

Fission Gas SciDAC 2

Simulation of Fission Gas in Uranium Oxide Nuclear Fuel

Project Summary

The objective of this project is to significantly advance the mechanistic understanding of fission gas behavior and release in UO_2 nuclear fuel by developing a mesoscale simulator that takes advantage of leadership class computers. An important aspect of our approach is to use the mesoscale insight gained via this tool to build an accurate and physically based fission gas release model for application in integrated fuel performance codes, as the fission gas models in standard fuel performance codes are a primary source of code uncertainty. Furthermore, the model development will be informed by results from massive atomistic and mesoscale simulations of the three stages of fission gas release, including diffusion and intra-granular bubble formation, bubble growth and coalescence on grain faces, and the transport of gas through interconnected grain edge tunnels to free surfaces. The simulation tools will also undergo rigorous uncertainty quantification and validation against existing experimental data.

This project builds upon (and partly overlaps with) our SciDAC-3 project: [Advancing Understanding of Fission Gas Behavior in Nuclear Fuel through Leadership Class Computing](#)

Publications and Presentations

Team

	Institution	Principal Investigator	Additional Participants
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Sponsor

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Key Partners

Program or Sponsor	Project	Project Point(s) of Contact	Partner Point(s) of Contact
SciDAC-4 Institutes	FASTMath – Frameworks, Algorithms, and Scalable Technologies for Mathematics	Barry Smith (ANL), Habib Najm (SNL)	
	RAPIDS - Resource and Application Productivity through computing, Information, and Data Science	David Bernholdt (ORNL), Phil Roth (ORNL)	
DOE Office of Nuclear Energy	Nuclear Energy Advanced Modeling and Simulation (NEAMS)		Steven L. Hayes (INL), Chris Stanek (LANL)
DOE Office of Nuclear Energy	Fuel Cycle R&D		Kurt A. Terrani (ORNL)

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