

SEAVEA Uncertainty Quantification Applications Meeting Agenda

Date: 12th December 2022, 10:00 - 17:00 (GMT), 11:00 - 18:00 (CET)

Locations:

1. Ground Floor, G5 Nyholm Room, Chemistry Department, UCL, 20 Gordon Street, London, WC1H 0AJ
2. Zoom online access: <https://ucl.zoom.us/j/97832318369>

09:30	Arrival and registration	
10:00	Opening and welcome	Peter Coveney (UCL)
10:05	Updates to the SEAVEA toolkit	Derek Groen (BUL)
Part 1:	Theory, algorithms and methods	
10:20	Application to the Met Office climate modelling	Daniel Giles (UCL)
10:40	The deep-active subspace method for high-dimensional uncertainty quantification	Wouter Edeling (CWI)
11:00	<i>Refreshment break</i>	
Part 2:	Applications I	
11:15	Uncertainty Quantification of the Glass Transition Temperature Predicted using Molecular Dynamics	Werner Roa Muller (UCL)
11:35	Aleatoric and Parametric Uncertainty in Molecular Dynamics Simulation	Shunzhou Wan (UCL)
11:55	<i>Lunch break (75 mins)</i>	
13:10	Early progress towards a particle-in-cell code based on SYCL and Nektar++ for ExCALIBUR-Neptune	James Cook (UKAEA)
13:30	Sensitivity Analysis of Flu And Coronavirus Simulator (FACS) Model	Arindam Saha (BUL)
13:50	Using Deep Active Subspace methods to calculate uncertainties related to atomic physics in SOLPS-ITER simulations of edge plasmas	David Coster (MPG)
14:10	<i>Refreshment break</i>	
Part 3:	Applications II	
14:25	Molecular and multiscale modelling of polymer nanocomposite mechanical properties	Maxime Vassaux (UCL)
14:45	Plasma turbulence in the edge of tokamak fusion reactors	John Omotani (UKAEA)

15:05	Reliability of and confidence in quantum simulations	Animesh Datta (Warwick)
15:25	Uncertainty Quantification in Quantum Error Mitigation	Tim Weaving (UCL)
15:45	A Multi-Objective Approach for Camp Location Selection in Forced Migration Scenarios	Yani Xue (BUL)
16:05	Space weather research programme for the Met Office	David Jackson, David (Met Office)
16:25	Towards VVUQ of a human cardiac population for in-silico trials to assess cardiac safety of drugs	Jazmín Aguado Sierra (BSC)
16:45	Panel session: wrap up and final remarks	Peter Coveney, Serge Guillas, Derek Groen
17:00	<i>End of meeting</i>	
18:00	<i>Dinner at: Spaghetti House, 15 Goodge St, London W1T 2PQ (Tottenham Court Road branch).</i>	