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 any of their employees, 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 authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof. Reference herein to any social initiative (including but not limited to Diversity, Equity, and Inclusion (DEI); Community Benefits Plans (CBP); Justice 40; etc.) is made by the Author independent of any current requirement by the United States Government and does not constitute or imply endorsement, recommendation, or support by the United States Government or any agency thereof.

Final Technical Report

Project Title: Conference Travel Fellowships: The 10th Annual International Conference on Multiscale Materials Modeling, Baltimore, Maryland, October 19-22, 2020

Principal Investigator:

Prof. Jaafar El-Awady
Department of Mechanical Engineering
Johns Hopkins University

Award Period: DOE Support Period: 07/01/2022 to 09/30/2024

Conference Dates: September 22-27, 2024

Location: Prague Congress Center, Czech Republic

Conference webpage: https://mmm11.ipm.cz/

1. Project Objectives

The original scope aimed to broaden participation in the 10th International Conference on Multiscale Materials Modeling (MMM 10) by supporting travel and accommodation for 10 junior scientists from U.S. Institutions. A funding request of $10,000 was submitted to partially offset the cost of registration and local accommodation for these early-career participants. Since the award was made close to the date MMM 10 was to be held, we requested a no-cost extension to defer this travel support to the 11th International Conference on Multiscale Materials Modeling (MMM 11), which was held in Prague Congress Center in the Czech Republic. The scope of the travel award remained the same: supporting travel and accommodation for 10 junior scientists from U.S. Institutions.

2. Project Significance and DOE Relevance

MMM 11 focused on cutting-edge multiscale materials modeling spanning mechanics, biology, manufacturing, and data-driven methods. The conference content aligned with DOE's Basic Energy Sciences (BES) priorities in topics such as:

- Synthesis and Processing Science
- Theoretical Condensed Matter Physics
- Physical Behavior of Materials
- Mechanical Behavior and Radiation Effects

The event fostered interaction among DOE-funded investigators, both among themselves and with international scientists, which helped advance DOE mission objectives by enabling collaborative, cross-institutional research exposure and dialogue.

3. **Description of the Event**

Held at the Prague Congress Center, Czech Republic , MMM 11 hosted around 750 international participants. It included:

- 7 Plenary Lectures by leading experts, including Ralf Drautz (Ruhr Universität and ICAMS Bochum, Germany), Hyoung Seop Kim (Pohang University of Science and Technology, South Korea), Tomáš Jungwirth (Institute of Physics of the CAS, Czechia & University of Nottingham, UK), Bob Coecke (Quantinuum Ltd. UK & Perimeter Institute, Canada), Chris Wolverton (Northwestern University, USA), Claire Wilhelm (Curie Institute & CNRS, France)
- 14 Technical Symposia on the following topics:
    - Quantum mechanical studies of structure and properties of materials
    - Ladislas Kubin memorial symposium on microstructure evolution across multiple length scales
    - Multiscale modeling of crystal plasticity of materials
    - Multiscale design of functional materials for energy conversion, harvesting and storage
    - Multiscale modeling of radiation effects and materials under extreme environments
    - Multiscale modeling of biological and soft-matter systems View G. Machine learning assisted materials discovery
    - Vaclav Vitek honorary symposium on atomistic simulations of materials
    - Multiscale and coarse-grained models of surfaces and interfaces
    - Multiscale insights into high and medium entropy alloys: From atomistic calculations to macroscopic applications
    - Damage mechanics across scales
    - Multiscale simulations of polymers and polymer composites

    - Advances in methodologies for understanding disorder and kinetics in complex materials
    - Multiscale and multi-physics modeling of metal additive manufacturing processes
- Two Poster Sessions with student poster competitions
- Industry exhibition and structured networking events

4. Award Implementation and Selection Process

Following DOE approval, the organizing committee:

- Published the travel fellowship opportunity through the conference email list
- Evaluated applicants received based on a ranked criterion, including:
    - Prior support history
    - Accepted papers or posters
    - Institutional diversity

Ultimately, every junior researcher who applied was supported either entirely or partially.

5. Outcomes and Impact

- All recipients attended the full conference and presented their work, either orally or as posters.
- Several of the awardees noted the event provided them with valuable professional exposure.
- Immediate research collaborations were initiated between attendees from different institutions.
- Positive feedback highlighted the impact of the DOE support on enabling career development.

6. Publications and Dissemination

The conference has arranged **peer-reviewed journal special issues** to publish selected papers from MMM 10 in

1. *Modelling and Simulation in Materials Science and Engineering*
2. *Materials Theory*

Award recipients were encouraged to contribute to these publications.

7. Conclusion

The DOE fellowship successfully facilitated the participation of early-career researchers at MMM 10, reinforcing BES's strategic goals in materials science and enhancing workforce diversity in the physical sciences. The event served as a springboard for future collaborations and the professional growth of junior scientists in multiscale materials modeling.