

Some mathematical and algorithmic aspects of computational materials science

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The talk will overview some recent mathematical contributions to computational materials science. First, the theoretical and challenging question of the passage from computational chemistry and microscopic solid state physics models (such as Hartree Fock type models) to continuum mechanics models for crystalline solids will be addressed. The discussion will be based upon a series of joint works with Xavier Blanc (Université Paris 6 and INRIA, Paris) and Pierre Louis Lions (College de France, Paris).

Second, some numerical aspects of the problem will be considered. Practical numerical approaches like the quasi-continuum method (a method coupling a discrete, atomistic description of matter, with a continuum mechanics description) will be examined from the perspective of numerical analysis. The second part of the talk is based on a series of works with Xavier Blanc and Frederic Legoll (LAMI-ENPC, Paris).