

Simul 6 – Free fast dynamic simulator of electrophoresis

Bohuslav Gaš*¹, Petr Bravenec²

¹ Faculty of Science, Charles University in Prague, Czech Republic

² Hobrosoft, s.r.o., Prague, Czech Republic

The separation process in capillary electrophoresis is of an inherently nonlinear nature. Though the equations describing electromigration of ions can easily be formulated, at least in its basic form, it is much more difficult to solve them due to their complexity and reveal all features of electrophoretic systems. The forceful development of computers paired with efficient numerical algorithms has enabled us to create software tools that are able to solve such equations numerically very rapidly and allow users to perform electrophoretic separations "virtually", not using a real instrument.

We have developed a series of efficient software for the numerical solution of the electromigration equations, Simul. Now we come with a largely reconstructed, latest version – Simul 6. Its computation core has been substantially redesigned in order to take full advantage of parallelization. The code has been rewritten in a fully standard-conformant C++ language using the Qt Cross-platform and is open under GNU General Public License, Version 3. Its computation speed is about 5 – 15 times faster than the previous generation. The Graphic User Interface allows for easily formulating separation tasks.

Practical examples have been provided to demonstrate the ability of the program, which can be downloaded from <http://echmet.natur.cuni.cz/>

Acknowledgments

The designing of Simul 6 was supported by the Czech Science Foundation, GAČR Grant No. 18-11776S and Agilent Foundation Research Gift No. 4135.