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Accelerating The Monte-Carlo Power Iteration Utilizing The Jacobian-Free Newton Krylov Methodology

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Abstract - *Nowadays, Monte-Carlo criticality analysis is performed utilizing the power iteration that calculates the fundamental eigenpair of the steady-state/k-eigenvalue form of the neutron transport equation. Whereas this method guarantees the convergence to the fundamental eigenmode, very often the convergence is slow. Consequently, it is of high interest to improve the convergence of the power iteration in order not only to increase the accuracy but also to reduce the computational cost. In this work an alternative version of the traditional Monte-Carlo power iterative algorithm is formulated, developed and analysed aiming to numerically accelerate the Monte-Carlo criticality analysis. More specifically, a Newton-based, matrix-free numerical method for solving non-linear systems, the Jacobian-Free Newton Krylov methodology, is adopted in the Monte-Carlo k-eigenvalue context attempting to accelerate the convergence. However, the computationally burdensome nature of a Monte-Carlo algorithm makes a straight forward implementation of this methodology rather impossible. The problem is overcome by suitably utilising a deterministic diffusion-based power iteration within the developed algorithm. Since the Monte-Carlo calculated quantities required by the introduced methodology are associated with statistical noise, a fact that creates questions about the performance of this new concept, the method is initially evaluated in simplified test-cases.*

I. INTRODUCTION

Nowadays, Monte-Carlo criticality (or k-eigenvalue) analysis is performed utilizing the power iteration that calculates the k-eigenvalue and the eigenvector of the eigenvalue form of the steady-state neutron transport equation. This method guarantees the convergence to the fundamental eigenmode but very often the convergence is slow; when the dominance ratio is near one. In practical problems this situation is often met. For this reason the improvement of the convergence of the Monte-Carlo k-eigenvalue iterative process is listed among the most important and challenging problems in computational neutron transport analysis as stated in [1] and [2] .

The convergence of the neutron source is a crucial point because it affects the accuracy of the results. This is the reason why the convergence of the source should be confirmed in order to avoid the contribution to the statistics, of cycles (or batches) that do not correspond to the converged region. The Shannon entropy, a concept from information theory, has been shown to be an effective diagnostic measure for characterizing the convergence of the neutron source ([3]-[5]). In practice, in every Monte-Carlo criticality calculation a problem-dependent number of cycles is skipped before tallying starts [6]. Another matter that is strongly bonded with the convergence of the source is the computational cost that generally imposes a constraint, especially when the problem requires a large number of cycles. As a consequence, it is of high interest to improve the convergence of the Power Iteration (PI) in order not only to increase the accuracy but also to reduce the computational cost.

One methodology that has been used for this purpose is the Coarse Mesh Finite Difference (CMFD) accelerated Monte Carlo proposed in [7]. According to this methodology, the multigroup diffusion equation in an eigenvalue form is solved per Monte-Carlo PI iterative step in order to find a better estimation of the current source distribution and to communicate it back to the next Monte-Carlo PI. Initially, CMFD methods were aiming to accelerate the neutron source convergence during the inactive cycles of a Monte-Carlo calculation. However the use of CMFD feedback in the active cycles is also investigated and applied. In [8] it is mentioned that the fission source that is affected by the CMFD parameters that are determined by the accumulated tallies of the previous cycles, suffers less from the inter-cycle correlation effect and can be an effective way to improve the global calculation.

In this work the first steps towards an alternative, numerically-accelerated, Monte-Carlo k-eigenvalue Power iterative algorithm is presented. More specifically, a Newton-based, matrix-free numerical method for solving non-linear systems, the Jacobian-Free Newton Krylov (JFNK) methodology [9] is adapted to a Monte-Carlo k-eigenvalue context aiming to accelerate the convergence of the calculated eigenpair. It should be mentioned that the JFNK has been implemented in the deterministic solution of the neutron transport equation [10]. However the stochastic and the computationally burdensome nature of a Monte-Carlo algorithm complicate significantly the problem and make a straight-forward implementation of JFNK rather impossible. As described below, JFNK requires the execution of some inner linear iterations per outer iteration that would increase the computational cost significantly in a Monte-Carlo simulation context. In order to overcome this problem, CMFD-based power iterations will be

utilized instead of Monte-Carlo ones within each inner linear iteration. Another important question is how the Monte-Carlo calculated quantities required by JFNK affect the global behaviour of the introduced algorithm. In this work, an initial step-by-step evaluation of the introduced methodology, developed on the OpenMC Monte-Carlo code [11], on simplified test-cases is performed.

II. METHODOLOGY

The k-eigenvalue form of the neutron transport steady-state equation is given by the following relation:

$$\begin{aligned}\boldsymbol{\Omega}\nabla\psi(\boldsymbol{r},\boldsymbol{\Omega},E)+\Sigma_t(\boldsymbol{r},E)\psi(\boldsymbol{r},\boldsymbol{\Omega},E)=\\ \iint\Sigma_s(\boldsymbol{r},E',\boldsymbol{\Omega}'\rightarrow E,\boldsymbol{\Omega})\psi(\boldsymbol{r},E',\boldsymbol{\Omega}')d\boldsymbol{\Omega}'dE'\\ +\frac{\chi(E)}{k_{eff}}\iint\nu(E')\Sigma_f(\boldsymbol{r},E')\psi(\boldsymbol{r},E',\boldsymbol{\Omega}')d\boldsymbol{\Omega}'dE'\end{aligned}\quad(1)$$

where $\boldsymbol{r}$ represents a point in $\mathbb{R}^3$, $\boldsymbol{\Omega}$ is a unit vector in $\mathbb{R}^3$ showing the direction of the neutron motion, E is the neutron energy, ψ is the angular flux that is connected with the the total flux ϕ by the relation $\phi=\int_{4\pi}\psi d\Omega$, and k_{eff} is the effective multiplication factor. Σ_t,Σ_s and Σ_f are the total, scattering and fission macroscopic cross-sections, ν is the mean number of neutrons produced per fission and χ is the fission energy distribution function. In operator form, that simplifies the notation, the equation can be written in the following relation:

$$(\mathbb{L}+\mathbb{T})\boldsymbol{\Phi}=\mathbb{S}\boldsymbol{\Phi}+\frac{1}{k_{eff}}\mathbb{M}\boldsymbol{\Phi}\quad(2)$$

where $\mathbb{L}$ is the leakage operator, $\mathbb{T}$ is the collision operator, $\mathbb{S}$ is the scatter-in operator and $\mathbb{M}$ is the fission multiplication operator and $\boldsymbol{\Phi}$ is the vector containing the scalar fluxes. After rearrangement of the involved terms it takes the following form:

$$(\mathbb{L}+\mathbb{T}-\mathbb{S})\boldsymbol{\Phi}=\frac{1}{k_{eff}}\mathbb{M}\boldsymbol{\Phi}\quad(3)$$

and finally:

$$\boldsymbol{\Phi}=\frac{1}{k_{eff}}\mathbb{F}\boldsymbol{\Phi}\quad(4)$$

Numerically this problem is traditionally solved by the Power Iteration:

$$\boldsymbol{\Phi}^{k+1}=\frac{1}{k_{eff}^{k}}\mathbb{F}\boldsymbol{\Phi}^{k}\quad(5)$$

where:

$$k_{eff}^{k+1}=k_{eff}^{k}\frac{\int\mathbb{M}\boldsymbol{\Phi}^{k+1}dr}{\int\mathbb{M}\boldsymbol{\Phi}^{k}dr}\quad(6)$$

and k denotes the k^{th} iterative step.

From this point on, the following idea is implemented. The PI, from a numerical point of view, can be seen as a fixed point iteration of the form:

$$\boldsymbol{u}^{k+1}=f(\boldsymbol{u}^{k})\quad(7)$$

where $\boldsymbol{u}$ is the vector of the solution that contains also the eigenvalue as a component of the solution:

$$\boldsymbol{u}=\begin{bmatrix}\boldsymbol{\Phi}\\ \lambda\end{bmatrix}\quad(8)$$

where $\lambda=\frac{1}{k_{eff}}$. f denotes the fixed point iteration as following:

$$f(\boldsymbol{u})=\begin{bmatrix}\lambda\,\mathbb{F}\boldsymbol{\Phi}\\ \overline{\lambda}(\boldsymbol{u})\end{bmatrix}\quad(9)$$

where $\overline{\lambda}(\boldsymbol{u})$ represents the updating procedure for λ. Instead of following the traditional PI methodology, a non-linear system is defined by setting:

$$\boldsymbol{r}(\boldsymbol{u})=\boldsymbol{u}-f(\boldsymbol{u})\quad(10)$$

where $\boldsymbol{r}$ is the vector of the nonlinear residual. A linearised form of Eq. 10 could be solved by setting, after a multivariate Taylor expansion about a current point $\boldsymbol{u}^k$, the delta/Newton form of the non-linear system:

$$\boldsymbol{J}\delta\boldsymbol{u}^{k}=-\boldsymbol{r}(\boldsymbol{u}^{k})\quad(11)$$

$$\boldsymbol{u}^{k+1}=\boldsymbol{u}^{k}+\delta\boldsymbol{u}^{k},\ \text{for } k=0,1...\quad(12)$$

where $\boldsymbol{u}$ is the vector of the unknowns, $\boldsymbol{u}^0$ is the initial guess, $\boldsymbol{r}(\boldsymbol{u}^k)$ is the vector of the non-linear residuals, $\boldsymbol{J}=\frac{\partial\boldsymbol{r}}{\partial\boldsymbol{u}}$ is its associated Jacobian matrix, and $\delta\boldsymbol{u}$ is the Newton correction vector. Because the construction of the Jacobian matrix is very expensive it can be avoided by using a linear solver that allows the solution of the linear system without the construction of the Jacobian matrix. Such a family of linear solvers constitute the Krylov solvers that require only the construction of matrix-vector products of the form $\boldsymbol{Jv}$ where $\boldsymbol{v}$ denotes a Krylov vector. These products can be approximated by the following relation:

$$\boldsymbol{Jv}=\frac{\boldsymbol{r}(\boldsymbol{u}+\varepsilon\boldsymbol{v})-\boldsymbol{r}(\boldsymbol{u})}{\varepsilon}\quad(13)$$

where ε is a small perturbation parameter. The scheme described by the Eqs 11-13 constitutes a JFNK scheme.

However, in a Monte-Carlo context, the implementation of this methodology would require the execution of some Krylov iterations per each Newton iteration that would be possibly proven computationally very expensive (consider that each Krylov iteration = one perturbed Monte-Carlo power iteration). In order to avoid the execution of some Monte-Carlo PIs per Newton iteration, the following idea is applied. Within each Newton iteration the performance of a perturbed Monte-Carlo power iteration for the calculation of the matrix-vector products will be replaced by PIs of a mutligroup diffusion-based method with transport-equivalent physics. Such a diffusion model methodology has been utilized in [12] within the context of CMFD acceleration. In operator form, this diffusion model can be written as following:

$$\mathbb{Q}\boldsymbol{\Phi}^{k+1}=\frac{1}{k_{eff}^{k}}\mathbb{P}\boldsymbol{\Phi}^{k}\quad(14)$$

where $\mathbb{Q}$ is the neutron loss matrix operator, $\mathbb{P}$ is the neutron production matrix operator, $\mathbf{\Phi}$ is the multigroup flux vector. These two operators are constructed by tallying the desired quantities within each Monte-Carlo cycle. As a consequence a diffusion PI, with physics constructed equivalently to the current Monte-carlo PI, is solved in a deterministic way using some linear solver.

Because the execution of deterministic diffusion Power iterations is considerably cheaper than the Monte-Carlo ones in terms of computational time, one could utilize a considerably large number of Krylov inner iterations per Newton outer iteration, in order to improve the convergence.

1. Krylov iteration

The main feature of Krylov methods which makes them suitable for use in the JFNK methods is that they need only matrix-vector products and so the creation of the expensive Jacobian matrix can be avoided. The general idea behind Krylov methodology is that it generates a chain of orthonormal vectors that are used as a basis of the subspace $\boldsymbol{K}_j$:

$$\boldsymbol{K}_j = span(\boldsymbol{r}_0^{linear}, \boldsymbol{A}\boldsymbol{r}_0^{linear}, \boldsymbol{A}^2\boldsymbol{r}_0^{linear}, ..., \boldsymbol{A}^{j-1}\boldsymbol{r}_0^{linear}) \quad (15)$$

This basis is used for the construction of the solution of a linear system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ where $\boldsymbol{r}_0^{linear} = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_0$ is the linear residual. The solution of the linear system is constructed iteratively as a linear combination of the Krylov vectors (Eq. 15) and can be written as:

$$\delta\boldsymbol{x}_j = \delta\boldsymbol{x}_0 + \sum_{i=0}^{j-1} \beta_i (\boldsymbol{J})^i \boldsymbol{r}_0^{linear} \quad (16)$$

where j is the Krylov iteration index and the scalars β_i are calculated to minimize the residual. The matrix-vector products required by Krylov methods can be approximated by Eq. 13 which is actually a first-order Taylor series expansion approximation to the Jacobian times a vector [9]. Although more than one Krylov methods exist, GMRES [13] is probably the most popular.

2. Setting a Monte-Carlo JFNK algorithm

The JFNK algorithm is suitable for a relatively simple implementation in an existing Monte-Carlo PI scheme. Actually only the difference between two successive PIs is needed in order to evaluate the vector of the non-linear residuals $\boldsymbol{r}(\boldsymbol{u})$. Consequently, all the details that concern the normalization and the update of the involved quantities will not be modified in this new context. It could be said that the new scheme acts as an acceleration of the traditional Monte-Carlo power iteration. As linear Krylov solver, GMRES method has been chosen. The implementation of the Krylov solver was done using Petsc library [14].

In order to apply the proposed methodology, a spatial/energetic mesh is required. In this work the CMFD coarse spatial mesh of OpenMC is used. Over that spatial mesh and the predifined energy groups, the neutron source, the non-linear residuals, the matrix-vector products as well as the JFNK-correction of the PI are evaluated. In addition a way for the communication between the Monte-Carlo particle distribution and the vector form of the information that is required by JFNK should be defined. In order to pass from a Monte-Carlo particle distribution to a cell-based vector form, the particle-weight per mesh cell is counted. In order now to communicate the JFNK correction back to Monte-Carlo, the expected number of neutrons to be born in a given cell and energy group calculated by JFNK is compared to the PI-calculated source distribution. This results to the generation of suitable weight adjusted factors ($f^g_{l,m,n}$) of the following form:

$$f^g_{l,m,n} = \frac{\sum_s^{JNFK} w_s}{\sum_s^{PI} w_s}; \quad s \in (g,l,m,n) \quad (17)$$

where w_s is the neutron's weight in a given cell (l,m,n) and energy group (g). Therefore the correction is communicated to the current neutron source by modifying the neutron weights per spatial cell and energetic group as following:

$$w'_s = w_s \times f^g_{l,m,n}; \quad s \in (g,l,m,n) \quad (18)$$

It should be noted that each particle's local coordinates and energy remain constant throughout this procedure. The algorithm developed in this work is summarised in Algorithm 1.

Algorithm 1 The introduced algorithm

do k = 1, Number of Power iterations
  Run the k_{th} Monte-Carlo cycle
   -Calculate $\boldsymbol{u}' = f(\boldsymbol{u}^{k-1})$
   -Tally the CMFD-required quantities
  Construct the residual: $\boldsymbol{r}^k = \boldsymbol{u}^{k-1} - \boldsymbol{u}'$
  Solve the linear system: $\boldsymbol{J}\delta\boldsymbol{u}^k = -\boldsymbol{r}^k$ (Krylov solver)
  -do j = 1, Number of Krylov iterations (Krylov solver)
    ...
    Perturb the solution (source and k_{eff}) : $\boldsymbol{u}_{per} = \boldsymbol{u}^{k-1} + \varepsilon\boldsymbol{v}$
    Run the diffusion based PI
    Calculate: $\boldsymbol{r}(\boldsymbol{u} + \varepsilon\boldsymbol{v}) = \boldsymbol{u}^{k-1} - \boldsymbol{u}_{per}$
    Calculate the matrix-vector product: $\boldsymbol{J}\boldsymbol{v} = \frac{\boldsymbol{r}(\boldsymbol{u}+\varepsilon\boldsymbol{v}) - \boldsymbol{r}(\boldsymbol{u})}{\varepsilon}$
    ...
  end do
  Update the global/Newton solution: $\boldsymbol{u}^k = \boldsymbol{u}^{k-1} + \delta\boldsymbol{u}^k$
  Communicate the new solution to the source bank
end do

III. TESTING THE DEVELOPED ALGORITHM - NUMERICAL EXPERIMENTS

As mentioned above, main aim of this work is to initially evaluate the performance of the introduced methodology (PI-JFNK) in the analysis of some simplified models. As a first step only the JFNK-corrected neutron fission source is communicated back to Monte-Carlo as an improved guess for the next Monte-Carlo cycle. JFNK-modified k_{eff} is tested only in the last test-case. Initially, this work evaluates the effect of PI-JFNK on the quality of the source. Afterwards, its effect

in complete calculations will be examined. Finally, the performance of the introduced algorithm is compared with those of the classical PI as well as the OpenMC's in-house CMFD accelerated PI (PI-CMFD). In this point it should be stated that the following test-cases are fictitious models with purpose to scout the performance of the introduced methodology.

1. A bare U-235 1-D slab case

The first test case is a simple 1-D slab with length equal 200 *cm* composed by just U-235 (1-D slab-1). A spatial mesh of 100 cells and 1 energy group have been utilized for this preliminary case (Table I). At the beginning, the effect of one PI-JFNK cycle on the neutron source is evaluated. More specifically after 19 skipped PI cycles, with 50k neutrons per cycle, the classical PI source of the 20^{th} step is compared with the source generated by PI-JFNK for the same cycle. Observing Fig. 1 it is obvious that PI-JFNK improves the neutron source distribution making the curve smoother and more similar to the well-converged source (Fig. 2) comparing with the classical PI. In this case the general shape of the source converges very fast, even with the classical PI, so a graph of Shannon entropy would not make any sense.

Now the impact of PI-JFNK on the convergence of the average eigenvalue, i.e. k_{eff}, is evaluated comparing with PI and PI-CMFD. These calculations are performed with 50k neutrons per cycle and 20 inactive cycles. For the PI-JFNK case a maximum number of 30 inner (linear) iterations are performed per outer (Power/Newton) step. Additionally, the converged eigenvalue of a PI with high statistics, that acts as a reference calculation, has been used for comparison. Fig. 3 shows that PI-JFNK improves the convergence of the average k_{eff} since it seems that this method generates a more stable, around the reference value, sequence of estimations of the average k-eigenvalue than the other two methodologies. Table II shows the final calculated k-eigenvalue; PI-JFNK gives the closest eigenvalue to the reference value.

Fig. 4 illustrates the behaviour of the Krylov iterative linear solver within some specific cycles. It can be seen that the magnitude of the linear residual converges to a continuously lower value ensuring that the global problem gradually converges. In addition it seems that a lower number of Krylov iterations could be selected since the convergence of the linear residual is achieved between the 10^{th} and the 15^{th} linear iteration with no significant improvement in the remaining iterations.

The converged neutron source generated by PI-JFNK is illustrated in Fig. 2; the very good quality of the calculated neutron source is ensured.

2. A bare UO_2 1-D slab case

In order to make the problem more difficult, the material properties of the fuel of 1-D slab-1 were modified in order to obtain a dominance ratio closer to unity. More specifically, the slab now contains UO_2; the atom densities and the material density are listed in Table I. This modified case is called 1-D slab-2.

Initially, three calculations are performed; one PI, one

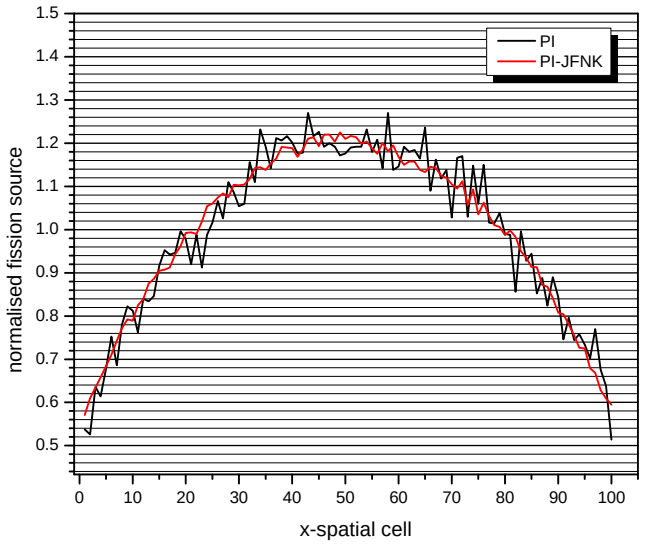

Fig. 1. Fission source of 1-D slab-1 for the 20^{th} cycle.

PI-CMFD and one PI-JFNK, all of them with 100k neutrons per cycle and 10 inactive cycles. Concerning PI-CMFD and PI-JFNK, CMFD and JFNK corrections are activated after 10 inactive cycles. For the PI-JFNK case a maximum number of 40 inner (linear) iterations are performed per outer (Power/Newton) step. Fig. 5 shows the evolution of the Shannon entropy for these three cases. It can be seen that PI needs around 100 cycles in order to achieve convergence. However even then it is characterised by a quite oscillatory behaviour of the Shannon entropy. On the other hand, the sources that correspond to PI-CMFD and PI-JFNK converge almost immediatelly after their activation; PI-CMFD source seems that converges somewhat faster than the one of PI-JFNK. As Fig. 5 suggests, an extra PI calculation is performed with 100, instead of 10, inactive cycles. The evolution of the average k_{eff} is depicted in Fig. 6. It can be seen that after 700 active cycles PI (100 inactive), PI-CMFD and PI-JFNK (both with 10 inactive) have converged approximately to the same value. However, it is illustrated that the PI-JFNK average k_{eff} converges faster than both PI and PI-CMFD. All methods diverge slightly (~ 25-35 pcm) from the reference value (PI with high statistics) but it is expected that after some extra cycles they would converge to that value. In addition, selection of higher Monte-Carlo statistics would improve the convergence of all methods. Figs 7-9 show the calculated fission sources in some

TABLE I. Slab models

	1-D slab-1	**1-D slab-2**
Length	200 *cm*	200 *cm*
# mesh cells	100	100
# energy groups	1	1
w_{235}	1	0.21
w_{238}	-	0.68
w_{16}	-	0.11
Density	0.00155 $\frac{atoms}{b-cm}$	19 g/cc

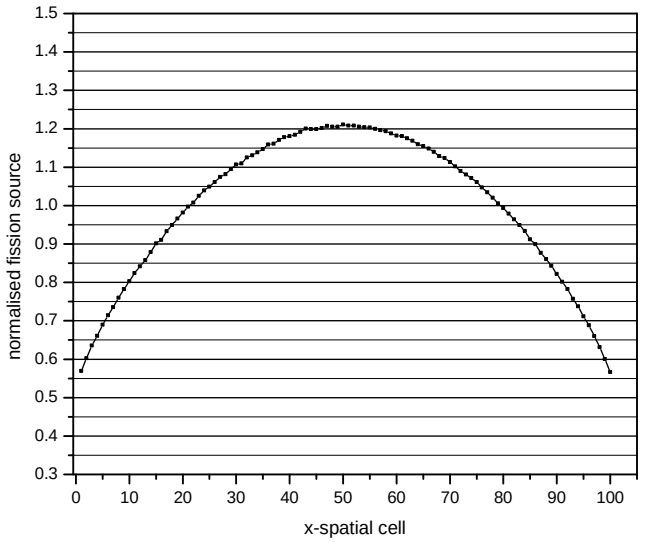

Fig. 2. Converged fission source of 1-D slab-1 with PI-JFNK.

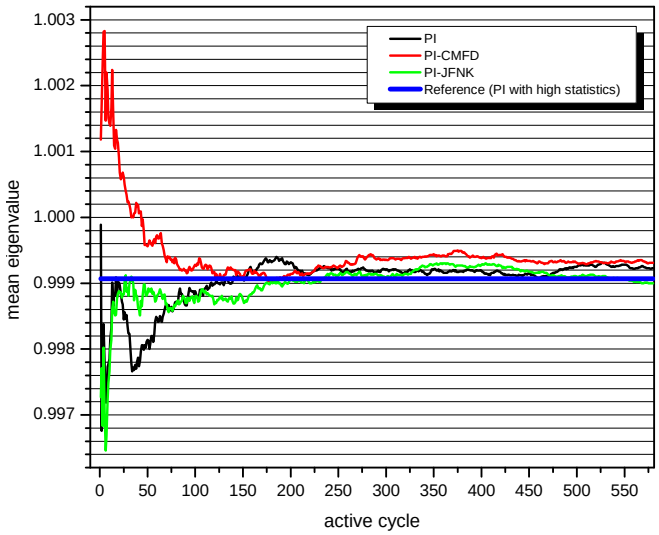

Fig. 3. Monte-Carlo calculated eigenvalue for 1-D slab-1.

specific cycles before and after JFNK correction within the same cycle. For cycle 11 it can be noticed that the neutron source has not converged at all. For both cycles 40 and 100 the general shape has converged. Higher quality is observed for cycle 100 as was expected. For both cases JFNK correction achieves its goal; it improves the pure PI guess within the same cycle.

Fig. 10 illustrates the behaviour of the Krylov iterative linear solver within some specific cycles. It can be seen that the magnitude of the linear residual converges to a continuously lower value ensuring again that the global problem gradually converges. It should be mentioned that the fact that this problem is more difficult than the previous case is also reflected to the fact that lower inner convergence levels (convergence

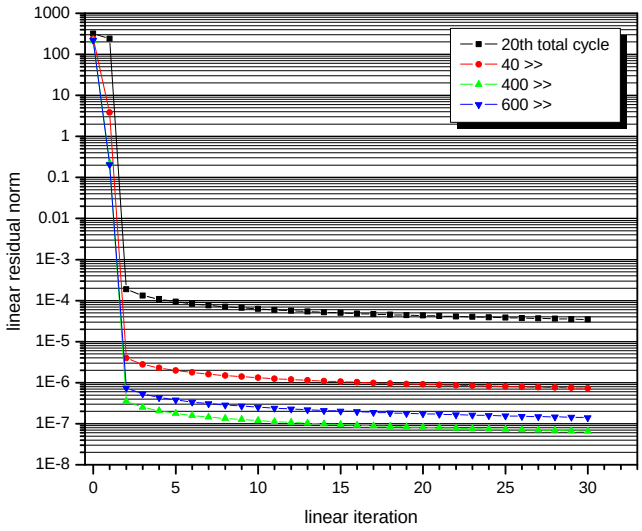

Fig. 4. Convergence of linear solver within some specific cycles for 1-D slab-1.

to higher values) are noticed in this case. Also in this case it seems that a significantly lower number of Krylov iterations could be selected since the convergence of the linear residual is achieved at the quite the early iterations with no significant improvement in the remaining iterations.

TABLE II. Calculated average eigenvalues (k_{eff}) for slab cases

	1-D slab-1	**1-D slab-2**
PI (20 inact.)	$0.99922 \pm 18pcm$	-
PI (100 inact.)	-	$1.60431 \pm 17pcm$
PI-CMFD	$0.99932 \pm 17pcm$	$1.60427 \pm 17pcm$
PI-JFNK	$\mathbf{0.99900 \pm 17pcm}$	$\mathbf{1.60424 \pm 17pcm}$
Reference (PI)	$\mathbf{0.99907 \pm 03pcm}$	$\mathbf{1.60398 \pm 05pcm}$

3. A single multi-region fuel pin

The third test case concerns a single-pin model with an axial variation of the fuel composition. The main features can be seen in Table (III). The fuel pin is surrounded by coolant-moderator. At the top and bottom there is a reflector. In the radial direction, reflective boundary conditions have been utilised whereas at the axial edges vacuum boundaries have been implemented. The fuel/moderator temperature as well as the moderator density profile have been calculated by some iterations of a coupled neutronic/Thermal-Hyduralic calculation [15] with 38 axial levels in the fuel region. The resulting strong density gradient is considered as a factor that complicates the solution of the Monte-Carlo k-eigenvalue calculation. Fig. 11 shows the coolant density profile that is used by this model.

In this case three calculations are performed; one PI, one PI-CMFD and one PI-JFNK. One PI with high statistics that acts as the reference calculation has also been performed. The spatial mesh that is used in PI-CMFD and PI-JFNK consists of 1×1×420 cells. In both PI-CMFD and PI-JFNK 10 inactive

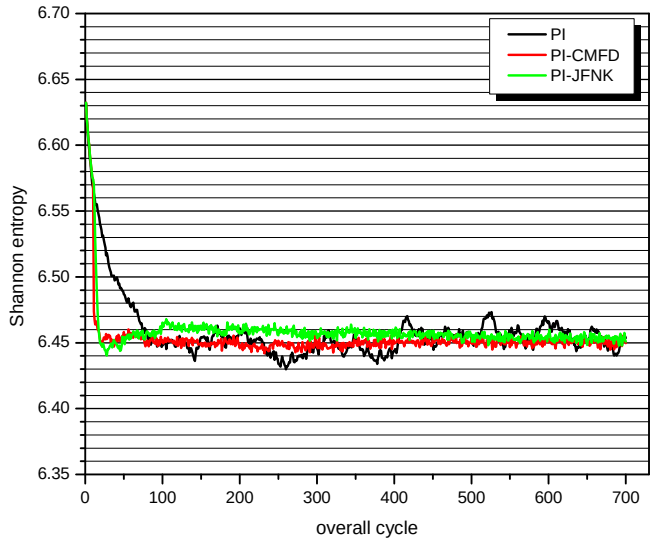

Fig. 5. Shannon entropy of the source of 1-D slab-2.

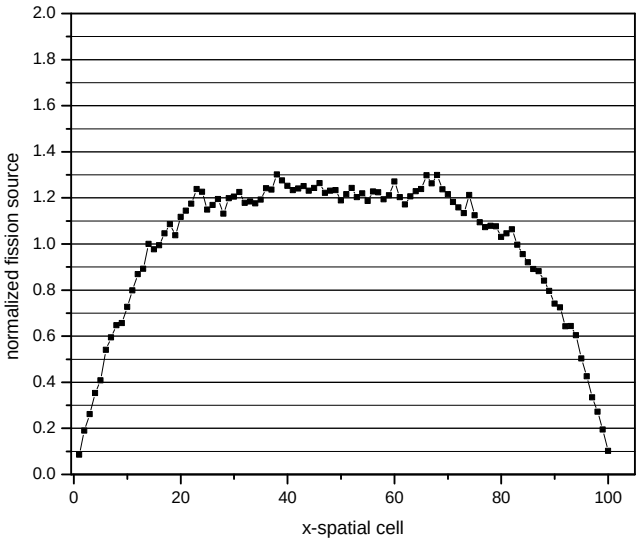

Fig. 7. Fission source of 1-D slab-2 for the 11^{th} cycle with PI-JFNK.

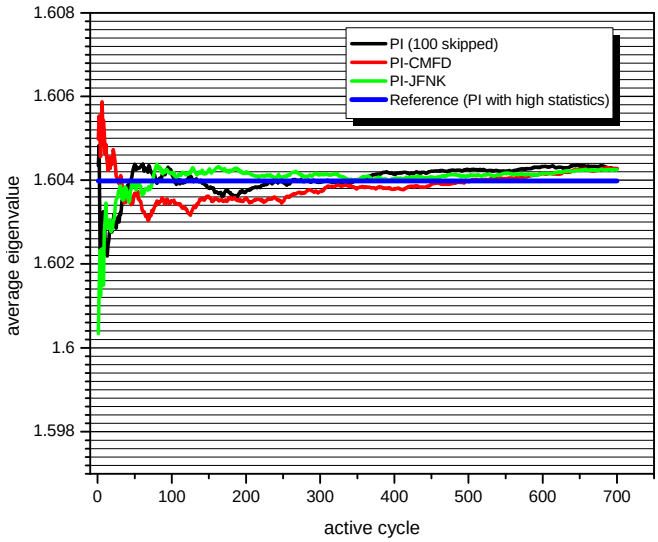

Fig. 6. Monte-Carlo calculated eigenvalue of 1-D slab-2.

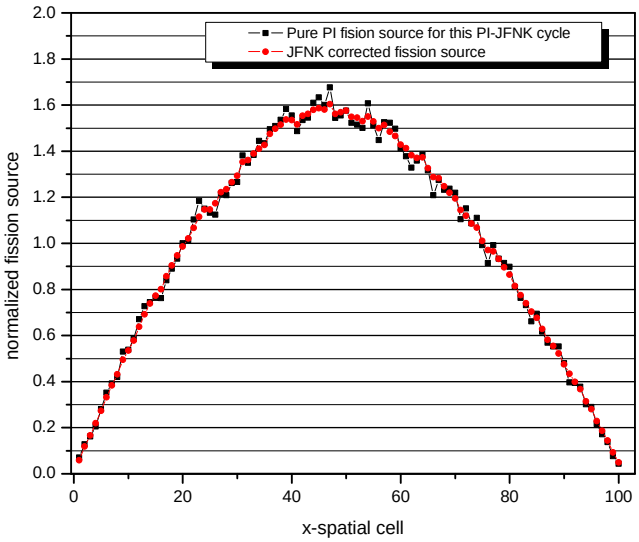

Fig. 8. Fission source of 1-D slab-2 for the 40^{th} cycle.

cycles are used and the acceleration feedback is activated in the 10^{th} cycle. The classical PI is performed with 150 inactive cycles. In both cases the initial neutron source guess is a spatially flat neutron distribution.

Fig. 12 shows that PI needs around 100 cycles to achieve convergence of the source. However even then PI is characterised by a somewhat oscillatory behaviour of the Shannon entropy. On the other hand the sources that correspond to PI-CMFD and PI-JFNK converge almost immediately after their activation. More specifically, PI-JFNK converges faster than PI-CMFD; PI-JFNK converges after ~70 overall cycles whereas PI-CMFD converges after ~100 overall cycles. Fig. 13 illustrates the evolution of the average k_{eff}. The converged eigenvalue calculated by the PI with high statistics is used as a reference. It can be seen that PI-JFNK converges after less than 100 active cycles, whereas PI (with ~150 inactive cycles) converges after 700 active cycles. PI-CMFD converges after ~200 active cycles. In addition Table (IV) shows that the PI-JFNK eigenvalue is the closest to the reference value.

At the end the introduced methodology is tested having activated the k_{eff} feedback additionally to the neutron source one. Two calculations run with a spatial mesh of 105 cells; one with only source feedback and one with both source and k_{eff} feedbacks. Fig. 14 shows the evolution of the Shannon entropy. It can be seen that in the case where the k_{eff} feedback

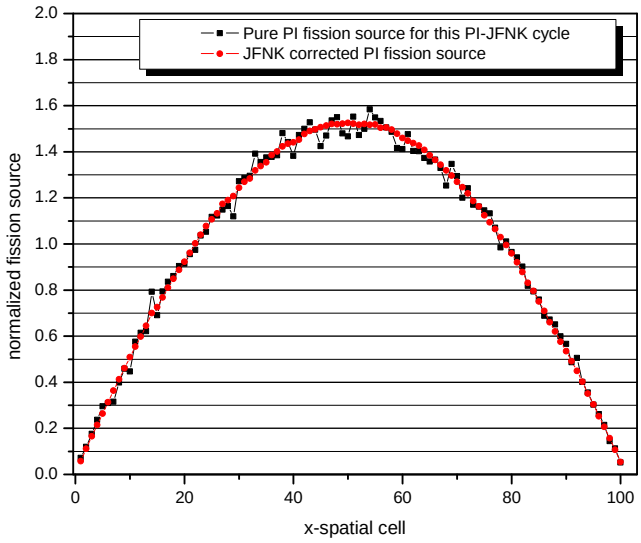

Fig. 9. Fission source of of 1-D slab-2 for the 100^{th} cycle.

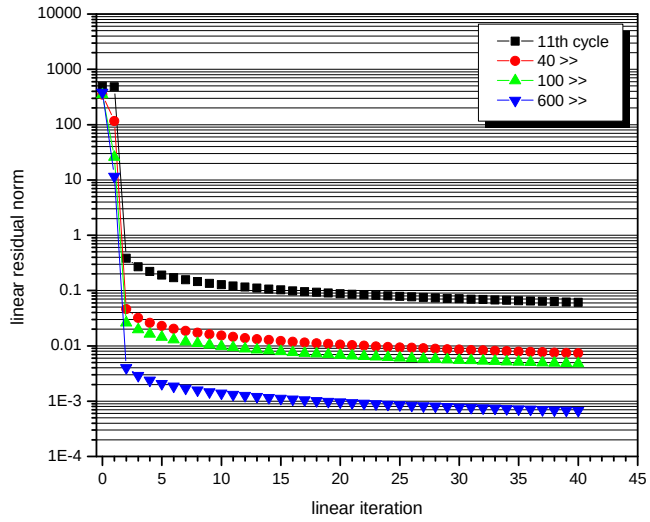

Fig. 10. Convergence of linear solver within some specific cycles for 1-D slab-2.

is activated the Shannon entropy converges faster, i.e. in less than 75 cycles, whereas the case without k_{eff} feedback needs about 150 cycles in order to achieve convergence.

4. Inner vs outer convergence

In this point it should be mentioned that the convergence of the outer Newton iteration can be linked to the one of the inner Krylov iteration by the following relation

$$\| \boldsymbol{J}^k \Delta \boldsymbol{u}^k + \boldsymbol{r}(\boldsymbol{u}^k) \|_2 < \gamma \| \boldsymbol{r}(\boldsymbol{u}^k) \|_2 \qquad (19)$$

where γ is a forcing term. Details about the role of this forcing term can be found in [16]. Here it should be stated that a proper trade-off should be found between the convergence

TABLE III. Single pin model

	Single multi-region pin
Active length (cm)	380
Total length (cm)	420
Pellet radius (cm)	0.5225
Pin radius (cm)	0.6125
Fuel enrichment (%)	0.71/3.3/7.7

TABLE IV. Calculated average eigenvalues (k_{eff}) for single-pin

	Single multi-region pin
PI (150 inact.)	$1.25800 \pm 17pcm$
PI-CMFD	$1.25804 \pm 16pcm$
PI-JFNK	$\mathbf{1.25820 \pm 17}\boldsymbol{pcm}$
Reference (PI)	$\mathbf{1.25815 \pm 08}\boldsymbol{pcm}$

level of the inner Krylov iteration and the one of the outer Newton iteration. Improper balance between the convergence of these two iterative procedures can result in the issue of "over-solving". Practically this means that a very low γ has been used in quite early Newton steps implying that a very accurate linear solution has been obtained to a quite inaccurate Newton correction. This can affect negatively the convergence of the outer Newton iteration. Discussion about this issue can be found in [17] and [18]. The analysis of the connection of these two norms was out of the scope of this work and constitutes subject for future research.

IV. CONCLUSION

This work introduces a new methodology that aims to accelerate the convergence of the classical Monte-Carlo Power iteration. This new methodology is based on the Jacobian-free Newton Krylov (JFNK) numerical technique. Because a

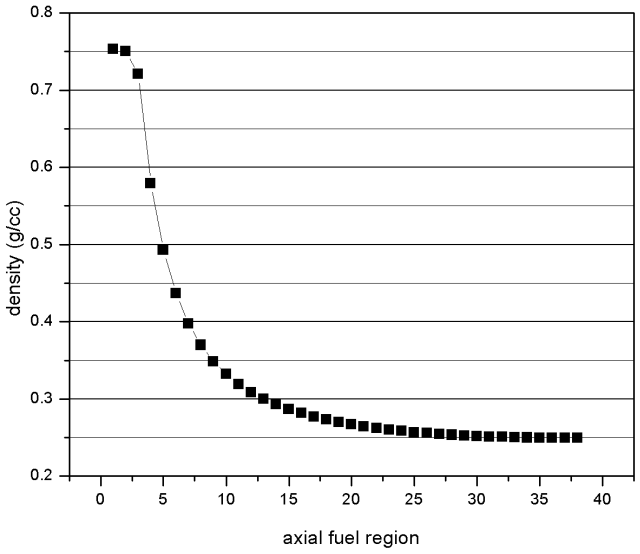

Fig. 11. Moderator density profile of the single-pin model (bottom to top).

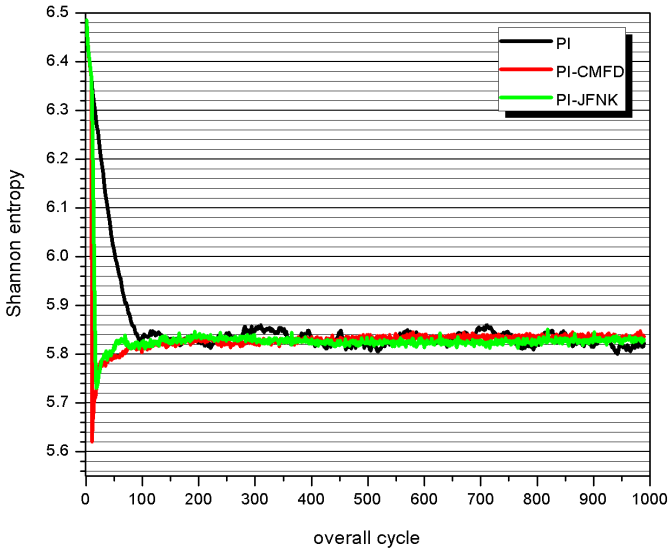

Fig. 12. Shannon entropy of the source of the single-pin.

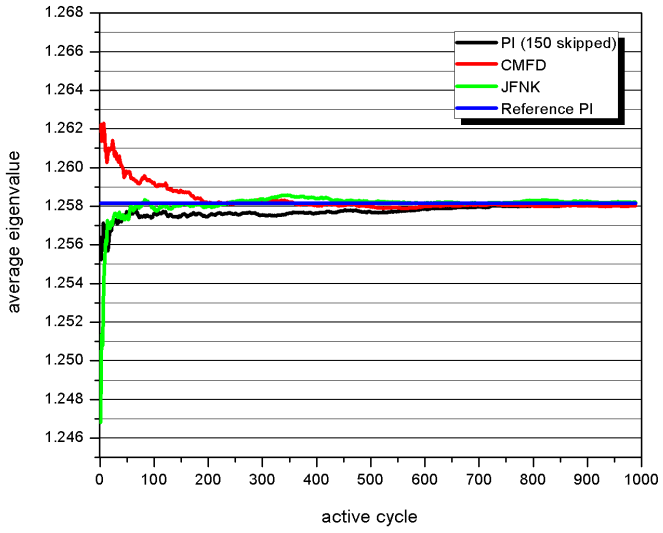

Fig. 13. Monte-Carlo calculated eigenvalue of the single-pin.

straight-forward implementation of JFNK in a Monte-Carlo context is rather impossible due to the high computational cost, the Coarsh Mesh Finite Difference (CMFD) diffusion technique was combined as an approximation with JFNK in order to alleviate this problem. Testing in simplified cases shows that the introduced methodology improves the quality of the neutronic solution update within each iteration comparing with the classical PI. This improved update in each iteration results in the acceleration of the convergence of the global problem. More specifically this methodology improves significantly the convergence comparing to the classical Power iteration. Furthermore, it seems that it behaves in a very satisfying way even comparing with CMFD; however further investigation is required.

Since JFNK involves a set of various numerical parameters, their optimal combination with the Monte-Carlo statistics should be investigated. In addition, the performance of the method in problems of larger scale should be examined and evaluated. Finally, the computational cost of this method should be investigated and compared with other methods. These issues constitute subject for future research.

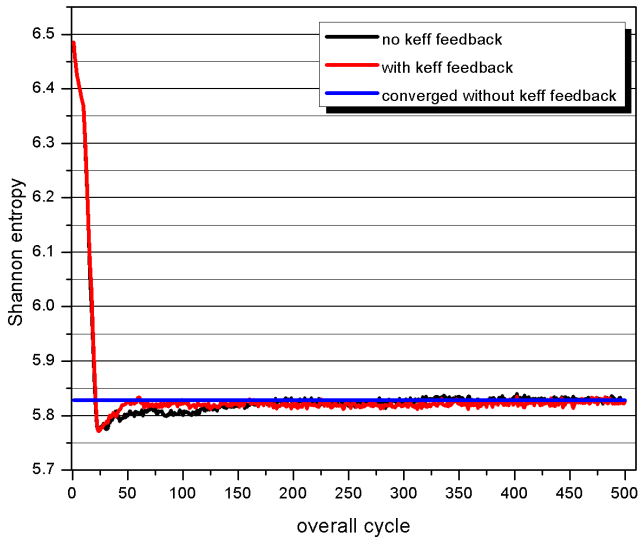

Fig. 14. Shannon entropy of the source of single-pin; PI-JFNK without and with k_{eff} feedback.

REFERENCES

1. N.Z. CHO, J. CHANG, “Some outstanding problems in neutron transport computation”, Nuclear Engineering and Technology, Special issue, 41, 4 (2009).
2. W. R. MARTIN, “Challenges and prospects for whole-core Monte Carlo analysis”, Nuclear Engineering and Technology, 44, 2 (2012).
3. T. UEKI , F.H. BROWN, “Stationarity and Source Convergence in Monte Carlo Criticality Calculations,” ANS Topical Meeting on Mathematics & Computation, Gatlinburg, TN April 6-11, (2003).
4. T. UEKI, F.B. BROWN , “Stationarity Modeling and Informatics-Based Diagnostics in Monte Carlo Criticality Calculations,” Nucl. Sci. Eng. 149, 38-50 (2005).
5. F.B. BROWN. “On the Use of Shannon Entropy of the Fission Distribution for Assessing Convergence of Monte Carlo Criticality Calculations,” proceedings PHYSOR-2006, Vancouver, British Columbia, Canada (2006).
6. F. BROWN, “A Review Of Best Practices For Monte Carlo Criticality Calculations,” American Nuclear Society, Nuclear Criticality Safety Topical Meeting, Richland, WA, 13-17 September (2009).
7. M.J. LEE, H.G. JOO, D. LEE K. SMITH,“Investigation of CMFD Accelerated Monte Carlo Eigenvalue Calculation with Simplified Low Dimensional Multigroup Formulation,” Proc. of the 2010 International Conference on the Physics of Reactors, May 9-14, 2010, Pittsburgh, PA, CD-ROM, American Nuclear Society (2010)

8. M.J. LEE, H.G. JOO, D. LEE, K. SMITH, "Coarse mesh finite difference formulation for accelerated Monte Carlo eigenvalue calculation", Ann. Nucl. Energy, 65, pp. 101-113 (2014).
9. D.A. KNOLL, D.E. KEYS, "Jacobian-free Newton-Krylov methods: a survey of approaches and applications," J. Comput. Phys., 193, 2004, pp. 357-397 (2004).
10. D.F. GILL, Y.Y. ASMY, "A Jacobian-Free Newton-Krylov Iterative Scheme For Criticality Calculations Based On The Neutron Diffusion Equation," Proc. Int. Conf. on Mathematics,Computational Methods and Reactor Physics, Saratonga Springs, New York, May 3-7 (2009).
11. P. K. ROMANO, B. FORGET, "The OpenMC Monte Carlo particle transport code," Nucl. Technol., 51, pp. 274-81 (2013).
12. B. R. HERMAN, B. FORGET, K. SMITH, "Progress toward Monte Carlo-thermal hydraulic coupling using low-order diffusion acceleration methods", Ann. Nucl. Energy, 84, pp. 63-72 (2015).
13. Y. SAAD, M.H. SCHULTZ, "GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems," SIAM J. Sci. Stat. Comput., 7, pp. 856-869 (1986).
14. S. BALAY, J. BROWN, K. BUSCHELMAN, W.D. GROPP, D. KAUSHIK, M.G. KNEPLEY, L.C. McINNES, B.F. SMITH, H. ZHANG, PETSc, http://www.mcs.anl.gov/petsc (2014).
15. A.G. MYLONAKIS, M. VARVAYANNI, D.G.E. GRIGORIADIS, P. SAVVA, N. CATSAROS, "Optimization of an Integrated Neutronic/Thermal-Hydraulic reactor core analysis model", 23rd International Conference Nuclear Energy for New Europe 2014, Portoroz, Slovenia, September 8-11 (2014).
16. R. DEMBO, S. C. EISENSTAT, T. STEIHAUG, "Inexact Newton methods", SIAM J. Numer. Anal. 19, 400-408 (1982).
17. J.N. SHADID, R.S. TUMINARO, H.F. WALKER, "An inexact Newton method for fully coupled solution of the Navier-Stokes equations with heat and mass transport", J. Comput. Phys. 137, 155-185 (1997).
18. R.S. TUMINARO, H.F. WALKER, J.N. SHADID, "On backtracking failure in Newton-GMRES methods with a demonstration for the Navier-Stokes equations", J. Comput. Phys. 180, 549-558 (2002).