POLITEHNICA UNIVERSITY OF BUCHAREST

The Doctoral School of <u>ELECTRICAL ENGINEERING</u>

Summary of PH. D. Thesis
MEMS Modeling and Simulation Techniques

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Contents

Abstract

Keywords: *multiphysic models, high performance computing, electromagnetic field, linear elasticity, functional analysis, weak formulations, finite elements, parallel processing*

The last three decades witnessed an exponential increase of the demand for computing power requested by both scientific community and commercial applications. Computer simulation became a *must* in the design process of modern high tech complex products. It's one of the main reasons that led to the development of a new science namely the *multiphysic modeling*. The process of modeling modern pieces of equipment imply simulating various physical phenomena including the coupling between them. One can frequently encounter the need of simulation the coupling between electromagnetic, mechanic, thermal and/or fluid flow phenomena.

This thesis describes a method to tackle multiphysic simulations by putting into interaction three essential scientific domains, namely: physics, mathematics and numerical computation. Actually, the method actually emphasizes the interdisciplinarity between the three mentioned sciences, which is now known as *Computational Science and Engineering (CSE).*

Chapter 1

High Performance Computing

This chapter exposes the hardware and software involved in the implementation process of the *CSE* algorithms. A short history of the development of the hardware CPU architectures is presented - starting with the Neumann architecture and ending with multicore microprocessors capable of parallel code processing. The high data volume that is usually involved in the multiphysic simulations is actually processed by means of clusters of paralleled multicore computers (see fig. 1.1).

In order to benefit of this tremendous hardware development new software design techniques have been developed. Two main programming models, both dedicated to implementing parallel algorithms, are discussed:

- the paralleling methodology first formalized by Foster în 1995 ([29]) according to the sequence: „Partition -> Communication -> Agglomeration -> Mapping” (PCAM);

- a paralleling methodology more general than Fosters's, formalized by Mattson [58] in 2004; this methodology aims to optimize the data structures and algorithms used to make an algorithm to be implemented on parallel processors.

Finally, the most popular software tools currently used for parallel programming:

- the Pthreads software library;

- the OpenMP software library;

- the Message Passing Interface (MPI) programming model;

For each of the above software tools the following aspects are discussed:

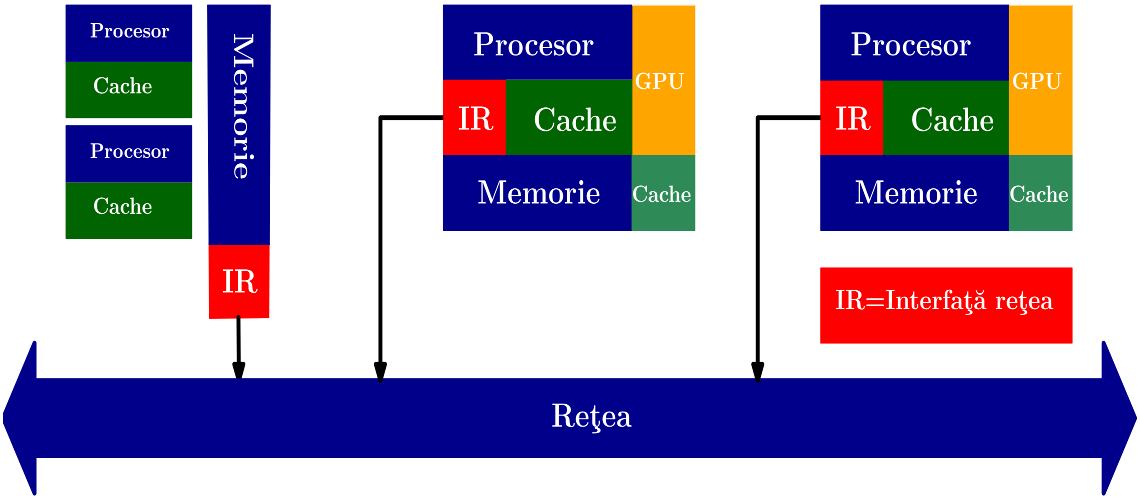

Figure 1.1: Computer cluster implying different types of multicore independent paralleled computers and distributed memory. In certain units the graphic processor (GPU) is used in parallel with the main multicore processor.

- the way in which, during execution, parallel threads are initiated, run, and ended;
- the way critical situations during parallel execution of processes are handled;
- the way the software tools are used;

Chapter 2

Physical Aspects

A multipysic universe can be decomposed in several overlapped or non-overlapped regions characterized by different material properties. In these regions several physical phenomena might simultaneously or sequentialy evolve. Each of these phenomenon is subject of a scientific theory characterized by:

- base physical quantities or derived physical quantities out of the base ones;
- an independent, consistent, and complete set of physical laws;
- a set of theorems, demonstrated on the basis of the previous mentioned laws.

This second chapters refers to the above mentioned physical theories which characterize the electromagnetic field theory and the linear elasticity theory.

Four space and time dependent vector fields locally characterize, from electromagnetic point of view, any point in space:

- the electric field intensity - $\mathbf{E}$;
- the electric displacement field (electric flux density) - $\mathbf{D}$;
- the magnetic field intensity - $\mathbf{H}$;
- the magnetic induction field (magnetic flux density) - $\mathbf{B}$.

The interaction between bodies and the electromagnetic field is locally characterized by the following quantities:

- the charge density (scalar) - ρ;
- the current density vector field - $\mathbf{J}$.

The electromagnetic field in bodies is globally characterized by scalar quantities which are obtained by integrating the local vector fields, and the scalar density charge, on several space varieties (C stands for 1D curves, S stands for 2D surfaces):

- the electric voltage - $u(t) = \int_C \mathbf{E}(\mathbf{r}, t) \cdot d\mathbf{r}$;
- the electric flux - $\psi(t) = \int_S \mathbf{D}(\mathbf{r}, t) \cdot \mathbf{n}\, dA$;
- the magnetic voltage - $u_m(t) = \int_C \mathbf{H}(\mathbf{r}, t) \cdot d\mathbf{r}$;
- the magnetic flux - $\phi(t) = \int_S \mathbf{B}(\mathbf{r}, t) \cdot \mathbf{n}\, dA$;
- the electric current intensity - $i(t) = \int_S \mathbf{J}(\mathbf{r}, t) \cdot \mathbf{n}\, dA$.
- the electric charge - $q(t) = \int_\Omega \rho(\mathbf{r}, t)\, d\Omega$, where Ω might be a 1D, 2D or 3D spatial variety.

The sources of electromagnetic field are described by its general laws: the electric flux law, the magnetic flux law, Faraday's law, the magnetic circuit law, the charge conservation law. Both local (differential) and global (integral) mathematical formulations are given. These laws are completed by the constitutive laws, which, based on material properties, establish the links between the vector fields intensities and flux densities:

- **D-E** by means of the electric permittivity ε,
- **B-H** by means of the magnetic permeability μ,
- **J** - $(\mathbf{E} + \mathbf{E}_i)$, where $\mathbf{E}_\mathrm{i}$ is the impressed electric field intensity, by means of the electric conductivity σ.

Finally the electromagnetic energy conservation theorem is pointed out. This theorem is further used to describe the generalized magnetic and electric forces that act on bodies under the influence of the electromagnetic field. These forces might be volume forces characterized by a volume force density, or surface forces characterized by Maxwell tensors.

According to the the mechanics of continua theory the action of forces upon bodies can be determined by knowing the stresses, strains and displacements. The forces can be locally characterized with space and time dependent vector fields:

- the volume force density - $\mathbf{b} = \lim_{\Delta V \to 0} \frac{\Delta \mathbf{F}_V}{\Delta V}$;
- the surface force density - $\mathbf{t} = \lim_{\Delta A \to 0} \frac{\Delta \mathbf{F}_S}{\Delta A}$;

- the volume torque density - $\mathbf{m}_V = (\mathbf{r}_V \times \mathbf{b})dV$;
- the surface torque density - $\mathbf{m}_A = (\mathbf{r}_A \times \mathbf{t})dA$;
- the stress tensor $\overline{\overline{\sigma}}$; this 2^{nd} order tensor is symmetric if there are no torque components in that point.

The global forces and torques are obtained by integrating the local vector fields over the appropriate space variety.

The strain is locally given by he strain tensor $\overline{\overline{\epsilon}}$. This tensor is related to the dispacement vector $\mathbf{u}$ by means of the geometric compatibility equation:

$$\overline{\overline{\epsilon}} = \frac{1}{2}\left([\nabla \mathbf{u}] + [\nabla \mathbf{u}]^T\right)$$

The link between stress and strain is given by the constitutive elasticity Hooke relation: $[\sigma] = [d] \cdot [\epsilon]$. $[d]$ is the rigidity matrix, that for linear, homogeneous, and isotropic materials depends only on specific material constants: longitudinal elasticity module E (Young's module), transverse elasticity module G and Poisson ratio ν.

The fundamental conservation laws of the mechanics of the continua are shown: the mass conservation law, the impulse conservation law, the torque impulse conservation law.

Finally the first principle of the thermodynamics is discussed and identified as one of the fundamental principle that frames both electromagnetic field and elasticity theories.

The different physical aspects, described by now, are depicted by means of scalar or vector fields which usually satisfy 2nd order partial derivative equations (PDE). The left hand side of the PDEs reflect the material (constitutive) properties of a certain region of the mutiphysic domain. The right hand side contains all quantities that represent the field sources, either internal or external to the problem domain.

Chapter 3

Mathematical Aspects

The third chapter of the present thesis deals with that part of mathematics that can be employed to naturally describe multiphysics models: the *functional analysis* with its fundamental concept, namely *the abstract spaces*. First, Banach spaces are taken into account. Sobolev spaces, which represent the PDEs' solutions spaces, are derived out of the Banach spaces. The Hilbert spaces are the only complete inner product Sobolev class spaces which consequently admit the definition of a norm. Furthermore the orthogonality condition can be stated. It is shown that Sobolev space elements can always be approximated, as well as needed, by means of $\mathbb{R}^N$ test functions.

According to functional analysis the so called *strong formulations* represented by the PDEs of a certain physical domain can be transformed into *weak formulations* characteristic to the abstract space corresponding to that physical domain. In order to do that, the equivalence between the PDEs of the strong formulation and the weak formulation equations, needs to be demonstrated. Actually one has to demonstrate that the transformation from the strong to the weak formulation preserves the weak continuity (according to the distribution theory) all over the problem domain. A special care should be taken on the domain borders, since these borders usually contain singularity points (corners, edges) - on which the functions are not continuous, hence not differentiable. It is the reason why the third chapter discusses the following:

- integer Sobolev spaces and the typical differential operators used to describe the weak formulations equivalent to the strong ones defined on the interior of the problem domain;

- fractional Sobolev spaces and the tipical surface differential operators used to describe the weak formulations equivalent to the strong ones defined on the borders of the problem domain;

- the *trace operators* which represent the link between the two above mentioned Sobolev spaces; actually they are restrictions on the domain border of the functions defined on the interior of the domain.

The weak formulation is obtained by projecting the strong formulation equations on a set of basis functions which span the associated abstract space. The weak formulation of the multiphysic problems assumes on the left hand side a bilinear functional $\mathcal{A}(u, v)$ and on the right hand side a linear functional $\mathcal{F}(v)$. Based on the weak formulation, the existence and uniqueness conditions of the solution are stated, according to the *Lax-Milgram* theorem. The weak formulations are expressed by means of the generalized differential operators (*grad, curl, div*). For each of these operators, one can find a compatible functional space, which preserves the weak continuity of the operators over the whole problem domain:

- The L^2 space formed by the functions with finite integral of their square:

$$L^2(\Omega) = \left\{ v : \int_\Omega |v(x)|^2 \, dx < +\infty \right\}; \qquad (3.1)$$

- The H^1 space which contains the functions from the space L^2 with generalized gradient being also in L^2:

$$H^1(\Omega) := \{\varphi \in \ L^2(\Omega) \,|\, \nabla\varphi \in [L^2(\Omega)]^d\}, \text{ where } d \in \{2,\, 3\}; \qquad (3.2)$$

- The $H(\mathbf{curl})$ space which contains the functions having their **curl** in L^2:

$$H(\mathbf{rot}, \Omega) := \{\vec{u} \in [L^2(\Omega)]^3 \,|\, \nabla \times \vec{u} \in [L^2(\Omega)]^3\}; \qquad (3.3)$$

- The $H(\mathbf{div})$ space which contains the functions having their divergence in L^2:

$$H(div, \Omega) := \{\vec{u} \in [L^2(\Omega)]^d \,|\, \nabla \cdot \vec{u} \in L^2(\Omega)\}. \qquad (3.4)$$

The relation between these spaces together with the construction method of one space from the previous one is pointed out by the exact *De Rham* sequence:

$$\mathbb{R} \to H^1(\Omega) \xrightarrow{\nabla} H(\mathbf{rot}, \Omega) \xrightarrow{\nabla\times} H(div, \Omega) \xrightarrow{\nabla\cdot} L^2(\Omega) \to \{0\}. \qquad (3.5)$$

The last two sections of chapter 3 contain a complete discussion of the functional treatment of an general elliptic equation: strong formulaton, weak formulation, solution uniqueness and existence particular cases. As a special case, a tipical linear elasticity equation system is discussed.

Chapter 4

Numerical Aspects

This 4^{th} chapter is dedicated to the numerical solving the weak form of PDEs, by means of the finite element method (FEM), using the Galerkin technique. The essential aspects that characterize the process of passing from the universe of continuous abstract spaces to the discrete digital space are emphasized:

- The initial opened domain Ω is approximated by the discretized finite domain $\Omega_h = \bigcup_{k \in \mathcal{T}_h(\Omega)} \Omega_k$, known as the *triangulation* $\mathcal{T}_h(\Omega)$. Accordingly, the approximate form of the weak formulation of the multiphysic problems will be described on the left hand side by the bilinear functional $\mathcal{A}(u_h, v_h)$ and on the right hand side by the linear functional $\mathcal{F}(v_h)$. u_h is the approximate numerical solution of the problem and v_h represent the elements of the approximate test functions space. The approximate solution in any point of Ω is an interpolation of the local solutions obtained for each finite element on its local space Ω_k;

- In the digital world, the notion of infinity is lost, being replaced by formulas which evaluate the infinity accuracy approximation. This accuracy is dependent on the refinement degree of $\mathcal{T}_h(\Omega)$ and on the degree of the polynomial interpolation mentioned above; in this thesis the simplest polynomials of first degree are considered;

- The finite element is an entity that summarizes both pure geometrical and functional characteristics: on the geometric domain two dual spaces are defined: one of the shape functions and the other one the space of degrees of freedom (DOF). According to the Galerkin technique both spaces are spanned by the same test functions basis.

- For each differential operator involved in the weak formulation one can establish finite elements conforming to the functional space described by that differential form. The shape functions and the DOF functional spaces can be defined on a reference master geometric element with unit coordinates. In this work a master triangle and a master tetrahedron are taken into account for 2D, respective for 3D problems. Using a continuously differentiable transformation the reference element can be mapped to the physical element. Conforming to the operator used to describe the weak formulation, the discrete numerical solution should be seeked in one of the following functional spaces:

- $\mathcal{W}_h^1$ for weak solutions seeked in $H^1(\Omega)$:
  $$\mathcal{W}_h^1 = \left\{ u_h(\mathbf{x}) \in H^1(\Omega) \,|\, u_h^k(\mathbf{x}) \in \mathrm{P}^{H1_k}(\Omega_k) \subset H^1(\Omega_k),\ \forall \Omega_k \in \mathcal{T}_h \right\},$$
  where $\mathrm{P}^{H1_k}(\Omega_k)$ is the space of the shape functions of the H^1 conforming finite element of first order defined on (Ω_k);
- $\mathcal{V}_{h,I}^1$ for weak solutions seeked in $H(\mathbf{curl}, \Omega)$:
  $$\mathcal{V}_{h,I}^1 = \left\{ \vec{u}_h(\mathbf{x}) \in H(\mathbf{curl}, \Omega) \,|\, \vec{u}_h^k(\mathbf{x}) \in R_k(\Omega_k) \subset H(\mathbf{curl}, \Omega_k), \forall \Omega_k \in \mathcal{T}_h \right\}.$$
  where $R_k(\Omega_k)$ is the space of the shape functions of the $H(\mathbf{curl})$ conforming finite element of 1st order (Nédélec of 1st order) defined on (Ω_k);
- $\mathcal{Q}_h^1$ for weak solutions seeked in $H(\mathbf{div}, \Omega)$:
  $$\mathcal{Q}_h^1 = \left\{ \vec{u}_h(\mathbf{x}) \in H(\mathbf{div}, \Omega) \,|\, \vec{u}_h^k(\mathbf{x}) \in D_k(\Omega_k) \subset H(\mathbf{div}, \Omega_k), \forall \Omega_k \in \mathcal{T}_h \right\}.$$
  where $D_k(\Omega_k)$ is the space of the shape functions of the $H(\mathbf{div})$ conforming finite element of 1st order (Raviart-Thomas 1st order) on (Ω_k);
- $\mathcal{S}_h^1$ for weak solutions seeked in L^2:
  $$\mathcal{S}_h^1 = \left\{ \varphi \in L^2(\Omega) \,|\, \varphi_h^k \in P_0(\Omega_k) \subset L^2(\Omega_k), \forall \Omega_k \in \mathcal{T}_h \right\}.$$
  where $P_0(\Omega_k)$ is the space of the shape functions of the L^2 conforming finite element of the first order defined on (Ω_k);

- The functional discrete spaces mentioned above can be ordered in the same exact *De Rham* sequence as their equivalents from the continuous world:
  $$\mathbb{R} \to \mathcal{W}_h^1 \xrightarrow{\nabla} \mathcal{V}_{h,I}^1 \xrightarrow{\nabla\times} \mathcal{Q}_h^1 \xrightarrow{\nabla\cdot} \mathcal{S}_h^1 \to \{0\}. \tag{4.1}$$

The sequence (4.1) leads to the following important conclusion: *The differential form that describes a local quantity, typical for a certain physical problem, represents the essential link between the physical, mathematical and numerical models of that particular problem.*

Chapter 5

Computational Aspects

In this chapter a multiphysic problem is discussed according to all the concepts presented in the former chapters. The problem deals with a multiphysic model of a capacitive microswitch. The device is part of the class of Micro Electro Mechanical Systems (MEMS).

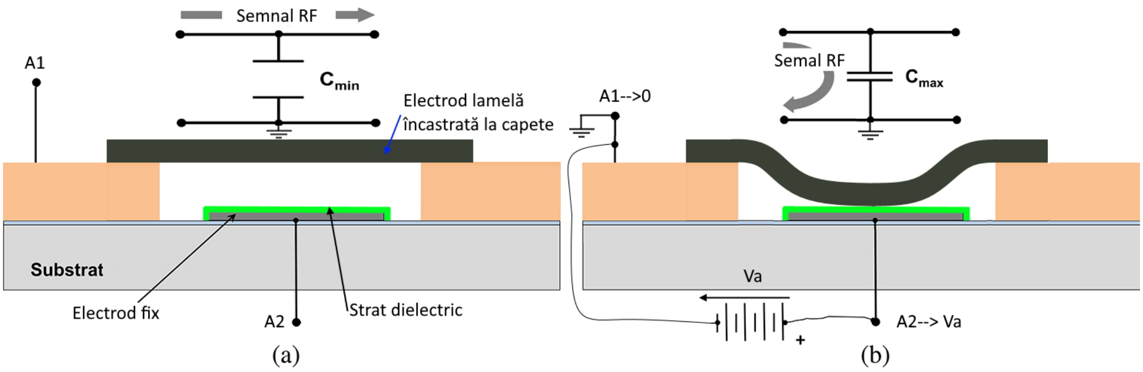

Figure 5.1: A capacitive microswitch. The switch is opened when there is no applied voltage V_a (a); the switch is fully closed when the critical voltage $V_a = V_{PI}$ is applied (b); the electrical capacity, hence the cut frequency can be voltage controlled for $0 < V_a \leq V_{PI}$.

During the modeling process the following steps were taken:

1. A 2D and a 3D conceptual models were constructed;

2. For both models the strong and weak formulations are written;

3. An 1D analytic model is described; the analytic solution of this model allows a qualitative evaluation of the device performance. There are two linear

problems - an electrical one (electrostatic regime) and a mechanical one (linear elasticity); their coupling is nonlinear because of two reasons:

(a) The electrostatic force which is the physical link between the two problems depends on the square of the applied voltage V_a; this force is computed by solving the electrostatic problem;

(b) The domain of the electric problem gets deformed because of the displacement of the elastic beam; this displacement is computed within the linear elasticity problem according to the value of the electrostatic force;

4. As a consequence to the above, an iterative algorithm is proposed to solve the problem;

5. Two FEM models corresponding to 2D and 3D domains are constructed by the means of **FreeFEM++** - a software dedicated to PDEs solving. **FreeFEM++** uses the weak formulation of the problems. Appendix 1 and 2 contain the listings of the programs written for the two models;

6. Simulations with H^1 conforming finite elements of the first and second degree are performed and the results are discussed;

7. Two methods are employed to determine the force acting on the elastic contact:

(a) by evaluating the components of Maxwell tensor on the elastic contact surface; actually these components are the components of the stress tensor that imposes the displacement of the elastic beam in the mechanical problem;

(b) using an energetic approach by calculating the force out of the variation of electrical energy determined by the elastic contact displacement;

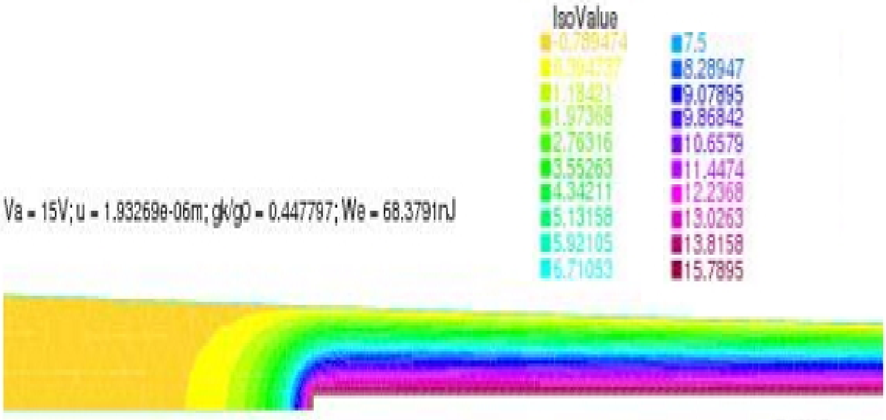

Figure 5.2: Electric potential distribution within the electrostatic problem domain for a command voltage $V_a = 15V$, and current displacement $u = 1,932\mu m$.

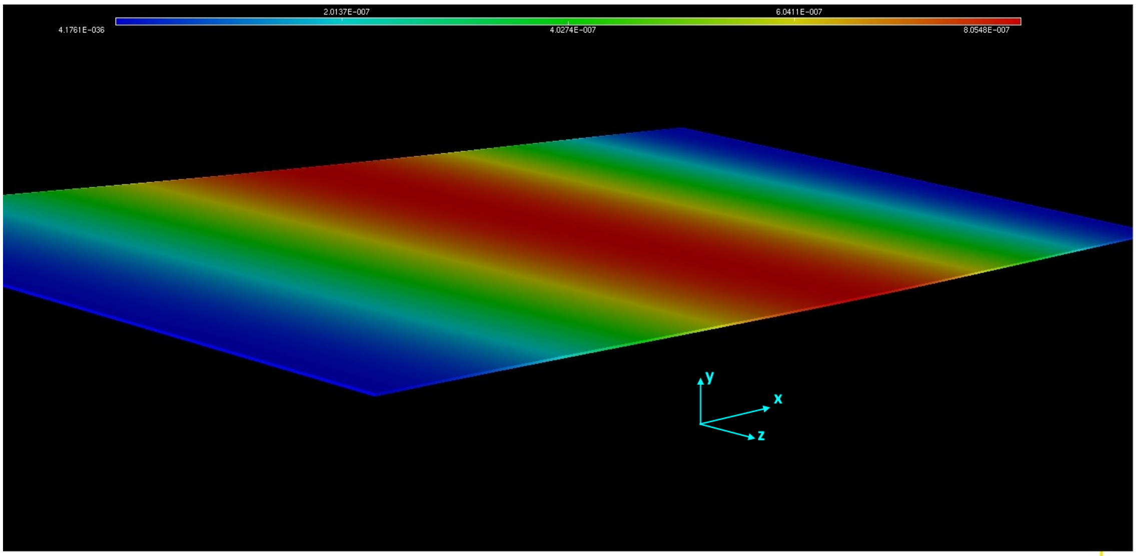

Figure 5.3: The vertical displacement component u_y of the elastic beam of the capacitive microswitch. The displacement is maximum in the middle of the beam. The command voltage is $V_a = 15V$.

8. The final goal of the simulations is to determine the critical *pull in voltage* V_{PI}
9. Comparisons are made between the 2D and 3D simulations (see. fig. 5.4); the main criteria are the accuracy of the solution and the solving time. The

3D simulation is more realistic than the 2D simulation, since it takes into account the fringing of the electrostatic field on the edges of the elastic beam. However, the 2D model implies solving a system of 5,100 equations which takes 148 seconds to solve, while the 3D model needs to solve a system of 1,160,000 equations that took 153 minutes to solve - almost 60 times more than the 2D case! The computations were performed on a Dell Inspiron laptop, with i7-8550U @1,80Ghz processor and 16Gb RAM, running under Windows10©.

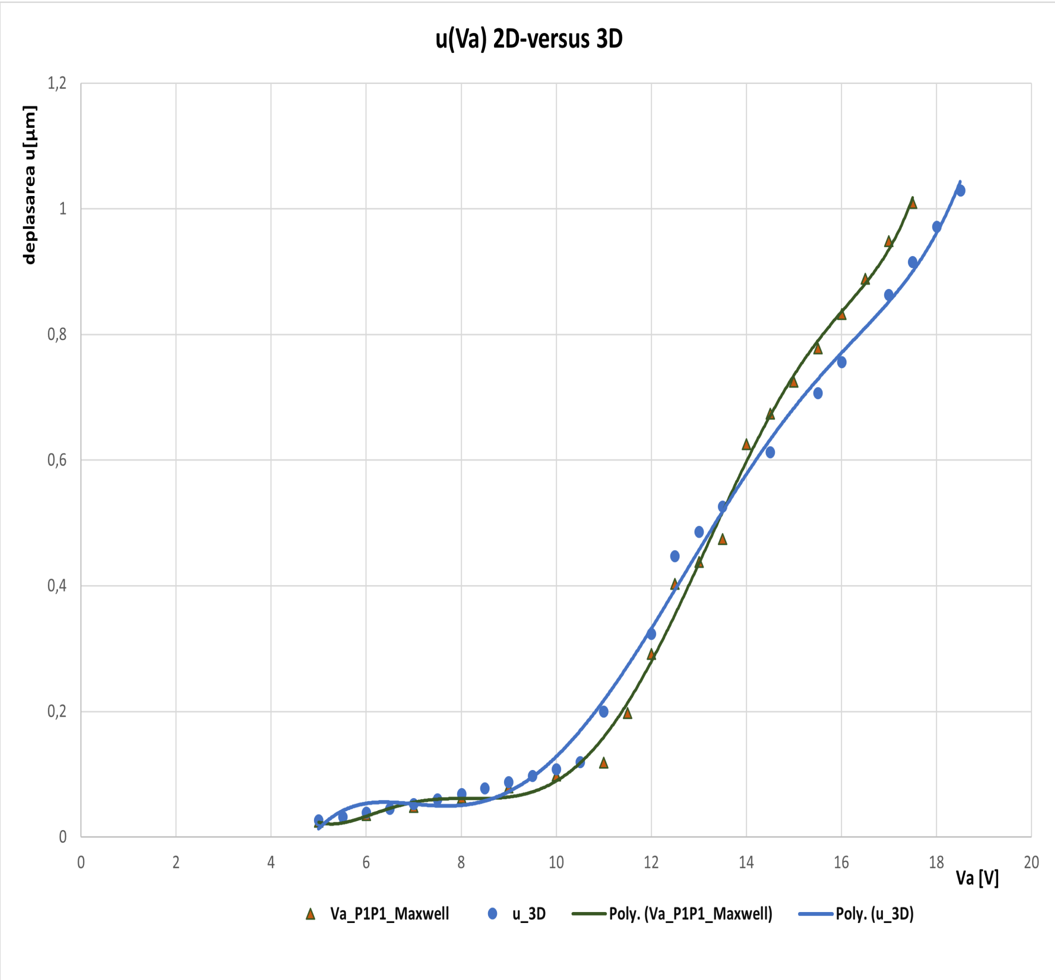

Figure 5.4: The displacement of the elastic beam u with respect to the command voltage V_a. Comparison between the curves determined with 2D (the green/triangular points curve) and 3D simulations (the blue/oval points).

10. Finally a domain decomposition method (DDM) is employed in order to make possible the use of a parallel algorithm to solve the problem; comparisons

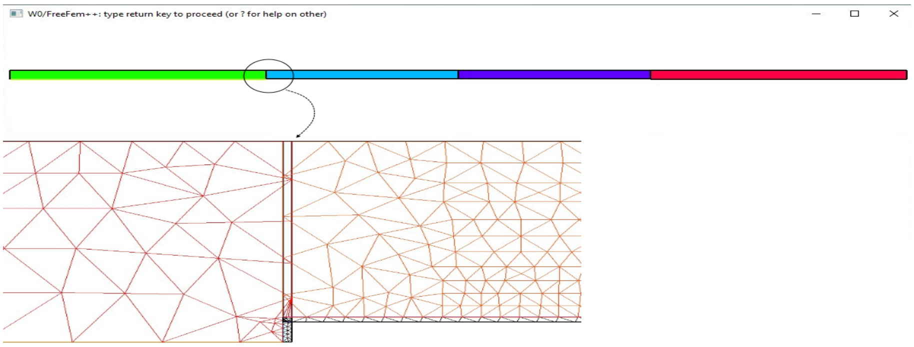

Figure 5.5: Domain Ω_E divided into 4 overlapping sub-domains.

are made between the time performance of the serial and parallel algorithms. The MEMS 2D electric problem model was divided into four overlapping sub-domains, corresponding to the 4 cores of the above mentioned processor (see fig.5.5). In order to solve the electric problem several iterations are performed. Finding the solution $v_i^{(k)}$ on the sub-domain Ω_i for iteration (k), uses as border conditions on the common border between sub-domains Ω_i and Ω_j the values $v_j^{(k-1)}$ calculated on Ω_j during the previous iteration. By the end of the process, the values of both v_i and v_j on that common border are very close. Figures 5.6 and 5.7 are relevant for this evolution.

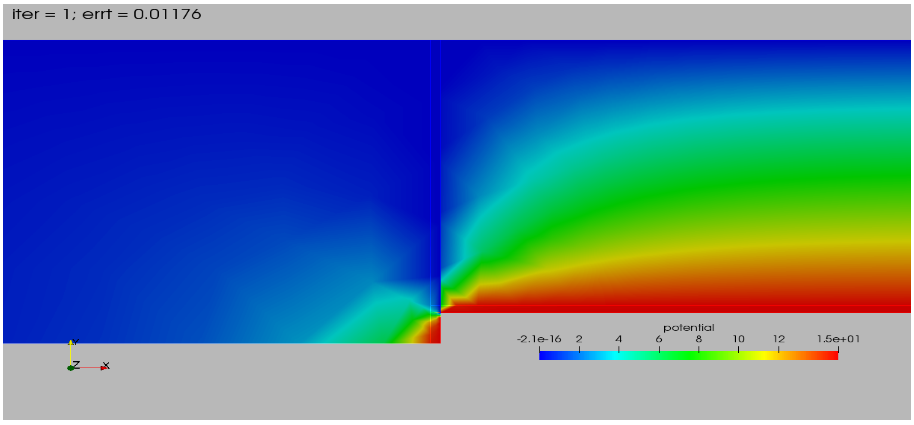

Figure 5.6: The electric potential distribution on the common border between sub-domains Ω_0 and Ω_1 after first iteration. Initially, on this common border, Dirichlet homogeneous conditions are imposed. The Euclidean error between $v_0^{(1)}$ and $v_1^{(1)}$ is of order 10^{-2}. The command voltage for the capacitive microswitch is $V_a = 15V$.

Process →	Serial			Paralel			
FE Order ↓	DOF	t [s]	t_{spec} [µs/DOF]	DOF	t [s]	t_{spec} [µs/DOF]	**S**
P1	4381	0,19	43	7073	0,13	18	2,39
P2	16492	0,86	52	26912	0,62	23	2,26

Table 5.1: Solving times for one iteration of the electric problem. A comparison is made between the serial and parallel approaches for H^1 conforming finite elements of first order (P1) and second order (P2). t_{spec} is the specific time per DOF.

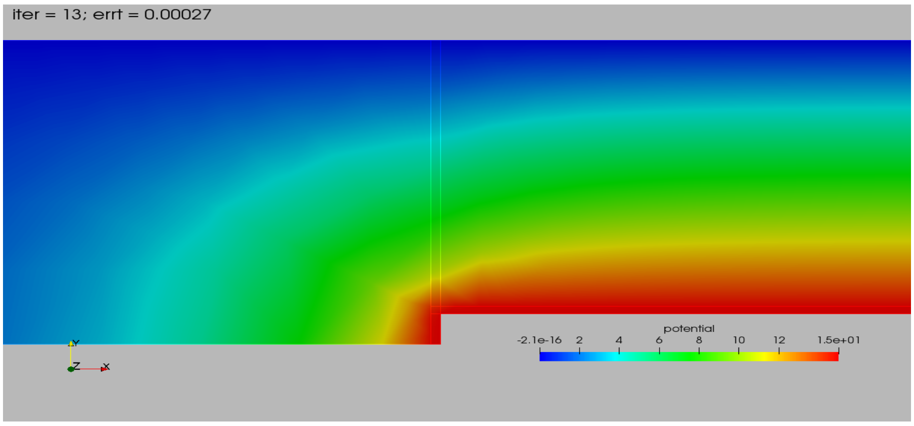

Figure 5.7: The electric potential distribution on the common border between sub-domains Ω_0 and Ω_1 after the last iteration. The Euclidean error between $v_0^{(1)}$ and $v_1^{(1)}$ is of order 10^{-4}. The command voltage for the capacitive microswitch is $V_a = 15V$.

Each sub-domain was automatically discretized by **FreeFEM++** , the final number of equations (7,073) being higher than the former single mesh case. Nevertheless, the solving time for the parallel process was almost 2.3 times smaller than in the serial case. The comparison was done by determining a *specific time* calculated as the ratio between the total solving time and the number of DOFs. Simulations were performed with H^1 conforming elements of first order (P1) and second order (P2)(see. tab.10).

Chapter 6

Conclusions

6.1 General

Nowadays we assist to an unprecedentedly demand for processing and storing increasingly higher amounts of data, in the shortest possible time. With respect to this phenomenon, the scientific community has a double role: on one hand to be a great consumer of computing resources and on the other to be the main developer of such resources. The first chapter of this thesis points out the milestones of the development of computer architectures.

At this very moment we are in a full process of expanding the use of parallel algorithms that run on parallel processors. The classic structured programming style now gives way to the new models of the parallel programming. However, this process does not give up the old style of serial programming techniques but embeds it in the new models of parallel software design. The most popular parallel software model of the present time is the „**S**ingle **P**rogram **M**ultiple **D**ata” (**SPMD**) model, because it best matches the actual multiphysic simulation requirements.

As a consequence a new science was born, namely the High Performance Scientific Computing (HPSC). The main characteristic of this new science is that it is highly*interdisciplinary*. Tackling it implies good knowledge of physics, engineering, mathematics, numerical methods and computer science.

Actually, this explains the themes of the following chapters of the thesis: physical aspects, mathematical aspects, numerical aspects and finally computational ones. The physic phenomena are described in every point of the physical domain by specific scalar or vector fields, space and time dependent, attached to basic physical quantities. The local behavior of these quantities is described by differential operators as gradient, curl, divergence. Furthermore we get the global quantities derived by integration of the basic ones on geometric varieties of first, second and third order, respectively curves, surfaces and volumes. There is a strong link between the above mentioned differential operators and these geometric varieties:

- the gradient applied to scalar functions, generates a conservative vector field which has a null integral on a closed curve (a first order geometric variety);
- the curl applied to vector fields generates another vector field which determines a null flux when integrated on a closed surface (second order geometric variety);
- the divergence applied to vector fields generates a scalar field of which integral performed on a third order geometric variety (volume), has the significance of a field source;

Each of the differential operators listed above, can generate an associated Hilbert space (see. (3.2), (3.3), (3.4)). These Hilbert spaces, along with the Hilbert real numbers space form an exact sequence called *De Rham sequence* (see. (3.5)). The importance of this sequence is that it shows on one hand that the linked spaces are isomorphic, and on the other hand it emphasizes a way of constructing one space form the other. Finally another important link can be made between the De Rham sequence and the Helmholtz fundamental vector field theorem, that states that each vector field allows an unique decomposition into a curl free vector field and a divergence free one.

The physical phenomena are mathematically described by PDEs of which the most encountered are the second degree ones. These PDEs represent the so called strong formulation which assumes the continuity of the solution in every point of the domain. By correctly identifying the Hilbert space in which the solution lives in, one can project the strong form equations on a basis that spans that Hilbert space in order to get the weak formulation of the problem. If the Hilbert space is properly chosen, the existence and uniqueness of the weak formulation solution can be demonstrated (see. the Lax-Milgram theorem). This solution still preserves the continuity property but in a generalized form - according to the distribution theory.

Taking a further step towards finding the numerical solution of the weak formulation equations, one needs to find an equivalent numerical formulation of the problem. This leads to the approximation of the domain - opened and eventually bounded - of the physical problem with a finite domain. Actually this latter domain is obtained by dividing the initial domain by means of a mesh, in finite geometrical elements with known shapes (triangular, tetrahedral, rectangular, cubes, etc.). On each of these finite sub-domains, a local interpolation function is defined in order to approximate the local solution. The local solution is called degree of freedom (DOF) and it is determined on certain geometric varieties of that finite domain. These can be:

- values in certain points (nodes) as zero order varieties;
- line integrals on edges as first order varieties;
- surface integrals (fluxes) on faces as second order varieties;
- scalars associated to volumes as third order varieties;

Any other solution value local to the finite element is found by using a local interpolation function. This interpolator is constructed by means of a shape function also defined on the finite element domain. As a cosequence one can define a finite element using three components:

- the finite element geometric domain;
- the space of DOFs which according to the above description can be scalars or functions;
- the space of shape functions defined on the finite element domain - dual of the DOFs space;

The solution in any point of the domain is then obtained by applying a global interpolation function to all DOFs. This can be possible iff the operators that describe the weak formulation can keep the continuity property even in their discrete form. This can be done if one keeps the proper association between the differential operators and the geometrical variety on which the DOFs are defined:

- *gradient* for DOFs defined on nodes;
- *curl* for DOFs defined as line integrals on edges;
- *divergence* for DOFs defined as surface integrals (fluxes) on faces;

As a consequence conforming finite elements (FE) spaces should be defined as follows:

- conforming H^1 FE space for DOFs defined on nodes;
- conforming $H(\mathbf{curl})$ FE space for DOFs defined as line integrals on edges;

- conforming $H(\mathbf{div})$ FE space for DOFs defined as fluxes on faces;
- conforming L^2 FE space for DOFs associated to every each element;

Now it can be emphasized the consistency of De Rham sequence applied either to the conforming FE spaces (see. (4.1)) either to conforming generalized differential operators spaces (see.(3.5)). The essential conclusion is the fact that the differential forms related to De Rham sequence represents the main interdisciplinary link between the physical, mathematical and numerical aspects of the multiphysic problems.

6.2 Original Contributions

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1. Several papers published within important conferences some of them ISI indexed:

   - „An Object Oriented Data Structure Designed for Multiphysics Simulations on Parallel Computers"; authors: Mihai Popescu, Aurel-Sorin Lup , Gabriela Ciuprina, Daniel Ioan; presented at the ATEE-2015 Conference (ISI), Bucharest [73] - *first author*. The work proposes an object oriented data structure suitable for the implementation of multiphysic simulation algorithms. The data structures were implemented in C++ and tested an a simple microswitch. This was the first setp towards a full class of objects dedicated to multiphysic simulation;
   - „Using Object Oriented Data Structures for Optimizing MEMS Devices on Parallel Computers"; authors: Mihai Popescu, Aurel-Sorin Lup, Ruxandra Bărbulescu, Gabriela Ciuprina and Daniel Ioan; lucrare presented la The XVII International Symposium on Electromagnetic Fields in Mechatronics, Electrical and Electronic Engineering (ISI), Valencia, Spain, 2015 [71]. The work presents the data structured discussed in the previous paper [73], but with significant improvements. This version allows dividing the problem domain in several sub-domains in order to be treated on parallel processors with little inter-processor communication. The results of the tests performed on our Numerical Modeling Laboratory were discussed;

- „Parametric Multiphysics 3D Modelling of a Bridge Type MEMS Capacitive Switch"; authors: Aurel-Sorin Lup, Gabriela Ciuprina, Mihai Popescu and Daniel Ioan; lucrare presented la The XVII International Symposium on Electromagnetic Fields in Mechatronics, Electrical and Electronic Engineering (ISI), Valencia, Spania, 2015 [53]. The work presents the 3D multiphysic sumulations performed for a capacitive microswitch with Comsol Multiphysics V4.4. The simulations were performed in both static and dynamic regimes;
- „Coupled multiphysics-RF reduced models for MEMS"; authors: Gabriela Ciuprina, Daniel Ioan, Aurel-Sorin Lup, Mihai Popescu, Ruxandra Barbulescu, Alexandra Stefanescu; presented la IEEE 1st International Conference on Power Electronics, Intelligent Control and Energy Systems (ICPEICES) (ISI) 2016- Dehli [17]. The work discusses the application of Model Order Reduction (MOR) techniques for an RF MEMS;
- „HPC in Multiphysics Analysis of RF-mems Capacitive Switches"; authors: Sorin Lup, Gabriela Ciuprina, Mihai Popescu and Daniel Ioan; lucrare presented la SIELA 2018 - The XXth International Symposium on Electrical Apparatus and Technologies (ISI), Burgas, Bulgaria [54]. The work presents a comparison between the nonlinear simulations of an RF MEMS, performed with two software packages: on one hand the commercial package Comsol Multiphysics V4.4, and on the other hand **FreeFEM++** - dedicated software for PDEs solving. Comsol used a serial algorithm, and on **FreeFEM++** was implemented a parallel one on 8 processors.
- „A Parallel Algorithm for Multiphysics Analysys of RF-MEMS"; authors: Mihai Popescu, Sorin Lup, Gabriela Ciuprina, Daniel Ioan and Ruxandra Bărbulescu, SCEE 2018 – The 12th International Conference on Scientific Computing in Electrical Engineering, 23 – 27 September 2018, Sicily, Italy [72]. The work uses the physical model used in the previous paper (SIELA), but described by means of the problem's weak formulation. Hence the implementation on the **FreeFEM++** was natural, the resulting parallel code being more efficient in this case. The comparisons where made against the Comsol Multiphysics model, solved with a parallel solver.

2. Synthetic discussion of the state of art in nowadays parallel data processing;

3. A coherent presentation of the very complex mathematical methods used

by the functional analysis to tackle the weak formulation of (multi)physic problems. The task was not an easy one because of the multitude of valuable sources in the field that was founded by the mathematicians of the first part of the 19$^{\text{th}}$ century. Any important relevant work usually brought its own symbols and demonstrations that sometimes makes their understanding difficult, especially when trying to connect the theory to the physical reality;

4. The exposure of the full mathematical methodology that leads to the use of conforming finite elements (FE). The methodology is used to construct triangular (2D) and tetrahedral (3D) first order conforming H^1, **curl**, and **div** finite elements. The importance of the *De Rham* sequence is emphasized.

   During the progress of this thesis several practical results were issued and published in the relevant conference papers mentioned above. However, using these results was not one of the goals of this present work; I preferred pointing out some main issues (without claiming full coverage) that might appear during a numerical simulation process and their possible causes. Knowledge of these issues is important for anyone who intends to work in the fascinating field of multiphysic simulations. Passing from the continuous real macroscopic world, mathematically described by the strong formulations, to the proper functional spaces that allow finding the weak formulation is not always straightforward, due to the need of preserving the continuity property. The same issue is even more challenging when passing to the finite discrete universe of the numerical formulations. Here, the importance of sequences as the De Rham one is crucial. Actually the work points out as one of its main conclusions that the De Rham sequence represents the main link between the physical, mathematical and numerical aspects of the multiphysic problems.

5. The main contribution of this thesis consists of the description of the full path that leads from a physical device to it's numerical simulated model. Following the example of a simple capacitive microswitch, presented in Chapter 5 of the thesis, other multiphysic simulations can be performed. This work emphasizes the crucial importance for every specialist, working in the field, to fully understand the functional analysis concepts and their application. It is worth stressing the fact that without this understanding, using dedicated software packages will be reduced to an interesting exercise but without any real practical utility.

6.3 Perspectives

The methodology presented in this work does not claim iit is unique. However, any method used to develop a multiphysic simulation should „touch” the following universes:

- quantities and laws used to describe the involved physical phenomena;
- functional analysis;
- numerical modeling;
- High Performance Computing (HPC).

The the present thesis, the last item in the previous list needs further research and more practical examples. This opens the perspective of future research:

- development of the present step by step method, by including automatic domain decomposition according to the available processing cores; the method should be illustrated with several practical examples from various physical fields;
- the present challenge is that the hardware development left quite far behind the software development. Thus, a recent produced software needs not necessarily to behave better on a brand new hardware system. That's the reason why complex simulation problems should be first run on different dedicated software packages in order to find the best match. With this respect, it will be useful to improve the experience of using three software platforms already used in our Numerical Modeling Laboratory of the Electrical Engineering Faculty, as follows:

  1. **FreeFEM++** , currently used in this thesis; the software recently got a new library dedicated to the domain decomposition methods, by using parallel algorithms (`https://doc.freefem.org/documentation/ffddm/`);
  2. **ONELAB** (`https://onelab.info/`), based on the **Gmsh** (`https://gmsh.info/`) [31] automatic mesh generator; this software has the advantage of an own graphical interface with sensible better performance than **FreeFEM++** ; ONELAB has its own solver but can be quite easily interfaced with standard mathematical libraries popular in the HPC world;

3. **COMSOL Multiphysics** ©(`https://www.comsol.com`) - a well known commercial package; the solver robustness, pre- and post-processing capabilities, and the good documentation which come altogether with such a piece of software, are shadowed by the lack of flexibility due to the impossibility to access the source code of the software.

Part of the above perspectives will be subjects of further works of the thesis author. Hopefully they will attract other specialists too, especial younger ones, to activate in the field of Computational Science and Engineering, which is not quite easy but has a great future.

Selective Bibliography

[1] ***. *OpenMP Application Program Interface*. OpenMP Architecture, July 2013. Version 4.0.

[2] ***. The guide to the program posix certified by ieee and the open group. Technical report, The IEEE Open Group, 2017.

[3] R.A. Adams and J.J.F. Fournier. *Sobolev Spaces*. Elsevier, 2003.

[4] Neculai Andrei. Modele matematice în mecanică. Research Institute for Informatics, Center for Advanced Modeling and Optimization, 2009.

[5] Donu Arapura. Introduction to differential forms, jun 2016.

[6] Stefan Banach. *Theorie des Operations Lineaires*. Z Subwencji Funduszu Kultury Narodowej, 1932.

[7] A. Behzadan and M. Holst. Sobolev-slobodeckij spaces on compact manifolds, revisited. Technical report, Departament of Mathematics, University of California San Diego, 2018.

[8] B. Blaise and L. Livermore. Posix threads programming. Technical report, Lawrence Livermore National Lab. HPC Tutorials, 2021.

[9] Alain Bossavit. *Electromagnetisme, en vue de la modelisation*. Springer Verlag Paris, 1993.

[10] Alain Bossavit. *Computational Electromagnetism*. Elsevier, Academic Press, 1997.

[11] H. Brezis. *Functional Analysis,Sobolev Spaces and Partial Differential Equations*. Springer, 2010.

[12] M. Brinskiy and M. Lubin. An introduction to mpi-3 shared memory programming. Technical report, Intel Corporation, 2018.

[13] Louis L. Bucciarelli. Solid mechanics. MIT Civil and Environmental Engineering Course 1.050., 2004.

[14] Theo Buhler and Dietmar Salamon. *FUNCTIONAL ANALYSIS*. ETH Zurich, 2017.

[15] Jean Cea. Annales de l'institut fourier. In *Approximation variationnelle des problèmes aux limites*, volume 14, pages 345–444. Imprimerie Durand, 28 - Luisant, 1964.

[16] P. G. Ciarlet. *The Finite Element Method for Elliptic Problems*. North-Holland Publishing Company, Amsterdam, 2nd edition, 1979.

[17] G. Ciuprina, D. Ioan, M. Popescu, Ș. Alexandra, and L. Sorin. Coupled multiphysics-rf reduced models for mems. In *IEEE 1st International Conference on Power Electronics, Intelligent Control and Energy Systems (ICPEICES) - Dehli*, 2016.

[18] Frank H. Clarke. Generalized gradients and applications. *Transactions of the American Mathematical Society*, 205, 1975.

[19] Keith Conrad. Bilinear Forms. Technical report, University of Connecticut, 2017.

[20] Bernard Dacorogna. *INTRODUCTION TO THE CALCULUS OF VARIATIONS*. Imperial College Press, 2004.

[21] Daniel. *Bazele Teoretice ale Ingineriei Electrice*. Editura 2000, 1989.

[22] Robert Resnick David Halliday and Jearl Walker. *Fundamentals of physics*. John Wiley & Sons, Inc., 9th edition, 2008.

[23] A.S. Demidov. *Generalized functions in mathematical physics Main ideas and concepts*. Nova Science Publishers, 2000.

[24] Leszek Demkowicz. *Computing With Hp-adaptive Finite Elements*. Institute for Computational Engineering and Sciences The University of Texas at Austin, 2005.

[25] Victorita Dolean, Pierre Jolivet, and Frédéric Nataf. An Introduction to Domain Decomposition Methods: algorithms theory and parallel implementation. HAL archives-ouvertes.fr, May 2016.

[26] J. V. Fernandez, W.H.A Schilders, and L. Miguel Silveira. Order reduction techniques for coupled multi-domain electromagnetic based models. Technical report, CASA, 2008.

[27] Richard Feynman. *Fizica modernă*, volume 1. Editura Tehnică, 1969.

[28] Mocanu Florentina. *Mecanica Mediilor Deformabile.* Universitatea Tehnică "Gheorghe Asachi" Iasi, 2000. Note de curs.

[29] I. Foster. *Designing and Building Parallel Programs: Concept and Tools for Parallel Software Engineering.* Addison-Wesley, 1995.

[30] M. Gander, F. Nataf, and L. Halpern. Optimized Schwartz Methods. *12th International Conference on Domain Decomposition Methods*, 2001.

[31] C. Geuzaine and J.F. Remacle. Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities. *International Journal for Numerical Methods in Engineering*, 79(11):1309–1331, 2019.

[32] V. Girault and P.A. Raviart. *Finite Element Methods for Navier-Stokes Equations: Theory and Algorithms.* Springer Berlin Heidelberg, 2012.

[33] C. Grossmann, H. Roos, and M Stynes. *Numerical Treatment of Partial Differential Equations.* Springer-Verlag Berlin Heidelberg, 3rd edition edition, 2007.

[34] S.D.A. Hannot. *Modeling Strategies for Electro–Mechanical Microsystems with Uncertainty Quantification.* Technische Universiteit Delft, 2010.

[35] F. Hecht. New development in freefem++. *Journal of Numerical Mathematics*, 20(3-4):251–256, 2012.

[36] F. Hecht. FreeFEM Documentation. Release 4.0, April 2019.

[37] R. Hiptmair. Finite elements in computational electromagnetism. *Acta Numerica*, 11:237–339, 2002.

[38] J. Necas I. Hlavácek. *Mathematical Theory of Elastic and Elasto-Plastic Bodies*, volume 3. ELSEVIER, 1st edition, 1981.

[39] Ronald H.W. Hoppe. Finite element methods. University of Huston - Webpage, 2016.

[40] Jacopo Iannacci. *RF-MEMS Technology for High-Performance Passives.* 2053-2563. IOP Publishing, 2017.

[41] D. Ioan and G Ciuprina. *Reduced Order Models of On-Chip Passive Components and Interconnects, Workbench and Test Structures*, chapter III.8, pages 447–467. Springer Berlin Heidelberg, 2008.

[42] D. Ioan, G. Ciuprina, and W.H.A. Schilders. *Model order reduction, applications*, chapter „Complexity reduction of electromagnetic systems", pages 145–200. De Gruyter, 2021.

[43] Marsden J.E. and Hughes Thomas J.R. *Mathematical Foundations of Elasticity.* Dover Publications Inc., 1983.

[44] D. Kanter. Inside nehalem: Intel's future processor and system. https://www.realworldtech.com/nehalem/, 2008.

[45] Robert C. Kirby, A. Logg, and A. Terrel. Common and unusual finite elements. http://www.logg.org/anders/pub/papers/KirbyLoggEtAl2012a.pdf, 2015.

[46] A.M. Krall. A review of orthogonal polynomials satifying boundary value problems. In *Othogonal Polynomials and their Applications*, volume 1329. Springer-Verlag, 1986.

[47] Erwin Kreyszig. *Introductory Functional Analysis with Applications.* Wiley & Sons, 1989.

[48] Cornelius Lanczos. *The Variational Principles of Mechanic.* University of Toronto Press, 1970.

[49] Peter D. Lax. *Functional Analysis.* John Wiley & Sons, Inc., 2002.

[50] G. Leoni. *A First Course in Sobolev Spaces*, volume v. 105. American Mathematical Society, 2009.

[51] Christian Lessig. A primer on differential forms. *Computing + Mathematical Sciences California Institute of Technology*, 2012.

[52] R.M. Lin and W.J. Wang. Structural dynamics of microsystems current state of research and future directions. In *Mechanical systems and signal processing*, volume 20, pages 1015–1043, 2006.

[53] S. Lup, G. Ciuprina, M. Popescu, and D. Ioan. Parametric multiphysics 3d modelling of a bridge type mems capacitive switch. In *ISEF*, 2015.

[54] S. Lup, M. Popescu, G. Ciuprina, and D. Ioan. Hpc in multiphysics analysis of rf-mems capacitive switches. In *XXth International Symposium on Electrical Apparatus and Technologies.*, 2018.

[55] N. et alii MacDonald. Writing message passingparallel programs with mpi. a two day course on mpi usage. Technical report, Edinburgh Parallel Computing Centre, 2013.

[56] Lawrence E. Malvern. *Introduction to the Mechanics of Continuous Medium.* Prentice-Hall, Inc, 1969.

[57] Tarek P.A. Mathew. *Domain Decomposition Methods for the Numerical Solution of Partial Differential Equations.* Springer, 2008.

[58] B. Mattson, B. Sanders, and B. Massingill. *Patterns for Parallel Programming.* Addison-Wesley Professional, 2004.

[59] W. McLean. *Strongly Elliptic Systems and Boundary Integral Equations.* Cambridge University Press, 2000.

[60] R. M. C. Mestrom. *Multiphysics Modelling and Experimental Validation of Microelectromechanical Resonator Dynamics.* PhD thesis, Technische Universiteit Eindhoven, 2009.

[61] C. I. Mocanu. *Teoria câmpului electromagnetic.* Editura Didactică și Pedagogică, București, 1981.

[62] Peter Monk. *Finite Element Methods for Maxwell's Equations.* Clarendon Press. Oxford, 2003.

[63] Jean-Claude Nédélec. Mixed finite element in 3d in $h(\text{div})$ and $h(\text{curl})$. *Equadiff 6*, Proceedings of the International Conference on Differential Equations and Their Applications held in Brno, Czechoslovakia, Aug. 26 - 30, 1985:321–325, August 1985.

[64] J. Necas. *Direct Methods in the Theory of Elliptic Equations.* Springer Monographs in Mathematics. Springer-Verlag Berlin Heidelberg, 2012.

[65] J. C. Nédélec. Mixed finite elements in $\mathbb{R}^3$. In *Numerical Mathematics.* Springer-Verlag, 1980.

[66] Patrick Newberry. Differential forms. Mathematics Department of the University of Colorado Boulder, sep 2016.

[67] Jarkko Niiranen. Finite Element Methods for 2d and 3d Elasticity. Aalto University, Helsinki, Engineering Computation and Simulation, 31.10.2016-20.12.2016, Course 9.

[68] Mícheál O'Searcoid. *Metric Spaces.* Springer Science & Business Media, 2006.

[69] P. S. Pacheco. *An Introduction to Parallel Programming.* Morgan Kaufmann Publishers, 2011.

[70] Iordan Petrescu. Introducere în metoda elementelor finite, cu aplicaţii în mecanica construcţiilor. Note de curs, 2012.

[71] M. Popescu, S. Lup, and R. Bărbulescu. Using object oriented data structures for optimizing mems devices on parallel computers. In *ISEF*, 2015.

[72] M. Popescu, S. Lup, G. Ciuprina, R. Bărbulescu, and D. Ioan. A parallel algorithm for multipysics analysys of rf-mems. In *SCEE 2018 – The 12th International Conference on Scientific Computing in Electrical Engineering*, 2018.

[73] M. Popescu, S. Lup, G. Ciuprina, and D. Ioan. An object oriented data structure designed for multiphysics simulations on parallel computers. In *ATEE*, 2015.

[74] M. Preda, P. Cristea, and F. Spinei. *Bazele Electrotehnicii*, volume I și II. Editura Didactică și Pedagogică, București, 1980.

[75] J.Y. Qian, G.P. Li, and F. De Flaviis. A parametric model of mems capacitive switch operating at microwave frequencies. In *IEEE MTT-S International Microwave Symposium digest*, 2000.

[76] A. Quarteroni and A. Valli. *Numerical Approximation of Partial Differential Equations.* Springer-Verlag Berlin Heidelberg, second edition, 2008.

[77] G. Rebeiz. Rf mems switches: Status of the technolgy. In *The 12th Conference on Solid State Sensors, Actuators and Microsystems*, 2003.

[78] G. M. Rebeiz. *RF MEMS: Theory, Design and Technology.* John Wiley & Sons, 2003.

[79] M. Rognes, Kirby R., et al. Efficient assembly of h(div) and h(curl) conformingfinite elements. *SIAM Journal on Scientific Computing*, 31(6):pp. 4130–4151, 2009.

[80] W. Rudin. *Functional Analysis.* McGraw-Hill, Inc, 2-nd edition, 1991.

[81] D Rusu. *Analiză funcţională.* Ed. Performantica, 2005.

[82] M. Rychlik. An introduction to orthogonal polynomials. Technical report, University of Arizona, 2009.

[83] W.H.A. Schilders, Henk A. van der Vorst, and J Rommes, editors. *Model order reduction: theory, research aspects and applications*, volume 13. Springer-Verlag Berlin Heidelberg, 1 edition, 2008.

[84] J. A. Scott. Some examples of the use of areal coordinates in triangle geometry. *The Mathematical Gazette*, 83(498):472–477, 1999.

[85] Marián Slodička. Partial Differential Equations. Lecture Notes for Master Courses - Department of Mathematical Analysis Ghent University, 2012.

[86] Barry Smith. *Domain Decomposition. Parallel Multilevel Methods for Elliptic Partial Differential Equations.* Cambridge University Press, 1996.

[87] Edwin H. Spanier. *Algebraic Topology, Cap. 4.5.* McGraw-Hill Book Company, 1995.

[88] Mircea Stan. *Mecanica mediilor continue.* Matrixrom, 2001.

[89] A. Timotin, V. Hortopan, A. Ifrim, and M. Preda. *Lecții de Bazele Electrotehnicii.* Editura Didactică și Pedagogică, 1970.

[90] F. M. G. Tomescu and A. Tomescu. *Bazele electrotehnicii. Câmp electromagnetic.* Matrix Rom, 2000.

[91] E. Tonti. The reason for analogies between physical theories. In C. Brebbia, editor, *Applied Mathematical Modelling*, volume 1, pages 37–50. IPC Science and Technology Press Ltd, UK, Dept. of Civil Engineering, University of Southampton, UK, 1976.

[92] J. Ubranic. Introduction to openmp. Technical report, Pittsburgh Supercomputing Center, 2021.

[93] Mark van Kraaij. Strain and deformation, a global overview, may 2006.

[94] Piero Villagio. *Mathematical Models for Elastic Structures.* Cambridge University Press, 1997.

[95] H. Whitney. *Geometric Integration Theory.* Princeton University Press, 1957.

[96] O. Windlund and A. Toselli. *Domain Decomposition Methods - Algorithms and Theory*, volume 34 of *Springer Series in Computational Mathematics.* Springer Verlag, 2005.

[97] Hugh Young and Roger Freedman. *University Physics with Modern Physics.* Addison-Wesley, the 13th edition, 2012.

[98] Sabine Zaglmayr. *High Order Finite Element Methods for Electromagnetic Field Computation.* PhD thesis, JOHANNES KEPLER UNIVERSITÄT LINZ, 2006.

[99] Bai Zhaojun, M. Patrick, Dewilde Roland, and W. Freund. Reduced-order modeling. *Handbook of Numerical Analysis*, 13, 2005.