Review of doctoral dissertation entitled "Efficient Algorithms for Three-Dimensional Computational Mesh Generations and Air Pollution Simulations Based on Hypergraph Grammars" by Mr. Krzysztof Podsiadło

Luis E. Garcia-Castillo
Universidad Carlos III de Madrid
legcasti@ing.uc3m.es

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General Statements / Summary

The doctoral dissertation "Efficient Algorithms for Three-Dimensional Computational Mesh Generations and Air Pollution Simulations Based on Hypergraph Grammars" by Mr. Krzysztof Podsiadło meets the requirements provided for in Article 13 of the Act of 14 March 2003 on Academic Degrees and Academic Title and Title in Art (Journal of Laws of 2017, item 1789).

The doctoral dissertation provides an original computational solution to the problem of modeling air pollution by using novel graph-grammar based mesh generation algorithms. Graph-grammar productions allow to take advantage of parallelism with irregular data structures and algorithm flows as it is the case with mesh generation and refinement. The methodology provided is applied to a real environment as it is the modeling of the air pollution in Lesser Poland where there is a severe public health problem. The doctoral dissertation also contains other specific scientific contributions as it will be reviewed, on a chapter basis, in the following. It is appreciated that the code developed in the context of the thesis is publicly available.

On the other hand, the writing and organization of the volume make it very difficult to read and understand what is exactly made and how.

The thesis has resulted in a publication indexed in the JCR in the first quartile (Q1) in which the doctoral candidate is the first author and which constitutes the core of his dissertation. He is also co-author of several publications in prestigious conferences and in one non-JCR journal. In total, he has 7 publications.

Chapter 1

Chapter 1 is devoted to describe the motivation, and main scientific contributions of the thesis, together with a brief state of the art in the different numerical and computational techniques used throughout the volume. The motivation is presented in a clear and concise manner. The state of the art, without being exhaustive, is correct. In any case, it does not seem to be sufficiently up to date, as there are very few references from the last few years.

Chapter 2

Chapter 2 is devoted to describe the methods and algorithms used in the thesis. It is a core chapter of the volume.

The chapter starts with a detailed description of the graph grammar representation for Ricara mesh refinement which is one of the main contributions of the thesis if not the most important one (see section 2.2). The description is easy to follow with the help of several plots and examples.

The parallel implementation (section 2.3) is carried out with GALOIS framework developed by group of Prof. Pingali's. The document shows (pages 32-36) sections of the code that are very illustrative. The downside is that the formatting is very bad visually; on the other hand, perhaps the code sections should have been included in an appendix separate from the main body of the document.

Section 2.4 is dedicated to the application of the graph-grammar productions to an advection-diffusion-reaction solver. The solver uses Crank-Nicolson time integration scheme and SPUG stabilization on tetrahedra "extruded" from the triangular mesh obtained by Ricara mesh refinement implemented through graph-grammar productions. The pesudocode for the refinement algorithm is shown in Algorithm 1, page 43. Apparently, the graph-grammar is only applied to the mesh refinement procedure, which is coupled with the solver itself. No reference is made to the use of graph-grammar for the calculation of the matrix coefficients or the matrix-by-vector multiplication processes of the GMRES-based algebraic iterative solver. Thus, it is not clear (actually, this reviewer is not sure) if graph-grammar is used only regarding mesh refinement or in other stages of the process. And more specifically, it is not clear if there is some form of error estimation, or if the algorithm simply refines the mesh until the accuracy limit is reached with which you have the starting terrain data.

A different solver is presented in section 2.5. In this case, an alternating direction solver on Navier-Stokes-Boussinesq Eqs. is presented to model the evolution of the air pollution. The alternating direction technique allows to obtain the solution of the problem with computational complexity $O(N)$ by expressing the matrices as Kronecker product of matrices corresponding to one-dimensional problems. In particular, Section 2.5.2 shows the extension to irregular terrain that is realized by imposing diagonal block diagonal entries in the corresponding matrices. The motivation for the inclusion of this solver in the thesis, if I understand correctly, is given in order to compare this solver with the one in Section 2.4 and earlier. Nevertheless, the comparison is a bit forced because they are very different approaches. In fact, page 53 of the Chap 4 describes the numerical experiments performed and only one experiment (the number 6) is related to this solver. Actually, later in Section 3.7 it is stated that although the alternating-direction solver runs in parallel (the PROMETHEUS supercomputer has been used) the memory requirements with small cell sizes make it not viable compared to a solution with an adapted mesh as is the case of the solver used in section 2.4 and earlier.

Although this chapter is reasonably well written there are some things that are not clear. Some of them have already been pointed out above. Others, for example, have to do with the mesh to be used with one solver and another. For example, figure 11 is quoted in the context of the solver of section 2.5 but shows the mesh which appears to be that of figure 27 obtained with graph-grammar on Ricara algorithm. On the other hand, some acronyms are used without having been previously expanded.

Chapter 3

Charter 3 contains the numerical experiments. Thus, it is a key part of the work.

There are a lot of worth displaying plots. However, in many cases, the plots are mixed with a few lines of text in same page page making the reading very difficult. In addition, new sections start before the plots associated to the previous sections ended.

Section 3.2. I miss further comments on the results shown in Table 2,

Section 3.3. Missing "Table" when referencing Table 3. As a MMS solution is used, there is no need to have any error estimator. Nevertheless, the criteria to divide or not an element is not given (Fig. 39-51). Any particular threshold that is used?

Section 3.4. Here we speak of topographic area of Lesser Poland but it is the same area as the one cited as "of Krakow" in other previous sections (same grid measures). It seems that here it is already 3D (tetrahedra extruded from triangular meshes) but it is not clear. On the other hand, the representation of Fig 56-65 should be further explained. For instance, what do the shadows on each tetrahedral face mean?

Section 3.5. Final simulation of the air pollution dynamics. They look great and useful! Are there records of experimental measurements that can be used for comparison/validation?

Section 3.6. Parallel implementation within GALOIS framework.

In the text, it is mentioned that the reports are for iterations 15-24 while in the caption of Table 4 is indicated for 10-24.

Chapter 4

Finally, chapter 4 contains the conclusions and some future works that might be considered.