Introducing GCex: a Tool for setup and Interactive Visual Exploration of geochemical simulations

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In this contribution we introduce a newly developed software tool, GCex, designed to visually help the geochemists in tasks such as uncertainty and sensitivity analysis, model calibration, parameter refinement and, in general, the in-depth exploration of large ensembles of geochemical models through a Graphical User Interface (GUI). This is a very challenging task since geochemical models are massively multivariate, with many input and even more output parameters, each possibly varying in scales spanning through several magnitude orders. The resulting analyses therefore often consist of several ten of thousand single model runs. Designed with flexibility and interactivity in mind as a visual data exploration tool, GCex implements a Visual Analytics approach combining hierarchical horizontal axis visualization (Stacked Parameter Relation, SPR) with semi-automatic guidance through linear sensitivity analysis. These conceptually simple but powerful methods allow the user to effectively identify the most significant effects on model's outputs in different regions of the input parameters space. The tool is based on open source components and the current implementation, altough in principle simulator-independent, covers the use of PHREEQC through the Rphree interface [1]. An additional GUI is provided for setting up the analysis, sampling the input parameter space, dispatching the calculations with automatic parallelization and gathering the results, thus greatly enhancing the user-friendliness of the whole workflow.

The use of GCex is demonstrated with a sensitivity analysis of a reaction involving the reductive dissolution of pyrite with precipitation of pyrrothite in presence of gaseous hydrogen. GCex enables exploring and visualizing at once a broad range of conditions, including extended range of temperature, pressure, background salinity, composition of the mineral assemblage, the presence of carbonate buffers and also comparing the effect of different thermodynamical databases. This study was a part of the german H2STORE research project investigating feasibility of hydrogen storage in porous media.

[1] De Lucia, M., Kühn, M. (2013): *Coupling R and PHREEQC: Efficient Programming of Geochemical Models*, Energy Procedia 40, p. 464-471, doi: 10.1016/j.egypro.2013.08.053