



Banff International Research Station for Mathematical Innovation and Discovery

Coupled Mathematical Models for Physical and Biological Nanoscale Systems and Their Applications

Workshop brief summary and outcomes in the following three areas:

- A.** Charge and spin transport in low-dimensional structures
- B.** Modeling biological phenomena from nano to macro scales
- C.** Mathematics for 2D materials and properties of confined nanostructures

In each of these areas we highlight open/critical problems, experimental achievements, current state-of-the-art modeling and feasibility of mathematical and computational methodologies. These problems require interdisciplinary efforts from different communities present at this workshop.



Some examples of synergies between fields that are the direct result of interactions during the workshop are:

- ▶ Better understanding of joint efforts required by mathematical modeling, physics, and computational science communities to treat challenging issues in the description of properties of nanostructures (e.g., nonlinear quantum mechanical phenomena, multiple spatial and temporal scales and their interactions, phonon description, transport in low dimensional nanostructure and non-local transfer operations, lack of periodicity in nanoscale systems with incommensurate structures as an example, identification and analysis of important control parameters for quantum information processing, etc)
- ▶ Cross-fertilization of ideas between these communities and life sciences in attacking new identified open/critical problems (including the development of new stochastic models for proliferation of bacterial colonies, biofilms; injection conditions from kinetic theory of semiconductors applied in the description of angiogenesis, transport in confined biological media, microtubules characteristics including electromechanics, information processing with biomolecules, etc)
- ▶ Consensus building towards a key role of refined mathematical models accounting for coupled effects and phenomena in the description of physical and biological systems, as well as the interaction of such systems with their environment (e.g., the issue of boundary conditions, the role of external fields and strain, heterogeneity of the environment and its treatment by the entropy, etc).
- ▶ Further clarification, refinement, and interpretation of the influence of important contributions by experimentalists on the development of new models, computational techniques, and the description of new phenomena, and vice versa (e.g., the issue of scalability for nanosystems; spin-orbit proximity effect in graphene and the Hall drag between two layers of this material; nonequilibrium single-molecule pulling experiment; unfolding pathway dynamics, etc).

One of the important outcomes was the creation of networks across disciplinary borders, and the initiation of several new ideas for collaborations.