Griffin [6] and passed to Pronghorn. Notably, the multidimensional velocity field is approximately one- dimensional in the core, which is achieved using an anisotropic friction coefficient blocking flow in the horizontal direction.





The SAM model includes the primary loop, the pump, and part of the secondary loop near the heat exchanger, shown in Figure 3. Figure 4 shows SAM's temperature profiles. Temperature rises as the molten salt undergoes fission through the core. The salt's temperature stays approximately constant from the core's outlet to the heat exchanger region where temperatures drops \sim 70 K. In this model, density, as a function of temperature, creates a buoyancy force.

The thermal-hydraulics and neutronics are strongly coupled by negative feedback; the MSRE core and primary loop are consequently coupled. The core conditions, such as temperature and precursor concentrations, determine the fission rate distribution, which in turn modifies the flow velocities and drives a change in core conditions. The varying neutronics feedback is not currently captured in the model.

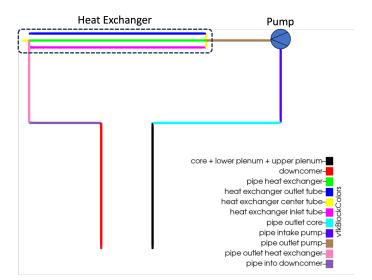


Fig. 3: SAM model of the MSRE primary and secondary circuits [1].

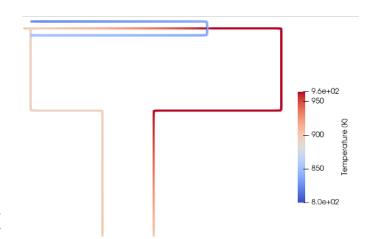


Fig. 4: Temperature distribution in the MSRE primary circuit and secondary loop (K) [1].

OVERLAPPING-DOMAIN COUPLING

Source [1] demonstrates that the Pronghorn-SAM ODC algorithm is: (1) numerically stable in a wide range of reactor operation conditions, (2) supports thermal-hydraulic coupling, (3) converges faster and is more accurate than the domain-segregated approach in fixed-point iterations, as shown in Figure 5, and (4) supports multiple boundaries in Pronghorn and SAM. The method successfully achieves these goals by solving three challenges: the abstraction of the systems-code topology in the overlapped SAM components, the information transfer (called iteration) between SAM and Pronghorn, and the correct computation of the source terms. The "source terms" refer to the volumetric source terms in the momentum, energy and precursors' equations that match the variables of interest, such as friction factor, volumetric heat transfer, and passive scalars, respectively.

The source terms are computed with two approaches: the

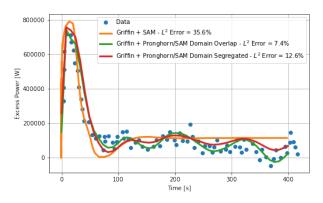


Fig. 5: Griffin coupled to thermal-hydraulics model results for reactivity insertion transient at 5 MW for MSRE [1].

Jacobi method and the update approach. The Jacobi method is used in a steady state relaxation to obtain the initial conditions for the update approach. The code provides the time the approach switches. The update approach then iterates on the coupling, converging different sources, until SAM and Pronghorn converge within a tolerance. This convergence is referred to as obtaining a consistent result between the solvers. The update approach uses the difference over a domain of the pressure drop, enthalpy balance, and passive scalar advection to iteratively update respective sources in SAM components, which drives the difference between Pronghorn's and SAM's integrated quantities to zero, thereby achieving equivalence between the overlapping loops.

ODC RESULTS

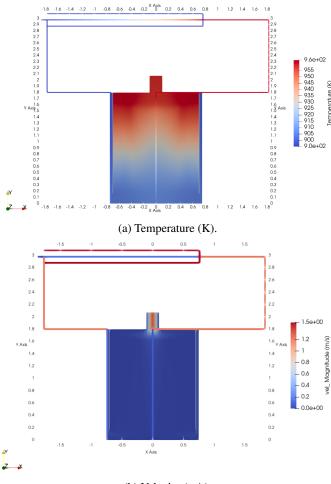
This coupling technique is accessible through a custom Action, a terminology used in MOOSE [7], labeled '[OverlappingDomainCouplings].' Provided the user has access to Pronghorn and SAM (both of which are available independently or via the BlueCRAB suite), the action will set up all additional required objects and equations. This Action approach adds versatility for many uses including the use of multiple inlets and outlets, and dealing with inertial forces implicitly, among others. The custom Action overlaps the following domains: downcomer, core, and plena. The Action automatically makes Pronghorn incorporate volumetric sources into the overlapped SAM components. The mass-flow-averaged predictions obtain a consistent result despite the exclusion of rigorous geometries in the coupling.

Figure 6 showcases this coupled approach. Here the vertical lines going up the middle of the core represent the corresponding SAM solution informed by the higher fidelity Pronghorn core model. SAM, being a one-dimensional representation of the core, models the interstitial velocity—the actual fluid properties in the core channels—whereas the Pronghorn model shows the superficial properties which includes the porosity treatment of the core.

Figure 6a shows how the temperature increases as the molten salt flows up from the downcomer, through the graphite stringers, and out the upper plenum. The velocity magnitude

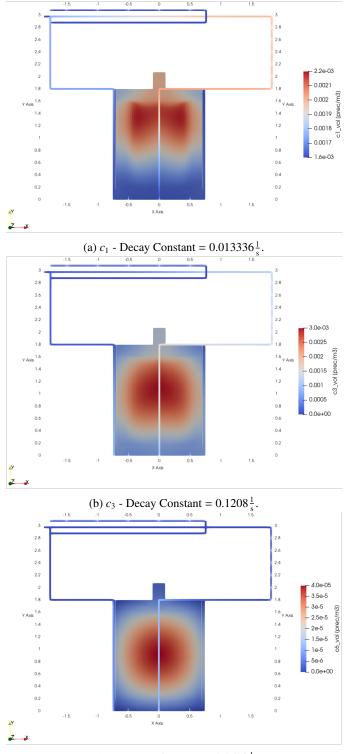
in Figure 6b corresponds to the cross-sectional area the salt flows through. The greater the area, the lower the velocity magnitude. Thus, the velocity magnitude plummets in the heat exchanger due to the shell-and-tube design, where the area the primary salt flows through is greatly increased in the shell.

The neutron precursor distribution yields almost-identical data in the overlapping SAM and Pronghorn loop components. Additionally, the ODC model exhibits exceptionally close agreement with experimental data compared with models just utilizing SAM or utilizing domain-segregated rather than domain-overlapping coupling [1]. As seen in Figure 5, the Pronghorn/SAM domain overlap coupling exhibits a 7.4% error compared with a 12.6% error from the domain-segregated solve. In Figure 7, we see the longer-lived precursors, group c_1 , almost make it around the entire primary loop before decaying. On the other hand, we see group c_6 precursors decay almost as soon as they are created.



(b) Velocity (m/s).

Fig. 6: Coupled Pronghorn-SAM thermal-hydraulics results for steady-state primary circuit and secondary cooling of MSRE [1].



(c) c_6 - Decay Constant = $2.8530\frac{1}{s}$.

Fig. 7: Coupled Pronghorn-SAM normalized neutron precursors concentration results for steady-state primary circuit of MSRE [1].

CONCLUSION

The implementation of the overlapping domain coupling on the MSRE model shows an approach to modeling advanced reactor primary loops. The ODC could ease previously taxing analyses for scientist and developers. Thanks to the release of the MSRE model on the VTB, researchers can use this coupling approach for their own purposes. The VTB's documentation of the model details each phase of the Pronghorn-SAM coupling. The underlying framework supports arbitrary geometries through the use of unstructured meshes. Additionally, the programs do not make implicit assumptions about the type of reactor being modeled. These reasons, among others, drive the applicability of the SAM-Pronghorn ODC to modeling other reactor types.

These NEAMS tools aim to serve the advanced nuclear reactor industry's simulation needs as companies set out to address energy infrastructure's challenges. Additional work is underway to incorporate reversals of flow over boundaries and increase capacity for transient events. Future work will include incorporating the thermal hydraulic feedback effect of delayed neutron precursors on the neutronics solve via Griffin for a tightly coupled multiphysics and ODC analysis.

REFERENCES

- S. SCHUNERT, M. T. RETAMALES, and M. JARA-DAT, "Overlapping Domain Coupling of Multidimensional and System Codes in NEAMS - Pronghorn and SAM," Tech. Rep. INL/RPT-23-72874, Idaho National Laboratory (2023).
- P. N. HAUBENREICH and J. R. ENGEL, "Experience with the Molten-Salt Reactor Experiment," *Nuclear Applications and Technology*, 8, 2, 118–136 (1970).
- I. DAVIS, O. COURTY, M. AVRAMOVA, and A. MOTTA, "High-fidelity multi-physics coupling for determination of hydride distribution in Zr-4 cladding," *Annals of Nuclear Energy*, **110**, 475–485 (2017).
- H. E. MCCOY and B. MCNABB, "Postirradiation examination of materials from the MSRE," (12 1972).
- M. FRATONI, D. SHEN, G. ILAS, and J. POWERS, "Molten Salt Reactor Experiment Benchmark Evaluation," (5 2020).
- M. JARADAT and J. ORTENSI, "Thermal Spectrum Molten Salt-Fueled Reactor Reference Plant Model," *Idaho National Laboratory*, **INL/RPT-23-72875** (07 2023).
- A. D. LINDSAY, D. R. GASTON, C. J. PERMANN, J. M. MILLER, D. ANDRŠ, A. E. SLAUGHTER, F. KONG, J. HANSEL, R. W. CARLSEN, C. ICENHOUR, L. HARBOUR, G. L. GIUDICELLI, R. H. STOGNER, P. GERMAN, J. BADGER, S. BISWAS, L. CHAPUIS, C. GREEN, J. HALES, T. HU, W. JIANG, Y. S. JUNG, C. MATTHEWS, Y. MIAO, A. NOVAK, J. W. PETER-SON, Z. M. PRINCE, A. ROVINELLI, S. SCHUNERT, D. SCHWEN, B. W. SPENCER, S. VEERARAGHAVAN, A. RECUERO, D. YUSHU, Y. WANG, A. WILKINS, and C. WONG, "2.0 - MOOSE: Enabling massively parallel multiphysics simulation," *SoftwareX*, 20, 101202 (2022).