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GEOMETRIC OPTIMIZATION OF NUCLEAR REACTOR CORES

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Abstract. Traditional designs of nuclear reactor cores, both for power and research reactors, rely on expert judgment and good practices with sound theoretical and experimental backgrounds. There are, however, come cases in which the decision of which design is the best for a certain application that cannot be easily answered and an engineering design optimization scheme ought to be applied. This work addresses some simple problems in which geometric parameters should be chosen in such a way to optimize a certain objective function—for example the location of irradiation chambers or boron injection nozzles—in order to understand how the different minimization algorithms works. The objective function to optimize may refer to performance such as maximize the neutron flux at a certain location, to economics for example to reduce as much as possible the construction and/or operations costs, or to a certain combination of both aspects. In particular, only two-dimensional few-group core-level problems are described in this article, because they are simple enough to be well understood and analyzed yet at the same time they maintain the basic physics and some of the geometric complexities found in full three-dimensional cases. The methodology developed for optimizing the simple problems addressed in this work can be extended to handle real cases of interest for the nuclear industry.

1 INTRODUCTION

When performing the conceptual engineering design phase of a new nuclear reactor, a number of decision have to be made in such a way to obtain the best performance, to reduce costs or—more often than not—even both at the same time. Many of these design decisions can be translated into a numerical values for certain parameters such as allowed content of boron in graphite or the required uranium enrichment of the fuel. In particular, the geometrical properties of the core fall within the scope of design parameters that ought to be optimized under both technical and economical points of view. In some cases, the values of the parameters that give the best results can be easily inferred by a cognizant engineer using a combination of common sense, best practices and particular expertise. However, there exist some parameters whose optimum value is not easily known beforehand and require the application of mathematical optimization techniques.

This article addresses a relatively simple problem of core-level neutronic design that at the same time presents the usual difficulties that are encountered in multidimensional minimization problems. In particular, it consists of finding where to locate a certain neutron absorber inside a simplified model of a two-dimensional reactor core in order to maximize its negative contribution to the overall reactivity. Even though the selected problem may seem fairly simple—which indeed it its—on the one hand it represents the first attempts to apply minimization algorithms to optimize nuclear reactor designs in the framework of the author's PhD thesis work and, on the other hand, the solution of the problem is not trivial and involves the application of state-of-the art numerical methods for solving both the neutron diffusion equation over unstructured grids (Theler, 2012) and the optimization problem (Theler et al., 2010).

2 THE FISH-IN-A-REACTOR PROBLEM

A classical problem in the nuclear reactor analysis academia (Lamarsh, 1966) consists of the following situation in two dimensions. Consider a circular bare homogeneous reactor of radius A that has an excess static reactivity equal to ρ_0. Now assume a small circular fish of radius $a \ll A$ is able to swim all over the reactor. The problem consists of finding the net reactivity change $\Delta\rho(r) = \rho(r) - \rho_0$ as a function of the location r of the fish—that acts mainly as a neutron absorber—with respect to the reactor center.

The traditional solution consists of employing perturbation techniques to the neutron diffusion theory to compute the reactivity change with respect to the analytical solution

$$\rho_0 = \frac{\nu\Sigma_{f0} - \Sigma_{a0} - D_0 \left(\frac{\nu_0}{A}\right)^2}{\nu\Sigma_{f0}} \tag{1}$$

where $\nu\Sigma_{f0}$ is the macroscopic ν-fissions cross section, Σ_{a0} is the one-group reactor macroscopic absorption cross section, D_0 the neutron diffusion coefficient, A is the reactor's radius and $\nu_0 = 2.4048\ldots$ is Bessel's zero-th order function first zero.

In the present work, not only do we solve the one-fish-in-a-reactor problem but we also address other fictitious cases involving optimization of the location of two and three fishes to accomplish a maximum negative reactivity contribution. Even though the multiple-fish problems can be solved using perturbation theory also, we solve the full neutron diffusion equation explicitly taking into account the location and size of the fish involved using a discretization scheme based on the finite element method using non-structured grids.

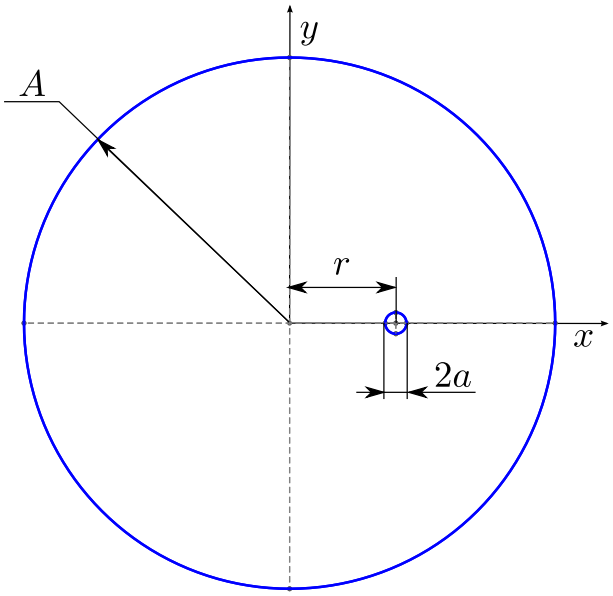


Figure 1: Continuous geometry containing a circular bare homogeneous reactor of radius A and a small neutron-absorbing circular fish of radius a located at a distance r of the reactor center.

2.1 One single fish: the S-curve

To solve the original one-fish problem—and at the same time to illustrate the procedure used to compute the objective function to optimize—we construct a planar geometry over the $x-y$ plane consisting of a big circle of radius A center at the origin and a small circle of radius a centered at $x = r$ and $y = 0$, as depicted in figure 1.

The dependance of $\Delta\rho$ with the position r can be obtained by parametrically varying r between zero and $A - a/2$ with a certain increment Δr. First, we need to generate a discrete grid corresponding to the continuous geometry of the problem for each value of $r \in [0, A-a/2]$. We use the free[1] program gmsh (Geuzaine and Remacle, 2009) to perform this step. Second, we have to solve the neutron diffusion equation. We use the free[2] program milonga (Theler, 2011) to obtain the net reactivity as a function of r. In fact, it is milonga the one that varies parametrically r in the selected range, builds a text file containing the continuous geometry of figure 1 for the particular value of r, calls gmsh, solves the diffusion equation using a finite-elements-based method and computes the difference between the numerical reactivity and the analytical result ρ_0 of equation (1). Indeed, it will be milonga the code that will optimize the problems using the scheme proposed in this work in the next sections.

To fix ideas, assume we choose the following non-dimensional values for the one-group macroscopic cross sections of the bare reactor:

$$\begin{aligned} D_0 &= 1 \\ \Sigma_{a0} &= 2 \times 10^{-2} \\ \nu\Sigma_{f0} &= 3 \times 10^{-2} \end{aligned}$$

and the following for the absorbing fish:

[1]Free as both in free speech and in free beer.
[2]Ibid.

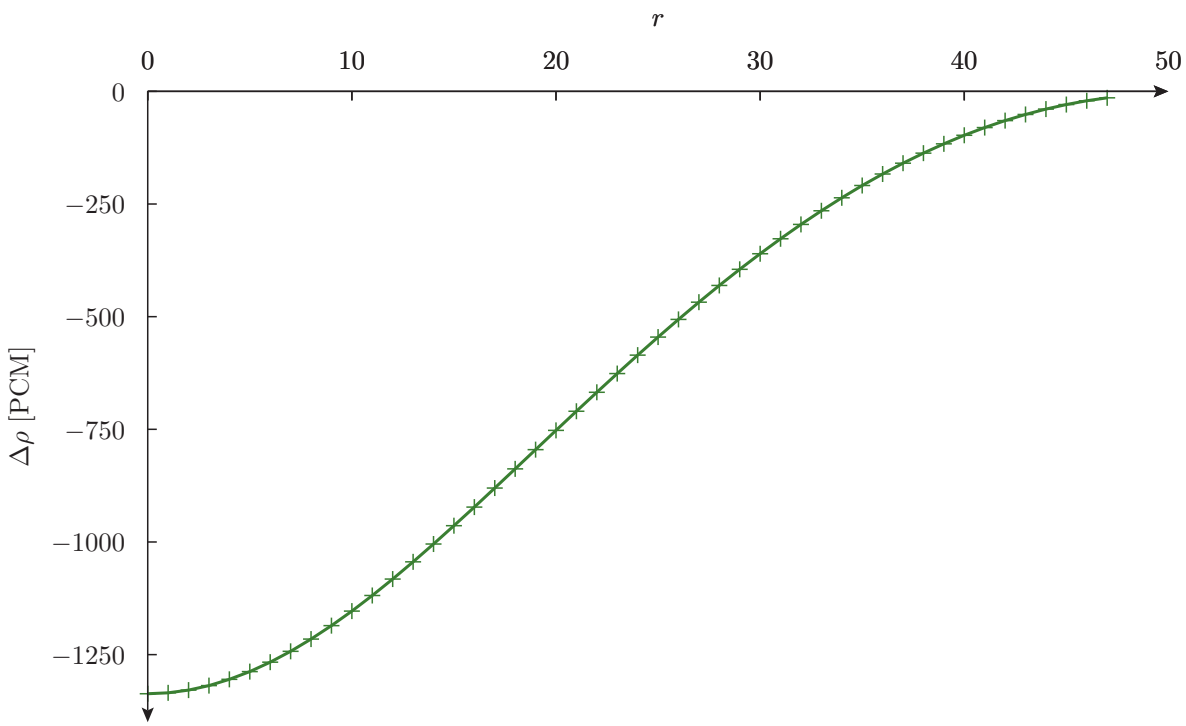


Figure 2: Dependance of the reactivity introduced by a single absorbing fish as a function of the distance r to the reactor center.

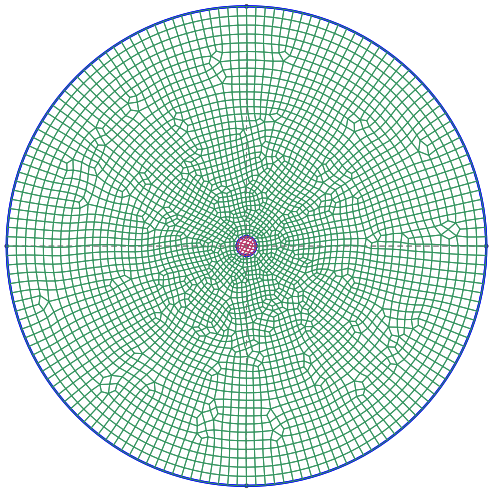
$$
\begin{aligned}
D_0 &= 0.9 \\
\Sigma_{a0} &= 1 \times 10^{-3} \\
\nu\Sigma_{f0} &= 0
\end{aligned}
$$

with the non-dimensional geometric parameters $A = 50$, $a = 2$ and $\Delta r = 1$. Then the dependance of $\Delta\rho$ with r is the one shown in figure 2. This result, due to its the characteristic shape, is known as an S-curve. When applied to the computation of the net reactivity insertion of real nuclear reactor control rods it is also known as the rod-worth curve. To further illustrate how figure 2 was obtained, consider figure 3 which shows three particular meshes used to obtain the overall reactivity $\rho(r)$ for $r = 0, 20, 40$.

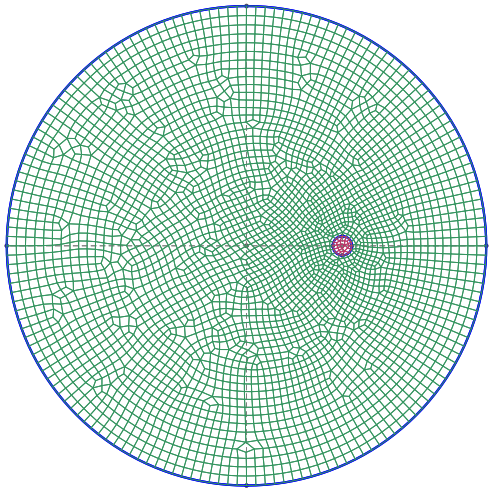
2.2 Two fish: shadowing and anti-shadowing effects

An extension to the single-fish problem consists of adding a second fish centered in a symmetric location from the first one with respect to the reactor center. In this case, the problem consists of finding again the reactivity change $\Delta\rho$ with respect to the fish-free reactor. However, a comparison of this result with respect to twice the reactivity inserted by the single fish discussed in the previous section leads to interesting spatial effects that are inherent of the way neutrons behave inside a nuclear reactor core. The corresponding continuous geometry for a generic r is shown in figure 4. To avoid problems with the mesh generator when overlapping both fish, we now vary r through the interval $[a + \Delta r/2, A - a/2]$. Three particular meshes for the cases $r = 2.5, 20, 40$ can be seen in figure 5.

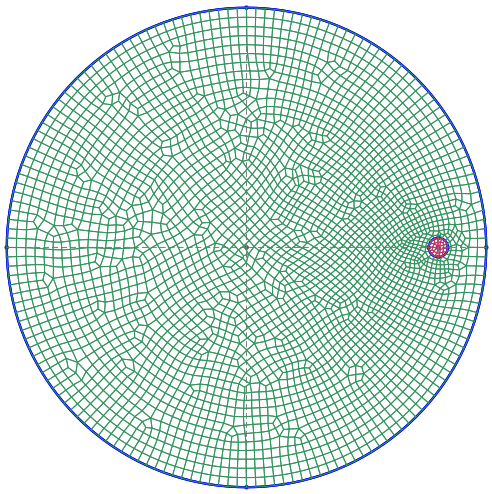
On the one hand, we observe that for large r the two curves in figure 6 coincide, indicating



(a) $r = 0$



(b) $r = 20$



(c) $r = 40$

Figure 3: Discrete grids used to solve the neutron diffusion equation for the one-fish problem for three different values of r.

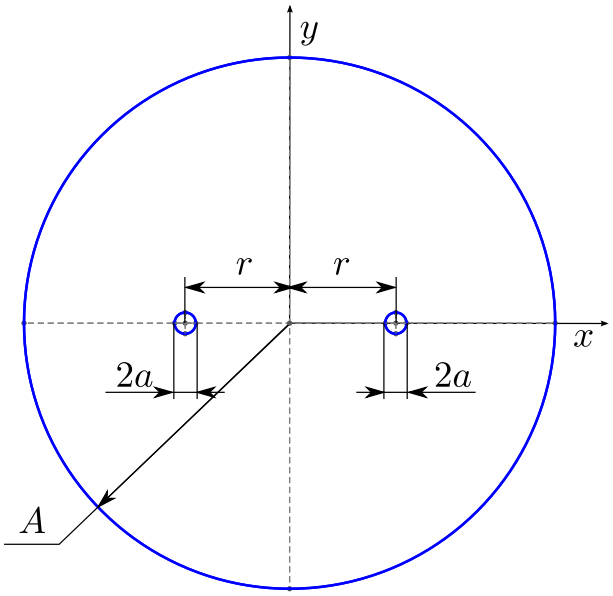


Figure 4: Continuous geometry containing a circular bare homogeneous reactor of radius A and two small neutron-absorbing circular fish of radius a symmetrically located at a distance r of the reactor center.

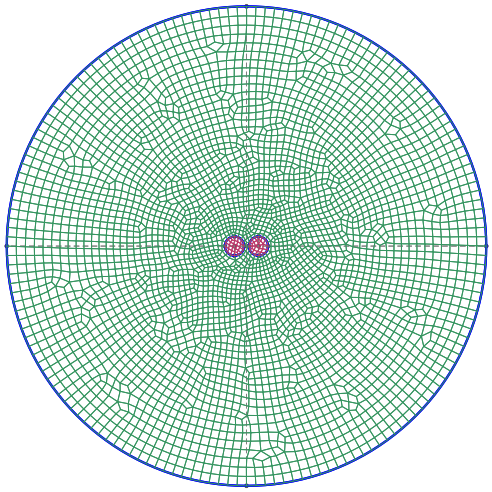
that the contributions to the net reactivity of each fish can be summed linearly. However, for small r, the net reactivity of both fish is lower than twice the one introduced by a single fish. This result is known as the "spatial shadowing effect", and is long discussed in the classical reactor analysis literature (Henry, 1975; Duderstadt and Hamilton, 1976). Less known is the fact that for moderate values of r, the net reactivity of two fish is more negative that twice the reactivity of one fish. This is called the "anti-shadowing effect" and is discussed by Lamarsh (1966), along with a semi-analytical derivation of figure 6. These two effects indicate that there is a value of r for which the net overall reactivity is minimum. Assuming this is a desirable feature—say for example that one designer is trying to determine where is the best location to insert a liquid neutron absorber for a fast reactor shutdown—then this case can be casted as a one-dimensional optimization problem. However, we defer the optimization discussion for the next section as in general the optimization of nuclear reactor design parameters are multi-dimensional problems which introduce a wide variety of caveats that are not present when minimizing functions of only one variable.

2.3 Three fish: geometry optimization

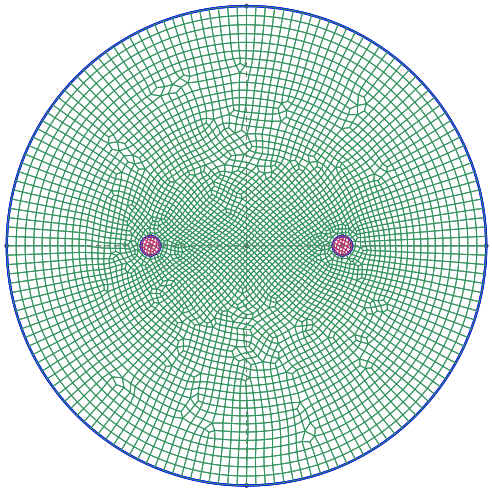
Consider now the fictitious case where three fish of radius a are introduced into the circular reactor of radius A but with the following particularity: two of them—namely fish one and fish two—are centered at fixed locations (x_1, y_1) and (x_2, y_2). The problem consists of finding the location (x_3, y_3) of the third fish that produces the most negative reactivity insertion (figure 7).

From the discussion of the results obtained in sections 2.1 and 2.2, it is clear that there is only one minimum of the reactivity change $\Delta\rho(x_3, y_3)$ and that is is located in the third quadrant with $x < 0$ and $y > 0$. Nevertheless, the proposed fictitious problem poses almost all of the complications contained in multidimensional optimization problem.

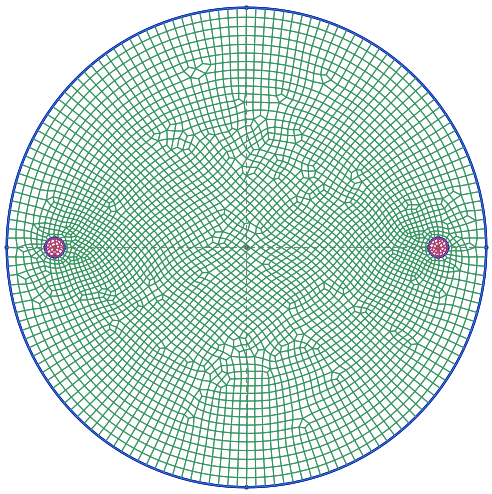
We set the locations of the two fixed fish to



(a) $r = 2.5$



(b) $r = 20$



(c) $r = 40$

Figure 5: Discrete grids used to solve the neutron diffusion equation for the two-fish problem for three different values of r.

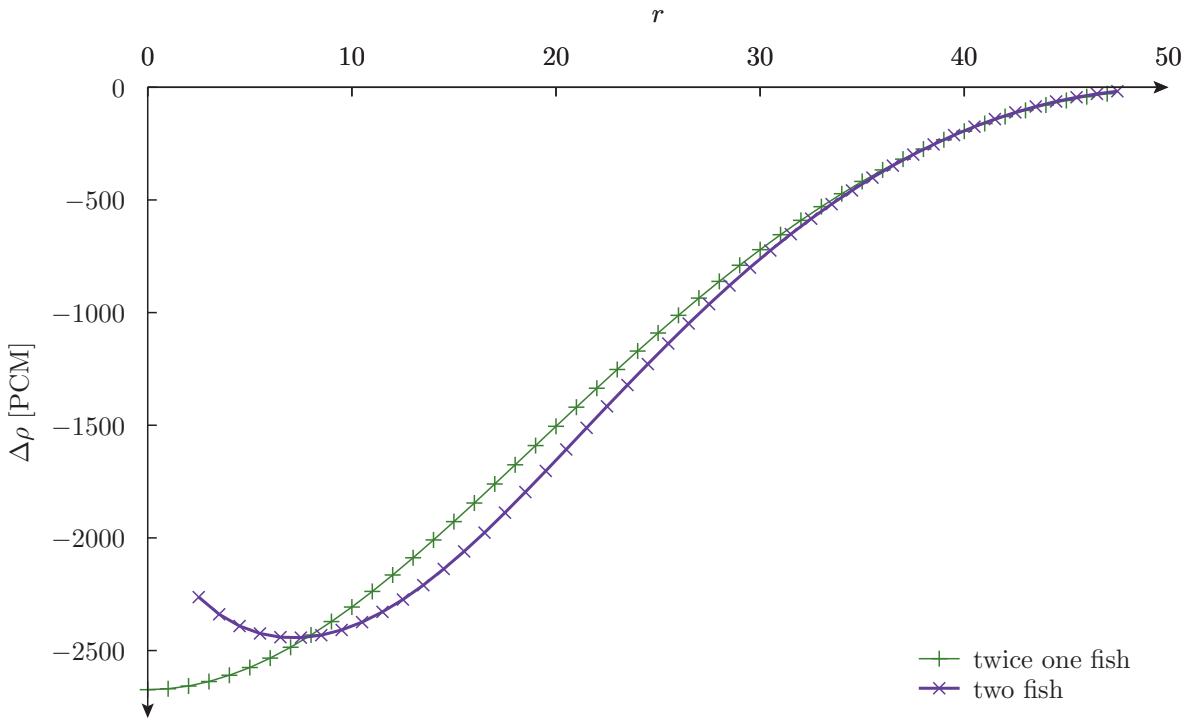


Figure 6: Dependance of the reactivity introduced by two symmetrically-located absorbing fish as a function of the distance r to the reactor center compared to twice the reactivity introduced by a single fish.

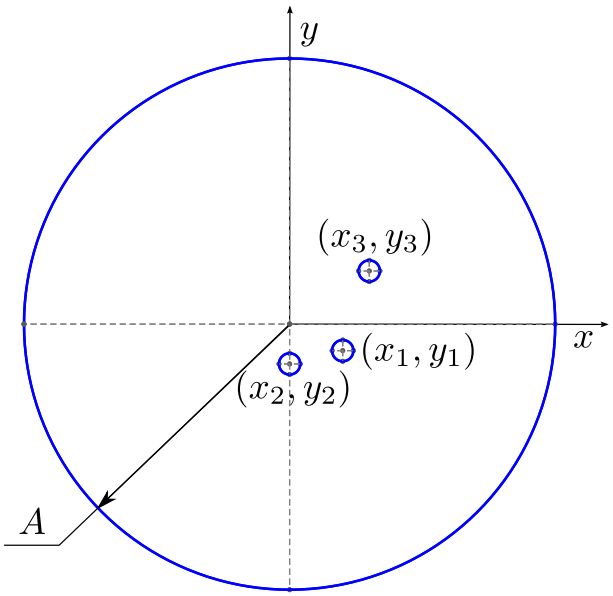


Figure 7: Continuous geometry containing a circular bare homogeneous reactor of radius A and three small neutron-absorbing circular fish of radius a. Two of these fish are fixed and the third one should be located in order to maximize the negative overall reactivity.

$$(x_1, y_1) = (0.2A, -0.1A)$$
$$(x_2, y_2) = (0, -0.15A)$$

and use the following initial guess for (x_3, y_3):

$$(x_3, y_3)_0 = (-0.6A, -0.6A)$$

which is explicitly located in the third quadrant and farther away from the reactor center than the other two fish to test if the optimization procedure is able to drive the third fish to the correct quadrant.

The computational code milonga interfaces with the GNU Scientific Library (Galassi et al., 2013) and—at least in its current version—uses the provided multidimensional minimization algorithms provided by said library. The available algorithms, as quoted from the documentation, are:

steepest_descent The steepest descent algorithm follows the downhill gradient of the function at each step. When a downhill step is successful the step-size is increased by a factor of two. If the downhill step leads to a higher function value then the algorithm backtracks and the step size is decreased. The steepest descent method is inefficient and is included only for demonstration purposes.

conjugate_fr This is the Fletcher and Reeves conjugate gradient algorithm. The conjugate gradient algorithm proceeds as a succession of line minimizations. The sequence of search directions is used to build up an approximation to the curvature of the function in the neighborhood of the minimum.

conjugate_pr This is the Polak and Ribière conjugate gradient algorithm. It is similar to the Fletcher-Reeves method, differing only in the choice of the coefficient β. Both methods work well when the evaluation point is close enough to the minimum of the objective function that it is well approximated by a quadratic hypersurface.

vector_bfgs2 This method use the vector Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. This is a quasi-Newton method which builds up an approximation to the second derivatives of the function using the difference between successive gradient vectors. By combining the first and second derivatives the algorithm is able to take Newton-type steps towards the function minimum, assuming quadratic behavior in that regio

nmsimplex2 This method use the Simplex algorithm of Nelder and Mead. Starting from the initial vector $\mathbf{x} = \mathbf{p}_0$, the algorithm constructs an additional n vectors $\mathbf{p}_i$ using the step size vector $\mathbf{s}$ as follows:

$$\begin{aligned}
\mathbf{p}_0 &= (x_1, x_2, \ldots, x_{n+1}) \\
\mathbf{p}_1 &= (x_1 + s_1, x_2, \ldots, x_{n+1}) \\
\mathbf{p}_2 &= (x_1, x_2 + s_2, \ldots, x_{n+1}) \\
&\vdots = \vdots \\
\mathbf{p}_n &= (x_1, x_2, \ldots, x_{n+1} + s_{n+1})
\end{aligned}$$

Method	Optimum (x_3, y_3)	$\Delta\rho$ [PCM]	Figure
Steepest Descent	$(-5.34, 8.58)$	-3406.5	8
Fletcher and Reeves	$(-6.12, 8.59)$	-3405.6	9
Polak and Ribière	$(-5.47, 8.27)$	-3406.6	10
Broyden-Fletcher-Goldfarb-Shanno	$(-5.17, 8.35)$	-3406.4	11
Nelder and Mead	$(-5.40, 8.67)$	-3406.5	12
Simulated Annealing	$(-5.59, 8.84)$	-3406.2	13

Table 1: Optimum location of fish #3 and reactivity increment $\Delta\rho$ for six different optimization methods.

These vectors form the $n+1$ vertices of a simplex in n dimensions. On each iteration the algorithm uses simple geometrical transformations to update the vector corresponding to the highest function value. The geometric transformations are reflection, reflection followed by expansion, contraction and multiple contraction. Using these transformations the simplex moves through the space towards the minimum, where it contracts itself.

siman The simulated annealing algorithm takes random walks through the problem space, looking for points with low energies; in these random walks, the probability of taking a step is determined by the Boltzmann distribution $p = \exp[-(E_{i+1} - E_i)/(kT)]$ if $E_{i+1} > E_i$, and $p = 1$ when $E_{i+1} \leq E_i$. In other words, a step will occur if the new energy is lower. If the new energy is higher, the transition can still occur, and its likelihood is proportional to the temperature T and inversely proportional to the energy difference $E_{i+1} - E_i$. The temperature T is initially set to a high value, and a random walk is carried out at that temperature. Then the temperature is lowered very slightly according to a cooling schedule, for example: $T \leftarrow T/\mu_T$ where μ_T is slightly greater than 1. The slight probability of taking a step that gives higher energy is what allows simulated annealing to frequently get out of local minima.

All of the methods start from the initial guess $(x_3, y_3)_0$ and then, according to the particular algorithm, choose a new evaluation point $(x_3, y_3)_1$ which should represent an improved (i.e. more negative) reactivity. After a number n of steps, if $\Delta\rho[(x_3, y_3)_n]$ cannot be further improved, the algorithm is considered to have converged. The actual convergence criteria depends on the particular method being used. The first four methods require the evaluation of the gradient of the objective function $\Delta\rho(x_3, y_3)$ which of course can only be obtained numerically by varying slightly and independently both x_3 and y_3 and re-computing the reactivity. However this overhead can be overcome by the fact that by knowing $\nabla(\Delta\rho)$ the next step of the iteration may improve significantly the solution. Except the simulated annealing method, all the other algorithms can only find local minima. However, as the three-fish problem has only one global minimum, if they converge then they will do it to said minimum.

Table 1 shows the results obtained with the code milonga Theler (2011) by employing the six optimization methods as implemented in the GNU Scientific Library Galassi et al. (2013). The steps taken by each algorithm are illustrated in figures 8–13. They all start at $(-30, -30)$ where the reactivity increment evaluates to $\Delta\rho_0 = -2218.2$ PCM, and immediately they all proceed in the direction of the third quarter. Gradient-based methods try to obtain directions in which to advance and step sizes to take, hoping that the next iteration will improve the solution. The numerical evaluation of $\nabla(\Delta\rho)$ is shown as a four-point stencil ($x_3 \pm \Delta x_3$ and $y_3 \pm \Delta y_3$) at each

step. If the next point results in a degradation of the solution, the method goes back through the last direction using a different step size and chooses a new direction in which to proceed. Gradient-free methods perform an educated random walk, also choosing the next point of the iteration in a clever way in order to improve the solution.

The actual number of evaluations of the target function $\Delta\rho(x_3, y_3)$–which is a measure of the computational effort needed to solve the problem—depends on the parameters that control how the different methods choose the next point and on the convergence criteria. These parameters are not the same for all the algorithms, and a fine analysis of their differences is beyond the scope of the current work.

3 CONCLUSIONS

The six multidimensional minimization algorithms implemented in the GNU Scientific Library (Galassi et al., 2013) that are used by the milonga neutronic code Theler (2011) to optimize nuclear reactor parameters are able to successfully solve the proposed fictitious three-fish problem. Even though the selected case is not trivial, as it involves the discussed shadowing and anti-shadowing effects over a two-dimensional domain that can be only seen with an accurate numerical solution of the neutron diffusion equation, it is fairly simple and none of the methods can be either chosen as the best choice or completely discarded for the particular problem discussed in this work. We expect that more complex problems involving either a bigger parameter space with multiple minima or in which the evaluation of the function to be minimized is significantly more expensive may render the utilization of certain algorithms useless. Future works will thus address more complex problems usually found in the conceptual engineering design of nuclear reactors. It is also expected that other optimization techniques such as genetic algorithms and neural networks can be employed to solve a wide variety of minimization problems resulting in some benefits with respect to traditional methods. Finally, the insertion of constrains may also require either the refinement of the algorithms discussed in this work or the introduction of completely new methods to aid the conceptual design of nuclear reactors.

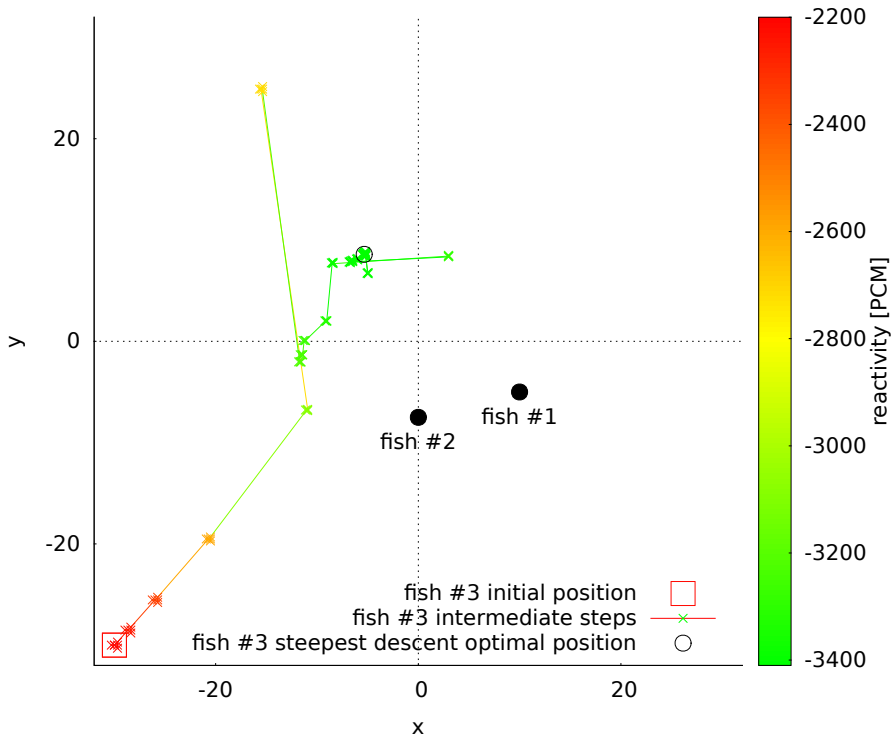


Figure 8: The three-fish problem solved with the Steepest Descent method

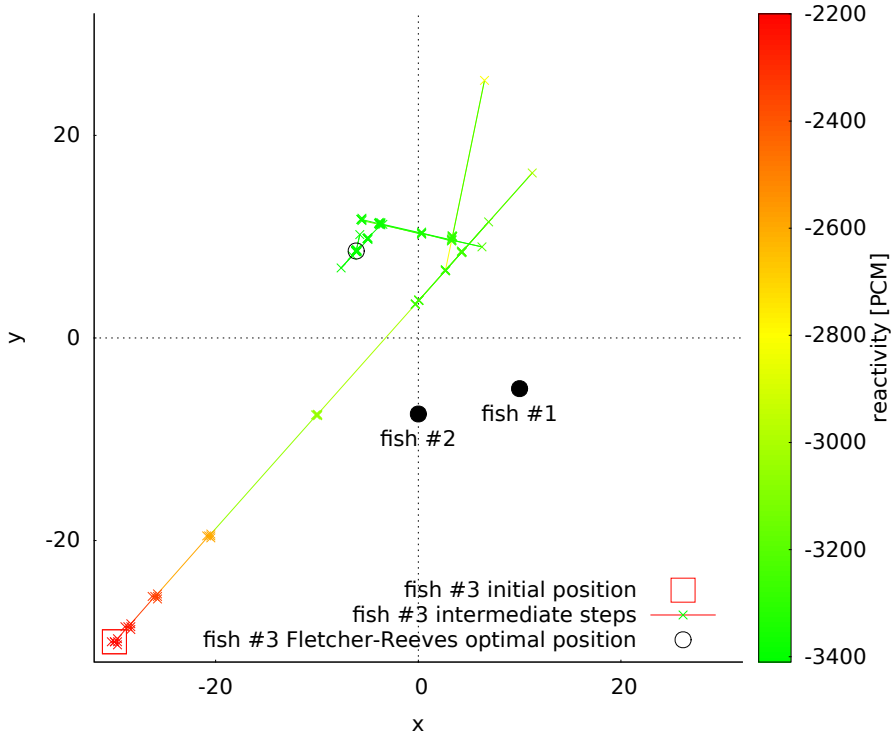


Figure 9: The three-fish problem solved with the Fletcher and Reeves method

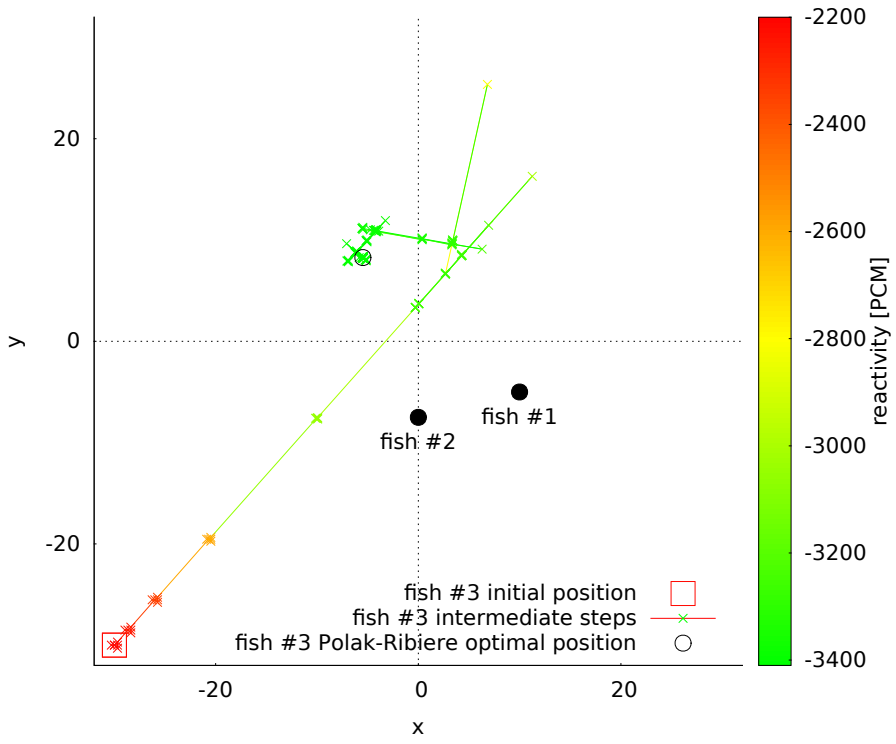


Figure 10: The three-fish problem solved with the Polak and Ribière method

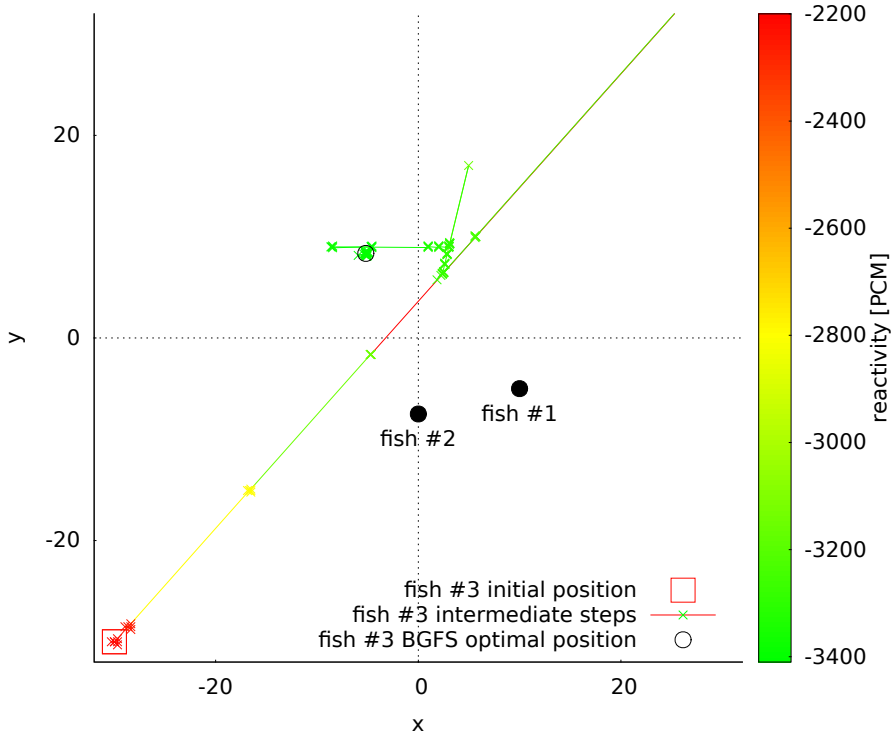


Figure 11: The three-fish problem solved with the Broyden-Fletcher-Goldfarb-Shanno method

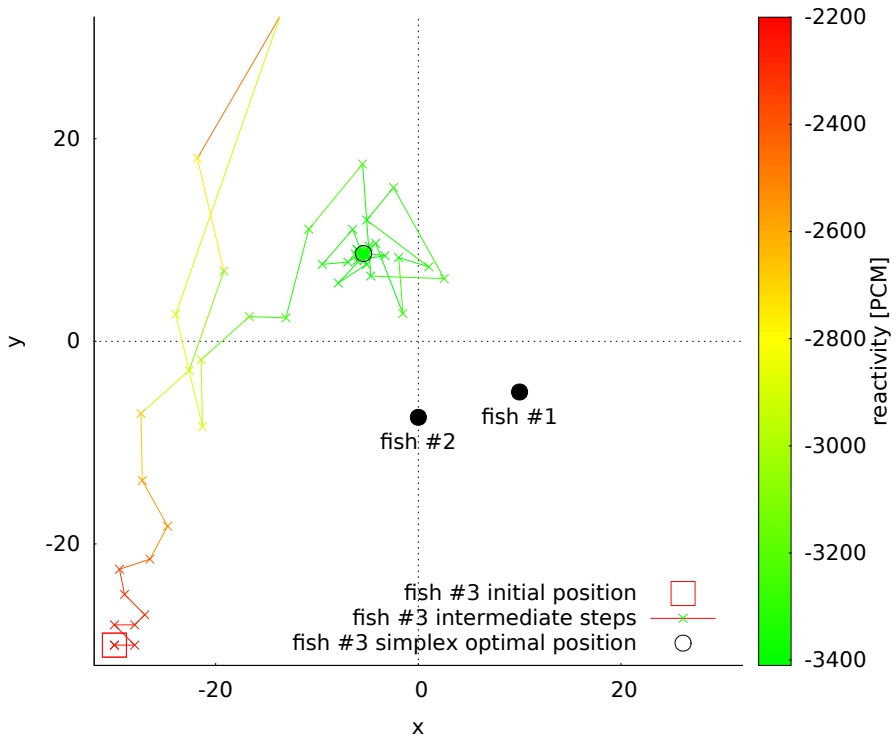


Figure 12: The three-fish problem solved with the Nelder and Mead method

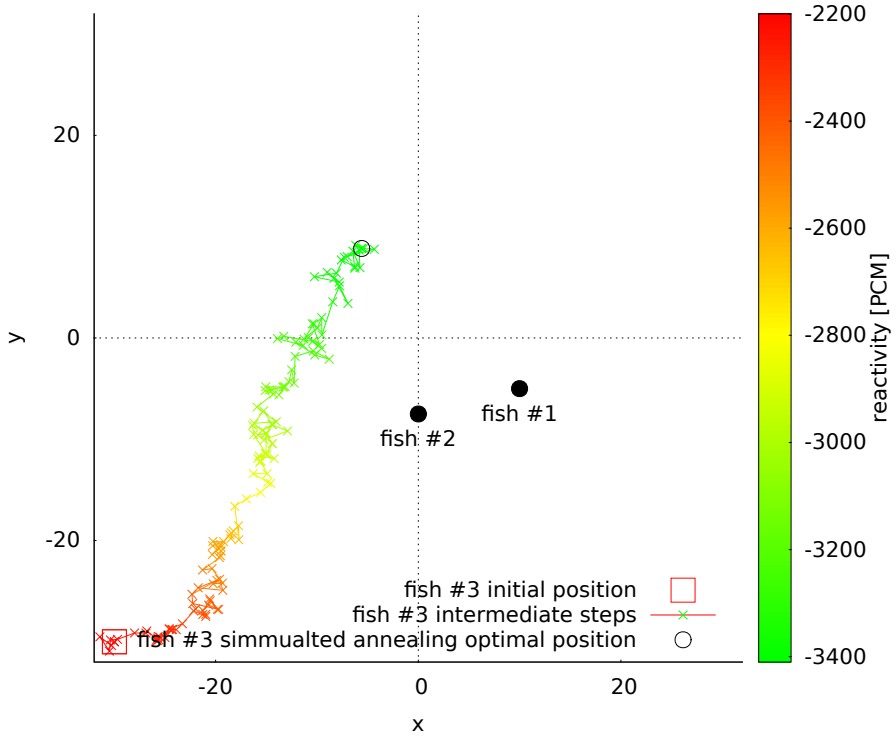


Figure 13: The three-fish problem solved with the Simulated Annealing method

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