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# The Jacobi–Davidson algorithm for large scale eigenvalue problems in heterogeneous materials

## Proposal for a master thesis

### Introduction

In strongly heterogeneous materials, such as structural glasses, sound has anomalous dispersion properties which are characterized by the Ioffe–Regel limit, and the universal phenomenon of the Boson peak. Molecular dynamics simulations are able to produce structural glasses in which the stable position of each atom is precisely known. Given such a computer generated atomic configuration, the corresponding vibrational properties can be investigated by solving an eigenvalue problem involving the Hessian of the potential energy landscape associated with material cohesion.

In this project, the Hessian obtained from a large scale molecular dynamics simulation of a model metallic structural glass involving half a billion atoms is to be constructed and 'diagonalized' to obtain a significant portion of the long-wavelength vibrational eigenmodes [1]. These eigenmodes will be analyzed to investigate the relationship between atomic-scale structure and the onset of the Boson peak regime. In order to calculate the vibrational frequencies, we have to solve the real symmetric eigenvalue problem

$$\boldsymbol{H}\boldsymbol{q} = \lambda \boldsymbol{q}, \tag{1}$$

where $\boldsymbol{H}$ is the given *Cartesian Hessian* that contains the second derivatives of the total electronic energy with respect to nuclear Cartesian coordinates. We are interested in the 100 to 1000 smallest eigenvalues $\lambda_k$ and associated eigenvectors $\boldsymbol{q}_k$ of (1). The corresponding vibrational frequencies are obtained by $\omega_k \sim \sqrt{\lambda_k}$. The simulation involves approximately $5 \cdot 10^8$ atoms leading to a matrix $\boldsymbol{H}$ of size about $1.5 \cdot 10^9$. In this thesis, the existing eigensolver FEMAXX [2, 3, 4] will be extended in order to solve this challenging problem.

Besides the challenging numerical and computational aspects, great insights into how sound breaks up in the material would immediately result from this thesis.

### Tasks

- Detailed formulation of the problem.
- Characterization of the eigenvalue problem.
- Adaptation of the existing Jacobi–Davidson algorithm FEMAXX to the problem at hand.
- Select an appropriate preconditioner for the solution of the correction equation (inner iteration).
- Optimize the convergence criterion for the inner iteration [5].

## Requirements

- Student in computational science or physics.
- Very good knowledge in numerical mathematics.
- Knowledge of parallelization techniques & C++ is advantageous.

## Milestones

The thesis starts on date $x$

- $x$: Literature search and study
- $x+2$ weeks: short 15 minute talk on: how you understand the problem, including a schedule with tasks & milestones
- $x+2$ months: presentation of status (less than 30 minutes)
- $x+5/6$ months: report handed in.
- Final presentation shortly after.

## Notes

- This project is a collaborative effort between PSI, ETH Zurich and MIT.
- A term project can precede the MSc thesis.

## Contact


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## References


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