Physics > Computational Physics

Computation of electron quantum transport in graphene nanoribbons using GPU

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The performance potential for simulating quantum electron transport on graphical processing units (GPUs) is studied. Using graphene ribbons of realistic sizes as an example it is shown that GPUs provide significant speed-ups in comparison to central processing units as the transverse dimension of the ribbon grows. The recursive Green's function algorithm is employed and implementation details on GPUs are discussed. Calculated conductances were found to accumulate significant numerical error due to single-precision floating-point arithmetic at energies close to the charge neutrality point of the graphene.

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