An efficient 'a priori' model reduction for boundary element models

D. Ryckelynck[a], L. Hermanns[b], F. Chinesta[a,*], E. Alarcón[b]

[a]*LMSP UMR 8106 CNRS-ENSAM-ESEM, 151 Boulevard de l'Hôpital, F-75013 Paris, France*
[b]*Departamento de Mecánica Estructural, ETSII—Universidad Politécnica de Madrid, Jose Gutierrez Abascal 2, E-28006 Madrid, Spain*

Abstract

The Boundary Element Method (BEM) is a discretisation technique for solving partial differential equations, which offers, for certain problems, important advantages over domain techniques. Despite the high CPU time reduction that can be achieved, some 3D problems remain today untreatable because the extremely large number of degrees of freedom—dof—involved in the boundary description. Model reduction seems to be an appealing choice for both, accurate and efficient numerical simulations. However, in the BEM the reduction in the number of degrees of freedom does not imply a significant reduction in the CPU time, because in this technique the more important part of the computing time is spent in the construction of the discrete system of equations. In this way, a reduction also in the number of weighting functions, seems to be a key point to render efficient boundary element simulations.

Keywords: Boundary element method; Model reduction; Karhunen-loève decomposition; Krylov's subspaces

1. Introduction

The Boundary Element Method (BEM) is a discretisation technique for solving partial differential equations, which offers, for certain problems, important advantages over domain techniques such as the finite element method [1]. One of the most interesting features of the method is the much smaller system of equations generated (which results full populated), due to the fact that the degrees of freedom are related to the nodes associated with the boundary mesh. Thus, a considerable reduction in the computing time, mainly for 2D or 3D problems, is expected. The BEM is also well suited for solving problems defined in unbounded domains, as encountered in mechanics, aerodynamics or hydrodynamics. The terms 'boundary element' indicates that the domain boundary is partitioned into a series of elements over which the unknown function is approximated like in the finite element method.

Despite the high CPU time reduction that can be achieved (despite the fact that the boundary models involve fully populated systems), some 3D problems remain today untreatable because the extremely large number of degrees of freedom—*dof*—involved in the boundary description. To alleviate this drawback, one possibility lies in the use of a model reduction (based on the Karhunen-Loève decomposition—KLD—, also known as proper orthogonal decomposition—POD—). Model reduction techniques proceed by approximating the problem solution using the most appropriate set of approximation functions, whose determination from the Karhunen-Loève decomposition and the use of the Krylov subspaces related to the residual of the governing equations will be addressed later in this paper.

Model reduction has been successfully applied in the finite element framework for modeling dynamic models of distributed parameters [2–6]. However, in these applications several direct problems must be solved to extract empirical functions that represent the system most efficiently. This set of empirical eigenfunctions is used as functional basis of the Galerkin procedure to lump the governing equation. Thus, for example, the resulting lumped parameter model can be used to obtain the solution when the boundary conditions are changing randomly. To avoid, these preliminary costly calculations, Ryckelynck proposed in [7] start the resolution process from any reduced basis, using the Krylov subspaces

generated by the governing equation residual for enriching the approximation basis, at the same time that a proper orthogonal decomposition extracts relevant information in order to maintain the low order of the approximation basis. This technique was applied in [8] for solving kinetic theory models.

However, a more 'philosophical' question can be addressed: if the reduced model makes use of a number of *dof* (n), lower than the initial one (N), one could expect that for computing the n degrees of freedom involved, the use of m weighting functions ($N \gg m > n$) could be enough. Thus, Ryckelynck has proved that there is an appropriate choice of a reduced number of weighting functions able to solve the problem efficiently. He has called this technique 'a priori model hyper-reduction' [9]. In the framework of the BEM, the reduction in the number of weighting functions seems to be essential, because in this technique the more important part of the CPU time is spent in the construction of the discrete system of equations.

In the present work, we will propose an efficient model reduction, especially well adapted for treating boundary element models. For the sake of simplicity, we will consider a potential problem defined in a 2D unbounded domain. The capabilities of both the reduced order modeling and the boundary element method will be outlined.

1.1. Boundary element discretization of a potential problem

We consider the potential function u verifying the following governing PDE

$$\Delta u = 0 \text{ in } \Omega \tag{1}$$

as well as the:

- Essential boundary conditions: $u = \bar{u}$ on Γ_1
- Natural boundary conditions: $q = \partial u/\partial n = \bar{q}$ on Γ_2

where the domain boundary Γ results $\Gamma = \Gamma_1 + \Gamma_2$.

The weighed residual expression related to the previous problem is

$$\int_{\Omega} \Delta u u^* \, \mathrm{d}\Omega = \int_{\Gamma_2} (q - \bar{q}) u^* \, \mathrm{d}\Gamma - \int_{\Gamma_1} (u - \bar{u}) q^* \, \mathrm{d}\Gamma \tag{2}$$

which integrating by parts, introducing the fundamental solution as weighting function, assuming the interpolation of u on the domain boundary defined from N nodal values, and performing the resulting integrals numerically (see [1] for more details concerning the standard discretization procedure) it results

$$\underline{\underline{H}}\,\underline{U} = \underline{\underline{G}}\,\underline{Q} \tag{3}$$

where $\underline{U}$ contains the nodal potentials and $\underline{Q}$ their normal derivatives. Effectively, at the nodes located on Γ_1 the potential is known, being its normal derivative known at the nodes located on Γ_2. Grouping at the left member the unknowns, Eq. (3) takes the final form

$$\underline{\underline{A}}\,\underline{X} = \underline{F} \tag{4}$$

where the size of $\underline{\underline{A}}$ is $N \times N$.

1.2. The Karhunen-Loève (KL) decomposition

We assume that the evolution of a certain field is known $u(\underline{x}, t)$. In practical applications this field is known in a discrete form, that is, it is known at the nodes of a spatial mesh and for some times $u(\underline{x}_i, t^p) \equiv u_i^p$. We can also write $u^p(\underline{x}) \equiv u(\underline{x}, t = p\Delta t)$; $\forall p \in [1,\ldots,P]$. The main idea of the KL decomposition is how obtain the most typical or characteristic structure $\phi(\underline{x})$ among these $u^p(\underline{x})$. This is equivalent to obtain a function $\phi(\underline{x})$ maximizing α defined by

$$\alpha = \frac{\sum_{p=1}^{p=P} \left[\sum_{i=1}^{i=N} \phi(\underline{x}_i) u^p(\underline{x}_i)\right]^2}{\sum_{i=1}^{i=N} (\phi(\underline{x}_i))^2} \tag{5}$$

The maximisation leads to

$$\sum_{p=1}^{p=P} \left[\left[\sum_{i=1}^{i=N} \tilde{\phi}(\underline{x}_i) u^p(\underline{x}_i)\right]\left[\sum_{j=1}^{j=N} \phi(\underline{x}_j) u^p(\underline{x}_j)\right]\right]$$

$$= \alpha \sum_{i=1}^{i=N} \tilde{\phi}(\underline{x}_i)\phi(\underline{x}_i); \quad \forall\, \tilde{\phi} \tag{6}$$

where $\tilde{\phi}(\underline{x})$ denotes the variation of $\phi(\underline{x})$. Eq. (6) can be rewritten in the form

$$\sum_{i=1}^{i=N} \left[\sum_{j=1}^{j=N} \left\{\sum_{p=1}^{p=P} u^p(\underline{x}_i) u^p(\underline{x}_j)\phi(\underline{x}_j)\right\} \tilde{\phi}(\underline{x}_i)\right]$$

$$= \alpha \sum_{i=1}^{i=N} \tilde{\phi}(\underline{x}_i)\phi(\underline{x}_i); \quad \forall\, \tilde{\phi} \tag{7}$$

Introducing a vector notation, Eq. (7) takes the following matrix form

$$\underline{\tilde{\phi}}^T \underline{\underline{k}}\,\underline{\phi} = \alpha \underline{\tilde{\phi}}^T \underline{\phi}; \quad \forall\ \underline{\tilde{\phi}} \Rightarrow \underline{\underline{k}}\,\underline{\phi} = \alpha \underline{\phi} \tag{8}$$

where the eigenvectors do not depend on time, i.e. $\phi(\underline{x})$. The two points correlation matrix $\underline{\underline{k}}$ is given by

$$k_{ij} = \sum_{p=1}^{p=P} u^p(\underline{x}_i) u^p(\underline{x}_j) \tag{9}$$

whose matrix form results

$$\underline{\underline{k}} = \sum_{p=1}^{p=P} \underline{u}^p (\underline{u}^p)^T \tag{10}$$

which is symmetric and positive definite.

If we define the matrix $\underline{\underline{Q}}$ containing the discrete field history:

$$\underline{\underline{Q}} = \begin{pmatrix} u_1^1 & u_1^2 & \cdots & u_1^P \\ u_2^1 & u_2^2 & \cdots & u_2^P \\ \vdots & \vdots & \ddots & \vdots \\ u_N^1 & u_N^2 & \cdots & u_N^P \end{pmatrix} \tag{11}$$

is easy to verify that the matrix $\underline{\underline{k}}$ in Eq. (9) results

$$\underline{\underline{k}} = \underline{\underline{Q}}\,\underline{\underline{Q}}^T \tag{12}$$

where the diagonal components are given by

$$\underline{\underline{k}}_{ii} = (\underline{\underline{Q}}\,\underline{\underline{Q}}^T)_{ii} = \sum_{j=1}^{j=P} (u_i^j)^2 \tag{13}$$

Thus, the functions defining the most characteristic structure of $u^p(\underline{x})$ are the eigenfunctions $\phi_k(\underline{x}) \equiv \underline{\phi}_k$ associated with the highest eigenvalues.

2. 'A posteriori' reduced modeling

2.1. Constructing the reduced model

If some direct simulations have been carried out previously, we can determine $u(\underline{x}_i, t^p) \equiv u_i^p$, $\forall\ i \in [1,\ldots,N]$, $\forall\ p \in [1,\ldots,P]$, and from that, the n eigenvectors related to the eigenvalues greater than an arbitrarily threshold value small enough. Thus, with the eigenvalues assumed ordered, if $\alpha_k > 10^{-10}\alpha_1$, $\forall\ k \in [1,\ldots,n]$, ($\alpha_1$ being the highest eigenvalue), we will consider the n eigenvectors defined by their nodal values: $\underline{\phi}_k = \phi_k(\underline{x}_i)$, $\forall\ i \in [1,\ldots,N]$, $\forall\ k \in [1,\ldots,n]$

Now, we can try to use these n eigenvectors for approximating the solution of a problem slightly different to the one that has served to define $u(\underline{x}_i, t^p) \equiv u_i^p$. For this purpose we need to define the matrix $\underline{\underline{B}}$

$$\underline{\underline{B}} = \begin{pmatrix} \phi_1(\underline{x}_1) & \phi_2(\underline{x}_1) & \cdots & \phi_n(\underline{x}_1) \\ \phi_1(\underline{x}_2) & \phi_2(\underline{x}_2) & \cdots & \phi_n(\underline{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\underline{x}_N) & \phi_2(\underline{x}_N) & \cdots & \phi_n(\underline{x}_N) \end{pmatrix} i \tag{14}$$

For the sake of simplicity, we consider, from now on, that the linear system (4) contains all the nodal potentials as unknowns, i.e. $\underline{X} = \underline{U}$. Thus we could write

$$\underline{U} = \sum_{i=1}^{i=n} \zeta_i \underline{\phi}_i = \underline{\underline{B}}\,\underline{\zeta} \tag{15}$$

from which

$$\underline{\underline{A}}\,\underline{U} = \underline{F} \Rightarrow \underline{\underline{A}}\,\underline{\underline{B}}\,\underline{\zeta} = \underline{F} \tag{16}$$

and multiplying both terms by $\underline{\underline{B}}^T$ it results

$$\underline{\underline{B}}^T\underline{\underline{A}}\,\underline{\underline{B}}\,\underline{\zeta} = \underline{\underline{B}}^T\underline{F} \tag{17}$$

which proves that the final system of equations is of low order, i.e. the size of $\underline{\underline{B}}^T\underline{\underline{A}}\,\underline{\underline{B}}$ is $n \times n$, with $n \ll N$, and the size of both $\underline{\zeta}$ and $\underline{\underline{B}}^T\underline{F}$ is $n \times 1$.

2.2. Alleviating the discrete system construction

Despite that Eq. (17) notices the reduction accomplished in the size of the linear system of equations that must solved at each iteration, in the boundary element method the construction of matrix $\underline{\underline{A}}$ is expensive from a computing time point of view. To alleviate the considerable computational efforts needed in the construction of $\underline{\underline{A}}$ we suggest to reduce the number of test functions used in the variational formulation weighting, in the framework of the hyper-reduction proposed by Ryckelynck in [9]. Several criteria exist for selecting these integration functions [9]. When the problem solution is smooth enough, the use of $m \approx 3n$ weighting functions (being n the number of unknowns involved in the reduced model) provides very accurate results.

$$(\underline{\underline{B}}^{\text{red}})^T\underline{\underline{A}}^{\text{red}}\underline{\underline{B}}\,\underline{\zeta} = (\underline{\underline{B}}^{\text{red}})^T\underline{F} \tag{18}$$

where the reduced matrix $\underline{\underline{A}}^{\text{red}}$ is $m \times N$; and the reduced matrix $\underline{\underline{B}}^{\text{red}}(m \times n)$ is computed from the truncated eigenvectors.

3. Reduced model adaptativity: an 'a priori' model reduction approach

In order to compute reduced model solutions without an 'a priori' knowledge, Ryckelynck proposed [7] to start with a low order approximation basis, using some simple functions (e.g. the initial condition in transient problems) or using the eigenvectors of a 'similar' problem previously solved. Now, we note by $\underline{\underline{B}}^{(r)}$ the approximation basis that has been updated r times. We compute S time steps of the evolution problem using the reduced model (17) (or (18) if the hyper reduction is considered) without changing the present approximation basis $\underline{\underline{B}}^{(r)}$. After each S time steps the linear system (16) is assembled, and the residual $\underline{R}$ is then evaluated:

$$\underline{R} = \underline{\underline{A}}\,\underline{U} - \underline{F} = \underline{\underline{A}}\,\underline{\underline{B}}^{(r)}\underline{\zeta}^{(r)} - \underline{F} \tag{19}$$

If the norm of the residual is small enough, $||\underline{R}|| < \varepsilon$, with ε a threshold value small enough, we can continue for other S time steps using the same approximation basis $\underline{\underline{B}}^{(r)}$, and the problem solution at this step $\underline{\zeta}_{pS}^{(r)}$ stocked (related to the approximation basis $\underline{\underline{B}}^{(r)}$ at the time step pS). On the contrary, if the residual norm is too large, $||\underline{R}|| < \varepsilon$, we need to enrich the approximation basis and compute again the last

S steps. This enrichment is built using some Krylov's subspaces $\{\underline{R}, \underline{\underline{A}}\underline{R}, \underline{\underline{A}}^2\underline{R}, \ldots\}$, which are added to the most representative information extracted from the previous solutions $\underline{\zeta}_{qS}^{(r)}$ (with the integer $q<p$), as well as from the solutions of 'a similar' problem (if it exists) up to the current time $\underline{\zeta}_{\text{sim},tS}^{(r)}$ ($t \geq p$). In both cases the superscript indicates that these reduced order solutions are expressed in the basis $\underline{\underline{B}}^{(r)}$. This information is extracted by applying the Karhunen-Loève decomposition to $\underline{\zeta}_{qS}^{(r)}$ and $\underline{\zeta}_{\text{sim},tS}^{(r)}(\forall q < p; \forall t \geq p)$, whose most representative eigenvectors define the matrix $\underline{\underline{V}}$. Then the evolution process is restarted for computing again the last S steps, using the enriched basis defined by: $\underline{\underline{B}}^{(r+1)} = \{\underline{\underline{B}}^{(r)}\underline{\underline{V}}, \underline{R}, \underline{\underline{A}}\underline{R}, \underline{\underline{A}}^2\underline{R}\}$ (we consider usually only the first three Krylov's subspaces). After each reduced basis modification, both the previous solutions and the ones related to the similar problem (when they exist) are projected into the new basis. Thus, one can write:

$$\underline{\zeta}^{(r+1)} = [(\underline{\underline{B}}^{(r+1)})^T \underline{\underline{B}}^{(r+1)}]^{-1} \underline{\underline{B}}^{(r+1)^T} \underline{\underline{B}}^{(r)} \underline{\zeta}^{(r)} \tag{20}$$

Remark. The application of the Karhunen-Loève decomposition to the reduced solutions instead to the nodal description has two advantages: (i) the eigenvalue problem has a lower dimension, and (ii) as the functions in $\underline{\underline{B}}$ verify the problem boundary conditions, then any low order solution $\underline{\zeta}$ determines a complete solution $\underline{\underline{B}}\underline{\zeta}$ satisfying these boundary conditions.

4. Numerical example

A potential problem defined in an unbounded domain is simulated, which consists of two cylinders moving as indicated in Fig. 1. The upper cylinder moves with a velocity of $\underline{v}$ along the x-axis meanwhile the lower cylinder remains at rest. If we assume that an inviscid and incompressible fluid occupies the unbounded domain Ω, and that no vorticity is generated by discontinuities or by the boundary, the fluid velocity can be expressed from the gradient of a certain potential function u. The normal derivative of the potential is prescribed on the cylinders boundaries to guarantee that the fluid does not penetrate the cylinders, that is $q = \partial u/\partial n = \underline{v} \cdot \underline{n}$, being $\underline{n}$ the unit outward vector defined on the cylinder surface and $\underline{v}$ the cylinder translation velocity. Thus, the problem can be defined from:

$$\begin{cases} \Delta u = 0 \quad \text{in} \quad \Omega \\ q = \dfrac{\partial u}{\partial n} = \underline{v} \cdot \underline{n} \quad \text{on} \quad \Gamma_{\text{upper}} \\ q = \dfrac{\partial u}{\partial n} = 0 \quad \text{on} \quad \Gamma_{\text{lower}} \end{cases} \tag{21}$$

where Γ_{upper} and Γ_{lower} denote the surface of the upper and lower cylinders, respectively.

This problem is solved firstly for a certain distance between both cylinders greater than d' using 25 time steps to cover the approximation and moving away stages. The approximation is performed using 300 nodes, which implies the same number of degrees of freedom. A direct problem is solved at each time step, from which the potential on each cylindrical surface is determined, defining the matrix $\underline{\underline{Q}}$ containing the discreet representation of these 25 solutions according to Eq. (11). From the solution of the associated eigenvalue problem (8) the most representative eigenvectors can be derived (those related to the eigenvalues greater than $10^{-8}\alpha_1$). Fig. 2 depicts the three most characteristic functions (after normalization), where the potential is represented on the surfaces. Fig. 3 shows the evolution of the weight of each one of these functions during the approximation and moving away stages, that is the evolution of the degrees of freedom of the reduced approximation basis. We can notice that the first eigenfunction is the most representative, and that only the first three eigenfunctions are required to describe accurately the evolution of the solution during these 25 time steps. Now, we consider the problem, where the distance between both cylinders is reduced to d' (see Fig. 1). Moreover, the approximation and moving away stages will be computed using 227 time steps instead of the 25 ones used to analyze the similar problem just described. Due to the potential smoothness on both cylinder surfaces, we consider only $3xn$ weighting functions (each one related to a certain node), where n denotes the number of degrees of freedom in the reduced approximation basis. For sharper solutions the determination of the most appropriate weighting functions requires a deeper analysis [9].

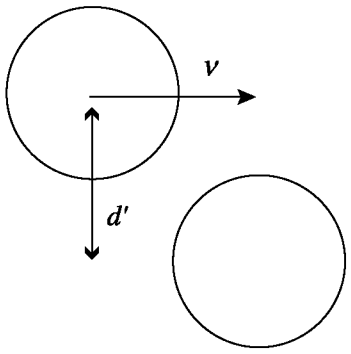

Fig. 1. Definition of the problem geometry.

In this case, the solution is performed starting from the reduced basis (containing the three eigenfunctions depicted in Fig. 2) obtained from the similar problem previously computed. After each 10 time steps the quality of the solution is checked, and when a residual higher than a threshold value is obtained, the basis is enriched from the three first Krylov's subspaces as described in Section 3. The use of this enrichment in tandem with the Karhunen-Loève decomposition to extract the relevant information from the previous history and from the 'future' solution of the similar problem-when it exists-(according to the scheme presented in Section 3) allows to maintain the low order of

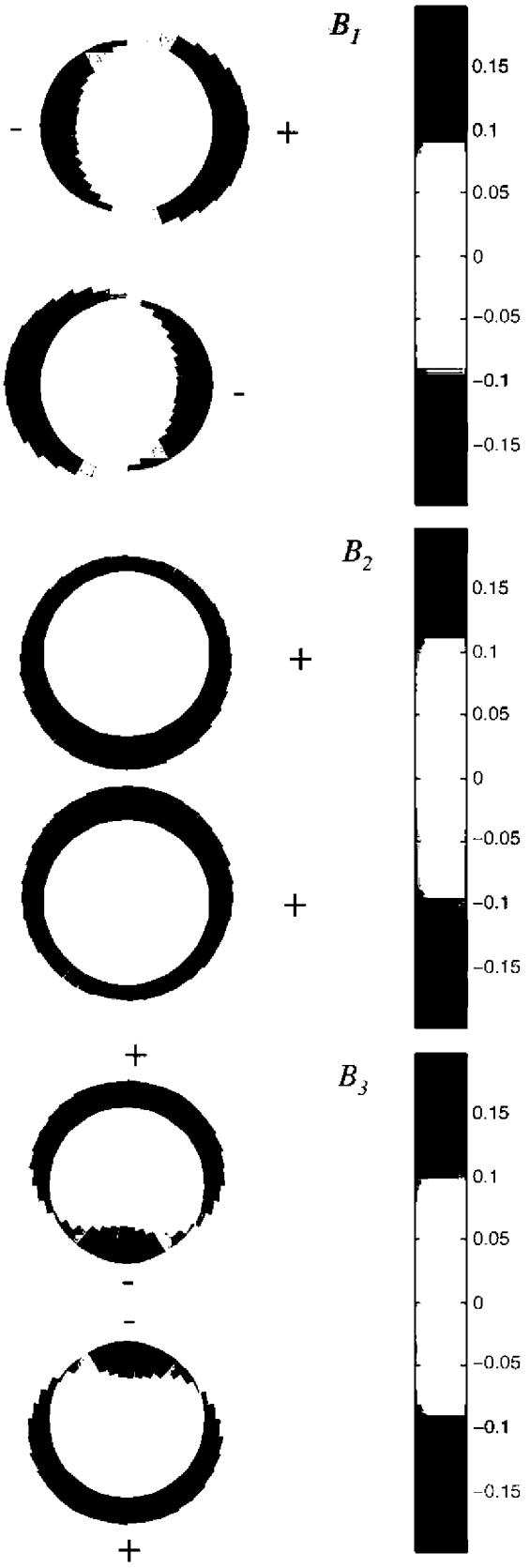

Fig. 2. Three first eigenfunctions.

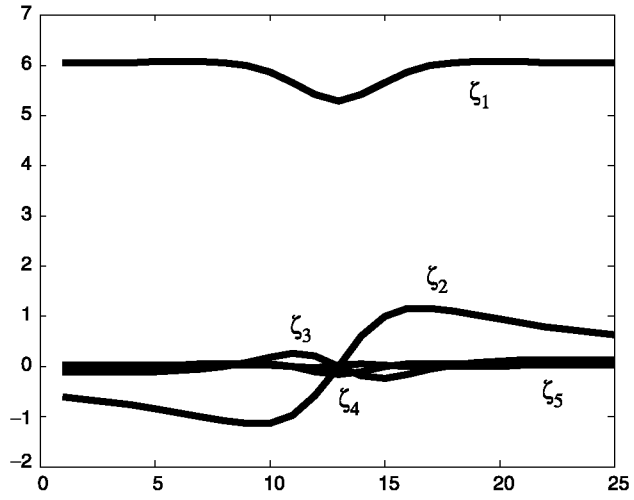

Fig. 3. Evolution of the weight of each eigenfunction in the solution (degree of freedom in the reduced approximation basis) during the approximation and moving away stages.

the approximation basis. Fig. 4 compares the evolution of the computed potential at a certain node using the full model (standard boundary element model)—continuous curve—with the one computed using the reduced approximation basis which contains less than 15 approximation functions circles-. As it can be noticed in this figure the quality of the low order solution is checked after each 10-time steps (blue circles). Moreover, the reduction in the number of weighting functions alleviates significantly the computing time. In the particular case analyzed here, the problem can be solved very accurately using only 15 degrees of freedom with an error lower than 0.1 per cent.

5. Conclusions

The reduction model strategy proposed in this paper, which combines a model reduction based on the *Karhunen-*

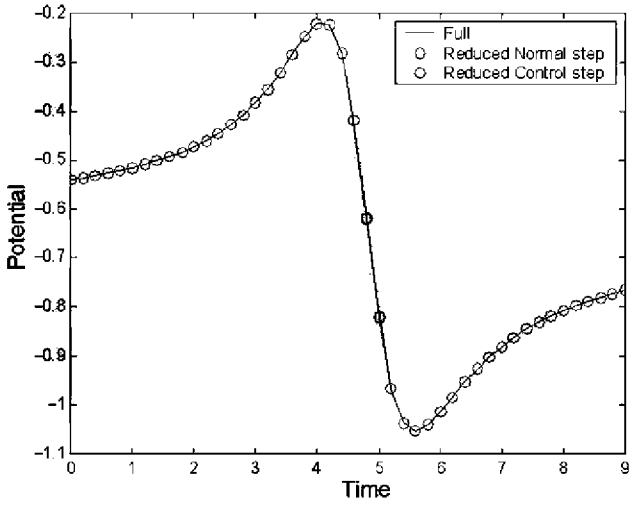

Fig. 4. Evolution of the potential at a certain node. Comparison between the full boundary element solution and the one obtained using a reduced approximation basis containing less than 15 degrees of freedom.

Loève decomposition with approximation basis enrichment, allows to accurate and fast resolution of boundary element models. Moreover, the CPU time is drastically reduced, as proved in [9], by using the concept of hyper-reduction, which lies in the use of a reduced number of weighting functions to determine the degrees of freedom involved by the reduced order approximation. The numerical example treated, despite of its simplicity, proves the potentiality of this numerical technique. The extension of this technique for solving models involving time derivatives as well as moving domains is a work in progress.

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