Study of Nuclear Reactor Reload Using Different Approaches of Quantum Inspired Algorithms

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Abstract: The purpose of this article is to show the performance of different approaches of quantum-inspired algorithms as optimization tool of Nuclear Reactor Reload of Brazilian Nuclear Power Plant. Nuclear Reactor Reload is a classical problem in Nuclear Engineering that has been studied for more than 40 years that focus on the economics and safety of the Nuclear Power Plant. The main goal of this article is to show the performance of Quantum Delta-Potential Well Based Particle Swarm Optimization Algorithm to solve the Nuclear Reactor Reload compared with its classical counterpart Particle Swarm Optimization with Random Keys method. Furthermore, others quantum inspired algorithms are also used to demonstrate the feasibility of quantum inspired algorithms to solve cycle 7 of Brazilian Nuclear Power Plant Angra 1. The results show that Quantum Delta-Potential Well Based Particle Swarm Optimization Algorithm found the best result with less computational effort than its classical counterpart. Besides shows that quantum inspired algorithm are well situated among the best alternatives for dealing with optimization problems that number of evaluations is crucial due to the high computational cost of the evaluations, such as Nuclear Reactor Reload.

1 INTRODUCTION

In the last few years, quantum-inspired algorithms have been developed and gained attention both in Physics, Mathematics, Computer Science and others fields. These algorithms are based on different theory of quantum mechanics and are created in order to increase the performance and velocity of traditional optimizations algorithms of the literature. Nuclear Reactor Reload Optimization Problem (NRROP) is a classical problem in Nuclear Engineering that consists in replacing part of the nuclear fuel of a Nuclear Power Plant (NPP). Generally, the remaining elements of previous cycles that can still be used are rearranged in the reactor’s core and the remaining positions are filled up with new fuel elements in order to provide operation of the NPP at nominal power. However, this is not a simple process. In the reactor core of Angra 1 NPP, for example, $10^{25}$ arrangements are possible, making it impossible to verify all the arrangements to determine the best one. Moreover, NRROP presents high-dimensionality, large number of feasible solutions, disconnected feasible regions in the search space as well as high computational cost of the evaluation function and lack of derivative information. For decades, the NRROP was carried out by specialists that used their knowledge and experience to build configurations of the reactor core to fulfill the requirements of the NPP.

The purpose of this article is to show the performance of different approaches of quantum-inspired algorithms as optimization tool of Nuclear Reactor Reload of Brazilian Nuclear Power Plant. The algorithm implemented in this study was Quantum Delta-Potential-Well-based Particle Swarm Optimization Algorithm (QDPSO) (J.Sun et al, 2004). Besides we use the results found by others quantum inspired algorithms such as Quantum Evolutionary Algorithm (QEA) (Nicolau et al, 2012) and Quantum PBIL (QPBIL)(Da Silva et al, 2011) to show the performance of this kind of technique in to solve hard optimization problems as NRROP. QDPSO uses the philosophy of “collective learning” of Particle Swarm optimization (PSO) (Kennedy and Eberhart, 1995) and are inspired on different theory of quantum mechanics. Uses quantum theory of mechanics to govern the movement of swarm
particles, thus the quantum state of a particle is depicted by wave function instead of the velocity and position functions which are in PSO. Inspired by analysis of convergence of the traditional PSO, assume that an individual particle moves in a Delta potential well in search space, of which the center is point $p$.

QEA is based on the most important concepts of Quantum computation: Q_bits and interference of quantum states. Different from QDPSO it uses the philosophy of Evolutionary Computation, more specifically on Genetic Algorithm (GA). QEA uses a population characterized by a chromosome formed by Q_bits, instead of a conventional binary representation as GA. Unlike GA which uses, for instance, the operator mutation and crossover, the population in QEA evolves based upon a variation operator known as Q-gate.

QPBIL is a new version of PBIL (Machado MD, 2005) that uses some basic concepts of quantum computing: Q_bit and the linear superposition of quantum states as QEA. In QPBIL as well as PBIL a whole population is created every generation from the vector probability distribution $P$. However, the vector $P$ of QPBIL consists of Q_bits.

This article is structured as follows: in the next section, we will present a brief summary of QDPSO, QEA and QPBIL algorithms compared with his classical counterpart PSO, GA and PBIL respectively. Section 3 describes the Nuclear Reactor Reload Optimization Problem. Section 4 presented the computational results and in Section 5 is presented the conclusion of this study.

2 METHODOLOGY

2.1 QDPSO Algorithm

QDPSO belongs to the class of Quantum-inspired algorithms that uses the philosophy of “collective learning” of Particle Swarm optimization (PSO) was proposed by Sun Jun, et al., 2004 and is based on the quantum theory of mechanics to govern the movement of swarm particles. Thus, the quantum state of a particle is depicted by wave function instead of the velocity and position which are in PSO. According to the statistical significance of the wave function, the probability of a particle’s appearing in a certain position can be obtained from the probability density function. And then the probability distribution function of the particle’s position can be calculated through the probability density function.

Inspired by analysis of convergence of the traditional PSO, assume that an individual particle moves in a Delta potential well in search space, of which the center is point $p$.

In Quantum Mechanics, the state of a particle with momentum and energy can be depicted by its wave function $\psi(x,t)$. For this, in QDPSO each particle is in a quantum state and is formulated by its wave function $\psi(x,t)$ instead of the position and velocity which are in PSO. Thus, the probability of a particle’s appearing in a certain position can be obtained from the probability density function $|\psi(x,t)|^2$. And then the probability distribution function of the particle's position can be calculated through the probability density function.

According to Sun Jun, et al., 2004, the wave function of the particle is defined as:

$$\psi(x) = \frac{1}{\sqrt{L}} e^{-\frac{x^2}{L}}$$

and the probability density function is defined by:

$$Q(x) = |\psi(x)|^2 = \frac{1}{\sqrt{L}} e^{-\frac{x^2}{L}}$$

where, $L$ is the most important variable, which determines search scope of each particle.

Due of quantum nature of these equations the measurements using classical computers should utilized the Monte Carlo method. The position of the particle can be defined by:

$$x = P \pm \frac{L}{2} \ln(1/u), \quad u = \text{rand}(0,1)$$

where, $u$ is a random number uniformly distributed in $(0,1)$. $L$ is defined as $L=(1/(g|x_k-p|)$ and $g$ is a parameter that is constrained by $g=\ln((2)^{1/2})$. QDPSO procedure is described in Sun Jun, et al., 2004.

2.2 QEA Algorithm

In QEA, similarly to Genetic Algorithm – GA, where a generic individual of the population is represented by a string of bit, a quantum individual $(q_i)$ is represented by a string of Q_bit. We can say that a Q_bit is a quantum representation of classical bit, where a generic Q-bit $|\psi\rangle$, might be represented not by an exact representation, but by a linear combination of the vectors $|0\rangle$ and $|1\rangle$ that assumes the values 0 and 1 simultaneously.

In such way that, $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$, where, $\alpha$ and
\( \beta \) are complex numbers that satisfy \( |\alpha|^2 + |\beta|^2 = 1 \).

The information stored in \( |\psi\rangle \) is a combination of all the possible states of \( |0\rangle \) and \( |1\rangle \). And a set of \( N \) Q-bits may be put in a superposition of \( 2^N \). But, when \( |\psi\rangle \) is measured, it is possible to find a unique state, on the other words, it is possible to find the state \( |0\rangle \) with a probability \( |\alpha|^2 \) or the state \( |1\rangle \) with a probability \( |\beta|^2 \).

The individual of the population is represented in two distinct phases. In the first phase, it is fully quantum, represented by a individual \( q_i(t) \) where his chromosome consisting of Q-bits, and assumes a superposition of states \( |0\rangle \) and \( |1\rangle \). After observation of quantum individual, creates a classical individual \( X_i(t) \) represented by a classic chromosome, which will be evaluated.

The population of solutions is represented by \( Q(t) = \{ q_1(t), q_2(t), ..., q_m(t) \} \), where \( m \) is the size of the population, \( m \) is the number of Q-bits, and \( q_i(t) \) is the quantum chromosome defined by:

\[
q_i(t) = \begin{bmatrix}
\alpha_{i1}(t) & \alpha_{i2}(t) & ... & \alpha_{in}(t) \\
\beta_{i1}(t) & \beta_{i2}(t) & ... & \beta_{in}(t)
\end{bmatrix}
\]

where,

\[
|\alpha_{ij}|^2 + |\beta_{ij}|^2 = 1
\]

In this way, any \( q_i^0 \) can represent the linear superposition of all the possible states with the same probability. In addition, the linear superposition of the Q-bits provides good diversity in the evolution process.

Classic individual \( X_i(t) \) is derived from the observation of quantum individual. This is a characteristic of the evolutionary algorithms of quantum computing adopting the theories of quantum mechanics. The classical population represented by:

\[
P(t) = \{ X_1(t), X_2(t), ..., X_m(t) \}
\]

and the candidate solutions \( X_i(t) \) with \( m \) bits, which will be evaluated by the fitness function, are represented by:

\[
X_i(t) = \{ x_{i1}(t), x_{i2}(t), ..., x_{im}(t) \}
\]

where \( x_{ij}(t) \) is the observed bit.

The best candidate solution of \( P(t) \) at each iteration \( t \) is stored in \( B(t) \), that is, \( B(t) = [b_{11}(t)b_{12}(t) ... b_{mn}(t)] \), where \( b_{ij}(t) \) represents the bits of the best solution.

Every bit of the binary string is obtained observing the step for construction of the population \( P(t) \). When all the states of \( Q(t) \) are observed, the value \( |x_{ij}(t)| = 0 \) or \( |x_{ij}(t)| = 1 \), from \( P(t) \) is determined by the probability \( |\alpha_{ij}(t)|^2 \). The pseudo-code for production of \( P(t) \) is according to Nicolau et al, 2012.

Unlike GA, which uses for instance the operators mutation and crossover, the population evolves based upon a variation operator known as Q-gate. This quantum gate operator, defined by the rotation matrix \( U(\Delta \theta) \), which is applied to each one of the columns of each individual's Q-bit. In practice, each pair of values \( \alpha_{ij} \) and \( \beta_{ij} \) is treated as a bi-dimensional vector and rotated using \( U(\Delta \theta) \) in such a way that:

\[
\begin{bmatrix}
|\alpha_{ij}(t+1)| \\
|\beta_{ij}(t+1)|
\end{bmatrix} =
\begin{bmatrix}
\cos(\xi(\Delta \theta_{ij})) - \sin(\xi(\Delta \theta_{ij})) & \xi(\Delta \theta_{ij}) \\
\sin(\xi(\Delta \theta_{ij})) & \cos(\xi(\Delta \theta_{ij}))
\end{bmatrix}
\begin{bmatrix}
|\alpha_{ij}(t)| \\
|\beta_{ij}(t)|
\end{bmatrix}
\]

with

\[
\xi(\Delta \theta_{ij}) = S(\alpha_{ij}, \beta_{ij}) \Delta \theta_{ij}
\]

Where the sign function \( S(\alpha_{ij}, \beta_{ij}) \) represents the direction of rotation and the pass \( \Delta \theta_{ij} \) represents the magnitude of the angle of rotation. Both \( \Delta \theta_{ij} \) and \( S(\alpha_{ij}, \beta_{ij}) \) are obtained in accordance with Nicolau et al, 2012.

### 2.3 QPBIL Algorithm

The QPBIL is a new version of the original PBIL that uses some basic concepts of quantum computing as QEA, like Q-bit and the linear superposition of quantum states.

According to Da Silva et al, 2011, as well as PBIL a whole population is created every generation from the vector probability distribution \( P \). However, the vector \( P \) of QPBIL consists of Q-bits. Such vector corresponds to the Q-bit individual described by [2], and for this reason, it shares all the quantum characteristics related to that one.

\[
P = \begin{bmatrix}
\alpha_1 & \alpha_2 & ... & \alpha_n \\
\beta_1 & \beta_2 & ... & \beta_n
\end{bmatrix}
\]

QPBIL acts in a binary space which turns it
capable of solving optimization problems in continuous search space. For this to be possible, however, it is necessary to covert the notation of Q_bits to conventional binary form, i.e, a string of zeros and ones. This is done from the observation of the probability distribution vector, $P$ that generates valid solutions shown in the form of binary strings. To determine in which quantum state the Q_bit will collapse, or what state it will be observed (0 or 1), a random number is generated according to the equation:

$$I_j = \begin{cases} 1 & \text{if } \text{rand} \geq \beta^2 \\ 0 & \text{if } \text{rand} > \beta^2 \end{cases}$$

where $I_j$ is the $j$th bit of the $i$th individual.

The goal is to make the new generated individuals to be increasingly look like the best individual and decreasingly as the worst one. The updating process is done by means of the quantum rotation gate $R(\theta_j)$:

$$R(\theta_j) = \begin{bmatrix} \cos(\theta_j) & -\sin(\theta_j) \\ \sin(\theta_j) & \cos(\theta_j) \end{bmatrix}$$

where $\theta_j$ represents how the Q_bits will approach the best individual. This gate works as follows: first, for each Q_bit $j$, is given a rotation that brings it to the best individual is given. The process is showed with more detail in Da Silva et al, 2011.

Then, a new quantum gate is used for the application of the angle $\omega_j$ in order to remove the next gate generation groups of the worst individual in accordance with Da Silva et al, 2011. Pseudocode of QPBIL is described in Da Silva et al, 2011.

3 NRROP

Started after the operation of the plant, the concentration of fissile material ($^{235}$U) fuel elements begins to decrease. After a time period, called operation cycle, it is not possible to maintain the NPP operating at the nominal power. The Fuel Assemblies (FA's) with low concentrations of $^{235}$U are replaced by new fuel elements and along with other FA's of the previous cycle compose the core of the subsequent cycle (Nicolaou et al, 2012).

NRROP consists in searching for the best loading pattern of FA's in the core, aiming to determine the permutation of FA's that optimizes the uranium utilization, with objective function evaluated according to specific criteria and methods of nuclear reactor physics. Thus, NRRP can be seen as a combinatorial problem: a number $n$ of FA's are permuted in $n$ positions of the core.

Although presenting a simple formulation the NRRP is a NP-Complete problem, whose difficulty grows exponentially with the number of FA's in the reactor core. The Nuclear Power Plant of Angra 1, for instance, contains 121 FA's and gives rise to approximately $8.09 \times 10^{200}$ (121!) loading patterns. However, due to 1/4 and 1/8 core symmetries and also to rules of placement of the FA's in the nucleus, this number falls to approximately $10^{25}$ loading patterns. This number is extremely high to solve this problem by enumeration. It would take approximately $5.8 \times 10^{19}$ years to test all these combinations with the Reactor Physics codes and today's computers, making it infeasible to check all these combinations to find the best. Besides these difficulties, this problem has nonlinear characteristics with discontinuities and multiple optima in the solutions search space.

For safe operation of a nuclear plant is necessary a loading pattern thoroughly being examined. For such, reactor physics codes are used, with implementations of the numerical resolution of Neutrons Transport or Diffusion models (Chapot et al, 2000). The direct use of these codes in an optimization process of reloading makes the process very slow. In this paper was used the Reactor Physics code RECNOD (Chapot et al, 2000).

Combination of these attributes: high-level combinations, nonlinear objectives and constraints, multimodality and high computational cost describe NRRP, which is challenging the traditional optimization methods and encouraging researchers to develop and implement more "intelligent" methods optimization in order to solve this problem.

4 COMPUTATIONAL RESULTS

For benchmarking QDPSO, the 7th reload cycle for Angra 1 NPP, PWR, designed by Westinghouse and operated by Eletronuclear, located at the Southeast of Brazil, has been selected. Angra 1 core gives 121 FA's and two main axis of symmetry dividing the core into four regions that, are called 1/4 (one-fourth) symmetry axis. These axis and two secondary diagonal axes divide the core into eight regions. Figure 1 shows Angra1 core (view from top) and the representation of 1/8 core symmetry (view from top).

In fact with 1/8 symmetry we reduce the complexity of the problem and works with 21 FA's: 1 at the center of the core, 10 over the lines of
Figure 1: Representation of Angra 1 core and 1/8 core symmetry. symmetry and 10 between the symmetry lines. In 1/8 core symmetry the quartets can only occupy the positions 1-10 and the octets must occupy only the positions 11-20. The central element is considered fixed and not part of the optimization process, as well as others approach in literature.

For this study QDPSO was developed in Matlab 6.5 with communication interface with RECNOD code. The simulations with the reactor physics code RECNOD (Chapot, et. al, 2000) used a low-leakage strategy with burnable poison. The QDPSO was used as a tool to determine the optimal boron concentration in 30 experiments with different random seeds. The population was 100. The objective function used to evaluate each individual of QDPSO is show bellow, as is the same function used in others woks in literature (Chapot, et. al, 1999, Machado MD, 2005, Meneses et. al, 2010, Da Silva et al, 2011, Nicolau et al, 2012).

\[
\text{Fitness} = \begin{cases} 
1/C_B & \text{if } P_{\text{rm}} \leq 1.395 \\
1/C_B^{\text{Max}} & \text{otherwise}
\end{cases}
\] (13)

where, \(C_B\) is the boron concentration and \(P_{\text{rm}}\) is the Maximum Normalized Assembly Power.

Thus, the optimization of this problem is closely related to the power plant cycle length as it maximizes the boron concentration yielded by the reactor physics code. At Angra 1 NPP, approximately 4ppm of soluble boron is consumed per Effective Full Power Day (EFPD). This relation indicates that increasing the boron concentration by an optimized core configuration will increase the NPP core operational days.

To do so, a candidate solution of the QDPSO is a vector that indicates a possible fuel rod configuration. In this vector, it’s possible to appear repetition of values. However, the repetition of FA’s does not stand as a valid configuration, because the same FA cannot be in more than one position in the core. In this way, Random Keys (Bean, 1994) model was used as well as in others woks in literature (Chapot, et. al, 1999, Machado MD, 2005, Meneses et. al, 2010, Da Silva et al, 2011, Nicolau et al, 2012). Thus, a candidate solution of the QDPSO converted by Random Keys method is a string with 20 elements that corresponds to the positions of the FA (where the quartets can only occupy the positions 1-10 and the octets must occupy the position 11-12).

Table 1 shows the best results of QEA implemented by Nicolau et al, 2012, GA implemented by Chapot, et. al, 1999, PSORK implemented by Meneses et al, 2010, PBIL implemented by Machado MD, 2005 and QPBIL implemented by Da Silva et al, 2011 every all applied to the NRROP of Angra 1 in the same conditions. The acquired results are analysed and compared with QDPSO developed in this study according to the value of \(C_B\) and number of evaluations.

![](image)

<table>
<thead>
<tr>
<th>Technique</th>
<th>(C_B) Average ((C_B))</th>
<th>Std* ((C_B))</th>
<th>Evaluations</th>
</tr>
</thead>
<tbody>
<tr>
<td>GA</td>
<td>1197</td>
<td>703</td>
<td>381.95</td>
</tr>
<tr>
<td>FPBIL</td>
<td>1428</td>
<td>1353</td>
<td>65</td>
</tr>
<tr>
<td>PSORK</td>
<td>1394</td>
<td>1168</td>
<td>95</td>
</tr>
<tr>
<td>QEA</td>
<td>1431</td>
<td>1385</td>
<td>35</td>
</tr>
<tr>
<td>QPBIL</td>
<td>1413</td>
<td>1383</td>
<td>45</td>
</tr>
<tr>
<td><strong>QDPSO</strong></td>
<td><strong>1441</strong></td>
<td><strong>1393</strong></td>
<td><strong>26</strong></td>
</tr>
</tbody>
</table>

*Std = Stand deviation

According to Table 1, the best result for \(C_B\) using QDPSO is higher than others results of the literature with less computational effort. The difference between the best value of \(C_B\) found by QDPSO (1424) and PSORK (1394) is equal to 30 ppm of boron. It’s corresponds to about 7 EFPD more. Also we can observe that QDPSO found the best result with 6,500 evaluations. Furthermore, we can observe that all others quantum inspired algorithms reported shows best results of the average boron concentration and lower standard deviation that his classical counterpart.

Figure 2, shows the evolution curve of QDPSO implemented. We can observe that at the beginning of the experiment QDPSO converges rapidly to values near \(9\times10^{-4}\), at this moment the search of QDPSO consists in find fitness values that guarantees the restriction \(P_{\text{rm}} \leq 1.395\), and then goes on to maximize the \(C_B\) value and consequently minimizes \(1/C_B\) (equation 13). In this case the best value for the fitness occurs near generation 140.
5 CONCLUSIONS

In this study we discuss about the efficiency of quantum-inspired algorithm in to solve the NRROP. In this case we implemented QDPSO algorithm in the same conditions of other optimization techniques presented in the literature. The results found by the QDPSO was best than its classical counterpart and compared with others quantum inspired algorithms is the best in relation to the number of evaluations. Furthermore, the results shown the superiority of quantum inspired algorithm compared with his classical counterpart presented in the literature for the NRROP. According to this study we can say that quantum inspired algorithms are well situated among the best alternatives for dealing with hard optimization problems that number of evaluations is crucial due to the high computational cost of the evaluations, such as NRROP.

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