

Singularities in PDE and the calculus of variations

Singularités en EDP et dans le calcul des variations

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Recent advances in orbital-free density functional theory

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Abstract

I will describe an efficient implementation of the Truncated-Newton method for energy minimization in the context of Orbital-free Density Functional Theory. I will illustrate the efficiency and accuracy of the method with numerical simulations in an Aluminium FCC lattice.