

Nonlinear optimization for reservoir characterization

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1. Abstract

At IFP, optimization problems are encountered in many different applications, such as seismic tomography, characterization of reservoirs, engine model calibration, etc. Many of them are expressed as inverse problems with a nonlinear forward problem that is generally time consuming. The size of those problems is varying: from 10 up to 10000. Moreover, the underlying optimization problems are often subject to inequality constraints. To solve these problems, we are currently developing a general software package, called SQPAL, which should be flexible enough to fit the large variety of requirements of the applications under study.

SQPAL is a Sequential Quadratic Programming algorithm developed to solve general nonlinear programming problems dealing with nonlinear equality and inequality constraints. The originality of our approach is to solve the osculating quadratic problem with linearized constraints by an augmented Lagrangian method, which has the potentiality to cope with many inequality constraints. The performances of SQPAL first on small and then on middle size NLP problems from the CUTER benchmark are illustrated.

The presented industrial application is a reservoir characterization problem, which aims at forecasting the production of an oil or gas field from available production data. Production data are measures of pressure, oil/water/gas rates at the wells and may be completed with 4D seismic data. Parameters to be determined in this inverse problem are for example, the petrophysical properties in some reservoir zones (permeability, porosity, ...) or the well productivity indexes. The associated forward problem is a fluid flow simulator for a given reservoir geological model, which may require a large computational time. The potential of the SQPAL solver for this industrial application is illustrated on a 2D realistic static problem including 2D seismic data.

2. Keywords: nonlinear optimization, SQP algorithm, augmented Lagrangian, CUTER benchmark, reservoir characterization.

3. Introduction

Optimization takes place in many IFP applications: estimating the parameters of numerical models from experimental data (earth sciences, combustion in engines), design optimization (networks of oil pipelines), optimizing the settings of experimental devices (calibration of engines, catalysis). These optimization problems consist in minimizing a functional that is complex (nonlinearities, noise) and expensive to estimate (solution to a numerical model based on differential systems, experimental measurements), and for which derivatives are often not available, with nonlinear constraints, and sometimes with several objectives among which it is necessary to find the best compromise. IFP has engaged an active research in this field for a number of years and develops its own optimization tools in order to match the needs of its applications as well as possible. The SQPAL solver is a sequential quadratic programming method suited to constrained nonlinear optimization problems. It has been developed in partnership with INRIA and industrialized for the TOMOinv1 and CondorFlow codes. Moreover, this solver has been successfully tested in two major fields of IFP applications: earth sciences and calibration of engines. We give below a list, which does not claim to be exhaustive, of the optimization problems solved with SQPAL in this two application fields.

- *Optimization problems in geophysics.* Two large scale nonlinear inverse problems have been tested in this discipline. The first one is the inverse problem of seismic reflection tomography [9]. It consists in determining a subsurface velocity model from the traveltimes of seismic waves reflecting

on geological interfaces. The optimization problem has a nonlinear least-squares objective and linear constraints. The size of the data space, of the model space and of the constraint space can be quite large (up to 106 data, 104 unknowns, and 104 constraints). The forward simulation is CPU time consuming. This problem has been solved with SQPAL using a Gauss-Newton method, the Jacobian matrix being sparse and computed at a negligible CPU time cost. The second problem of this discipline is the prestack elastic waveform inversion. Its aims at determining a subsurface elastic model (P-impedance, S-impedance, and density) from prestack seismic data. It is formulated as a nonlinear least-squares optimization problem with bound constraints. For 3D real applications, the number of data, unknowns and constraints are each larger than 107. The forward simulation is CPU time consuming and only the gradient is available (the Jacobian matrix cannot be stored in memory). This problem is classically solved with a nonlinear conjugate gradient algorithm. The SQPAL solver has been tested on this problem using a BFGS Hessian approximation.

- *Optimization problems in geology and more particularly the stratigraphic inversion of sedimentary basins.* This problem consists in determining the geometry, facies, and petrophysical properties of sedimentary layers from geological data (subsidence rate, sea-level variations, bathymetry range). This is a large scale nonlinear optimization problem with nonlinear constraints. The gradient is computed by the adjoint-state method. This problem is solved using the SQPAL solver with a Gauss-Newton method.
- *Optimization problems in calibration of engines.* It aims at finding the best control parameters of an engine over multiple objectives such as jointly minimizing polluting agent emission and fuel consumption. It is a multi-objective nonlinear constrained optimization problem where analytical gradients are not available. Luckily, the size of the problem is small: less than 50 unknowns and around 100 constraints. Numerical gradient are computed thanks to an approximated model of the cost function and a solution can be found with SQPAL using a BFGS Hessian approximation.

In Section 4, we briefly describe the SQPAL package and give a particular attention to two new implemented techniques: second order correction of the line-search globalization algorithm and elastic programming. Both techniques are crucial when dealing with nonlinear optimization avoiding respectively Maratos Effect and constraint infeasibility. The robustness of this solver is illustrated in Section 5 on small and middle size optimization problems of the CUTER benchmark. The results are compared to ones obtained from other solvers. In Section 6, we test SQPAL on a new industrial application: a reservoir characterization problem issued from reservoir engineering discipline.

4. SQPAL: a package for general constrained optimization problem

We consider the general constrained optimization problem

$$\min_{x \in \Omega} f(x) \quad \text{subject to } c_E(x) = 0, \quad c_I(x) \leq 0, \quad (1)$$

where a real-valued function $f : \Omega \rightarrow \mathbb{R}$ is defined on an open set Ω in \mathbb{R}^n , c_E and c_I are the vectors of equality and inequality constraint functions, respectively. We further define the feasible set

$$X = \{x \in \Omega : c_E(x) = 0, \quad c_I(x) \leq 0\}$$

and assume that f, c_E and c_I are differentiable functions. Moreover, c'_E is surjective or onto for all x in the open set Ω . Presently, numerical methods to solve (1) can be gathered into two classes:

- the class of penalty methods, which includes the augmented Lagrangian approaches and the interior point (IP) approaches,
- the class of direct Newtonian methods, which is mainly formed of the sequential quadratic programming (SQP) approach.

Often, actual algorithms combine elements of the two classes, but their main features make them belonging to one of them. The choice of the class of algorithms strongly depends on the features of the optimization problem to solve. The key issue is to balance the time spent in the simulator (to evaluate the functions defining the nonlinear optimization problem) and in the optimization procedure (to solve the linear systems or the quadratic programs). In the seismic reflection tomography application we argue that the SQP approach is the best fitted (see Delbos *et al.* [9]). Generally, this is particularly

true for applications where the forward modeling is CPU time consuming and where the number of iterations with a Newton-like algorithm is less smaller than the one generated with IP algorithms. This type of conditions are widely encountered at IFP, and particularly in inverse problems issued from earth sciences. This is our main motivation for developing the SQPAL solver, which implements an SQP-like algorithm.

4.1. Description of the SQPAL solver

Sequential quadratic programming (SQP) is one of the most effective methods for solving nonlinearly constrained optimization problems. The approach was first suggested by Wilson [23] for the special case of convex optimization, then popularized mainly by Biggs [3], Han [15], and Powell [19, 20] for general nonlinear constraints. Gould and Toint [14] survey the recent development in SQP. The main idea of the SQP approach is to solve the nonlinearly constrained problem using a sequence of quadratic programming (QP) subproblems. In each QP subproblem, the constraints are obtained by linearizing the constraints in the original problem, and the objective function is a quadratic approximation to the Lagrangian function.

SQPAL is a software developed for the general nonlinear optimization problem (1). Quasi-Newton techniques are used for the approximate the Hessian of the Lagrangian. Two types of quasi-Newton methods are implemented into the solver:

- the BFGS method, which is adapted to applications where second order derivatives of the cost function are not available but where gradient can be estimated.
- the Gauss-Newton method, which is suitable for least-squares applications in which Hessian is not available, while the Jacobian matrix of the forward problem can be computed.

To be practical, an SQP method must be able to converge from remote starting points. Two class of methods can be used at this point: line-search or trust regions. Several line-search algorithms are supplied in SQPAL. They use the l_1 exact penalty function as merit function. On the other hand, trust regions can also be used to globalize the Gauss-Newton algorithm, even when bound constraints are present. In subsection 4.2, we describe how to avoid the Maratos effect using a second order correction technique. To overcome the difficulty linked to linear constraint infeasibility, we follow the elastic mode idea proposed in the SNOPT program [13]; we will be more specific on this technique in section 4.3.

An originality of our SQP implementation is to use the augmented Lagrangian (AL) method to solve the QPs [9]. This is a well-established method to solve nonlinear optimization problems. Since it can be implemented in such a way that it does not need any matrix factorization, it is adapted to large problems. The difficulty linked to the augmentation parameter determination is based on a precise theoretical study [8], which has led us to design a suitable and effective heuristics [9]. The inner subproblems are solved by a technique combining gradient projection, active set, and conjugate gradient.

4.2. Avoiding the Maratos effect by second order corrections

The l_1 exact penalty function used in SQPAL can prevent the rapid local convergence of SQP by truncating steps that judged inadequate although they make good progress toward the solution. This is called the Maratos effect (see, for instance, Counter-example 15.6 in [5]). To avoid this difficulty, we use a second-order correction (SOC). This one provides further decrease in the constraints and is added to the usual SQP step.

Let us be more specific. If the SQP step is d_k , the second order correction w_k is defined by (see [18])

$$w_k = -M_k^T (M_k M_k^T)^{-1} \tilde{c}(x_k + d_k), \quad (2)$$

where $M_k^T = [\nabla \tilde{c}_i(x_k)]$ and $\tilde{c}(x)$ denotes the active constraint functions. In fact, w_k is the minimum-norm solution to the following equation $M_k w_k + \tilde{c}(x_k + d_k) = 0$.

We describe the Armijo algorithm with second order correction as Algorithm 1. First the Jacobian matrix M_k of active constraints at x_k is formed and the constraint function \tilde{c} is evaluated at $x_k + d_k$. We note that the step w_k can be defined by

$$w_k = -Y_k \tilde{c}(x_k + d_k), \quad (3)$$

where Y_k is some right inverse of the Jacobian matrix M_k (see [5]), which is assumed to be surjective. We assume that $M_k^T \in \mathbb{R}^{n \times n_c}$, $n \geq n_c$, where n is the number of parameters and n_c the number of active constraints. To compute matrix Y_k , we make a QR factorization of the matrix

$$M_k^T = QR,$$

where $Q \in \mathbb{R}^{n \times n_c}$ is an orthogonal matrix, $R \in \mathbb{R}^{n_c \times n_c}$ is an upper triangular matrix, using the modified Gram-Schmidt algorithm. By setting

$$Y_k = Q(R^T)^{-1}$$

and (3), w_k can be obtained (see [1] for more details).

The inefficiencies caused by Maratos effect can also be avoided by occasionally accepting steps that increase the merit function. But if a sufficient reduction of the merit function has not been obtained within a certain number of iterates of the relaxed step, then we return to the iterate before the relaxed step and perform a normal step, using a line-search or some other techniques to force the reduction of the merit function. This technique is called watchdog strategy (see [18]). Another way is to change the merit function. For instance, Fletcher's augmented Lagrangian merit function does not suffer the Maratos effect; see [5, 18] for more details.

Algorithm 1. Armijo algorithm with second order correction.

data: $\alpha_k = 1$, newpoint=false;

while not newpoint **do**

if Armijo condition is satisfied **then**

$x_{k+1} = x_k + \alpha_k d_k$, newpoint=true;

if Armijo condition is not satisfied and $\alpha_k = 1$ **then**

 compute w_k from (2);

if Armijo condition is satisfied for $x_{k+1} = x_k + \alpha_k d_k + \alpha_k^2 w_k$ **then**

$x_{k+1} = x_k + \alpha_k d_k + \alpha_k^2 w_k$, newpoint=true;

else

 choose new α_k ;

end

if Armijo condition is not satisfied and $\alpha_k < 1$ **then**

if Armijo condition is satisfied for $x_{k+1} = x_k + \alpha_k d_k + \alpha_k^2 w_k$ **then**

$x_{k+1} = x_k + \alpha_k d_k + \alpha_k^2 w_k$, newpoint=true;

else

 choose new α_k ;

end

else

 choose new α_k ;

end

end

4.2. Elastic programming: a technique to deal with infeasible QP subproblems

A difficulty arises in the SQP algorithm when the linearized constraints are incompatible, since then the QP subproblem is infeasible. Let us consider a simple example

$$x^2 + y^2 = 10, \quad x \geq 1, \quad \text{and} \quad y \geq 1.$$

These constraints are compatible ((1, 3) satisfies them). Now if the linearization point is $x = y = -10$, then the linearized constraints read

$$20d_x + 20d_y = 190, \quad d_x \geq 11, \quad \text{and} \quad d_y \geq 11.$$

It is clear that this system is inconsistent. To overcome this difficulty, we can define a relaxation of the SQP subproblem that is guaranteed to be feasible. Thus, the so-called elastic programming, which

is proposed in the SNOPT program [13], is used in SQPAL. When the QP subproblem is found to be infeasible, SQPAL solves the following auxiliary problem

$$\begin{aligned}
& \min_x f(x) + \beta e^T w \\
& \text{subject to } c_E(x) + w = 0, \\
& \quad c_I(x) + w \leq 0, \\
& \quad w \geq 0,
\end{aligned} \tag{4}$$

where e is the vector of ones and the penalty parameter β is chosen sufficiently large. The choice of β requires a heuristics and the condition $\|\lambda\|_\infty \leq \beta$ should be satisfied. We let the initial value of β to be

$$\beta = \max(10^4 \|\nabla f(x_s)\|_\infty, \epsilon_\beta),$$

where x_s is the first iterate at which inconsistent linearized constraints were detected and ϵ_β is a small positive threshold. In order to enforce the condition $\|\lambda\|_\infty \leq \beta$, the penalty parameter β is updated using the same algorithm as the one that updates the penalty weights of the merit function.

5. Small and middle size examples of the CUTER benchmark

CUTER [4] is a versatile testing environment for optimization and linear algebra solvers. The package contains a collection of test problems intended to help developers design, compare and improve new and existing solvers. In order to test the SQPAL solver, an interface has been built with this environment. This interface furnishes most of the input informations that SQPAL needs to solve an optimization problem (such as the evaluation of the function and gradient, the constraint Jacobian matrix, etc). SQPAL needs also several user-defined optimization parameters such as the required accuracies to reach the first-order optimality conditions, the maximum number of SQP iterations and the violation threshold of constraints. Note that, if these parameters are not defined, SQPAL can initialize them to standard values. Table 1 summarizes the SQPAL run-time options chosen for this study. Gradients are externally computed through CUTER tools. A BFGS method with Powell's correction has been chosen to approximate the Hessian matrix. The method is globalized thanks to an Armijo line-search with second order corrections. Finally, KKT thresholds are all fixed to 10^{-6} .

Table 1: SQPAL run-time options

gradient estimation method	no internal gradient estimation
Hessian matrix estimation/update method	BFGS method with Powell's correction
globalization method	Armijo line-search with SOC
maximum number of SQP iterations	800
Lagrangian gradient threshold	1.0e-6
equality constraint violation threshold	1.0e-6
inequality constraint violation threshold	1.0e-6
Lagrangian multipliers threshold for inequality constraints	1.0e-6
complementarity conditions threshold	1.0e-6

The results presented in this section focus on two different classes of the CUTER benchmark: the small size problems of Hock and Schittkowski [16] and the middle size problems. They can be selected from the complete benchmark and uploaded online*. Although these classes do not contain large scale problems, it is not an easy task, even for commercial optimization solvers, to solve them correctly (i.e. to fulfill the KKT conditions up to a defined accuracy). For each class, we present next the solver results in term of failure number. We then compare the SQPAL results with the ones obtained from three other optimization solvers: SNOPT [13], KNITRO [6] and LOQO [22].

The class of Hock and Schittkowski test problems contains 124 nonlinear optimization problems. Figure 1 shows that these problems are small size: the number of unknowns and constraints are respectively

*<http://numawww.mathematik.tu-darmstadt.de:8081/opti/select.html>

less than 30 and 40. Figure 2 shows that only SNOPT reach perfect results with no failure. SQPAL failed to find a solution for only 4 examples of this benchmark (the *hs13*, *hs16*, *hs17* and *hs61* examples). Note that this number of failures is in the order of the failures generated by the other optimization solvers. The use of a second order correction technique with a line-search globalization algorithm helps in solving more test of this benchmark. We particularly observe that 4 tests (the *hs12*, *hs27*, *hs47* and *hs49* examples) cannot be solved without the use of this technique.

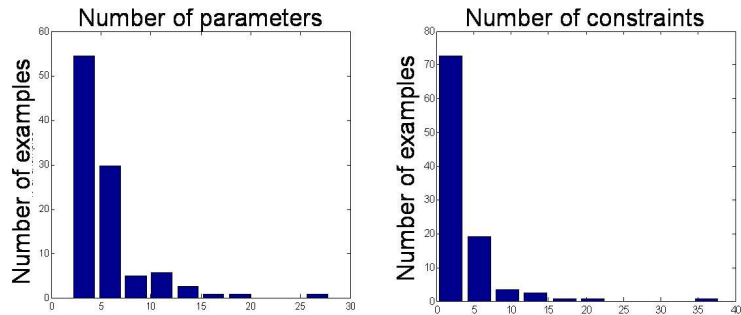


Figure 1: Description of the small size examples (Hock & Schittkowski examples) of the CUTer benchmark

Solver	SQPAL	SNOPT	KNITRO	LOQO
Failures	4/121	0/121	7/121	1/121

Figure 2: Results obtained with different optimization solvers on the small size examples of the CUTer benchmark (SNOPT, KNITRO and LOQO results can be found from LOQO website <http://www.princeton.edu/~rvdb/bench.htm>)

The class of middle size problems contains 319 general constrained optimization problems (linear or nonlinear, equality, inequality and bound constraints). Optimization problems of this class have less than 5000 unknowns and less than 350 constraints (see figure 3). The results of SQPAL compared to the other solvers are plotted in figure 4. We notice a good behavior of SQPAL with a small failures number (42 over 319) which is in the order of the other solvers. For this class, LOQO has the best results with 10 failures.

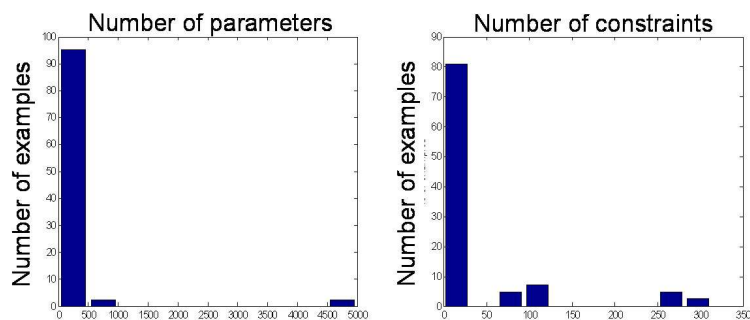


Figure 3: Description of the middle size examples of the CUTer benchmark

Solver	SQPAL	SNOPT	KNITRO	LOQO
Failures	42/319	24/319	57/319	10/319

Figure 4: Results obtained with different optimization solvers on the middle size examples of the CUTER benchmark (SNOPT, KNITRO and LOQO results can be found from LOQO website <http://www.princeton.edu/~rvdb/bench.htm>)

6. Application of SQPAL for reservoir characterization

The goal of reservoir characterization is the estimation of the unknown reservoir parameters by integrating all kinds of available data. These reservoir parameters could be classified in two classes: those related to the geological modeling (spatial distribution of porosity, permeability, faults) and those related to the fluid flow modeling (relative permeability curves, productivity index of the wells). Those parameters could be determined directly by measurements (or only locally using well logs), this is the reason why this parameter estimation problem is formulated as an inverse problem with some forward simulators that depend on those parameters and compute some measurable data: production data acquired at production/injection wells (bottom-hole pressure, gas-oil ratio, oil rate), time lapse seismic data (more precisely compressional and shear wave impedances for different seismic campaigns at different calendar times during the production of the field). The associated forward problems are on one hand a fluid flow simulator, on the other hand, a petro-elastic model (PEM) based on rock physic Gassmann equations. For further details on this application see Fornel *et al.* [12] and Feraille *et al.* [11].

In the presented example, the dataset is composed of 2D seismic impedances (P and S-impedance) associated with a cross section of a reservoir built up of two block units (see figure 5 for P and S-impedance data). Its size is 3240m in x-direction and 90m in z-direction. The unknown parameters are the mean porosity of the two units and some parameters which control the spatial variations of the porosity (gradual deformations of Gaussian stochastic models of porosity, see Hu *et al.* [17]). It ends up with 18 parameters and 15000 measurements. This is a small test case with no repeated seismic (only one 2D seismic survey). This allows to compare easily different optimization methods. A realistic case will be larger: especially the number of measurements will be much larger (up to $1M$, Berthet *et al.* [2]). The formulation is a classical least-square formulation which measures the mismatch between the observed data and the modelled data, some weights are introduced to handle the uncertainties associated with the different types of data.

An important point is that the gradient of the objective function is not available in the forward simulator, the derivatives are computed thanks to finite differences. Then, a key point is the choice of the perturbation: we have adopted an adaptive step depending on the size of the trust region. If the size of the trust region is small, the step size is reduced. A too small step size leads to difficulties, some numerical instabilities in the forward simulator being observed. On this application, we have tested three methods (figure 6): BFGS quasi-Newton method coupled with a line search method for globalization, a Levenberg-Marquardt Gauss-Newton method and a Gauss-Newton Dog-Leg trust region approach, three options available in SQPAL. The two latter methods are very similar, the Levenberg-Marquardt coefficient being tuned from the comparison of the reduction of the quadratic model of the cost function with the effective reduction of the cost function as in the trust-region method. We notice that the two Gauss-Newton approaches give slightly better results than BFGS method which is not surprising for least-square problems. However, these methods are not applicable for realistic cases of $1M$ of measurements (with the computation of the huge Jacobian matrix). BFGS quasi-Newton is the appropriate method for this type of problem. On figures 7 and 8 are respectively plotted the P-impedance and S-impedance residuals associated to the initial and optimal model of the BFGS method. Both figures shows that residuals are smaller on the optimal model than on the initial one, which shows the good behavior of the optimization process.

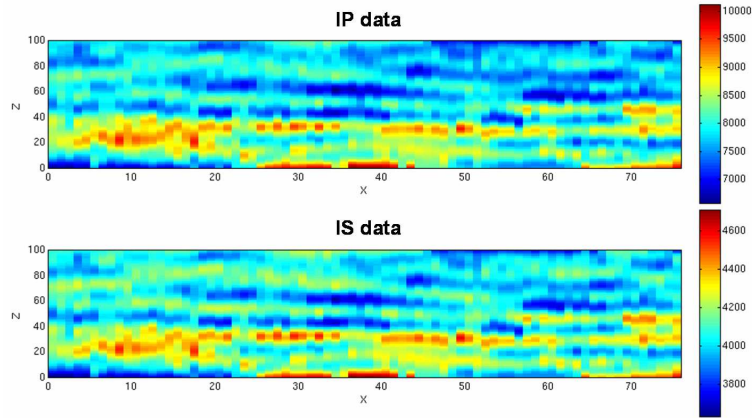


Figure 5: Ip and Is data

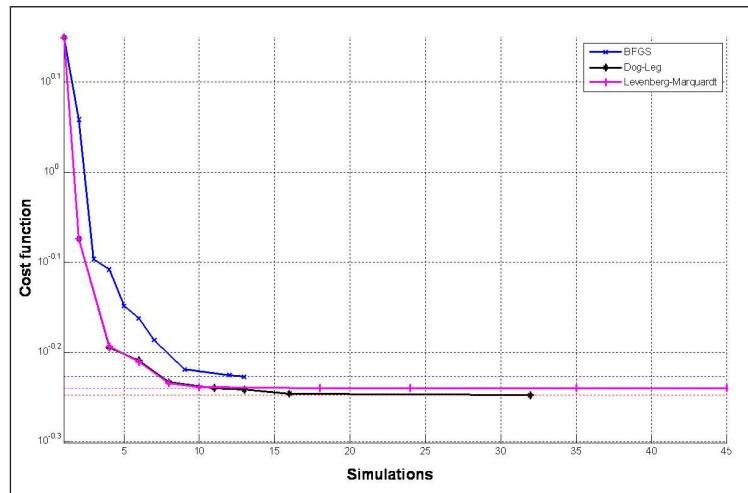


Figure 6: Cost function versus simulation numbers for 3 optimizations performed with BFGS method with line search globalization (in blue), with Levenberg-Marquardt Gauss-Newton method (in pink) and with Dog-Leg trust region method (in black). Each tag on the curves indicates one nonlinear iteration, the simulations needed to compute the numerical gradients being not taken into account here. The total number of simulations are: 193 for BFGS method (9 iterations), 181 for Dog-Leg method (8 iterations) and 227 for Levenberg-Marquardt Gauss-Newton method (9 iterations).

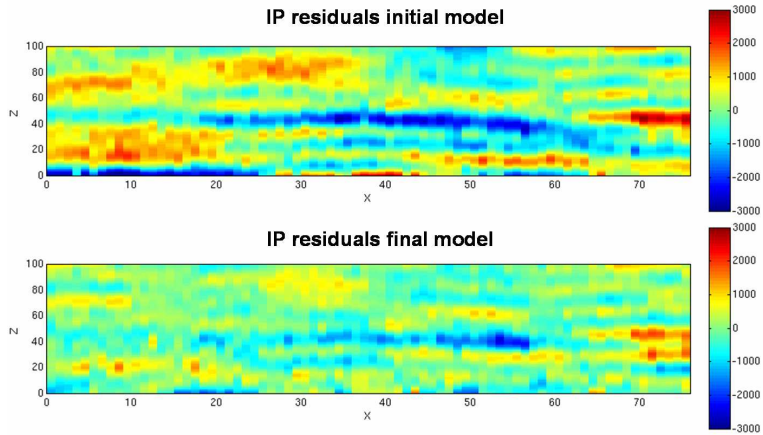


Figure 7: Residuals between Ip data and Ip modelled by the forward PEM simulator for the final model obtained by BFGS method.

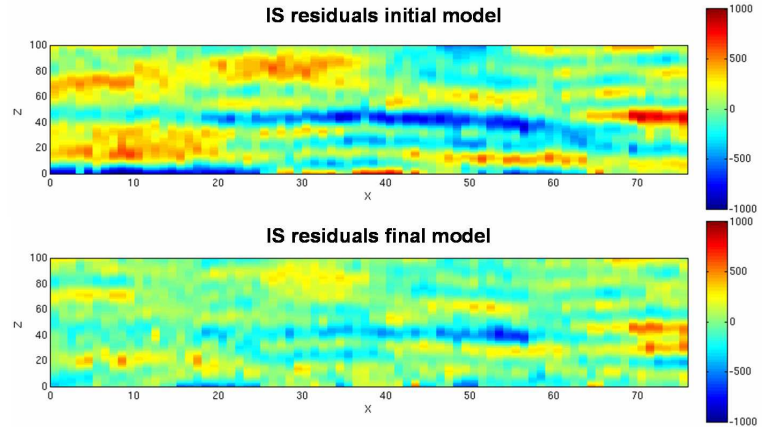


Figure 8: Residuals between Is data and Is modelled by the forward PEM simulator for the final model obtained by BFGS method.

5. Conclusions

The results obtained with our SQPAL solver are promising: it gives good global results on small and medium size problems of the CUTER benchmark. The techniques of elastic programming and line-search second order corrections are crucial to correctly solve more problems of the benchmark. Note that, to better estimate the potential of SQPAL over other solvers a performance profile analysis should be undertaken (see Dolan [10]). A Further step would be to investigate the efficiency of this solver for the large size problem of the CUTER benchmark. This study may require a limited storage algorithm like the l-BFGS algorithm which is not yet implemented in SQPAL.

For the static problem of our reservoir characterization application, SQPAL gives a reliable solution. The next step will be to apply it to the dynamic problem which includes 4D seismic data. As the number of unknowns and data is much larger in the dynamic problem, SQPAL should be used with the l-BFGS algorithm. Moreover, the computation of numerical gradient is an obstacle to a large number of parameters (simulations are time consuming, especially fluid flow simulator). A study of surrogate optimization techniques as Derivating Free Optimization approach proposed by Conn *et al.* [7] and Powell [21] is in progress.

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