



Parallel, fully automatic *hp*-adaptive 2d finite element package

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Abstract

This paper presents a description of par2Dhp—a 2D, parallel fully automatic *hp*-adaptive finite element code. The parallel implementation is an extension of the sequential code 2Dhp90, which generates fully automatic *hp*-approximations for solutions of various boundary value problems. The presented work addresses parallelization of each stage of the automatic *hp*-adaptive algorithm, including decomposition of the computational domain, load balancing and data re-distribution, a parallel frontal solver, and algorithms for parallel mesh refinement and mesh reconciliation. The application was written in Fortran 90 and MPI, and the load balancing is done through an interface with the Zoltan library. Numerical results are presented for the model L-shape domain problem, and a highly anisotropic heat conduction (battery) problem from Sandia National Laboratories.

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1. Introduction

1.1. *hp*-Finite elements

In the most flexible version of the Finite Element Method, elements may have a locally varying element size h , and polynomial order of approximation p . A rationale for using *hp* elements may have different origins. In singularly perturbed problems, e.g. elastic thin-walled structures, elements with $p \geq 5$ allow for

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avoiding locking [27]; for wave propagation problems, high order elements help to minimize the dispersion (pollution) error [1]. At the same time, small elements are necessary to capture geometrical details present in real world problems. The *hp* elements allow for combining small elements of lower order with large elements of high order in the same mesh. The main motivation of this work, however, comes from using *hp*-adaptive discretizations where the distribution of element size *h* and order *p* is optimized to deliver the smallest possible problem size (number of *degrees-of-freedom* (d.o.f.)) meeting a prescribed error tolerance criterion. After over a decade of research, a fully automatic, problem independent, *hp*-strategy has been constructed [7–9] that delivers a sequence of optimally refined *hp* meshes and *exponential convergence*—the error decreases exponentially fast, both in terms of problem size and actual CPU time [7–9].

The presented work is motivated with solutions of large Electromagnetic scattering problems involving geometrical singularities (diffraction on edges and points) and scattering from resonating cavities, see e.g. [4]. Resolution of geometric singularities in 2D requires many levels of *h*-refinements (the ratio of the smallest to largest elements may be 10^{-6}). Additionally, resolution of boundary layers (skin effects in EM computations) and edge singularities in 3D calls for anisotropic mesh refinements.

1.2. Parallelization of adaptive methods

Parallelization of adaptive codes is difficult. Most implementations for distributed memory parallel computers are based on Domain Decomposition (DD) concepts. The domain of interest is partitioned into sub-domains with each of the sub-domains delegated to a single processor. To maintain scalability, only local sub-domain information about the mesh may be stored in each processor's memory. The situation is different for Boundary Element (BE) computations where high order discretizations result in a “small” but dense stiffness matrix, and a copy of a mesh supporting data structure can be stored on each processor; the main effort then is directed at parallelizing the integration of element matrices and a linear solver [30].

Among major undertakings to develop a general infrastructure to support DD based parallelization of PDE solvers, one has to list first of all the Sierra Environment [28,11–13] developed by Sandia National Labs. Designed to support *h*-adaptivity, the Sierra framework has been used to parallelize several FE codes developed at Sandia [13]. The Sierra environment allows for an arbitrary domain partitioning of a current mesh but it does not support anisotropic mesh refinements.

General environments to support local mesh refinements have been developed in the groups of Joe Saltz, see e.g. [16], Scott Baden, see e.g. [20] and, more recently, Kathy Yelick [32,25]. None of them, unfortunately, turned out to be applicable directly to our *hp* codes.

The only parallel *hp* codes that we are aware of, have been developed by Joe Flaherty at RPI [26] in the context of Discontinuous Galerkin (DG) methods, and Abani Patra at SUNY at Buffalo [18,3,17].

In our first attempt to develop a parallel *hp* code, we managed to develop only a parallel two-grid solver for *hp* meshes and 2D Maxwell equations [2], but we failed miserably with the parallelization of the actual code. This failure motivated us to develop new data structures better suited for parallelization [5,6].

The presented concept of parallelization is based on the assumption that in the DD based parallel code, each of the processors is executing the sequential code with only minimal upgrades added (to support communication between sub-domains). In order to maintain the load balance during refinements, the mesh has to be frequently repartitioned, and the data structure arrays supporting the new sub-domains, must be generated. In simple terms—elements and nodes are assigned new numbers. This requires reproducing horizontal information, like element-to-nodes connectivities with new numbers, a nightmare for adapted meshes with hanging nodes. To avoid the problem, the new *hp* data structures include the horizontal information *only* for the initial mesh elements and nodes. All other information on elements and nodes resulting from *h* or *p*-refinements is reproduced from *nodal trees* relating parent and children nodes only *vertically*. Contrary to the horizontal information, the trees are much easier to regenerate.

The use of trees has forced us to partition the domain using the initial mesh elements only. In this context, the complexity of the DD step and data regeneration is only slightly higher than for static FE meshes with classical data structures.

An alternative technique, better suited for parallel implementation, was presented in [18]. There, the elements and nodes are assigned individual keys (identifiers) with the whole connectivity information specified in terms of the assigned keys. The actual information about the mesh entities is stored using the hash tables, with the definition of the hash function based on the space filling curve technique. Domain Decomposition does not alter then the connectivity information. Hash functions are redistributed by “cutting off” segments of the space filling curve.

1.3. Wave propagation problems

The main motivation for developing a parallel version of the *hp* methodology is the solution of large wave propagation problems. The very first issue in addressing this class of problems is the resolution of the wave form of the solution. High order methods turned out to be the most powerful tool in minimizing the *dispersion error*, and other preasymptotic convergence range artifacts classified in the FE community under the common name *pollution error*. As mentioned in the beginning, resolution of complex geometries requires the use of very nonuniform meshes. Employing the same, high order of approximation for both small and large elements is very inefficient and unnecessary. Only the *hp* elements allow for adjusting the element order to its size, and satisfaction of dispersion error criteria in an efficient way [1].

Another issue is rooted in the Galerkin method itself which, for time-harmonic wave propagation problems, becomes stable only asymptotically. The actual *approximation error* becomes equal to the *best approximation error* characterizing approximation properties of a mesh, only for sufficiently fine meshes. Entering the asymptotic region of convergence depends upon wave number k , and occurs later with larger k , i.e. the “meeting point” of the approximation and best approximation error occurs at a smaller level of the best approximation error with growing wave number k . Once in the asymptotic convergence region, the Galerkin method becomes stable, and further mesh optimization can then be used to capture geometric singularities or near resonance behavior. The *hp* strategy discussed in this paper is based on an interaction between a coarse and fine mesh. The fine mesh is obtained from the coarse mesh through a global *hp*-refinement, where each element of the coarse mesh is broken into 4 sons in 2D or 8 sons in 3D, and order of approximation is uniformly raised by one. In other words, the fine grid is $\frac{1}{2}h$ and $p + 1$ of the coarse. This results in 30–40 times larger number of d.o.f. in 3D case. One of the main points about our strategy is that *only the fine mesh must be in the asymptotic convergence region*; the solution on the coarse mesh may be completely meaningless (hundreds of percent of error) when the mesh optimization process begins, compare [8,9]. The difficulty is that in this situation, the main engine of making the strategy possible—our two-grid solver used to solve the fine grid problem [21], fails to converge. It is only after the coarse grid enters the asymptotic convergence range, that the two-grid iterations become effective. On the practical side, this implies that in the beginning of the mesh optimization process we are forced to use the direct solver for both the coarse and fine mesh solves, and only later we can switch to the orders of magnitude more efficient two-grid iterations. This motivates the development of the parallel version of the algorithm, based on a direct solve for both coarse and fine grids, presented in this contribution.

1.4. Challenges

Besides the DD and data structure regeneration issues, the parallelization of our *hp* codes involved two more main challenges—parallelization of the linear solvers, and mesh reconciliation. Even if the decision on optimal *hp*-refinements is made fully in parallel (which may be impossible, as we will discuss later), the

execution of optimal *hp*-refinements on the sub-domains results in meshes that are globally illegal. The *hp* meshes supported by our codes satisfy two main regularity assumptions—they must be 1-irregular (no multiply constrained nodes are allowed) and they must satisfy the *minimum rule* (order for edges is set to the minimum of orders for the neighboring elements). Enforcing both regularity assumptions *a-posteriori*, is commonly called the *mesh reconciliation*, and presents one of major challenges for the parallel implementation of the *hp* methods discussed in this paper.

The current implementation does not support mesh unrefinements. This will be essential for time dependent and non-linear problems, or for solving a sequence of similar problems with different load data.

2. Flowchart for the parallel *hp* algorithm

The input data for the parallel version of the *hp* code includes the following items.

- *Geometry* of the domain is prescribed within the *Geometry Modeling Package* [31]. A 2D domain is described as a union of curvilinear GMP “rectangles” forming a FE-like mesh. Each of the rectangles is identified with the image of reference square $(0,1)^2$ through an explicit or implicit parameterization supported by GMP. For adjacent rectangles, the corresponding parameterization are compatible with each other, i.e. they yield an identical parameterization for the common edge.
- *Data for (an initial) mesh generation*. Each of the reference squares is covered with a uniform mesh of $m_1 \times m_2$ elements of uniform order $\mathbf{p} = (p_1, p_2)$. The number of horizontal m_1 and vertical m_2 subdivisions must be compatible with the adjacent rectangles, so that the resulting initial mesh is regular. The *minimum rule* is used to determine the order of approximation for edges shared by two rectangles.
- *Material and load data*. It is assumed that the coefficients of the differential equation and boundary operators, as well as source term f and boundary data g , are constant within each GMP rectangle. If the exact (manufactured) solution is known, the load data is determined from the differential equation and boundary conditions.
- *Additional data for post-processing*: definition of elements sets, sections etc., all done within GMP logic.

The *hp* algorithm produces a sequence of *coarse* and corresponding *fine* meshes that deliver exponential convergence.

In Figs. 3 and 4, different colors denote different orders of approximations, as presented in Fig. 2. Each element may have different orders of approximation on its edges, and different horizontal and vertical order of approximation assigned to its middle-node. For example, for the upper element located on the right-hand side picture in Fig. 3, the order of approximation assigned to its nodes is as follows. The middle node “horizontal” order is 1 and “vertical” 3, the left edge has order 3, the right edge has order 2, and both horizontal edges are of order 1.

The initial mesh is the coarse mesh for the first iteration. The algorithm performs the following iterations, see Fig. 1. The coarse mesh is globally refined in both element size h (each quad element is divided into four element sons in 2D) and order of approximation $\mathbf{p} = (p_1, p_2)$ (raised uniformly by one), to obtain the fine mesh, see Fig. 3. Load balancing using the Zoltan library [33] is performed at the beginning of each iteration step. The problem is solved twice, once on the current coarse mesh, and once on a fine mesh. The FE error on the coarse grid is estimated by simply evaluating (norm of) the difference between the coarse grid and fine grid solutions. If error exceeds a preset tolerance, the coarse grid is *hp*-refined in an optimal way. The optimal *hp*-refinements (see Fig. 3) are obtained by minimizing the coarse grid *projection based interpolation error* of the fine grid. Both coarse and fine grid solution are stored in element fashion, using elements’ local coordinates systems. This localization principle allows us to compute projections of global

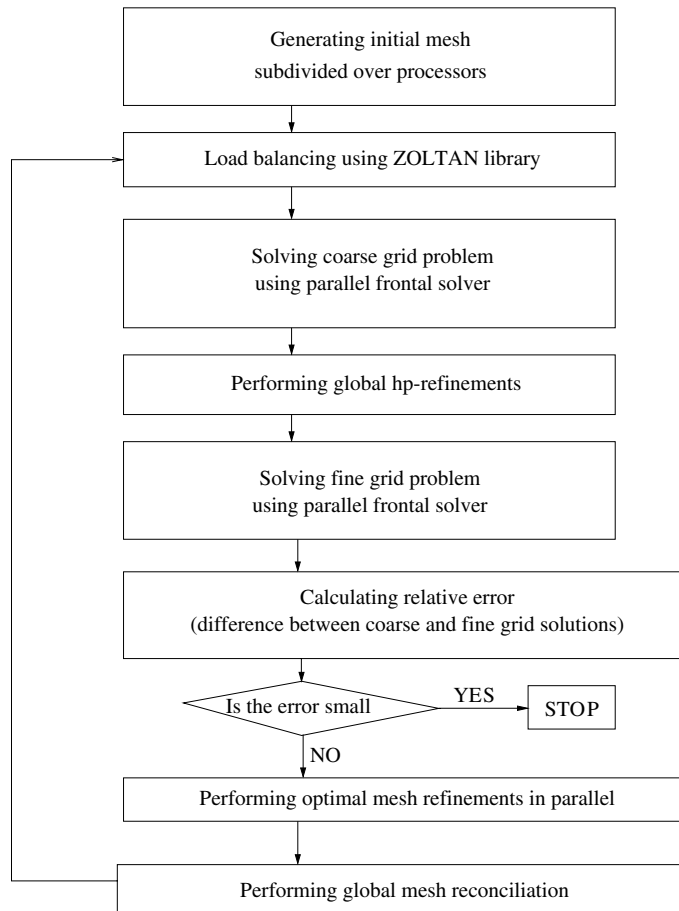
Fig. 1. Flow chart for parallel fully automatic hp -adaptive finite element algorithm.

Fig. 2. Orders of approximation over elements.

interpolants locally, over particular elements. The optimal mesh obtained in the current step constitutes the coarse mesh for the next step, see Fig. 4. The iterations are stopped when the estimated error is sufficiently small.

3. Parallel data structures and load balancing

Since the parallel code described in this paper was developed as an extension of the serial code 2Dhp90, we will begin with a short description of the data structures in the serial code, and discuss how they have been modified in the parallel code. The data structures are organized into three layers with geometry

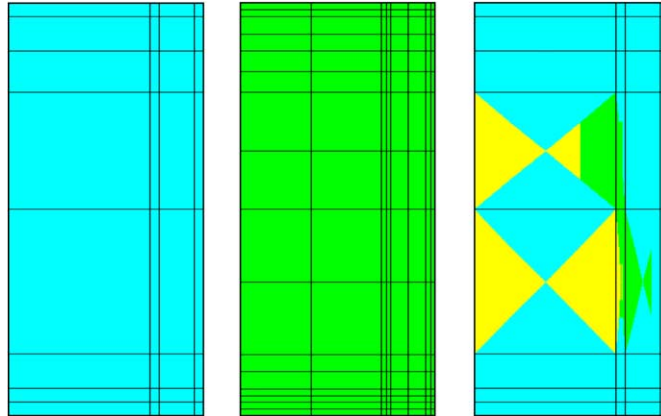


Fig. 3. Left picture: Initial mesh = coarse mesh. Middle picture: Fine mesh in the first iteration. Right picture: Optimal mesh after the first iteration.

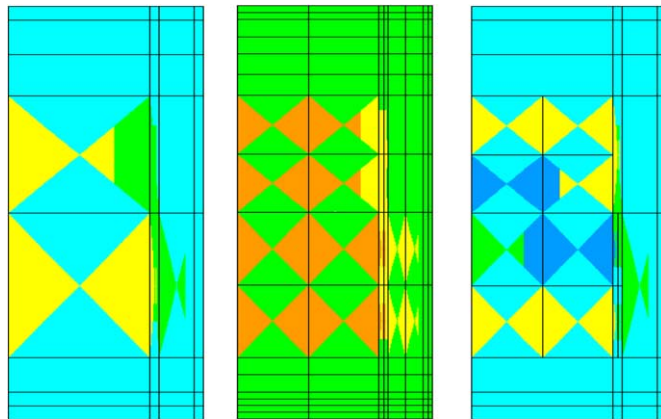


Fig. 4. Left picture: Optimal mesh after the first iteration = coarse mesh for the second iteration. Middle picture: Fine mesh in the second iteration. Right picture: Optimal mesh after the second iteration.

representation at the bottom, initial mesh elements in the middle, and refinement trees on top, see Fig. 5. In general, geometry and initial mesh elements are static, while refinement trees are grown dynamically. In the parallel version, the geometry is global, while initial mesh elements and refinement trees are local. This will be clarified in the following discussion.

The lowest level, geometry representation, is provided by the Geometrical Modeling Package (GMP, [31]). The geometry is represented as a collection of points, curves, and rectangular figures. In the parallel version, geometry is global, i.e. each processor constructs an identical copy of the geometry for the entire computational domain.

At the next initial mesh level, a truly parallel execution begins. Each processor takes responsibility for a part of the global geometry, and generates initial mesh elements only for that part. For each initial mesh element we store the following data,

`nodes` local pointers to four vertex nodes, four edge nodes, and a single middle node (to be described below),

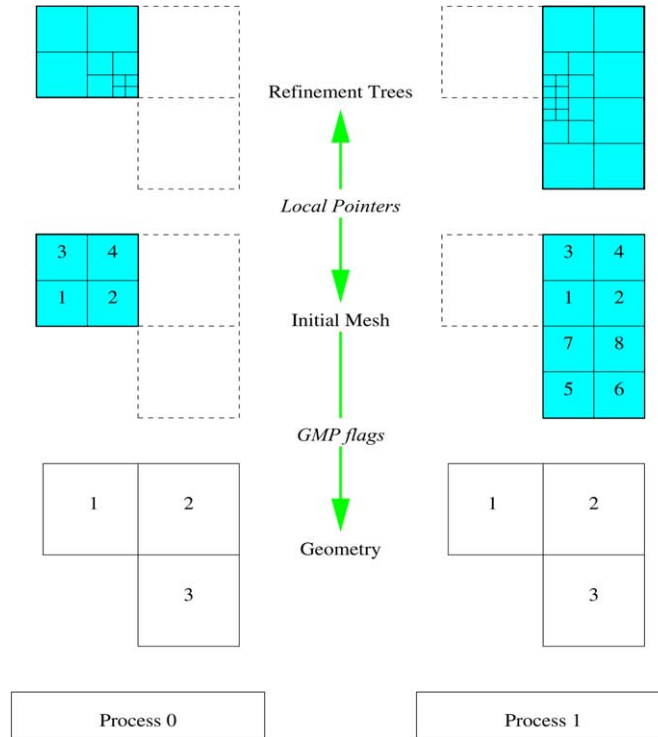


Fig. 5. Global geometry, divided initial mesh, and refinements.

orient orientations for the four edge nodes,
 bcond boundary condition flags for the four edges,
 neig local pointers to the four neighboring initial mesh elements, or zero if a particular neighbor resides on another processor or doesn't exist because the element is adjacent to the boundary,
 geom_intf an interface to GMP that identifies the geometric figure in which the element resides and its local element number within that figure.

Because the global geometry is known to each processor, the `geom_intf` flag is a unique global identifier for each element, and provides the basis for communication between processors. For example, when we need to find all the neighbors for an element, we can first look at the local pointers `neig` to identify all neighbors that reside on the same processor. If one of these is zero we can jump down one layer into the geometry data and either discover that the element is adjacent to the boundary, or that the neighbor simply resides on another processor, in which case we can identify it by using its `geom_intf` flag.

With initial mesh elements thus constructed, each processor initializes the final layer, refinement trees, by adding vertex, mid-edge, and mid-quad nodes to the mesh. For vertices we store the following information,

bcond a boundary condition flag,
 father for initial mesh vertices, this is a pointer to one of the initial mesh elements containing the vertex;
 for vertices resulting (later) from the refinement of mid-edge or mid-quad nodes, this is a pointer to the parent node that was refined,

`coord` geometric coordinates,
`zdofs` solution degrees of freedom.

For mid-edge and mid-quad nodes alike, we store,

`type` identifies the node as mid-edge or mid-quad,
`order` polynomial order of approximation (possibly anisotropic for mid-quad nodes),
`bcond` a boundary condition flag,
`ref_kind` h -refinement flag,
`sons` for nodes that have been h -refined, we store pointers to the nodes generated by that refinement; a mid-edge node may have zero or three sons (two mid-edge nodes and a vertex), and a mid-quad node may have zero, three (two mid-quads and a mid-edge), or nine (four mid-quads, four mid-edges, and a vertex) sons,
`coord` geometry degrees of freedom,
`zdofs` solution degrees of freedom.

Notice that nodes do not store horizontal connectivities, i.e. a mid-quad node does not store pointers to the adjacent vertices or mid-edge nodes. Only father-son relationships are stored, and efficient algorithms are used to dynamically reconstruct horizontal connectivities in the refined mesh.

While the initial mesh is distributed evenly across all processors, adaptive refinements lead to load imbalance and we must obtain a new domain decomposition to rebalance the load. The most general approach would allow for any partitioning of the current active mesh. However, this would be an enormous departure from the serial code. Instead, we only allow a partitioning along lines in the initial mesh, i.e. each initial mesh element, along with its refinement trees, is treated as a unit.

Our data decompositions are obtained through a simple interface with the Zoltan library [33]. For each initial mesh element, we provide Zoltan with the corresponding global identifier (the `geom_interf` flag), spatial coordinates of the element centroid, and a weight representing the computational cost for that element and its refinement tree (currently we use a weight that scales with the order of approximation p like the cost for element stiffness matrix integration, i.e. $O(p^4)$ in 2D).

Having gathered this information from each processor, Zoltan employs one of its load balancing algorithms providing a new decomposition of the domain with the weights equitably distributed between subdomains. Currently, we are using a Hilbert space filling curve-based algorithm, based on a non-intersecting curve passing through the element centroids, see Fig. 6. This curve is cut into segments (one for each processor) in such a way that the computational weights are equitably distributed between segments. Because

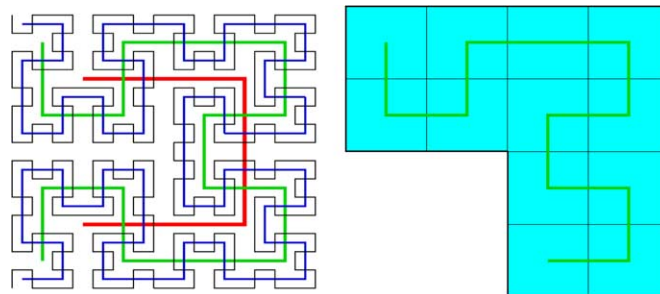


Fig. 6. Refinement levels for a Hilbert space filling curve, and the one that passes through initial mesh elements.

the initial mesh is static, this curve never changes; only the weights and therefore the cuts change as the mesh is refined. The new data decomposition is returned to each processor in the form of a list of elements to be exported (and to which processor) and a list of elements to be imported (and from which processor). We perform the necessary data migration using the Message Passing Interface (MPI).

The communication cost of data migration after load balancing can be described in terms of *h-relation personalized communication* where each processor has possibly different amount of data to share with a subset of other processors such that each processor is the origin or destination of at most h messages. We have proposed the communication strategy for *h-relation personalized communication* based on a bipartite graph coloring algorithm [22] with an overall complexity $O\left(\tau h + \frac{n}{p}\sigma\right)$, where τ is the message initialization time, n is total amount of data assumed to be distributed in $\frac{n}{p}$ portions over p processors, and σ is the time per byte at which processor can send or receive data through the network ($\frac{1}{\sigma}$ is the bandwidth of the network). The core of our communication strategy is a *concurrent point-to-point communication*, which can be effectively performed on clusters, as we have demonstrated in [22].

After data migration each processor has to reassemble those elements it did not export to other processors, and those elements it imported from other processors, into a single data structure. The elements are sorted based on their `geom_interf` flags, first by geometric figure numbers, and then by local element numbers within a figure. The new data structure is then assembled, element by element. This process is actually quite simple since the refinement trees do not store horizontal connectivities. We only need to reconstruct the horizontal connectivities (i.e. pointers to neighbors) on the initial mesh level and the refinement trees are assimilated automatically!

An alternative strategy demonstrated in [23] is to migrate parent elements, then perform the refinements on target processors. The strategy is motivated with a simple observation that the mesh repartition is done on a smaller mesh which reduces the complexity and communication cost. We intend to make these modifications in our next implementation.

4. Parallel frontal solver

Both the coarse mesh and fine mesh problems are solved using a parallel frontal solver. (In the future a parallel version of a two grid solver will be developed for solving the fine mesh problem [21].) The frontal solver is an extension of the Gaussian elimination algorithm, where assembly and elimination are performed together on the so-called frontal sub-matrix of the global matrix [14].

The solver performs forward elimination first, and then backward substitution (just like the standard Gaussian elimination scheme). It visits each element, assembles the element contribution into the frontal matrix, and performs elimination of those degrees of freedom that won't be visited in the future (whose final contribution comes from the current element).

We have implemented a parallel version of the solver, using the domain decomposition approach [29]. The computational domain is subdivided into d sub-domains and d.o.f. are enumerated in the following way,

- All internal d.o.f. from 1-st sub-domain,
- All internal d.o.f. from 2-nd sub-domain,
- ...,
- All internal d.o.f. from d -th sub-domain,
- All d.o.f. from the global interface.

The structure of the global stiffness matrix is (see also Fig. 7)

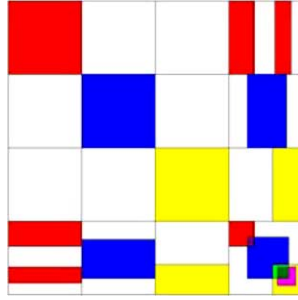


Fig. 7. Global matrix after the domain decomposition.

$$\begin{bmatrix} A_1 & \dots & B_1 \\ & A_2 & B_2 \\ & \dots & \dots \\ & & A_d & B_d \\ C_1 & C_2 & \dots & C_d & A_s \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_d \\ x_s \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_d \\ b_s \end{bmatrix}, \quad (4.1)$$

or equivalently,

$$\begin{bmatrix} A_I & B^T \\ C & A_s \end{bmatrix} \begin{bmatrix} x_I \\ x_s \end{bmatrix} = \begin{bmatrix} b_I \\ b_s \end{bmatrix}. \quad (4.2)$$

The Schur complement of system (4.2) is

$$\hat{A}x_s = \hat{b}, \quad (4.3)$$

$$\hat{A} = A_s - CA_I^{-1}B^T, \quad (4.4)$$

$$\hat{b} = b_s - CA_I^{-1}b_I, \quad (4.5)$$

$$A_I x_I + B^T x_s = b_I. \quad (4.6)$$

The resulting global matrix has sparse form, except for the part connected with d.o.f. from the global interface. Upon the static condensation of the sub-domains' interior d.o.f. (computation of the Schur complements), we formulate and solve the global wire-frame problem. Finally, we solve a local interior problem on each sub-domain in parallel, using the wire-frame problem solution.

A practical implementation is achieved by adding a so-called “fake” element [29] at the end of the list of elements browsed by the frontal solver on each sub-domain. The “fake” element contains all interface d.o.f. from that sub-domain (see Fig. 8), and tricks the frontal solver into leaving the associated d.o.f. in the front. In other words we perform the following operations:

- Run the forward elimination stage of the frontal solver in parallel. Stop the elimination stage *before* processing fake elements. The final front matrices obtained on each sub-domain are precisely the sub-domain contributions to the global Schur complement.
- Assembly obtained matrices and solve the wire-frame problem (sequential).
- Run the backward substitution stage over each sub-domain in parallel.

Going into details, let

n = total number of d.o.f.,

$n_{\text{internal}}^{(i)}$ = number of interior d.o.f. of sub-domain i ,

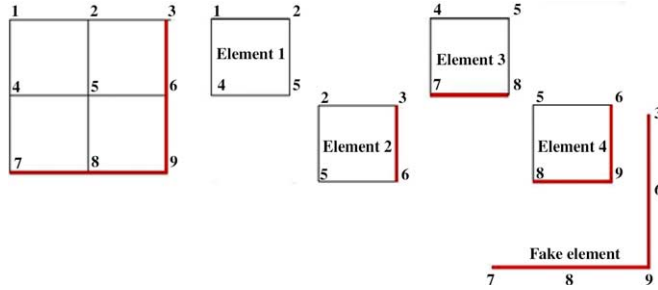


Fig. 8. Finite elements together with the fake element over a sub-domain, processed by the parallel frontal solver.

$n_{\text{interface}}^{(i)}$ = number of interface d.o.f. of sub-domain i ,
 $n_{\text{interface}}$ = global number of interface d.o.f.

We define the following inclusions:

$$P_i: M\left(n_{\text{internal}}^{(i)} + n_{\text{interface}}^{(i)} \times n_{\text{internal}}^{(i)} + n_{\text{interface}}^{(i)}\right) \rightarrow M(n \times n), \quad (4.7)$$

$$P_{bi}: M\left(n_{\text{interface}}^{(i)} \times n_{\text{internal}}^{(i)}\right) \rightarrow \left(n_{\text{interface}}^{(i)} + n_{\text{interface}}^{(i)}\right), \quad (4.8)$$

$$P_{ib}: M\left(n_{\text{internal}}^{(i)} \times n_{\text{interface}}^{(i)}\right) \rightarrow \left(n_{\text{interface}}^{(i)} + n_{\text{interface}}^{(i)}\right). \quad (4.9)$$

The global matrix can then be represented by the following decomposition

$$A = \sum_{i=1}^p P_i A^{(i)} P_i^T, \quad (4.10)$$

where

$$P_i A^{(i)} P_i^T \begin{bmatrix} 0 & & & & \\ & \dots & & & \\ & & A_i & & P_{ib} B_i P_{ib}^T \\ & & & \dots & \\ & P_{bi} C_i P_{bi}^T & & & P_{bb} A_s^i P_{bb}^T \end{bmatrix}. \quad (4.11)$$

The global matrix can be stored in a distributed manner, over d processors (see Fig. 9).

The forward elimination stage of the frontal solver can be run over each sub-domain to assemble the system,

$$\begin{bmatrix} A_i & B_i \\ C_i & A_s^i \end{bmatrix} \begin{bmatrix} x_i \\ x_s^i \end{bmatrix} = \begin{bmatrix} b_i \\ b_s^i \end{bmatrix}, \quad (4.12)$$

where A_i , B_i , C_i and b_i are fully assembled, and A_s^i is partially assembled.

The frontal solver eliminates all internal d.o.f., but keeps all interface d.o.f. After processing all elements except the fake element, the front is A_s^{i*} , see Fig. 10.

The global wire-frame interface matrices are then computed, comp. (4.13) and (4.14), see Fig. 10.

$$\hat{A} = \sum_{i=1}^p P A_s^{(i)*} P^T, \quad (4.13)$$

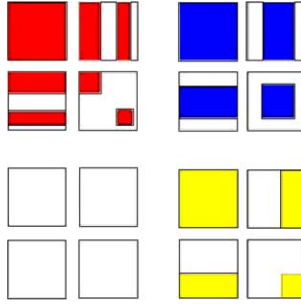


Fig. 9. Distribution of the global matrix into processors.

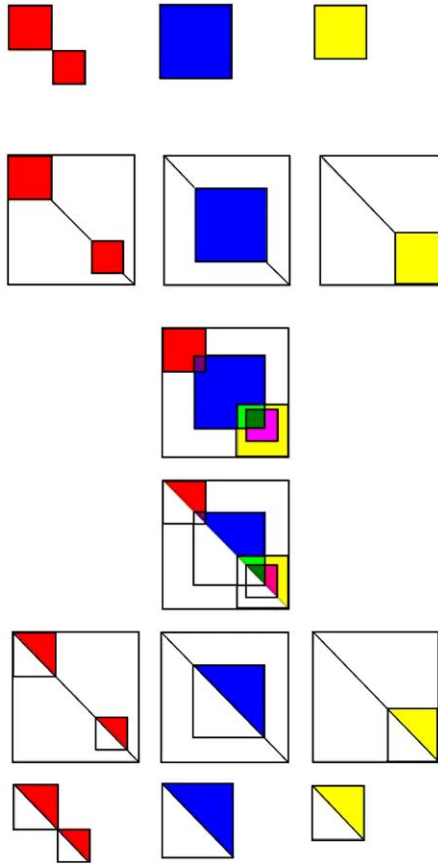


Fig. 10. First row: Front matrices $A_s^{(i)}$ in contributing slave processors. Second row: $P_{bb}A_s^{(i)T}P_{bb}^T$ distribution of the interface problem part of the global matrix into processors. Third row: The interface problem $\hat{A} = \sum_{i=1}^p P_{bb}A_s^{(i)T}P_{bb}^T$ formulated on a master processor. Fourth row: Global interface problem after forward elimination stage. Fifth row: Distribution of the upper triangular form of the interface problem into processors. Sixth row: Upper triangular forms of front matrices on slave processors.

$$\hat{b} = \sum_{i=1}^p P_{bb}A_s^{(i)T}P_{bb}^T. \quad (4.14)$$

The wire-frame problem is currently formulated and solved on a separate processor sequentially.

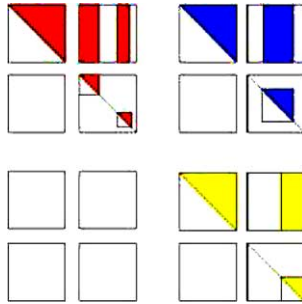


Fig. 11. Distributed global matrix before the parallel backward substitution.

The interface problem should be parallelized using an iterative solver as this can be a very large bottleneck for even a modest number of processors. The parallel multi frontal solver using PLAPACK [24] was successfully done by [10,3]. For large numbers of processors the interface problem is also quite sparse and the PLAPACK may not be sufficient, since it has been designed for dense matrices. In our current work we review a number of better alternatives including the massively parallel multi frontal solver MUMPS [19].

Finally, the backward substitution stage runs on each sub-domain separately, see Fig. 11.

5. The sequential *hp*-algorithm

In this section we discuss the 2D version of our *hp* mesh optimization algorithm. The logic of the algorithm is the same for both elliptic and Maxwell problems, only the projections used are different.

5.1. Mesh regularity

- A mesh, consisting of quads, is called *regular*, if the intersection of any two elements in the mesh is either empty, reduces to a single vertex, or consists of a *whole* common edge shared by the elements.
- An *isotropic h-refinement* occurs (in 2D) when an existing element is broken into four son elements.
- An *anisotropic h-refinement* occurs when an existing element is broken into two son elements, in either the horizontal or vertical direction.
- An edge consists of two vertices and one mid-edge node. When an element is refined, in isotropic or anisotropic manner, some of its edges are broken.
- During the isotropic *h-refinement*, an element is broken into four smaller sons, as presented in Fig. 12. As a result of the refinement, a *big* element, shown in Fig. 12 on the right, has two smaller *neighbors*. In such a situation, two mid-edge nodes of smaller elements and one common vertex of both smaller elements remain constrained with no new nodes generated in global data structure arrays *NODES* and *NVERS*. The d.o.f. of constrained nodes are *forced* to match appropriate linear combinations of *parent nodes* d.o.f. in order to enforce the continuity of the approximation (hence the name) but they do not exist in the data structure arrays.
- A mesh with constrained nodes is called an *irregular mesh*. It may happen that smaller elements need to be broken once again, as it is presented in Fig. 13. In such a case newly created constrained nodes are said to be *multiply constrained*.

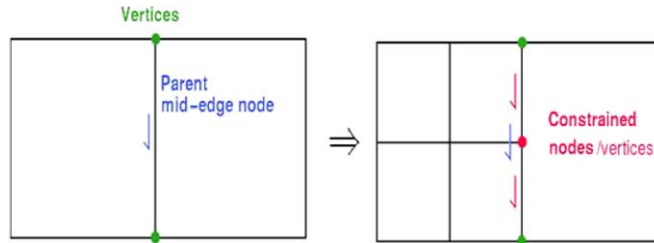


Fig. 12. Isotropic refinement of a finite element. mid-edge nodes and one common vertex of two newly created elements are called *constrained nodes*.

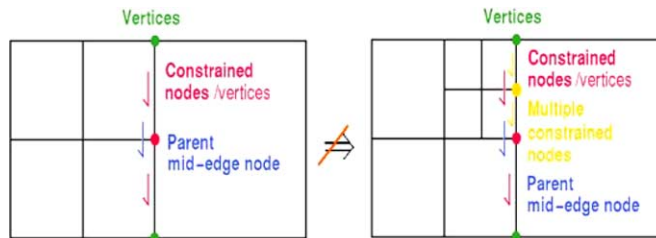


Fig. 13. Next refinement leads to the *multiply constrained nodes*.

- It is desirable for many reasons to avoid multiply constrained nodes, and limit ourselves to 1-*irregular* meshes only. We enforce this 1-*irregularity rule* by breaking only those elements, which do not contain constrained nodes. In the case of quads, it is necessary to check if any adjacent mid-edge nodes are constrained. If a constrained node is found on some element edge, we must first break the neighboring element, as shown in Fig. 14.
- The fine grid solution is stored locally within each coarse grid element. Translating global d.o.f. into an element local d.o.f. involves using element to nodes connectivities, taking into account global orientations of mid-edge nodes, and the whole machinery of constrained approximation. Calculation of the element local d.o.f. is one of the essential components of the *hp* codes.
- The determination of optimal *hp*-refinements based on *projection-based interpolation* takes place *locally* over each element of the coarse mesh, without any communication with neighboring elements or any other data structures.

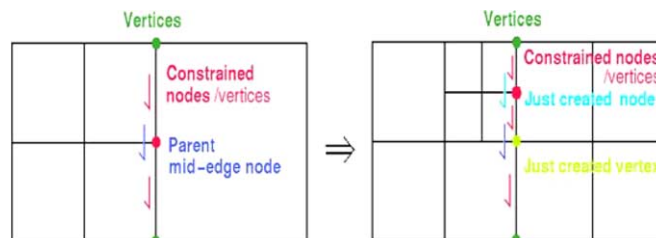


Fig. 14. Enforcing breaking neighboring elements, in order to enforce 1-*irregularity rule*.

5.2. The *hp* algorithm

We continue now with a short discussion of operational aspects of the algorithm focusing on those aspects that will be modified in the parallel version.

The main idea of the algorithm is to use the fine grid solution to stage a competition between various possible refinements, by comparing the corresponding decrease rates of the projection-based interpolation error,

$$\text{rate} = \frac{\|u_{h/2,p+1} - w_{hp}\| - \|u_{h/2,p+1} - w_{hp}^{\text{new}}\|}{\text{ndof}_{\text{added}}}. \quad (5.15)$$

Here $u_{h/2,p+1}$ denotes the fine grid solution, w_{hp} is the current coarse grid interpolant, w_{hp}^{new} is the interpolant corresponding to a (new) grid being tested, and $\text{ndof}_{\text{added}}$ denotes the *number of local d.o.f. added*, and represents the cost of investment. The mesh optimization is done hierarchically, first optimal edge refinements are determined, and then optimal refinements for (interiors of) elements are found. In the current version of the algorithm, the topology of the new mesh (*h*-refinements) is determined entirely by optimal edge refinements, and so called *isotropy flags* for coarse grid elements. The isotropy flags reflect the isotropic/anisotropic character of the error function, and are calculated during the evaluation of the global error [7,8]. The mesh optimization over elements (refined or not in *h*) consists only of determining the optimal assignment of element orders of approximation.

The algorithm consists of the following main steps:

1. For each element in the coarse grid, the difference between coarse and fine grid solutions is computed, and the corresponding isotropy flags indicating the need for isotropic or anisotropic refinements are determined.
2. For each edge in the coarse mesh, the locally optimal refinement is determined (the edge may be *p*-refined, or *h*-refined with optimal orders for the new mid-edge nodes selected), and the corresponding error decrease rate is computed. The computation of the rate requires accessing information about elements neighboring the edge (element size h_1, h_2).
3. Looping over all edges in the mesh, the maximum edge error decrease rate is computed. This requires some global communication. Once the optimal rate is determined, all edges are revisited, and we invest into refining only those edges that deliver error decrease rates within a prescribed percentage of the maximum rate.
4. Based on optimal edge refinements and element isotropy flags, a decision is made about how (and if) to *h*-refine each element. The optimal *h*-refinements are made, enforcing the 1-irregularity rule.
5. As a result of enforcing the 1-irregularity rule, some coarse grid edges are *involuntarily h*-refined. Those edges are visited again, and the optimal distribution of orders is determined for the new edges, based on comparing the resulting error decrease rates with the maximum rate. The approximation on all coarse grid edges, refined or not, must be fully known before the element stage of the algorithm.
6. Optimal element error decrease rate for each coarse grid element (*h*-refined or not) is determined. Looping over all elements in the mesh, we compute the maximum element rate. We revisit all elements again and use the maximum element rate to select optimal distribution of orders *p* for all refined elements.

6. Parallel mesh refinements and mesh reconciliation

We turn now our attention to the parallelization of the *hp* mesh optimization algorithm.

The parallel version of the algorithm requires a global mesh reconciliation step after refinements have been performed over each sub-domain in parallel. The mesh must be globally consistent. Maintaining

the 1-irregularity of the mesh (to avoid the logical nightmare of multiply constrained nodes) requires that an element edge can be broken only once without also breaking the neighboring element. The ultimate goal is to enforce the same rules for element edges situated on the global interface as for those within a sub-domain interior. A final step enforces the minimum rule to ensure that the order of approximation for each edge is set to the minimum of the orders of approximation in the neighboring element interiors.

Our mesh reconciliation algorithm requires an exchange between processors of the following items: refinement trees for edges located on the interface, locations of newly created constrained nodes situated on the interface edges, and the interior orders of approximation for elements adjacent to the interface.

We can summarize the main logic of the algorithm in the following stages:

1. determine the optimal refinements (almost entirely in parallel) and perform them in parallel,
2. exchange information about edge refinement trees, constrained nodes and orders of approximation along the interface,
3. mesh reconciliation.

A repetition of stages (2) and (3) may be required if some of the interface edges were modified during the last iteration.

6.1. Example of the parallel mesh refinements

Let us consider the following example. We focus on three initial mesh elements, each one located in a separate sub-domain. The element from sub-domain 1, is adjacent to the element from sub-domain 2, along its right edge, and to the element from sub-domain 3, along its bottom edge, as shown in Fig. 15. Only the element from sub-domain 3 is broken. The edges located on the global interface are treated in the same way as internal nodes, so the constrained node is created on the upper edge of the element.

The next *hp*-refinement iteration is started, and the element from sub-domain 3 is broken once again, see Fig. 16. The upper edge of the element is located on the global interface, so the edge needs to be treated in the same way as an internal edge. The interface edge must be broken, since the mesh must remain 1-irregular, and multiply constrained nodes are not allowed. Next, a new constrained node is created on the interface edge, see again Fig. 16.

The mesh must be globally consistent, so the element neighboring the edge in sub-domain 1 must be broken, see Fig. 17. This is done in a *mesh reconciliation* routine, which is called after parallel mesh refinements.

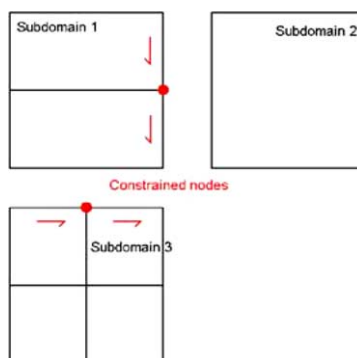


Fig. 15. Example of mesh reconciliation process: starting mesh.

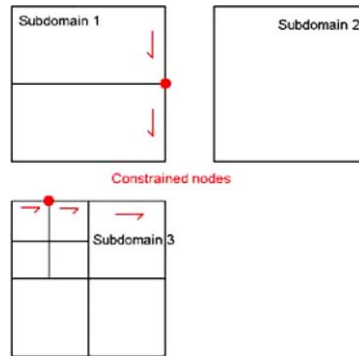


Fig. 16. Example of mesh reconciliation process: mesh after refinements process.

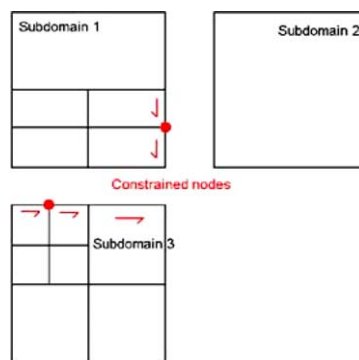


Fig. 17. Example of mesh reconciliation process: mesh after the first run of reconciliation routine.

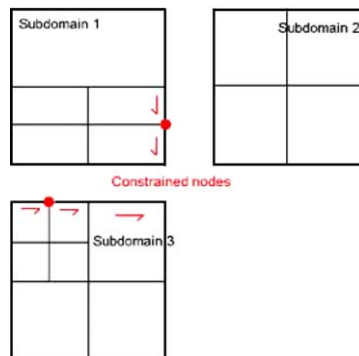


Fig. 18. Example of mesh reconciliation process: mesh after the second run of reconciliation routine.

But the mesh is still not globally consistent. The mesh reconciliation algorithm must be called once again, in order to break the element located on the second sub-domain, see Fig. 18.

This example illustrates one important problem, which arose during implementation of the parallel mesh refinements algorithm. The problem is related to the need for exchanging refinement tree data over the

interface edges. In other words, it is necessary to make the mesh globally consistent, and enforce the breaking of appropriate elements adjacent to the global interface.

Other problems, follow from the need to break interface edges with constrained nodes, as illustrated in Fig. 16. These are related to the need for establishing orders of interface edges with constrained nodes, correction factors, and the problem of constrained nodes located at the same place on both sub-domains. All of those problems are explained in detail in the following sub-sections.

6.2. Coding the refinement trees

The refinement trees are exchanged between neighboring sub-domains in a compressed binary format. For example, let us consider the binary description of two refinement trees located on the interface edge, presented in Fig. 19. Code 1 denotes a broken edge, while code 0 denotes an edge that is not broken. There is an isomorphism between refinement trees and their binary descriptions, so it is enough to exchange binary descriptions between neighboring sub-domains, compare a description of a refinement tree from current sub-domain with a received description of a refinement tree from neighboring sub-domain, and break some edges in the current refinement tree, if they are different from received ones. The above example shows that the refinement trees need to be exchanged as long as there were any changes made to interface edges during the current step of the mesh reconciliation process.

6.3. Orders of approximation for interface edges with constrained nodes

Let us consider a situation, when one edge of an element neighboring interface edge with constrained node was set to be broken in one sub-domain, but in the other sub-domain the interface edge is not to be refined, as in Fig. 20 on the left. The element is broken, and the interface edge with constrained node is also broken, as in Fig. 20 on the right. To establish orders of approximation for the broken mid-edge node sons, it is necessary to interpolate the fine grid solution over the broken edge. But on the current sub-domain there is no active finite element having entire edge that has just been broken. It is necessary to ask neighboring sub-domain for orders of approximation of just broken interface edge. This example illustrates a need for:

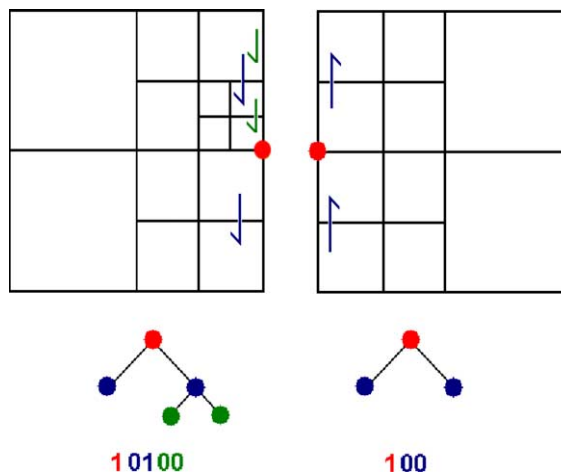


Fig. 19. Refinement trees and their representation (before mesh reconciliation).

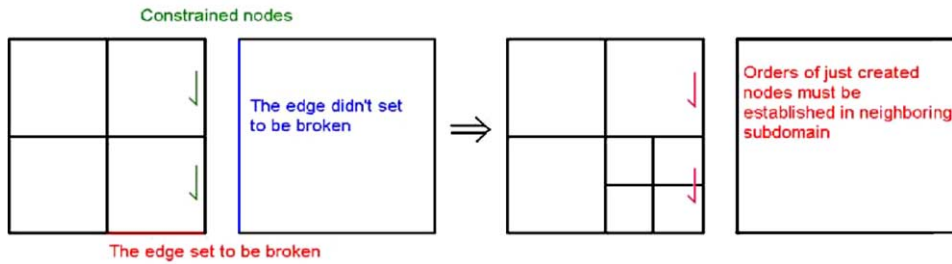


Fig. 20. Breaking an element having constrained node on the interface (before mesh reconciliation).

- sending/receiving data for interface edges constrained nodes to neighboring sub-domains,
- calculating the propositions of orders of approximation that can be use on neighboring sub-domain, in a case when the interface edge with constrained node will be broken,
- sending these propositions to neighboring sub-domains.

6.4. Correction factors

The third problem, that is hidden inside the sequential code, is connected with the need of calculating some correction factors over elements neighboring an interface edge. The decision of the refinement kind over an edge situated on the global interface is made using an interpolation of the fine grid solution projected onto the edge, with some *correction factor*. The factor is defined as a function of the area of elements neighboring the edge. Thus, a communication is required in order to obtain the correction factors from elements neighboring the interface edge, located on some other sub-domain.

6.5. Constrained nodes located at the same place on both neighboring sub-domains

The last problem arose from the methodology of treating interface edges. When an interface edge is broken, then a constrained node is created, since interface edges are treated in the same way as internal edges. If the same interface edge is broken on both adjacent elements located on two neighboring sub-domains, then a constrained node will be created at the same place on the edge, in both sub-domains. The refinement trees are identical for this edge, however these constrained nodes must both become unconstrained nodes. Thus, a communication is required in order to locate and replace those constrained nodes, which are located at the same place on both neighboring sub-domains, by newly created unconstrained node.

7. Results and discussion

7.1. L-shape domain problem

We begin with numerical results for the standard L-shape domain [6] problem. The par2Dhp code was run for the initial mesh presented in Fig. 21, over 4 processors, with 3 sub-domains and 1 processor responsible for the wire-frame problem solution. After 8 iterations of automatic parallel *hp*-adaptive strategy the optimal mesh was reached, presented in Fig. 22. The optimal mesh delivers a solution shown in Fig. 23 with a 1% relative error (in energy norm).

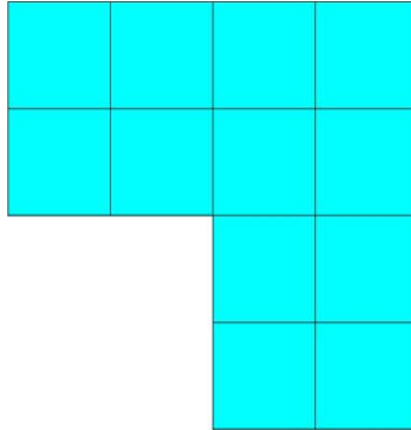


Fig. 21. Initial mesh for the Laplace equation over the L-shape domain problem.

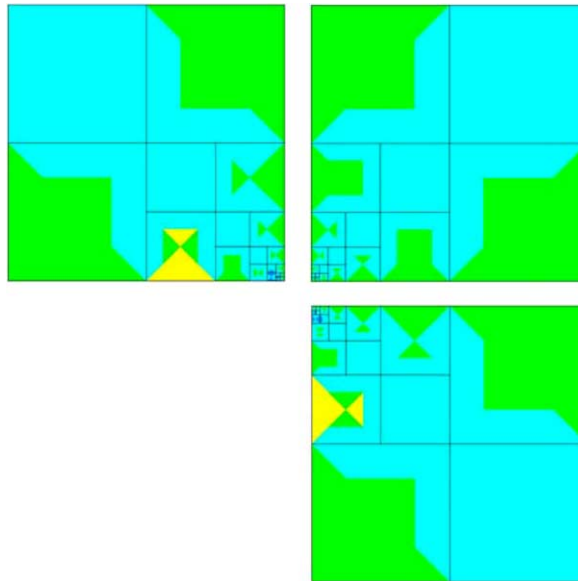


Fig. 22. Optimal hp mesh delivering accuracy of 1% error.

7.2. The Sandia battery problem

The second problem presented here is a battery problem from Sandia National Laboratories. The problem consists in solving orthotropic heat equation,

$$\nabla(K\nabla u) = f, \quad (7.16)$$

$$K = \begin{bmatrix} K_x & 0 \\ 0 & K_y \end{bmatrix} \quad (7.17)$$

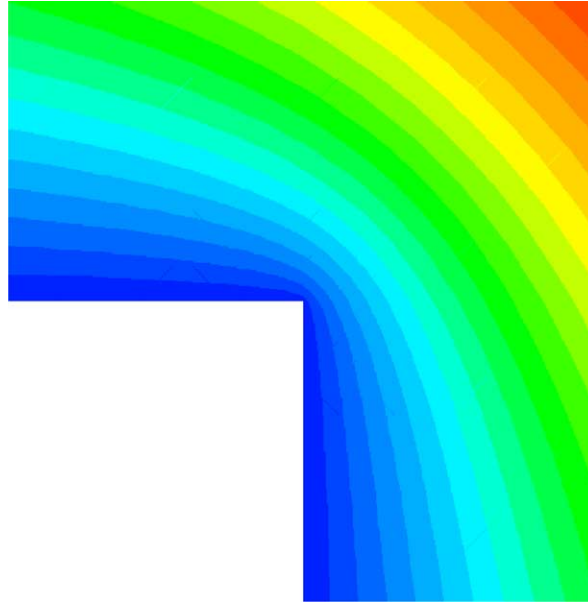


Fig. 23. Solution of the Laplace equation over the L-shape domain with 1% relative error. Exponential convergence is obtained to the accuracy of 1% relative error.

over the domain with 5 different materials, some orthotropic, some not, see Fig. 24. There is a large number of jumps in the material data, which generate singularities. Determining an optimal mesh requires highly anisotropic refinements.

The par2Dhp code was run for the initial mesh presented in Fig. 25, over 16 and 32 processors, with 15 or 31 sub-domains respectively, and processor 1 responsible for the wire-frame problem solution. The optimal hp mesh was reached after 45 iterations, together with the corresponding mesh partition shown in Figs. 26 and 27. The solution on optimal mesh, see Fig. 28, has a 0.1% relative error. The sequence of refined meshes delivers exponential convergence rates, illustrated in Fig. 29.

7.3. Discussion on the efficiency of the parallel algorithm

In this section we discuss the efficiency of our parallel algorithm, using the Sandia's battery problem, report the total computational time for different processors numbers, in Fig. 30, relative efficiency $E = \frac{T_1}{pT_p}$, in Fig. 31 and relative speedup $S = \frac{T_1}{T_p}$, in Fig. 32. Here T_1 is the total sequential code time, T_p

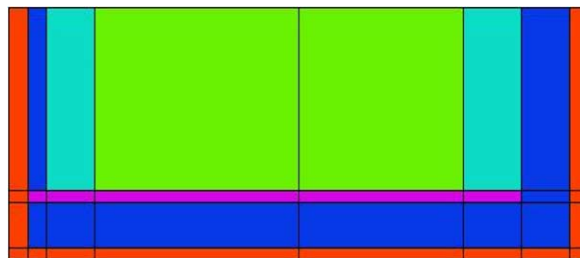


Fig. 24. Different materials on the battery problem domain.

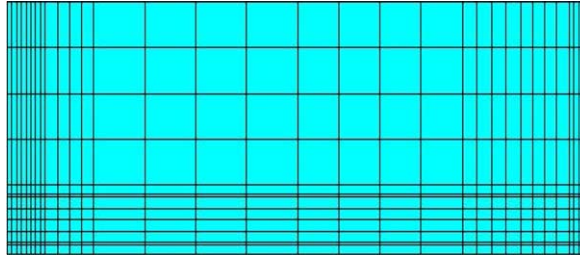


Fig. 25. Initial mesh for the battery problem.

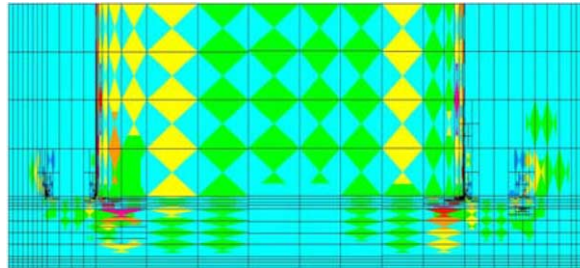


Fig. 26. The optimal mesh giving 0.1% relative error of the solution for the battery problem.

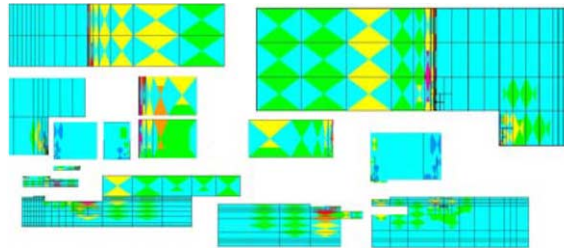


Fig. 27. Subdivision of the optimal mesh into processors.

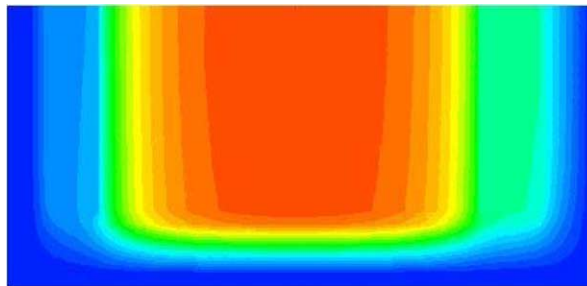


Fig. 28. Solution of the battery problem with 0.1% relative error.

is the total parallel code time for p processors [15]. In order to investigate the lost of speedup for large number of processors, we have performed detailed measurements for 16 and 32 processors, presented below.

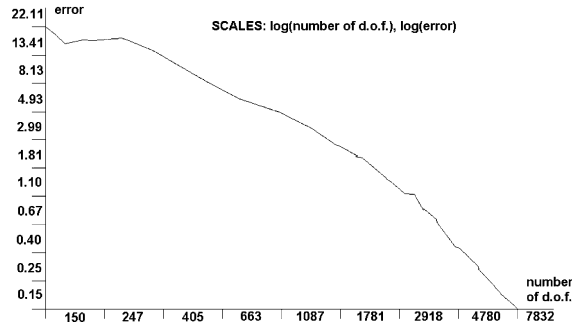


Fig. 29. Exponential convergence rate for the parallel calculations of the anisotropic battery problem from Sandia National Laboratories.

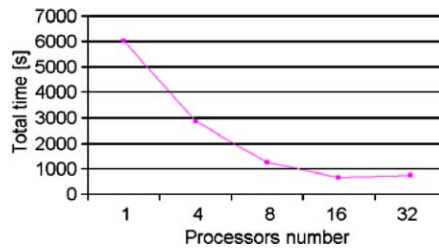


Fig. 30. Total computational times for different number of processors.

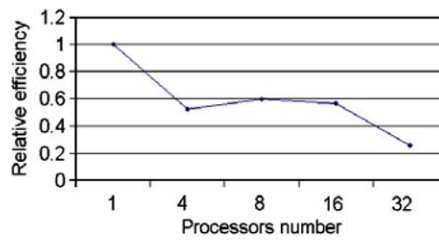


Fig. 31. Relative efficiency $E = \frac{T_1}{pT_p}$ for different number of processors p .

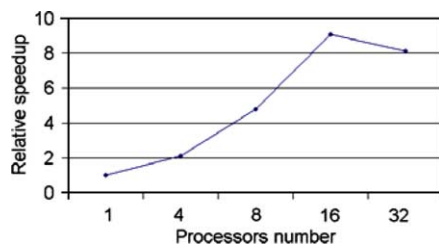


Fig. 32. Relative speedup $S = \frac{T_1}{T_p}$ for different number of processors.

We measured the computation time for each part of the sequential code, during all performed iterations, as presented in Fig. 33. The total computation time varied from 23 s in the first iteration, up to 124 s in the

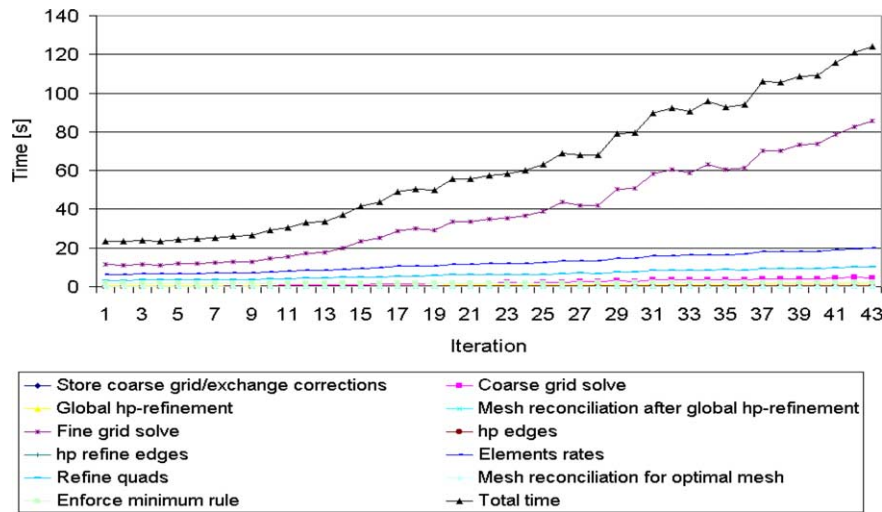


Fig. 33. Computation time for each part of the sequential code, measured during each iteration.

last one. The highest influence in the total computation time had the “Fine grid solve” part as expected. That time was uniformly raising from 11 s in the first iteration, when the fine grid problem size was 20.000 d.o.f. up to 85 s, when the fine grid problem size was about 80.000 d.o.f. The next most expensive part was the “Elements rate” part, where optimal refinements for each finite element are determined, by comparing error decrease rates for all possible *hp* refinements. The algorithm requires solution of some local systems of equations over each particular finite element, and its cost is raising with the number of degrees of freedom. The next most expensive components were “Refine quads” routine, estimating optimal orders of approximation for each finite element, and the “Coarse grid solve”.

We compare now the graph with a similar result for the parallel execution using 16 processors, as presented in Fig. 34. We observe that the number of iterations required in order to obtain the same 0.1% accuracy as in the serial code, was lower, equal to 37. This can be explained by the better accuracy of the parallel frontal solver, in comparison with the sequential one, see Section 8. The total computation time for the parallel execution varied from about 4 s in the first iteration up to 18 s in the last one. Again, the most expensive part was the “Fine grid solve” part, for which execution time varied from about 2 s up to about 9 s. Next most expensive components were “*hp* refine edges” and “Enforce minimum rule” routines, where inter-processors communication is required. The “Refine quads” part was still essential, and the reason for that will be explained. Next, we plot a similar representation for the parallel execution using 32 processors, shown in Fig. 35. Surprisingly, the overall shape of the 32 processors case is similar to that drawn for 16 processors.

We have also measured times for particular stages of the dominating fine grid problem solve part. These are: forward elimination and backward substitution for all slave processors, and the interface problem solution for the master processor (including communication during assembling of the interface problem matrix). We present computation times for both 16 and 32 processors, shown in Figs. 36 and 37. We can conclude from these Figures, that the interface problem solution time dominates for 32 processors run, and this motivates our future work plans on using the MUMPS parallel solver [19].

In order to investigate the problem with a lack of significant difference between computation times for 16 and 32 processors, we performed some measurements of loads over all processors, during particular iteration. Fig. 38 presents measured distribution of computational load (as input into ZOLTAN load balancing library), for each of 32 processors, in particular iterations. The great surprise was that after 6 iterations,

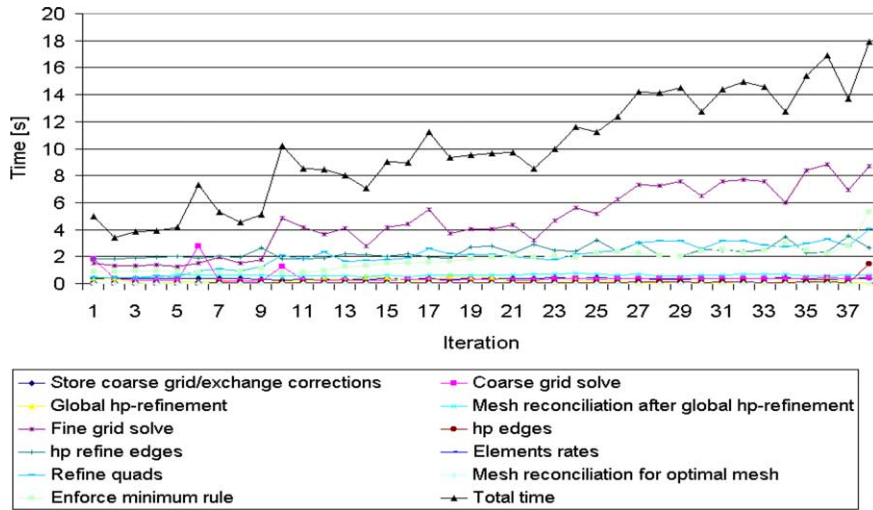


Fig. 34. Computation time for each part of the parallel code executed over 16 processors, measured during each iteration.

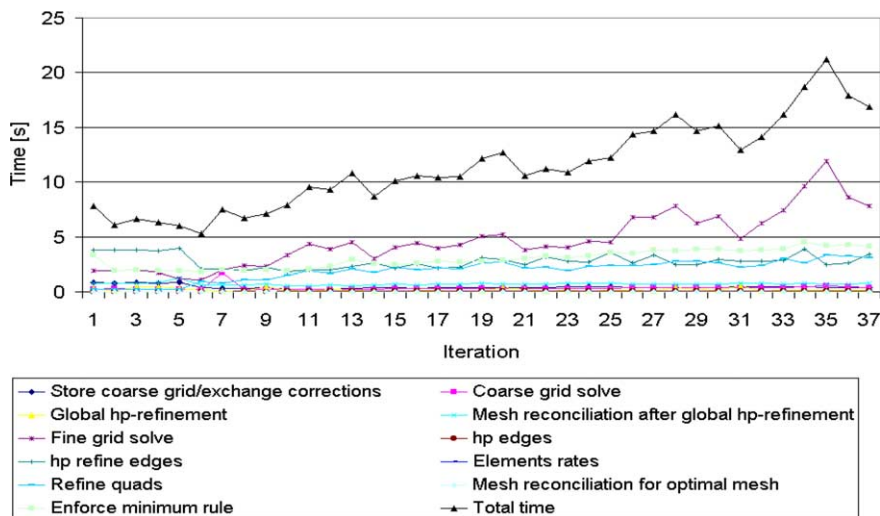


Fig. 35. Computation time for each part of the parallel code executed over 32 processors, measured during each iteration.

when load was almost uniformly distributed over each processor, the load began to rise dramatically on about 14 processors, whilst other processors had zero load and empty sub-domains. The reason for such behavior can be explained by the following example. Let us consider a case, when there are 10 initial mesh elements, and the load on the first element is equal to 10, whilst the load on each other element is equal to 1. The optimal load balancing for the case of 4 processors, as presented in Fig. 39 is that processor one has the first element with the highest load, and all other nine elements are assigned to processor 2. In other words, processors 3 and 4 have empty sub-domains!

In our *hp*-adaptive code the load balancing is done on the level of initial mesh elements only. In the Sandia battery problem there are about four areas in our computational domain where singularities are

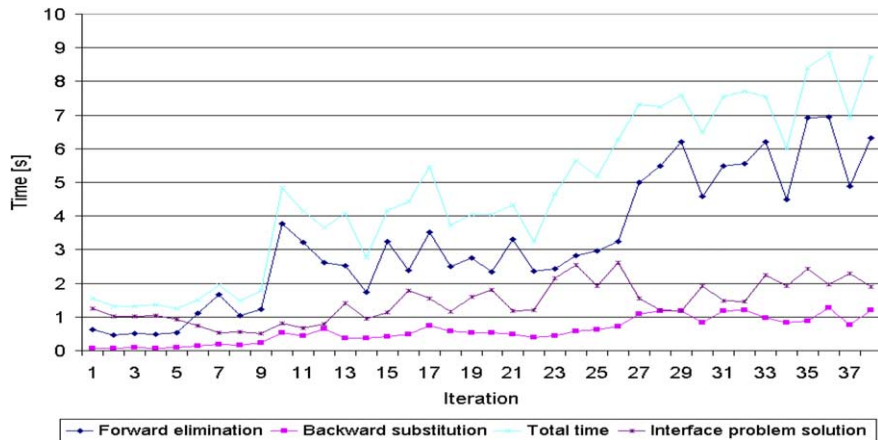


Fig. 36. Computation time for each part of the fine grid problem solver, executed on 16 processors, measured during each iteration.

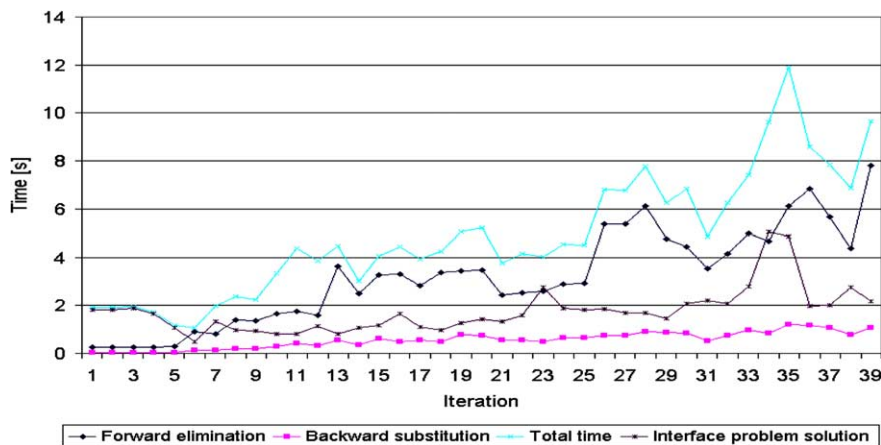


Fig. 37. Computation time for each part of the fine grid problem solver, executed on 32 processors, measured during each iteration.

present, and most of the hp -refinements was required in the neighborhood of these areas. There are about twelve initial mesh elements which completely cover these areas with singularities. After some initial steps, where global hp -refinements take place, the algorithm starts strong hp -refinements around the detected singularities, as presented in Fig. 40. These refinements are performed exclusively within these twelve initial mesh elements. The load for some of these elements is one order of magnitude higher than overall load for all other elements. The optimal load balancing proposed by ZOLTAN resulted in using only fourteen sub-domains: some with only one initial mesh element with high load, and others with remaining initial mesh elements, whose total load was smaller than the load of those highly hp -refined initial mesh elements.

In conclusion, the use of large number of processors is therefore motivated for problems with large number of singularities. In order to effectively utilize a large number of processors the initial mesh must have a correspondingly large number of elements that can be distributed among the processors.

Our numerical experiments indicate that the cost of resolving a point singularity with a 0.1% accuracy in our current implementation is about 20 s. We believe that this will extend to more complicated cases provided the number of processors match number of singularities to be resolved.

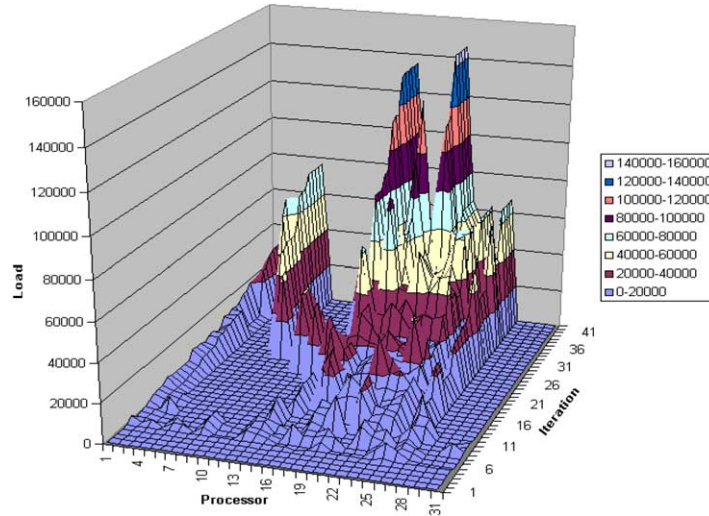


Fig. 38. Load distribution over 32 processors during particular iterations.

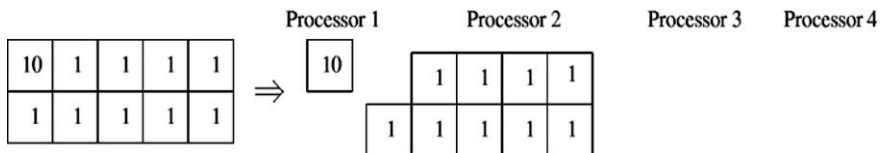
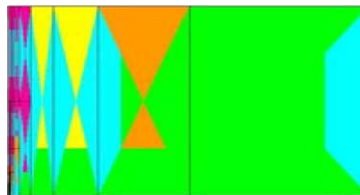


Fig. 39. Optimal load balance for mesh containing one finite element with load higher than total load of all other finite elements.

Fig. 40. Highly *hp*-refined initial mesh element in the neighborhood of a strong singularity.

8. Study on the accuracy of parallel and serial solvers

It was observed that the number of iterations required in order to obtain the same 0.1% accuracy was lower in the parallel code than in the serial one. We compared the refinement history for parallel and serial computations. The first difference appears in sixth iteration, as presented in Fig. 41. The difference results from numerically different error estimations for the same finite element. In the parallel code, the error estimation for the element was equal to 0.11031×10^{-07} , while the estimation in the serial code was 0.14381×10^{-07} . The difference in the eighth digit results in a different *p*-strategy chosen by the element. The next relevant difference appears in the seventh iteration, as presented in Fig. 42, and follows again from

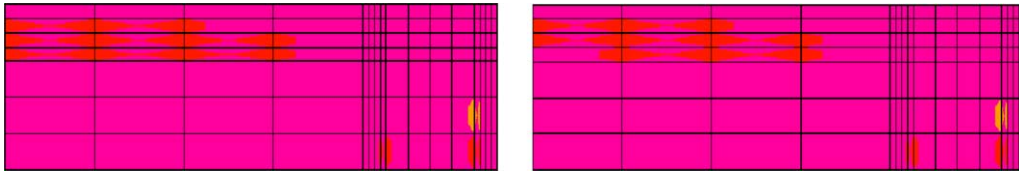


Fig. 41. First little difference in the mesh obtained by the parallel and the serial codes, in the sixth iteration. Left-hand side picture: Serial code. Right-hand side picture: Parallel code.

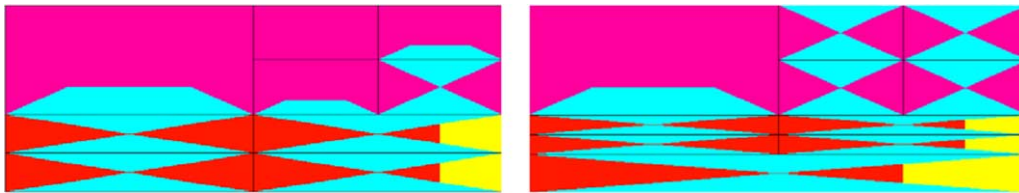


Fig. 42. Next difference in the mesh obtained by the parallel and the serial codes, in the seventh iteration. Left-hand side picture: Serial code. Right-hand side picture: Parallel code.

numerically different error estimations for some finite elements. The error estimation is calculated as a difference between coarse and fine grid solutions. We postulate therefore that the better accuracy of the parallel frontal solver, in comparison with the serial one, leads to slightly better choices in the refinement algorithm. The number of differences grows with increasing number of iterations, and it results in faster convergence of the parallel code.

9. Conclusions and future work

In the paper, a parallel version of the fully automatic *hp*-adaptive FE method, has been presented. The three main technical challenges in parallelizing the sequential version of the code included:

- mesh repartitioning accompanied by regeneration of *hp* data structure arrays after each mesh refinement, necessary to maintain load balancing,
- parallelization of a (sequential) frontal solver,
- parallel execution of optimal *hp* mesh refinements and following mesh reconciliation to enforce mesh regularity rules.

The par2Dhp package can be run on any parallel machine, equipped with Fortran 90 compiler, MPI communication platform, and a C++ compiler, required for rebuilding of the ZOLTAN library.

It is possible to select required load balancing algorithm by simply changing value of “LB_METHOD” parameter in ZOLTAN library interface. Thus, load balancing algorithms can be fit to a specific problem requirements.

Mesh is refined fully in parallel, and the algorithm enforces the rule that nodes located on the global interface are treated at the same manner as internal nodes. The 1-*irregularity* rule of the refined mesh is enforced in the parallel version of the code. This implies that the parallel mesh refinements algorithm delivers a similar sequence of refined meshes as the serial one.

We discuss now shortly our current and future work.

9.1. Parallelization of the 3D code

First and foremost, the presented work has been a ‘warm up project’ before starting the actual parallelization of the 3D *hp* code [21]. Both 2D and 3D codes share an identical data structure which gives us a hope to overcome the complexity of the 3D *hp* coding. The Zoltan/MPI framework has passed the 2D exam and seems to be an optimal environment for doing the 3D work as well.

9.2. Solvers

The linear solver presented in this paper does not scale with the number of sub-domains. This is due to the solution of the wire-frame interface problem on a single processor. We are in process of replacing this step with the parallel dense solver from *PLAPACK* [24]. An ideal choice to solve the wire-frame problem—a parallel iterative solver, in context of non-definite wave-propagation problems, is not available. We are also in process of parallelizing our two grid solver. The distributed memory implementation calls for a different logic of implementation, compared with the workstation version. The main bottle neck in terms of resources is the memory available on a single processor.

9.3. Selecting the number of processors with respect to the number of singularities

From the presented discussion it follows that the use of large number of processors is motivated for problems with large number of singularities. We therefore conclude that some initial analysis of the problem should be performed in order to estimate reasonable number of processors, with respect to the number of singularities detected in the computational domain. It can be done automatically, by returning some processors back to system, when the load balancing algorithm starts turning off some sub-domains because of large load associated with other sub-domains where strong singularities are detected.

9.4. New approach to *hp*-adaptivity

Finally, we mention our continuing work on determining optimal *hp* refinements. The determination of optimal mesh refinements is done in stages: for coarse mesh edges, then faces, and finally element interiors. In our current implementation, each stage is followed with the execution of the optimal refinements, e.g. the optimal refinements for faces are determined *after* performing optimal refinements for edges. Enforcement of 1-irregular meshes produces *unwanted refinements* changing the scenarios and complicating tremendously the logic of the algorithm, especially for a parallel implementation. In order to resolve the problem, we are working on a new version of the algorithm in which none of the refinements takes place until all optimal edge, face and element interiors refinements are determined. The determination of optimal refinements will take place in a stand alone code which should facilitate the parallel implementation as well.

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