WORKSHOP PROGRAM 2018

SCOPING

Dissipative particle dynamics: Where do we stand

on predictive application?

24 - 26 April, Daresbury Laboratory, UK R. Anderson (STFC), M. Noro (STFC), M. Seaton (STFC), P. Warren (Unilever), W. Swope (IBM)

Solubility prediction

14 - 15 May, ENS Lyon, France

E. Sanz (UCM), C. Michel (ENS Lyon), D. Frenkel (U. Cambridge), P. Meenan (Pfizer), R. Docherty (Pfizer)

Building the bridge between theories and software:

SME as a boost for technology transfer in

industrial simulative pipelines

23 - 25 May, IIT Genova, IT S. Decherchi (IIT), A. Cavalli (IIT), S. Bonella (EPFL)

STATE OF THE ART

Improving the accuracy of ab-initio predictions for

materials

17 - 20 September, MdIS Saclay, France

C. Pierleoni (U. L'Aquila), D. Aflé (UCL), D. Ceperley (UIUC)

Centre Européen de Calcul Atomique et Moléculaire

Large scale activated event simulations

1 - 3 October, U. Vienna, Austria

C. Dellago (U.Vienna), P. Bolhuis (UvA), G. Kahl (TU Vienna)

EXTENDED SOFTWARE DEVELOPMENT *

Atomistic, Meso- and Multiscale Methods on HPC

Systems

14 - 18 May 2018, JSC, Germany

G. Sutmann(JSC), I. Pagonabarraga(EPFL), B. Duenweg (MPIP)

Quantum dynamics



F. Agostini (U. Paris-sud), B. Curchod (Durham U.), A.P. Seitsonen (ENS Paris)

Intelligent high throughput computing for scientific

applications

16 - 20 July, Polytechnic University of Turin, ItalyD. Swenson (UvA), A. O'Cais (JSC)

Scaling Electronic Structure Applications

7 - 18 January 2019, UCD, Ireland
N. Papior (DTU), Y. Pouillon (UNICAN), M. Oliveira (MPSD), V.
Blum (Duke U), F. Corsetti (QuantumWise), E. Artacho (U.Cambridge)

Full event listing at: www.e-cam2020.eu/events

* These are multi-part events and we indicate the date for the first meeting. Dates of follow ups are decided during the first event.



European Centre of Excellence

Supporting HPC simulations in industry and academia, through software development, training and discussios in simulation and modelling

CONTACT

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WORKSHOPS

STATE OF THE ART WORKSHOPS

workshops will These survey algorithmic new methods and developments in simulation and establish the codes and software modules that should be included in the E-CAM library. They will establish the current state-of-the-art and highlight developments the immediate required.

Workshops take place every two years in each of our four scientific areas.

These workshops are open to academics and industrial partners.

S C O P I N G W O R K S H O P S

Industrial partners and academics will work together to sharpen and focus the work plan for the project.

Academic beneficiaries will outline the major advances to be expected in each area with an emphasis on application.

Industrial partners will outline, in general terms, the areas that they wish to see developed and the kind of consultancy that they require.

These workshops are open to academics and industrial partners.

EXTENDED SOFTWARE DEVELOPMENT WORKSHOPS

These workshops will train scientists in the development of modular codes for high performance machines.

Documentation and testing are key components of the workshops and the associated on-line manuals and test cases will be made available through a web platform as part of the E-CAM software library.

ESDWs are open to postdocs, senior graduate students and early career researchers in industry and academia.

E-CAM2020.EU