Parallelizations of TFETI-1 coarse problem using PETSc
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Report contains the main results reached by dual method TFETI using our library FLLOP (FETI Light Layer On top of PETSc) [1] on the Cray XE6 machine HECToR – joint work with Václav Hapla. As a benchmark, model 2D elastostatic problem of the steel traverse was chosen.

The FETI methods having as the input primal data of decomposed problem into $N_s$ subdomains with block-diagonal stiffness matrix, vector of forces, block-diagonal null space matrix (which can be formed directly from the mesh without any computation in TFETI case) and constraint matrix for subdomains’ gluing

$$
K = \begin{bmatrix} K^1 & \cdots & \hat{K} & \cdots & K^{N_s} \end{bmatrix}, f = \begin{bmatrix} f^1 \vdots f^{N_s} \end{bmatrix}, R = \begin{bmatrix} R^1 & \cdots \hat{R} & \cdots & R^{N_s} \end{bmatrix}, B = [B^1 \cdots B^{N_s}]
$$

blend iterative and direct solvers. The dual problem

$$
PF\lambda = Pd
$$

is solved iteratively using e.g. CG or PCG method; in each iteration, the auxiliary problems related to the application of an unassembled system matrix $PF$ (subdomain problems’ solutions and projector application in dual operator) are solved directly. Here dual objects are denoted by

$$
F = BK^+B^T, G = R^TB^T, P = I - Q, Q = G^T(GG^T)^{-1}G, e = R^Tf, d = BK^+f - F\hat{G}^T(GG^T)^{-1}e.
$$

The first auxiliary problem is the stiffness matrix’s pseudoinverse $(K^+: KK^+K = K)$ application $K^+v$. It is parallelizable without any data transfers because of a nice block-diagonal structure. The second one is the coarse problem (CP) solution

$$
GG^Tx = y
$$

appearing in the application of the projector $P$ onto the kernel of so called natural coarse space matrix $G$. However, this problem does not possess such a nice structure suitable for parallel processing; some communication is needed in this case.

Natural effort using the massively parallel computers is to maximize number of subdomains so that sizes of subdomain stiffness matrices are reduced which accelerates not only their factorization and subsequent pseudoinverse application but also reduces the number of iterations. Negative effect of that is an increase of dual and null space dimension, which decelerate the CP solution, so that the bottleneck of the TFETI method is the application of the projector.

We have suggested and compared several strategies of CP solution. These strategies of the projector application can be viewed from two points (see [2]):

I. how $G$ is distributed and its action carried out:
A) horizontal blocks,
B) vertical blocks.
II. how the CP is solved which implies the level of preprocessing of $G$ and $GG^T$:
1) iteratively using CG by the master process,
2) directly using Cholesky/LU factorization by the master process,
3) applying explicit inverse of $GG^T$ in parallel,
4) the CP is eliminated, provided that the rows of $G$ are orthonormalized.

All B cases have a big advantage - we can parallelize all dual vectors and operations with them. Numerical experiments confirm as best choice the strategy B4 and then B3.

<table>
<thead>
<tr>
<th>Number of subdom.</th>
<th>192</th>
<th>768</th>
<th>1728</th>
<th>3072</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of cores</td>
<td>192</td>
<td>768</td>
<td>1728</td>
<td>3072</td>
</tr>
<tr>
<td>Primal dim.</td>
<td>12,580,224</td>
<td>50,320,896</td>
<td>114,476,544</td>
<td>201,283,584</td>
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<td>Dual dim.</td>
<td>129,984</td>
<td>537,216</td>
<td>1,228,464</td>
<td>2,183,424</td>
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<td>Kernel dim.</td>
<td>576</td>
<td>2304</td>
<td>5184</td>
<td>9216</td>
</tr>
<tr>
<td>$G_{rank}$</td>
<td>1.001e-02</td>
<td>1.152e-02</td>
<td>1.489e-02</td>
<td>1.527e-02</td>
</tr>
<tr>
<td>broadcast of $G$ to all cores</td>
<td>9.102e-00</td>
<td>3.710e-00</td>
<td>8.353e-00</td>
<td>1.389e+00</td>
</tr>
<tr>
<td>B1: $GG^T$ assembing</td>
<td>6.710e-02</td>
<td>2.469e-01</td>
<td>7.155e-01</td>
<td>1.203e+00</td>
</tr>
<tr>
<td>B2: $GG^T$ Chol. fact.</td>
<td>8.090e-00</td>
<td>1.042e-00</td>
<td>8.108e-00</td>
<td>2.004e+00</td>
</tr>
<tr>
<td>B3: inverse</td>
<td>1.767e-01</td>
<td>1.149e+00</td>
<td>6.401e+00</td>
<td>9.264e+00</td>
</tr>
<tr>
<td>B4: orthonormalization</td>
<td>9.669e-02</td>
<td>5.983e-00</td>
<td>3.262e+00</td>
<td>4.652e+00</td>
</tr>
<tr>
<td>B1: $Q_G$ action</td>
<td>1.070e-02</td>
<td>6.934e-02</td>
<td>3.204e-01</td>
<td>6.424e-01</td>
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<td>B3: $Q_G$ action</td>
<td>5.822e-03</td>
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<td>1.760e-01</td>
<td>3.621e-01</td>
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<tr>
<td>B4: $Q_G$ action</td>
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<td>2.694e-02</td>
<td>6.424e-02</td>
<td>9.874e-02</td>
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</table>

Acknowledgements
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References