Linear Computational Cost Graph Grammar Based Direct Solver for 3D Adaptive Finite Element Method Simulations

Anna Paszyńska, Piotr Gurgul, Marcin Sieniek, and Maciej Paszyński

Abstract—In this paper we present a new graph grammar based direct solver algorithm delivering linear $O(N)$ computational cost and linear $O(N)$ memory usage for adaptive finite element method simulations. Classical direct solvers on regular grids deliver $O(N^{1.5})$ complexity for 2D problems and $O(N^2)$ in 3D ones. The linear computational cost of our solver is obtained by generating graph representation of the adaptive mesh and by utilizing dynamic construction prescribing the solver algorithm as graph grammar productions.

Index Terms—Direct solvers, graph grammar, adaptive finite element method.

I. INTRODUCTION

Direct solver is the core part of several challenging engineering applications performed by means of the Finite Element Method (FEM) [1]-[3]. Exemplary problems involve generation of acoustic waves over the model of the human head [4] or borehole resistivity simulations [5]. The process of solving finite element engineering problems starts with generation of the mesh describing the geometry of the computational problem. Next, the physical phenomena governing the problem is described by some Partial Differential Equation (PDE) with boundary and / or initial conditions. Then, PDE is discretized into a system of linear equations using FEM. At this point, the solver algorithm is executed in order to provide the solution to the system of linear equations. The aforementioned engineering problems generate huge linear systems with several million unknowns, and the solver algorithm is the most expensive part of the process in terms of the computational cost. Multi-frontal solver is the state-of-the art algorithm for solving linear systems of equations [6], [7] using the direct solver approach. The multi-frontal algorithm constructs an assembly tree based on the analysis of the connectivity data or the geometry of the computational mesh. Finite elements are merged into pairs and fully assembled unknowns are eliminated within frontal matrices associated to multiple branches of the tree. This process is repeated until the root of the assembly tree is reached. Finally, the common interface problem becomes solved and partial backward substitutions are recursively called on the assembly tree.

Classical direct solvers executed on regular grids deliver $O(N^{1.5})$ complexity for two dimensional problems and $O(N^2)$ complexity for three dimensional problems [8]. In this paper we propose a new graph grammar based direct solver, delivering linear $O(N)$ time and memory complexity for computational problems with point singularities.

II. MODEL PROBLEM

The L-shape domain problem is a model academic problem formulated by Babuška in 1986 [9, 10], to test the convergence of the $p$ and $hp$ adaptive algorithms. The problem consists in solving the temperature distribution over the L-shape domain, presented in Fig. 1 with fixed zero temperature in the internal part of the boundary, and the Neumann boundary condition prescribing the heat transfer on the external boundary.

![Fig. 1. The L-shape domain model problem.](image1)

![Fig. 2. The solution of the L-shape domain model problem.](image2)
There is a single singularity in the central point of the domain (the gradient of temperature goes to infinity, compare Fig. 2), so the accurate numerical solution requires a sequence of adaptations in the direction of the central point.

The problem can be summarized as follows:

Find the temperature distribution

$$u : \mathbb{R}^2 \supset \Omega \ni x \rightarrow u(x) \in \mathbb{R}$$

such that

$$\sum_{i=1}^2 \frac{\partial^2 u}{\partial x_i^2} = 0 \text{ in } \Omega$$

with boundary conditions

$$u = 0 \text{ on } \Gamma_D$$

$$\frac{\partial u}{\partial n} = g \text{ on } \Gamma_N$$

with $n$ being the unit normal outward to $\partial \Omega$ vector, and being defined in the in the radial system of coordinates with the origin point $O$ presented in Fig. 1. Equation (5) is actually based on the exact solution to the L-shape problem.

$$g(r, \theta) = r^{\frac{3}{2}} \sin \left( \frac{\theta + \pi}{2} \right)$$

III. FICHERA PROBLEM

The Fichera problem constitutes the generalization of the L-shape domain problem into three dimensions. It can be summarized in the following way: Find the temperature distribution $u : \mathbb{R}^3 \supset \Omega \ni x \rightarrow u(x) \in \mathbb{R}$ over the domain presented in Fig. 3 such that

$$\sum_{i=1}^3 \frac{\partial^2 u}{\partial x_i^2} = 0 \text{ in } \Omega$$

with boundary conditions

$$u = 0 \text{ on } \Gamma_D$$

$$\frac{\partial u}{\partial n} = g \text{ on } \Gamma_N$$

with $n$ being the unit normal outward to $\partial \Omega$ vector, and $g$ is the exact solution of the L-shape problem.

IV. AUTOMATIC HP-ADAPTATION

A. Exponential Convergence

The presented problems have been solved by both self-adaptive $hp$-FEM and $h$-FEM (with constant polynomial approximation level $p=5$). Only $hp$-adaptive FEM is guaranteed to deliver exponential convergence of the numerical error with respect to the mesh size [2], [3]. See Table I to compare convergence rates for both methods.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1206</td>
<td>5.06</td>
</tr>
<tr>
<td>8261</td>
<td>3.18</td>
</tr>
<tr>
<td>13726</td>
<td>2.46</td>
</tr>
<tr>
<td>19191</td>
<td>2.23</td>
</tr>
<tr>
<td>35586</td>
<td>2.15</td>
</tr>
<tr>
<td>665</td>
<td>9.75</td>
</tr>
<tr>
<td>846</td>
<td>6.18</td>
</tr>
<tr>
<td>1093</td>
<td>4.58</td>
</tr>
<tr>
<td>1577</td>
<td>3.55</td>
</tr>
<tr>
<td>2247</td>
<td>2.91</td>
</tr>
<tr>
<td>3493</td>
<td>2.51</td>
</tr>
</tbody>
</table>

The basic idea behind $hp$-FEM has been explored further in this paragraph.
B. Mesh Refinements

Generally, the quality of the solution can be improved by the expansion of the approximation base. In FEM terms, this could be done thanks to two kinds of mesh refinements:

1) **P-refinement** – increase order of the basis functions on the elements where the error rate is higher than desired. More basis functions in the base mean smoother and more accurate solution but also more computations and the use of high-order polynomials often leads to undesirable side-effects (e.g. Runge effect).

2) **H-adaptation** – split the element into two or four in order to obtain finer mesh. This idea arose from the observation that the domain is usually non-uniform and in order to approximate the solution fairly some places require more precise computations than others, where the acceptable solution can be achieved using small number of elements. The crucial factor in achieving optimal results is to decide if a given element should be split into two parts horizontally, into two parts vertically, into four parts (both horizontally and vertically) or not split at all. The refinement process is fairly simple in 1D but in 2D and 3D many refinement rules to follow are being enforced.

C. Automated Hp-Adaptation Algorithm

Neither p- nor h-adaptation guarantee error rate decrease that is exponential with a step number. This can be achieved by combining these two methods. In order to identify the most sensitive areas at each stage dynamically, and improve the acceptable solution can be achieved using small number of elements. The crucial factor in achieving optimal results is to decide if a given element should be split into two parts horizontally, into two parts vertically, into four parts (both horizontally and vertically) or not split at all. The refinement process is fairly simple in 1D but in 2D and 3D many refinement rules to follow are being enforced.

```plaintext
1: function adaptive_fem(mesh_initial, err_desired)
2:   mesh_coarse = mesh_initial
3:   repeat
4:     u_coarse = compute solution on mesh_coarse
5:     mesh_fine = copy mesh_coarse
6:     divide each element of mesh_fine into two new elements
7:     increase order of functions on each element of mesh_fine by 1
8:     u_fine = compute the solution on mesh_fine
9:     for each element K of mesh_fine do
10:        err_K = compute error decrease rate on K
11:     end do
12:     mesh_adapted = copy mesh_coarse
13:     for each element K of mesh_adapted do
14:        if err_K > threshold * err_max then
15:           divide K
16:        end if
17:     end do
18:     enforce mesh_adapted integrity
19:     mesh_coarse = mesh_adapted
20:     until err_max < err_desired

Alg. 1. hp-adaptive PBI pseudocode
```

We iterate until the solution on the given mesh reaches satisfactory error rate (lines 3-20). First, we compute the solution on the initial mesh, called coarse mesh. Next, we create its copy called fine mesh and perform both h- (line 6) and p-refinement (line 7) on each element K. Then, we compute the solution fine mesh and for each element K we evaluate relative error decrease. If it is satisfactory (here we can assume threshold = 0.3, see line 14), we keep the hp refinement on that element, since it was a justified decision. Otherwise, we skip the refinement for such element. More details can be found in [2].

V. GRAPH GRAMMAR MODEL

The input for the solver algorithm is the locally refined computational mesh represented as a graph. The mesh is obtained by executing a sequence of graph grammar productions, summarized in Fig. 6 and 7.

![Fig. 6. Graph grammar production for generation rectangular finite element](image)

The computational mesh is further h-refined, which is expressed by graph grammar production summarized in Fig. 8. Selected rectangular elements are broken into 8 new son elements with 12 new faces.

In addition to that, the solver algorithm obtains a sequence of element matrices, one matrix for each sub-graph of the mesh representing a single finite element, resulting from discretization of the computational problem. The solver algorithm browses the graph representation of the mesh from bottom elements up to the root elements, and it merges the element matrices into only one frontal matrix. It first identifies fully assembled nodes located within each level of the graph representation of the mesh, eliminates them, and then it iterates the process by going up to the next level. This pattern for elimination ensures that the size of a single frontal matrix involved in the solver algorithm remains constant.

The solver algorithm is expressed as graph grammar productions coloring graph nodes, as it is presented in Fig. 9, 10 and 11.
VI. LINEAR COMPUTATIONAL COST OF THE SOLVER ALGORITHM

Since the cost at each step (level of the elimination tree) is constant, the total cost of the algorithm is proportional to the number of levels, which by grid construction is proportional to the number of unknowns. As a result, we obtain a solver algorithm with linear computational cost with respect to the number of unknowns.

This theoretical estimation has been verified experimentally, as it is presented in Fig. 12. It must be also clearly stated that the theoretical proof of the linear cost has been so far conducted only for h-FEM with fixed $p$ only. For hp-FEM, where $p$ may be different for each element, linear complexity has not been proven yet. On the other hand, experimental results show that solver’s complexity is for hp-FEM is very close to linear, compare Fig. 13.

Although the linear solver code that was used to produce the results was only a proof-of-concept, not optimized implementation, it already has delivered very promising performance.

The presented linear cost solver can help to dramatically lower the computational intensity of the existing h- and hp-FEM solutions. In terms of future work, it is important to transform the solver algorithm into efficient production code that could be easily applied to the large scope of problems.
Fig. 11. Coloring of graph nodes for elimination of the top level in the adaptive mesh. This time both red (internal) and yellow (boundary) nodes are fully assembled and can be eliminated.

Fig. 12. Linear computational cost of the h-adaptive solver algorithm

Fig. 13. Almost linear computational cost of the h-adaptive solver algorithm

REFERENCES


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A graph grammar model of the hp adaptive three dimensional Finite Element Method. P. 1 / Anna Paszyńska, Ewa Grabiska, Maciej Paszynski // Fundamenta Informaticae ; 2012 vol. 114 no. 2 s. 149–182 IF: 0.522

A graph grammar model of the hp adaptive three dimensional Finite Element Method. P. 2 / Anna Paszyńska, Ewa Grabiska, Maciej Paszynski // Fundamenta Informaticae ; 2012 vol. 114 no. 2 s. 183–201 IF: 0.522

Graph grammar based model for three dimensional multi-physics simulations / Maciej Paszynski, Anna Paszyńska, Robert Schaefer, Advances in intelligent modeling and simulation : simulation tools and applications, Berlin ; Heidelberg : Springer-Verlag, 2012, s. 299–324

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