International Conference
Nuclear Energy for New Europe 2005
Bled, Slovenia, September 5-8, 2005

NEW SPARSE MATRIX SOLVER in the KIKO3D 3-DIMENSIONAL REACTOR DYNAMICS CODE

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ABSTRACT

The goal of this paper is to present a more effective method Bi-CGSTAB for accelerating the large sparse matrix equation solution in the KIKO3D code. This equation system is obtained by using the factorization of the improved quasi static (IQS) method for the time dependent nodal kinetic equations. In the old methodology standard large sparse matrix techniques were considered, where Gauss-Seidel preconditioning and a GMRES-type solver were applied. The validation of KIKO3D using Bi-CGSTAB has been performed by solving of a VVER-1000 kinetic benchmark problem. Additionally, the convergence characteristics were investigated in given macro time steps of Control Rod Ejection transients. The results have been obtained by the old GMRES and new Bi-CGSTAB methods are compared.

1 INTRODUCTION

KIKO3D [1, 2] is a three-dimensional reactor dynamics code for coupled neutron kinetics and thermal-hydraulics calculation of VVER type pressurized water reactor cores. The code has been developed in KFKI Atomic Energy Research Institute. Main applications of KIKO3D are the calculation of asymmetric accidents in core, e.g. Control Rod Ejection, Inadvertent Control Rod Withdrawal. The above – so called – middle-fast transients play an important role in the safety analyses.

Recently, there has been a tendency to use new simulation methods in the field of nuclear energy. Our interest is focused on uncertainty analysis methods, which need a lot of computer running. Hence, by using more effective iteration techniques for the solution of large sparse equations result in saving a good amount of time.

2 DERIVATION OF THE LARGE SPARSE MATRIX EQUATION

In the KIKO3D code [1] the core is subdivided into nodes. Six delayed neutron groups are considered. The time dependent neutron balance in each node is written into the following form:

$$\mathbf{T}(\mathbf{r},t)\Psi(\mathbf{r},t)=\left(\frac{1}{\mathbf{v}}\frac{\partial}{\partial t}-\chi\beta\,\mathbf{F}(\mathbf{r},\mathrm{t})\right)\Psi(\mathbf{r},t)+\chi\sum_{j=1}^{6}\lambda_j \mathrm{C}_j(\mathbf{r},t)\,, \qquad (1)$$

$$\frac{\mathrm{d}C_j(\mathbf{r},t)}{\mathrm{d}t} = -\lambda_j C_j(\mathbf{r},t) + \beta_j \mathbf{F}(\mathbf{r},t)\Psi(\mathbf{r},t), \tag{2}$$

where the left hand side of Eq. (1) comprises the terms of the static neutronic equation (for example the two-group diffusion equation) and

- **F(r**, t**)** is the fission operator,
- Ψ**(r**, t**)** is the two-group scalar flux,
- β_j and β are the delayed neutron fractions,
- C_j**(r**, t**)** are the precursor densities,
- χ is the fission spectrum.

As a result of the applied advanced nodal method [1] the time dependent nodal equation for the whole reactor can be derived, where the unknowns are the time dependent amplitudes $\mathbf{O}_j$ and the face integrated fluxes **F**. The factorization of the improved quasi static (IQS) method is introduced as

$$\mathbf{F}(t) = \mathrm{A}(t)\mathbf{f}(t), \tag{3}$$

where A(t) is the amplitude function, and **f(***t***)** is the shape function changing slowly with the time. Finally, we get the point kinetic equations for the amplitude function and a large sparse matrix equation for the shape function using backward differential scheme:

$$\left[\mathbf{G}_0 - \beta\mathbf{G}_\mathrm{f} - \frac{\frac{\mathrm{dA}}{\mathrm{d}t}}{\mathrm{A}}\mathbf{G}_\alpha\right]\mathbf{f}(t_i^{macro}) - \mathbf{G}_\alpha\frac{\mathbf{f}(t_i^{macro}) - \mathbf{f}(t_{i-1}^{macro})}{\Delta t} + \frac{1}{\mathrm{A}}\sum_{j=1}^{6}\lambda_j\mathbf{G}_\mathrm{f}\mathbf{O}_j = 0, \tag{4}$$

where $\mathbf{G}_\mathrm{x}$ (x = "0", "α", "f") are the generalized response matrices defined in [1].

This equation can be written mathematically in the following matrix form:

$$\mathbf{A}\mathbf{x} = \mathbf{b}. \tag{5}$$

The shape function equations are solved so called macro step – by - macro step and the point kinetic equations are solved micro step – by – micro step between two macro steps.

3 NUMERICAL SOLUTION OF THE LARGE SPARSE EQUATION SYSTEM BY THE GMRES AND BI-CGSTAB ALGORITHMS

Eq. (5) defines a large sparse equation system where matrix **A** is usually non-symmetric so we have to apply such numerical techniques which are applicable for solving this problem. The sparse matrix comes from the condition that each node is connected with a restricted number of nodes in its neighbourhood but not with nodes that lie farther away.

In the old methodology Eq. (5) was solved with standard large sparse techniques, where Gauss-Seidel preconditioning and a Generalized Minimal Residual (GMRES)-type solver were applied. According to the goal – accelerating the large sparse matrix equation solution – in the new procedure the BiConjugate Gradient Stabilized (Bi-CGSTAB) [4] was selected and built into the KIKO3D code. It must be mentioned that in both cases we used Gauss-Seidel preconditioning in KIKO3D so that in fact one has to solve:

$$\left(\mathbf{I} + (\mathbf{L}+\mathbf{D})^{-1}\mathbf{U}\right)\mathbf{x} = \tilde{\mathbf{A}}\mathbf{x} = (\mathbf{L}+\mathbf{D})^{-1}\mathbf{b} = \tilde{\mathbf{b}}. \tag{6}$$

Both GMRES and Bi-CGSTAB algorithms are so called Krylov-subspace methods characterized by the subspaces in which the iterates lie. The Krylov-subspace can be given as

$$\mathcal{K}_m(\mathbf{A},\mathbf{r}_0) \equiv span\left\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \ldots, \mathbf{A}^{m-1}\mathbf{r}_0\right\}, \tag{7}$$

where $\mathbf{r}_0 = \mathbf{b}\text{-}\mathbf{A}\mathbf{x}_0$ is the initial residual vector.

The theories of these methods are discussed in book of Saad [5] and a deeper discussion of Krylov-subspace methods can be found in a new book of Broyden and Vespucci [6].

In case of GMRES, applying the modified Gram-Schmidt orhtogonalization to the Krylov-subspace one can build an orthonormal basis. This procedure is called Arnoldi's method [7], which brings matrix **A** with an orthonormal similarity transform to an upper Hessenberg matrix. Matrices of upper Hessenberg form have zeros below the lower codiagonal positions, i. e. $h_{ij} = 0$, $i - j > 1$. It can be shown that this method can be applied to solving the eigenvalue problem and even the large sparse linear system. In the literature there are two variants to realize the GMRES method.

On the one hand, a GMRES method was published by Saad and Schults [8] for solving linear system, which minimizes the Euclidean norm of the residual vector using the orthonormal basis of $\mathcal{K}_m(\mathbf{A}\ \mathbf{r}_0)$ in each iteration cycle.

On the other hand Walker and Zhou [3] published a simpler variant of GMRES which minimizes the Euclidean norm of the residual vector using the orthonormal basis of $\mathbf{A}\mathcal{K}_m(\mathbf{A}\ \mathbf{r}_0)$. Our method corresponds to this latter one. This algorithm bring matrix **A** at once into the form of an upper triangular matrix so that programming and using of that is easier.

In the KIKO3D code the error of the solution is estimated in Chebyshev norm as:

$$\left\|\mathbf{x} - \mathbf{x}_{k+1}\right\|_\infty \approx \frac{\left\|\mathbf{r}_k\right\|_1 \left\|\mathbf{r}_k\right\|_2}{\left(\sum_{j=1}^{k} h_{jk}^2\right)^{1/2}}, \tag{8}$$

where h_{jk} comes from the modified Gram-Schmidt othogonalization procedure. This is not an exact estimation for this problem and one can found its derivation using of $\mathbf{A}^T\mathbf{A}$ vectors in [9].

According to the goal we have investigated other Krylov-subspace methods [5, 6] for the solution of Eq. (5). These were Conjugate Gradient (CG), Biconjugate Gradient (Bi-CG) and BiConjugate Gradient Stabilized (Bi-CGSTAB). The algorithms to be applied can be seen in Table 1.

For comparison, CG can be only used for problems where the matrix is symmetric and positive definite but it is also suitable for non-symmetric matrices by introducing the normal equations:

$$\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b}\,. \tag{9}$$

However, it has a lot of disadvantages because of the squaring of the condition number which leads usually a slow convergence.

In case of Bi-CG method the biorthogonality relations are satisfied and the algorithm to be applied is defined in Table 1. One can recognize that the algorithm is very similar to the CG but now one has to solve the adjoint problem, as well.

Numerical investigations have showed that the convergence of Bi-CG can become irregular or it can stagnate and may also break down.

Table 1: The CG, Bi-CG and Bi-CGSTAB algorithms

	CG	Bi-CG	Bi-CGSTAB
The problem to be solved	$\mathbf{Ax} = \mathbf{b}$	$\mathbf{Ax} = \mathbf{b}, (\mathbf{A}^{\mathrm{T}}\mathbf{x}^* = \mathbf{b}^*)$	$\mathbf{Ax} = \mathbf{b}, (\mathbf{A}^{\mathrm{T}}\mathbf{x}^* = \mathbf{b}^*)$
Initial assumptions	$\mathbf{r}_0 := \mathbf{b} - \mathbf{Ax}_0$ $\mathbf{p}_0 := \mathbf{r}_0$	$\mathbf{r}_0 := \mathbf{b} - \mathbf{Ax}_0$ Choose so that $\mathbf{r}_0^* \Rightarrow (\mathbf{r}_0, \mathbf{r}_0^*) \neq 0$ $\mathbf{p}_0 := \mathbf{r}_0, \mathbf{p}_0^* := \mathbf{r}_0^*$	$\mathbf{r}_0 := \mathbf{b} - \mathbf{Ax}_0$ Choose so that $\mathbf{r}_0^* \Rightarrow (\mathbf{r}_0, \mathbf{r}_0^*) \neq 0$ $\mathbf{p}_0 := \mathbf{r}_0, \mathbf{p}_0^* := \mathbf{r}_0^*$
For $j = 0,\ldots$ until conver.			
Weighting factor for the solution	$\alpha_j := \frac{\left\|\mathbf{r}_j\right\|^2}{(\mathbf{Ap}_j, \mathbf{p}_j)}$	$\alpha_j := \frac{(\mathbf{r}_j, \mathbf{r}_j^*)}{(\mathbf{Ap}_j, \mathbf{p}_j^*)}$	$\alpha_j := \frac{(\mathbf{r}_j, \mathbf{r}_0^*)}{(\mathbf{Ap}_j, \mathbf{r}_0^*)}$
New solution vector	$\mathbf{x}_{j+1} := \mathbf{x}_j + \alpha_j \mathbf{p}_j$	$\mathbf{x}_{j+1} := \mathbf{x}_j + \alpha_j \mathbf{p}_j$	$\mathbf{s}_j := \mathbf{r}_j - \alpha_j \mathbf{Ap}_j$ $\omega_j := \frac{(\mathbf{As}_j, \mathbf{s}_j)}{(\mathbf{As}_j, \mathbf{As}_j)}$ $\mathbf{x}_{j+1} := \mathbf{x}_j + \alpha_j \mathbf{p}_j + \omega_j \mathbf{s}_j$
New residual vectors	$\mathbf{r}_{j+1} := \mathbf{r}_j - \alpha_j \mathbf{Ap}_j$	$\mathbf{r}_{j+1} := \mathbf{r}_j - \alpha_j \mathbf{Ap}_j$ $\mathbf{r}_{j+1}^* := \mathbf{r}_{j+1}^* - \alpha_j \mathbf{A}^{\mathrm{T}}\mathbf{p}_j^*$	$\mathbf{r}_{j+1} := \mathbf{s}_j - \omega_j \mathbf{As}_j$
Weighting factor for the search Directions	$\beta_j := \frac{\left\|\mathbf{r}^{j+1}\right\|^2}{\left\|\mathbf{r}^{j}\right\|^2}$	$\beta_j := \frac{(\mathbf{r}_{j+1}, \mathbf{r}_{j+1}^*)}{(\mathbf{r}_j, \mathbf{r}_j^*)}$	$\beta_j := \frac{(\mathbf{r}_{j+1}, \mathbf{r}_0^*)}{(\mathbf{r}_j, \mathbf{r}_0^*)} \times \frac{\alpha_j}{\omega_j}$
New search directions	$\mathbf{p}_{j+1} := \mathbf{r}_{j+1} + \beta_j \mathbf{p}_j$	$\mathbf{p}_{j+1} := \mathbf{r}_{j+1} + \beta_j \mathbf{p}_j$ $\mathbf{p}_{j+1}^* := \mathbf{r}_{j+1}^* + \beta_j \mathbf{p}_j^*$	$\mathbf{p}_{j+1} := \mathbf{r}_{j+1} + \beta_j(\mathbf{p}_j - \omega_j \mathbf{Ap}_j)$
End for			

Avoiding this problem Van der Vorst [4] published a new method called Bi-CGSTAB. This method can be derived from Bi-CG algorithm and from GMRES algorithm without recurrence. The method is such that locally a residual vector is minimized. The algorithm can be seen in Table 1. Here one can also recognize that this algorithm is very similar to the Bi-CG but one does not have to solve the adjoint problem explicitly. Another difference is that there are a new vector $\mathbf{s}_j$ and a new scalar ω_j. The latter one is associated with the condition of local minimum of residual vector. Another improvement in Bi-CGSTAB compared to the Bi-CG is that there is no matrix-vector product with transpose matrix.

Taken into account the above discussed arguments the Bi-CGSTAB algorithm has been built in the KIKO3D where the error of the solution is estimated by the following term:

$$\frac{\left\|\mathbf{x} - \mathbf{x}_k\right\|_2}{\left\|\mathbf{x}\right\|_2} \approx \frac{\left\|\mathbf{r}_k\right\|_2}{\left\|\mathbf{b}\right\|_2} \tag{10}$$

This is a rough estimation of the real error and its effectiveness must be tested. This is one of the topics of the following chapter. However, it must be mentioned that according to

the literature it can not be considered a satisfactory estimation being generally effective for the real error in case of using Bi-CGSTAB algorithm.

4 EXAMPLES

The KIKO3D code was validated and benchmarked in the frame of the AER international co-operation, where new hexagonal VVER-440 type benchmark problems were defined [2]. Now the verification of the Bi-CGSTAB algorithm and validation of the KIKO3D code using that will be presented in three cases. In these cases the convergence behaviours of the respective algorithms including the speed of the convergence were tested.

First of all, a brief description will be given about the simulation of a rod ejection transient in a Russian pressurized VVER-440 reactor. Such transients are considered in Cases 1 and 2. The core is in steady state before the transient, each elements of the control rod group are at 50 cm position, the power is 10^{-3} % of the nominal value. The transient starts with control rod ejection due to a rapid cross break of the control assembly drive mechanism. A very fast and large asymmetric reactor power increasing follows, and then the fast decreasing of power due to the Doppler effect, before the SCRAM can be observed.

Additionally, in the VVER-440 core there are 349 assemblies and the lattice pitch is 14.7 cm. Each node corresponds to a part of the axially divided assembly, which is of height 25cm.

***Case 1*:** Firstly, in a given macro step (at the beginning of the transient) of a rod ejection transient the linear equation system given by Eq. (5) was extracted. This equation system was solved by both GMRES and Bi-CGSTAB algorithms and reference solution was prepared, as well. The dimension of the matrix **A** was 15408*15408 with 423216 non-zero elements.

The estimated relative errors depending on the CPU time are shown in Fig. 1. In case of using GMRES the relative error was estimated so that the right hand side of Eq. (8) was divided by the Chebyshev norm of the estimated solution. The notation 'DIM' refers to the dimension of the subspace where the residual vector is minimised. It can be seen that the speed of the estimated convergence is attractive in case of preconditioned Bi-CGSTAB algorithm and also in case of Bi-CGSTAB algorithm without preconditioning.

In order to get information about the relationship of the estimated and the 'real' relative error the latter one was considered in Chebyshev norm as

$$\frac{\left\| \mathbf{x}_k - \mathbf{x}_{ref} \right\|_\infty}{\left\| \mathbf{x}_{ref} \right\|_\infty}, \tag{11}$$

where $\mathbf{x}_k$ is the estimated solution in step k calculated by the respective algorithm and $\mathbf{x}_{ref.}$ is the pre-calculated reference solution.

In Fig. 2 the estimated and the real relative errors depending on time are compared. In this Figure only the case of DIM = 12 is considered but the other GMRES calculations with different dimensions show similar time characteristics. The main conclusion is that the estimated relative error is very close to the real relative error in case of preconditioned Bi-CGSTAB but the real relative error is conservatively overestimated by the estimated relative error (approximately with 2 order of magnitude) in case of preconditioned GMRES. It can be also seen that the real relative errors of the solutions obtained by GMRES or Bi-CGSTAB are in fact closer together in a given time than the estimated relative errors.

***Case 2*:** Recently an uncertainty analysis [10] has been performed in case of a control rod ejection accident. In the course of performance of this analysis the input parameters were varied and a lot of (100) computer running were performed. In one case of 100 runs, where physically extreme input data are applied, the KIKO3D code using Bi-CGSTAB algorithm

(henceforth KIKO3D-Bi-CGSTAB) was not able to achieve the solution. The KIKO3D code using GMRES algorithm with a dimension of 12 (henceforth KIKO3D-GMRES) calculated the solution but it was usually (the convergence problems appeared in each macro step) not able to reach the given prescribed relative error and the results could not have been interpreted physically.

The calculation of the transient was performed firstly only by KIKO3D-GMRES (number of the iterations at the static problem are 26) but later the convergence problems were solved by iterating the steady state solution better (number of the iterations at the static problem are 35). It must be mentioned that the iteration is stopped in KIKO3D if the estimated relative error of the solution reaches a given tolerance (it is 10^{-3} in case of KIKO3D-GMRES and it is 10^{-6} in case of KIKO3D-Bi-CGSTAB) but another condition must be realized. Iterating the solution (shape factor) sometimes we recalculate the reactivity. A linear convergence is assumed for the reactivity and the prescribed absolute error tolerance is $5*10^{-6}$ in case of GMRES and it is 10^{-6} in case of Bi-CGSTAB.

Some results of the calculation are presented in Figs. 3, 4, and 5. In Fig. 3 the nuclear power depending on time is given. It is well seen that physically false results are obtained if one applies only 26 static iterations. Fig. 4 shows the relative deviation between the two kinds of solution using 35 static iterations and it can be stated that there is a satisfactory agreement between the two kinds of results. In Fig. 5 it can be seen that KIKO3D-Bi-CGSTAB is faster than KIKO3D-GMRES in most cases. Main conclusions of this step are that the Bi-CGSTAB applied in KIKO3D converged to the solution safely and KIKO3D-Bi-CGSTAB was app. 7 % (in case of conservative calculation, which is not presented here, it was app.12 %) faster than KIKO3D-GMRES.

***Case 3*:** The validation of the KIKO3D code using Bi-CGSTAB algorithm was carried out in the case of a Control Rod Withdrawal kinetic process measured on a critical facility corresponding to a VVER-1000 core. The transient and the obtained results are detailed in [11]. Now we give only a short description about the transient. Starting from a V-1000 steady state with all control rods withdrawn, a transient was initiated by inserting a single cluster and then withdrawing it again. The reactivities of the reactimeters PIR1 and PIR2 were determined by inverse point kinetics from the signals of two out-core ionisation chambers KNK-56, placed at opposite sides of the radial core edge. Additionally, in the VVER-100 core there are 163 assemblies and the hexagonal assembly lattice pitch is 23.6cm. Good agreement was found between the calculated and measured relative powers at detector positions taken into account the uncertainties of the input data and the measurements.

Additional information to the comparison of the KIKO3D-GMRES and KIKO3D-Bi-CGSTAB calculations is that the dimension of the matrix **A** was 10951*10951 with 152743 non-zero elements. In Figs. 6, and 7 the measured and calculated (by KIKO3D-GMRES and KIKO3D-Bi-CGSTAB) relative powers and their deviation are given at the detector position (126L) where the single-cluster motion happened. In Fig. 8 the measured (defined above) and calculated (by inverse point kinetics from KIKO3D results) reactivities of the reactimeters PIR1 and PIR2 are shown. It can be seen that KIKO3D slightly overestimated the measured reactivity. A good agreement can be seen between the two kinds of calculation results of reactivity taken into account the additional uncertainty coming from the inverse point kinetics calculation. In Fig. 9 it can be seen that KIKO3D-Bi-CGSTAB is in each step faster than KIKO3D-GMRES. Main conclusions of this step are that KIKO3D-Bi-CGTAB converged to the solution safely and it was app. 10 % faster than KIKO3D-GMRES. The other results of this calculations (not presented here) show similar features than above.

5 SUMMARY

In this paper the focus was on the presentation of a more effective method Bi-CGSTAB for accelerating the large sparse matrix equation solution in the KIKO3D code. The mathematical backgrounds of the applied algorithms were detailed. The verification of the algorithm and the validation of KIKO3D-Bi-CGSTAB were shown by examples. It was concluded that the real relative errors of the solutions obtained by GMRES or Bi-CGSTAB algorithms are in fact closer together than the estimated relative errors. In case of transients the main conclusions were that KIKO3D-Bi-CGSTAB converges safely and it is 7-12 % faster than KIKO3D-GMRES.

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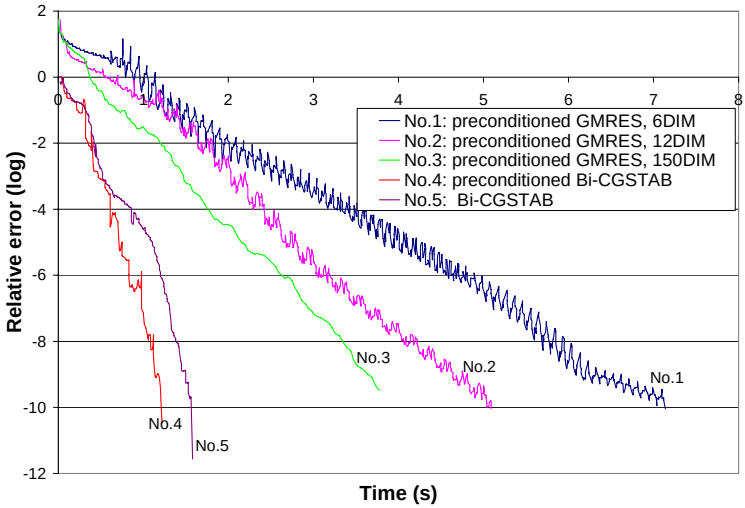

Figure 1: Estimated relative errors depending on CPU time, Case 1

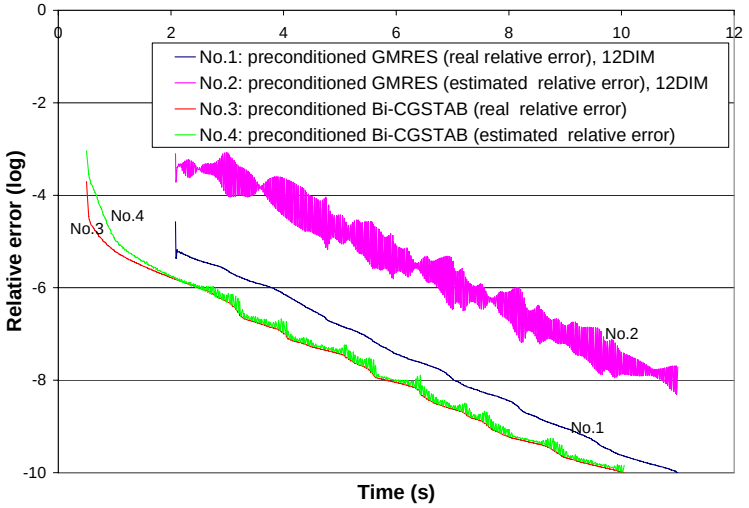

Figure 2: Estimated and real relative errors depending on time, Case 1

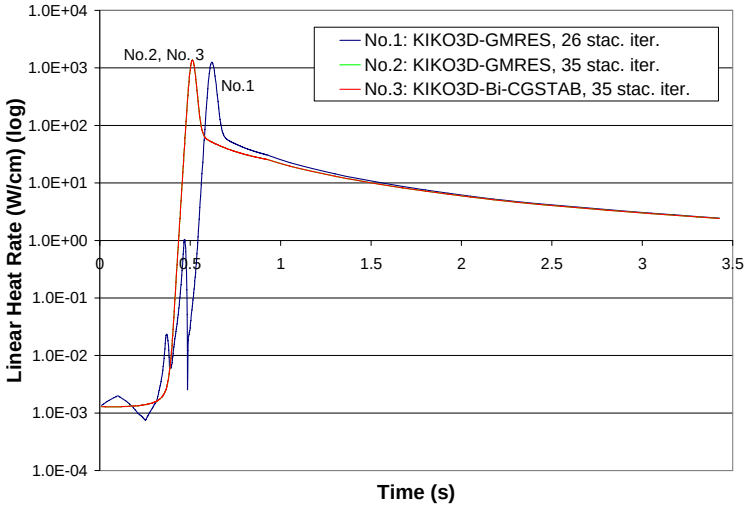

Figure 3: Nuclear power, given in core averaged linear heat rate, Case 2

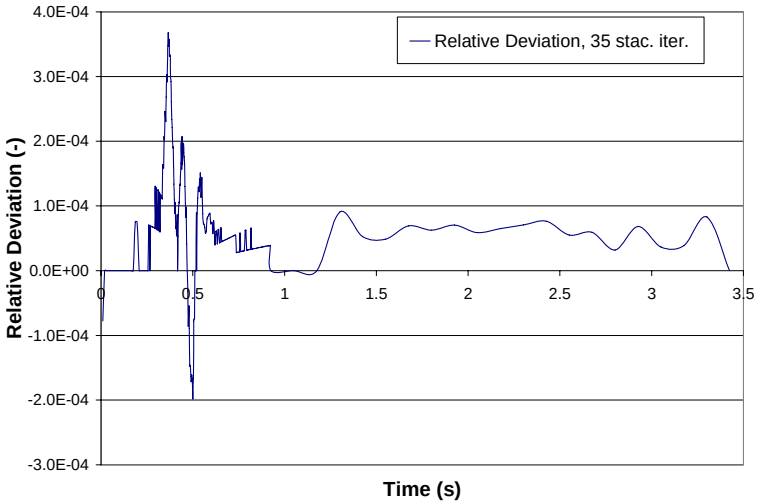

Figure 4: Relative deviation of the nuclear powers calculated by KIKO3D-GMRES and KIKO3D-Bi-CGSTAB, Case 2

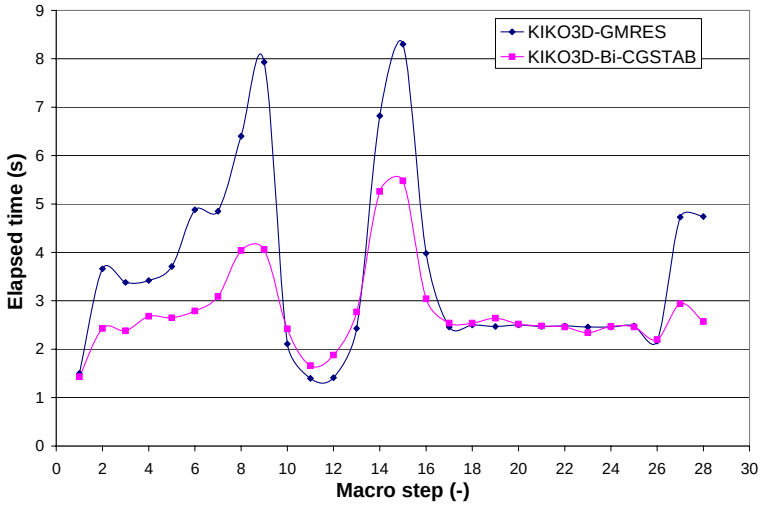

Figure 5: Elapsed time in macro step, Case 2

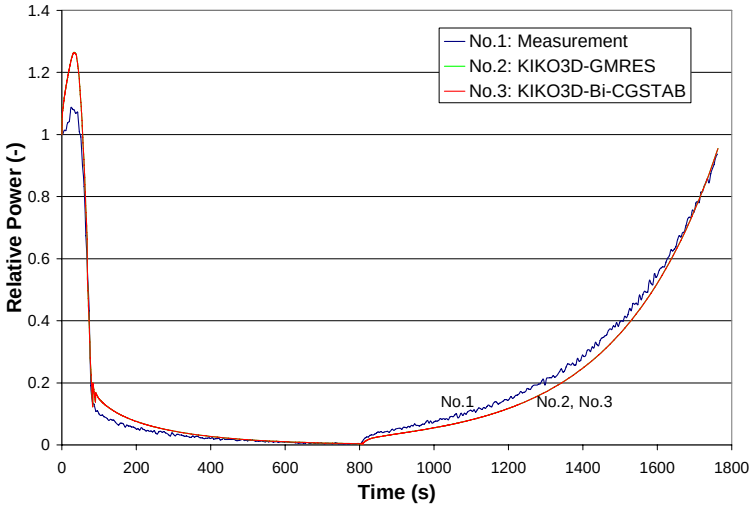

Figure 6: Measured and calculated relative powers at detector position 126L, Case 3

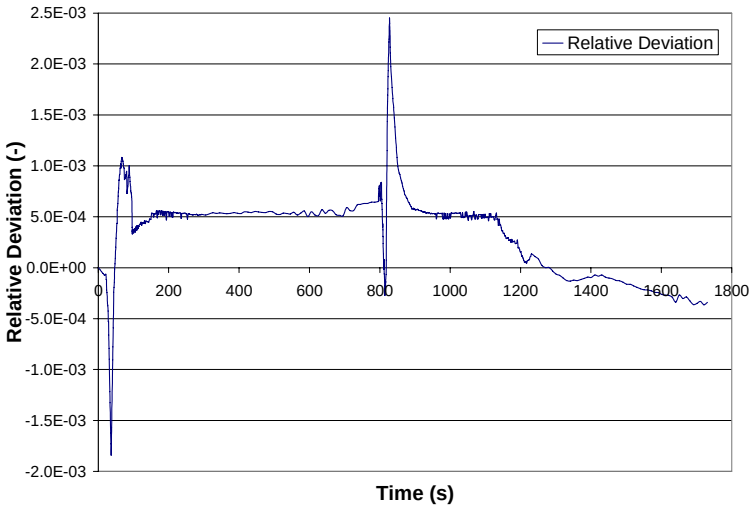

Figure 7**:** Relative deviation of the relative powers at detector position 126L calculated by KIKO3D-GMRES and KIKO3D-Bi-CGSTAB, Case 3

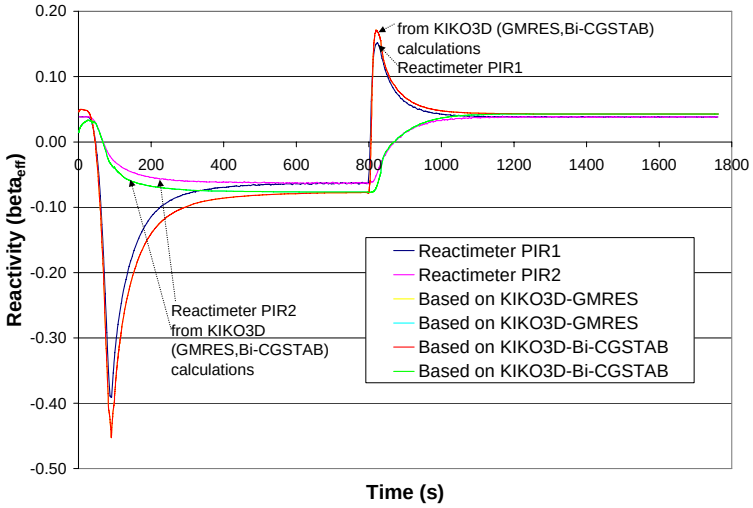

Figure 8**:** Reactivity obtained from inverse kinetic calculations (used KIKO3D results) and reactivity obtained from the signal of ionization chambers, Case 3

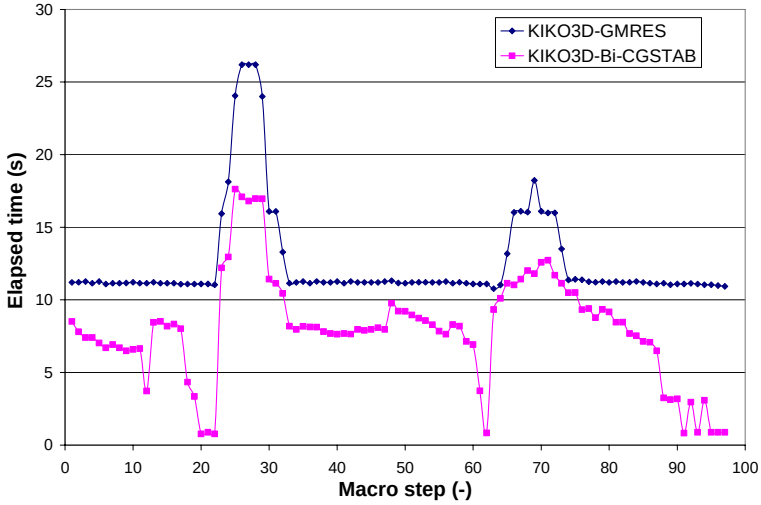

Figure 9**:** Elapsed time in macro step, Case 3