



Agenda for the MAGICS Workshop, March 2-4, 2018 at the Radisson Hotel at USC

Friday, March 2, 2018

Time	Event
12:00 pm	Registration
1:30 pm – 2:00 pm	HPC Account Setup
2:00 pm – 2:15 pm	Introduction to MAGICS workshop Priya Vashishta, USC
2:15 pm – 3:00 pm	Lecture: Introduction to classical molecular dynamics and thermal conductivity computation Instructor: Priya Vashishta, USC
3:15 pm – 4:15 pm	Hands-on: Thermal conductivity plugin download and set up. Instructors: Aravind Krishnamoorthy, Pankaj Rajak, Ankit Mishra, Nitish Baradwaj, Nick Grabar USC
4.15 pm - 4.30 pm	Break
4:30 pm – 6:00 pm	Hands-on: Thermal conductivity computation and visualization Instructors: Aravind Krishnamoorthy, Pankaj Rajak, Nitish Baradwaj, Ankit Mishra, Nick Grabar USC
6:00 pm – 7.00 pm	Reception



Saturday, March 3, 2018

Time	Event
7:30 am– 8:15 am	Breakfast
8:30 am– 8:45 am	Overview of the Day Priya Vashishta, USC
8:45 am– 9:45 am	Lecture: Reactive Force Field (ReaxFF) Instructors: Sungwook Hong and Ken-ichi Nomura, USC
9:45 am– 10:45 am	Hands-on: RXMD Software Introduction Instructors: Ken-ichi Nomura, Sungwook Hong, Pankaj Rajak, Chunyang Sheng, Subodh Tiwari, USC
10:45 am–11:00 am	Break
11:00 am– 12:30 pm	Hands-on: RXMD Software Hands on I Instructors: Ken-ichi Nomura, Sungwook Hong, Pankaj Rajak, Chunyang Sheng, Subodh Tiwari USC
12:30 pm– 1:30 pm	Lunch

2:00 pm– 3:00 pm	Lecture: Reactive Forcefield (ReaxFF) and More Instructors: William Goddard III and Saber Naserifar, California Institute of Technology
3:00 pm– 4:00 pm	Hands-on: RXMD Software Hands on II Instructors: Ken-ichi Nomura, Sungwook Hong, Pankaj Rajak, Chunyang Sheng, USC
4:00 pm– 4:30 pm	Break
4:30 pm– 6:00 pm	Hands-on: RXMD Software Hands on II Instructors: Ken-ichi Nomura, Sungwook Hong, Pankaj Rajak, Chunyang Sheng, USC
6:30PM-8PM	Dinner/Banquet

Sunday, March 4, 2018

Time	Event
7:30 am– 8:15 am	Breakfast
8:15 am– 8:30 am	Overview of the day
8:30 am– 9:30 am	Lecture: Quantum Molecular Dynamics Instructor: Aiichiro Nakano, USC
9:30 am– 10:30 am	Hands-on: Introduction to QXMD Software Instructors: Subodh Tiwari, Aravind Krishnamoorthy, Lindsay Bassman, Ken-ichi Nomura, USC
10:30 am– 10:45 am	Break
10:45 am– 11:30 am	Hands-on: QXMD Software Hands on I Instructors: Subodh Tiwari, Aravind Krishnamoorthy, Lindsay Bassman, Ken-ichi Nomura, Hiroyuki Kumazoe USC
11:30 am– 12:30 pm	Hands-on: QXMD Software Hands on I - Continued Instructor: Subodh Tiwari, Aravind Krishnamoorthy, Lindsay Bassman, Ken-ichi Nomura, Hiroyuki Kumazoe USC
12:30 pm– 1:30 pm	Lunch

2:00 pm– 2:45 pm	Lecture: Exfoliation Simulation using ReaxFF Instructors: Rajiv K. Kalia USC
2:45 pm– 4:00 pm	Hands-on: Exfoliation Simulation using ReaxFF Instructors: Rajiv K. Kalia USC
4:00 pm– 4:30 pm	Break
4:30 pm– 6.00 pm	Demo: GEARS Using virtual reality in visualizing simulations
4.30 pm– 6.00 pm	Discussion on Research Collaboration with USC and Workshop Report
6.00 pm	Dinner and Closing Remark