# A thermo-mechanical MD-FE coupling based on the generalized Langevin equation and digital filters approximations

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**ABSTRACT**

The main motivation of this work is to reduce the computational expenses of Molecular Dynamics (MD) simulations by means of a direct multi-scale approach. At its early age, the multi-scale coupling methods between molecular dynamics and continuum methods considered only low temperatures, mainly for simplicity reasons. However, the coarsening of a finite element mesh away from the atomic region can trap a part of the kinetic energy which would introduce a non-realistic overheating in the fine scale model. A homogeneous temperature can be enforced, as many authors did, by employing classical thermostats. However, a large heat generation, as it occurs in the case of sliding friction, release a lot of kinetic energy that needs to be transported at the adequate conduction speed through the coupling interface. The nature of heat in itself is a difficulty: at the atomic scale, mechanical waves and heat constitute the dual facets of the same phenomenon. Only marginal coupling approaches are nowadays capable of handling finite temperatures and heat fluxes.

We present a technique of spectral separation of waves[1]. The aim is to transmit mechanically to the continuum model only the waves for which enough degrees of freedom are available. Concretely, only the lowest frequencies serve as a boundary condition to the finite element model which represents the mechanical deformations. On the contrary, the high frequency part that was not transmitted cannot remain trapped in the atomic region. A selective damping approach allowed us to damp only that targeted range of frequencies and constitutes the heat flux going from atomic regions towards continuum regions. Also, the continuum must have a flux that injects thermal energy to the molecular dynamics model. The sum of both these heat flows is the net heat flux through the coupling interface. An adequate flux balance equation has been designed and enforced using the general Langevin dynamics formalism with the constraint that it acts only on the desired frequency band. This allows a two-way coupling of thermal energy, with total energy conservation (within the thermal noise precision) within a coupling between molecular dynamics, thermal and mechanical continuum representations.

A prototype of the method as been implemented and validated[2] in the LibMultiScale open-source framework. Nevertheless, the high computational cost of the convolution operation necessary to achieve a proper spectral filtering calls for approximations and compromises between accuracy and speedup. In this talk, we present the fundamentals of the employed coupling strategy followed with a study of possible filtering approximations, such as adaptive coarsening and FFT, which renders this approach fully functional.

## References

[1] S. B. Ramisetti, G. Anciaux, and J. F. Molinari. Spatial filters for bridging molecular dynamics with finite elements at finite temperatures. 253:28–38.

[2] S. B. Ramisetti, G. Anciaux, and J. F. Molinari. A concurrent atomistic and continuum coupling method with applications to thermo-mechanical problems. 97(10):707–738.