dr hab. inż. Krzysztof Banaś
Katedra Informatyki Stosowanej i Modelowania
Wydział Inżynierii Metali i Informatyki Przemysłowej
Akademia Górniczo-Hutnicza im. Stanisława Staszica w Krakowie

Kraków, 12.10.2015r.

Review of PhD Thesis
„ADAPTIVE STRATEGIES FOR MULTISCALE PROBLEMS"
submitted by mgr inż. Marcin Sieniek

The subject of the thesis

The subject of the thesis belongs to the domain of computational science. The thesis concerns the application of adaptive finite element strategies to simulations that aim at solving difficult multi-scale problems. Simulation based science and engineering is an important field of research, both from practical and theoretical point of view. Adaptive strategies are fundamental to the successful realization of simulations, where accurate and reliable results should be provided in optimal time.

On the other hand, the fields of adaptive methods and multi-scale problems are broad and the thesis must concentrate on specific, selected problems. The applications presented in the thesis belong to such diverse domains as electronics and material science. They concern important problems, currently investigated by many researchers in the field. The results presented in the thesis constitute a timely contribution to the research. This fact is confirmed by several articles in international journals, of which the PhD candidate was the author or a co-author, where the ideas, described in the thesis, were presented originally. The articles on which the thesis is based are listed in the dissertation, with their high total impact factor and MNISW score numbers.

The presentation of the thesis

The thesis consist of 103 pages, with 3 chapters presenting the main material of the dissertation, 3 appendices with auxiliary, technical content, the presentation of the accomplishments of the PhD candidate, the bibliography and the lists of figures and algorithms.

The first chapter presents briefly the main thesis of the dissertation, the state of the art for the field of investigations and the statement of identified open problems, that the thesis attempts to solve.

The next chapter is the longest part of the dissertations and, in subsequent eight sections and several subsections, describes the achievements of the PhD candidate. The consecutive subsections treat the problem of pre-processing mesh and initial condition for adaptive finite element simulations, the problem of solving systems of linear equations, arising from finite element discretizations, in the case when several parts of the computational domain have the identical structure and the problem of discrete-continuous coupling, where different discretizations are used in different parts of the computational domain.

The problem of initial data pre-processing is presented in the context of modelling of metals, where the structure of the investigated material may be defined by a bitmap obtained from e.g. MRI scans. The problem consist in finding the optimal mesh for the solution of the approximation problem and, at the same time, providing the optimal interpolation of initial data on the mesh. The author presents two algorithms to solve the problem. The first one is the simplified version of the projection based interpolation (PBI) method, introduced by Demkowicz, where the simplifications consist in keeping the same degree of approximation during the whole process. This allows for obtaining closed formulae for coefficients of a linear combination that defines the approximating function. Thanks to this, the process of initial data pre-processing becomes faster. For the cases when the accuracy is more important that the execution time, the author presents the full hp-adaptive algorithm. 2D and 3D examples are shown as proof of concept, with hexahedral and tetrahedral elements in 3D.

The problem of optimization of the multi-frontal direct solver in the cases when parts of the computational domain have the same structure, both in terms of local element topology, as well as local degree of approximation, is solved by reusing the suitable parts of elimination tree. The problem is solved in practice, by providing the implementation that is later tested for computational examples. The technique is also analysed using graph transformations, that provide the theoretical background for the algorithm and allow for assessing its correctness and complexity.

The last problem investigated in the dissertation is the discrete-continuous coupling, that often appears in the multi-scale modelling. The author presents the algorithms, as well as data structures (in Appendix C) that can be used to solve the problem. The proposed solutions are tested for the problem of modelling Step-and-Flash Imprint Lithography (presented in Appendix B).

The short conclusions (Chapter 4) summarize the main achievement of the thesis.

The assessment of the dissertation

The author presents the solutions to three different problems associated with the attempts to solve multi-scale problems using the adaptive finite element method. The first problem, the problem of construction of optimal initial data for simulations with discrete input data sets, is solved using two variations of the same method, that uses projection based interpolation. The first variant is aimed at cost-effective solution, with the constant degree of polynomials for approximated data, while the second uses full hp-adaptivity, to get the most accurate results.

The second problem is associated with the optimal realization of calculations, specifically with the optimization of the direct solver of linear equations, that often constitute the most important part of finite element codes, from the point of view of minimizing execution time. The author presents a variant of the sophisticated, state-of-the-art multi-frontal direct solver, that improves the existing standard versions, in the cases when the computational domain contains the parts with identical structure (due e.g. to similar singularities).

The last problem results from the often encountered necessity of coupling discrete and continuous descriptions of a modelled process. The solution presented by the author combines two important techniques, mesh adaptivity in finite element modelling and coupling of different models defined in different parts of the computational domain.

The solutions to the problems are original and innovative, showing the substantial knowledge of the PhD candidate, both concerning the field of investigations, as well as the methodology of conducting research in computational science.

The discussion and comments

Apart from several minor remarks concerning the notation (e.g. the lack of explanation for the symbols used in Table 1, page 19), the language (e.g. the use of "paralleled" instead of "parallelized" or "divide variables" instead of "share variables"), the repetitions (e.g. for several references in the bibliography or several definitions, like the definitions of shape functions on pages 12-15, 80 and 85 or the weak statement for the linear elasticity problem – pages 70 and 74) and the omissions (e.g. in the description of the frontal solver algorithm on page 43), there are several concerns of more general character.

One of the drawbacks of the dissertation is the lack of extensive introduction, with the comprehensive literature review and the broader presentation of the state of the art, from which the motivation for the research may arise. Such introduction would serve as a proof of the PhD candidate's knowledge. For the submitted thesis, the reviewers must assess this knowledge based on the results of the research only, and not on the presentation of the field of investigations. Moreover, from the short introduction in the thesis it cannot be concluded how often and in which situations the problems investigated in the thesis appear in multi-scale modelling and how severe obstacles they impose for applying adaptive strategies, especially the adaptive finite element method.

A similar comment concerns the rest of the dissertation. The content concentrates on the results of investigations, the solutions to the particular problems considered (with some parts explicitly taken from research articles), with the lack of a broader, unifying context and a single flow of presentation, linking together the different sections of the work. It would be good to have a single multi-scale problem solved, where all the presented achievements could be applied.

Finally the thesis lacks the broader discussion of results. As a consequence, the importance of the research for the field is not fully depicted in the thesis. The contribution of the results presented in the dissertation for solving the particular problems defined in the introduction as open problems is evident, but a more general influence of the results on the domain of applying adaptive methods for solving multi-scale problems with discrete input data is not fully investigated. Especially there are no comparisons with other methods of pre-processing discrete input data (e.g. based on simple adaptive strategies with geometrical criteria for initial mesh construction), other adaptive strategies than the automatic hp-strategy based on interpolation error estimates, other methods of solving systems of linear equations (e.g. iterative with different preconditioning) or other methods of coupling different scales in multi-scale modelling, apart from discrete-continuous coupling described in the thesis.

The conclusion

Despite several critical remarks, the general assessment of the PhD thesis by mgr inż. Marcin Sieniek is positive. The PhD candidate has shown satisfactory level of general, computer science related, knowledge as well as specific knowledge, concerning adaptive strategies and multi-scale problems. In my opinion the dissertation fulfils the requirements of the law („Ustawa o stopniach i tytule naukowym oraz o stopniach i tytule w zakresie sztuki" from March 14th, 2003) and I recommend to admit the thesis to the defence.

Krzysztof Banaś