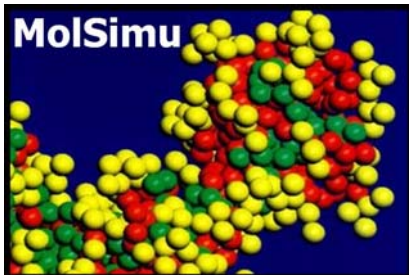

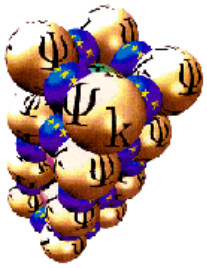

MARIE CURIE ACTIONS

Tutorial "Quantum Simulation of Liquids and Solids"

October 30, 2006 to November 10, 2006

(Provisional Report)

(14 January 2009)

Introduction

The tutorial “Quantum Simulaiton of Liquids and Solids” took place from October 30, 2006 to November 10, 2006 at CECAM, located on Ecole Normale Supérieure de Lyon Campus, 46, Allée d’Italie, 69007 Lyon, France

This course is aimed at giving an introduction in the simulation of electronic structure in condensed phase materia, solids and liquids. A first series of lectures will be devoted to the basics of Density Functional Theory and to the solution of the electronic structure problem in solids using plane wave basis sets and Green's function technique. This part of the tutorial was based on the book by R. M. Martin "Electronic Structure. Basic Theory and Practical Methods" (Cambridge University Press, Cambridge, 2004). A second series of lecture will then focus on the simulation of liquid systems using ab initio Molecular Dynamics. These will also include an introduction to advanced techniques including simulation of reactive processes in liquids and coupling of quantum and classical simulations (so-called QM/MM). The morning sessions are lectures introducing the methods and in the afternoons there are computer exercises in which these methods will be applied. During these practical classes the students will run a few simulations using existing packages, like CPMD, CP2K, KKR-ASA and VASP, to apply the techniques discussed in the morning lectures and be acquainted with these packages. They will also write a simple program to solve a one dimensional Schrodinger equation with a periodic potential using a plane wave basis set. In addition, a miniworkshop will be organized, where participants can present results of their research. The course does not assume any previous knowledge in molecular simulations. However, elementary knowledge in quantum and statistical physics is assumed. Support for participation (travel and lodging) is available via the Marie Curie Action MolSimu.

The tutorial was organized by:

- Evert Jan Meijer (University of Amsterdam, Netherlands),
- Igor Abrikosov (Linköping University, Sweden),
- Rodolphe Vuilleumier (Université Pierre et Marie Curie, France)
- Sergei Simak, (Linköping University, Sweden)

Invited lecturers were :

- François-Xavier Courdert (Université Paris 6, France)
- Elske Leenders (University of Amsterdam, Netherlands)
- Bjoern Alling, IFM, Linköping University, Sweden
- Ralf Everaers, ENS-Lyon, France
- Marivi Fernandez Serra, CECAM, Lyon, France
- Arkady `Mikhaylushkin, Uppsala University, Sweden`
- Ivano Tavernelli, EPFL, Lausanne, Switzerland
- Joos Vandevondele, EPFL, Lausanne, Switzerland

The morning sessions were lectures introducing the methods and in the afternoons there were computer exercises in which these methods were applied.
Support for participation (travel and lodging) was available via the Marie Curie Action “MolSimu”.

40 participants (of which 11 conference organizers and invited lectures) were selected, representing 11 European countries:
Algeria (2), Austria (1), Belgium (2), France (5), Germany (3), Greece (1), India (1), Italy (7), Netherlands (2), Russia (6), Spain (1), Sweden (5), UK (2), Ukrain (1), USA (1).

Participants

Eligible researchers

In Appendix I a complete list of participants is given. Table 1 compares the expected number of eligible researchers with the realized ones.

Table 1: Participation Tutorials

	Expected	Realized
Group 1		22
Group 2		10
Group 3		0
Non-eligible		8
Total		40

Clearly, our School has attracted more Group 1 researchers than expected; the total number of participants was well above the target.

The number of third country nationals was 11 (27,5%), which is well below the allowed maximum of 30%. In addition, The school attracted participants from 15different nationalities. The largest number of participants with the same nationality was Italy (7), (17,5%), which is well below the allowed 30%.

Gender issues

From the 40 participants 4 were Female (=10%). Although this is below the target value of 40%, we were very pleased with such a number of female participants given the very small number of Female students in this field.

Participation in school

Table 2 indicates how the event participants were involved in the tutorials. The keynote speakers include the lectures, while the oral contributions include the researchers involved in the computer exercises.

Table 2: Involvement of participants in the tutorial

	Number of event participants (including non funded)			
	Active participation			Passive participation
	Keynote Speech	Oral Contribution	Poster	
Early Stage Researchers [1]	1	1	0	20
More Experienced Researchers	7	3	0	8

[1] For the definition of Early Stage Researchers, etc., refer to the definitions in Annex III to your contract.

European Researchers active outside Europe	0	0	0	0
Third country nationals [2]	2	0	0	9

[2] Including Third Country nationals already listed under “Early Stage” and “More Experienced Researchers”

	F. Name	Name	Citizenship	Ge	Gr	3rd	Institute	
1	**Abrikosov**	Igor	Russia	M	X	1	IFM, Linköping University	Sweden
2	**Adjaoud**	Omar	Algeria	M	1	1	Bayerisches Geoinstitut	Germany
3	**Allesch**	Markus	Austria	M	1		Graz University of Technology	Austria
4	**Alling**	Bjoern	Sweden	M	1		IFM, Linköping University	Sweden
5	**Artyukhov**	Vasilii	Russia	M	1	1	Moscow Institute for Physics and Technology	Russian Federation
6	**Aschauer**	Ulrich	Germany	M	1		EPFL	Switzerland
7	**Baykov**	Vitaly	Russia	M	2	1	Royal Institute of Technology	Sweden
8	**Beglitis**	Nikolaos	UK	M	1		University College London	UK
9	**Colonna**	Francesco	Italy	M	1		HIMS, University of Amsterdam	Netherlands
10	**Coudert**	François Xavier	France	M	2		Université Paris Sud	France
11	**de Meyer**	Frédérick	Belgium	M	1		CECAM, Lyon	France
12	**Di Pietro**	Elisa	Italy	F	1		Università degli Studi di Firenze	Italy
13	**Everaers**	Ralf	Germany	M	X		ENS-Lyon	France
14	**Fernandez serra**	Marivi	Spain	F	2		CECAM, Lyon	France
15	**Hénin**	Jérôme	France	M	2		University of Pennsylvania, Philadelphia	USA
16	**Isayev**	Olexandr	Ukrain	M	1	1	Jackson State University	USA
17	**Ivanov**	Sergei	Russia	M	2	1	Ruhr-Universität Bochum	Germany
18	**Jouanna**	Paul	France	M	X		MSE	France
19	**Kefaelides**	Christos	Greece	M	1		Aristotle University of Thessaloniki	Greece
20	**Koci**	L	Sweden	M	1		CMT, Uppsala University	Sweden
21	**Leenders**	Elske	Netherlands	F	1		University of Amsterdam	Netherlands
22	**Leetma**	Mikael	Sweden	M	1		Fysikum, Stockholm University	Sweden

23	**Ljungberg**	Mathias	Sweden	M	1		Stockholm University	Sweden
24	**Lounis**	Samir	Algeria	M	1	1	IFF, Forschungszentrum, Juelich	Germany
25	**Mazzi**	Giacomo	Italy	M	1		University of Edinburgh	UK
26	**Meijer**	Evert Jan	Netherlands	M	X		University of Amsterdam	Netherlands
27	**Mikhaylushkin**	Arkady	Russia	M	2	1	Uppsala University	Sweden
28	**Moretti**	Roberto	Italy	M	2		INGV Osservatorio Vesuviano	Italy
29	**Poissier**	Adrien	France	M	1		CECAM, lyon	France
30	**Rasander**	Mikael	Sweden	M	1		Department of Physics, Uppsala University	Sweden
31	**Saal**	James	USA	M	1	1	Penn State University	USA
32	**Sena**	Alessandro	UK	M	1		University College London	UK
33	**Sibasis**	Acharya	India	M	2	1	Technical University, Clausthal	Germany
34	**Simak**	Sergei	Russia	M	X	1	IFM, Linköping University	Sweden
35	**Simeoni**	Mirko	Italy	M	1		University of L'Aquila	Italy
36	**Tavernelli**	Ivano	Italy	M	X		EPFL	Switzerland
37	**VandeVondele**	Joost	Belgium	M	2		University of Zürich	Switzerland
38	**Vetuschi**	Marino	Italy	M	X		DIPTERIS, University of Genova	Italy
39	**Vuilleumier**	Rodolphe	France	M	X		LPTL, Université Paris 6	France
40	**Zimmermann**	Janina	Germany	F	1		Fraunhofer Institut für Werkstoffmechanik	Germany

Appendix II: Program

IAA : Igor A. Abrikosov, Linköping University, Sweden
B.A :Bjoern Alling, Linköping University, Sweden.
S. I. S : Sergei I. Simak, Linköping University, Sweden
A. M. : Arkady Mikhaylushkin, Uppsala University, Sweden

Monday, October 30

9.00 - 9.45 General information and introduction into the tasks of the tutorial (IAA)
10.00-10.45 Basics of the electronic structure theory (IAA)
10.45 - 11.15 Coffee
11.15-12.00 Periodic solids and
12.15-12.45 electronic bands (SIS)

12.45 - 14.00 Lunch

14.00-14.45 Introduction into computational tasks (BA and AM)
15.00-15.45 Computer classes
15.45 - 16.15 Coffee
16.15-17.00 Computer classes
17.15-18.00 Computer classes

Tuesday, October 31

9.00 - 9.45 Many-body problem and
10.00-10.45 density functional theory (IAA)
10.45 - 11.15 Coffee
11.15-12.00 Self-consistent band structure
12.15-12.45 calculations for periodic solids (SIS)

12.45 - 14.00 Lunch

14.00-14.45 Introduction into computational tasks (BA and AM)
15.00-15.45 Computer classes
15.45 - 16.15 Coffee
16.15-17.00 Computer classes
17.15-18.00 Computer classes

Wednesday, November 1

9.00 - 9.45 Introduction into the multiple-
10.00-10.45 scattering theory (IAA)
10.45 - 11.15 Coffee
11.15-12.00 Theory of the pseudopotentials
12.15-12.45 and PAW technique, part 1 (SIS)

12.45 - 14.00 Lunch

14.00-14.45 Introduction into computational tasks (BA and AM)
15.00-15.45 Computer classes
15.45 - 16.15 Coffee
16.15-17.00 Computer classes
17.15-18.00 Computer classes

Thursday, November 2

9.00 - 9.45 Green's function technique and
10.00-10.45 the coherent potential approximation (IAA)
10.45 - 11.15 Coffee
11.15-12.00 Introduction into the pseudopotential
12.15-12.45 and PAW technique, part 2 (SIS)

12.45 - 14.00 Lunch

14.00-14.45 Introduction into computational tasks (BA and AM)
15.00-15.45 Computer classes
15.45 - 16.15 Coffee
16.15-17.00 Computer classes
17.15-18.00 Computer classes

Friday, November 3

9.00 - 9.45 Linear scaling methods
10.00-10.45 for the electronic structure calculations (IAA)
10.45 - 11.15 Coffee
11.15-12.00 Alloy phase stabilities from
12.15-12.45 Monte-Carlo simulations (IAA)

12.45 - 14.00 Lunch

14.00-15.45 Presentation of the computational projects (BA and IAA)
15.45 - 16.15 Coffee
16.15-18.00 Presentation of the computational projects (BA and IAA)

Appendix III Evaluation form

Quantum Simulations of Liquids and Solids
October 30, 2006 to November 10, 2006
All participants were asked to fill in the form given in Appendix III in addition to the EC form. Out of the 40 participants a response of 26 participants was received.

Overall Impression of the lecture
Quality of the lectures
unacceptable/poor/acceptable but needs improvement/good/very good 1/2/3/4/5
4,3/5

Level of the lectures
Appropriate(25)/Too easy(1)/Too difficult(0)

Ratio Lectures/Exercices
Appropriate(24)/To many lectures(0)/To many exercises(2)

Remarks and comments:

Overall Impression of the computer exercises
Quality of the computer exercises
unacceptable/poor/acceptable but needs improvement/good/very good 1/2/3/4/5
3,7/5

Connection with lectures
unacceptable/poor/acceptable but needs improvement/good/very good 1/2/3/4/5
3,8/5

Computer facilities
unacceptable/poor/acceptable but needs improvement/good/very good 1/2/3/4/5
3,5/5

Level of the exercises
Appropriate(23)/Too easy(3)/Too difficult(0)

Support with exercises
unacceptable/poor/acceptable but needs improvement/good/very good 1/2/3/4/5
3,7/5

Remarks and comments:

Overall Impression of the local arrangements (hotel,food)
*Information prior to arrival**
unacceptable/poor/acceptable but needs improvement/good/very good 1/2/3/4/5
3,6/5

Accomodation
unacceptable/poor/acceptable but needs improvement/good/very good 1/2/3/4/5
3,8/5

Molsimu support sufficient
unacceptable/poor/acceptable but needs improvement/good/very good 1/2/3/4/5
4,1/5

Remarks and comments:

Overall mark of the course
*Did the course meet your expectations?** **yes(25)/no(1)**
*Would you recommend the course to a colleague?** **yes(24)/no(2)**

Appendix IV: Individual comments of the participants

Remarks and comments regarding lecturers

[1.] The lectures were very good, however the exercises didn't learn me much in function of the time they took. In practice exercices were just finding the right input file and run the program. It doesn't bring you much real insight. But the lectures were really good. For the liquid part (second week) I expected more complex liquid exaples with biomolecules.

[2.] The organization of the exercise session could be prepared better.

[3.] I really enjoyed this event. Work in teams is nice experience.

[4.] Although my overall experience of the tutorial lectures was a good one. However in future I think that the description of the tutorial should be defined in more detail beforehand and then more rigidly adhered to. Some of the lectures, whilst intersting were not directly relevant to many peoples' field of study.

[5.] WEEK 1
I think the lectures were informative, but lacked focus between the two lecturers. I believe having more planning in the future (perhaps having the entire set of lectures created together) would help.
WEEK 2
The quality of the lectures was very good, but handouts were needed to be able to better keep notes.

[6.] The lectures were very interesting, in particular because they followed a progressive improvement of the level of difficulty.

[7.] Very good tutors.

[8.] Specially during the second week, too many exercises about the same code....

[9.] During the second week of the school, hard copies of the lectures were not available before the talks and this made it difficult to follow the lecturers. It would be nice if electronic copies of the lectures are available on the website of the tutorial.

[10.] Motivated and well-prepared lecturers

[11.] It would be nice to go deeply in the field on the lectures. Probably this requires higher background level of the participants.

[12.] The course consists of nice lectures with very good practical exercises.

[13.] Towards the end level of lectures was too high

[14.] The first week more organized than the 2nd one. The 2nd week was started and the programm and the copies of presentation were not yet ready.

Remarks and comments regarding computer exercises

[1.] see above

[2.] The exercises could be explained better before the sessions.

[3.] Some exercises take quite a bit time. Perhaps dedicated computational cluster is needed for them.

[4.] In the first week the set up was better. The setting of projects that had to be completed and then presented is a very good way of doing things. However, the projects were not very well described and a number of things were difficult to accomplish. Consequently the support staff were stretched very thin. In the second week the opposite was the case. The problems were very well described and consequently the staff support was more than adequate. However, the general approach could have been more structures. Combining the best parts of both would lead to an excellent system.

[5.] The lectures had little connection with the exercises. Rather than learning how various programs work, we were given exercises in only how to use them. In the end, we received only a superficial understanding of the programs. I was particularly disappointed that we did not write any code, as was described in the description of the tutorial. The exercises, particularly in the first week, were not fully tested. Several of the input files of our calculations had unexplained errors and there was obviously not enough time to complete the work in the time given (although it was expected). In the first week, more people were needed to offer help to the participants. My group found ourselves waiting for one of the two helpers much too often.

[6.] The number of the computer exercises was too big, because no more time to make an appropriate analysis of the data remained. The idea to make a miniworkshop about our works was good but it would be better organized.

[7.] More tutors with a better preparation are needed! A more detailed and complete script for the exercises would be useful. There must be much more instructions for the whole computer class exercises.

[8.] More support and discussions during the exercises would be nice

[9.] In the first week, we had research projets. At the end of the week, each group present the results that they have found during all the week. I think that it will be good if it was the same for the second week.

[10.] The course was very much divided up into two halfs. The first week the computer exercises were on a good level and felt meaningfull. They had good connection with the lectures and with the exercises from the day before.
The week after there was much less structure. More like "try some things and see what happens" instead of any well defined tasks. I tend to like the organisation of the first weeks exersices more.
Then there was a problem with lack of available computers. Quite often, many

groups had to work simultaneously on the same procrssor, making things go very slow.

Remarks and comments regarding information, accomodation

[1.] not appropriate

[2.] Nice location in city center.

[3.] There was no sunday event as such. The mini workshop held at the end of the first week was very good. The hotel was fine and the serving of breakfast much appreciated. Lunch was similarly fine. Communication as to whether hotels need to be booked and whether we will be funded beforehand could be made to us more promptly.

[4.] I'm not sure what the event on Sunday refers to. I think right when we find out we have been accepted to the tutorial, an short introductory email should be sent to let us know how to proceed. I found myself wondering how to proceed. The hotel was pretty good, and overall my stay was enjoyable.

[5.] The information about the program, the hotel and the possibility to present a poster or a talk were a little bit late. The Sunday's event didn't exist.

[6.] There wasn't any Sunday Event!

[7.] what do you mean with sunday's event?

[8.] There was no sunday event.

[9.] The organization was very poor: the (few!) forward informations arrived very late (program arrived 2 days before tutorials beginning); missing/incomplete answers to my emails. The accomodation was completely unacceptable: the hotel was dirty and unhygienic, and there was missing a wardrobe. Never seen such a bad-kept hotel before There was no Sunday's event!!

[10.] Might be I missed something, but there were no Sunday's events.

[11.] Information about tutorial was sent out very late.

[12.] The information given prior to arrival should have come a few weeks earlier. I don't know what sunday activity means, since there was no arranged activity one neither saturday or sunday. But, eitherway, it was nice to have some free time for sightseeing...

Remarks and comments regarding expectations of the course

[1.] Special aknowledgements to CECAM adm. team for help with visa issues.

[2.] Overall my experience at the tutorial was a very good one and would recommend other people in my position to attend a similar event at CECAM. Hopefully my comments will help to improve the tutorials still further. Many thanks.

[3.] I think the course needs improvement, particularly the computer exercises. If offered again next year, I would perhaps try to increase the level of involvement of the exercises. Perhaps merge lectures with the exercises. The level of the exercises must be brought in line with the lectures, because in the end the exercises did not help much at all.

[4.] It was amazing!

[5.] reading the description of the tutorial, I expected that a part of it should be dedicated to the development of a code....this the main failure of the tutorial in my opinion

[6.] The teaching and the lectures where very good, the contents of the tutorial met my expectations. But I would recommend the course only if the environment and organization are improved.

[7.] This was a very good course, with excellent lectures. (Special credits to Igor.)