A Metropolis Algorithm Combined with the Hooke-Jeeves Method Applied to a Nuclear Reactor Core Design Optimization Problem

Wagner F. Sacco, Hermes Alves Filho, Nélio Henderson
Depto. de Modelagem Computacional, IPRJ, UERJ
28630-050, Nova Friburgo, RJ
E-mail: {wfsacco, halves, nelio}@iprj.uerj.br

Ana Carolina Rios-Coelho
Programa de Pós-Graduação em Modelagem Computacional, IPRJ, UERJ
28630-050, Nova Friburgo, RJ
E-mail: acrios@iprj.uerj.br

Abstract: *A hybridization of the recently introduced Particle Collision Algorithm (PCA) and the Hooke-Jeeves algorithm is applied to a nuclear reactor core design optimization problem which was previously attacked by other metaheuristics. The optimization problem consists in adjusting several reactor cell parameters, such as dimensions, enrichment and materials, in order to minimize the average peak-factor in a three-enrichment-zone reactor, considering restrictions on the average thermal flux, criticality and sub-moderation. The new metaheuristic performs better than the canonical PCA, thus demonstrating its potential for other applications.*

1. Introduction

The Particle Collision Algorithm (PCA, Sacco and de Oliveira, 2005; Sacco *et al.*, 2006) is a Metropolis-based algorithm (Metropolis *et al.*, 1953) that was introduced as an alternative to Simulated Annealing (Kirkpatrick *et al.*, 1983). The main motivation behind the PCA was that in spite of being very powerful, simulated annealing is too sensitive to the choice of free parameters, such as, for example, the annealing schedule and initial temperature (Carter, 1997). The PCA does not rely on user-supplied parameters to perform the optimality search, being thus more robust. This algorithm is loosely inspired by the physics of nuclear particle collision reactions (Duderstadt and Hamilton, 1976), particularly scattering and absorption. Thus, a particle that hits a high-fitness nucleus is absorbed and explores the boundaries. On the other hand, a particle that hits a low-fitness region is scattered to another region of the search space.

In this article, we use a hybridization of the Particle Collision Algorithm and the Hooke-Jeeves direct search algorithm (Hooke, Jeeves, 1961). The aim is to perform a wide search in the solution space using a stochastic optimization algorithm (the PCA) and then scan the promising areas with a local search technique (Hooke-Jeeves). This searching is performed iteratively until a certain number of objective- function evaluations is reached.

This hybrid algorithm, called the Hooke-Jeeves Particle Collision Algorithm (HJPCA, Sacco *et al.*, 2008a), is applied to a nuclear core design optimization problem that was introduced by Pereira *et al.* (1999), and has subsequently been attacked by other authors (Pereira and Lapa, 2003, Sacco *et al.*, 2004, Sacco *et al.*, 2006, for example). The NMPCA is compared with the PCA, which performed better than the genetic algorithm and simulated annealing (Sacco *et al.*, 2006).

The remainder of the paper is organized as follows. In the next section the original Particle Collision Algorithm is outlined, the Hooke-Jeeves algorithm is described in detail and the new algorithm is presented. Section 3 presents the reactor design optimization problem. In section 4, the implementation of the algorithm is briefly described and the results are shown. Finally, in section 5, the conclusions are made.

2. HJPCA

2.1 PCA

The PCA resembles in its structure that of simulated annealing: first an initial configuration is chosen; then there is a modification of the old configuration into a new one. The qualities (i.e., objective-function values) of the two configurations are compared. A decision then is made on whether the new configuration is acceptable . If it is, it serves as the old configuration for the next step. If it is not acceptable, the algorithm proceeds with a new change of the old configuration. PCA can also be considered a Metropolis algorithm, as a trial solution can be accepted with a certain probability. This acceptance may avoid the convergence to local optima.

A summary of PCA is given below. The algorithm's default is for maximization problems. For minimization problems, just multiply the objective-function by -1 and invert the ratio in $p_{scattering}$.

Initialization Step

Generate an initial random solution *Old_Config.*

Main Step

Do until termination criterion is reached:

1. Generate a stochastic perturbation *New_Config* of the solution *Old_Config.*
2. If Quality(*New_Config*)>Quality(Old_*Config*), let *Old_Config* ← *New_Config* and go to *Exploitation*.
Otherwise, go to *Scattering*.

End-Do

Exploitation

Do for one-hundred iterations:

1. Generate a small stochastic perturbation *New_Config* of the solution *Old_Config.*
2. If Quality(*New_Config*)>Quality(*Old_Config*), let *Old_Config* ← *New_Config.*

End-Do

return

Scattering

1. Calculate
$$p_{scattering} = 1 - \frac{\text{Quality}(New\_Config)}{Current\_Best\_Quality}$$
2. If $p_{scattering}$>random(0,1), let *Old_Config* receive a random solution.
Otherwise, go to *Exploitation.*

return

2.2 The Method of Hooke and Jeeves

The method of Hooke and Jeeves performs two types of search: an exploratory search and a pattern search. A summary of the method is given below (from Bazaraa *et al.*, 1993). At this time, the algorithm's default if for a minimization problem.

Initialization Step

Let $\vec{d}_1, \ldots, \vec{d}_n$ be the coordinate directions. Choose a scalar $\epsilon > 0$ to be used for terminating the algorithm. Furthermore, choose an initial step size, $\Delta \geq \epsilon$, and an acceleration factor, $\alpha > 0$. Choose a starting point $\vec{x}_1$, let $\vec{y}_1 = \vec{x}_1$, let $k = j = 1$, and go to the main step.

Main Step

1. If $f(\vec{y}_j + \Delta \vec{d}_j) < f(\vec{y}_j)$, the trial is termed a *success*; let $\vec{y}_{j+1} = \vec{y}_j + \Delta \vec{d}_j$, and go to step 2. If, however, $f(\vec{y}_j + \Delta \vec{d}_j) \geq f(\vec{y}_j)$, the trial is deemed a *failure*. In this case, if $f(\vec{y}_j - \Delta \vec{d}_j) < f(\vec{y}_j)$, let $\vec{y}_{j+1} = \vec{y}_j - \Delta \vec{d}_j$, and go to step 2; if $f(\vec{y}_j - \Delta \vec{d}_j) \geq f(\vec{y}_j)$, let $\vec{y}_{j+1} = \vec{y}_j$, and go to step 2.
2. If $j < n$, replace j by $j+1$, and repeat step 1. Otherwise, go to step 3 if $f(\vec{y}_{n+1}) < f(\vec{x}_k)$, and go to step 4 if $f(\vec{y}_{n+1}) \geq f(\vec{x}_k)$.
3. Let $\vec{x}_{k+1} = \vec{y}_{n+1}$, and let $\vec{y}_1 = \vec{x}_{k+1} + \alpha(\vec{x}_{k+1} - \vec{x}_k)$. Replace k by $k+1$, let $j = 1$, and go to step 1.
4. If $\Delta \leq \epsilon$, stop; $\vec{x}_k$ is the solution. Otherwise, replace Δ by $\Delta/2$. Let $\vec{y}_1 = \vec{x}_k$, $\vec{x}_{k+1} = \vec{x}_k$, replace k by $k+1$, let $j = 1$, and repeat step 1.

Steps 1 and 2 above describe an exploratory search. In step 3, there is an acceleration along the direction $\vec{x}_{k+1} - \vec{x}_k$. Finally, in step 4 the step size Δ is reduced.

2.3 The PCA with Hooke_Jeeves

The principle behind our hybrid metaheuristic is quite simple: the PCA explores the search space and when a better-than-previous solution is found, it is used as an initial point for the Hooke-Jeeves direct search method. Thus, function Exploitation in the original algorithm was replaced by the Hooke-Jeeves method in the HJPCA, as summarized below.

Initialization Step
Generate an initial random solution *Old_Config*.

Main Step
Do until termination criterion is reached:
1. Generate a stochastic perturbation *New_Config* of the solution *Old_Config*.
2. If Quality(*New_Config*)>Quality(Old_*Config*), let *Old_Config* ← *New_Config* and go to *Hooke-Jeeves*.
Otherwise, go to *Scattering*.
End-Do

Hooke-Jeeves
1. Apply the HJ method to the solution *Old_Config*, as described in section 2.2.
2. If -Quality(*New_Config*)>-Quality(*Old_Config*), let Old_Config ← New_Config.
return

Scattering
1. Calculate

$$p_{scattering} = 1 - \frac{\text{Quality}(New\_Config)}{Current\_Best\_Quality}$$

2. If $p_{scattering}$>random(0,1), let *Old_Config* receive a random solution.
Otherwise, go to *Exploitation*.
return

Note that as the Hooke-Jeeves method was conceived as a minimization algorithm, we had to change the signs of the objective-function values in function Hooke-Jeeves in order to fit the PCA.

3. Problem Description

Our optimization problem will be briefly described here: consider a cylindrical 3-enrichment-zone PWR, with typical cell composed by moderator (light water), cladding and fuel. The problem consists in adjusting several reactor cell parameters, such as dimensions, enrichment and materials, in order to minimize the average peak-factor in a 3-enrichment-zone reactor, considering restrictions on the average thermal flux, criticality and sub-moderation.

The design parameters that may be changed in the optimization process, as well as their variation ranges are shown in Table 1.

Parameter	Range
Fuel Radius (R_f,cm)	0.508 to 1.270
Cladding Thickness (Δ_c,cm)	0.025 to 0.254
Moderator Thickness (R_e,cm)	0.025 to 0.762
Enrichment - Zones 1, 2, 3 (E_1, E_2, E_3, %)	2.0 to 5.0
Fuel Material (M_f)	{U-Metal, UO_2}
Cladding Material (M_c)	{Zircaloy-2, Aluminum, SS-304}

Table 1: Parameters range

The objective of the optimization problem is to minimize the average power-peaking factor, f_p, of the proposed reactor, considering that the reactor must be critical $(k_{eff}=1\pm1\%)$ and sub-moderated, for a given average flux ϕ_0. Let $\vec{D}=\{R_f, \Delta_c, R_e, E_1, E_2, E_3, M_f, M_c\}$ be the vector of design variables. Then, the optimization problem can be written as follows:

Minimize
$f_p(\vec{D})$
s.t.

$$\phi(\vec{D})=\phi_0; \qquad (1)$$

$$0.99 \le k_{eff}(\vec{D}) \le 1.01; \qquad (2)$$

$$\frac{d\,k_{eff}}{d\,V_m} > 0; \qquad (3)$$

$$D_i^l \le D\,i \le D_i^u,\; i=1,2,..,6; \qquad (4)$$

$$M_f = \{\text{UO}_2 \text{ or U-metal}\}; \qquad (5)$$

$$M_c = \{\text{Zircaloy-2, Al or SS-304}\} \qquad (6)$$

4. Implementation and Results

4.1 Implementation

In our tests, the canonical PCA and HJPCA were set up for 100,000 objective-function evaluations, so that the results were obtained with the same computational effort. For each algorithm, ten independent runs were made. Each execution took 10h in a

Pentium IV PC with 1 Gb RAM, as the reactor physics code is the system s bottleneck.

The Hooke-Jeeves routine inside HJPCA was set up with $\Delta=10^{-3}$, $\epsilon=10^{-3}$ and $\alpha=0.8$.

Following Pereira s implementation (Pereira *et al.*, 1999), the optimization algorithm sends to the Reactor Physics code HAMMER (Suich and Honeck, 1967) a solution and receives back power-peaking, average thermal flux and the effective multiplication factor. This information is translated to the algorithm by means of an objective-function that, if all constraints are satisfied, has the value of the average peak factor. Otherwise, it is penalized proportionally to the discrepancy on the constraint.

4.2 Results

Table 2 shows the best objective-function values (i.e., lowest power-peaking factor values) obtained by the PCA and by HJPCA in ten independent experiments. Note that HJPCA's worst result is better than PCA's best.

Experiment	PCA[a]	HJPCA
#1	1.2827	1.2784
#2	1.2876	1.2783
#3	1.2964	1.2784
#4	1.2874	1.2784
#5	1.2829	1.2779
#6	1.2791	1.2777
#7	1.2975	1.2780
#8	1.2865	1.2783
#9	1.2908	1.2784
#10	1.2845	1.2787
Average	1.2875	1.2783

[a] Sacco et al., 2006.

Table 2: Results for 100,000 objective-function evaluations.

Table 3 shows the best configurations obtained by both algorithms, plus the objectives achieved and constraint values. The parameters obtained by each algorithm are quite different, suggesting that they may have reached different regions of the search space.

Parameters	PCA[a]	HJPCA
f_p	1.2791	1.2777
Avg. flux	8.06×10^{-5}	8.67×10^{-5}
k_{eff}	0.991	1.001
R_f (cm)	0.5497	0.7833
Δ_c (cm)	0.1450	0.1145
R_e, (cm)	0.6111	0.7581
E_1 (%)	2.7953	2.2179
E_2 (%)	2.9469	2.3252
E_3 (%)	5.0000	4.0227
M_f	U-Metal	U-Metal
M_c	SS-304	SS-304

[a] Sacco et al., 2006.

Table 3: Best configurations obtained by each algorithm.

5. Conclusions

With this work, we show that a hybridization of stochastic optimization and direct search optimization methods can be quite effective, as the former promote a thorough exploration of the search space and the latter exploit its promising areas. We do believe that the future in optimization lies in hybrid algorithms. In fact, there have been many recent efforts in this research field (see, for example, Oliveira and Lorena, 2007).

Moreover, we ratify the conclusion of Sacco *et al.* (2006), who recommended that the PCA should be applied to other optimization problems in the nuclear engineering field.

We are planning to apply the HJPCA to the nuclear core reload optimization problem (Poon and Parks, 1992), and also to a nuclear power plant surveillance tests optimization (Sacco *et al.*, 2008b).

Acknowledgements

The authors gratefully acknowledge Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ): A.C. Rios-Coelho is supported by grant E-26/100.452/2008 (Bolsa de Mestrado Aluno Nota Dez) and our research group is supported by grant E-26/171.107/2006.

References

M.S. Bazaraa, H.D. Sherali, C.M. Shetty, Nonlinear Programming Theory and Algorithms , John Wiley and Sons, New York, 1993.

J.N. Carter, Genetic Algorithms for Incore Fuel Management and other recent developments in optimization , in: Advances in Nuclear Science and Technology, Volume 25, Plenum Press, New York, 1997.

J.J. Duderstadt, L.J. Hamilton, Nuclear Reactor Analysis , John Wiley and Sons, New York, 1976.

R. Hooke, T.A. Jeeves, “Direct Search” Solution of Numerical and Statistical Problems, Journal of the ACM, vol. 8, pp. 212-229 (1961).

S. Kirkpatrick, C.D. Gelatt, M.P. Vecchi, Optimization by Simulated Annealing, Science, vol. 220, pp. 671-680 (1983).

N. Metropolis, A.W. Rosenbluth, M.N. Teller, E. Teller, Equations of State Calculations by Fast Computing Machines, Journal Chem. Phys., vol. 21, pp. 1087-1092 (1953).

A.C.M. Oliveira, L.A.N. Lorena, Hybrid Evolutionary Algorithms and Clustering Search , in: Studies in Computational Intelligence, Volume 75, Springer Verlag, Berlin, 2007.

C.M.N.A. Pereira, C.M.F. Lapa, Coarse-grained parallel genetic algorithm applied to a nuclear reactor core design optimization problem, Annals of Nuclear Energy, vol. 30, pp. 555-565 (2003).

C.M.N.A. Pereira, R. Schirru, A.S. Martinez, Basic Investigations Related to Genetic Algorithms in Core Designs, Annals of Nuclear Energy, vol. 26, pp. 173-193 (1999).

P.W. Poon, G.T. Parks, Optimizing PWR Reload Core Designs , in: R. Männer, B. Manderick (Eds.), Proc. 2nd Int. Conf. Parallel Problem Solving from Nature PPSN 2, North-Holland, Amsterdam, 1992.

W.F. Sacco, C.R.E. de Oliveira, C.R.E., A New Stochastic Optimization Algorithm based on Particle Collisions , in: Transactions of the American Nuclear Society, 92, 2005 ANS Annual Meeting, San Diego, CA, June, 2005.

W.F. Sacco, C.R.E. de Oliveira, Two stochastic optimization algorithms applied to nuclear reactor core design, Progress in Nuclear Energy, vol. 48, pp. 525-539 (2006).

W.F. Sacco, C.M.F. Lapa, C.M.N.A. Pereira, H. Alves Filho, A Metropolis Algorithm applied to a Nuclear Power Plant Auxiliary Feedwater System surveillance tests policy optimization, Progress in Nuclear Energy, vol. 50, pp. 15-21 (2008b).

W.F. Sacco, M.D. Machado, C.M.N.A. Pereira, R. Schirru, The fuzzy clearing approach for a niching genetic algorithm applied to a nuclear reactor core design optimization problem, Annals of Nuclear Energy, vol. 31, pp. 55-69 (2004).

W.F. Sacco, A.C. Rios-Coelho, N. Henderson, M. Ali, “A Metropolis Algorithm Combined with Hooke-Jeeves Local Search Applied to Continuous Global Optimization Test Problems”, in: Proceedings of the International Workshop on Stochastic and Applied Global Optimization (SAGO 2008), Skukuza, South Africa, 19-22 July, 2008a (to appear).

J.E. Suich, H.C. Honeck, The HAMMER System Heterogeneous Analysis by Multigroup Methods of Exponentials and Reactors , Savannah River Laboratory, Aiken, South Carolina, 1967.