

**About an analytical approach to a quasicontinuum method via  
 $\Gamma$ -convergence**

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**Abstract**

Quasicontinuum (QC) methods are computational techniques to reduce the complexity of atomistic simulations in a static setting. The main idea is to couple atomistic and continuum models.

I will present recent results with A. Schlömerkemper, where we aim at a mathematically rigorous verification of a QC method in the context of fracture mechanics. To this end, we start from a one-dimensional system and consider a chain of atoms with nearest and next-to-nearest neighbour interactions of Lennard-Jones type and focus on the so called quasinonlocal quasicontinuum approximation. We derive a development by  $\Gamma$ -convergence of this QC approximation and compare the limiting functional and its minimizers with those obtained for a fully atomistic system. In particular, it turns out that the discretization in the continuum region has an impact on the validity of the QC approximation. See arXiv:1405.6122 for details.