

## An improvement in preconditioned BiCGStab method

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In order to solve linear equations

$$A\mathbf{x} = \mathbf{b}, \quad (1)$$

preconditioned BiCGStab (PBiCGStab) method<sup>3)</sup> is often used. PBiCGStab brings well convergence, further, its calculation cost is not a lot and its required memory size is a little. However, conventional representation of PBiCGStab has a mathematical inadvisability on its preconditioning conversion for the shadow residual vector  $\mathbf{r}_0^\sharp$ .

A preconditioned system of eq.(1) is

$$(AK^{-1})(K\mathbf{x}) = \mathbf{b}, \quad (2)$$

this residual vector is  $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ . Here,  $K$  ( $\approx A$ ) is a preconditioner. The preconditioned dual system is  $(K^{-T}A^T)\mathbf{x}^\sharp = K^{-T}\mathbf{b}^\sharp$ , this (shadow) residual vector is  $K^{-T}\mathbf{r}^\sharp = K^{-T}\mathbf{b}^\sharp - (K^{-T}A^T)\mathbf{x}^\sharp$ . That is, this preconditioning conversion for shadow residual vector is

$$\tilde{\mathbf{r}}_0^\sharp \Rightarrow K^{-T}\mathbf{r}_0^\sharp, \quad (3)$$

but conventional typical algorithm<sup>3)</sup> is based on

$$\tilde{\mathbf{r}}_0^\sharp \Rightarrow \mathbf{r}_0^\sharp. \quad (4)$$

Eq.(3) is proper in mathematical, this is common characteristic to Lanczos biorthogonalization type algorithms<sup>2)</sup>.

Conventional preconditioning conversion for eq.(2) is as follows:

$$\tilde{\mathbf{p}} \Rightarrow \mathbf{p}, \tilde{\mathbf{t}} \Rightarrow \mathbf{t}, \tilde{\mathbf{r}} \Rightarrow \mathbf{r}, \tilde{\mathbf{r}}_0^\sharp \Rightarrow \mathbf{r}_0^\sharp.$$

On the other hand, our conversion manner for eq.(2) is,

$$\tilde{\mathbf{p}} \Rightarrow K\mathbf{p}, \tilde{\mathbf{t}} \Rightarrow \mathbf{t}, \\ \tilde{\mathbf{z}} \Rightarrow K\mathbf{z}, \tilde{\mathbf{r}} \Rightarrow \mathbf{r}, \tilde{\mathbf{r}}_0^\sharp \Rightarrow K^{-T}\mathbf{r}_0^\sharp,$$

then the following PBiCGStab is obtained.

Algorithm 1. An improved preconditioned BiCGStab method:

$\mathbf{x}_0, \mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0, \mathbf{r}_0^\sharp = K^{-1}\mathbf{r}_0, \beta_{-1} = 0,$

For  $k = 0, 1, 2, \dots$ , until convergence, Do:

$$\mathbf{p}_k = K^{-1}\mathbf{r}_k + \beta_{k-1}\mathbf{z}_{k-1}, \quad (5)$$

$$\alpha_k = \frac{\langle \mathbf{r}_0^\sharp, K^{-1}\mathbf{r}_k \rangle}{\langle \mathbf{r}_0^\sharp, K^{-1}A\mathbf{p}_k \rangle}, \quad (6)$$

$$\mathbf{t}_k = \mathbf{r}_k - \alpha_k A\mathbf{p}_k,$$

$$K^{-1}\mathbf{t}_k = K^{-1}\mathbf{r}_k - \alpha_k K^{-1}A\mathbf{p}_k, \quad (7)$$

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$$\zeta_k = \frac{(AK^{-1}\mathbf{t}_k, \mathbf{t}_k)}{(AK^{-1}\mathbf{t}_k, AK^{-1}\mathbf{t}_k)},$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k + \zeta_k K^{-1}\mathbf{t}_k,$$

$$\mathbf{r}_{k+1} = \mathbf{t}_k - \zeta_k AK^{-1}\mathbf{t}_k,$$

$$\mathbf{z}_k = \mathbf{p}_k - \zeta_k K^{-1}A\mathbf{p}_k, \quad (8)$$

$$\beta_k = \frac{\alpha_k}{\zeta_k} \times \frac{\langle \mathbf{r}_0^\sharp, K^{-1}\mathbf{r}_{k+1} \rangle}{\langle \mathbf{r}_0^\sharp, K^{-1}\mathbf{r}_k \rangle}, \quad (9)$$

End Do

Here,  $\langle \mathbf{u}, \mathbf{v} \rangle$  means “scalar product without metric”, and  $(\mathbf{u}, \mathbf{v})$  means “inner product with metric”.

Alg.1 has two technical interesting items on preconditioning conversion. First, there are three preconditioning operations in alg.1,  $K^{-1}\mathbf{t}_k, K^{-1}\mathbf{r}_k, K^{-1}A\mathbf{p}_k$ . But calculating cost of  $K^{-1}\mathbf{t}_k$  is almost nothing, because  $K^{-1}\mathbf{t}_k$  is composed of  $K^{-1}\mathbf{r}_k$  and  $K^{-1}A\mathbf{p}_k$  by using eq.(7), these latter operations are already calculated by eqs.(9)(6), respectively. Second, eq.(5) is separated in two eqs. (5)(8) in alg.1.

Numerical results by systematic performance evaluation<sup>1)</sup> shows advantage of our algorithm. We will show them at the HPCS2011. Our PBiCGStab algorithm will be implemented in Xabclib<sup>4)</sup>.

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