Geophysical Research Abstracts
Vol. 18, EGU2016-16066, 2016
EGU General Assembly 2016


# Parameter estimation and uncertainty quantification in a biogeochemical model using optimal experimental design methods

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The statistical significance of any model-data comparison strongly depends on the quality of the used data and the criterion used to measure the model-to-data misfit. The statistical properties (such as mean values, variances and covariances) of the data should be taken into account by choosing a criterion as, e.g., ordinary, weighted or generalized least squares. Moreover, the criterion can be restricted onto regions or model quantities which are of special interest. This choice influences the quality of the model output (also for not measured quantities) and the results of a parameter estimation or optimization process.

We have estimated the parameters of a three-dimensional and time-dependent marine biogeochemical model describing the phosphorus cycle in the ocean. For this purpose, we have developed a statistical model for measurements of phosphate and dissolved organic phosphorus. This statistical model includes variances and correlations varying with time and location of the measurements. We compared the obtained estimations of model output and parameters for different criteria.

Another question is if (and which) further measurements would increase the model's quality at all. Using experimental design criteria, the information content of measurements can be quantified. This may refer to the uncertainty in unknown model parameters as well as the uncertainty regarding which model is closer to reality. By (another) optimization, optimal measurement properties such as locations, time instants and quantities to be measured can be identified.

We have optimized such properties for additional measurement for the parameter estimation of the marine biogeochemical model. For this purpose, we have quantified the uncertainty in the optimal model parameters and the model output itself regarding the uncertainty in the measurement data using the (Fisher) information matrix. Furthermore, we have calculated the uncertainty reduction by additional measurements depending on time, location and tracer.

The high computational effort of a model evaluation was encountered by using the transport matrix method with spatial parallelization, advanced derivative-based optimization algorithms and a cost saving approximation of the derivative. Globalization techniques were used to overcome local minima. Due to a special software interface, coupling of arbitrary water-column biogeochemical models is possible. In the talk, we present the used methods together with results for this exemplary model.