26th International Congress on Modelling and Simulation, Adelaide, SA, Australia, 30 Nov–4 Dec 2025
mssanz.org.au/modsim2025

PEST++SQP: a new, non-intrusive, open-source package for high-dimensional non-linear optimisation under uncertainty

Reygie Q Macasieb [a b], **Matthew J Knowling** [c d], **Jeremy T White** [e]

[a] *INTERA Geosciences, Perth, Western Australia, Australia, 6000*
[b] *School of Earth and Oceans, The University of Western Australia, Crawley, Western Australia, Australia, 6009*
[c] *School of Architecture and Civil Engineering, The University of Adelaide, South Australia, Australia, 5001*
[d] *School of Agriculture, Food and Wine, The University of Adelaide, South Australia, Australia, 5001*
[e] *INTERA Inc., Austin, Austin, Texas, USA*
Email: rqmacasieb@intera.com

Abstract: Real-world environmental resource management problems are often complex, involving many decision variables as well as uncertainty and nonlinearity in objectives and constraints. Application of formal quantitative approaches to address such problems remains prohibitive, especially with the increasing complexity and thus computational expense associated with environmental simulation models.

Sequential quadratic programming (SQP) is an approach that has been proven in the petroleum industry to explicitly handle very high dimensional problem sequencing and resource development with both nonlinear constraints and objective function. An active set approach is often used in solving a reduced quadratic programming subproblem in order to handle both equality and inequality constraints in an effective and tractable manner, and a practical line search method is used to determine the optimal parameter upgrade.

While interest in formal management optimisation is growing in applied environmental modelling, there remain few large-scale applications to date, largely reflecting the fact that available software do not provide robust, scalable and generalised SQP capabilities.

We have implemented the SQP algorithm within the open-source community-driven software ecosystem of PEST++. This enables: (i) a non-intrusive and parallelised application programming interface that allows the tool to be applied to a wide range of models and provides flexibility in problem definition, (ii) support for both finite-difference and ensemble-based gradient approximations, and (iii) on-demand switching to other algorithms with PEST++ such as the iterative ensemble smoother to seek/maintain feasibility.

We will present theory and concepts related to the SQP algorithm, its implementation within the PEST++ suite, how it handles model input uncertainty, and how it can provide posterior prediction uncertainty estimates. We will demonstrate an example application of PEST++SQP in a groundwater management optimisation problem with a large number of decision variables and nonlinear constraints.

Keywords: *Decision support, optimisation under uncertainty, nonlinear constraints, sequential quadratic programming, resource management*