

Ab Initio Modelling in Applied Bio-Sciences: Structure, Dynamics & Function

SCIENTIFIC REPORT-1973

Summary:

A joint Psi-k/SimBioMa Workshop (co sponsored by Uppsala University, CNR-INFN-Democritos-National Simulation Center)

Location: Department of Physics, Ångström Laboratory, Uppsala University, Sweden

Dates: 11-12 December 2008

Organisers:

P. M. Panchmatia, Department of Physics and Materials Science, Uppsala University, Sweden/
Department of Chemistry, University of Bath, UK

B. Sanyal, Department of Physics and Materials Science, Uppsala University, Sweden

P. M. Oppeneer, Department of Physics and Materials Science, Uppsala University, Sweden

O. Eriksson, Department of Physics and Materials Science, Uppsala University, Sweden

A. Magistrato, INFN-DEMOCRITOS and SISSA Trieste, Italy

P. Carloni, SISSA and INFN-DEMOCRITOS, Trieste, Italy

Understanding biological phenomena often requires a precise understanding of interactions at atomic scale where quantum mechanics plays an important role. This is particularly important for applied biosciences (bionanotechnology, pharmacology) where QM approaches are being used with increasing success. In particular, the integration of different electronic-structure methods allows us to directly compare calculations with experiments and sometimes to explain them. The workshop allowed experts in the field of applied biological sciences to interact, exchange and compare the various methodologies and show the potentialities and the limitation of state-of-the art quantum-mechanics-based computational techniques. Emphasis was given to topics and approaches for which direct contact with experiments can be made. Here we sought a sum of 5,500 Euros to support young participants, for travel and accommodation. This encouraged participation from younger scientists, who presented a poster on receiving a bursary. It is of utmost importance to boost younger scientist participation in meetings of such inter-disciplinary nature. We also felt that supporting students who did not have money was inspiring both to them as upcoming scientists as well as to the workshop as a whole. Their contributions were valuable to the understanding and advancement of multi-disciplinary fields.

Scientific Content and Discussion:

The conference was divided into 4 sessions:

- Magnetic Properties of Biomaterials
- Methods Development & Hybrid Methods for Very Large Systems
- Drug Design and Bio-Material Design
- Biological Reactivity

The program attached below details the speakers under each session. Of the main list of speakers, Prof. Leif Eriksson cancelled at the last moment due to sickness. However his students and post-docs attended the meeting and presented posters.

Unfortunately, the main organiser, Dr. Pooja Panchmatia was also not present at the last moment, due to her father suddenly falling ill in India. She had to fly to India on the 8th December 2008, for her fathers' open heart surgery on the 11th December 2008, which was later postponed to 15th December 2008. She did answer all queries by e-mail and phone. The feedback section proves that despite this mishap, the participants were well looked after by the hosts (Prof. Olle Eriksson and Dr. Biplab Sanyal) at Uppsala University and the organisation was more than satisfactory.

PROGRAM DETAILS

Arrival of participants Wednesday 10th December, Accommodation: Hotel Uppsala & Vandrarhem

Thursday 11th December: Polhelmsalen, Angstrom Laboratoriet

Time	Duration	Speaker	Chair
8:00 – 8:45	Registration		
8:55	Opening		
Session: Methods Development & Hybrid Methods			
9:00	Lect 1	Nicola Marzari	Lars Nordstrom

9:30	Lect 2	Juerg Hutter	
10:00	Lect 3	Daniel Sebastiani	
10:30	Coffee		
11:00	Lect 4	Claudia Filippi	David Van der Spoel
11:30	Lect 5	Bernd Einsing	
12:00	Lect 6	Leonardo Guidoni	
12:30	Lunch		
13:30	Lect 7	Matteo Del Parero	Karin Larsson
14:00	Lect 8	David Van der Spoel	
14:30	Lect 9	Anders Niklasson	
15:00	Lect 10	Daniele Varsano	
15:30	coffee		
Session: Magnetic Properties of Bio-Materials			
16:00	Lect 10	Heiko Wende	Peter Oppeneer
16:30	Lect 11	Thomas Jung	
17:00	Lect 12	Stefano Sanvito	
17:30	Lect 13	Kevin Leung	
18:00-19:30	Poster Session		
19:45	Conference Dinner	Eklundshof	

Friday 12th December: Polhelmsalen, Angstrom Laboratoriet

Time	Duration	Speaker	Chair
Session: Biological Reactivity			
9:00	Lect 1	Ivano Tavernelli	Biplab Sanyal
9:30	Lect 2	Carme Rovira	
10:00	Lect 3	Ulf Ryde	
10:30	Coffee		
11:00	Lect 4	Margareta Blomberg	Paolo Carloni
11:30	Lect 5	Md. Ehesan Ali	
11:50	Lunch		
Session: Drug Design and Bio-Materials Design			
13:00	Lect 6	Johan Aqvist	Alessandra Magistrato
13:30	Lect 7	Paolo Carloni	
14:00	Lect 8	Simone Raugei	
14:30	Coffee		
15:00	Lect 9	Leif Eriksson (Cancelled)	Johan Aqvist
15:30	Lect 10	Stefano Fabris	
16:00	Lect 11	Alessandra Magistrato	
16:20	Closing	Paolo Carloni	

.The scientific content of the workshop was very appropriate to the interest and expertise of the audience. This was a perfect meeting point between the biological physics and materials science. The similarities in methodologies between the two communities (materials scientists and bio scientists) was apparent (e.g. ab-initio molecular dynamics and quantum Monte Carlo simulations) , but it was also clear that the scientific questions raised in a specific field has pushed the technology in a specific direction. Hence it became clear that there are also possibilities from one community to learn from the developments of the other community. As an example it could be mentioned that DFT based theories applied to bio-relevant questions rely to a much larger extent on Gaussian functions compare to simulations in the materials community. Overall, the lectures on the development of new methodologies were very instructive and opened an excellent way of future collaboration. The lectures containing the applications to several topics on biological problems clearly showed the power of today's supercomputing facilities to tackle such complex issues. Discussions were very nice during the sessions as well in the coffee and lunch breaks. The poster session was

very interactive, with most young scientists presenting excellent research results.

Assessment of Results:

The strong interaction between the participants of the workshop and the lively discussions are a clear signal of the fruitfulness of the meeting. The healthy participation of scientists at all lectures is also an excellent sign of well prepared and well received lectures at the workshop.

We expect a big impact of this event in near future. The two communities learned from each others scientific questions as well as the technical means with which they try to give answers to these questions. We anticipate new collaborations germinated from the workshop. Also, follow up meetings on these topics were discussed and will most likely be implemented.

Feedback:

From: Biplab Sanyal <biplab.sanyal@fysik.uu.se> (Uppsala University)
To: Pooja Panchmatia <pooja.panchmatia@fysik.uu.se>
Date: 11/12/2008 17:06
Subject: workshop
Hej Pooja,

The workshop is running quite smoothly. People were discussing about you.
Thanks for making it so good.

Biplab

From: sebastia@mpip-mainz.mpg.de
To: "Pooja Panchmatia" <pooja.panchmatia@fysik.uu.se>
Date: 12/12/2008 08:25
Attachments: uppsala08-Sebastiani.pdf
Subject: pdf file of talk
Dear Pooja,

thanks again for your excellent work organizing the workshop in Uppsala!
The organizers suggested to collect the PDF files of all the talks, and named you as the person to whom we should send the files - so here you go.

Best regards,

Daniel

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From: Olle Eriksson <olle.eriksson@fysik.uu.se>
To: Pooja Panchmatia <pooja.panchmatia@fysik.uu.se>
Date: 12/12/2008 09:14
Subject: Re: Thank you

Pooja Panchmatia skrev:

> Thank you for still making it happen.

>

> My dad has had a set back yesterday and so his operation has been postponed to Monday due to complications. Its very stresful at the moment. Please keep him in your thoughts.

>

> Glad its all worked out there.

>

> -Pooja

>

Dear Pooja,

I will keep both him and you in my thoughts. Hope it all works out. The conference is a great success! People ask for you, too bad you couldn't make it.

Best Olle

From: "Heiko Wende" <heiko.wende@uni-due.de>
To: "Pooja" <pooja.panchmatia@fysik.uu.se>
Date: 12/12/2008 20:05
Subject: great success!

Dear Pooja,

now the workshop is over, and I think that it was really a great success. I enjoyed the talks and discussions very much. It is really unfortunate that you could not join. Really everyone at this conference knew that you did all the work. You organized everything perfectly! I hope that we can meet in the

near future. I wanted to invite you to present a talk at our department in Duisburg. Are you in Germany by chance in the near future?

All the best,

Heiko

=====
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=====

From: "Paolo Carloni" <carloni@sissa.it>
To: "Pooja" <pooja.panchmatia@fysik.uu.se>
Date: 14/12/2008 16:32
Subject: RE: FINAL reminder- dietary requirements

Dear Pooja,

I am writing you now from the airport of Stockholm. I just wanted to thank you for all the work you did at the conference. I also wanted to tell you that everything went smoothly, thanks indeed to such excellent organization.

I wish you all the best in this difficult moment.

Kind regards, Paolo

From: "Leung, Kevin" <kleung@sandia.gov>
To: Pooja <pooja.panchmatia@fysik.uu.se>
Date: 15/12/2008 07:13
Subject: RE: computers available

Dear Pooja,

Thanks very much again for your assistance. Sorry not to be able to meet you at the workshop -- hope all is well!
I look forward to another opportunity to chat with you.

Sincerely,
Kevin

From: "I-Chun" <ichun0@gmail.com>
To: Pooja <pooja.panchmatia@fysik.uu.se>
Date: 15/12/2008 07:57
Subject: reimbursement

Dear Pooja,

Could you please clarify if the travel reimbursement includes only the flight or also the train ride to the airport? Thank you very much for your help! I really enjoyed the workshop.

Regards,

I-Chun

From: "Leonardo Guidoni" <l.guidoni@gmail.com>
To: "Pooja Panchmatia" <pooja.panchmatia@fysik.uu.se>
Date: 15/12/2008 22:01
Subject: thanks!

Dear Pooja,

I really enjoyed the conference in Uppsala !!!!!

I found the meeting very interesting and very well organised. I imagine you had hard work to do that and it was a pity that you could not come. As you probably know, I (together with Angel Rubio) just become the spokenperson of the biology Psi-k working group. Paolo Carloni left after 10 years. I would first like to update the web pages and it would be nice if you can send me the complete list of the participants with e-mails.

Thanks a lot for your help

All the best

leo

--
Leonardo Guidoni
Universita' degli studi dell'Aquila
Dipartimento di Chimica, Ingegneria Chimica e Materiali
<http://bio.phys.uniroma1.it>

From: Maria Fyta <mfyta@deas.harvard.edu>
To: Pooja <pooja.panchmatia@fysik.uu.se>
Date: 16/12/2008 08:37
Attachments: mfyta_airtick.pdf
Subject: workshop reimbursement

Hi Pooja,

it's a pity we didn't get to meet at the workshop, but I hope you are all well. It was a well organized and interesting workshop and you did a great job organizing it. I also heard about your work and would like to talk to you about it ... maybe some other time.

Regarding the reimbursements (I guess you must be getting too many e-mails about this, sorry for also bugging you with this...). I guess what you need from me is the airplane ticket, which I attach (it's for two people, but the amount is clearly shown in USD next to my name). Let me know, if there is anything else I need to do.

many thanks,
maria

From: "Shanthi Pandian" <Shanthi.Pandian@postgrad.manchester.ac.uk>
To: pooja.panchmatia@fysik.uu.se, biplab.sanyal@fysik.uu.se, Olle.Eriksson@fysik.uu.se
Date: 19/12/2008 10:33
Subject: Thanks

Dear Organizers,

I would like to thank you for giving me a chance to attend the Conference at the Uppsala University last week. It was very useful and interesting to know about scientific members and their field of research.

I would like to take this opportunity to wish you all Merry Christmas and Prosperous New Year.

Thanks and Regards
Shanthi.

Full List of Speakers and Participants:

All participants received tickets for lunch. Tea and coffee were served during breaks. The conference dinner for all participants was also financed from funding received from other sources. Accommodation for 2 nights (10th and 11th Dec) and travel bursary (250 Euros per student) was awarded to 12 participants (All those who have a (B) next to their name on the list), from the funding of ESF.

Name	Email	Country	Institute	Talk/Poster
Olle Eriksson	Olle.Eriksson@fysik.uu.se ,	Sweden	Uppsala University	Organiser
Biplab Sanyal	Biplab.Sanyal@fysik.uu.se ,	Sweden	Uppsala University	Organiser/chair
Pooja Panchmatia	Pooja.Panchmatia@fysik.uu.se ,	Sweden/UK	Uppsala University/Univ. of Bath	-
Peter Oppeneer	Peter.Oppeneer@fysik.uu.se ,	Sweden	Uppsala University	Organiser/chair
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Alessandra Magistrato	alema@sissa.it	Italy	SISSA	talk/chair
Md. Ehesan Ali	ehesan.ali@fysik.uu.se	Sweden	Uppsala University	talk
Stefano Sanvito+Wife+son	sanvitos@tcd.ie	Ireland	Trinity college	talk
Kevin Leung	kleung@sandia.gov	US	Sandia National Lab	talk
Nicola Marzari	marzari@MIT.EDU	US	MIT	talk
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Daniel Sebastiani	sebastia@mpip-mainz.mpg.de	Germany	MPI, Mainz	talk
Heiko Wende	heiko.wende@uni-due.de	Germany	Duisburg University	talk
Thomas A. Jung	thomas.jung@psi.ch	Switzerland	Paul Scherrer Institute	talk
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Carne Rovira	crovira@pcb.ub.es	Spain	University of Barcelona	talk
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Stefano Fabris	fabris@democritos.it	Italy	DNSC	talk
Anders Niklasson	amn@lanl.gov	US	Los Alamos National Lab	talk
Margareta Blomberg	mb@physto.se	Sweden	KTH	talk
Ulf Ryde	Ulf.Ryde@teokem.lu.se	Sweden	Lund University	talk
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