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MULTISCALE/MULTIPHYSICS COMPUTATIONAL MODELS FOR LAB-ON-CHIP TECHNOLOGY APPLICATIONS

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ABSTRACT

In this communication, we propose and investigate multiphysics and multiscale computational models for the simulation of complex problems in Lab-On-Chip technology applications [1].

The aim of the research is *i*) to devise a mathematical model capable of accounting for the electrical, fluid-mechanical and bio-chemical phenomena simultaneously occurring in complex bio-electronic systems like bio-chips or bio-reactors; *ii*) to devise computational techniques for an efficient, accurate and stable numerical approximation of the above mentioned model; *iii*) to incorporate models and numerical methods in a general-purpose simulation tool that can be easily adapted to cover a wide variety of applications, including the areas of interest of Micro and Nano Fluidics [2], Bio-Electronics [3], Tissue Engineering [4] and Electrophysiology [5].

To accomplish the above objectives, we consider the nonlinear Poisson-Nernst-Planck/Navier-Stokes (PNP/NS) system of PDEs [6], suitably coupled with generation/reaction zero-order terms, reduced-order ODE systems and interface transmission conditions to treat the problems at hand according to a heterogeneous multi-domain formulation [7,8,9].

For the numerical solution of the PNP/NS system, we use a fixed-point solution map for system decoupling and linearization, which generalizes the classical Gummel's algorithm used in semiconductor

device simulation [10]. Discretization of each decoupled subproblem is carried out using Galerkin hybridized finite elements, because of their capability of ensuring flux conservation, sharp fronts and discrete maximum principles.

We discuss several numerical examples to validate the proposed methodologies in the simulation of realistic bio–chips and bio–reactors.

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