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PARALLELIZABILITY OF TASKS USING SUPERCOMPUTER TO SOLVE LARGE TASKS OF CIVIL ENGINEERING - A CASE STUDY

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ABSTRACT

Supercomputers are widely used across variety of industries. Civil Engineering methods of numerical modelling are conservative and new technologies are used only occasionally. As numerical models become more complex with more detailed material models and a more extensive construction model, the limits of standard workstations are often reached. When a large task with many unknowns and nonlinearities needs to be solved, the demands on hardware requirements are high. In such cases supercomputers are convenient because they allow to solve larger tasks then a standard workstation Low computational time is another advantage of a supercomputer. Finally, the supercomputer doesn´t need a huge investment from the user, because only computing time is rented. Appropriate resource allocation is essential to maximize the computational potential of a supercomputer. The task in this article is aimed on a soil-foundation interaction. The Ansys HPC commercial software was used for the calculations on the Anselm cluster in the National Supercomputing Center IT4Innovations in VSB-Technical University of Ostrava. The optimal method of resources allocation was observed and discussed with regard to task size and a calculation time. The article consists of two examples. First example was computed on 16 nodes with the 16 Ansys HPC licenses with various methods of resources allocation. The second example evaluated using all available HPC licences in the National Supercomputing Center IT4Innovations. The maximal possible task size was evaluated in all used methods.

Keywords: ansys, finite element method, layered half-space, soil modelling, supercomputer.

INTRODUCTION

Numerical modelling of soil-structure interaction entails uncertainties of solution including choice of computational model of a construction, of a soil and their mutual interaction. The choice of computational model of building materials like concrete or steel is based on their uniformed parameters and characteristics which are approximated same in the whole volume and can be assumed quite precisely based on normalized classes. The biggest issue is related to the soil model because the soil is compound of heterogeneous particles with different characteristics mixed and distributed unevenly in different uniformity and in layers with uneven widths. Detailed description of geological profile under the construction side is needed to obtain precise calculation. The input parameters are not very precise even with this knowledge and the soil modelling alone brings uncertainties about a size of the soil model, type of a calculation model or its interaction with structure. All these parameters have huge impact to the computed results. Combination of experimental testing and numerical modelling is crucial part of deepening the theoretical basis and developing new procedures.

Experimental testing and studies are performed all over the whole world and provide the deformations of the soil trough the concrete slab (Tomasovicova and Jendzelovsky, 2017), (Cajka, Labudkova and Mynarcik, 2016), (Aboutalebi *et al.*, 2014), (Cajka, 2014) punching of slab (Halvonik and Majtanova, 2018), (Hegger *et al.*, 2007), (Kotsovou and Vougioukas, 2016), the tension inside of the soil (Hrubesova, Mohyla and Lahuta, 2018) and related processes such reinforced concrete from composite materials (Madi, Guenfoud and Nouaouria, 2014), response of foundations (Pavlou, 2015) as well as numerical modelling of partial problems as models of pre-stressed concrete (Abdul Rahman and Abed, 2017) or heterogeneous structures (Ninouh, 2014) or of construction near excavation (Chehade *et al.*, 2015) These recorded experiments are first and crucial part for developing computational models and confirming them.

It is essential to create a numerical model that takes into account the model in the context of its subsoil for design of monumental structures with difficult foundation conditions. Model designed this way is computationally demanding. Standard workstation is insufficient for solving such task. Therefore, use of supercomputer may be required to design larger structures (Patzák, 2012). To use supercomputers, it is necessary to adapt the task for possible use of parallel calculations (Adnane and Medromi, 2014). Certain limitations are related to use of supercomputer (Neuwirthova and Cajka, 2019). Some limitations are related to used cluster and others to computational program. Commercial software Ansys, which is widely used all over the world (Kralik, Rosko and Kralik, 2018), (Youbi and Rougui, 2015), needs specific way of allocating resources. Correct and reasonable method of allocation resources is essential to maximize the potential of supercomputers. Inconsiderate allocation can result in weeks of waiting to run the task or other complication. The situation is even more complex using Ansys software while allocation of HPC licenses are an important part of the system.

This article is focused on a case study of parallelizability of a task using supercomputer. The task is based on experimental test of concrete slab tested on special testing equipment. A numerical model is developed based on the experiment. The model is simplified to a soil model while neglecting all other parts.

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The article consists of two examples. First example was computed on 16 nodes with the 16 Ansys HPC licenses with various method of allocation resources. The maximal possible task size was evaluated for each method. The recommendations for allocation process of similar tasks are concluded at the end. The second example evaluated the largest possible task size using all available HPC licences in the National Supercomputing Center IT4Innovations.

METHODS

The experimental test was performed at the Faculty of Civil Engineering at VŠB - Technical University of Ostrava on a special testing equipment (Cajka and Labudkova, 2014). A representative numerical model of the experiment was created using finite elements. In order to run tasks on supercomputer the Anselm cluster in National Supercomputing Center IT4Innovations in the VSB-Technical University of Ostrava was selected. Ansys HPC was used to perform computing. Supercomputing calculations are limited by the number of available Ansys licenses and therefore the number of cores used for parallel computing (Neuwirthova and Cajka, 2019). There is an assumption that allocation of more cores than are actually used for parallel computing can positively affect the calculations. This assumption was verified in this article.

Experimental testing layout

The concrete slab was tested using special testing equipment (Cajka and Labudkova, 2014). The slab dimensions are 2000 x 2000 x 150 mm. A material is a plain concrete mixture class C25/30 (Figure-1). The slab was loaded by 25 kN through a distribution plate with dimensions of 400 x 400 mm. The load enlarged by 25 kN every 30 minutes was applied until maximal bearing capacity of the slab was reached (Figure-2). The failure occurred at force of 345 kN and 21.68 mm deformation.

Figure-1. Loading of the slab.

Figure-2. Broken slab.

Numerical model

A numerical model of the subsoil was based on the Boussinesq´s theory as linear elastic, isotropic, homogeneous. The Semi-infinite assumption in the Boussinesq theory was replaced by a cube of finite dimensions. All finite elements are linear hexahedrons.
The subsoil is fixed at its bottom side. Vertical displacements are allowed on the sides of the soil while horizontal displacements are fixed as shown in Figure-3. The Elastic modulus of the soil model was 6.8 MPa with the Poisson ratio 0.35. It was based on a static load test, which was performed before the actual experiment. The model is loaded by pressure according to the experiment. The actual slab was neglected in the model (Figure-4) as well as self-weight. The parameters remain constant throughout all computations.

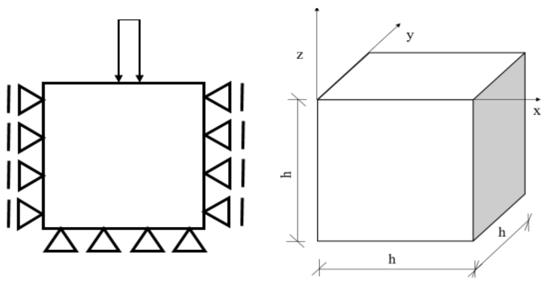

Figure-3. a -Assumed boundary conditions; b - geometry of parametric task.

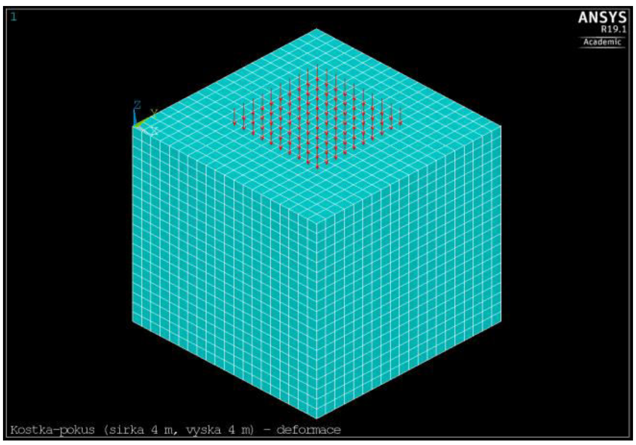

Figure-4. Typical numerical model layout. Cube with dimensions of 4 x 4 x 4 m with finite element size 0.2 m. Loaded by 345kN trough area of 2 m x 2 m.

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Anselm supercomputer

The Anselm cluster is one of two supercomputers located at National Supercomputing Center IT4Innovations in VSB-Technical University of Ostrava. This cluster is the smaller one but it is sufficient for civil engineering tasks.

The Anselm consists of 209 computational nodes. 180 of them are regular nodes. The rest are GPU accelerated, MIC accelerated, and fat nodes. Each of the regular nodes is a computer with 16 cores and at least 64GB of RAM memory. The calculations were carried out on the regular nodes.

An active account and an active project with nonzero computing resources are needed to be able to use one of the supercomputers. An allocation of resources is needed to submit a task. The number of nodes as well as the number of cores per node and the time of calculation had to be allocated in the standard allocation procedure for this study. In addition, the number of cores per node needed to perform the actual computing is required. For use of the Ansys HPC, an allocation of Ansys HPC licenses is required as well.

There are only 512 Ansys HPC licenses available at VSB-Technical University of Ostrava for both supercomputer clusters. Therefore, the calculation cannot be run on more than 512 cores. However, with 512 licenses shared amongst more users, allocation of all the licenses for a single user is practically impossible.

RESULTS AND DISCUSSIONS

It was proved (Neuwirthova and Cajka, 2019) that the main limiting element of a task size is lack of available memory. One way of counteracting this phenomenon is an allocation of extra cores which serve as a memory buffer. The unused but allocated cores are then called passive cores.

Selected task was computed on 16 cores. The used cores were set to 16 since a single node of the Anselm supercomputer carries 16 cores, as mentioned in the chapter II.3. Each allocated core requires one Ansys license; therefore 16 Ansys HPC licenses were used. The intention was to find the dependence of the distribution of the cores on different numbers of allocated nodes. Calculations were performed repeatedly using different amounts of allocated nodes. Therefore, various amounts of cores from each node were used for the calculations. The total amount of nodes remained uniform through all calculations.

Five variants of calculations were created to investigate the benefit of passive cores. The 16 cores were divided gradually through 1-16 nodes.

- One single node was used for the first case (marked as 1x16c). There are no passive cores in this case.
- Two nodes with eight active cores and eight passive cores on each node were used for the second case (marked as 2x8c).
- Four nodes with four active cores were used in the third case (marked as 4x4c).
- Eight nodes were allocated in the four case incorporating only two active cores per node (marked as 8x2c).
- Full 16 nodes were allocated the last case with 1 active and 15 passive cores per node (marked as 16x1c).

Computing times were recorded in each case for further comparison. The number of degrees of freedom of each task was recorded to track the parallelism of the task (Table-1, Table-5).

The largest task computed within first case (1x16c) has 512 000 degrees of freedom. Its calculation time was 245.7 seconds (Table-1). Any larger task could not be computed for insufficient memory.

Table-1. Time of calculation using 16 cores through 1 node (1x16c).

Size of the task [m x m x m]	Degrees of freedom	Time of calculation [s]
4	8 000	2.5
6	27 000	2.2
8	64 000	6.8
10	125 000	19.9
12	216 000	52.3
14	343 000	119.3
16	512 000	245.7

The largest task using two computational nodes (variant 2x8c) had 1 million degrees of freedom (Table-2). This task was almost two times larger (195.3%) than the largest task from the 1x16c case.

The largest solved task using 4 nodes (4x4c) had 1 331 000 degrees of freedom (Table-3).

Table-2. Time of calculation using 16 cores through 2 nodes (2x8c).

Size of the task [m x m x m]	Degrees of freedom	Time of calculation [s]
4	8 000	2.2
6	27 000	3.6
8	64 000	8.6
10	125 000	22.0
12	216 000	54.1
14	343 000	116.3
16	512 000	238.1
18	729 000	447.6
20	1 000 000	805.2

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Table-3. Time of calculation using 16 cores through 4 nodes (4x4c).

Size of the task [m x m x m]	Degrees of freedom	Time of calculation [s]
4	8 000	1.3
6	27 000	2.7
8	64 000	7.4
10	125 000	20.3
12	216 000	51.7
14	343 000	110.9
16	512 000	229.4
18	729 000	436.2
20	1 000 000	777.6
22	1 331 000	1422.8

The largest solved task on 4 nodes (8x2c) had 1.72 million of degrees of freedom (Table-4).

Table-4. Time of calculation using 16 cores through 8 nodes (8x2c).

Size of the task [m x m x m]	Degrees of freedom	Time of calculation [s]
4	8 000	0.8
6	27 000	2.0
8	64 000	6.6
10	125 000	18.7
12	216 000	49.2
14	343 000	110.4
16	512 000	222.7
18	729 000	426.5
20	1 000 000	762.1
22	1 331 000	1370.4
24	1 728 000	2338.5

The largest allocated amount of nodes was 16 (Table-5) with 16 active cores and 240 passive cores. This case had the largest memory buffer. The largest task using 16nodes (16x1c case) had 2 197 000 degrees of freedom. The task is larger by 469 000 degrees of freedom when compared to the degrees of freedom to the 8x2c case.

Table-5. Time of calculation using 16 cores through 16 nodes (16x1c).

Size of the task [m x m x m]	Degrees of freedom	Time of calculation [s]
4	8 000	0.5
6	27 000	1.7
8	64 000	6.0
10	125 000	17.7
12	216 000	49.1
14	343 000	108.1
16	512 000	224.1
18	729 000	426.2
20	1 000 000	768.2
22	1 331 000	1390.3
24	1 728 000	2365.3
26	2 197 000	3606.7

The numbers of degrees of freedom were compared for the largest tasks of the 1x16c and 16x1c cases. The task from the 16x1c case is larger by 1 685 000 degrees of freedom than the 1x16c case.

It can be concluded that additional allocation of passive cores has a positive effect on the maximal possible size of the computed task.

The results were summarized in the Table-6. First three columns recap previously published results. The results are limited to maximal solved tasks. The fourth column shows an absolute gain. The absolute gain was computed (1) as an increase between the number of degrees of freedom of the largest task of the 16x1c case and the largest tasks from the other cases (1x16c, 2x8c, 4x4c and 8x2c). The 16x1c case was assumed as base for all calculations. The last column shows a relative gain between each two consecutive cases (2).

$$I_A = \frac{D_{f(i)} \cdot 100}{D_{f(16x1c)}} \quad (1)$$

$$I_{Ri} = \frac{D_{fi} \cdot 100}{D_{f(i-1)}} \quad (2)$$

Table-6. Maximum degrees of freedom based on allocated computational nodes.

Variant	Degrees of freedom D_f	Absolute gain I_A [%]	Relative gain I_R [%]
1x16c	512 000	23.3	
2x8c	1 000 000	45.5	195.3
4x4c	1 331 000	60.5	133.1
8x2c	1 728 000	78.6	129.8
16x1c	2 197 000	100.0	127.1

The largest relative gain is between the 1x16c and the 2x8c cases. Then it decreases. The size of the task is increased twice between the 2x8c and the 16x1c cases. Using the 16x1c case can be very constructive for solving larger tasks if there are insufficient Ansys HPC licenses.

The measured times and sizes of tasks (Table-6) were evaluated in a graphical comparison (Figure-5). The vertical axis shows the degrees of freedom. The horizontal axis shows the calculation times in logarithmic scale.

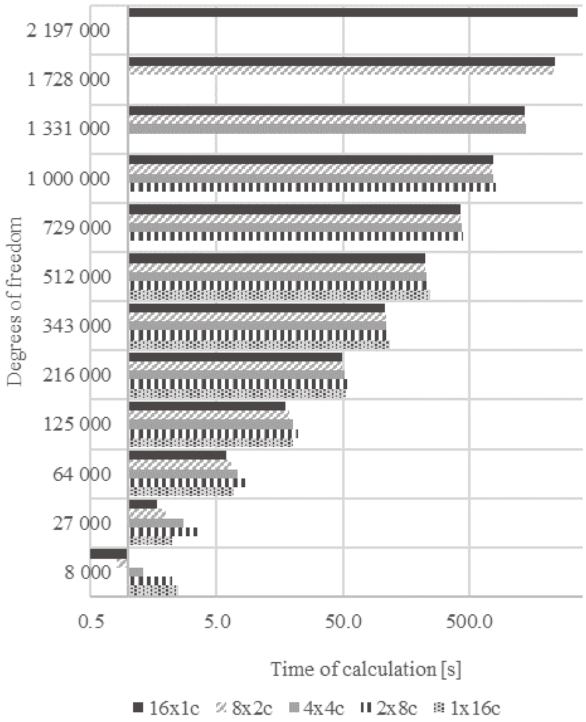

Figure-5. Graphical evaluation of results.

Calculation times are significantly faster on the 16 nodes despite the necessary communication between the nodes in small tasks (125 000 degrees of freedom). The times become more balanced with increased size of the task.

The time of the calculations of the middle size tasks are balanced across all cases, therefore allocation of smaller amount of nodes might seem sufficient. It is worth noting that some cases can compute larger tasks than the others. e.g. allocation of more cores completes the task calculation more reliably.

The graphical comparison in Figure-6 reflects the total amount of all allocated cores across all cases. The aim of the investigation was the dependence of the task size, i.e. number of degrees of freedom on an amount of allocated cores. The absolute gain from Table-6 is also provided in the graph.

The horizontal axis shows the number of allocated cores is in logarithmic scale. The left vertical axis shows the number of degrees of freedom and the right vertical axis shows the absolute gain in logarithmic scale.

Significantly larger tasks were computed by increasing allocated sources. Passive cores have an important role of a memory buffer and should cover at least half of all allocated cores.

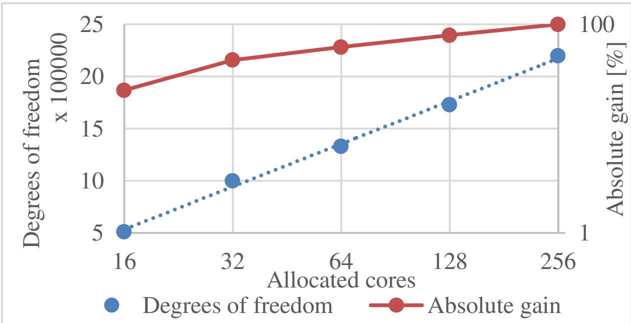

Figure-6. Graphical evaluation of results in terms of total allocated cores.

Application to larger task

The maximal task size on the Anselm supercomputer was calculated before (Neuwirthova and Cajka, 2019). It was 17.5 million of degrees of freedom (Tab. VII) using all 512 available HPC Ansys licenses distributed on 32 nodes. However, allocating all 512 licenses is a tedious process and it is accomplished very rarely.

Using data from this research, the original research task (Neuwirthova and Cajka, 2019) (32 nodes) was computed with different amounts of HPC licenses-128 and 256 respectively (Tab. IX).

In another task, 128 licenses and full 64 were used. (Table-8). It was possible to compute 24 million unknowns. The measured data were evaluated in a graph (Figure-7).

It is obvious that the maximal size of a computed task depends rather on the total amount of allocated cores (both passive and active) than on the number of licenses. The number of allocated licenses only affects the total solution time.

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Table-7. Maximal task using 512 licenses on 32 nodes on HPC.

Model size		Time of calculation	
Dimension [m x m x m]	**Number of degrees of freedom**	**[min]**	**[s]**
30	10 125 000	11	7
32	12 288 000	21	17
34	14 739 000	26	0
36	17 496 000	37	33

The conclusion from the previous work (Neuwirthova and Cajka, 2019) needs to be revised. The largest possible task on the Anselm supercomputer would require using all 512 HPC licenses with 128 nodes, which is politically impossible.

The Salomon cluster consists of 576 regular compute nodes. Therefore, theoretical allocation of the 512 nodes with 512 licenses (one active core per node) would lead to the largest possible task computed on the Ostrava supercomputers.

Table-8. Maximal task using 128 licenses on 64 nodes on HPC.

Model size		Time of calculation	
Dimension [m x m x m]	**Number of degrees of freedom**	**[min]**	**[s]**
30	10 125 000	21	17
32	12 288 000	30	51
34	14 739 000	48	56
36	17 496 000	75	11
38	20 577 000	107	46
40	24 000 000	134	7

Table-9. Maximal task using 128 and 256 licenses on 32 nodes on HPC.

Model size	Time of calculation 128 cores		Time of calculation 256 cores	
Number of degrees of freedom	**[min]**	**[s]**	**[min]**	**[s]**
10 125 000	21	46	13	46
12 288 000	31	13	27	53
14 739 000	55	33	31	41
17 496 000	98	37	46	57

When an in-core memory is exhausted, an out-of-core memory is required for the calculation. The calculation using an out-of-core memory is way slower since the use of the external memory extends the communication between nodes.

The out-of-core memory impact is apparent on the tasks with 32 and 64 nodes and 128 licenses (Figure-7). There was a 30% difference in computational time between the two while solving 17.5 million unknowns since the 32 nodes calculation had insufficient in-core-memory, but both tasks took the same time for solving 10 million unknowns.

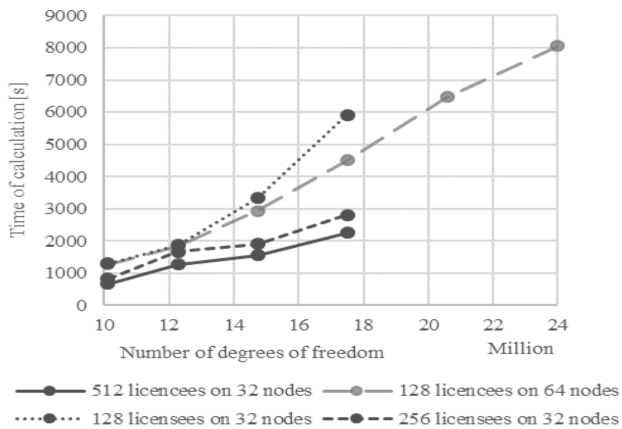

Figure-7. Comparison of calculations.

CONCLUSIONS

The main limiting element of a task size is lack of available memory. The allocation of extra cores as a memory buffer was used to counteract this phenomenon. Several ways of resource allocation, each with a different amount of passive cores was examined and compared in this paper. It was inspected how it affects the maximal task size as well as the influence to the computational time.

The task was computed on the 16 cores coupled with the 16 Ansys HPC licenses. Calculations were performed repeatedly using different amounts of allocated nodes using various amounts of cores from each node were used for the calculations. The total amount of nodes remained uniform through all calculations. Five allocation cases were compared.

The larger task can be calculated while using more passive cores. This approach reduces usage of valuable HPC licensees.

The defined conclusions were applied within second part of this paper to the earlier authors' work (Neuwirthova and Cajka, 2019) examining the maximum size of a task using the supercomputer Anselm. Same procedure was repeated as in the original paper (Neuwirthova and Cajka, 2019) while lower amount of HPC licenses were allocated. Three allocation arrangements were tested. First two calculations ran parallel on 32 nodes and 64 nodes respectively using 128 HPC licences. The third case runs on the 32 nodes using 256 HPC licences.

Allocation of HPC licences for each allocated core is not the optimal solution. This way of allocation is not economical, user waits longer for the calculation start and the calculation time is not so much better with comparison to other allocation procedure. A least 50% of allocated cores needs to be passive for optimal allocation.

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