Dislocation Dynamics Simulations : trends and challenges

Proposed date and place

2 days workshop (from noon 1st day to noon 3rd day) ; December 10-12th in Paris ; 40 participants (including 20 invited lectures)

I. Organizers

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II. Proposal

For structural materials, a key challenge is to relate the mechanical behaviour to the physics at the origin of the plasticity so that the material constitutive equations are valid for a large domain of applications. In many cases however, experiments can be costly and difficult to implement (e.g. irradiated materials, small sized samples, confined plasticity, extreme loading conditions, etc...). For these cases, numerical modeling is an alternative which has demonstrated to advantageously replace the experiments.

In the case of crystalline materials, Discrete Dislocation Dynamics (DDD) simulations has became an essential step of multi-scale approach to plasticity. DDD codes consists in modeling the behaviour of dislocation lines which are the carrier of plasticity at the grain scale. Thus, DDD simulations nicely fill the gap between molecular dynamics simulation at the atomic scale and finite elements simulations at the continuum scale. Born in France in the 90's, three dimensional dislocation dynamics is reaching its maturity as testified by world-wide efforts to develop this numerical method. Recently, many improvements have been performed in the different groups. As an example, the most recent 3D DDD codes can now handle elastic anisotropy, some have been coupled to finite element codes in order to enforce complex boundary conditions, others have been optimized in order to allow larger strain in bigger

sample sizes, ...

The aim of this international workshop is to bring together leading researchers working in the numerical simulation of dislocations and to provide a forum of dissemination, discussion and networking. Three main topics will be addressed :

1) Mathematics of 3D dislocation dynamics (time algorithm, force integration, stress fields, multipoles, etc...)

2) Parallelization strategies (OpenMP, MPI, hybrid scheme, GPU, etc...)

3) Simulation challenges based on experimental needs (irradiated materials, polycrystals, dislocation patterning, etc...)

III. Tentative list of lecturers

from USA :

- Stanford : Wei Cai : caiwei@stanford.edu
- LLNL : Jaime Marian : marian1@llnl.gov
- UCLA : Nasr Ghioniem : ghoniem@seas.ucla.edu
- GeorgiaTech : Laurent Capolungo : laurent.capolungo@georgiatech-metz.fr

from Great Britain :

- Oxford/Mathematics department : Steve Fitzgerald : fitzgerald@maths.ox.ac.uk
- Oxford/Material department : Steve Roberts : steve.roberts@materials.ox.ac.uk

from Germany :

- KIT : Daniel Weygand : Daniel.Weygand@kit.edu
- HZG : Erica Lilleodden : Erica.Lilleodden@hzg.de
- ICAMS : Alexandre Hartmaier : Alexander.Hartmaier@icams.rub.de
- Max Planck : Dierk Raabe : d.raabe@mpie.de

from France :

- CEA-DAM : Ronan Madec : ronan.madec@cea.fr
- CEA-DAM : Aurelien Vattre : Aurelien.vattre@cea.fr
- CEA-SRMP : Emmanuel Clouet : Emmanuel.Clouet@cea.fr
- CEA-SRMA : Christian Robertson : Christian.Robertson@cea.fr
- Onera-LEM : Benoit Devincre : devincre@onera.fr
- EDF : Ghiath Monnet : Ghiath.Monnet@edf.fr
- MinesParistech-CdM : Vladislav Yastrebov : vladislav.yastrebov@mines-paristech.fr
- Ponts : Regis Monneau : monneau@cermics.enpc.f
- Metz-LEM3 : Vincent Taupin : vincent.taupin@univ-lorraine.fr
- Lyon-Mateis : Jonathan Amodeo : Jonathan.Amodeo@insa-lyon.fr

— Toulouse-CEMES : Joel Douin : douin@cemes.fr

IV. Financial Support

The workshop is organized by a team of researchers involved in the ANR project OPTIDIS. This ANR program will support most of the expenses.

We plan to cover the full cost for 20 invited lecturers with an average enveloppe of 1000 euros per participant.

We also would like to open the workshop to students (Ph.D and postdoc) and we ask for additional support from CFCAM : 4000 euros which will support lunches and accommodations for them.