TIME TABLE

TIME	Monday	Tuesday	Wednesday	Thursday	Friday
	May 26	**May 27**	**May 28**	**May 29**	**May 30**
9.00 - 9.45	Registration	Yip	Cleri	Tadmor	Tadmor
9.45 - 10.30	Yip	Yip	Cleri	Tadmor	Cleri
11.00 - 11.45	De Simone	De Simone	Tadmor	Cleri	Bocquet
11.45 - 12.30	Colombo	De Simone	Tadmor	Cleri	Falk
14.30 - 15.15	Yip	Colombo	Bocquet	Falk	
15.15 - 16.00	Yip	Colombo	Bocquet	Falk	
16.30 - 17.15	Colombo	De Simone	Falk	Bocquet	
17.15 - 18.00	Colombo	De Simone	Falk	Bocquet	

ADMISSION AND ACCOMMODATION

Applicants must apply at least one month before the beginning of the course. Application forms can be sent by post or on-line through our web site: http://www.cism.it. A letter of confirmation will be sent to accepted participants.

The registration fee is 600,00 €.

A limited number of participants from universities and research centres who are not supported by their own institutions can be offered board and/or lodging in a reasonably priced hotel. Requests should be sent to CISM Secretariat by **March 26, 2008** together with the applicant's curriculum and a letter of recommendation by the head of the department or supervisor confirming that the institute cannot provide funding. Preference will be given to applicants from countries which sponsor CISM.

The Deutsche Forschungsgemeinschaft offers scholarships to German students (please contact Dr-Ing. Marcel Urban, DFG, Kennedyallee 40, 53175 Bonn, Germany, tel. +49 (228) 885 2655, e-mail: Marcel.Urban@dfg.de - web site: http://www.dfg.de).

Information about travel and accommodation are available at http://www.cism.it/cism/travel-reach.htm, or can be mailed upon request.

For further information please contact:

CISM
Palazzo del Torso - Piazza Garibaldi 18
33100 Udine (Italy)
tel. +39 0432 248511 (6 lines)
fax +39 0432 248550
e-mail: cism@cism.it
http://www.cism.it

Centre International des Sciences Mécaniques
International Centre for Mechanical Sciences

ACADEMIC YEAR 2008
The Krajcinovic Session

BRITTLE FRACTURE AND PLASTIC SLIP: FROM THE ATOMISTIC TO THE ENGINEERING SCALE

Advanced School coordinated by

Luciano Colombo
Università di Cagliari
Italy

Antonio De Simone
SISSA, Trieste
Italy

Udine, *May 26 - 30,* 2008

INdAM "Francesco Severi"
Research project on
"Mathematical Challenges in
Nanomechanics"

INdAM
Istituto Nazionale di Alta Matematica
Francesco Severi

BRITTLE FRACTURE AND PLASTIC SLIP: FROM THE ATOMISTIC TO THE ENGINEERING SCALE

In recent years new techniques - complementing the traditional approaches based on experiment and on continuum theories - have become available to study, understand, and control those mechanical phenomena occurring when deformations organize in spatially localized patterns. On the one hand, atomistic simulations have reached the scale and resolution necessary to perform numerical experiments describing extended defects and their interaction. On the other hand, new mathematical tools have made it possible to model in microscopic detail the evolution of those singularities (dislocations, shear bands, cracks), which control the inelastic response of solids at the macroscopic level. The occurrence of such conceptually diverse developments has led to a new generation of numerical models, aimed at interfacing the atomistic and continuum description. Here, the wide range of length and time scales that need to be resolved creates a situation where a single set of methods/approaches cannot be used. Rather, different tools are employed to deal with a hierarchy of sub-problems. In such a multiscale theoretical device, phenomenological models are typically used to incorporate the properties at a finer scale within calculations at a larger scale. The ability to couple atomic-scale (or, even, electronic-level) simulations with macroscopic modeling represents a revolutionary step forward towards the ability to predict bulk material properties from first principles, so that constitutive laws need no longer to be postulated for describing the mechanical behaviour of a given system. Similarly, the incorporation of microstructural inhomogeneities and the explicit resolution of cracks and shear bands in finite element simulations at the continuum scale have led to significant improvements in our understanding of material response.
The aim of this course is to present the above recent developments by highlighting both strengths and limitations of each single method, and emphasizing the necessity of bridging between different time and length scales. Focus will be put on:

i. advances in atomistic simulations offering the possibility to span time intervals typical of some interesting mechanical phenomena;
ii. coarsening of spatial degrees of freedom, namely, a key issue for bridging disparate lengths;
iii. mechanisms of fracture in brittle solids and of plastic deformation in amorphous materials (in particular, shear banding in metallic glasses), examined both at the atomistic and at the continuum scale.

The course is addressed to Master and Ph.D. students, post-docs and research associates in applied mathematics, physics, materials science, mechanical sciences, and structural (e.g., civil, mechanical,…) engineering.

PRELIMINARY SUGGESTED READINGS

Atomistic simulations:
D. Frenkel and B. Smit
"Understanding Molecular Simulation" (Academic Press, 1996) Chapters: 2.1 to 2.2; 4.1 to 4.3; 6.1.

Plasticity theory:
L.M. Kachanov
"Fundamentals of the Theory of Plasticity" (Dover, 2004)
Chapters: 1, 2, and 5.

Materials modelling:
S. Yip "Handbook of Materials Modelling" (Springer, New-York-Berlin, 2005)
Chapters: 2.19 to 2.25; 3.1 to 3.4; 6.7 to 6.13; 7.1 + 7.6 + 7.11
Chapters: 2.19 to 2.25; 3.1 to 3.4; 6.7 to 6.13; 7.1 + 7.6 + 7.11.

Quasicontinuum method:
E.B. Tadmor e R.E. Miller
"The theory and implementation of the Quasicontinuum Method"
In: S. Yip, "Handbook of Materials Modelling" (Springer, New-York-Berlin, 2005).

LECTURES

All lectures will be given in English. Lecture notes can be downloaded from CISM web site, instructions will be sent to accepted participants.

INVITED LECTURERS

Lyderic Bocquet - Université Lyon I, France
5 Lectures on: Rheology of glassy materials and molecular materials. Experimental and theoretical progress in the description and understanding of flows in glassy materials exhibiting strongly non-Newtonian and solid-like behavior; occurrence of shear bands.

Fabrizio Cleri - Univ. de Science et Technologie de Lille, France
5 Lectures on: Simulation of extended defects in materials at all length scales. Structural and topological characterization of extended defects in materials. Theoretical description (atomistic simulations, coarse-grained and mesoscopic models) of the behavior of a population of defects: defect-defect interaction , and microstructure evolution.

Luciano Colombo - Università di Cagliari, Italy
5 Lectures on: Atomistic simulations for materials mechanics. Basic concepts and algorithms underlying atomistic simulations. Numerical implementation. Border conditions. Interatomic potentials. Atomic-scale formulation of continuum concepts.

Antonio De Simone - SISSA, Trieste, Italy
5 Lectures on: Continuum plasticity: a primer on plastic flow and shear bands. Continuum description of strain and stress. Constitutive equations. Yield surfaces and flow rules. Strain localization and shear banding.

Michael Falk - University of Michigan, Ann Arbor, MI, USA
5 Lectures on: Using atomic-scale simulation for investigating plasticity and failure in non-crystalline solids. Development of constitutive models for plastic deformation and failure in amorphous solids using molecular dynamics simulation. Data analysis and relationship between structure and strain rate. Constitutive laws based on the shear transformation zone.

Ellad Tadmor - University of Minnesota, Minneapolis, MN, USA
5 Lectures on: Coupling atoms to continuum: The quasicontinuum method. Introduction to the theory and the practical issues underlying quasi-continuum (QC) simulations. QC is a multiscale method based on the idea of representative atoms and finite element interpolation.

Sidney Yip - MIT, Cambridge, MA, USA
5 Lectures on: Delivering on the promise of computational materials. Computational materials research through the linking of models. Simulation methods across length and time scale. Challenges of molecular modeling of technological processes.

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Udine, May 26 - 30, 2008
Application Form
(Please print or type)

Surname _____

Name _____

Affiliation _____

Address _____

_____

E-mail _____

Phone _____ *Fax* _____

Method of payment upon receipt of confirmation (Please check the box)

The fee of Euro 600,00 includes IVA/VAT tax and excludes bank charges

❑ *I shall send a check of Euro* _____

❑ *Payment will be made to CISM - Bank Account N° 094570210900, VENETO BANCA - Udine (CAB 12300 - ABI 05418 - SWIFT AMBPIT2M - IBAN CODE IT83Z 05418 12300 09457 0210900).*
Copy of the receipt should be sent to the secretariat

❑ *I shall pay at the registration counter with check, cash or VISA Credit Card (Mastercard/Eurocard, Visa, CartaSi)*

IMPORTANT: CISM is obliged to present an invoice for the above sum. Please indicate to whom the invoice should be addressed.

Name _____

Address _____

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C.F.* _____

VAT/IVA* No _____

(*) Only for EU residents or foreigners with a permanent business activity in Italy.

Only for Italian Public Companies

❑ *I ask for IVA exemption (ex law n. 537/1993 - art. 14 comma 10).*

Privacy policy: I understand that data received via this form will be used only to provide information about CISM and its activities, within the limits set by the Italian legislative decree no. 196/2003 and subsequent amendments.
Complete information on CISM's privacy policy is available at www.cism.it.

I have read the "Admission and Accommodation" terms and conditions and agree.

Date _____ Signature _____