



Geometrical optimization of PWR spacer grids using GeN-Foam and Genetic Algorithms

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Abstract: This paper presents the results of Computational Fluid Dynamics (CFD) oriented geometrical optimization using the GeN-Foam solver applied to subchannels of the fuel assembly in a PWR-type nuclear reactor. GeN-Foam is a coarse mesh OpenFOAM solver designed to study nuclear engineering problems involving the coupled solution of thermohydraulics, neutronics and thermomechanics. However, the solver could be used for complex geometry simulations, enabling multi-scale coupled simulations. To use GeN-Foam under these conditions, the results of the code for complex geometry simulation had to be evaluated. This assessment involved comparing the results obtained with the solver and those presented in a literature reference study. Despite the higher numerical diffusivity of the solver, this comparison demonstrated that GeN-Foam is capable of studying the fluid dynamics of fuel assemblies in nuclear reactors for both coarse and refined geometry conditions. After GeN-Foam was assessed, optimization was performed on subchannels of a fuel assembly using Genetic Algorithms (GA), evaluating the influence of geometric parameters of the spacer grids to minimize pressure drop and maximize secondary flow. Pareto Front solutions were assessed to identify a geometry that best balanced these two objectives. The optimized model showed better results than the reference study, as expected. However, the results also highlight the need to incorporate thermal physics and neutronics to ensure that the optimized solution meets the subchannel's flow and heat exchange requirements. All tools used in this work are well-established in the literature, free, and open-source.

Keywords: GeN-Foam, spacer grids, PWR, optimization.









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Otimização geométrica de grades espaçadoras de reatores PWR usando GeN-Foam e Algoritmos Genéticos

Resumo: Este trabalho apresenta os resultados da otimização geométrica orientada à fluidodinâmica computacional (CFD) utilizando-se o solver GeN-Foam aplicados a subcanais do elemento combustível de um reator nuclear do tipo PWR. O GeN-Foam é um solver do OpenFOAM para malhas grosseiras desenvolvido para estudar problemas de Engenharia Nuclear envolvendo soluções acopladas de termohidráulica, neutrônica e termomecânica. Entretanto, o solver poderia, teoricamente, ser utilizado para simulações com geometrias completas, o que permitiria simulações acopladas multi-escalas. Para utilizar o GeN-Foam sob estas condições, os resultados do código para uma simulação de geometria complexa tiveram que ser avaliados. Esta avaliação envolvei a comparação inicial dos resultados obtidos com o *solver* e aqueles apresentados em um trabalho de referência na literatura. Apesar de uma maior difusividade numérica do solver, esta comparação demonstrou que o GeN-Foam é adequado para o estudo da fluidodinâmica do elemento combustível em reatores nucleares para ambas as condições de geometria grosseira e refinada. Após o GeN-Foam avaliado, foi realizada uma otimização em subcanais de um elemento combustível, através da utilização de Algoritmos Genéticos (AG), na qual foi avaliada a influência de parâmetros geométricos das grades espaçadoras, buscando minimizar a perda de carga e maximizar o fluxo secundário. As soluções da Frente de Pareto foram avaliadas para identificar uma geometria que melhor equilibrasse esses dois objetivos. O modelo utilizado apresentou resultados melhores do que o estudo de referência, como esperado. No entanto, os resultados também evidenciam a necessidade de incorporar aspectos térmicos e neutrônicos para garantir que a solução otimizada atenda às necessidades de escoamento e troca de calor dentro do subcanal. Todas as ferramentas utilizadas neste trabalho são consolidadas na literatura, gratuitas e de código aberto.

Palavras-chave: GeN-Foam, grades espaçadoras, PWR, otimização.







1. INTRODUCTION

The fuel assembly in the core of a PWR reactor consists of two nozzles and a bundle of rods containing a fissile material arranged in pellets, as shown in Figure 1. The rods inside the fuel assembly can be organized differently and maintained in fixed positions using spacer grids so that the refrigerant flows through them to cool the rods. The arrangement of the fuel rods and spacer grids, some of which have mixing devices, is made to ensure that heat removal occurs most efficiently. It is important to emphasize that the spacer grid's structure also increases pressure loss in the circuit, which corresponds to the difference at the inlet and outlet. Therefore, when developing spacer grids, an optimal compromise must be achieved between the turbulence of the fluid for its cooling and the corresponding pressure loss [1].



Figure 1: Example of a fuel assembly with its components.



Inside a fuel assembly, the space between the rods filled with refrigerant fluid is designated subchannels. Spacer grids, which determine the arrangement of the rods and the behavior of the fluid, can be of different types and have various mixing devices. This results in different effects on the fluid flow inside and through these subchannels. As a result, the thermo-hydraulic performance of a fuel assembly and its efficiency in heat transfer are largely determined by the geometric features of the spacer grid and the mixing vanes [2].

Components of a nuclear reactor core can be simulated numerically using Computational Fluid Dynamics (CFD) [3], which is a method employed to analyze systems involving fluids, heat transfer, and other related phenomena [4]. CFD is a versatile tool with applications across various industrial sectors, and it plays a crucial role due to its capability to analyze systems where performing controlled experiments is challenging or even impossible. In the case of numerical simulation of nuclear reactor components, it is mostly desirable to include neutronics. However, the available solvers are typically used to simulate neutronics and thermal-hydraulics in a loose coupled way, which can increase the complexity and is computationally time-consuming [5].

GeN-Foam [6] is a CFD tool designed to solve nuclear engineering problems involving the coupled solution of thermohydraulics, neutronics and thermomechanics, based on OpenFOAM® [7], which is an open-source software in the C++ language used to solve partial differential equations. GeN-Foam was developed to work on scales more significant than the solvers available in OpenFOAM®; through the porous-medium model. This model is a standard approach for studying complex structures using a coarser, less refined mesh with dedicated models to simulate fluid interaction with subscale structures. Using the porous-medium technique reduces the complexity of numerical problems, such as stability or numerical diffusion problems, which occur when trying to couple different solutions for different meshes or using different solvers [5]. To evaluate GeN-Foam for subscale, the first objective of this work was to perform a comparison of the fluid dynamics solution for a subchannel of a PWR nuclear fuel assembly with the results obtained by Karoutas *et al.* [8] and Chun and Oh [9].

In studying nuclear reactor components, improving the neutronic and thermalhydraulic parameters of these components towards one or more objectives through optimization techniques is possible. Optimization evaluates the influence of specific parameters on achieving maximum or minimum values for the associated objectives [10]. In order to do this, the Genetic Algorithms (GAs) were the chosen technique, which corresponds to a class of Evolutionary Algorithms that use computational techniques based on the mechanisms of Darwinian evolution to solve optimization problems [11]. GAs evaluate populations of candidate solutions, where each individual represents a potential solution to the problem being addressed [12]. Over successive iterations, these populations evolve as the algorithm searches for the optimal solution [13]. In this sense, the second objective of this work was to run GeN-Foam solver in the numerical simulation of fluid dynamics coupled with GA to improve the spacer grid geometry of a nuclear fuel assembly to achieve the best possible performance based on the fluid dynamics properties considered.

To address this problem, GAs were applied to optimize a spacer grid with mixing vanes for a subchannel, focusing on two objectives related to the flow within a section containing four subchannels of the assembly. To achieve this, the velocity and pressure of the flow were measured during the simulation. After the optimization was performed, the set of solutions with the best compromises between these two objectives was obtained, called the Pareto Front [14]. The flow behavior of these solutions was analyzed, and the selected solution was compared with the results from Karoutas *et al.* [8] to evaluate the improvements achieved.



2. MATERIALS AND METHODS

CFD was employed to conducte numerical simulations associated with different geometries of the spacer grid and to understand their influence on fluid dynamics phenomena. The chosen tool was GeN-Foam, which addresses thermo-hydraulic problems by combining traditional RANS (Reynolds Averaged Navier-Stokes) equations, using the porous-medium model by adding a porosity term γ to the governing equations. This approach is used for a simplified treatment of the structures of a nuclear reactor when the interest is the representation of the macroscopic treatment, due to its simple formulation and ease of implementation [15].

Besides the porosity term, the equations also include the terms F_{SS} and \dot{Q}_{SS} , that represent the effects of subscale structures on the fluid flow, corresponding to the drag force made by the subscale structures on the fluid and the heat transferred between the fluid and the subscale structure, respectively. The conservation equations used by the solver are given by the Equations 1, 2 and 3. Without considering porous media, the equations are reduced to standard RANS equations, making them capable of simulating complex structures as a regular CFD solver. This feature theoretically enables multi-scale simulations using GeN-Foam.

$$\frac{\partial \gamma \rho}{\partial t} + \nabla \cdot (\gamma \rho \mathbf{u}) = 0 \tag{1}$$

$$\frac{\partial(\gamma\rho u)}{\partial t} + \nabla \cdot (\gamma\rho u \mathbf{u}) = -\frac{\partial\gamma p}{\partial x} + \nabla \cdot (\mu \nabla \mathbf{u}) + \gamma S_M + \gamma F_{SS}$$
(2)

$$\frac{\partial(\gamma\rho u)}{\partial t} + \nabla \cdot (\gamma \mathbf{u}(\rho i + p)) = \nabla \cdot (\gamma k \,\nabla T) + \gamma \mathbf{F}_{SS} \mathbf{u} + \gamma \dot{Q}_{SS}$$
(3)

Discretizing the target domain to solve equations 1, 2 and 3 using the finite volume method is necessary. To evaluate the use of GeN-Foam for complex geometries, such as fuel element spacer grids, the computational modeling of the problem requires the creation of the geometry of the subchannel with the spacer grid and the subsequent creation of the mesh.



For this study, the spacer grid geometry investigated by Karoutas *et al.* [8] was used as a reference for defining the parameters used in the numerical simulation and as a benchmark for comparing the results obtained. Table 1 presents the geometric parameters for the the computational modeling of the problem, considering a section with four subchannels of the fuel assembly of a PWR nuclear reactor. The arrangement of the vanes in the mixing device of the spacer grid corresponds to the same as in the work of Karoutas *et al.* [8].

Characteristic	Value	
Section length	0.660 m	
Rod configuration	2 x 2	
Number of subchannels	4	
Rod diameter	9.5 mm	
Pitch distance	12.7 mm	
Spacer grid height	grid height 40.0 mm	
Thickness of spacer grid and vanes	0.48 mm	
Number of vanes	8	
Vane base width	4.5 mm	
Vane height	10.0 mm	
Vane angle relative to the grid normal	25°	
Distance from spacer grid base in relation to inlet	0.1 m	

Table 1 : Fuel	assembly	section	characte	eristics.
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Previous work developed by Santos [2] was used as a reference for the mesh generation. The mesh was generated using OpenFOAM® native capabilities through BlockMesh, SurfaceFeatureExtract and SnappyHexMesh [7]. The mesh generated and its refinement, including viscosity layers near to the rod walls, are presented in Figure 2, resulting in 3,665,127 cells in the mesh.

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Figure 2: Top view of the used mesh and its details for the spacer grid.

Source : author.

After the comparison with Karoutas *et al.* [8], the defined methodology was employed for a geometrical optimization process. The spacer grid geometry was studied regarding pressure drop and secondary flow. These are the main parameters defining the spacer grid's fluid-dynamic characteristics. A low pressure drop and high secondary flow are desired.

The initial step in spacer grid optimization using GeN-Foam was to automate the generation of geometries for CFD simulations based on provided parameters. To achieve this, the proposed method uses a file in JSON (JavaScript Object Notation) dictionary format, in which all configurations were informed. The code for creating parametrized geometries was developed in Python [16] and uses libraries available on the SALOME platform [17] to create the geometry of the subchannel, including the spacer grid with vane. A mesh was generated for each geometry created. This parameterization is necessary for the optimization algorithm to find the optimal solution.

To simulate GeN-Foam, it was necessary to define the parameters for the numerical solution. These parameters include boundary conditions and initial conditions for each component, in addition to the physical properties of the refrigerant fluid. For the problem addressed in this work, the rod surfaces and the spacer grid were set as fixed and non-slip



walls, as highlighted in blue in Figure 3. The inlet was located on the lower face of the subchannel section, the outlet was on the upper face and the sides of the domain were modeled with translational cyclic periodicity. Cyclic periodicity boundary conditions are highlighted in green in Figure 3.



Figure 3: Boundary conditions and cyclical periodicity.

The other boundary conditions and the physical properties of coolant water were the same as those used in the experiments by Karoutas et al. [8], as presented in Table 2.

Tuble = (Doulidary contaitions and physical properties)			
Characteristic	Value		
Flow velocity at inlet	6.79 m/s		
Turbulent intensity	5%		
Static pressure at outlet	1.0x105 Pa		
Coolant temperature	temperature 26.67 °C		
Coolant pressure	4.83 bar		
Coolant density	15ity 996.7781 kg/m ³		
Coolant enthalpy	Coolant enthalpy 112,264.0483 J/kg		
Coolant entropy	390.4827 J/kg.K		
Coolant specific heat	oolant specific heat 4,180.0924 J/kg.K		
Coolant viscosity	8.5713x10 ⁻⁴ Pa.s		

Table 2: Boundary conditions and physical properties

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Once the boundary conditions and the physical properties were defined, numerical simulation was performed using GeN-Foam to obtain the numerical solution. As in Karoutas *et al.* [8], the evaluation of the numerical simulation result in this work considers the following parameters:

- Difference of Pressure or Pressure Drop (DP): It corresponds to the pressure difference between two distinct measurement points;
- Secondary Flow (SF): It corresponds to the average lateral movement of the refrigerant fluid that flows through the fuel assembly and is measured in a cross section. The calculation of the secondary flow related to each volume control present in the cross-section is performed by Equation 4. The average SF is obtained by calculating the simple average, where U_x and U_y correspond to lateral velocities and U_z is the axial velocity of the fluid in the subchannel.

$$SF = \frac{\sqrt{(U_x^2 + U_y^2)}}{U_z}$$
(4)

To evaluate the results obtained in this work, the same measurement positions were considered as in the work of Karoutas *et al.* [8] along the flow section. Therefore, the axial and lateral velocity profiles were measured along two subchannels at the positions indicated in Figure 4 to obtain the average secondary flow. It graphically presents these positions along the nuclear fuel assembly and the representation of the velocity measurement line at each position. The pressure is measured at positions O, A and G to calculate the pressure drop.







Source : Santos [2].

The computational optimization technique, Genetic Algorithms (GA), was used to obtain an optimized spacer grid. Figure 5 depicts a simple GA structure, where the optimal solution is identified after a finite number of iterations, each of which a set of potential solutions to the problem is evaluated. In this technique, one feasible solution is encoded in a set of values for the problem parameters, or design variables, and this encoding is called an individual. The quality of each solution related to the problem is assessed using a fitness function that must be chosen so that the individuals with the highest quality in terms of solving the problem have a greater probability of being selected for the next iteration. The individuals representing a set of solutions in an iteration are called a population. Genetic operators are applied in each iteration to diversify the population and incorporate the best individuals features through subsequent iterations. The algorithm concludes its execution when a termination condition, or stopping criterion, is achieved, like convergence or number of iterations [13].





Figure 5: Genetic Algorithms.

Source : author.

To conduct the optimization, a case study was executed focusing on optimizing the steady-state fluid flow within the section of the fuel assembly. The two objectives were to minimize pressure drop and maximize secondary flow. This assembly section comprises four subchannels, with a spacer grid featuring a mixing device located at the top. The mixing device consists of four pairs of vanes, with one pair positioned in each subchannel, as illustrated in Figure 6(a). In the computational modeling, each pair of vanes can be oriented along either the X-axis or the Y-axis, as depicted in Figure 6(b), with each vane forming an angle α with the normal to the axis on which it is positioned. The vanes have a length of 10 mm, and the angle α can vary independently for each vane between -37° and 37°.





Figure 6: Example of spacer grid for the case study.

Source : author.

The other geometric parameters of the model used in this study, except the section length, were the same as those used in comparing the GeN-Foam simulation with the benchmark, as shown in Table 1. Section length was reduced from 0.660 m to 0.360 m to reduce the computational cost of the various numerical simulations required during the GA iterations without compromising the optimization results. This reduction in length decreased the number of total cells in each mesh to the range of 1,117,158 to 1,127,518 elements and an average of 1,121,955. Data collection for the reduced fuel assembly section was carried out up to position E, as indicated in Figure 4.

Since the optimization performed in this work aims to minimize the pressure drop (DP) and maximize the secondary flow (SF), these are the two objectives to be evaluated in the GA, and the resolution of the problem needs to consider its multiobjective nature. Therefore, the implementation of MOGA (MultiObjective Genetic Algorithm) available in version 6.17 of the DAKOTA platform [18] was used, which is open source under the GNU LGPL (GNU Lesser General Public License) license and available for free download. MOGA uses the Pareto Front to find optimized solutions that balance two or more



objectives. The meta parameters for running a Multi-Objective Genetic Algorithm (MOGA) are detailed in Table 3. The 12 simulation variables correspond to the angles of each of the eight vanes and the orientation of each one of the four pairs of vanes on the spacer grid.

Meta parameter	Value	
Number of generations	Not defined	
Maximum number of mutations	120	
Initial population size	12	
Number of variables	12	
Number of objective functions	tions 2	
Type of crossover	2 points binary	
Crossover application rate	0.8	
Type of mutation	Uniform replacement	
Mutation application rate	0.1	

Table 3 : MOGA configuration for the case study.

The genetic operator called binary recombination with 2-point crossover was employed in processing MOGA for the case study. This method involves randomly selecting two crossover points within each encoding and swapping the values between these points between individuals in a pair. In this study, the crossover rate applied to each pair of individuals was 80%. The genetic operator mutation used in this study was a uniform mutation, where variation in the features was introduced by randomly selecting a design variable from an individual chosen randomly from the population and then altering its value to a new random value within the domain for that variable.

For the numerical simulation performed in the evaluation of each individual *x* during the MOGA iterations, the two objective functions evaluated as fitness function are:

f₁(x) = profile obtained by the secondary flow (SF) values collected in the plane transverse to the flow in each measurement positions A to E indicated in Figure 4. The objective function f₁(x) must be maximized;



f₂(x) = difference between the pressure measured at the inlet and at the outlet of the flow. The pressure at each position is obtained calculating the weighted sum of the pressure by the surface area of the elements in the plane. The objective function f₂(x) must be minimized.

Figure 7 illustrates the diagram of the operation of the DAKOTA tool for multiphysics optimization, including the coupling between the Genetic Algorithm and the numerical simulation used to evaluate each individual. The result is the set of optimized solutions of the Pareto Front.





Source : author.



The results obtained from the running of MOGA coupled with GeN-Foam were compared with those from Karoutas *et al.* [8] for the selected thermal-hydraulic parameters.

3. RESULTS AND DISCUSSIONS

Figure 8 compares the results obtained at the measurement positions after the spacer grid for lateral velocity (a) and axial velocity (b) to evaluate whether the results produced by GeN-Foam correspond with those from the benchmark study. Figure 8(a) indicates that, at the position A after the spacer grid, the results from GeN-Foam shows-similar behavior to those reported by Karoutas *et al.* [8], and as the flow progresses further from the spacer grid within the rod bundle GeN-Foam exhibits damping of the flow due to numerical diffusivity or turbulence model effects.

In Figure 9, the chart compares the pressure drop of the present work and the values calculated using the semi-empirical methodology developed by Chun and Oh [9], which estimates the pressure difference with 15% uncertainty. The chart shows the pressure losses between position O and G, which includes the spacer grid indicated in the gray region. It can be seen that the behavior in both cases is the same, with the present work showing slightly higher values for pressure drop along the evaluated domain.

For the optimization process, the impact of the numerical diffusivity of GeN-Foam can be disregarded as it is consistently present across all processed solutions, exerting the same influence on each comparison throughout the iterations of the Genetic Algorithm.

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Figure 8: Comparison of simulation results with experimental and numerical studies for lateral (a) and axial (b) velocities.

Figure 9: Comparison of simulation results with a numerical study for pressure drop.





Figure 10 presents a graph with the solutions obtained during the execution of MOGA and the set of optimized solutions of the Pareto Front. Each point on the graph represents a solution x, with the axes indicating the values of the objective functions $f_1(x)$ and $f_2(x)$ for each solution. The individuals in the Pareto Front represent the optimization results, which include a set of 12 solutions. The red line in the graph highlights the Pareto Front solutions, numbered according to the sequence in which the GA generated then. The points labeled PIS and NIS represent the solutions with the best and worst values for each objective function considering the solutions in Pareto Front, respectively. Solution number 92 is identified as having the best compromise between the objectives, based on the TOPSIS method [19].



Figure 10: Solutions obtained with the simulation.

Source : author.



Among the solutions on the Pareto Front, solution number 92, chosen using the TOPSIS method, corresponds to the vane as shown in Figure 11(a). The values obtained for this solution's functions $f_1(x)$ and $f_2(x)$ were 0.025584168254172954 and 32752.18990156341, respectively. Figure 11(b) illustrates the magnitude and direction of the lateral movement obtained from the simulation along the cross section at location A.



Figure 11: Solution 92, obtained by TOPSIS method.

Source : author.

In Figure 11(b) shows that, in the region closest to the vanes, the optimal solution exhibits a predominance of fluid movement in a single direction, from left to right, with minimal variation between the upper and lower subchannels. In a nuclear fuel assembly with such geometric characteristics and considering the thermal aspect, this flow pattern could form hot spots on the rod walls between the upper and lower subchannels, affecting heat transfer. However, it is important to note that this case study focused exclusively on fluid dynamics, and the solution obtained met the proposed objectives.

To compare the results of the CFD simulation using the vane layout of solution number 92 with those of the simulation based on the vane arrangement from Karoutas *et al.* [8], a CFD simulation was conducted incorporating the configurations obtained with MOGA and the vane angles from benchmark.



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Table 4 illustrates the vane arrangement in the spacer grid and the lateral flow obtained at measurement positions A, C, and E for the same vane angles as those used by Karoutas *et al.* [8] and the ones by solution number 92.



The comparative graph of the secondary flow profile between the two layouts at measurement points A through E is shown in Figure 12.



Figure 12: SF profile with rods of Solution 92 and Kaoutas et al.

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Additionally, Table 5 compares pressure drop values for the two vane layouts, with a flow length of 0.36 meters considered in both cases.

Table 5 : Pressure drop between the inlet and outlet faces and secondary flow at positions A and B for the configuration proposed by Karoutas *et al.* and solution 92.

Layout	Pressure Drop (Pa)	SF (A) (m/s)	SF (E) (m/s)
Karoutas <i>et al.</i>	32,219.93	0.19196	0.01445
Solution 92	32,752.19	0.24227	0.09086
Difference	1.65%	26.21%	528.79%

Based on the comparative results presented in Figure 11 and Table 5, it is observed that, although the pressure drop of layout 92 from the case study is 1.65% higher than that of the layout from Karoutas *et al.* [8], the magnitude of the lateral movement was improved by 26.21% at position A and by 528.79% at position E compared to the results obtained with the layout from Karoutas *et al.* [8].

4. CONCLUSIONS

The assessment of GeN-Foam for the study of nuclear fuel assemblies in subscale was performed by comparing its results in this work with those of Karoutas *et al.* [8], when higher numerical diffusivity was observed in the results obtained with the solver. This characteristic, present in all solutions generated by GeN-Foam, does not impact its use in the optimization process, as it uniformly affects all generated solutions during the iterations. Regarding the optimization objectives, minimizing pressure drop and maximizing secondary flow, the best solution obtained with the Genetic Algorithm outperformed the results of Karoutas *et al.* [8]. The pressure drop obtained with the spacer grid geometry of this best solution is higher than that of the benchmark study. However, the significant increase in secondary flow at all measurement positions highlights the potential of applying computational optimization



techniques to improve the performance of nuclear reactors, through the determination of the best geometric configurations for their components.

This study achieved its objectives of comparing the use of GeN-Foam with the benchmark study and applying optimization techniques to enhance the fuel assembly of a PWR nuclear reactor. However, the results also indicate the need to incorporate neutronic and thermal aspects to optimize the fuel assembly comprehensively. Therefore, this will be considered in future work.

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CONFLICT OF INTEREST

All authors declare that they have no conflicts of interest.

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