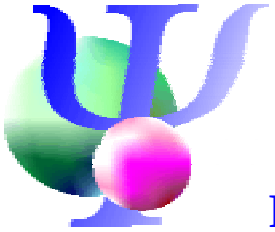

Research School in Multiscale Materials Modelling

University of Sidi-Bel-Abbes, Algeria

August 25th to 31st , 2001

Physical properties of materials are the result of processes operating at various space and time scales, ranging respectively from nanometers to meters and from femtoseconds to seconds. At thermodynamic equilibrium, values for quantities of interest (free energy and its derivatives) are computed analytically or numerically, as space and/or time averages of the appropriate microscopic observables within the framework of statistical thermodynamics.

Under conditions not far from equilibrium, studying physical properties is still a possible task by using linear response theory and mean field approaches. Examples are the calculation of transport coefficients via the Green-Kubo formulae, the mean field prediction of phase transformations and of microstructural changes.

However, the processing and applications of materials occur often under strong gradients of pressure and temperature, i.e. very far from equilibrium. As a consequence, material properties become "history" dependent (because an equation of state does not exist) and highly non-linear. It is worth mentioning that the non-linearity is often due to the collective behavior of structural equilibrium (point defects) and metastable (dislocations, grain boundaries) defects.

Numerical simulation provides a means for studying the properties of materials under such non-equilibrium conditions. Starting from physically founded cohesion models or from an ab-initio description of atomic bonding, atomic scale simulation techniques (Molecular Dynamics and Monte Carlo) give insight to the behavior of the materials studied. This can help improving the quality of materials for technological applications and possibly to the development of new materials and/or fabrication processes. Unfortunately, the scales of most properties relevant for applications are fundamentally different from these of atomistic simulations. The challenge therefore consists for numerical simulations in bridging the gaps of space and time scales that separate atomic and macroscopic material properties.

This school aims at bringing together researchers with expertise in different areas of condensed matter and material physics. It is thereby expected to meet the following twofold objective:

1. To address issues related to methods for bridging space and time scales in specific sub-fields and to identify the most promising directions of development of appropriate theoretical and numerical tools.
2. To offer participants an overview of methods used in specific sub-fields they may not be aware or familiar with and thereby promote new ideas and collaborations.

Topics

1) Classical MD - Simulations on Massively Parallel Supercomputers with Application to Shock Waves in Solids.

Johannes ROTH,
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2) Theory and procedures of embedded atom method (EAM) series ; the method to calculate energy of multi-atomic systems

Kunio TAKAHASHI,

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3) Potentials functions

Sakir ERKOC

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4) **Hartree-Fock and Crystal**

Sylvia CASSASA
University of Torino
Italy

5) Classical Molecular Dynamics

Ahmed Lazreg
University of Sidi Belabbes
Algeria

6) Ab initio Pseudopotential Calculations

Bachir Bouhafs,
University of Sidi Bel-abbes
Algeria

Abbar Boucif,
University of Sidi Bel-abbes
Algeria

7) Tight Binding Total Energy

Amel Laref,
University of Sidi Bel-abbes
Algeria

8) Finite Element Method

Goumri-Said Souraya,
University of Sidi-Bel-Abbes
Algeria

9) MultiScale Materials Modelling

Hafid Aourag,
University of Sidi Bel-abbes
Algeria

Course Timetable

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Venue: Link Building Seminar Room unless indicated

Saturday 25 August

09.00 - 10.30 **H. Aourag :** ***Scope of multiscale modelling***
10.30 - 12.00 **A. Lazreg** ***Classical Molecular Dynamics***

13.00 - 14.00 **Lunch**
14.30 - 17.30 **Computing Laboratory** : ***Theory and procedures of MD***
Mr Amriou, Mr Aouas; Dr Lazreg

Sunday 26 August

08.30 - 10.00 **S. Erkoc** ***Potential Functions***
10.30 - 12.00 **J. Roth** ***MD on massively parallel computing***

13.00 - 14.00 **Lunch**
14.00 - 15.30 **J. Roth :** ***Shock waves***
16.00-18.00 **S.Cassasa** ***Hartree Fock Theory and Crystal***

Monday 27 August

08.30 - 10.00 **K. Takahashi** : ***History of EAM Series***

10.30 - 12.30 **S.Cassasa : *Use of Crystal***
12.30 - 13.30 **Lunch**

14.30 - 17.30 **Computing Laboratory** : ***Crystal98***
Dr Cassasa, Mr Sayede

Tuesday 28 August

08.30 - 10.30 **K. Takahashi** : ***EAM , calculation procedure***
11.00 - 12.30 **Computing Laboratory** :***Use of EAM***
Prof Takahashi, Miss Ferouan

12.30 - **Excursion to oran and the seacoast**

Wednesday 29 August

08.30 - 10.30 **B. Abbar** : ***DFT***
11.00 - 12.30 **B. Bouhafs** : ***ab initio pseudopotential calculations***

12.30 - 13.30 **Lunch**
14.30 - 17.30 **Computing Laboratory : *Execution and visualization of EAM***
Prof Takahashi, Miss Feraoun PWSCF code

Thursday 30 August

08.30 - 10.30 **A. Laref** ***Tight Binding Total Energy***
11.00 - 12.30 **S. Goumri-Said : *Finite Element Methods***

12.30 - 13.30 **Lunch**
14.00 - 17.30 **Computing Laboratory** : ***PWSCF***
Mrs Sayede, Amriou, Lakdja and Miss Dridi

Friday 31 August

08.30 - 10.30 **H. Aourag *Multi Scale Modelling*** ***(lecture notes)***
10h30- 12.30: **Computing Laboratory :**TBTE code
Miss Laref and Netadjer
13.00 : **Lunch**
15.00 : **Closing Ceremony**

Every evening there will be some extra courses and computer practice on some other available software (Wien, Abinit, Crysdens, EAMLD...) check the programme avery day .

Social Programme

Friday 24 August 2001

20.00 : Get Together party

Saturday 25 August 2001

22.00 : Trio Tahadi (Sketchs)

Sunday 26 August 2001

22.00 : Folkloric Danses

Monday 27 August 2001

22.00 : traditionnal Music

Tuesday 28 August 2001

22.00 : Algerian Music (groupe Raina Rai)

Wednesday 29 August 2001

22.00 : Traditionnal Danses

Thursday 30 August 2001

22.00 : theatre