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Petr Tichý; Jan Zítko

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DERIVATION OF BICG FROM THE CONDITIONS DEFINING  
LANCZOS' METHOD FOR SOLVING A SYSTEM  
OF LINEAR EQUATIONS

PETR TICHÝ, JAN ZÍTKO, Praha

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*Abstract.* Lanczos' method for solving the system of linear algebraic equations  $Ax = b$  consists in constructing a sequence of vectors  $x_k$  in such a way that  $r_k = b - Ax_k \in r_0 + AK_k(A, r_0)$  and  $r_k \perp \mathcal{K}_k(A^T, \tilde{r}_0)$ . This sequence of vectors can be computed by the BiCG (BiOMin) algorithm. In this paper is shown how to obtain the recurrences of BiCG (BiOMin) directly from this conditions.

*Keywords:* biorthogonalization, linear equations, biconjugate gradient method

*MSC 2000:* 65F10, 65F25

## 1. INTRODUCTION

The application of recursive biorthogonalization to the numerical solution of eigenvalue problems and linear systems goes back to Lanczos ([Lancz-50], [Lancz-52]) and is therefore referred to as the *Lanczos process*. In its basic form [Lancz-50], the process generates a pair of biorthogonal bases for a pair of Krylov spaces, one generated by the matrix  $A$  and the other by the matrix  $A^T$ . This process is characterized by a three-term recurrence and is here called the *Lanczos biorthogonalization (BiO) algorithm* [Gutkn-97]. A variation of it, described already in the second Lanczos paper [Lancz-52] under the section heading “*The Complete Algorithm for Minimized Iterations*”, applies instead a pair of coupled two-term recurrences and is here referred to as BiOC algorithm [Gutkn-97], because it produces additionally a second pair of biconjugate bases.

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An application of the BiOC for solving linear algebraic systems was already presented in the above mentioned Lanczos paper. This algorithm was later reformulated by many authors and is named BiOMin [Gutkn–97] or *Biconjugate gradient* (BiCG) *algorithm* [Fletcher–76]. Block formulation of BiCG is due to [Leary–80].

Let  $\mathcal{K}_k(A, r_0) = \text{span}\{r_0, Ar_0, \dots, A^{k-1}r_0\}$  be the *Krylov space* spanned by a nonsingular matrix  $A \in \mathbb{R}^{n \times n}$  and a vector  $r_0 \in \mathbb{R}^n$ . Let  $x_0$  be any initial guess for the solution of the system  $Ax = b$ ,  $r_0 = b - Ax_0$  the starting residual and  $\tilde{r}_0$  an arbitrary nonzero vector. The *Lanczos' method* for solving this system consists in the construction of a sequence of vectors  $x_k$  and residuals  $r_k = b - Ax_k$  ( $k \geq 1$ ) such that

- $x_k \in x_0 + \mathcal{K}_k(A, r_0)$ ,
- $r_k \perp \mathcal{K}_k(A^T, \tilde{r}_0)$ .

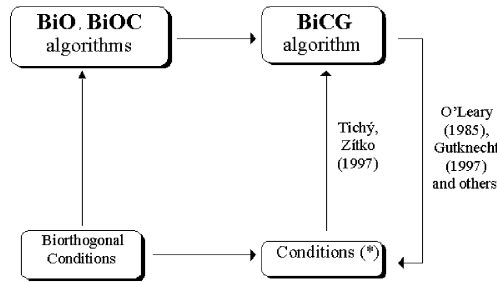


Figure 1: In 1950, Lanczos introduced an algorithm (BiO) that generates a pair of biorthogonal vector sequences. Lanczos (1952) suggested under the section heading “The Complete Algorithm for Minimized Iterations” an alternative algorithm (BiOC) for computing these sequences of vectors generated by the BiO algorithm. In the same paper an algorithm for solving linear algebraic systems was presented. Many authors ([Leary–80], [Gutkn–97]) showed that the vectors  $x_k$  and  $r_k$  generated by the BiCG algorithm fulfil the conditions (\*)  $x_k \in x_0 + \mathcal{K}_k(A, r_0)$  and  $r_k \perp \mathcal{K}_k(A^T, \tilde{r}_0)$ . In this paper we show how to obtain the recurrences of BiCG directly from these conditions.

For deriving BiCG we need to define auxiliary vectors  $\tilde{r}_k$  ( $k \geq 1$ ) under conditions

- $\tilde{r}_k \in \tilde{r}_0 + A^T \mathcal{K}_k(A^T, \tilde{r}_0)$ ,
- $\tilde{r}_k \perp \mathcal{K}_k(A, r_0)$ .

If we substitute the residual  $r_{i+1}$  in the form

$$r_{i+1} = r_0 + A \sum_{j=0}^i b_j^{(i)} A^j r_0 \quad (i = 0, \dots, k-1)$$

into conditions  $r_{i+1}^T A^{Tj} \tilde{r}_0 = 0$  ( $j = 0, \dots, i$ ) we find that the coefficients  $b_j^{(i)}$  fulfil the system of linear equations

$$- \begin{pmatrix} (\tilde{r}_0, r_0) \\ (\tilde{r}_0, Ar_0) \\ \vdots \\ (\tilde{r}_0, A^i r_0) \end{pmatrix} = \begin{pmatrix} (\tilde{r}_0, Ar_0) & (\tilde{r}_0, A^2 r_0) & \dots & (\tilde{r}_0, A^{i+1} r_0) \\ (\tilde{r}_0, A^2 r_0) & (\tilde{r}_0, A^3 r_0) & \dots & (\tilde{r}_0, A^{i+2} r_0) \\ \vdots & & & \\ (\tilde{r}_0, A^{i+1} r_0) & (\tilde{r}_0, A^{i+2} r_0) & \dots & (\tilde{r}_0, A^{2i+1} r_0) \end{pmatrix} \begin{pmatrix} b_0^{(i)} \\ b_1^{(i)} \\ \vdots \\ b_i^{(i)} \end{pmatrix}.$$

The determinant of the matrix of this system is called the *Hankel determinant* and is denoted by  $d_{i+1}$ . If  $d_{i+1} \neq 0$  then the residual  $r_{i+1}$  exists and is unique. By analogy, it can be shown that if  $d_{i+1} \neq 0$ , the vektor  $\tilde{r}_{i+1}$  exists, is defined uniquely and can be written in the form

$$\tilde{r}_{i+1} = \tilde{r}_0 + A^T \sum_{j=0}^i b_j^{(i)} (A^T)^j \tilde{r}_0 \quad (i = 0, \dots, k-1).$$

Moreover, if  $\tilde{r}_j^T r_j \neq 0$  ( $j = 0, \dots, i$ ) then the vectors  $r_j$  and the vectors  $\tilde{r}_j$  are linearly independent,

$$(1) \quad \text{span}\{r_0, \dots, r_i\} = \mathcal{K}_{i+1}(A, r_0), \quad \text{span}\{\tilde{r}_0, \dots, \tilde{r}_i\} = \mathcal{K}_{i+1}(A^T, \tilde{r}_0)$$

and the vectors  $r_{i+1}$  and  $\tilde{r}_{i+1}$  can then be written as

$$r_{i+1} = r_i + A \sum_{j=0}^i \gamma_j^{(i)} r_j \quad \text{and} \quad \tilde{r}_{i+1} = \tilde{r}_i + A^T \sum_{j=0}^i \gamma_j^{(i)} \tilde{r}_j \quad (i = 0, \dots, k-1).$$

It will be shown in Lemma 1 and in Theorem 1 that if  $d_{j+1} \neq 0$  and  $\tilde{r}_j^T r_j \neq 0$  for  $j = 0, \dots, i$  then all coefficients  $\gamma_j^{(i)}$  are different from zero and the vectors  $r_{i+1}$  can be written in the form

$$r_{i+1} = r_i + \gamma_i^{(i)} A \left( r_i + \frac{\gamma_{i-1}^{(i)}}{\gamma_i^{(i)}} \left( r_{i-1} + \frac{\gamma_{i-2}^{(i)}}{\gamma_{i-1}^{(i)}} \left( r_{i-2} + \dots + \frac{\gamma_1^{(i)}}{\gamma_2^{(i)}} \left( r_1 + \frac{\gamma_0^{(i)}}{\gamma_1^{(i)}} r_0 \right) \dots \right) \right) \right)$$

and the ratio  $\gamma_{j-1}^{(i)}/\gamma_j^{(i)}$  does not depend on  $i$ . If we set  $\alpha_i = -\gamma_i^{(i)}$  and  $\beta_{i-1} = \gamma_{i-1}^{(i)}/\gamma_i^{(i)}$ , then  $r_{i+1}$  can be written as

$$r_{i+1} = r_i - \alpha_i A (r_i + \beta_{i-1} (r_{i-1} + \beta_{i-2} (r_{i-2} + \dots + \beta_1 (r_1 + \beta_0 r_0) \dots))) \quad (i = 0, \dots, k-1).$$

If we define  $p_0 = r_0$ ,  $p_{j+1} = r_{j+1} + \beta_j p_j$  for  $j = 0, \dots, i-1$ , then

$$\begin{aligned} r_{i+1} &= r_i - \alpha_i A p_i, \\ x_{i+1} &= x_i + \alpha_i p_i. \end{aligned}$$

Likewise, if we define  $\tilde{p}_0 = \tilde{r}_0$ ,  $\tilde{p}_{j+1} = \tilde{r}_{j+1} + \beta_j \tilde{p}_j$ , we obtain recurrences for vectors  $\tilde{r}_{i+1}$  in the form

$$\tilde{r}_{i+1} = \tilde{r}_i - \alpha_i A^T \tilde{p}_i.$$

The classical form of coefficients  $\alpha_i$  and  $\beta_i$  will be obtained by using biorthogonal relations.

## 2. RECURRENCES FOR THE BICG ITERATES

**Lemma 1.** *Let us suppose that  $d_j \neq 0$  for  $j = 1, \dots, k+1$  and  $\tilde{r}_i^T r_i \neq 0$  for  $i = 0, \dots, k$ . Then there exist real numbers  $\gamma_j^{(i)} \neq 0$ ,  $0 \leq j \leq i \leq k$ , such that*

$$(2) \quad r_{i+1} = r_i + A(\gamma_i^{(i)} r_i + \gamma_{i-1}^{(i)} r_{i-1} + \dots + \gamma_1^{(i)} r_1 + \gamma_0^{(i)} r_0),$$

$$(3) \quad \tilde{r}_{i+1} = \tilde{r}_i + A^T(\gamma_i^{(i)} \tilde{r}_i + \gamma_{i-1}^{(i)} \tilde{r}_{i-1} + \dots + \gamma_1^{(i)} \tilde{r}_1 + \gamma_0^{(i)} \tilde{r}_0).$$

Moreover, the numbers  $\gamma_j^{(i)}$  are determined uniquely.

*Proof.* The vectors  $r_{i+1}$  and  $r_i$  fulfil

$$r_{i+1} = r_0 + b_1^{(i+1)} A r_0 + b_2^{(i+1)} A^2 r_0 + \dots + b_{i+1}^{(i+1)} A^{i+1} r_0,$$

$$r_i = r_0 + b_1^{(i)} A r_0 + b_2^{(i)} A^2 r_0 + \dots + b_i^{(i)} A^i r_0,$$

and thus

$$r_{i+1} = r_i + A((b_1^{(i+1)} - b_1^{(i)}) r_0 + \dots + (b_i^{(i+1)} - b_i^{(i)}) A^{i-1} r_0 + b_{i+1}^{(i+1)} A^i r_0).$$

According to (1), there exist uniquely determined real numbers  $\gamma_0^{(i)}, \dots, \gamma_i^{(i)}$  such that

$$(4) \quad r_{i+1} = r_i + A(\gamma_i^{(i)} r_i + \gamma_{i-1}^{(i)} r_{i-1} + \dots + \gamma_1^{(i)} r_1 + \gamma_0^{(i)} r_0).$$

Analogously we obtain equality (3).

Now, we have to prove that the real numbers  $\gamma_j^{(i)}$  are different from zero. Let us define  $c_{i,j} = \tilde{r}_i^T A r_j$ . It is easy to see that  $c_{i,j} = 0$  when  $|i - j| > 1$ . For  $i = 0, \dots, k$  we have

$$(5) \quad r_i = r_{i-1} + A(\gamma_{i-1}^{(i-1)} r_{i-1} + \dots + \gamma_0^{(i-1)} r_0).$$

If we multiply the equation (5) from the left by the vector  $\tilde{r}_i^T$  we obtain

$$\tilde{r}_i^T r_i = \gamma_{i-1}^{(i-1)} \tilde{r}_i^T A r_{i-1}.$$

Since  $\tilde{r}_i^T r_i \neq 0$  we have  $\tilde{r}_i^T A r_{i-1} \neq 0$  and hence  $c_{i,i-1} \neq 0$ . Likewise, if we write  $\tilde{r}_i$  in the form (3), we get  $c_{i-1,i} \neq 0$ . Let us multiply the equation

$$r_{i+1} = r_i + A(\gamma_i^{(i)} r_i + \dots + \gamma_0^{(i)} r_0)$$

from the left by the vectors  $\tilde{r}_i^T, \dots, \tilde{r}_0^T$ . Then we get for the real numbers  $\gamma_j^{(i)}$  the identity

$$(6) \quad - \begin{pmatrix} \tilde{r}_i^T r_i \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} c_{i,i} & c_{i,i-1} & & & \\ c_{i-1,i} & c_{i-1,i-1} & c_{i-1,i-2} & & \\ & c_{i-2,i-1} & c_{i-2,i-2} & c_{i-2,i-3} & \\ & & \ddots & \ddots & \ddots \\ & & & c_{1,2} & c_{1,1} & c_{1,0} \\ & & & & c_{0,1} & c_{0,0} \end{pmatrix} \begin{pmatrix} \gamma_i^{(i)} \\ \gamma_{i-1}^{(i)} \\ \vdots \\ \gamma_0^{(i)} \end{pmatrix}.$$

The matrix in (6) is nonsingular because if a vector  $(\hat{\gamma}_i, \hat{\gamma}_{i-1}, \dots, \hat{\gamma}_0)^T$  fulfils the identity (6) then the vector  $\hat{r}_{i+1} = r_i + A(\hat{\gamma}_i r_i + \dots + \hat{\gamma}_0 r_0)$  is orthogonal to  $\tilde{r}_0, \dots, \tilde{r}_i$  and lies in  $r_0 + AK_{i+1}(A, r_0)$ . But the uniqueness implies that  $\hat{r}_{i+1} = r_{i+1}$  and thus  $\hat{\gamma}_j = \gamma_j^{(i)}$ ,  $j = 0, \dots, i$ . The matrix in the identity (6) has to be nonsingular. If we denote the three-diagonal matrix in identity (6) as  $V_i$ , then  $\det(V_i) \neq 0$  for  $i = 0, \dots, k$ . Let us denote by  $V_i^{(j)}$  the matrix that arises from the matrix  $V_i$  if we substitute the  $j$ th column of the matrix  $V_i$  by the left hand side of identity (6). Then according to the Cramer rule for  $j = 0, \dots, i$  we have

$$\gamma_j^{(i)} = \frac{\det(V_i^{(i+1-j)})}{\det(V_i)}.$$

If we define  $V_{-1} = 1$ , then we can write  $\det(V_i^{(j)})$  in the form

$$(7) \quad \det(V_i^{(j)}) = (-1)^j \cdot \tilde{r}_i^T r_i \cdot \prod_{l=i-j+1}^{i-1} c_{l,l+1} \cdot \det(V_{i-j}), \quad j = 1, \dots, i+1.$$

From (7) it follows that  $\det(V_i^{(i+1-j)}) \neq 0$  and hence  $\gamma_j^{(i)} \neq 0$  for  $j = 0, \dots, i$ .  $\square$

**Theorem 1.** *Let us suppose that  $d_i \neq 0$  for  $i = 1, \dots, k+1$ ,  $\tilde{r}_i^T r_i \neq 0$  for  $i = 0, \dots, k$  and  $p_0 = r_0$ ,  $\tilde{p}_0 = \tilde{r}_0$ . Then we can compute the vectors  $r_{i+1}$ ,  $\tilde{r}_{i+1}$  and  $x_{i+1}$  for  $i = 0, \dots, k$  from the recurrences*

$$(8) \quad r_{i+1} = r_i - \alpha_i A p_i,$$

$$(9) \quad \tilde{r}_{i+1} = \tilde{r}_i - \alpha_i A^T \tilde{p}_i,$$

$$(10) \quad p_{i+1} = r_{i+1} + \beta_i p_i,$$

$$(11) \quad \tilde{p}_{i+1} = \tilde{r}_{i+1} + \beta_i \tilde{p}_i,$$

$$(12) \quad x_{i+1} = x_i + \alpha_i p_i,$$

where

$$(13) \quad \alpha_i = \frac{\tilde{r}_i^T r_i}{\tilde{p}_i^T A p_i}, \quad \beta_i = \frac{\tilde{r}_{i+1}^T r_{i+1}}{\tilde{r}_i^T r_i}.$$

**P r o o f.** According to relation (5) (we know that  $\gamma_j^{(i)} \neq 0$  for  $j \leq i \leq k$ ) we can write

$$(14) \quad \begin{aligned} r_{i+1} &= r_i + \gamma_i^{(i)} A \left( r_i + \frac{\gamma_{i-1}^{(i)}}{\gamma_i^{(i)}} r_{i-1} + \frac{\gamma_{i-2}^{(i)}}{\gamma_i^{(i)}} r_{i-2} + \dots + \frac{\gamma_0^{(i)}}{\gamma_i^{(i)}} r_0 \right) \\ &= r_i + \gamma_i^{(i)} A \left( r_i + \frac{\gamma_{i-1}^{(i)}}{\gamma_i^{(i)}} \left( r_{i-1} + \frac{\gamma_{i-2}^{(i)}}{\gamma_{i-1}^{(i)}} r_{i-2} + \dots + \frac{\gamma_0^{(i)}}{\gamma_{i-1}^{(i)}} r_0 \right) \right) \\ &= r_i + \gamma_i^{(i)} A \left( r_i + \frac{\gamma_{i-1}^{(i)}}{\gamma_i^{(i)}} \left( r_{i-1} + \frac{\gamma_{i-2}^{(i)}}{\gamma_{i-1}^{(i)}} \left( r_{i-2} + \dots + \frac{\gamma_1^{(i)}}{\gamma_2^{(i)}} \left( r_1 + \frac{\gamma_0^{(i)}}{\gamma_1^{(i)}} r_0 \right) \dots \right) \right) \right). \end{aligned}$$

We can rewrite all residuals ( $i = 0, \dots, k$ ) in the form (14). Let us prove that

$$(15) \quad \frac{\gamma_{i-1}^{(l)}}{\gamma_i^{(l)}} = \frac{\gamma_{i-1}^{(j)}}{\gamma_i^{(j)}} \quad \text{for } 1 \leq i \leq l \leq k, \quad 1 \leq i \leq j \leq k$$

holds. We have

$$\begin{aligned} \frac{\gamma_{i-1}^{(l)}}{\gamma_i^{(l)}} &= \frac{\det(V_l^{(l+2-i)})}{\det(V_l^{(l+1-i)})} = \frac{(-1)^{l+2-i} \cdot \tilde{r}_l^T \tilde{r}_l \cdot \prod_{j=i-1}^{l-1} c_{j,j+1} \det(V_{i-2})}{(-1)^{l+1-i} \cdot \tilde{r}_l^T \tilde{r}_l \cdot \prod_{j=i}^{l-1} c_{j,j+1} \det(V_{i-1})} \\ &= -c_{i-1,i} \frac{\det(V_{i-2})}{\det(V_{i-1})}. \end{aligned}$$

We can see that the right-hand side does not depend on the index  $l$ . Likewise we can write

$$\frac{\gamma_{i-1}^{(j)}}{\gamma_i^{(j)}} = -c_{i-1,i} \cdot \frac{\det(V_{i-2})}{\det(V_{i-1})}$$

and (15) holds. Let us define real numbers  $\alpha_i$  and  $\beta_i$  as

$$\alpha_i = -\gamma_i^{(i)} \quad \text{and} \quad \beta_{i-1} = \frac{\gamma_{i-1}^{(i)}}{\gamma_i^{(i)}}.$$

Then according to relations (15) and (14), we can rewrite the residuals  $r_{i+1}$  ( $i = 0, \dots, k$ ) in the form

$$(16) \quad r_{i+1} = r_i - \alpha_i A(r_i + \beta_{i-1}(r_{i-1} + \beta_{i-2}(r_{i-2} + \dots \beta_1(r_1 + \beta_0 r_0) \dots))).$$

If we define

$$p_0 = r_0, \quad p_{j+1} = r_{j+1} + \beta_j p_j \quad \text{for } j = 0, \dots, i-1,$$

we can rewrite (16) in the form

$$(17) \quad r_{i+1} = r_i - \alpha_i A p_i \quad \text{for } i = 0, \dots, k.$$

Since  $\alpha_i \neq 0$  we have that  $\tilde{p}_i^T A p_i = -\tilde{r}_i^T r_i / \alpha_i \neq 0$ . Let us derive now the well-known forms of the real numbers  $\alpha_i$  and  $\beta_i$ . We find that

$$\tilde{p}_i^T r_{i+1} = \tilde{p}_i^T r_i - \alpha_i \tilde{p}_i^T A p_i$$

and thus we obtain for  $\alpha_i$  the formula

$$\alpha_i = \frac{\tilde{p}_i^T r_i}{\tilde{p}_i^T A p_i}.$$

Since

$$\tilde{p}_i^T r_i = \tilde{r}_i^T r_i + \beta_{i-1} \tilde{p}_{i-1}^T r_i = \tilde{r}_i^T r_i,$$

we obtain

$$\alpha_i = \frac{\tilde{r}_i^T r_i}{\tilde{p}_i^T A p_i}.$$

Let us carry on the derivation of  $\beta_i$ . We have

$$\tilde{r}_i^T p_{i+1} = \tilde{r}_i^T r_{i+1} + \beta_i \tilde{r}_i^T p_i$$

and therefore

$$\beta_i = \frac{\tilde{r}_i^T p_{i+1}}{\tilde{r}_i^T r_i}.$$

Since

$$\tilde{r}_{i+1}^T r_{i+1} = \tilde{r}_{i+1}^T p_{i+1} = \tilde{r}_i^T p_{i+1} - \alpha_i \tilde{p}_i^T A p_{i+1} = \tilde{r}_i^T p_{i+1} + \frac{\alpha_i}{\alpha_{i+1}} \tilde{p}_i^T (r_{i+2} - r_{i+1}) = \tilde{r}_i^T p_{i+1},$$

we get

$$\beta_i = \frac{\tilde{r}_{i+1}^T r_{i+1}}{\tilde{r}_i^T r_i}.$$

The forms (9) and (11) can be proved analogously. The form (12) we get from

$$b - A x_{i+1} = b - A x_i - \alpha_i A p_i.$$

□



According to the previous theorem, we can formulate Algorithm of BiCG.

### Algorithm BiCG

**Input**  $x_0$ ,  $A$ ,  $b$ ,  $\tilde{r}_0 \neq 0$ ,  $\varepsilon$ ;

$r_0 = b - Ax_0$ ;

$p_0 = r_0$ ;  $\tilde{p}_0 = \tilde{r}_0$ ;

$k = 0$ ;

**while**  $\frac{\|r_k\|}{\|r_0\|} > \varepsilon$  **do**

**begin**

$\alpha_k = \frac{\tilde{r}_k^T r_k}{\tilde{p}_k^T A p_k}$ ;

$x_{k+1} = x_k + \alpha_k p_k$ ;

$r_{k+1} = r_k - \alpha_k A p_k$ ;

$\tilde{r}_{k+1} = \tilde{r}_k - \alpha_k A^T \tilde{p}_k$ ;

$\beta_k = \frac{\tilde{r}_{k+1}^T r_{k+1}}{\tilde{r}_k^T r_k}$ ;

$p_{k+1} = r_{k+1} + \beta_k p_k$ ;

$\tilde{p}_{k+1} = \tilde{r}_{k+1} + \beta_k \tilde{p}_k$ ;

$k = k + 1$

**end**;

$x^* = x_k$ .

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*Authors' address: Petr Tichý, Jan Zítko*, Department of Numerical Mathematics, Faculty of Mathematics and Physics, Charles University of Prague, Malostranské náměstí 25, 118 00 Praha 1, Czech Republic, e-mail: [tichy@menza.mff.cuni.cz](mailto:tichy@menza.mff.cuni.cz), [zitko@ms.mff.cuni.cz](mailto:zitko@ms.mff.cuni.cz).