

## Charge and phonon transport in graphene

Vittorio Romano,  
University of Catania, Italy

The last years have witnessed a great interest for 2D-materials due to their promising applications. The most investigated one is graphene which is considered as a potential new material to exploit in nano-electronic and optoelectronic devices.

Charge transport in graphene can be described with several degrees of physical complexity. At quantum level an accurate model is represented by the Wigner equation but in several cases its semiclassical limit, the Boltzmann equation, constitutes a fully acceptable model. However, the numerical difficulties encountered in the direct solution of both the Wigner and the semiclassical Boltzmann equation has prompted the development of hydrodynamical, energy transport and drift diffusion models, in view of the design of a future generation of electron devices where graphene replaces standard semiconductors like silicon and gallium arsenide. Moreover, thermal effects in low dimensional structures play a relevant role and, therefore, also phonon transport must be included.

Interesting new mathematical issues related to the peculiar features of graphene arise. The main aspects will be discussed and recent results [1-9] illustrated in the perspective of future developments, in particular the optimization of graphene field effect transistors.

- [1] A. Majorana, G. Nastasi, V. Romano, Simulation of bipolar charge transport in graphene by using a discontinuous Galerkin method, *Comm in Comp. Physics* (2018).
- [2] L. Luca, V. Romano, Comparing linear and nonlinear hydrodynamical models for charge transport in graphene based on the Maximum Entropy Principle, *Int. J. of Non-Linear Mech.* (2018).
- [3] M. Coco, A. Majorana, V. Romano, Cross validation of discontinuous Galerkin method and Monte Carlo simulations of charge transport in graphene on substrate, *Ricerche mat.*, 66, 201—220, 2017.
- [4] A. Majorana, V. Romano, Numerical Solutions of the Spatially Homogeneous Boltzmann Equation for Electrons in n-Doped Graphene on a Substrate, *J. of Computational and Theoretical Transport* 46(3), 176-185, 2017.
- [5] G. Mascali, V. Romano, Charge transport in graphene including thermal effects, *SIAM J. Applied Math.* Vol 77 (2), 593-613 (2017).
- [6] M. Coco, G. Mascali, V. Romano, Monte Carlo Analysis of Thermal Effects in Monolayer Graphene, *J. of Computational and Theoretical Transport* 45(7), 540-553, 2016.
- [7] A. Majorana, G. Mascali, V. Romano, Charge transport and mobility in monolayer graphene, *J. Math. Industry* 7:4, <https://doi.org/10.1186/s13362-016-0027-3>, 2016.
- [8] M. Coco, A. Majorana, V. Romano, DSMC method consistent with the Pauli exclusion principle and comparison with deterministic solutions for charge transport in graphene, *J. Comput. Phys.* 302, 267-284, 2015.
- [9] V. D. Camiola, V. Romano, Hydrodynamical Model for Charge Transport in Graphene, *J. Stat. Phys.* 157, 1114-1137, 2014.