# 2018 Scientific Discovery through Advanced Computing (SciDAC-4) Principal Investigator Meeting

## Sponsored by the U.S. Department of Energy Office of Advanced Scientific Computing Research

Hilton Washington DC/Rockville
Rockville, MD
July 23 - 24, 2018

## Agenda

The agenda is also available as a PDF file (143 KB). All presentations linked to the agend are in PDF fiormat.

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## Monday, July 23, 2018

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| 7:00am - 8:00am | Continental Breakfast | | Plaza Ballroom Foyer |
| 8:00am - 5:30pm | Poster Session | **Mark Pederson** | Atrium |
| 8:15am - 8:35am | ASCR Welcome | **Ceren Susut, Randall Laviolette** US Department of Energy | Plaza Ballroom Foyer |
| 8:35am - 10:00am | Program Overviews: | **Program Managers** | Plaza Ballroom Foyer |
| | *8:36 - 8:48 Advanced Scientific Computing Research (ASCR)* (1.02 MB) | **Ceren Susut, Randall Laviolette** | |
| | *8:48 - 9:00 Fusion Energy Sciences (FES)* (3.03 MB) | **John Mandrekas** | |
| | *9:00 - 9:12 High Energy Physics (HEP)* (2.16 MB) | **Lali Chatterjee** | |
| | *9:12 - 9:24 Biological & Environmental Research (BER)* (2.16 MB) | **Dorothy Koch** | |
| | *9:24 - 9:36 Office of Nuclear Energy (NE)* (435 KB) | **Dan Funk** | |

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| | *9:36 - 9:48 Basic Energy Sciences (BES)* (1.33 MB) | **James Davenport** | |
| | *9:48 - 10:00 Nuclear Physics (NP)* (391 KB) | **Ted Barnes** | |
| 10:00am - 10:15am | Break | | Plaza Ballroom |
| 10:15am - 12:00pm | Institutes – Rob Ross (RAPIDS) (4.14 MB), Lori Diachin (FASTMath) (4.34 MB) | **Ceren Susut** US Department of Energy | Plaza Ballroom |
| 12:00pm - 1:30pm | Lunch | | Plaza Ballroom |
| 1:30pm - 4:00pm | *Breakout Sessions:* | | |
| | ***1:30 – 4:00 – Basic Energy Sciences (BES)***<br>1:30 – **Thomas Devereaux**, SLAC: "Superconductivity and CDWs in the doped Hubbard & t-J models: pairing Without quasiparticles"<br>2:00 – **Martin Head-Gordon**, Lawrence Berkeley National Laboratory: "Advancing Catalysis Modeling: From Atomistic Chemistry to Whole System Simulation" (9.49 MB)<br>2:30 – **Thomas Maier**, Oak Ridge National Laboratory: "S-wave pairing from repulsive interactions: Quantum Monte Carlo study of systems with incipient bands" (9.49 MB)<br>3:00 – **Todd Martinez**, SLAC National Accelerator Laboratory: "Scaling Quantum Mechanics and First Principles Dynamics for Accuracy and Efficiency" (5.47 MB)<br>3:30 – Poster Session<br>5:30 – Adjourn | **James Davenport** | Eisenhower |
| | ***1:30 – 3:30 – Nuclear Physics (NP)***<br>1:30 PM – 2:00 PM<br>TEAMS Nuclear Astrophysics Project (8.75 MB)<br>**Raph Hix** (ORNL) 30 mins (25+5)<br>2:00 PM – 2:30 PM<br>LQCD Lattice Quantum Chromodynamics Project (4.53 MB)<br>**Robert Edwards** (TJNAF) 30 mins (25+5)<br>2:30 PM – 3:00 PM - Break | **Ted Barnes** | Regency |

3:00 PM – 3:30 PM
NUCLEI Nuclear Computational Low Energy Initiative Project (4.46 MB)
**Joe Carlson** (LANL) 30 mins (25+5)

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| | ***3:30 – 4:00 – Office of Nuclear Energy (NE)*** Simulation of Fission Gas in Uranium Oxide Nuclear Fuel (4.27 MB) (20 minute talk + 10 min Q&A) **David Andersson** | **Dan Funk** | Regency |
| 5:30pm | *Adjourn* | | |

## Tuesday, July 24, 2018

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|---|---|---|---|
| 7:00am - 8:00am | Continental Breakfast | | Plaza Ballroom Foyer |
| 8:00am - 5:30pm | Poster Session | **Mark Pederson** | Atrium |
| 8:15am - 9:15am | SciDAC-4-ASCR Facilities Discussion (1.02 MB) | **Ceren Susut, Randall Laviolette** US Department of Energy | Plaza Ballroom |
| 9:15am - 9:30am | Break | | Plaza Ballroom Foyer |
| 9:15am - 12:00pm | *Breakout Sessions:* | | |
| | ***9:30 – 12:00 – High Energy Physics (HEP)*** 9:30 – 9:50: **Jim Amundson**, ComPASS4 (533 KB) (15+5min) 9:50 – 10:10: **Salman Habib**, Inference and Machine Learning (3.5 MB) (15+5 min) 10:10 – 10:30: **Jim Kowalkowski**, HEP Data Analytics (1.89 MB) (15+5 min) 10:30 – 10:45: **Giuseppe Cerati**, Pilot - Event Reconstruction (7.8 MB) (10+5 min) 10:45 – 11:00: **Stephan Hoeche**, Pilot - Monte Carlo Event Generators (1.66 MB) (10+5 min) 11:00 – 11:15: Break 11:15 – 12:00: Discussion: Future Plans - HEP Cross-Cut Computing Challenges, CCE Engagement, SciDAC Coordinating Committee | **Lali Chatterjee** | Regency |

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| | activities; Lessons Learned (45 min) | | |
| | ***9:30 – 12:00 – Fusion Energy Sciences (FES) α***<br>9:30 – 9:45: opening remarks, John Mandrekas, Randall Laviolette<br>9:45 – 10:15: **David Green**, ORNL, "Center for Integrated Simulation of Fusion Relevant RF Actuators" (6.75 MB)<br>10:15 – 10:45: **Jeff Candy**, General Atomics, "Advanced Tokamak Modeling Environment (AToM)" (7.15 MB)<br>10:45 – 11:00: Break<br>11:00 – 11:30: **CS Chang**, PPPL, "Partnership Center for High-fidelity Boundary Plasma Simulation (HBPS)" (1.91 MB)<br>11:30 – noon: **Xianzhu Tang**, LANL, "Tokamak Disruption Simulation" (5.83 MB) | **John Mandrekas** | Eisenhower |
| 12:00pm - 1:30pm | Lunch | | Plaza Ballroom Foyer |
| 1:30pm - 5:00pm | *Breakout Sessions cont.* | | |
| | ***1:30 – 5:00 – Biological & Environmental Research (BER)***<br>1:30 Opening 10 minutes: Dorothy, Randall, Kate<br>1:40 ProSPect (4.09 MB) 20 minutes – **Steve Price**<br>2:00 CANGA (2.88 MB) 20 minutes – **Phil Jones**<br>2:15 NH-dycore (1.48 MB) 15 min – **Peter Bosler**<br>2:30 Break<br>2:45 UQ-sensor (3.74 MB) 15 min – **Daniel Ricciuto**<br>3:00 Sea-ice (444 KB) 15 min – **Adrian Turner**<br>3:15 Atmos physics convergence (1.33 MB) 15 min – **Hui Wan**<br>3:30 Vertical grids (1.29 MB) 10 min – **Tak Yamguchi**<br>4:40 3D-Flow (1.87 MB) 10 min – **Gautam Bisht**<br>4:50 Discussion<br>5:00 Adjourn | **Dorothy Koch** | Regency |
| | ***1:30 – 5:00 – Fusion Energy Sciences (FES) β*** | **John Mandrekas** | Eisenhower |

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| | 1:30 – 2:00: **David Hatch**, University of Texas, "Partnership for Multiscale Gyrokinetic (MGK) Turbulence" (3.29 MB)<br>2:00 – 2:30: **Steve Jardin**, PPPL, "Center for Tokamak Transients Simulations (CTTS)" ( MB)<br>2:30 – 3:00: **Zhihong Lin**, University of California, Irvine, Integrated Simulation of Energetic Particles in Burning Plasmas (ISEP)" (3.16 MB)<br>3:00 – 3:15: Break<br>3:15 – 3:45: **Brian Wirth**, University of Tennessee, Knoxville / ORNL, "Plasma Surface Interactions: Predicting the Performance and Impact of Dynamic PFC Surfaces" (4.66 MB)<br>3:45 – 4:15: **Mark Shephard**, RPI, "Unstructured Mesh Technologies for Fusion Simulation Codes" (3.04 MB)<br>4:15 – 5:00: All, Discussion / Whole-Device Modeling (WDM) integration" | | |
| 5:00pm - 5:30pm | Wrap up and Farewell | **Ceren Susut, Randall Laviolette**<br>US Department of Energy | Plaza Ballroom |
| 5:30pm | Adjourn | | |