A massively parallel and memory efficient FEM toolbox with A Hybrid Total FETI solver with accelerator support

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Abstract

In this paper we present the ESPRESO FEM library, which includes a FEM toolbox with interfaces to professional and open-source simulation tools, and a massively parallel Hybrid Total FETI (HTFETI) solver which can fully utilize the OLCF Titan supercomputer, and achieves super-linear scaling. This paper presents several new techniques for FETI solvers designed for efficient utilization of supercomputers with a focus on: (i) performance - we present a fivefold reduction of solver runtime for the Laplace equation by redesigning the FETI solver, and offloading the key workload to the accelerator. We compare Intel Xeon Phi 7120p and Tesla K80 and P100 accelerators to Intel Xeon E5-2680v3 and Xeon Phi 7210 CPUs; and (ii) memory efficiency - we present two techniques which increase the efficiency of the HTFETI solver 1.8 times, and pushes the limits of the largest possible problem ESPRESO can solve from 124 to 223 billion unknowns for problems with unstructured meshes. Finally we show that by dynamically tuning hardware parameters we can reduce energy consumption by up to 33 %.

Keywords

FEM, Hybrid Total FETI, GPU, Xeon Phi, KNC, KNL, massively parallel, sparse linear solver

1 Introduction

In this paper we present the ExaScale PaRallel FETI SOLver (ESPRESO) Finite Element Method (FEM) library which contains (i) a FEM preprocessor (ESPRESO FEM) and (ii) a Finite Element Tearing and Interconnecting (FETI) solver. The ESPRESO FEM preprocessor requires a mesh generated by 3rd party software together with definition of groups of elements, we call them sets, onto which boundary conditions are prescribed. The boundary conditions are described by an ESPRESO configuration file. We support the input formats of one commercial and two open-source tools for mesh and sets data. The commercial tool is ANSYS Workbench (ANSYS, 2017) and the open-source tools are ELMER (IT Center for Science, CSC, 2017), and OpenFOAM (Jasak et al., 2007).

When using the standard toolchain, the ESPRESO FEM assembles all FEM matrix objects and passes them to the FETI solver. As of now the ESPRESO FEM contains assemblers for structural mechanics (heat transfer and linear elasticity) problems, but new physics are being continuously implemented. At the end, mesh and simulation results are stored in the VTK format (Visualization Toolkit), see Shroeder et al. (1998). Moreover, in collaboration with ELMER developers at CSC - IT Center for Science, we have developed an API which transfers all necessary FEM objects. In this case ESPRESO serves only as a massively parallel linear solver.

The interface that allows our library to connect with other FEM tools enables our scalable solvers to be used by the listed tools. The solver also supports modern many-core architectures, the Intel Xeon Phi and the NVIDIA GPU,

using methods described in Section 3. Section 4.2 then presents solver performance.

One of the key components of the library is the massively parallel linear solver. It is based on the Finite Element Tearing and Interconnecting method (FETI, for more detail see, e.g., in Farhat et al. (1994a); Gosselet and Rey (2006)) which are successfully used in the engineering community for very large problems.

In this method the original structure is decomposed into several non-overlapping subdomains. Mutual continuity of primal variables between neighboring subdomains is enforced afterwards by dual variables, i.e., Lagrange multipliers (LM). They are usually obtained iteratively through certain Krylov subspace methods, then the primal solution is evaluated locally on each subdomain. Dostál et al. (2006) introduced a new variant of an algorithm called Total FETI (TFETI) in which the Dirichlet boundary condition is enforced by LM as well.

ESPRESO contains both the original TFETI method as well as its variant called HTFETI (Hybrid TFETI). The HTFETI method is a variant of hybrid FETI methods for FETI and FETI-DP, introduced by Klawonn and Rheinbach (2010). In this approach a number of subdomains is

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combined into clusters, which can be seen as a three-level domain decomposition approach.

The main advantage of HTFETI is its potential to solve problems decomposed into a large number of subdomains due to reduction of the main bottleneck of the FETI methods, the coarse problem. In this paper we show that our implementation in one of the presented examples uses 81.2 million subdomains organized into 17,576 clusters processed by the 17,576 compute nodes of the Titan supercomputer installed in the Oak Ridge Leadership Computing Facility, OLCF (2017). This means that: (i) the solver is able to solve extremely large problems (over 223 billion unknowns for the 3D Laplace equation); (ii) the solver can decompose smaller problems of approximately 1 billion unknowns into small subdomains, which improves memory efficiency (faster Cholesky factorization of small matrices) and the performance of the solver in terms of the FETI numerical scalability (a smaller number of iterations).

To further improve the memory efficiency of our HTFETI solver we propose two techniques: (i) a repeated factorization technique and (ii) an iterative solver technique to solve subdomain stiffness matrices. Both techniques eliminate the high memory utilization caused by the LU or Cholesky decomposition done by the sparse direct solvers that are used in all FETI solvers. The problems presented in this paper use unstructured meshes, and a significant part of the memory is therefore used by the mesh and the stiffness matrices.

Scalable implementations of domain decomposition methods have been presented in several works. Klawonn et al. (2016b) combined FETI-DP methods with a parallel algebraic multigrid as a solver for the coarse problem, to increase the scalability. The authors focused on 2D linear elasticity and nonlinear hyperelasticity problems, and demonstrated scalability to more than 10 billion DOFs and 500,000 MPI ranks. The total memory consumption was approximately 256 TB. In comparison, we present a 3D linear elasticity problem with 70 billion unknowns using 560 TB of memory. Similarly, Klawonn et al. (2016a) presented a solution used micro-macro scale bridging in the simulation of dual-phase steel. The 3D solver is able to scale up to 786,432 cores, solving problems with more than 19 billion unknowns, using 768 TB of memory.

Highly scalable implementations of the Balancing Domain Decomposition by Constraint (BDDC) method are presented in Badia et al. (2014) and Sistik and Cirak (2015). The former paper outlines the solution of 3D Poisson and linear elasticity problems with up to 1 billion unknowns on 27 thousand cores consuming 110 TB of RAM. The latter focuses on the simulation of low Reynolds number flows around fixed and moving rigid bodies in 3D. The largest solved problem, reaching 3.3 billion unknowns, was solved using 65,500 cores and 65 TB of memory. These results demonstrate the abilities of non-overlapping domain decomposition methods to utilize computational resources of current multi-petascale supercomputers for solution of various kinds of problems.

However, large numbers of supercomputers are now equipped with many-core accelerator technologies. Therefore, in addition to the scalable HTFETI implementation, the paper presents acceleration using the Intel Xeon Phi coprocessors or GPU accelerators, which enables us to fully utilize

Figure 1. A cantilever beam in 2D.

the computational power of these accelerated machines; see the list in Table 2.

FETI methods are based on sparse matrices, and the most time consuming operation is the solve routine of the sparse direct solver. This is called for all subdomain matrices repeatedly in every iteration of the Preconditioned Conjugate Projected Gradient (PCPG) solver. We present two approaches to accelerating this operation: (i) maintain the sparse matrices by using a sparse direct solver on the accelerator; and (ii) use our proposed approach, which converts sparse data to dense. Then instead of using the solve routine on sparse data, the dense general matrix-vector (GEMV) multiplication operation is used. The size of the new dense matrix is similar to the size of the Cholesky decomposition of the original sparse matrix.

The first approach can be used efficiently for Intel Xeon Phi, both the Knights Corner (KNC) and the Knights Landing (KNL) generations, since the MKL PARDISO sparse direct solver is well optimized for these. However for GPUs we have not found any suitable alternative. The second approach converts the sparse data into dense using the local Schur complement (LSC) method for HTFETI, presented in the Section '2.2' which was originally presented for Total FETI in Riha et al. (2016b). The main advantage of the LSC method is that GEMV operation provides regular memory access and is therefore able to fully utilize the high memory bandwidth of the accelerator.

2 Methods

In this section we introduce the Hybrid Total FETI method, the key element for the scalability of the ESPRESO solvers, and the local Schur complement method as a key tool for efficient acceleration of the HTFETI method.

2.1 Hybrid Total FETI method

The principle of the HTFETI method is explained in contrast to the classical TFETI method.

2.1.1 Total FETI method We will shortly introduce the TFETI method for a two-dimensional linear elasticity problem given by a cantilever beam (see Figure 1.a). After discretization and domain decomposition, the i -th set of nodal equilibrium equations related to i -th subdomain is

$$\mathbf{K}_i \mathbf{u}_i = \mathbf{f}_i - \mathbf{B}_i^T \boldsymbol{\lambda} \quad i \in (1, 2, 3, 4) \quad (1)$$

where $\mathbf{K}_i$ is the local subdomain stiffness matrix and $\mathbf{f}_i$ is the local right-hand side vector, both are assembled only

from elements belonging to i -th subdomain. λ is a vector of LMs (reaction forces enforcing the continuity between neighbouring subdomains) and B_i is the constraints matrix. These four systems of linear equations are complemented by the compatibility condition

$$B_1 u_1 + B_2 u_2 + B_3 u_3 + B_4 u_4 = c. \quad (2)$$

All of these local matrices B_i appearing in (2) can be collected in one global object

$$B = B_{1:4} = \begin{pmatrix} B_1 & B_2 & B_3 & B_4 \end{pmatrix} \quad (3)$$

which enforces the continuity on the decomposed structure, and also the Dirichlet boundary condition. Introducing the block diagonal matrix $K = K_{1:4} = \text{diag}(K_1, K_2, K_3, K_4)$, the global right-hand side vector $f^\top = f_{1:4}^\top = (f_1^\top, f_2^\top, f_3^\top, f_4^\top)$, and the global vector of unknowns $u^\top = u_{1:4}^\top = (u_1^\top, u_2^\top, u_3^\top, u_4^\top)$, the linear system representing the discretized equilibrium equations of the cantilever beam can be written as follows:

$$\begin{pmatrix} K & B^\top \\ B & O \end{pmatrix} \begin{pmatrix} u \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ c \end{pmatrix}. \quad (4)$$

In the text above, we also introduced the interval selection of matrices and vectors. For instance, $K_{i:j}$ means the block diagonal stiffness matrix containing local stiffness matrices of subdomains number $i, i+1, i+2, \dots, j$.

Eliminating primal variable u by

$$u = K^+ (f - B^\top \lambda) + R\alpha \quad (5)$$

and utilizing the orthogonality condition

$$R \perp f - B^\top \lambda \quad (6)$$

we arrive at the Schur complement system

$$\begin{pmatrix} F & G \\ G^\top & O \end{pmatrix} \begin{pmatrix} \lambda \\ \alpha \end{pmatrix} = \begin{pmatrix} d \\ e \end{pmatrix}, \quad (7)$$

where $F = BK^+B^\top$ is the TFETI operator, $G = -BR$ is a transformation matrix, and $d = BK^+f - c$ and $e = -R^\top f^\top$ are parts of the dual right hand side vector. The matrix $R = R_{1:4} = \text{diag}(R_1, R_2, R_3, R_4)$ consists of the vectors that create the basis of the null space of the stiffness matrix K . From the statics point of view, the basis stored in matrix R describes rigid body movements (RBM) of all subdomains. The vector α contains their amplitudes.

It is worth noting that the new system (7) is better conditioned than (4), and it will be solved by the PCPG method. In the algorithm, the gradient is projected at each iteration by the orthogonal projector

$$P = I - G(G^\top G)^{-1}G^\top, \quad (8)$$

where $G = -BR$. The part of the projector $G^\top G \in \mathbb{R}^{n_G \times n_G}$ called the coarse problem is usually orthogonalized or factorized to improve the performance. Its dimension

$$n_G = n_{sub} \cdot d, \quad (9)$$

proportionally depends on the number of subdomains n_{sub} . The parameter d (number of RBMs of a single floating

subdomain) is 3 in 2D and 6 in 3D. If the number of subdomains is too large, the coarse problem can be a serious bottleneck for the TFETI method. Concretely for the simple beam benchmark (see Figure 1.b left), the size is given by

$$n_G = (4 \text{ subdomains}) \times (3 \text{ RBM}) = 12. \quad (10)$$

The possible ways to overcome it will be shown in the next section.

2.1.2 The HTFETI method We apply the HTFETI method to the same problem in order to demonstrate how the size of the coarse problem can be decreased. Firstly, we introduce the new object

$$B_c = \begin{pmatrix} B_{c,1:2} & O \\ O & B_{c,3:4} \end{pmatrix} = \begin{pmatrix} B_{c,1} & B_{c,2} & O & O \\ O & O & B_{c,3} & B_{c,4} \end{pmatrix} \quad (11)$$

similar to the constraint matrix B . The first diagonal block $B_{c,1:2}$ consists of constraints that lock all mutual rigid movements between subdomains number one and two. This group will be denoted as cluster number one. The second block $B_{c,3:4}$, locks mutual movements between subdomains number three and four (see Figure 1.b right). The block structure of B_c will be utilized in an algorithm later on. The cluster of subdomains in the HTFETI method can be viewed in the same manner as a single subdomain in the classical TFETI method. The collection of LMs that enforce the required locking effect is denoted as $\tilde{\lambda}_c^\top = (\tilde{\lambda}_{c,1}^\top, \tilde{\lambda}_{c,2}^\top)$.

The extended linear system (nodal equilibrium equations of the cantilever beam with additional constraints) can be written as follows:

$$\begin{pmatrix} K & B_c^\top & B^\top \\ B_c & O & O \\ B & O & O \end{pmatrix} \begin{pmatrix} u \\ \lambda_c \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ o \\ c \end{pmatrix}. \quad (12)$$

and the choice of B_c is realized in a way that the primal solution u is the same as u in the original (4). In other words, the additional set of constraints in B_c does not violate the primal solution linked to constraints stored in B . Thanks to the block-structure of B_c , the system may be reordered according to clusters 1 and 2 into

$$\left(\begin{array}{ccc|ccc|c} K_1 & O & B_{c,1}^\top & O & O & O & B_1^\top \\ O & K_2 & B_{c,2}^\top & O & O & O & B_2^\top \\ B_{c,1} & B_{c,2} & O & O & O & O & O \\ \hline O & O & O & K_3 & O & B_{c,3}^\top & B_3^\top \\ O & O & O & O & K_4 & B_{c,4}^\top & B_4^\top \\ O & O & O & B_{c,3} & B_{c,4} & O & O \\ B_1 & B_2 & O & B_3 & B_4 & O & O \end{array} \right) \begin{pmatrix} u_1 \\ u_2 \\ \lambda_{c,1} \\ u_3 \\ u_4 \\ \lambda_{c,2} \\ \lambda \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ o \\ f_3 \\ f_4 \\ o \\ c \end{pmatrix} \quad (13)$$

and consistently with the line partitioning rewritten into

$$\left(\begin{array}{c|c|c} \tilde{K}_1 & O & \tilde{B}_1^\top \\ O & \tilde{K}_2 & \tilde{B}_2^\top \\ \hline \tilde{B}_1 & \tilde{B}_2 & O \end{array} \right) \begin{pmatrix} \tilde{u}_1 \\ \tilde{u}_2 \\ \tilde{\lambda} \end{pmatrix} = \begin{pmatrix} \tilde{f}_1 \\ \tilde{f}_2 \\ \tilde{c} \end{pmatrix}. \quad (14)$$

Clearly, $\lambda = \tilde{\lambda}$ and $c = \tilde{c}$. One can interpret the system (14) as a problem solved by the TFETI method with two subdomains where matrices $\tilde{K}_1$ and $\tilde{K}_2$ are the

corresponding (cluster) stiffness matrices. Denoting $\tilde{\mathbf{K}} = \text{diag}(\tilde{\mathbf{K}}_1, \tilde{\mathbf{K}}_2)$, $\tilde{\mathbf{B}} = (\tilde{\mathbf{B}}_1, \tilde{\mathbf{B}}_2)$, $\tilde{\mathbf{f}}^\top = (\tilde{\mathbf{f}}_1^\top, \tilde{\mathbf{f}}_2^\top)$, and $\tilde{\mathbf{u}}^\top = (\tilde{\mathbf{u}}_1^\top, \tilde{\mathbf{u}}_2^\top)$, the system (14) is simplified into

$$\begin{pmatrix} \tilde{\mathbf{K}} & \tilde{\mathbf{B}}^\top \\ \tilde{\mathbf{B}} & \mathbf{O} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{u}} \\ \tilde{\boldsymbol{\lambda}} \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{f}} \\ \tilde{\mathbf{c}} \end{pmatrix}. \quad (15)$$

Using the steps and substitutions (here with tilde) applied in (4), (5), (6), and (7), we derive the dual Schur complement also for the HTFETI method in the form

$$\begin{pmatrix} \tilde{\mathbf{F}} & \tilde{\mathbf{G}} \\ \tilde{\mathbf{G}}^\top & \mathbf{O} \end{pmatrix} \begin{pmatrix} \tilde{\boldsymbol{\lambda}} \\ \tilde{\boldsymbol{\alpha}} \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{d}} \\ \tilde{\mathbf{e}} \end{pmatrix} \quad (16)$$

which is solvable by the same iterative solvers as in the TFETI method case. However the current coarse problem $\tilde{\mathbf{G}}^\top \tilde{\mathbf{G}} \in \mathbb{R}^{n_{\tilde{\mathbf{G}}} \times n_{\tilde{\mathbf{G}}}}$ is smaller because it newly depends on the number of clusters and not of subdomains. With the same meaning of parameter d as in (10), the size is given by

$$n_{\tilde{\mathbf{G}}} = (2 \text{ clusters}) \times (3 \text{ RBM}) = 6, \quad (17)$$

as illustrated in Figure 1.b right. Obviously, the beam problem used as an example does not contain a large number of subdomains. Nevertheless, it is ‘large’ enough to demonstrate how the size of the coarse problem is managed by the HTFETI method.

However, the HTFETI method does not bring only positive changes. For the same discretized and decomposed problem, the assembled system of linear equations in the HTFETI method is not as well-posed as the one assembled for the TFETI method. Therefore, one can expect the number of iterations to be slightly higher.

There are at least two important points that should be mentioned in contrast to the original TFETI method:

First, the orthogonal projection by $\tilde{\mathbf{P}} = \mathbf{I} - \tilde{\mathbf{G}} (\tilde{\mathbf{G}}^\top \tilde{\mathbf{G}})^{-1} \tilde{\mathbf{G}}^\top$ in the HTFETI case can be performed for the same number of subdomains efficiently, due to the locking effect of specific RBM (the coarse problem requires less memory for its storage and maintenance).

Second, the application of the generalized inverse of the stiffness matrix $\tilde{\mathbf{K}}$ (for more details see, e.g., Riha et al. (2016a)), the most expensive operation appearing in the operator $\tilde{\mathbf{F}}$, contains additional operations. To see the differences, the application of the HTFETI operator (matrix vector product)

$$\mathbf{v} = \tilde{\mathbf{F}}\mathbf{p} = \sum_{I=1}^{n_{\text{clust}}} \tilde{\mathbf{F}}_I \mathbf{p} = \sum_{I=1}^{n_{\text{clust}}} \tilde{\mathbf{B}}_I \tilde{\mathbf{K}}_I^+ \tilde{\mathbf{B}}_I^\top \mathbf{p} \quad (18)$$

written with the objects introduced for the TFETI method plus $\mathbf{B}_c$ is

$$\mathbf{v} = \underbrace{\sum_{I=1}^{n_{\text{clust}}} \mathbf{B}_{j:k} \mathbf{K}_{j:k}^+ \mathbf{B}_{j:k}^\top \mathbf{p}}_{\text{TFETI}} + \underbrace{\mathbf{B}_{j:k} \mathbf{R}_{j:k} \mathbf{R}_{j:k}^\top \beta_I - \mathbf{B}_{j:k} \mathbf{K}_{j:k}^+ \mathbf{B}_{c,j:k}^\top \boldsymbol{\mu}_I}_{\text{HTFETI}}. \quad (19)$$

The first product is the same as in the case of the classical TFETI method. The only difference is in the second and third products, which relate to the clusters. The meaning of β_I and $\boldsymbol{\mu}_I$ is described together with the special Schur complement $\mathbf{S}_{c,I} = \mathbf{G}_{c,I}^\top \mathbf{F}_{c,I}^{-1} \mathbf{G}_{c,I}$ in more detail, e.g., in Riha et al. (2016a). It is worth noting that always only one triplet of $\beta_I, \boldsymbol{\mu}_I$ and $\mathbf{S}_{c,I}$ relates to one cluster.

2.2 The local Schur complement method

TFETI solver processing can be divided into two stages: (i) preprocessing and (ii) solver run time. During the preprocessing stage the most time consuming tasks include assembling the distributed inverse matrix of the coarse problem $(\mathbf{G}^\top \mathbf{G})^{-1} = (\mathbf{R}^\top \mathbf{B}^\top \mathbf{B} \mathbf{R})^{-1}$ and factorization of the subdomain stiffness matrices $\hat{\mathbf{K}}_i$. While the coarse problem processing time is mainly given by the number of subdomains, the $\hat{\mathbf{K}}_i$ factorization times are given by the subdomain sizes. The solver run time stage executes the PCPG method and its execution time is therefore given by the number of iterations and the iteration time. The most time consuming part of a single iteration is the execution of the solve routine (forward and backward substitutions) of the sparse direct solver using the Cholesky decomposition of the $\hat{\mathbf{K}}_i$. This operation can take up to 95% of the iteration time (more detail can be found in Riha et al. (2016a)). The main focus of this paper is to describe a method to speed up this operation using accelerators.

Sparse data structures cannot take full advantage of accelerators which are equipped with high number of single instruction multiple data (SIMD) units. To reach the full potential of such architectures, a dense representation of sparse stiffness matrices $\hat{\mathbf{K}}_i$ and their Cholesky decomposition is required.

In the TFETI solver, prior to calling the solve routine with $\hat{\mathbf{K}}_i$, the vector of the LMs (the dual variables $\boldsymbol{\lambda}$) must be converted to primal variables using the gluing matrix $\mathbf{B}^\top$. The result of the solve routine (primal variables) has to again be converted into dual variables using $\mathbf{B}$. This operation appears during the initialization stage of the PCPG and then once at each iteration (in the regular conjugate gradient method it is equivalent to the matrix-vector multiplication with the system matrix). It contains two calls of sparse matrix vector multiplication from sparse BLAS (SpMV with $\mathbf{B}_i$), and one call of the solve routine of a sparse direct solver (e.g., the PARDISO solver (Kuzmin et al., 2013; Schenk et al., 2008, 2007)) - the action of generalized inverse $\mathbf{K}^+$. Instead of executing these three operations on sparse matrices, we can directly assemble the i -th contribution $\mathbf{F}_i$ to the global TFETI operator $\mathbf{F}$ from

$$\mathbf{A}_i = \begin{pmatrix} \hat{\mathbf{K}}_i & \mathbf{B}_i^\top \\ \mathbf{B}_i & \mathbf{0} \end{pmatrix} \quad (20)$$

by eliminating the primal variables and assembling the negative Schur complement $\mathbf{F}_i = \mathbf{B}_i \mathbf{K}_i^+ \mathbf{B}_i^\top = \mathbf{B}_i \hat{\mathbf{K}}_i^{-1} \mathbf{B}_i^\top$. In (20), the matrix $\hat{\mathbf{K}}_i$ is appropriately modified to $\mathbf{K}_i$, satisfying the equality $\hat{\mathbf{K}}_i^{-1} = \mathbf{K}_i^+$. We call this approach for replacing sparse operations with a multiplication by a single dense matrix the local Schur complement method.

An efficient approach to assemble the $\mathbf{F}_i$ matrix is to use an incomplete factorization method implemented in the PARDISO solver. When the factorization is stopped after the elimination of the (1,1) block of the system in (20), the Schur complement $-\mathbf{B}_i \hat{\mathbf{K}}_i^{-1} \mathbf{B}_i^\top = -\mathbf{F}_i$ will be available in the block (2,2). The numerical experiments presented in Table 4 show that the assembly of the $\mathbf{F}_i$

*Please note that when assembling the Schur complement the matrix $\mathbf{B}_i$ is used in its ‘‘condensed’’ form (only the non-zero rows are kept)

matrix is significantly slower than the factorization of the stiffness matrix. On the other hand, the multiplication by the dense Schur complement matrix on accelerators with high bandwidth memory is significantly faster than the sparse solve on the CPU. Before using the method, it is therefore necessary to evaluate the tradeoff between the preprocessing time which is executed just once, and the iterative solver run time in which the local Schur complements are processed repeatedly in every iteration. These results are presented in Tables 3 and 4.

2.2.1 The local Schur complement method for the HTFETI Operator In the previous section a method to accelerate the TFETI operator is described. However, in this paper we use primarily the HTFETI method. The application of the HTFETI operator is more complex, as shown in (19), and in order to get the contribution $\tilde{\mathbf{F}}_I \mathbf{p}$, the auxiliary variables β_I (rigid body motions amplitudes) and μ_I (LM) have to be calculated at each iteration. It requires two additional factorizations of objects; $\mathbf{F}_{c,I}$ and $\mathbf{S}_{c,I}$ per each cluster in the preprocessing.

The non-negligible feature of the HTFETI method is that the first product $\mathbf{B}_{j:k} \mathbf{K}_{j:k}^+ \mathbf{B}_{j:k}^\top \mathbf{p}$ in (19) can be executed on the accelerator (as described in the next section) independently of the remaining parts in (19), which can be performed concurrently on the CPU. The set of Schur complements $(j, j+1, \dots, k)$ belonging to the I -th cluster denoted as

$$\mathbf{F}_I = \sum_{i=j}^k \mathbf{F}_i = \mathbf{B}_{j:k} \mathbf{K}_{j:k}^+ \mathbf{B}_{j:k}^\top = \mathbf{B}_{j:k} \hat{\mathbf{K}}_{j:k}^{-1} \mathbf{B}_{j:k}^\top \quad (21)$$

is obtained one by one, the same way as in the TFETI method using (20).

3 Acceleration of the HTFETI Solver

In this section we present two approaches for improving HTFETI solver performance using accelerators. The first approach employs a sparse direct solver running on the accelerator, the second, and more suitable one, uses the LSC method.

3.1 Acceleration approaches

As described in Section 2, we need to solve linear systems with symmetric positive definite matrices. There are only a few suitable sparse direct solvers which support accelerators as required by HTFETI method. For the Intel Xeon Phi (Jeffers and Reinders, 2013, 2014, 2015), we use the Intel version of the PARDISO solver (Kuzmin et al., 2013; Schenk et al., 2008, 2007), which is included in the Intel Math Kernel Library (MKL (Intel Corporation, 2003–2017)). The solver is optimized for many-core coprocessor architecture by the vendor. For the GPU accelerators, there are, e.g., the SuperLU library, which is suitable for nonsymmetric systems only, and the SuiteSparse (Rennich et al., 2016) and PaStiX (Casadei et al., 2008–2017) libraries. These unfortunately provide acceleration for the factorization stage only. To utilize the GPU accelerators in HTFETI we need acceleration of the solve stage as well. Therefore the only option we found is the NVIDIA cuSolver library, which however is

not yet optimized from both the performance and memory utilization points of view. The library is part of the CUDA toolkit, documented by NVIDIA Corporation (2006–2017).

3.1.1 Direct sparse solve on Intel Xeon Phi (KNC) using MKL PARDISO To accelerate the TFETI and HTFETI computation one can offload the sparse solve with the subdomain stiffness matrices $\hat{\mathbf{K}}_i$ during the application of the operators $\mathbf{B}_i \hat{\mathbf{K}}_i^{-1} \mathbf{B}_i^\top$ to the coprocessor. This consists of several steps:

1. During the preprocessing, after the subdomain stiffness matrices are assembled, their CSR data are collected into three contiguous arrays to minimize the number of individual data transfers via the PCI-Express bus.
2. The data are offloaded to a coprocessor. Additional memory is allocated on the device (for input/output vectors, sparse solver auxiliary arrays, etc.).
3. Matrices are factorized on the coprocessor.
4. Within each iteration, the right hand side (RHS) vectors are collected into a single array and offloaded to the device, where the solve is performed within an OpenMP parallel region with up to 244 threads.

3.1.2 Direct sparse solve on NVIDIA GPU using cuSolver In the preprocessing stage of the ESPRESO solver, a new instance of the sparse cuSolver context is initialized for each subdomain. To overlap the kernel execution and data transfers, a set of CUDA streams is created, and each stream is associated with group of subdomains. After the setup of the cuSolver context, the reordering of the $\hat{\mathbf{K}}_i$ matrix using the Symmetric Approximate Minimum Degree Algorithm (SYMAMD (Amestoy et al., 1996)) provided by the cuSolver library is performed. This operation reduces the zero fill-in during the following symbolic and numeric Cholesky factorization. While reordering of the matrix is performed by the CPU, the factors are computed using the GPU accelerator and kept in the GPU memory.

In each PCPG iteration the RHS vector is reordered by the CPU and transferred to the GPU memory. The solve routine of the cuSolver is executed on the GPU. The solution vector is transferred back to the host memory and reordered. Due to the CUDA streams, everything is asynchronous with CPU processing.

3.1.3 The local Schur complement method The main disadvantage of the approach presented in the previous section is the usage of sparse data structures, which leads to an irregular memory access pattern. To make use of the full potential of the many-core architecture we use the local Schur complement method presented in Section 2.2. This enables us to replace the sparse solve with dense matrix-vector multiplication within each iteration of the PCPG solver. The workflow is similar to the case of the sparse solve (see Figure 2). The following steps differ according to the architecture of the accelerator.

Knights Corner coprocessors In the case of the Knights Corner coprocessor, the matrices of Schur complement $\mathbf{F}_i = \mathbf{B}_i \mathbf{K}_i^+ \mathbf{B}_i^\top = \mathbf{B}_i \hat{\mathbf{K}}_i^{-1} \mathbf{B}_i^\top$ are assembled on the host using the PARDISO solver, stored in a contiguous array, and the array is then offloaded to the accelerator.

Figure 2. Acceleration using the local Schur complement method.

Within each iteration of the CG-based solver the multiplied vectors are collected into a single array and offloaded to the device. The dense matrix-vector multiplication is performed within an OpenMP parallel region on a device with up to 244 threads. The offloaded computation is done asynchronously, and at the same time the host performs its computation (i.e., application of additional HTFETI operators or processing of subdomains that do not fit into coprocessor's memory). After multiplication the results are sent back to the host within a single contiguous array.

GPU acceleration In the case of the GPU accelerator, the total size of Schur complement matrices is first computed. Considering the available amount of device memory, an appropriate number of subdomains are marked for processing on the GPU using the LSC method, while the rest of them remain on the CPU. According to the solver configuration, the subdomains on the CPU can be processed either using the LSC method, or with a sparse direct solver. The Schur complement F_i is then assembled for particular marked subdomains in parallel on the CPU, using the PARDISO solver.

To perform the fast symmetric matrix-vector multiplication using the cuBLAS library (NVIDIA Corporation, 2006–2017), and to use the device memory efficiently, we combine the Schur complements of the two neighboring subdomains in the following manner. If the size of F_i is greater than the size of F_{i+1} , the upper triangular part of F_i is preserved in the original array, and the lower part is overwritten by the lower part of F_{i+1} . In the opposite case, when the size of F_i is lower than the size of F_{i+1} , the larger array with the lower triangular part of F_{i+1} is preserved and the upper part is overwritten by the upper part of F_i . In cases where the size of both matrices is equal, a new larger array is allocated to fit both triangular matrices including their diagonals, and filled with the upper part of F_i and the lower part of F_{i+1} .

The pointer to the first element of each triangular matrix and its leading dimension is stored along with the array and used during the cuBLAS method call. After the Schur complements are combined, the shared arrays are transferred to the GPU memory. The GPU memory and the pinned host memory is also preallocated for the corresponding vectors of the multiplication.

In each PCGP iteration, before the $F_i p_i$ multiplication, the p_i vector is transferred from the pinned host memory to the device memory using an asynchronous memcpy operation in a separate CUDA stream from a streams pool. The resulting vector is transferred back to the pinned host memory in an analogous manner.

In both cases, converting sparse data structures to dense ones enables us to use optimized and vectorized dense BLAS routines with a regular and coalesced memory access pattern. This is essential in order to be able to utilize accelerators' fast memories and wide SIMD units. As will be seen from the numerical experiments, the iteration time can be significantly reduced in comparison with the original CPU code. On the other hand, the preprocessing time is increased, since the Schur complement computation is more demanding than the factorization of the sparse matrix. This makes the method more suitable for problems requiring a large number of PCGP iterations, e.g. transient or ill-conditioned problems.

3.1.4 Acceleration of the preconditioner application The Dirichlet preconditioner (Farhat et al., 1994b) has the form

$$F^{D-1} = \sum_{s=1}^{N_s} B_s \begin{pmatrix} 0 & 0 \\ 0 & S_s^{bb} \end{pmatrix} B_s^\top,$$

where S_s^{bb} is a dense Schur complement matrix

$$S_s^{bb} = K_s^{bb} - (K_s^{ib})^\top (K_s^{ii})^{-1} K_s^{ib}.$$

Here i are the indices of the local stiffness matrix K_s associated with interior degrees of freedom and b represents

Table 1. Acceleration of the Dirichlet preconditioner on Intel Xeon Phi 7120p. For comparison we also present the performance of the LSC method.

	Intel Xeon E5-2680v3 time [s]	Intel Xeon Phi 7120p time [s]	speedup
FETI operator	0.125 s	0.062 s	2.03
Dirichlet prec.	0.075 s	0.043 s	1.75

Figure 3. Load balancing of the iterative solver between the CPU (2x Xeon E2-2680v3) and the MIC (2x Xeon Phi 7120P)

indices of the boundary degrees of freedom. Since the matrix of the preconditioner is dense, it is suitable to offload its application to the coprocessor together with the action of the HTFETI operator. The preconditioner blocks are assembled using the host CPU during the preprocessing phase, stored in a contiguous array, and copied to the coprocessor. Then, during each iteration the `gemv` routine from the MKL is called to apply the preconditioner.

3.1.5 Load balancing While the offloaded computation is being performed, the host processor can simultaneously continue its work. It can perform tasks which are independent of the output of the coprocessor's computation (mainly in the case of the HTFETI method) or apply its portion of the blocks of the system matrix. The portion of matrix-vector multiplication processed by the coprocessor and host can easily be adjusted after every iteration using the following formula:

$$r_d^{\text{new}} = \frac{r_d^{\text{old}} t_h}{r_d^{\text{old}} t_h + t_d (1 - r_d^{\text{old}})},$$

where r_d is the ratio of work done by the device and t_h, t_d are computational times on the host and device respectively, in the previous iteration. In order to avoid expensive transfers of matrices between host and device after each iteration, the matrix data are duplicated on both. Using this simple approach we can automatically adjust workload distribution at the price of higher memory requirements.

3.2 Architecture evaluation

In Table 3 and Table 4 we present the processing times of the sparse direct solver and the local Schur complement method, comparing the selected architectures presented in Table 2. The problem sizes of the particular tests were selected to occupy the same amount of accelerator memory that was limited by the memory size of one NVIDIA Tesla K80 chip (12 GB). The key operations that are required by the HTFETI

solver are presented. The following observations can be made from these tables: (i) MKL PARDISO on all Intel architectures performs significantly better than cuSolver on NVIDIA architectures; (ii) in the case of linear elasticity, the Xeon Phi 7210 is the fastest for both the factorization and solve, with a speedup of up to 2x with respect to the Xeon E5-2680v3, whereas in other cases, the sparse solvers on accelerators brought no speedup; (iii) the LSC method is fastest on the Tesla P100 with speedup up to 5.3x due to its high memory bandwidth. The difference of solve runtime follows the difference in memory bandwidth between the Tesla P100 and the Xeon Phi 7210, since the most time-consuming part performs the memory bound GEMV operation.

4 Memory efficient implementation

The most memory consuming objects of the FETI solvers in general are the Cholesky factors of the stiffness matrices $\mathbf{K}^+$. To eliminate these objects we propose two techniques in this section: (i) the repeated factorization technique and (ii) the iterative solver technique. Both techniques are able to reduce memory consumption for the cost of additional per iteration time of the PCPG solver.

4.1 The repeated factorization technique

This technique allows the user to select a set of subdomains for which the factorization is not performed during the preprocessing, but is performed within the action of the HTFETI operator. This means that in every PCPG iteration, both the factorization and the solve routine of MKL PARDISO are performed, and at the end the Cholesky decomposition objects are deleted. From a performance point of view the factorization is approximately 10 times slower for linear elasticity and 20 times slower for heat transfer than the solve routine. The effect of the repeated factorization is shown in Figure 4 where the number of kept factors goes from 100 % (all factors are kept) to 85 %. The single iteration time increases from 1.66 s to 4.87 s, and the amount of saved memory is 2.8 GB. If one keeps no factors in the memory, the solver will save 16 GB of RAM and the single iteration time will be 15.7 s (factorization and solve runtime).

4.2 The iterative solver technique

The second technique uses the iterative CG solver instead of the sparse direct solver, therefore no preprocessing is required. The disadvantage of this method is that its performance is data dependent. The convergence of the iterative solver depends on the condition number of subdomain matrices. No preconditioner is used in order to keep the memory profile as low as possible.

Since the subdomain matrices for the 3D heat transfer (Laplace equation) are well conditioned, this method is more efficient for such problems than repeated factorization. Using this method we were able to solve the largest possible problem yet with our FEM package: 223 billion unknowns on the 17,573 compute nodes of Titan, approximately 12.8 million unknowns per compute node with 32 GB RAM. Please note that this is a problem with an unstructured mesh where assembled matrices are kept in the memory. In total

Table 2. Key properties of the hardware architectures selected for the paper. Note: SP - single precision, DP - double precision; [1] only one GPU chip of the dual chip Tesla K80 accelerator; [2] PCI Express version of the Tesla P100 accelerator for PCIe-based servers.

	Fabrication process [nm]	Clock frequency [GHz]	Number of cores	Peak floating point performance SP/DP [GFLOPS]	Peak power consumption [W]	Perf. per Watt SP/DP [GFLOPS/W]	Theoretical Memory Bandwidth [GB/s]	Memory type
Intel Xeon E5-2680v3 (Intel Corporation, 2017a)	22	2.5	12	960 / 480	120	8.0 / 4.0	68	DDR4
Intel Xeon Phi 7120p (Intel Corporation, 2017b)	22	1.24	61	2420 / 1210	300	8.1 / 4.0	352	GDDR5
Intel Xeon Phi 7210 (Intel Corporation, 2017c)	14	1.3	64	5325 / 2662	215	24.8 / 12.4	102 / 400	DDR4/MCDRAM
NVIDIA Tesla K80 (1 chip ^[1]) (NVIDIA Corporation, 2017b)	22	0.56	1597 SP / 533 DP	4365 / 1455	150	29.1 / 9.7	240	GDDR5
NVIDIA Tesla K20X (Titan) (NVIDIA Corporation, 2017a)	28	0.732	2688 SP / 896 DP	3950 / 1310	235	16.8 / 5.6	250	GDDR5
NVIDIA Tesla P100 (PCIe ^[2]) (NVIDIA Corporation, 2017c)	16	1.328	3584 SP / 1792 DP	8345 / 4217	250	33.4 / 16.9	720	HBM2

Table 3. Performance of the sparse solve on various many-core architectures. Solve times are measured for 100 iterations of the PCPG solver. Note: [1] only one GPU chip of the dual chip Tesla K80 accelerator is used; [2] values for the Tesla P100 are extrapolated due to the excessive memory consumption of the cuSolver; [3] with respect to MKL PARDISO sparse solve on CPU.

			Intel Xeon E5-2680v3		Intel Xeon Phi 7120P		Intel Xeon Phi 7210		NVIDIA Tesla K80 (1 chip ^[1])		NVIDIA Tesla P100 ^[2]		All architectures
	# of sub-domains	DOFs per subdomain	preprocess [s]	solve [s]	preprocess [s]	solve [s]	preprocess [s]	solve [s]	preprocess [s]	solve [s]	preprocess [s]	solve [s]	solve speedups ^[3]
Heat transfer problem													
TFETI	125	8000	1.23	5.54	7.75	7.04	1.36	8.14	26.50	92.02	20.79	135.54	0.8/0.7/0.06/0.04
	512	2744	1.48	4.43	23.27	6.45	1.6	6.78	15.25	123.37	12.31	120.15	0.7/0.7/0.04/0.04
HTFETI	125	8000	1.22	6.18	7.31	7.74	1.38	7.67	26.46	92.99	22.82	139.29	0.8/0.8/0.07/0.04
	512	2744	1.21	5.83	22.97	7.92	1.57	6.84	15.35	122.57	12.46	121.44	0.7/0.9/0.05/0.05
Linear elasticity problem													
TFETI	125	5184	0.97	5.38	7.77	6.49	0.69	3.45	18.71	75.14	15.16	100.75	0.8/1.6/0.07/0.05
	512	2187	1.15	5.68	24.94	7.84	0.94	3.50	17.27	130.52	13.52	117.42	0.7/1.6/0.04/0.05
HTFETI	125	8000	0.97	5.95	8.50	6.95	0.76	3.52	18.93	75.64	14.70	82.14	0.9/1.7/0.08/0.07
	512	2187	1.17	7.67	27.07	9.56	0.86	3.92	17.18	138.20	13.72	130.26	0.8/2.0/0.06/0.06

Table 4. Performance of the local Schur complement method on selected architectures. Solve times are measured for 100 iterations of the PCPG solver. Note: [1] with respect to MKL PARDISO sparse solve on CPU.

			Intel Xeon E5-2680v3 MKL PARDISO		Intel Xeon E5-2680v3 LSC		Intel Xeon Phi 7120P LSC		Intel Xeon Phi 7210 LSC		NVIDIA Tesla K80 (1 GPU) LSC		NVIDIA Tesla P100 LSC		All architectures
	# of sub- domains	DOFs per subdomain	preproce- ssing [s]	solve [s]	preproce- ssing [s]	solve [s]	solve [s]	preproce- ssing [s]	solve [s]	solve [s]	solve [s]	solve [s]	solve [s]		solve speedups ^[1]
Heat transfer problem															
TFETI	125	24389	5.32	27.3	142.05	19.01	15.57	57.57	10.19	16.08	5.20	5.20	5.20		1.4/1.8/2.7/1.7/5.3
	512	6859	3.82	21.4	49.42	16.42	10.25	32.14	9.71	14.70	5.29	5.29	5.29		1.3/2.1/2.2/1.5/4.0
HTFETI	125	24386	5.32	30.5	139.68	22.81	15.96	57.67	11.37	17.14	6.46	6.46	6.46		1.3/1.9/2.7/1.8/4.7
	512	6859	3.8	26.0	45.49	21.53	10.68	31.98	10.62	16.72	7.49	7.49	7.49		1.2/2.4/2.5/1.6/3.5
Linear elasticity problem															
TFETI	125	12288	3.07	20.2	92.29	16.48	12.9	48.79	6.87	12.55	4.12	4.12	4.12		1.2/1.6/2.9/1.6/4.9
	512	3993	2.31	20.4	55.70	18.18	11.30	34.23	8.09	16.18	5.85	5.85	5.85		1.1/1.8/2.5/1.3/3.5
HTFETI	125	12288	3.08	20.9	92.62	18.65	14.15	48.98	6.18	13.54	5.14	5.14	5.14		1.1/1.5/3.4/1.5/4.1
	512	3993	2.31	21.2	55.99	22.36	11.50	34.28	9.02	18.12	7.93	7.93	7.93		0.9/1.8/2.4/1.2/2.7

we are using approximately 560 TB of the CPU memory (we cannot utilize the GPU memory now). The size can potentially be 3 times greater when executed on machines like Sequoia with 1.57 PB of memory (Lawrence Livermore National Laboratory, LLNL, 2017) or the K computer

with 1.41 PB of memory (RIKEN Advanced Institute for Computational Science, AICS, 2017).

Large scale memory efficient evaluation. Figure 8 (bottom) shows the weak scalability evaluation of the HTFETI solver for the 3D heat transfer problem. This test uses the iterative solver technique presented in the previous

Figure 4. Evaluation of the repeated factorization technique on 1000 nodes of the OLCF Titan machine for 3D linear elasticity.

Table 5. The maximum problem that can be solved on the Titan supercomputer with ESPRESO. Note: [1] Depends on the condition number of subdomain matrices.

Heat Transfer problem (Laplace equation in 3D)	single iteration time [s]	the largest possible problem [billion unknowns]
Factorization in preprocessing	2.5	124
Factorization + LSC on GPU	3.5	136
Iterative solver technique	18 ^[1]	223
Repeated factorization	34	223

section. One can see that the CG iterative solver takes up the majority of time and we have significantly longer per-iteration time, approximately 18 s, which is caused by the HTFETI operator. With respect to the scalability, we can see that both parallel scalability (see single iteration time), and numerical scalability (see number of iterations for different problem sizes), perform as expected and are very good.

Finally Table 5 shows a comparison of the presented techniques and (i) a general FETI approach (Cholesky decomposition in preprocessing), which is able to solve 124 billion unknowns, (ii) the combination of the previous approach plus utilization of the GPU memory by LSC, which increases the size of solvable problem by 10 %, and (iii) the presented techniques themselves, which can solve 223 billion unknowns.

To sum up, we can state that the proposed memory efficient technique allows us to solve 1.8 times larger problems (124 vs 223 billion unknowns) on the same supercomputer. However, the cost is 7.2 to 13.6 times slower solution time (2.5s vs 18s – 34s), depending on how well conditioned the subdomain matrices are.

5 Improving energy efficiency using dynamic tuning

In this section we present how to reduce the energy consumption of a supercomputer while running the ESPRESO library. Our approach is based on dynamically tuning selected hardware parameters, called *tuning parameters*, during the application runtime. The tuning parameters are: (i) the CPU core frequency using Dynamic Voltage and Frequency Scaling (DVFS), (ii) the CPU uncore frequency[†] (Intel Corporation, 2012) and (iii) the number of OpenMP threads. Tuning itself is not performed by ESPRESO, but using a set of external tools. The concept of dynamic tuning is introduced by the

H2020 READEX (2018) project and is described in more by Schuchart et al. (2017).

In short, the process of dynamic tuning is performed in following three steps:

- *Step 1:* identify and annotate the significant regions of an application (see Figure 5 for regions that have been used for tuning of the ESPRESO library).
- *Step 2:* find the optimal settings for the tuning parameters for each of these regions to minimize energy consumption[‡].
- *Step 3:* dynamically switch to the optimal settings of tuning parameters during the application runtime.

Step 1 is done manually by a code developer. The goal is to identify the regions with different workloads (compute bound, memory bound, I/O bound, communication bound, etc.) and annotate them in the source code. Annotated regions, also called *significant regions*, are evaluated in step 2, which is called the analysis phase. During the analysis, the application is executed multiple times with all combinations of the tuning parameters to find the optimal settings for each significant region.

After manual annotation, the analysis is performed automatically using our in-house tools MERIC (performs parameter tuning and energy measurements) and RADAR (analyzes the measurements and creates the tuning model), see Vysocky et al. (2017). The optimal settings are then saved into a file called *tuning model*, which is used in step 3. Finally, the production runs are done in step 3, in which the dynamic tuning is performed by the MERIC tool. At application startup, MERIC reads the tuning model from the file, and at the beginning of each significant region it changes the tuning parameters to the optimal settings for that particular region. At the end of the region the settings are changed back to the optimal ones for the parent region.

We evaluated the effect of dynamic tuning on the Salomon supercomputer equipped with two Intel Xeon E5-2680v3, two Intel Xeon Phi 7120p, and 128GB RAM per node (IT4Innovations National Supercomputing Centre, IT4I, 2017). The potential of this approach is presented in Table 6. Results were measured using a heat transfer problem with 3.5 million DOF generated by the mesh generator (see Figure 6 d.). We used this rather small problem to show that this approach can (i) save energy; up to 33 %; (ii) reduce processing time; up to 22 %; and (iii) improve the strong scalability. Please note, that for 1 to 16 nodes, the energy savings are paid for with extra processing time. However for 32 to 128 nodes both energy and time savings are achieved due to fact that the workload per node is significantly smaller, most of the data fits into L3 caches, and some significant regions use a smaller number of cores.

[†]The uncore region of the Intel Xeon E5-2600v3 CPUs include QPI controllers, L3 cache, a snoop agent pipeline, an on-die memory controller, etc.

[‡]The energy consumption of the CPU and DDR memory is measured using Intel RAPL counters at rate of 1000 samples per second. The energy consumption of the remaining hardware of the compute node is used as a baseline. The baseline of a compute node of the IT4I Salomon supercomputer is between 70-85W based on node utilization. We use a simple linear model to estimate the baseline based on the energy consumption of its CPUs.

Figure 5. Significant regions of the ESPRESO library used for dynamic tuning in order to reduce the energy consumption.

Table 6. Energy savings analysis for the strong scalability test of the ESPRESO library when running the cube benchmark (see Figure 6 d.).

number of nodes	no tuning		dynamic tuning		total savings	
	time [s]	energy [kJ]	time [s]	energy [kJ]	time [%]	energy [%]
1	129.3	37.2	143.7	34.3	-11.1	8.0
2	68.6	39.8	75.5	36.5	-10.1	8.2
4	33.2	38.0	35.6	34.3	-7.2	9.8
8	21.5	49.6	22.9	44.7	-6.8	9.9
16	13.4	60.8	14.3	53.5	-6.3	12.1
32	7.7	62.2	7.2	50.6	6.1	18.7
64	4.0	69.9	3.6	52.4	9.3	25.0
128	3.6	119.6	2.8	80.1	22.2	33.0

6 Parallel scalability results

In this section we present large scale tests generated from a built-in mesh generator which is able to generate extremely large meshes with geometric decomposition (cubical problems decomposed into cubical domains, see Figure 6 d). This tool is used for all huge scalability tests of the HTFETI solver in this paper because it is able to generate multi-billion unknown problems in tens of seconds. In addition we use three real-world problems generated by Ansys and ELMER.

6.1 Large Scale Tests with Mesh Generator

We used two types of problems/physics for scalability evaluation: heat transfer (3D Laplace equation) and 3D linear elasticity, both widely used in structural mechanics. Please note, that in order not to consume too many core-hours, the stopping criteria for the PCPG solver was set to 10^{-3} for all large scale tests.

Large Scalability Tests. We evaluated both the strong and weak scalability of the HTFETI solver on up to 17,576 compute nodes of the Titan supercomputer. Figure 7 shows the strong scalability for a 20 billion unknowns heat

transfer problem and an 11 billion unknowns linear elasticity problem, respectively. The figure shows that due to the numerical properties of the HTFETI solver, the number of iterations decreases as problem size per compute node/MPI process/HTFETI cluster decreases. Therefore we can state that due to the combination of numerical and parallel scalability in our implementation, we have achieved super-linear scaling.

Figure 8 demonstrates the weak scalability of the heat transfer problem on the full OLCF Titan machine. The top chart uses all PARDISO for CPU memory and LSC for GPUs (causing longer preprocessing times) and solves up to 136 billion unknowns. The bottom chart uses the memory efficient iterative solver technique, and it is able to solve up to 223 billion unknowns. In both cases we can observe almost flat scalability. Figure 9 shows a similar comparison for 3D linear elasticity. The top chart is the smallest problem test but has the fastest solution, and uses only PARDISO on the CPU. The middle chart is the test using PARDISO on the CPU and LSC on the GPU, which increases the maximum solvable problem size to 91 billion unknowns. If a repeated factorization technique with 90% of factors kept in memory is applied, the maximum solvable problem size is 100 billion unknowns (bottom chart). In none of these tests do we use an accelerator to increase the performance, but rather to increase the problem size.

6.2 Real World Structural Mechanics Problems

The Ansys Workbench Benchmark. To evaluate the solver on complex geometry we created a 300 million unknowns benchmark shown in Figure 6 a). It is a 3D elasticity benchmark with the following material properties: Young's modulus $E = 2 \times 10^{11}$ Pa, Poisson's ration $\mu = 0.3$, density $\rho = 4900$ kg/m³, loaded by standard Earth gravity $g = 9.8066$ ms⁻² and additional external forces. The same configuration is also used for other linear elasticity benchmarks.

We decomposed the mesh into 512, 1024, 2048, 4096, and 8192 clusters. Each MPI process owns one cluster and there are 22 MPI processes per node. We used the Salomon supercomputer mentioned in Section 5.

We compared TFETI and HTFETI to show that for a smaller number of MPI processes, TFETI with better convergence is more efficient. Due to the limited parallel scalability of TFETI (caused by the coarse problem) HTFETI is more efficient for larger numbers of clusters.

Intel Xeon Phi Acceleration. The model used for this benchmark is a 120 million unknowns linear elasticity problem shown in Figure 6 b). Here we compare the performance of two Xeon E5-2680v3 and two Xeon Phi 7120p per node. The CPU is using MKL PARDISO, while the MIC is using LSC. The Dirichlet preconditioner is also accelerated. The table presents two experiments with decompositions into 128 and 512 subdomains per MPI rank. The optimal decomposition is into 128 subdomains, and speedup is 2.04 times. For these tests, load balancing between the CPU and the accelerator was enabled.

The ELMER FEM Benchmarks. For this test we used the Winkel benchmark, which is part of the ELMER

Figure 6. A set of benchmark problems used in this paper for structural mechanics. Real world problems generated by Ansys Workbench a) a 300 million unknowns problem; b) a 120 million unknowns problem and scalability benchmarks c) the Winkel benchmark in ELMER and d) the Massively Parallel Benchmark from ESPRESO.

Figure 7. Results of the strong scalability test for heat transfer and linear elasticity problems with 20 and 11 billion unknowns.

Figure 8. Results of the weak scalability test for the heat transfer problem. Top: a problem with up to 130 billion unknowns solved by a combination of PARDISO on the CPU and LSC on the GPU. Bottom: a problem with 223 billion unknowns solved using the iterative solver for subdomain matrices.

Figure 9. Results of the weak scalability evaluation for the linear elasticity problem with up to 70, 92 and 100 billion unknowns. Top: PARDISO only; middle: PARDISO and LSC on the GPU; bottom: PARDISO with repeated factorization (90%) and LSC on the GPU.

Table 7. Results of the performance evaluation of the Intel Xeon Phi acceleration of the real world problem.

# of domains per MPI rank	# of iterations	solver runtime E5-2680v3 [s]	solver runtime Phi 7120p[s]	speedup
128	295	88	42.9	2.04
512	363	96.5	54.9	1.78

Figure 10. Results of the strong scalability evaluation for a 3D linear elasticity problem with 300 million unknowns, see Figure 6 a).

Figure 11. Results of the weak scalability evaluation for 3D linear elasticity problems with up to 745 million unknowns generated by ELMER, including a comparison of the HTFETI solver in ESPRESO, the FETI solver in ELMER, and the ML multigrid solver from Trilinos. All solvers are called directly from ELMER.

package. The large problem size was achieved by the mesh-multiplication technique implemented in ELMER. We compared our HTFETI solver with the FETI solver implemented in ELMER, and the ML multigrid solver from Trilinos (Heroux et al., 2005). For smaller problems the Trilinos ML solver is faster. However, the scalability of the HTFETI solver is better for large problems. The results are shown in Figure 11, with achieved speedup of 4.5 times with respect to Trilinos ML, and 2.45 times with respect to ELMER FETI.

7 Conclusions

This paper presents the ESPRESO library and its FEM preprocessing package as well as the modern HTFETI solver. We have demonstrated techniques that can utilize the fast HBM memory of the latest NVIDIA Tesla P100, bringing a speedup of 5.3x for TFETI / 4.7x for HTFETI and 4.9x for TFETI / 4.1x for HTFETI for heat transfer (the 3D Laplace equation) and linear elasticity respectively, when compared to Intel Haswell Xeon E5-2680v3. The difference between the Tesla P100 and Xeon Phi 7210 is mainly caused by different memory bandwidths, since the bandwidth of the P100 is 1.8 times higher. We also have to take into account that the 7210 must do all the work, while the P100 has a CPU to perform some tasks.

An essential part of our HTFETI solver is its numerical and parallel scalability. The solver achieved superlinear strong scaling from 2744 compute nodes to 17,576 compute nodes for both linear elasticity and heat transfer problems.

We have also presented new techniques that push the boundaries of the HTFETI solver towards larger problems with unstructured meshes. The two techniques can increase the problem size that can be solved by a factor of 1.8, to 223 billion unknowns on 17,576 nodes with 560 TB of memory. These approaches have been demonstrated using weak scalability tests.

Using the ESPRESO FEM tools we can solve real-world problems with complex meshes from Ansys Workbench, ELMER, and OpenFOAM. We have demonstrated the superlinear scalability with a combination of TFETI and HTFETI solvers. For these problems, we have also presented the load-balancing technique, and the accelerated Dirichlet preconditioner.

We have also shown that by dynamically tuning the hardware parameters the ESPRESO library can reduce energy consumption by up to 33 %, and save up to 22 % of runtime, while also improving its strong scalability.

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Declaration of conflicting interests

The Authors declare that there is no conflict of interest.

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