December 14, 2020

INL/PRO-20-60699

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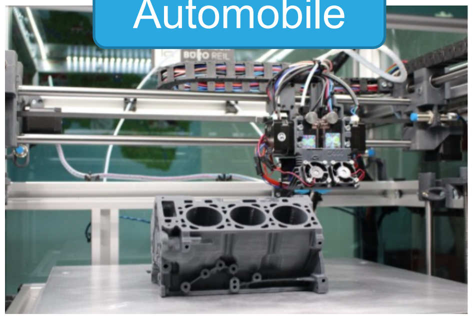
Extended Finite Element Based Approach in Additive Manufacturing Modeling for Optimizing Highly Complex Manifold in Protonic Ceramic Electrochemical Cells

Idaho National Laboratory

How to Improve Additive Manufacturing (AM) Processing and Modeling Capabilities at INL?

Aerospace

Automobile



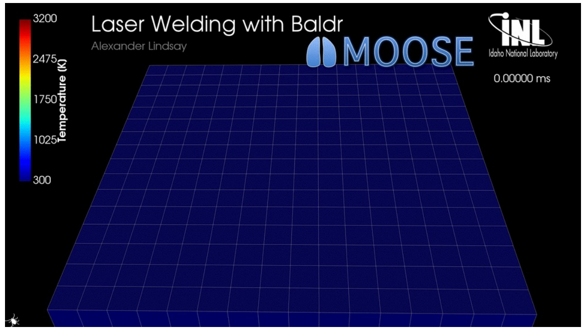
Medical

Construction

Education

➢ AM's application to a variety of fields (images from *addit3dprinting.com* and *ge.com*)

Modeling & Simulation



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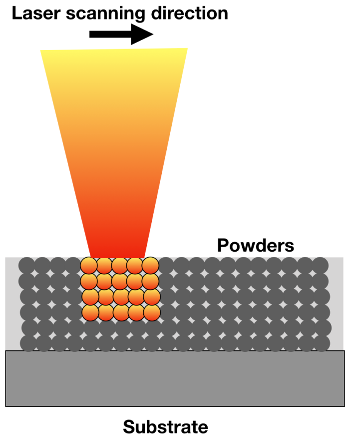
Experimental Realization



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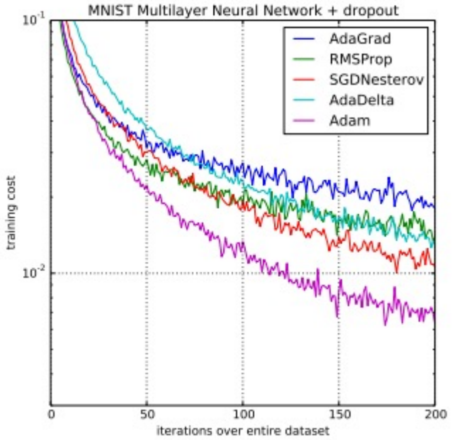
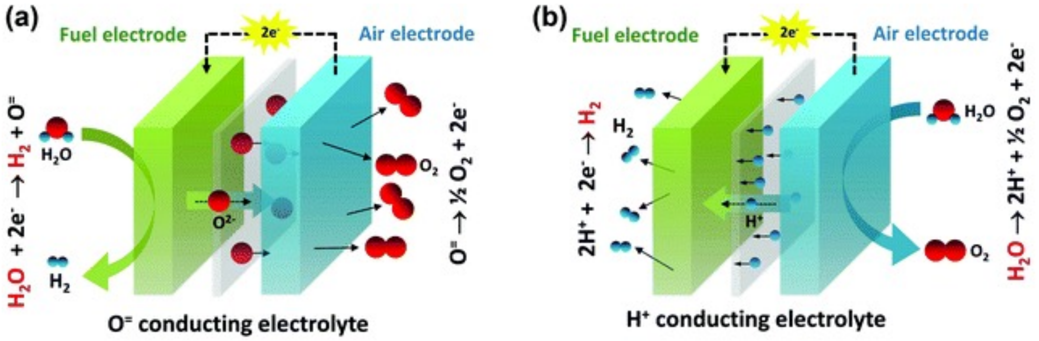
Parameter Optimization



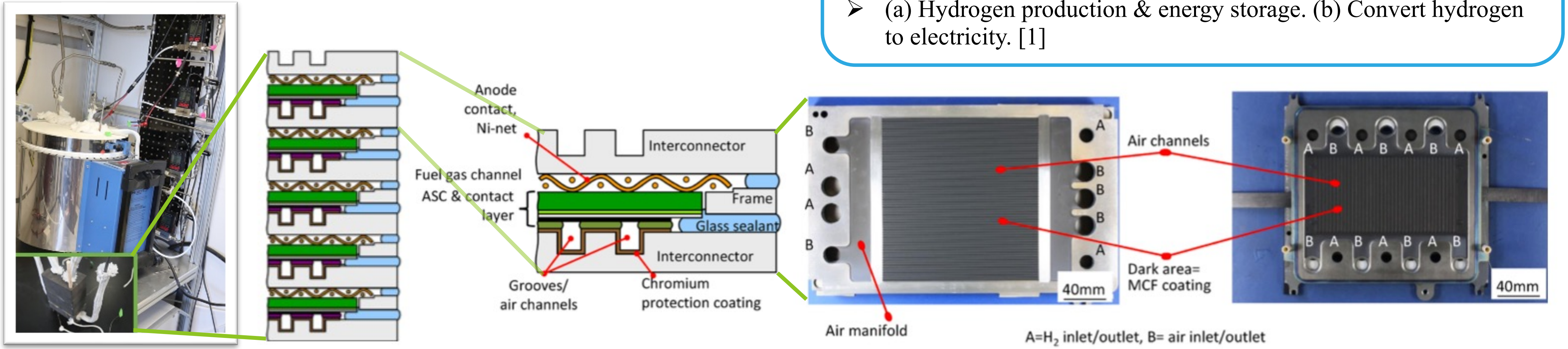
AM Modeling for PCEC Manifold and Interconnector

- Applications for INL's protonic ceramic electrochemical cell (PCEC) development include
  - hydrogen production through water electrolysis
  - ammonia electrosynthesis
- Commercialization requires a scaled-up stackable production
  - manifold and Interconnector design & fabrication is critical
  - successful usage of stainless steel can lower the overall cost (from 20 - 30% to 8 - 10%)
- Modeling the AM process guides and ensures the success of the design and manufacturing processes

How PCEC works



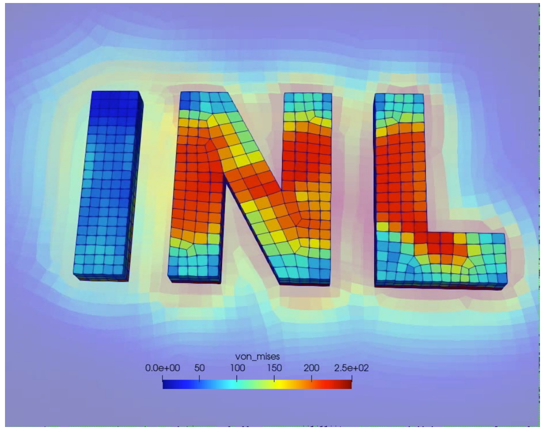
➢ (a) Hydrogen production & energy storage. (b) Convert hydrogen to electricity. [1]

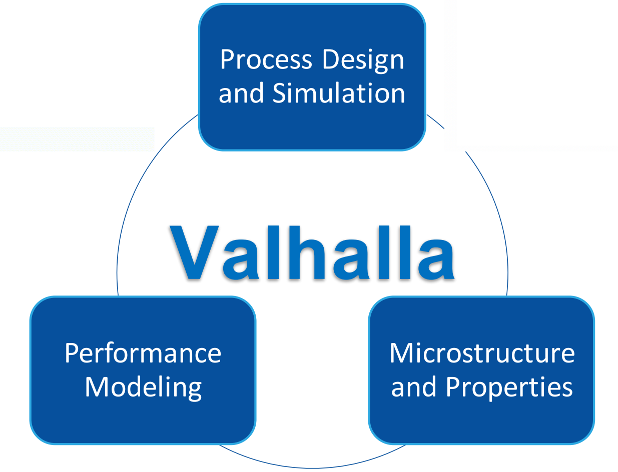


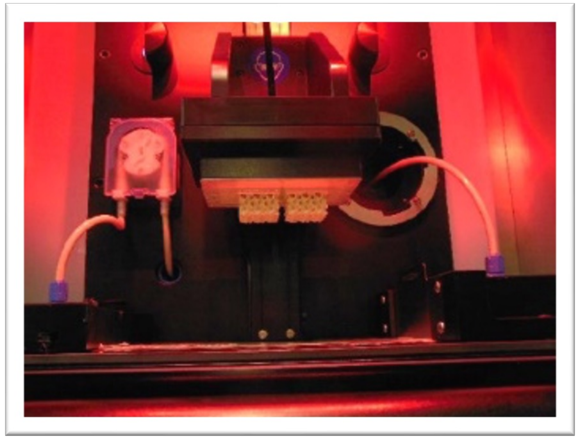
➢ INL's PCEC assembly capability. A stack repetition units [2]. One PCEC unit with interconnector [2]. Two types of interconnector [2].

AM Modeling Development at INL & Challenges

- **AM simulation capability – Valhalla**
  - Simulates material deposition (not optimal)
  - Includes physics modules (parameters not verified or validated)
- **AM processing capability (for model validation)**
  - Material discovery (not used in complex structures)







➢ (left) INL's AM process to make advanced nuclear fuels. (right) Digital light processing 3D printer at EIL.

➢ (top) AM modeling of the INL logo printing process. (bottom) Valhalla–A MOOSE-based application for simulating AM processes.

AM Modeling Development Challenges

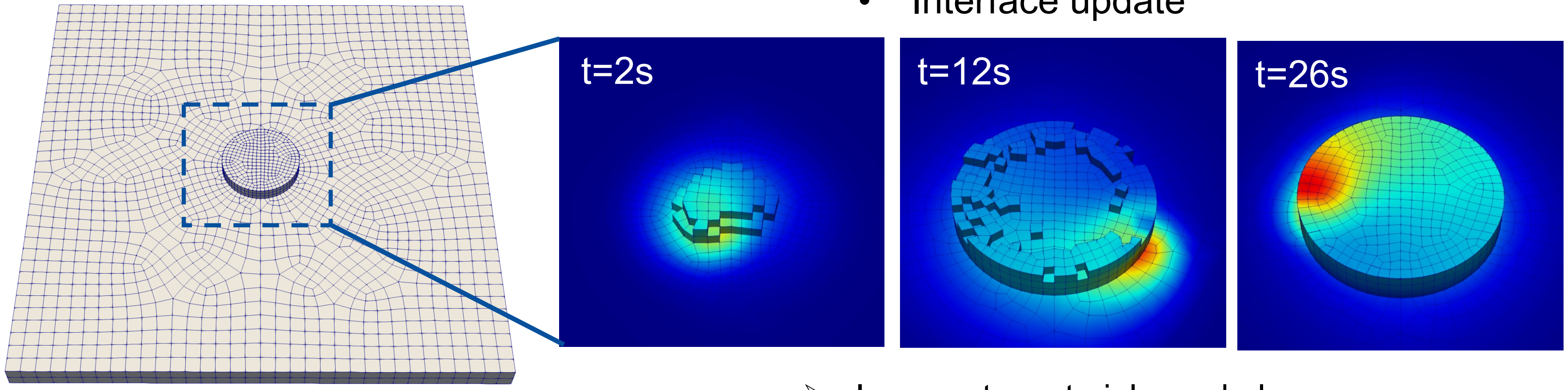
Modeling the Moving Interface

Preprocessing

- Meshing

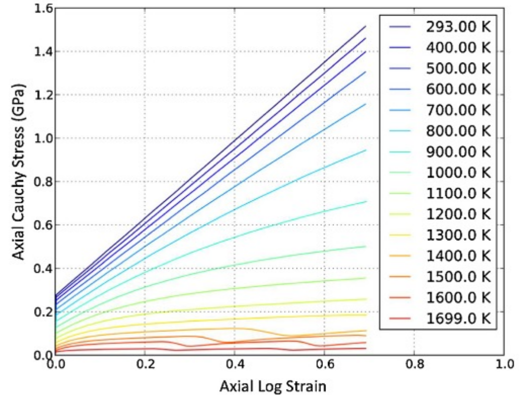
Processing

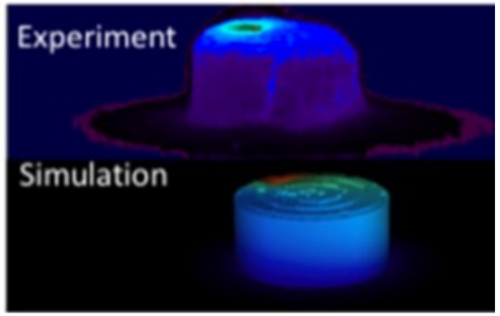
- Element activation
- Interface update



- ➢ Highly refined mesh around the product
- ➢ Inaccurate material morphology
- ➢ Predefined material boundary

Verification & Validation



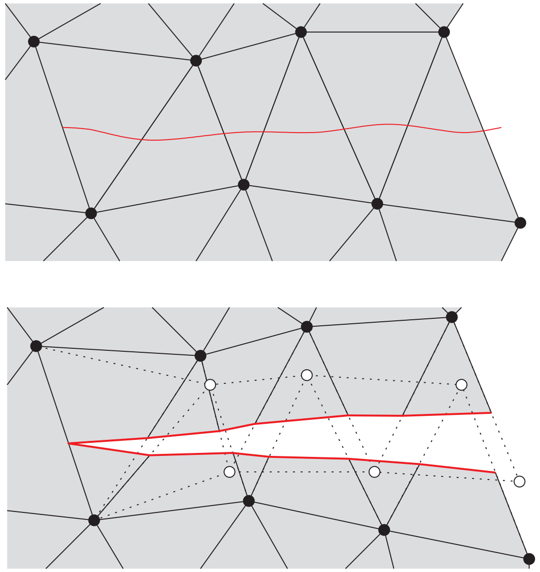


Integration & Modulization

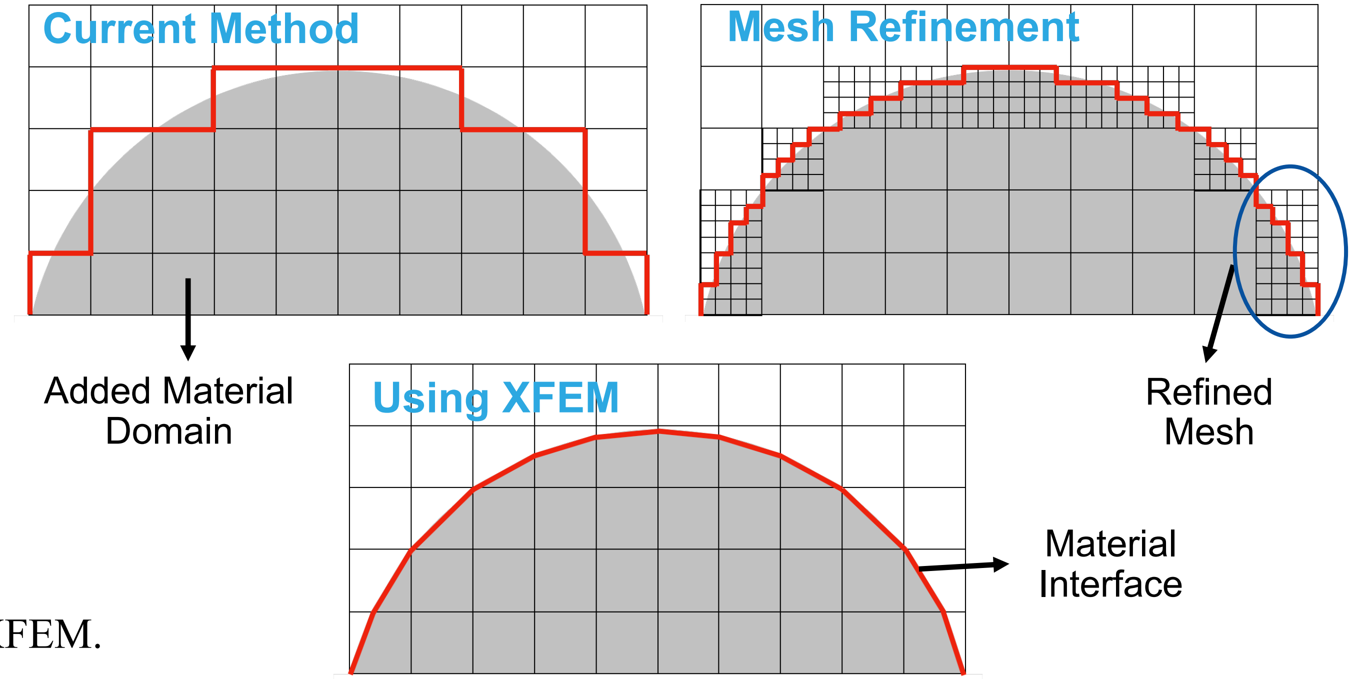
MOOSE Valhalla RAVEN Slic3r Open source 3D printing toolbox

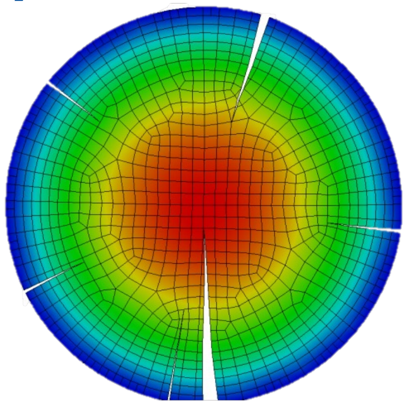
- ➢ Physics-based simulation
- ➢ Optimization
- ➢ Printing path planning

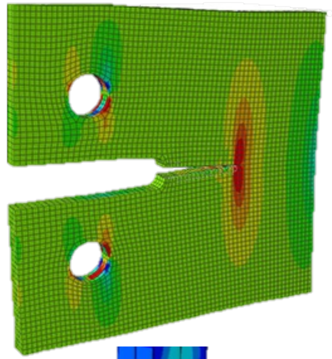
What Is Extended Finite Element Method (XFEM) & How Can It help?

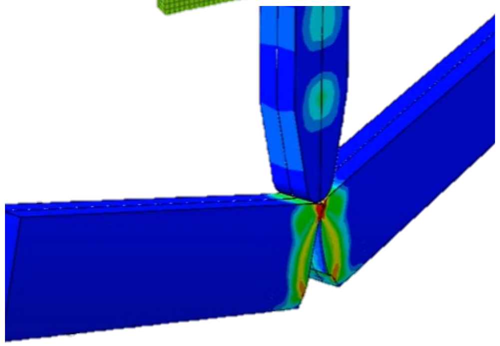


➢ Mesh cutting for modelling crack in XFEM.









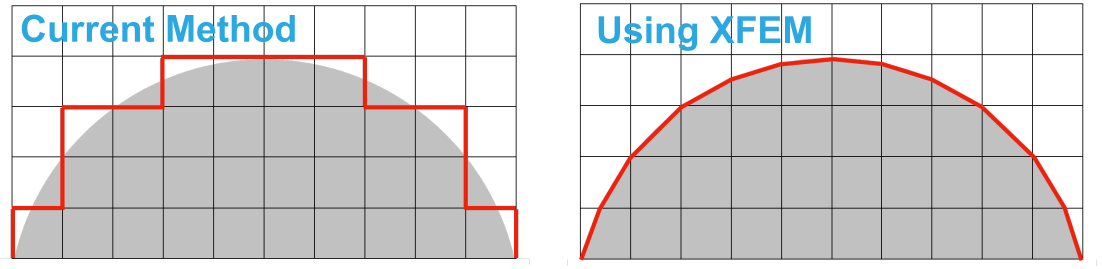
Benefits for using XFEM in modeling moving interface:

- Enables accurate descriptions of the product configuration
- Reduces the computation cost caused by highly refined meshes
- Removes unrealistic assumptions brought by predefining the material boundaries

What We will Do

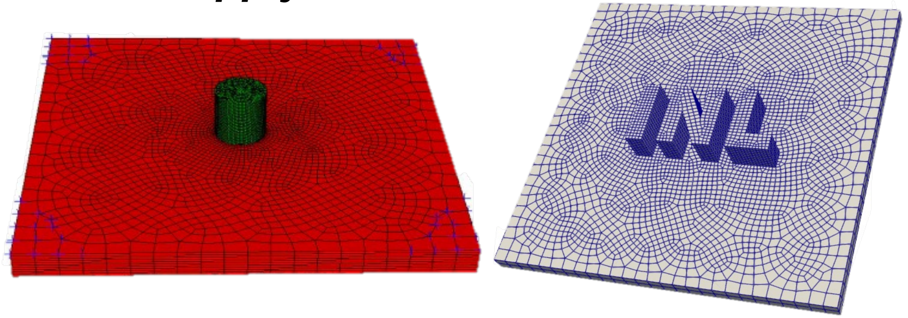
Task 1: Method Development

Accurately Model Material Boundaries

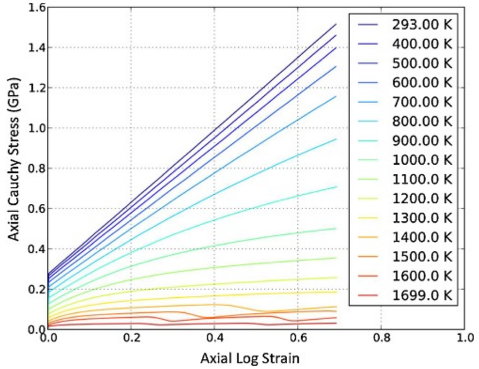


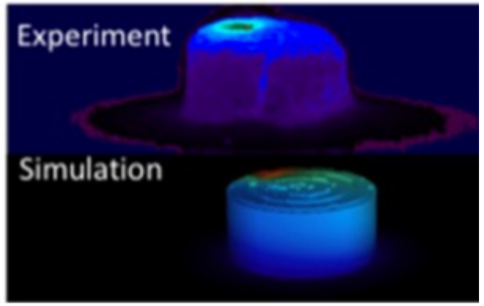
Task 2: Simulation & Optimization

Apply in Current Test Cases



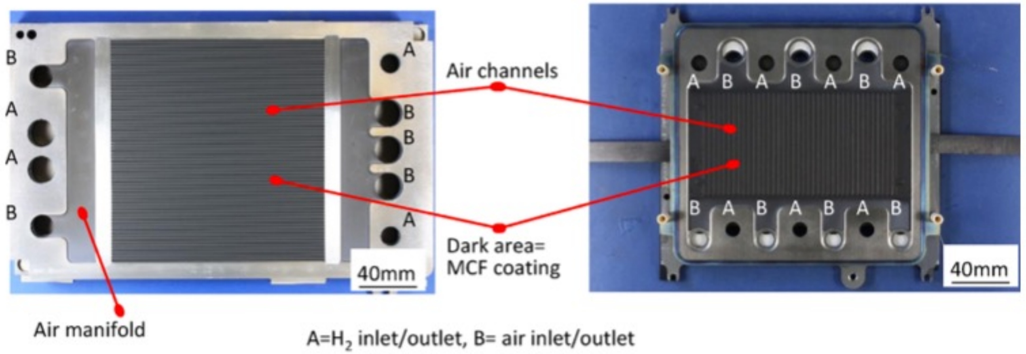
Task 3: Verification & Validation



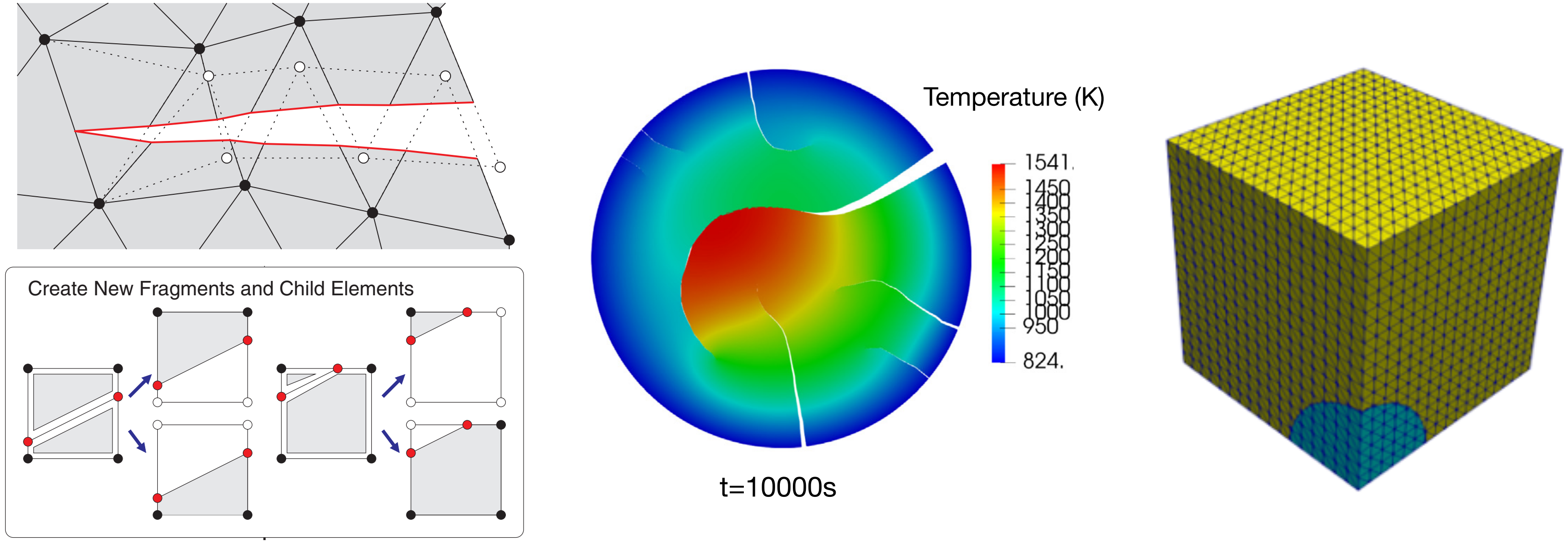


Deployment

Extend to Complex Structures



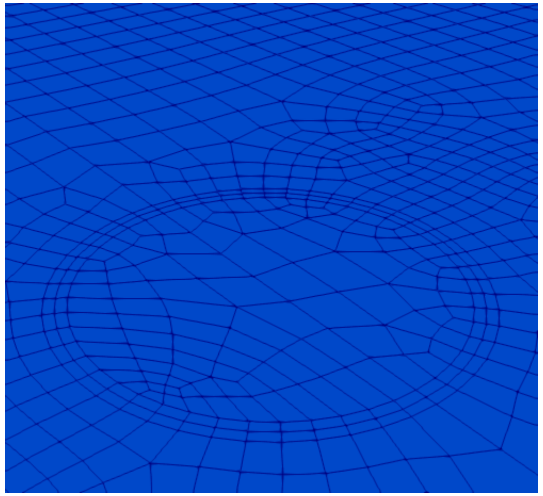
Method Development Plan

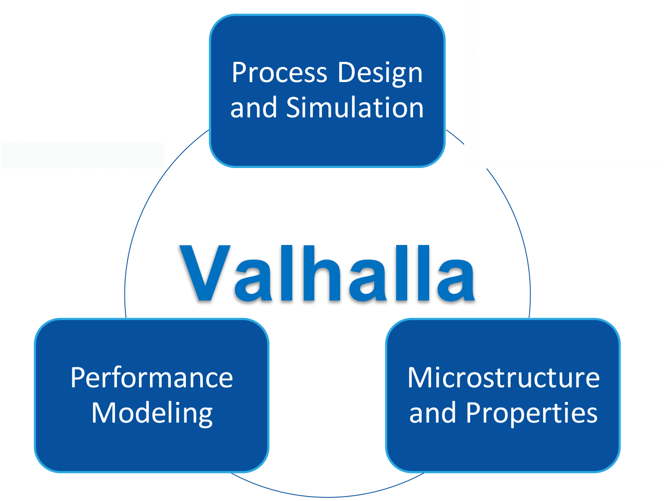


➢ (left) Schematic of the mesh cutting process in XFEM. (center) Simulation of propagating cracks in a fuel pellet using XFEM. (right) Use of XFEM to model a moving interface between two materials.

- Add the ability to represent moving material surfaces with XFEM
- Develop simple 3D test cases and evaluating the accuracy of the approach
- Apply boundary conditions
- Improve the integration accuracy (moment fitting method)

Simulation & Optimization Plan

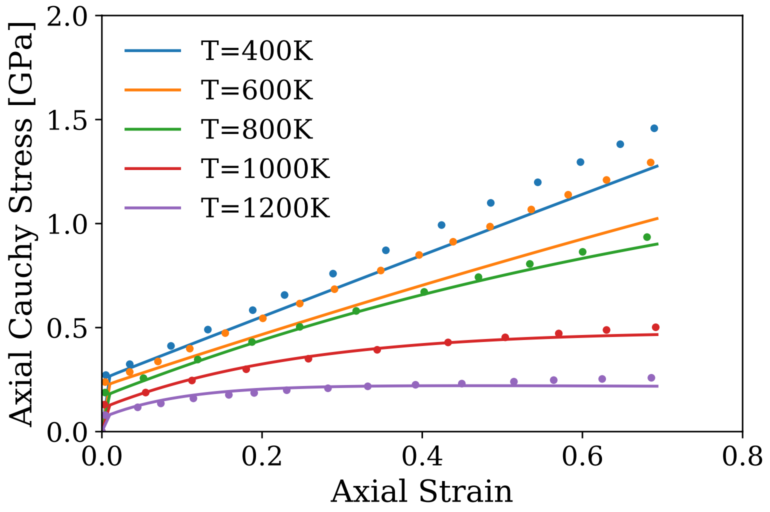


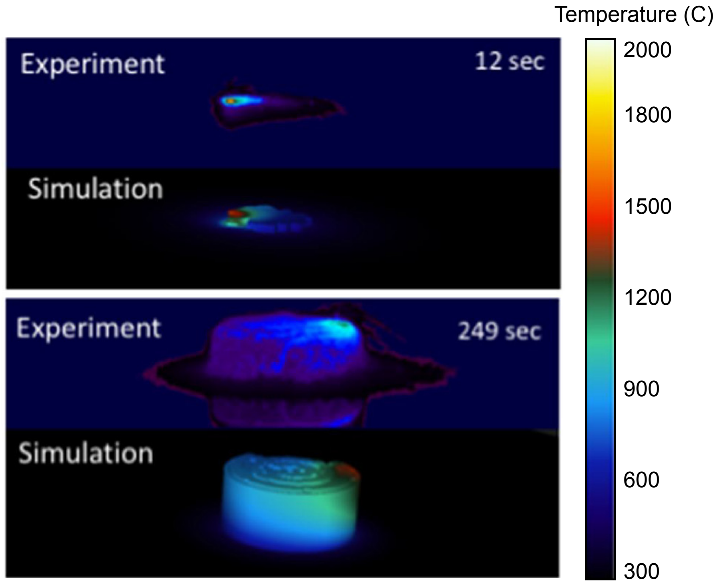


➢ (left) Valhalla – A MOOSE-based application for simulating AM processes. (right) AM simulation of printing a INL logo using Valhalla.

- Valhalla will be used to simulate the mesoscale AM process
- Analysis of the residual stress, distortion, porosity, and parameter sensitivity
- Iteration between V&V for optimizing the AM parameters and product design
- Use PCEC manifold processing as a proof of concept

Verification & Validation Plan





- ➢ (left) Verification example for a high temperature plasticity model. (middle) Experimental setting from [3]. (right) Example validation of the temperature field in [3].
  - Compare and match simulation results in literatures

    (temperature field, residual stress, distortion)
  - Compare and match existing AM-processed metal parts and experimental data

Timeline & Deliverables

Q1: Initial method development
- Investigate and implement improvements to the XFEM-based moving interface approach
- Demonstrate the advantages of this approach on simple test cases

Q2–Q3: Model development and validation
- Develop the full system model for the AM process
- Verify the numerical model with literature
- Validate material and AM processing parameters with experimental data

Q4: Model and design optimization
- Iterate between optimizing the design and the numerical model for the optimal performance of the product
- Prepare and report to INL LDRD office

- ➢ A new XFEM-based approach for modeling moving interface
- ➢ A verified and validated model for AM process modeling and product optimization
- ➢ One peer-reviewed publication in a high-impact journal in this field and delivery of one conference presentation

Customers & Opportunities

DOE offices:

- Office of Nuclear Energy (NE) programs

  (fuels design, fabrication, and modeling)

- Office of Energy Efficiency & Renewable Energy
  - Advanced Manufacturing Office

    (AM processing of other types of metals, ceramics, and composites)

  - Hydrogen and Fuel Cell Technology Office

    (PCEC stack production)

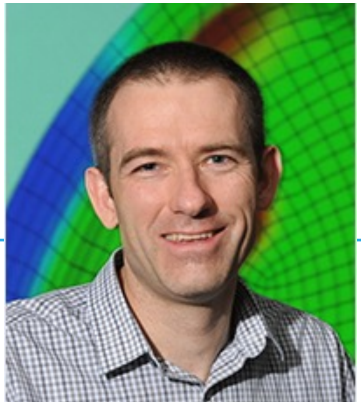
Industry:

- Westinghouse
- General Electric

We will Enable Success

Dewen Yushu,
Postdoctoral Research Associate

Expertise in computational solid mechanics, mechanical contact, constitutive modeling, numerical solver and preconditioner, and multigrid methods.



Benjamin Spencer,
Computational Scientist

Expertise in developing and applying computational methods for fracture, contact, constitutive modeling, and structural dynamics. PI of LDRD that originally developed XFEM in MOOSE.

Dong Ding,
Group Lead

Expertise in materials discovery, manufacturing, and electrochemistry with prospective visions in ADM and IES. PI for AMO, FCTO, DOD, FE, and LDRD projects > $10M

Budget Summary

A: Research Tasks	FY-21 ($k)	FY-22 ($k)	Total ($k)
Task 1: Method development	40	0	40
Task 2: Numerical analysis and design optimization	48	0	48
Task 3: Model verification and validation	0	32	32
Total Task Budget	88	32	120
B: Budget by Researcher	**FY-21 ($k)**	**FY-22 ($k)**	**Total ($k)**
Dewen Yushu	60	20	80
Benjamin Spencer	20	10	30
Dong Ding	8	2	10
Total INL Labor	88	32	120
Total Budget Request	**88**	**32**	**120**

INL

Idaho National Laboratory

References

[1] Choi, Sihyuk, Timothy C. Davenport, and Sossina M. Haile. 2019. "Protonic Ceramic Electrochemical Cells for Hydrogen Production and Electricity Generation: Exceptional Reversibility, Stability, and Demonstrated Faradaic Efficiency." Energy & Environmental Science 12(1): 206–215.

[2] Harboe, S., A. Schreiber, N. Margaritis, L. Blum, O. Guillon, N.H. Menzler. 2020. "Manufacturing Cost Model for Planar 5 kWel SOFC Stacks at Forschungszentrum Jülich." International Journal of Hydrogen Energy 45(15): 8015–8030.

[3] Stender, Michael E., Lauren L. Beghini, Joshua D. Sugar, Michael G. Veilleux, Samuel R. Subia, Thale R. Smith, Christopher W. San Marchi, Arthur A. Brown, Daryl J. Dagel. 2018. "A Thermal-Mechanical Finite Element Workflow for Directed Energy

[4] Deposition Additive Manufacturing Process Modeling." Additive Manufacturing 21: 556–566.

Paolini, Alexander, Stefan Kollmannsberger, and Ernst Rank. "Additive manufacturing in construction: A review on processes, applications, and digital planning methods." Additive Manufacturing 30 (2019): 100894.

[5] Schoinochoritis, Babis, Dimitrios Chantzis, and Konstantinos Salonitis. "Simulation of metallic powder bed additive manufacturing processes with the finite element method: A critical review." Proceedings of the Institution of Mechanical Engineers, Part B: Journal of Engineering Manufacture 231.1 (2017): 96-117.

[6] Beaman, J. J., et al. "Additive Manufacturing Review: Early Past to Current Practice." Journal of Manufacturing Science and Engineering 142.11 (2020).

[7] Weimar, Mark R., et al. Cost study for manufacturing of solid oxide fuel cell power systems. No. PNNL-22732. Pacific Northwest National Lab.(PNNL), Richland, WA (United States), 2013.

[8] Harboe, S., et al. "Manufacturing cost model for planar 5 kWel SOFC stacks at Forschungszentrum Jülich." International Journal of Hydrogen Energy 45.15 (2020): 8015-8030.

[9] Battelle Memorial Institute. "Manufacturing Cost Analysis of 100 KW and 250 KW Fuel Cell Systems for Primary Power and Combined Heat and Power Applications." (2016).

References

[10] Bandyopadhyay, Amit, and Kellen D. Traxel. "Invited review article: Metal-additive manufacturing—Modeling strategies for application-optimized designs." Additive manufacturing 22 (2018): 758-774.

[11] Z. Zhang, W. Jiang, J. E. Dolbow, and B. W. Spencer. "A modified moment-fitted integration scheme for X-FEM applications with history-dependent material data". Computational Mechanics, 62.2 (2018):233–252.

[12] W. Jiang, B. W. Spencer, and J. E. Dolbow. "Ceramic nuclear fuel fracture modeling with the extended finite element method." Engineering Fracture Mechanics 223 (2020): 106713.