Computational Tools for Advanced Molten Salt Reactors Simulation

Andrei Rykhlevskii, PI: Kathryn Huff Advanced Reactors and Fuel Cycles Group

University of Illinois at Urbana-Champaign

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About ARFC Fission basics Motivation

Insights at Disparate Scales





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Nuclear Fission Reaction





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Nuclear Fission Chain Reaction





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Nuclear Power Plant



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Why Molten Salt Reactors?





Main advantages of liquid-fueled Molten Salt Reactors (MSRs) [1]

- 1 High coolant temperature (600-750 $^{\circ}$ C).
- Various fuels can be used (²³⁵U, ²³³U, Thorium, U/Pu).
- Increased inherent safety.
- High fuel utilization ⇒ less nuclear waste generated.
- 6 Online reprocessing and refueling.

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Challenges in simulation MSR

- ① Contemporary burnup codes cannot treat fuel movement.
- 2 Neutron precursor location is hard to estimate.
- 3 Operational and safety parameters change during reactor operation.
- Ø Power generation strongly depends on fuel temperature and vica versa.



Figure 1: Challenges in simulating MSR (Courtesy of Manuele Aufiero, 2012).



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Research objectives



Goal #1: Tool for online reprocessing depletion simulation (SaltProc)[2]

- ① Create high-fidelity full-core neutronics model of MSBR.
- ② Develop online reprocessing simulation code, SaltProc, which expands the neutronics code capability for simulation liquid-fueled MSR operation.
- Analyse Molten Salt Breeder Reactor (MSBR) neutronics and fuel cycle performance.

Goal #2: Tool for multiphysics simulation of MSR (Moltres)[3]

- Demonstrate steady-state coupling of neutron fluxes, precursors, and thermal-hydraulics.
- 2 Implement advective movement of delayed neutron precursors.
- 3 Demonstrate capabilities with 2D axisymmetric and 3D mesh.





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Moderator element geometry (Zone I)



Figure 2: Molten Salt Breeder Reactor Zone I unit cell geometry from the reference [4] (left) and SERPENT 2 (right).

Full-core SERPENT model of MSBR



Figure 3: Plan (left) and elevation (right) view of MSBR model.

Core Zone II



Figure 4: Detailed plan view of graphite reflector and moderator elements.

Online reprocessing method





Figure 5: Flow chart for the SaltProc.

SaltProc capabilities

- Remove specific isotopes from the core with specific parameters (reprocessing interval, mass rate, removal efficiency)
- · Add specific isotopes into the core
- Maintain constant number density of specific isotope in the core
- Store stream vectors in an HDF5 database for further analysis or plots
- Generic geometry: an infinite medium, a unit cell, a multi-zone simplified assembly, or a full-core

MOOSE Framework





Figure 6: Multi-physics Object-Oriented Simulation Environment (MOOSE).

- Fully-coupled, fully-implicit multiphysics solver
- MOOSE interfaces with libMesh to discretize simulation volume into finite elements
- Residuals and Jacobians handed off to PetSc which handles solution of resulting non-linear system of algebraic equations
- Automatically parallel (largest runs >100,000 CPU cores!)
- Built-in mesh adaptivity
- Intuitive parallel multiscale solves





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Effective multiplication factor for full-core MSBR model



Figure 7: k_{eff} during a 20 years depletion simulation.



Power and breeding distribution





Figure 9: 232 Th neutron capture reaction rate normalized by total flux

²³²Th refill rate





- Fluctuation due to batch-wise removal of strong absorbers
- Feed rate varies due to neutron energy spectrum evolution
- 232 Th consumption is 100 g/GWh_e

Figure 10: $^{232}\mathrm{Th}$ feed rate over 20 years of MSBR operation

Multiphysics simulation results (2D)



Multiphysics simulation results (2D) (2)



Figure 12: Temperature in channel obtained using Moltres [3].

Multiphysics simulation results (3D)



Figure 13: Cuboidal MSR steady-state temperature and fast neutron flux [5].





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Conclusions



- New tool SaltProc was developed to simulate fuel depletion in the MSR.
- **SaltProc** was tested for MSBR conceptial design, equilibrium fuel salt composition was found and verified against recent studies.
- Average ^{232}Th refill rate throughout 20 years of operation is approximately 2.39 kg/day or 100 g/GWh_e.

Moltres

- New tool Moltres was developed for modeling coupled physics in novel molten salt reactors.
- 2D-axisymmetric and 3D multiphysics models are presented.
- **Moltres** demonstrated strong parallel scaling (up to 384 physical cores) but further optimization required.
- Over 55,000 node-hours were consumed on **Blue Waters** to perform this research.

Future research



Future research effort

- Equilibrium state search for Transatomic MSR (>30,000 node-hours).
- Fuel cycle performance analysis for load-following regime (>40,000 node-hours).
- Light Water Reactor (LWR) fuel transmutation in MSR viability (>30,000 node-hours).
- Start exploring transients in Moltres, e.g. explore responses to reactivity insertion or gaseuos poisons removal (>70,000 node-hours).





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Processing options for MSR fuels

HIDERGEN H Lin Soomu Na	Be Be Mg	 Elements that escape from fuel salt Elements that can be removed without processing Elements that can be removed only by chemical processing of fuel salt B C N O F A Si P S CI 															HELLUM He ARON ARON ARON AR
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	ASSINC	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Мо	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те		Хе
Слезиин	Ва		Hf	Та	TUNISTICS W	Re	OSWILLN OS	lr	PLATINUM	Au	Hg	THALLIUM	Pb	Bi	Poo	Attent	Rn
FRANCEIM	Ra		Rf	Db	Sg	Bh	HASSEE	Mt	Ds	Rg	Сореннистии	Unit	Filler	University	Lv	UNUNGEREIGEN	Uuo
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Но	Er	Tm	Yb	Lu	
		Астична	Those units	Pa		NPTUMUM	PUTONUM	Am	Cm	Bk	CALIFORMUM	Es	FERMIUM	Md	North		

BUBBLE GENERATOR AND GAS SEPARATOR for MSBR



Chemical processing facility for MSBR



Multiplication factor dynamics during Rb, Sr, Cs, Ba removal (3435days)



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MSBR neutron energy spectrum for different regions



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Fissile isotopes producing in MSBR core





MSBR plain view





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Generation IV Reactors



Goals for Generation IV Nuclear Energy Systems

- Sustainability
- 2 Economics
- **3** Safety and Reliability

Proliferation Resistance and Physical Protection Generation I

