

Forcefields: Status, challenges & vision

Daresbury Laboratory, 28-29 of January 2019



Organizers: Albert Bartok-Partay, Alin Elena, Tom Keal, Barbara Montanari, Leon Petit, and Gilberto Teobaldi

Fifty speakers and delegates took part in the event. The aim of this workshop was to bring together experts in classical and ab-initio simulations and experimentalists, to get an overview of the different methodologies used for potential generation and usage and to take stock of the current state of the art. Future development strategies in the field were discussed, and collaborative ways of moving forward in partnership with our sponsoring communities CCP5, CCP9, UKCP, MCC, CCPBioSim and CECAM-UK Daresbury

The 16 talks varied covering from traditional potentials, to modern machine-learning driven ones to very specific problem driven ones. Gabor Csanyi, Richard Graham, Paul Popelier and James Kermode presented the new generation of potentials that use machine learning and gaussian processes to capture chemistry and physics of interest. Colin Freeman, Scott Woodley, Michael Rushton and John Harding explained how traditional form potentials are still of interest in modelling from ceramics to nuclear materials. Pooja Goddard, Dorothy Duffy, Jonathan Essex and Karen Johnston showed how there is a continuous need to develop new model potentials to study new phenomena. Peter Coveney and Peter Brommer demonstrated the importance of being able to validate and quantify the uncertainty of forcefields in order to be able to trust the results obtained. Caitlin Bannan spoke about the US emergent efforts in the field of centralizing biomolecular forcefield via OpenFF initiative in US.

During the lively panel discussions a number of points/requirements were noted:

- the necessity of critical review of the subject, although it was recognised that concentrating on a subset of applications is more viable rather than all the field.
- the need of a curated database of high quality papers describing forcefields can be beneficial to community
- a database of parameters in formats ready available for different codes is required , see as example Scott Woodley's db
- a collection of Machine learned potentials easy available to community
- CoSeC will follow up with the participants for a full list of wishes
- workflows that can automate the creation of parameters with easy access for community
- having well defined reference data sets for fitting/learning, that can be used for validation or regeneration of new potentials.
- finding suitable funding avenues for such initiatives
- is a study equivalent to "Comparing Solid State DFT Codes, Basis Sets and Potentials" feasible for forcefields simulation software?
- organising an international workshop on the subject possibly via CECAM, in order to try to interact and collaborate with international efforts in the field.

Programme

Monday 28th of January 2019

09:30 - 10:00: Registration and coffee

10:00 - 10:30: **Paul Popelier** (University of Manchester) **FFLUX: Pushing the boundaries of atomistic potentials**

10:30 - 11:00: **Michael Rushton** (Bangor University) **The development of actinide potential models**

11:00 - 11:30: **Peter Coveney** (UCL) **Verification, validation and uncertainty quantification: the role of force fields**

11:30 - 12:00: **Gábor Csányi** (University of Cambridge) **Machine learning approaches lead to a new dawn for interatomic potentials**

12:00 - 13:00: lunch

13:00 - 13:30: **Tristan Youngs** (ISIS) **Neutron Diffraction as a Resource for Generating Interatomic Potentials?**

13:30 - 14:00: **Colin Freeman** (University of Sheffield) **Forcefields for the interface between Organic and Inorganic Worlds**

14:00 - 14:30: **Mark Wilson** (Durham University) **Development of coarse-grained force fields: insights from top-down and bottom-up approaches**

14:30 - 15:00: **Karen Johnston** (University of Strathclyde) **Evaluation and Optimisation of Interface Force Fields for Water on Gold Surfaces**

15:00 - 15:30: Coffee Break

15:30 - 16:00: **Pooja Goddard** (Loughborough University) **Development of Anionic and Poly Oxyanionic forcefields for energy materials applications**

16:00 - 16:30: **Peter Brommer** (University of Warwick) **Uncertainty quantification for force-matched effective potentials**

16:30 - 17:00: **Caitlin Bannan** (UC Irvine) **SMIRNOFF and The Open Force Field Initiative's Progress and Plans for Parameterization**

17:00 – 18:00: **Discussion**

18:30 - 21:30: Conference Dinner

Tuesday 29th of January 2019

09:00 - 09:30: **Richard Graham** (University of Nottingham) **Interpolation of intermolecular potentials using a Machine Learning Algorithm**

09:30 - 10:00: **Dorothy Duff** (UCL) **Including electronic effects in classical simulations using electronic temperature dependent potentials**

10:00 - 10:30: Coffee break

10:30 - 11:00: **John Harding** (University of Sheffield) **Forcefields in ceramics: where are we and where do we go from here?**

11:00 - 11:30: **James Kermode** (University of Warwick) **Targeting quantum mechanical accuracy for thermally activated processes in chemomechanical systems**

11:30 - 12:00: **Scott Woodley** (University College London) **Interatomic Potentials**

12:00 - 13:00: lunch

13:00 - 13:30: **Daniel Cole** (University of Newcastle) **Quantum Mechanical Bespoke Potentials for Computer-Aided Drug Design**

13:30 - 14:00: **Jonathan Essex** (University of Southampton) **How well does the AMOEBA force field reproduce protein electrostatics?**

14:00 - 15:00: **panel discussion** (includes coffee)