

Proposal for a workshop on the simulation of water

Basic organisation.

Workshop title: *Water, water everywhere; nor any drop to drink.*
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Scientific Content.

There remain basic problems in the simulation of the pure phases of water (liquid and the many ice phases) by *ab initio* and potential-based methods. However, water appears as a constituent in a tremendous range of scientific problems. Biological problems almost by definition involve the aqueous phase. Geological processes such as weathering require the consideration of the solution chemistry, the aqueous/mineral interface and chemical reactions involving water. All oxides when exposed to air react (usually immediately) with water (and often with carbon dioxide also) to produce a complex surface phase.

While *ab initio* methods are suitable for the bulk phases and the simpler interface problems, the multiple length and timescales in interface (and particular bulk interface) systems means that descriptions of water at different levels of sophistication are essential. First there is the move the classical potentials, then to schemes where the water is considered as a dielectric continuum, finally to implicit schemes where the effect of the solvent is (hopefully) included within the particle-particle interactions. Ideally, there should be a hierarchy whereby the coarser-grained schemes are parametrised in terms of the more fundamental descriptions. In constructing models of water itself, much progress has been made. However, when we wish to consider water interacting with surfaces matters are much less far advanced. An absolutely basic problem is to find a reasonable description of water in acidic or alkaline conditions that can be used for classical dynamical simulations. Few systems of interest have a pH that is rigidly equal to seven and most of them are too large or complex for *ab initio* simulations to be a realistic possibility

The workshop will bring together experimentalists and theorists working on water (and problems that involve water) to discuss what the real problems are and what needs to be done to solve them. Since we want a discussion of the *current* problems, not a presentation of past results, the format proposed is rather different from many workshops. The programme is divided into eight sessions, each guided by a chairman. Participants will be invited to bring a few powerpoint slides to illustrate a current problem(s) and asked to spend a few minutes outlining the issue. This will be in the context of a round-table discussion of the session topic. An outline of the workshop programme is given below. These discussions will bring together experimentalist and theorists and (we hope) lead to new inter-disciplinary collaborations.

Speakers and participants

It is not intended to have a workshop planned as a conventional conference. Therefore there are no “speakers” as such. Instead, we intend to have sessions on various topics chaired by

people who will give a short introduction and then guide the resulting discussion. All participants will be invited to bring material (a few powerpoint slides) on current interests and problems to add to the discussion. A list of suggested participants is appended, together with a draft schedule

Tutorial element / new researchers

Since the intention of the workshop is to survey the simulation of water in a wide range of contexts from new *ab initio* methods to biosimulations, it is not likely that anyone will be expert over the whole field. We also intend to invite researchers at various stages in their careers. We therefore intend to begin with a general session whose purpose is both to introduce people to different areas of the field (and also to each other!) and to enable people to ask the “simple” questions about the area that often need asking. The person chairing this session will be asked to make the initial presentation a general introduction to the field and include tutorial material.

Sponsorship for the workshop.

The seed-corn funding for the workshop comes from an EPSRC (UK Science Research Council) Grant GR/S80103/01 “Structural Modelling of the Biological Interface with Materials” headed by one of the organisers (John Harding). This is part of an EPSRC initiative designed to focus and develop the UK molecular modelling capacity. However, this development must involve strong interactions with other European colleagues to exchange and develop ideas and, if possible, set up new collaborations. We therefore wish to hold a meeting with a strong presence from other European countries and are therefore approaching both CECAM and Psi-k to enable this. We set out the possible participant list below.

Budget for the workshop

Cost for board and lodging of 40 participants in Sheffield 4-6 th Jan 2006	9500
Travel expenses for 40 participants at an average of €150 each (UK Participants) and €300 each (other European participants)	9000
TOTAL	18500

We have already funds available from an EPSRC grant to fund a meeting at Sheffield (£5000 ≈ €7000)

We therefore wish to apply for €11500 to cover the balance of funding the workshop. Since we are applying both to CECAM and to Psi-k, we request €5750 from each of these bodies, with the proviso that, if one of them declines to fund the request, we wish to apply for the full €11500 from the other.

Location and date of workshop.

Sheffield, UK on 4-6th January 2006

U.S. participants.

We would like to bring Mike Klein (Penn State) and Ulrike Diebold (Tulane). We will discuss this with Mike Klein (who is visiting at the end of September).

DRAFT PROGRAMME

4th January

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12:00 - 13:30	Lunch
13:30 - 15:00	SESSION 1: The state of the question: what do we want to do with water simulations?
15:00 - 15:30	Tea
15:30 - 17:45	SESSION 2 Developments in <i>Ab initio</i> calculations
18:00	Dinner

5th January

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07:30 - 08:45	Breakfast
9:00 - 10.30	SESSION 3: The state of water potentials: classical simulations
10.30 - 11.00	Tea
11.00 - 12.00	SESSION 4 Solutions: ions, molecules and pH.
12:00 -13:30	Lunch
13:30 - 15:00	SESSION 5 Aqueous mineral interfaces
15:00 - 15:30	Tea
15:30 - 17:45	SESSION 6 Biological systems and water
18:00	Dinner

6th January

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07:30 - 08:45	Breakfast
9:00 - 10.30	SESSION 7 Ice structures
10.30 - 11.00	Tea
11.00 - 12.00	SESSION 8 Common challenges and new perspectives
12:00 -13:30	Lunch

LIST OF SUGGESTED PARTICIPANTS

Please note that this list of proposed participants is not final; we intend to invite approximately equal numbers of UK and non-UK participants

ORGANISERS

John	Harding*	Sheffield
Philip	Lindan*	Kent

UK Participants

Maria	Alfredsson*	Univ. Coll. London
Jamshed	Anwar*	Bradford
Emilio	Artacho*	Cambridge
David	Cooke*	Cambridge
Nora	DeLeeuw*	Birkbeck
John	Finney*	Univ. Coll. London
Mike	Gillan*	Univ. Coll. London
Dewi	Lewis*	Univ. Coll. London
Massimo	Mella*	Cardiff
Carla	Molteni*	Kings Coll. London
Steve	Parker*	Bath
Matt	Probert*	York
Mark	Roger*	Warwick
Dave	Sherman*	Bristol
Ben	Slater*	Royal Institution
Neal	Skipper*	Univ. Coll. London
Pat	Unwin*	Warwick
Tiffany	Walsh*	Warwick
Mark	Wilson*	Durham

Other European participants

Alain	Allouche*	Marseille
Marie-Claire	Bellissent-Funel	Saclay
Marcel	Besnard	Bordeaux
Sandro	de Vita*	Trieste
Alex	De Vries	Groningen
Maria	Grillo	Accelrys, Munich
Victor	Kempter*	TU Clausthal
Siewert	Marrink	Groningen
Angelos	Michaelides	Berlin
Raffaele	Resta	Trieste
Ursula	Roethlisberger	Lausanne
Matthias	Scheffler	Berlin
Berend	Smit	Lyon