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Development and implementation of the Kinetic Monte Carlo algorithms from scratch

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The widespread use of personal computers and laptops brough our generation to a new digital era of science. Nowadays we have an excellent opportunity to save time and money on expensive experiments and use computer power for generating “labs-on-the-chips”. Geochemical systems can be modeled and simulated up to molecular details. This approach does not substitute experiments and field studies but can help us to substantially improve their scientific efficiency. The widespread availability of computational software for numerical simulations, such as Matlab, Mathematica, and open-source codes for modelling geochemical systems across the scales, allows us and our students to implement any system or process of interest.

The major obstacle, however, in generating “digital geochemical systems on a chip” is not technical. It is educational: most geoscience programs are not equipped yet with in-depth courses for computational modelling and algorithm design. The issue is that design of algorithms and their implementation for the purposes of special scientific problems require building skills for long periods of time. This time gap impedes the progress of the students in their research tasks involving computer simulations.

Here I share my experience and expertise on writing Kinetic Monte Carlo models for simulations of reactions at mineral-fluid interfaces. I write codes in FORTRAN for number-crunching tasks as well as scripts in Python for data processing and workflow management. In this presentation I share my strategies on writing efficient codes from scratch. I discuss how to help yourself and your students in overcoming the following commonplace issues: the fear of coding, the “black box” treatment of open-source codes and software, difficulties in translating research problems from the “language of nature” to the “language of Boolean logic”, and final technical implementations.