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Summary of Dissertation

Computational aspects of the FEM for solving boundary value problems

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Abstrakt

Předkládaná disertační práce *Výpočetní hlediska řešení okrajových úloh použitím MKP* se zabývá použitím metody konečných prvků (MKP) v úlohách termomechaniky. MKP se běžně používá k prostorové diskretizaci parciálních diferenciálních rovnic popisujících takové úlohy. Výsledkem je soustava obyčejných diferenciálních rovnic, která se některým ze standardních postupů numerické integrace převede na soustavu algebraických rovnic, již je nutné řešit v každém časovém kroku. Pokud je tato soustava nelineární nebo příliš velká, mohou při jejím řešení nastat problémy.

Práce sestává ze dvou částí. První část se zabývá nelineární úlohou vedení tepla v pevném tělese, cílem je zlepšit numerickou stabilitu výpočtu. Modifikovaná Newton-Raphsonova metoda je rozšířena o lineární akceleraci (line-search) a jsou navrženy dva způsoby rozhodování, kdy se má aktualizovat tangenciální matice. Pro obě varianty se zjišťuje vliv lineární akcelerace na zrychlení konvergence a zvýšení numerické stability.

Druhá část se věnuje použití metod rozkladu oblasti bez překrývání (nonoverlapping domain decomposition). Práce se soustředí především na metodu BDDC (Balancing Domain Decomposition by Constraints) a její efektivní implementaci pro řešení velkých soustav lineárních rovnic v úlohách elasticity.

Algoritmy uváděné v obou částech byly zabudovány do standardního systému používajícího MKP a byly vyzkoušeny na úlohách inženýrské praxe v oblasti nelineárního vedení tepla a lineární elasticity.

Abstract

The thesis *Computational aspects of the FEM for solving boundary value problems* The thesis is devoted to the computational aspects of the Finite Element Method (FEM) applied to problems of thermomechanics. FEM is a commonly used method for spatial discretization of partial differential equations that govern these problems. The resulting system of ordinary differential equations is then numerically integrated using standard techniques, which leads to the solution of the system of algebraical equations at every time step. Difficulties can occur when the system to be solved is either nonlinear, or very large, or both.

The thesis has two main sections. The first section treats nonlinearity in heat conduction in solids with the aim to enhance the numerical stability of the computation. The common Modified Newton-Raphson method is complemented by line-search. Two decision criteria of when to update the tangential matrix are proposed and compared with regard to better convergence and numerical stability properties. They are compared also to the Newton-Raphson method without line-search.

The second section deals with the application of nonoverlapping domain decomposition methods, namely Balancing Domain Decomposition by Constraints (BDDC). The aim is to reduce computational time needed for solving large problems in elasticity.

Algorithms discussed in both sections were implemented using parts of a standard FEM software and tested on practical problems in nonlinear heat conduction and linear elasticity.

Contents

Abbreviations

BDD	Balancing Domain Decomposition
BDDC	Balancing Domain Decomposition by Constraints
DD	Domain Decomposition
FEM	Finite Element Method
FETI	Finite Element Tearing and Interconnecting
FETI-DP	Finite Element Tearing and Interconnecting, Dual–Primal
GMRES	Generalized Minimal Residual Method
LS	Line Search
MNR	Modified Newton-Raphson method
PCG	Preconditioned Conjugate Gradients
PDE	Partial Differential Equations
ODE	Ordinary Differential Equations
SPD	Symmetric Positive Definite

Chapter 1

Introduction

1.1 Motivation

The thesis is devoted to computational aspects of the Finite Element Method (FEM) applied to problems of thermomechanics. FEM is a commonly used method for a spatial discretization of partial differential equations that govern these problems. The resulting system of ordinary differential equations is then numerically integrated using standard techniques, which leads to the solution of a system of algebraic equations at every time step. Difficulties can occur when the system to be solved is either nonlinear, or very large, or both.

The thesis has two main parts. The first part treats nonlinearity in heat conduction in solids with aim to enhance the numerical stability and efficiency of the computation.

The second part deals with an application of nonoverlapping domain decomposition methods, especially Balancing Domain Decomposition by Constraints (BDDC).

1.2 State of the art

Numerical solution of problems in linear and nonlinear mechanics often leads to solving of large, sparse, unstructured linear systems.

Direct methods are often applied to solution of these systems, like a frontal algorithm by IRONS [10] – a variant of the Gauss elimination especially designed for the FEM. Its more recent generalization suitable for parallel computers, a multifrontal algorithm, was proposed by DUFF AND REID [6]. The direct solvers usually need a lot of memory and also computational time increases fast with data size.

Iterative solvers like Preconditioned Conjugate Gradients (PCG) are less expensive in terms of memory and computational time, but they do not guarantee convergence for ill-conditioned systems. The convergence rate of iterative methods deteriorates with growing condition number of the solved linear system. The condition number of linear systems obtained by discretization of many problems in mechanics typically grows as $O(h^{-2})$, where h is the meshsize of the triangulation, so the larger the problem, the better preconditioner is usually needed.

Linear systems derived from huge problems are hard to solve by direct solvers because of their size and their lack of structure. They are also hard to solve by iterative solvers because of their large condition number. Most efficient recent methods use combination of both approaches, often together with some hierarchy in meshing. Domain Decomposition (DD) methods are powerful tools to handle large linear systems arising from the discretization of differential equations. They have many common traits with another efficient tool, the multigrid methods.

Historically, they emerged from the analysis of partial differential equations, beginning with the work [26] of SCHWARZ in 1870. A general approach of DD methods is to decompose the underlying domain into subdomains and use this information for splitting the original large linear system into number of smaller and numerically more convenient ones. Most often DD methods are used as very efficient preconditioners for an iterative metod like PCG. The intrinsic parallelism of DD algorithms and the straightforward distributability of the associated data makes this approach suitable for parallel computing.

1.3 Aims of the work

The main concern of the presented Ph.D. thesis are aspects of the FEM applied to problems of thermomechanics, namely treating slow convergence and stability of iterative methods in nonlinear problems and treating large, sparse, unstructured linear systems.

The common tool for dealing with nonlinearity in algebraic equations is the Newton-Raphson method or the Modified Newton-Raphson method. These are iterative methods which convert a solution of a nonlinear algebraic system to the successive solution of linear algebraic systems. Sometimes problems occur concerning slow convergence and numerical stability of these methods. Several algorithms are tested for handling of these problems.

Domain decomposition methods represent a promising way of parallelization of problems in thermomechanics.

1.4 Commentary

The subject of the presented Ph.D. thesis consists of main results achieved by the author and published in selected articles:

- **[1A]** Čertíková, M. and Dobiáš, J.: Numerical Solution of Nonlinear Heat Conduction on Solids, *Engineering Mechanics 4, 2 (1997)* , 95–106.

- **[2A]** Čertíková, M.: Parallel Implementation and Optimization of Balancing Domain Decomposition in Elasticity, *Science and Supercomputing in Europe (2006)* , 591–596.

- **[2B]** Burda, P., Čertíková, M., Novotný, J. and Šístek, J.: BDDC method with simplified coarse problem and its parallel implementation, *Proceedings of MIS 2007, Josefův Důl, Czech Republic, January 13–20* , 3–9.

- **[2C]** Šístek, J., Burda, P., Čertíková, M. and Novotný, J.: On Construction of The Coarse Space in the BDDC Method, *Proceedings of Seminar Programs and Algorithms of Numerical Mathematics 14, PANM'08, Dolní Maxov, Czech Republic, June 1 – 6 (2008)* , 177–184.

- **[2D]** Šístek, J., Novotný, J., Mandel, J., Čertíková, M. and Burda, P.: BDDC by a frontal solver and stress computation in a hip joint replacement, *Math. and Comp. Simulation (Elsevier), spec. issue devoted to Computational Biomechanics and Biology 2009, in print*.

The full text of these articles is involved in the Appendix.

Chapter 2

Nonlinear heat conduction problem

2.1 Problem to be solved

PDE governing nonstationary nonlinear heat conduction problem can be written as

$$\rho\, c\, \frac{\partial T}{\partial t} - \operatorname{div}(\lambda \operatorname{grad} T) = g,$$

where T represents unknown temperature and t represents time. The thermophysical parameters c – heat capacity, ρ – mass density, and λ – heat conductivity, and the right-hand side g – density of heat sources, can depend not only on spatial coordinates, but also on the temperature: $c \equiv c(x,T)$, $\rho \equiv \rho(x,T)$, $\lambda \equiv \lambda(x,T)$, and $g \equiv g(x,T)$.

The PDE is transformed to the weak form and discretized with regard to spatial unknowns by means of FEM, which results in a system of ODEs. Its subsequent numerical integration using a general one-step method (LAMBERT [17]) leads to the system of algebraic equations, which can be formally written as

$$\mathbf{K}_{j+1}\, \mathbf{u}_{j+1} = \mathbf{q}_{j+1}\,. \tag{2.1}$$

The system has to be solved at every time step $\mathbf{t}_{j+1}$ for unknown vector $\mathbf{u}_{j+1}$. Both the matrix $\mathbf{K}_{j+1} \equiv \mathbf{K}_{j+1}(\mathbf{u}_{j+1})$ and the right-hand side $\mathbf{q}_{j+1} \equiv \mathbf{q}_{j+1}(\mathbf{u}_{j+1})$ can in general depend on the unknown vector $\mathbf{u}_{j+1}$ (beyond an explicit dependence on $\mathbf{t}_{j+1}$ and values computed at the previous time step $\mathbf{t}_j$). This dependence of $\mathbf{K}_{j+1}$ and $\mathbf{q}_{j+1}$ on $\mathbf{u}_{j+1}$ makes the system nonlinear. The nonlinearity originates in dependence of thermophysical material and heat transfer properties on temperature and also can be caused by certain types of boundary conditions, for instance radiation.

Components of $\mathbf{u}_{j+1}$ are often called *degrees of freedom* and they represent values of temperature at time $\mathbf{t}_{j+1}$ at mesh nodes of an underlying domain. Components of the right-hand side $\mathbf{q}_{j+1}$ can be interpreted as a heat flux concentrated to mesh nodes.

2.2 Modified Newton-Raphson method

The modified Newton-Raphson method (MNR) is a common iterative technique for solving nonlinear systems of algebraic equations (GRIFFITHS AND SMITH [9]). Assume that equation

(2.1) is solved at time step $\mathbf{t}_{j+1}$. Let us drop the index $_{j+1}$ in the rest of this section and let us emphasize the nonlinearity by rewritting the equation (2.1) as

$$\mathbf{K}(\mathbf{u})\,\mathbf{u} = \mathbf{q}(\mathbf{u})\,. \tag{2.2}$$

One iterative step of the full Newton-Raphson method for equation (2.2) then can be formulated as to find $\mathbf{u}^{i+1}$ such that

$$\mathbf{J}(\mathbf{u}^i)\,(\mathbf{u}^{i+1} - \mathbf{u}^i) = \mathbf{q}(\mathbf{u}^i) - \mathbf{K}(\mathbf{u}^i)\mathbf{u}^i\,, \tag{2.3}$$

where $\mathbf{J}(\mathbf{u}^i)$ is the Jacobian (tangential) matrix of the residual $\mathbf{K}(\mathbf{u}^i)\mathbf{u}^i - \mathbf{q}(\mathbf{u}^i)$. The iteration process is usually started with $\mathbf{u}^0 = \mathbf{u}_j$ and the sequence $\mathbf{u}^i$ is expected to converge to $\mathbf{u}_{j+1}$. The iteration process (2.3) requires the forward Gauss elimination to be performed in every iteration.

In MNR the system matrix of equation (2.3) is kept unchanged for several iterations in order to reduce the number of forward Gauss eliminations, usually at the expense of slower convergence. One iterative step of MNR can be formulated as to find $\mathbf{u}^{i+1}$ such that

$$\mathbf{J}(\mathbf{u}^m)\,(\mathbf{u}^{i+1} - \mathbf{u}^i) = \mathbf{q}(\mathbf{u}^i) - \mathbf{K}(\mathbf{u}^i)\mathbf{u}^i\,, \tag{2.4}$$

where $m \in < 0, \ldots, i >$ is fixed for several iterations.

BATHE [2] recommends using the matrix $\mathbf{K}(\mathbf{u}^m)$ as a good approximation of $\mathbf{J}(\mathbf{u}^m)$, so the equation

$$\mathbf{K}(\mathbf{u}^m)\,(\mathbf{u}^{i+1} - \mathbf{u}^i) = \mathbf{q}(\mathbf{u}^i) - \mathbf{K}(\mathbf{u}^i)\mathbf{u}^i \tag{2.5}$$

is solved instead of (2.4).

The question remains as when to update m to the current value of i and recompute the matrix $\mathbf{K}(\mathbf{u}^m)$ on the left-hand side of (2.5). One possibility is to update m in every M-th iteration step (the choice of $M = 1$ leads to the method of successive approximations for equation (2.2)). Another possibility is to choose M as an upper bound for the number of iterations between two successive updates and update m on the basis of actual convergence rate.

2.3 Line Search

The Line Search (LS, LEE [19]) is a general method that applies to any iterative method. In every iteration step of (2.5) we can try to improve the actual approximation $\mathbf{u}^{i+1}$ of the solution of (2.2) by searching a better approximation $\mathbf{u}(\beta)$ on the line determined by the last two approximations $\mathbf{u}^i$, $\mathbf{u}^{i+1}$ as

$$\mathbf{u}(\beta) = \mathbf{u}^{i+1} + \beta(\mathbf{u}^{i+1} - \mathbf{u}^i)\,. \tag{2.6}$$

The appropriate β is obtained as a root of the real function

$$r(\beta) = (\mathbf{u}^{i+1} - \mathbf{u}^i) \cdot \mathbf{R}(\mathbf{u}(\beta))^{\mathrm{T}}\,, \tag{2.7}$$

where the dot denotes the scalar product and $\mathbf{R}(\mathbf{u}) = \mathbf{K}(\mathbf{u})\,\mathbf{u} - \mathbf{q}(\mathbf{u})$ is the residual of (2.2). The root need not be computed too accurately, it is suitable to take any β satisfying

$$|r(\beta)| < \epsilon\,|r(-1)|\,, \tag{2.8}$$

with ϵ chosen somewhere in the interval $< 0.3\,,\, 0.5 >$ (LEE [19]).

If a suitable β is found and if in addition $|\mathbf{R}(\mathbf{u}(\beta))| < |\mathbf{R}(\mathbf{u}^{i+1})|$ in the Euclidean norm, the approximation $\mathbf{u}(\beta)$ is chosen instead of $\mathbf{u}^{i+1}$ and the iteration process (2.5) continues by the next step. The line search is carried out only if $\mathbf{u}^{i+1}$ itself is not "good enough" in a sense that the condition (2.8) is not fulfilled for $\beta = 0$.

2.4 Results

The methods described in paragraphs **2.2** and **2.3** above were incorporated into standard FEM software package and extensively tested on practical problems.

Three algorithms were tested and compared:

1. The method (2.4) with m updated after every M iteration steps. No line search.
2. The method (2.4) with m updated if either $|\mathbf{R}(\mathbf{u}^i)| < |\mathbf{R}(\mathbf{u}^{i+1})|$ or M iteration steps passed since the last updating. No line search.
3. The method (2.4) with m updated if either $|\mathbf{R}(\mathbf{u}^i)| < |\mathbf{R}(\mathbf{u}^{i+1})|$ or M iteration steps passed since the last updating. The line search was added.

It was found that it is difficult to estimate in advance the appropriate number of iterations between two successive updating in Algorithm 1 and that the wrong choice sometimes causes even failure of the convergence of the method.

On the contrary, if the time of updating of the tangential matrix was controlled by the norm of residual as in Algorithms 2 and 3, both the stability of the method and the number of iterations were improved. Our experience shows that the number M should be selected big enough not to interfere with the residual criterion.

The best results were achieved with Algorithm 3 with the line search involved, which lowered not only the number of iterations, but also the number of updates of the tangential matrix.

A typical performance of these three algorithms is demonstrated on three illustrative examples presented in article **[1A]** given in Appendix of the Ph.D. thesis. Table 2.1 bellow shows this typical preformance on one of the examples. The three columns of the table represent the three algorithms described above, the table compares the total number of iterations of MNR and the number of Gauss factorizations (the numbers are separated by a slash).

M	Algorithm 1	Algorithm 2	Algorithm 3
1	10 / 10	10 / 10	15 / 15
2	17 / 9	14 / 7	24 / 12
3	34 / 12	11 / 5	15 / 6
4	27 / 9	10 / 4	25 / 9
5	34 / 7	59 / 21	18 / 6
6	28 / 5	20 / 7	11 / 4
7	58 / 9	13 / 4	12 / 4
8	27 / 4	13 / 4	12 / 4
9	41 / 5	14 / 4	12 / 4
10	49 / 5	14 / 4	12 / 4
11	43 / 4	14 / 4	12 / 4

Table 2.1: A comparison of the results of the three algorithms on a nonlinear problem: The total number of iterations of MNR / The number of Gauss factorizations

Full text of the article **[1A]** is involved in Appendix of the Ph.D. thesis.

Chapter 3

Substructuring DD methods

Basic ideas of an important class of the DD methods, namely the *substructuring DD methods*, sometimes also called *nonoverlapping*, are described here, with an emphasis on two of the recent leading DD algorithms, BDDC and FETI-DP.

Substructuring methods rely on splitting the domain into nonoverlapping subdomains, or substructures, tied-up together by means of some interface communication.

There are two basic approaches to interconnection among the subdomains, a *primal* and a *dual* one (see Section 3.4), with the interface problem formed by a Schur complement problem. The Schur complement problem and its decomposition is described in detail in Sections 3.2 and 3.3, respectively. DD methods are generally used as preconditioners; that is why they are formulated here as Richardson methods. In Section 3.6 the general use of Richardson methods as preconditioners is described.

Troughout this text we assume that investigated domains are already meshed and divided into nonoverlapping subdomains and the original equations are already discretized by means of FEM. For a better insight, algebraic formulations are illustrated on an example of a 2D Poisson equation, one of the most common partial differential equations encountered in various areas of engineering.

DD methods have developed a lot during past twenty years and the literature of the field is quite extensive. Let us mention just some important summary texts here. A good introduction to the field is the monograph by LE TALLEC [18]; it introduces the model problem in solid mechanics, presents its mathematical formulation and describes the principles of the DD methods in several forms: differential, operator and matrix form. The monograph by TOSELLI AND WIDLUND [28] is a modern comprehensive 400-pages book with a list of nearly 500 related references. An excellent textbook on iterative methods generally is SAAD [25], a whole chapter in his textbook is devoted also to DD. A comprehensive overview and comparison of substructuring DD methods can be found in SOUSEDÍK [27]. A more practical point of view on domain decomposition methods is presented by KRUIS [16]. In a recent book [5] by DOSTÁL, application of FETI-DP method to solution of a coercive variational inequality can be found together with a wide introduction to the field, developed in several chapters starting with linear algebra.

3.1 Problem to be solved

After a discretization of a linearized partial differential equation of elliptic type in a given domain Ω, a system of linear algebraic equations

$$\mathbf{K}\mathbf{u} = \mathbf{f} \tag{3.1}$$

is to be solved with a matrix $\mathbf{K}$ and a right-hand side $\mathbf{f}$ for the unknown vector $\mathbf{u}$. Components of $\mathbf{u}$ are often called *degrees of freedom*.

The discretizad domain is split into nonoverlapping subdomains so that every element belongs to exactly one subdomain. Two types of nodes can now be distinguished: *interior nodes* belonging to just one "closed" subdomain and *interface nodes* belonging to boundary of more than one subdomain.

3.2 Schur complement problem for the interface

The Schur complement problem represents a reduction of the original problem to the *interface unknowns* (unknowns linked to the interface nodes) by eliminating all *interior unknowns* (unknowns linked to the interior nodes); this reduction is sometimes called a *static condensation*.

In order to get a suitable structure for Schur complement system, let us rearrange the system $\mathbf{K}\mathbf{u} = \mathbf{f}$ and rewrite it in a block form, with the first block corresponding to interior unknowns ordered subdomain after subdomain and the second block corresponding to interface unknowns:

$$\begin{bmatrix} \mathbf{K}_{\mathrm{oo}} & \widehat{\mathbf{K}}_{\mathrm{or}} \\ \widehat{\mathbf{K}}_{\mathrm{ro}} & \widehat{\mathbf{K}}_{\mathrm{rr}} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{\mathrm{o}} \\ \widehat{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{\mathrm{o}} \\ \widehat{\mathbf{f}} \end{bmatrix}, \tag{3.2}$$

where $\widehat{\mathbf{u}}$ represents all the interface unknowns. The hat symbol $\widehat{\ }$ is used to denote global interface quantities.

Different subdomains have disjoint sets of interior unknowns with no connections among them, so $\mathbf{K}_{\mathrm{oo}}$ is block diagonal. Interface unknowns cannot be separated in this way, as every of them belongs to two or more subdomains.

After eliminating all the interior unknowns from (3.2) we get

$$\begin{bmatrix} \mathbf{K}_{\mathrm{oo}} & \widehat{\mathbf{K}}_{\mathrm{or}} \\ \mathbf{0} & \widehat{\mathbf{S}} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{\mathrm{o}} \\ \widehat{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{\mathrm{o}} \\ \widehat{\mathbf{g}} \end{bmatrix}, \tag{3.3}$$

where $\widehat{\mathbf{S}} = \widehat{\mathbf{K}}_{\mathrm{rr}} - \widehat{\mathbf{K}}_{\mathrm{ro}}\mathbf{K}_{\mathrm{oo}}^{-1}\widehat{\mathbf{K}}_{\mathrm{or}}$ is the *Schur complement* of (3.2) with respect to interface and $\widehat{\mathbf{g}} = \widehat{\mathbf{f}} - \widehat{\mathbf{K}}_{\mathrm{ro}}\mathbf{K}_{\mathrm{oo}}^{-1}\mathbf{f}_{\mathrm{o}}$ is sometimes called *condensed right-hand side*.

Problem (3.3) can be split into subdomain problems

$$\mathbf{K}_{\mathrm{oo}}\mathbf{u}_{\mathrm{o}} = \mathbf{f}_{\mathrm{o}} - \widehat{\mathbf{K}}_{\mathrm{or}}\widehat{\mathbf{u}}\,, \tag{3.4}$$

and a *Schur complement problem*

$$\widehat{\mathbf{S}}\,\widehat{\mathbf{u}} = \widehat{\mathbf{g}}\,. \tag{3.5}$$

Problem (3.4) represents N independent subdomain problems with Dirichlet boundary conditions $\mathbf{u}_{\mathrm{r}}^i$ prescribed on the interface

$$\mathbf{K}_{\mathrm{oo}}^i\mathbf{u}_{\mathrm{o}}^i = \mathbf{f}_{\mathrm{o}}^i - \mathbf{K}_{\mathrm{or}}^i\mathbf{u}_{\mathrm{r}}^i\,, \tag{3.6}$$

where $\mathbf{u}_{\mathrm{r}}^i$ represents $\widehat{\mathbf{u}}$ restricted to the interface of Ω_i and $\mathbf{K}_{\mathrm{or}}^i$ is a block of $\widehat{\mathbf{K}}_{\mathrm{or}}$ corresponding to Ω_i (when using the FEM for discretization, $\mathbf{K}_{\mathrm{oo}}^i$ and $\mathbf{K}_{\mathrm{or}}^i$ are assembled from element matrices for elements contained in Ω_i only).

The Schur complement problem (3.5) represents a problem for interface unknowns $\widehat{\mathbf{u}}$ only. Its decomposition to subdomain problems is handled in the next section, as it is not so straightforward.

3.3 Decomposition of the Schur complement problem

If the original problem is too large, even the Schur complement problem (3.5) might be too large and ill-conditioned to be solved by standard algebraic methods. An advantage of using iterative substructuring DD methods for solving (3.5) is that the Schur complement problem is not assembled and solved as a whole. Instead only *local Schur complement problems* on subdomains are repeatedly solved and in every iteration step just interface information between neigbouring subdomains is exchanged. Moreover, even local Schur complement problems need not be assembled; subdomain problems with Dirichlet and Neumann boundary conditions on the interface can be solved instead.

The local Schur complement operator S^i operates only on the interface unknowns of the subdomain Ω_i. The local Schur complement problem is obtained as in the previous section, the only difference is that the process is performed on the subdomain Ω_i rather than on the whole domain Ω. Let us consider problem (3.2) restricted to Ω_i:

$$\begin{bmatrix} \mathbf{K}^i_{\mathrm{oo}} & \mathbf{K}^i_{\mathrm{or}} \\ \mathbf{K}^i_{\mathrm{ro}} & \mathbf{K}^i_{\mathrm{rr}} \end{bmatrix} \begin{bmatrix} \mathbf{u}^i_{\mathrm{o}} \\ \mathbf{u}^i_{\mathrm{r}} \end{bmatrix} = \begin{bmatrix} \mathbf{f}^i_{\mathrm{o}} \\ \mathbf{f}^i_{\mathrm{r}} \end{bmatrix}, \tag{3.7}$$

where $\mathbf{u}^i_{\mathrm{r}}$ represents interface unknowns belonging to Ω_i and $\mathbf{K}^i_{\mathrm{rr}}$, $\mathbf{K}^i_{\mathrm{ro}}$, and $\mathbf{K}^i_{\mathrm{or}}$ represent a local contribution of Ω_i to the global blocks $\widehat{\mathbf{K}}_{\mathrm{rr}}$, $\widehat{\mathbf{K}}_{\mathrm{ro}}$, and $\widehat{\mathbf{K}}_{\mathrm{or}}$, respectively (when using FEM for discretization, $\mathbf{K}^i_{\mathrm{rr}}$, $\mathbf{K}^i_{\mathrm{ro}}$ and $\mathbf{K}^i_{\mathrm{or}}$ are assembled from element matrices for elements contained in Ω_i only). However, it is not clear how to determine local interface forces $\mathbf{f}^i_{\mathrm{r}}$.

After eliminating all the interior unknowns from (3.7) we get

$$\begin{bmatrix} \mathbf{K}^i_{\mathrm{oo}} & \mathbf{K}^i_{\mathrm{or}} \\ \mathbf{0} & \mathbf{S}^i \end{bmatrix} \begin{bmatrix} \mathbf{u}^i_{\mathrm{o}} \\ \mathbf{u}^i_{\mathrm{r}} \end{bmatrix} = \begin{bmatrix} \mathbf{f}^i_{\mathrm{o}} \\ \mathbf{g}^i \end{bmatrix}, \tag{3.8}$$

where $\mathbf{S}^i = \mathbf{K}^i_{\mathrm{rr}} - \mathbf{K}^i_{\mathrm{ro}}(\mathbf{K}^i_{\mathrm{oo}})^{-1}\mathbf{K}^i_{\mathrm{or}}$ is the *local Schur complement* of (3.7) with respect to the relevant part of the interface and $\mathbf{g}^i = \mathbf{f}^i_{\mathrm{r}} - \mathbf{K}^i_{\mathrm{ro}}(\mathbf{K}^i_{\mathrm{oo}})^{-1}\mathbf{f}^i_{\mathrm{o}}$. Problem (3.8) can be split into two problems: the local subdomain problem (3.6) and the *local Schur complement problem*

$$\mathbf{S}^i\,\mathbf{u}^i_{\mathrm{r}} = \mathbf{g}^i. \tag{3.9}$$

In order to establish relations between the Schur complement $\widehat{\mathbf{S}}$ and the local Schur complements $\mathbf{S}^i$, function spaces $\widehat{W}$, W, and W^i and operators R and R^i are introduced in a standard manner (see MANDEL, DOHRMANN, AND TEZAUR [23]):

- $\widehat{W}$ is a space of functions with minimal energy on subdomains, continuous across the interface. Function $\widehat{u} \in \widehat{W}$ is represented by a vector $\widehat{\mathbf{u}}$ of values at global degrees of freedom at interface.
  W^i is a space of functions from $\widehat{W}$ restricted to Ω_i; $u^i_{\mathrm{r}} \in W^i$ is represented by a vector $\mathbf{u}^i_{\mathrm{r}}$ of values at local degrees of freedom at interface of Ω_i.

- $W = W^1 \times W^2 \times \cdots \times W^N$ is a space of functions with minimal energy on subdomains, possible discontinuous ("teared apart") across the interface. Function $u_{\mathrm{r}} \in W$ is represented by a vector $\mathbf{u}_{\mathrm{r}}$ of values at union of independent instances of all local interface unknowns from all subdomains (so for every global interface unknown belonging to m subdomains there can be m different local values coming from different subdomains).

- $\widehat{W}'$, $W^{i\prime}$, and W' ... dual spaces to $\widehat{W}$, W^i, and W, respectively.

The Schur complement operator $\widehat{S}$: $\widehat{W} \to \widehat{W}'$ is represented by the Schur complement $\widehat{\mathbf{S}}$, the local Schur complement operator S^i: $W^i \to W^{i\prime}$ is represented by the local Schur complement $\mathbf{S}^i$.

- R^i: $\widehat{W} \to W^i$ is the operator of a restriction from Ω to Ω_i. The operator R^i is represented by a matrix $\mathbf{R}^i$ that keeps only those components of a vector that belong to the closure of Ω_i. Note that the operator of a restriction R^i defined here keeps also interface components that lie on the boundary of Ω_i.

- $\mathrm{R}^{i\mathrm{T}}$: $W^{i\prime} \to \widehat{W}'$ is the operator of a prolongation from Ω_i to Ω. It is represented by the transpose $\mathbf{R}^{i\mathrm{T}}$ to the matrix $\mathbf{R}^i$, which takes a variable from Ω_i and represents it as the corresponding variable in Ω.

- R: $\widehat{W} \to W$ is the operator of tearing interface unknowns apart to independent subdomains. It is represented by the matrix

$$\mathbf{R} = \begin{bmatrix} \mathbf{R}^1 \\ \mathbf{R}^2 \\ \vdots \\ \mathbf{R}^N \end{bmatrix} \tag{3.10}$$

  which m-times copies every global unknown belonging to m subdomains.

- R^{T}: $W' \to \widehat{W}'$ is a transpose of the operator R. It is represented by the matrix $\mathbf{R}^{\mathrm{T}}$, which sums local interface values from adjacent subdomains.

3.4 Primal and dual methods

Let us suppose in this section that every diagonal block of $\mathbf{S}$, formed by local Schur complement $\mathbf{S}^i$, is invertible (floating subdomains will be treated in the next section).

Both *primal* (*Neumann-Neumann*, *BDD* type) and *dual* (*FETI* type) methods are iterative methods for solving the Schur complement problem (3.5) using the decomposed problem (3.9). Only local Schur complement problems are solved, although repetitively.

3.4.1 Primal methods

The primal DD methods iterate on the primal space $\widehat{W}$. For algebraic description of the primal method we need to introduce an operator E for averaging displacements discontinuous across the interface:

- E: $W \to \widehat{W}$ is the operator of averaging of interface values from adjacent subdomains; it is represented by a matrix $\mathbf{E}$.

- E^{T}: $\widehat{W}' \to W'$ is the operator of distributing of global interface forces to subdomains, represented by the transpose $\mathbf{E}^{\mathrm{T}}$ of the matrix $\mathbf{E}$.

The simple example of E is an arithmetic average: value at interface node is set as an arithmetic average of values at the corresponding node from all subdomains containing that node. For more sophisticated choices of E see MANDEL, DOHRMANN AND TEZAUR [23] or KLAWONN AND WIDLUND [13].

Primal (Neumann-Neumann) method can be formulated as a Richardson method for the Schur complement problem (3.5):

$$\widehat{\mathbf{u}}^{(k+1)} = \widehat{\mathbf{u}}^{(k)} + \mathbf{E}\mathbf{S}^{-1}\mathbf{E}^{\mathrm{T}}\widehat{\mathbf{r}}^{(k)}, \tag{3.11}$$

where $\mathbf{S}$ is a block-diagonal matrix with blocks formed by local Schur complements $\mathbf{S}^i$.

3.4.2 Dual methods

The dual DD methods iterate on the dual space W' or, strictly speaking, on a space of the Lagrange multipliers. More details and references can be found in the Ph.D. thesis.

3.5 BDDC and FETI-DP

The primal (Neumann-Neumann) and dual (FETI type) methods, as described in the previous section, have two main drawbacks. First, no floating subdomains are allowed in order to have local Schur complements invertible. Second, there is no global communication as in each iteration step information is exchanged between neighbouring subdomains only. This leads to deteriorating of the convergence rate with growing number of subdomains.

There have been many different attempts to tackle the first drawback. Let us mention just two successful methods from early 1990s, the FETI method by FARHAT AND ROUX [8] and the BDD method by MANDEL [21].

Most advanced recent methods seem to be the BDDC (Balancing Domain Decomposition by Constraints) developed by DOHRMANN [4] and the FETI-DP (FETI Dual-Primal) introduced by FARHAT ET AL. [7]. Both methods are described and compared in an abstract algebraic setting in MANDEL, DOHRMANN, AND TEZAUR [23] and in MANDEL AND SOUSEDÍK [24], or in a functional analytic framework in BRENNER AND SUNG [3]. A detailed description of the BDDC method with emphasis on implementation can also be found in ŠÍSTEK [29].

Both BDDC and FETI-DP methods construct a new space $\widetilde{W} \subset W$ by imposing some continuity constraints across the interface in *coarse degrees of freedom* so that $\widehat{W} \subset \widetilde{W}$ and the local Schur complement problems (3.9) restricted to $\widetilde{W}$ are invertible. Then methods from previous section are used on $\widetilde{W}$ instead of W: primal method in the case of BDDC and dual method in the case of FETI-DP.

It was shown that a smart choice of the coarse degrees of freedom resolves even the second drawback. It can not only improve convergence properties, but also make convergence independent of the number of subdomains (see TOSELLI AND WIDLUND [28] or MANDEL AND DOHRMANN [22]).

3.5.1 The coarse degrees of freedom

The interface nodes can be divided into three types of classes of equivalence: faces, edges, and corners. A *face* contains all nodes shared by two given subdomains (and not shared by any other subdomain), an *edge* contains all nodes shared by a given set of three or more subdomains (and not shared by any other subdomain), a *corner* is a degenerated edge with only one node.

According to this definition, every interface node belongs to exactly one subset: either to a face, or to an edge, or it is a corner. More details on this can be found in the work of ŠÍSTEK [29] or KLAWONN ET AL. [14].

A choice of the coarse degrees of freedom usually starts by a selection of some nodes on the interface as *coarse nodes*, typically corners of subdomains are chosen first and then other nodes are added as needed. Values at coarse nodes are used as coarse degrees of freedom. The space $\widetilde{W} \subset W$ consists of functions continuous across the interface at coarse nodes, represented by functions in W for which values at coarse degrees of freedom coincide.

For better convergence properties not only values at coarse nodes are used as coarse degrees of freedom, but also weighted averages of values over edges and faces of adjacent subdomains. More details can be found for instance in MANDEL AND DOHRMANN [22], KLAWONN, WIDLUND, AND DRYJA [15], KLAWONN AND RHEINBACH [12] or in LI AND WIDLUND [20], where a change of variables is used for treating averages so that each average corresponds to an explicit degree of freedom, like a coarse node.

Let us denote by

- $\widetilde{\mathrm{R}}^{\mathrm{T}}$: $\widetilde{W}' \to \widehat{W}'$ a restriction of the operator R^{T} to $\widetilde{W}'$,
- $\widetilde{\mathrm{R}}$: $\widehat{W} \to \widetilde{W}$ transpose of the operator $\widetilde{\mathrm{R}}^{\mathrm{T}}$,
- $\widetilde{\mathrm{E}}$: $\widetilde{W} \to \widehat{W}$ a restriction of an average operator E to $\widetilde{W}$.

3.5.2 BDDC (Balanced Domain Decomposition by Constraints) method

The BDDC method is the primal method rewritten for partially decomposed problem in the space $\widetilde{W}$ instead of totally decomposed problem in the space W. It can be expressed as a Richardson method, similarly as (3.11):

$$\widehat{\mathbf{u}}^{(k+1)} = \widehat{\mathbf{u}}^{(k)} + \widetilde{\mathbf{E}}(\widetilde{\mathbf{S}})^{-1}\widetilde{\mathbf{E}}^{\mathrm{T}}\,\widehat{\mathbf{r}}^{(k)}. \tag{3.12}$$

3.5.3 FETI-DP (Finite Element Tearing and Interconnecting Dual-Primal) method

The FETI-DP method is the dual method rewritten for partially decomposed problem in the space $\widetilde{W}'$ instead of totally decomposed problem in the space W'. More details can be found in the Ph.D. thesis.

3.6 DD methods as preconditioners

DD methods usually are not used on their own. They are used as outstanding preconditioners, specifically tailored to the given problem. The original problem (3.1), or the Schur complement problem (3.5), are actually solved using some other iterative method, typically PCG for symmetric problems and GMRES for nonsymetric ones.

A preconditioner $\mathbf{M}$ for a given problem $\mathbf{A}\,\mathbf{x} = \mathbf{b}$ is sought so that it has two concurrent properties:

- the problem $\mathbf{M}\mathbf{A}\,\mathbf{x} = \mathbf{M}\mathbf{b}$ has good spectral properties (in this sense $\mathbf{M}$ can be regarded as some approximation of $\mathbf{A}^{-1}$), and

- a preconditioned residual $\mathbf{p} = \mathbf{M}\mathbf{r}$ is "cheap" to obtain for any given $\mathbf{r}$.

A good preconditioner improves the convergence of the iterative method; without a preconditioner the iterative method may even fail to converge. More about preconditioners and iterative methods can be found in SAAD [25] or BARRET ET AL. [1].

Next idea is adopted from LE TALLEC [18]: DD methods in preceeding sections are formulated as Richardson iterative methods with a preconditioner $\mathbf{M}$ for the problem $\mathbf{A}\,\mathbf{x} = \mathbf{b}$ as

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \rho\,\mathbf{M}\mathbf{r}^{(k)}, \tag{3.13}$$

where $\mathbf{r}^{(k)} = \mathbf{b} - \mathbf{A}\,\mathbf{x}^{(k)}$ is a residual at k-th iterative step and $\rho = 1$. Any such method can be understood as a recipe for computing a preconditioned residual $\mathbf{p}$ by using only second term of (3.13) as $\mathbf{p} = \mathbf{M}\mathbf{r}$. This is the way how DD methods are used in practice.

From (3.12) it follows that the BDDC preconditioner for problem (3.5) can be written as

$$\mathbf{M}_{\mathrm{BDDC}} = \widetilde{\mathbf{E}}\widetilde{\mathbf{S}}^{-1}\widetilde{\mathbf{E}}^{\mathrm{T}}\,. \tag{3.14}$$

3.7 Application of BDDC to linear elasticity

Several practical problems from mechanical engineering, like the problem described bellow, were computed in order to test different implementations of the BDDC method ported to different computers.

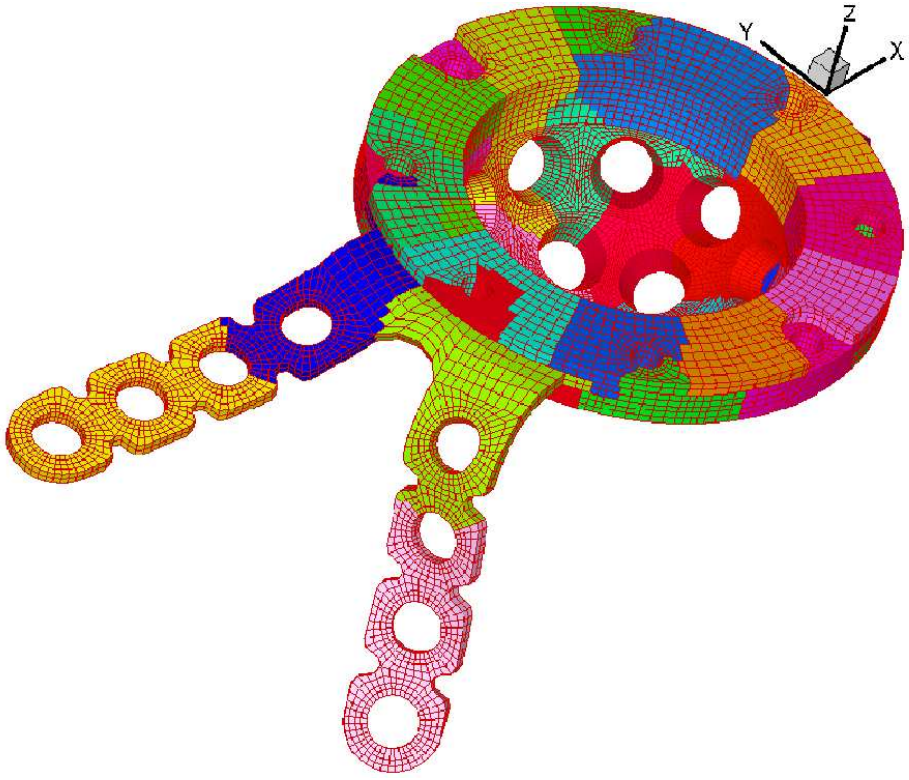

Figure 3.1: Replacement of a hip joint. FEM discretization: 27 586 elements, 154 247 nodes, 551 720 degrees of freedom. Domain is decomposed into 31 subdomains coloured by different colours.

Hip joint replacement

One practical problem from engineering is a problem of structural analysis of a replacement of a hip joint construction loaded by pressure from body weight. The global mesh consists of 27 586 quadratic isoparametric elements and 154 247 nodes that represent 551 720 degrees of freedom (Fig. 3.1). The problem and the computational mesh were provided by Jaroslav Novotný, Institute of Thermomechanics of the Czech Academy of Sciences.

The domain was decomposed into 31 subdomains using the METIS package [11]. For 1 600 coarse nodes randomly selected from interface nodes PCG converged after 46 iterations. The two most time consuming parts of the computations are the factorization of problems on subdomains and coarse problem and the PCG solution of the interface problem.

The computation of stress in the construction needs about 36 hours when using serial frontal solver. Two parallel implementations described in the articles **[2A]** and **[2B]** are compared in the two tables bellow. Table 3.1 shows results for coarse problem solved in parallel with the subdomain problems. Processor 0 is reserved only for the coarse problem. The problems on the subdomains are divided among the remaining processors. Table 3.2 shows results for coarse problem processed in serial mode with the subdomain problems. The problems on the subdomains are divided among all the processors. The processor 0 solves in addition also the coarse problem.

number of processors	5	9	17	32
number of subdomains per processor	8	4	2	1
time spent by factorization	44	30	27	21
time spent by pcg iterations	68	35	18	12
total time	113	66	45	33

Table 3.1: Scaling results for the problem at Figure 3.1 (time in minutes), coarse problem is solved in parallel with subdomain problems.

number of processors	4	8	16	32
number of subdomains per processor	8	4	2	1
time spent by factorization	53	35	30	23
time spent by pcg iterations	67	32	22	15
total time	120	68	52	38

Table 3.2: Scaling results for the problem at Figure 3.1 (time in minutes), coarse problem is solved in serial mode with subdomain problems.

Presented results were obtained on the Lomond server (Sun Fire E15k) of EPCC, University of Edinburgh.

Results obtained by different choices of the coarse problem are published in the articles **[2C]** and **[2D]**.

Full text of the articles **[2A]** – **[2D]** is involved in Appendix of the Ph.D. thesis.

Chapter 4

Conclusion

The presented thesis summarizes results published in articles **[1A]** – **[2D]** (see Section 1.4). It consists of two parts.

The first part is concerned with nonlinearity in heat conduction in solids. The aim is to enhance the numerical stability and efficiency of the computation. The problems are treated by a suitable choice of the criterion when to update the tangential matrix in MNR and by the line-search method, as described in Chapter 2.

The second part deals with an application of Balancing Domain Decomposition by Constraints (BDDC) – nonoverlapping domain decomposition method, described in Chapter 3. The aim is to get efficient algorithms for solving large, sparse, unstructured linear systems that stem from numerical solution of practical problems from engineering.

Algorithms discussed in both parts were implemented using components of a standard FEM software and tested on practical problems in nonlinear heat conduction and linear elasticity.

My main original results and achievements are:

- Proposing and implementing two criteria for updating the tangential matrix into Modified Newton-Raphson method and implementing the line-search into a standard FEM software package. Comparing the methods on nonlinear heat conductivity problems with regard to better convergence and numerical stability properties.
- Parallelizing solution of the coarse problem of the BDDC method in the previous implementation (the first implementation done in ŠÍSTEK [29]) and comparing the efficiency of both variants.
- Based on deeper insight into the subject of domain decomposition methods, I made several propositions dealing with implementation of constraints across the interface.

Results of work in the thesis were presented at the following international conferences:

- LSSC 6 – Large-Scale Scientific Computations, Sozopol, Bulgaria, June 5 – 9, 2007
- ICCBB 1 – International Conference on Computational Biomechanics and Biology, Plzeň, Czech Republic, September 10–13, 2007
- PANM 14 – Progams and algorithms of numerical mathematics, Dolní Maxov, Czech Republic, June 1 – 6, 2008

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