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ANALYSIS OF DIFFERENT ADAPTIVE MESH STRATEGIES FOR NUMERICAL SIMULATIONS OF ELECTROPHORETIC SEPARATIONS

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Abstract. Electrophoretic separations comprise a set of analytical techniques based on the application of an electric field to explode different physicochemical characteristics of molecules in order to discriminate and identify them. In recent years these techniques have been extremely important in the development of different fields of bioanalytical chemistry such as genomics, proteomics and metabolomics.

Numerical simulations of electrophoretic separations have contributed to the development of these techniques since the beginning of their academic and commercial use in the early 80's. They provide information about the influence of the different experimental conditions as well as crucial information about the behavior of different sample components, and the overall analytic performance of the studied methods. In general, numerical simulations of electrophoretic separations are challenging due to its multiphysics nature (the solution of the electric, mass transport and fluidic problems are required), the large amount of different substances (numerically, degrees of freedom) interacting in the separations, and the extremely fast migration process during the transient phases of the separations that generates extremely high local Peclet number (up to 2000). Due to these particular characteristics, adaptive mesh refinement is a powerful tool in order to improve the accuracy and the computational cost of these simulations enabling the analysis of the performance of different experimental conditions in a reasonable computing time. In this work we present a study of performance for two different adaptive mesh refinement strategies: node relocation and h-adaptivity for the solution of numerical simulation of the three most common electrophoretic techniques used in practice: capillary electrophoresis, isotachophoresis and isoelectric focusing.

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