



Midwest Integrated Center
for Computational Materials

All Hands Meeting

Time: December 4, 2020, 1:30-5pm US central

Location: virtual

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| 1:30pm | <i>Introduction</i> Giulia Galli (UChicago & ANL) |
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| | Code coupling Chair: Marco Govoni |
| 1:50pm | <i>Coupling strategy, and WEST-Qbox coupling</i> Marco Govoni (ANL & UChicago) |
| 2:05pm | <i>SSAGES-Qbox coupling</i> Elizabeth Lee (UChicago) & Jiale Shi (UNotreDame) |
| 2:15pm | <i>SSAGES-COPSS coupling (applications)</i> Siva Dasetty (UChicago) |
| 2:25pm | <i>iPI-Qbox coupling</i> Arpan Kundu (UChicago) |
| 2:35pm | Discussion |
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| | GPU porting & path towards Exascale Chair: Francois Gygi (UCDavis) |
| 3:00 pm | <i>WEST GPU-related activities</i> Marco Govoni (ANL & UChicago) |
| 3:10 pm | <i>SSAGES GPU-related activities</i> Pablo Zubieta (UChicago) |
| 3:20 pm | <i>Qbox GPU-related activities</i> Francois Gygi (UC Davis) |
| 3:30pm | Discussion |

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| | Verification, Validation, Data Chair: Maria Chan |
| 4:00pm | Update on V&V and data activities Giulia Galli (UChicago) |
| 4:10pm | <i>Calculations of photoluminescence spectra: verification & validation</i> Yu Jin (UChicago) |
| 4:20 | Discussion on V&V& Data, followed by general discussion |
| 4:55pm-5pm | <i>Summary</i> Giulia Galli (UChicago & ANL) |