Moving heterogeneities and elastodynamic wave propagation: simulation and detection

Proposed dates and place:

Spring 2013, Institut Henri Poincaré, Paris

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1. Proposal

1.1 Introduction and motivation

Acoustic emission (AE), i.e., the emission of elastodynamic waves, has long been used as a method of detection and analysis of fast, irreversible, structural modifications in materials, induced by plastic deformation (dislocation motion and slip, in the bulk or at grain boundaries), fracture, and less commonly bulk phase transformations of the martensitic type. Applications range from metallurgy to glaciology, seismology and rock mechanics, and industrial testing.

From the theoretical standpoint, AE is produced during motion of singularities such as linear defects in plasticity (dislocations), surface front lines in fracture or twinning, and volume-bounding surfaces in phase transformations.

The problem can be roughly summarized as follows. Under applied stresses or strains, acoustic waves produced by defect motion propagate subsequently in a heterogeneous medium, with heterogeneities consisting of previously existing defects. The problem thus involves on the one hand, the issue of which equations govern fast defect motions (e.g., in plasticity, non-local-in-time inertial effects should be accounted for) under the action of dynamically evolving local stresses, and on the other hand, elastodynamic wave propagation in a complex environment with multiple scatterings. In addition, in plasticity or fracture, collective depinning of defect lines gives rise to avalanche-type of breakdown events, a purely dynamical phenomenon involving a wide range of spatial and time scales. Fracture processes involve additional complexities associated with branching instabilities.

Simplified models are used by experimentalists to interpret AE in rock mechanics, metallurgy or glaciology, mostly by correlating the observed signals to failure events. While efficient large-scale elastodynamic wave propagation codes are developed by seismologists, the numerical simulation of dynamic defect propagation at the mesoscopic scale remains a very difficult challenge. For instance, there exists by now a few three-dimensional dynamic codes for martensitic phase transformations, but no such codes are available for plasticity or fracture, although notable progresses have been made in the two-dimensional case.

While some well-known international conferences are targeted towards AE in general, mostly with focus on applications, and others are devoted to wave propagation and transport in random media, purely dynamical effects are currently only marginally represented in conferences devoted to dislocations, phase transformations, or continuum mechanics at the mesoscopic scale. It thus appears that there is room for an event specialized in such questions.

1.2 State of the art

An enormous amount of theoretical work has been devoted over decades to elastodynamic wave interaction with scatterers: wave propagation in random media, scattering of waves by dislocation lines, etc.

Although a great deal of work has been done here also, relatively less explored is the emission of stress fields from moving singularities: while general field equations have been established in the sixties up to the eighties, their numerical exploitation has scarcely been initiated, and simplified models (such as the Rouby model, for instance) are sometimes used to interpret AE data by experimentalists. Most of such models assume infinite rectilinear defect lines.

The same situation prevails for the equations governing the motion of singularities (the so-called ``self-force problem”), the theory of which is still under development. For instance, in the domain of dislocation dynamics (DD) codes aimed at performing mass-scale calculations, the simplest approach to dynamical questions to date (explored by a few workers only) has been to consider that inertia in dislocation motion is governed by an inertial mass computed at constant velocity, and effects of wave interaction in depinning processes and avalanches are poorly understood. In this dynamical problem, crystal anisotropy poses computational issues, too, due to the complexity of the equations involved. Twinning in shock loadings poses an outstanding theoretical and computational problem also.

Transonic and supersonic transitions for defect motion have been explored by means of molecular dynamics (some of them including absorbing boundary conditions), or experimentally. Though notable efforts have been directed towards the computation of the driving self-force (e.g., of dislocations), no fully dynamical analytical model is at the present time able to account for such transitions.

On the other hand, phase-field-type codes have been introduced in the last decade to handle dislocation motion as individual lines, from general field formulations of the problem in the continuum, and numerical solution of the Navier equation (by finite elements). The potential of such codes is nowadays limited to handling only a few dislocations. Compared to molecular dynamics, an alternative approach to the study of such systems, the phase field method, which is free of thermal noise, can be considered as a test bench for comparisons with numerical solutions of equations for dynamic defect motion. However, such comparisons have scarcely been attempted.

Actually, the privileged application domain of such phase-field type codes seems to be that the dynamics of martensitic phase transformations, a subject still in its infancy. Notably, existing finite-element codes operating at the mesoscopic scale do not include absorbing boundary conditions, so that wave reflection at the boundary of the simulation volume --or the size of the latter, when using periodic boundary conditions-- restrict the usable time window of simulations. Confrontations between calculations and experimental detection of acoustic emission have apparently never been carried out so far.

Concerning wave-propagation codes used in seismology, the finite-difference methods used in the beginnings have by now been superseded by finite-element ones, and absorbing boundary conditions seem to be routinely used. Multipole methods have been introduced to handling boundary conditions. It is not clear, however, which of these approaches would be the best to use in the perspective, e.g., of coupling DD codes to wave propagation processes.

1.3 Objectives

This interdisciplinary Discussion Meeting aims at gathering scientists concerned with acoustic emission phenomena: materials science physicists involved with dislocations and/or fast fracture, metallurgists, glaciologists, seismologists, theorists of elastodynamic wave propagation in heterogeneous media, experts in wave propagation codes, and in molecular dynamics, and willing to discuss informally questions (modelling, exploitation) relevant to dynamical defect propagation and acoustic emission at the mesoscopic scale.

The focus will be on summarizing the existing state-of-the-art, pointing out limitations of current models and techniques, and identifying possible convergence domains between communities. Furthermore, the opportunity of organizing in France an international conference on these questions will be examined, discussing what could be its appropriate format, possibilities for funding, and key leaders to be contacted. Its purpose would be to promote interdisciplinary discussions, and the development of dynamic simulation codes for defect propagation, with interactions with experimentalists.

Specific topics that should ideally be surveyed and discussed are:

- numerical techniques for wave-propagation codes (e.g., finite differences vs. finite elements, absorbing boundary conditions)
- acoustic emission and phase transformations: phase-field methods; experiments
- possible strategies towards coupling Discrete Dislocation Dynamic codes (currently quasi-static) to wave propagation effects
- models for dynamical fracture
- transonic and supersonic defect motion (experimental evidence, simulation)
- equations governing defect motion in the dynamical regime
- means of detecting acoustic emission: types of waves; limitations of models currently employed in interpreting experiments
- equations governing dynamical defect motion
- dynamic motion of defects at the microscopic scale: molecular dynamics techniques
- simulation of avalanches
- dynamical homogenization methods

Speakers are expected to present their contributions on these questions in synthetic talks. The goal is to host, during 3 half days, around 15 talks of 30 mins with sufficient time devoted to exchanges and discussion.

A one-hour discussion will be devoted to the perspective of organizing a larger conference.

1.4 Participant List

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All of the above participants have given their agreement of principle for attending the meeting A few others (3~4) not mentioned in the list may still be contacted.

2 Financial Support

Transport (avion, train) : 1300 Euros
7 nuits d'hôtel dans un hôtel convenable du Quartier Latin : 875 Euros
Un déjeuner en commun au restaurant + pauses café : 825 Euros
Total : 3000 Euros requested to CFCAM