VSB TECHNICAL UNIVERSITY OF OSTRAVA | FACULTY OF CIVIL ENGINEERING | DEPARTMENT OF MATHEMATICS

Opponent's review of the dissertation thesis "Parallel Numeric Solution of Differential Equations" by Ing. Gabriela Nečasová

1. Meeting the objectives

In this work, the student employed the semi-discretization method of lines, which discretizes the spatial domain using a suitable approximation of the derivative while keeping the time domain continuous. Consequently, the given partial differential equation (PDE) is transformed into a system of ordinary differential equations (ODE), leading to the solution of the initial problem. The resulting system of ODE is solved using Runge-Kutta methods, commonly employed in practice, as well as a newly proposed higher-order method based on Taylor expansion. This method utilizes a variable integration step and order determined by the recurrent computation of Taylor series terms at each time interval. A crucial feature of the method is its ability to automatically select the order based on the integration step size.

The student aimed to demonstrate that extensive systems of ODE, arising from PDE through the method of lines, can be more efficiently solved using a parallel method based on Taylor expansion compared to conventional state-of-the-art numerical methods. In this study, numerical experiments were conducted on a specific selected class of problems modeled by second-order PDE. These included the heat conduction equation, the wave equation, and the telegraph equation. In the spatial domain, both of three-point and five-point central finite differences were used. The sizes of the systems of ODE ranged from 128,000 to 2,048,000. Both Taylor series methods and Runge-Kutta methods were employed to solve these systems. The numerical experiments were performed on the Barbora supercomputer at IT4Innovations National Supercomputing Center in Ostrava.

The objectives of the work have been achieved; however, I would appreciate to see the real limits of the developed methods and the current implementation.

2. Solution process and results, specific benefits

I have several comments regarding the organization of the work, with a particular focus on the length of the proposed thesis. While I am not acquainted with the limits defined by Faculty of Information Technology at Brno University of Technology, submitting a thesis that spans 268 pages may not be reasonable. To be more clear - considering the limited time available to academic staff, it's essential to make the most of their resources; the deep study of such a long thesis can be time-consuming and inefficient. A more optimal approach would be to aim for a Ph.D. thesis that contains between 100 and 120 pages of refined content, with a strong focus on the student's core research problem from the outset. In this context, Chapter 5 (Parallel and distributed computing) may appear as an optional addition. As an opponent of the thesis, I appreciate the historical context and the overview of supercomputer architectures presented in the work, however, it's worth noting that while this information is interesting, there appears to be a lack of corresponding testing and results computed on the presented architectures. It might be beneficial to consider the relevance of this historical and architectural content in relation to the thesis's core objectives or simply remove this chapter; these sections of the thesis may be extraneous, diverting the opponent's attention away from the paper's

central focus. Another aspect that affect the quality of the work is the presence of subsections 6.5.3, 6.5.4, 6.6.2, 6.6.3, 6.6.4,6.7.2, 6.7.3, 6.7.4, 6.8.2, 6.8.3, 6.8.4, 6.9.6, 6.9.7, which solely consist of pictures and lack accompanying text. Furthermore, these images are not referenced in the text. Based on my expertise, it is essential to include references to images and charts in the text to ensure their relevance and contribution to the work.
In this work, the focus is on solving 1D PDE, which align with straight-line methods. It would be intriguing to explore how the presented MTSM and MTSM_PREC algorithms would perform when applied to 2D or even 3D problems and whether the efficiency remains comparable to other existing approaches. However, please, consider this as a suggestion for the student's future work rather than a critique of the current thesis.

3. Significance for practice and development of the discipline

The dissertation’s topic hold serious relevance within the field of science and practice. I would like to commend the student for the numerous contributions to major international conferences and publications in leading international publishers. The internship at the supercomputing center in Lugano further underscores the importance of the work that has been accomplished.

4. Formality, language level

The work is written in English, and I was highly impressed with the overall quality. I noticed very few typos and errors in the text. However, I found some room for improvement in the mathematical formulations and the definition of variables. The thesis would benefit from a thorough review and consistent use of alphabet characters, whether Greek or classical, for variable notation. Additionally, I have minor formatting concerns regarding some of the graphs and figures. It would be helpful to include a list of abbreviations in the thesis, as it would enhance navigation and prevent labeling duplications.

5. Comments on the student's publications

I greatly admire the student's publishing achievements, with 21 entries in the Scopus database, including 3 articles. This is an excellent result, complemented by a notable number of citations and an H-index of 3. From this perspective, the Ph.D. student's publication activity alone is commendable and demonstrates significant dedication. In the future, I recommend focusing more on publications in journals with an impact factor to further enhance their academic contributions.

6. Additional questions and comments

Questions:

- Why does the abstract mention that Nicolaus Bernoulli first used PDE in the 18th century, while this historical context is not present in the introduction?
- Why are there no references in Chapter 1?
- Based on my experiences, it is common practice to number only those equations subsequently cited in the text. Are all the numbered equations in the text referenced?
- The thesis would benefit from a preface that outlines general rules for labeling and citations. It should specify that articles and conference papers where the student is an author will be cited in the thesis in a certain format. This addition would enhance clarity and prevent confusion.

- On page 62, the text mentions that Figure 3.12 displays the Verner Runge-Kutta method, but the legend and caption indicate the Fehlberg method. Are these methods equivalent?
- Equations (3.116) to (3.119) appear to be identical to equations (3.124) to (3.127). Is it possible to refer to the former equations and thus shorten the text?
- What was the purpose of experiments 1 to 5 on pages 72 to 78?
- In the results tables, you list efficiency speedup against various factors, but I require the average solution times. While you have these times plotted on graphs, it can be challenging to discern the exact values from the graphs. Would it be possible to include these times for one selected example in the tables?
- In Section 6.9, Figure 6.40 displays the fill rate of sparse matrices, where matrix A is nearly one percent and A with a canopy is over 53 percent, which raises questions about whether A with a 53 percent fill rate can still be considered a sparse matrix. Additionally, it would be valuable to compare both the memory requirements and the preprocessing times for building these matrices. I recommend providing a detailed explanation in the presentation to clarify why the MTSM_PRECALC method is significantly faster and more efficient than MTSM.

Comments:

- On page 20, Equation (2.2): Is the variable y` independent of time t?
- On page 20: The following equation h_i = t_(i+1) - t_i do not include the domain of index i. It is not defined anywhere.
- On page 20: At the end, you have the formula h=(b-a)/n; here, it should not be n but k.
- On page 21, Definition 2.0.2.: This definition is repeated in the text and the formulas on page 20. It is unfortunate.
- On page 21: At the end of the page, you have f(t,y) without indices i. Is this correct, or are you missing indices?
- On page 22: In Definition 2.0.7, you have an equation and a term in the sum f(t_(i+1-k), y_(i+1-k)) that can be written before the sum because there is no index j to be added over. Is this a case, or should the index j be instead of the index k?
- On page 22: At the end of Definition 2.0.9, I recommend to mention that this is true for all k of the set of numbers from 1 to n.
- On page 23: You have the text "The local in each time step...". Here, you talk about the “time” for the first time. Therefore - what does the variable t means in your conception? I would appreciate more clarification.
- On page 23: I am afraid I have to disagree with the statement that i should be greater than or equal than 0. There must be an upper bound, or it will fly out of the box.
- On page 23: Why are you using h going to zero here? It needs to be more precise. Additionally, the variable h was defined for an equidistant network.
- On page 24: If we are talking about the nth order, I recommend writing n-th and not n to th in italics, where someone may confuse it with n being augmented to th.
- On page 24: Is the variable t a time or a point?
- On page 27, Equation (2.29): sum values i=1, why it cannot go from zero? The upper bound is set to s, but the variable s is not defined anywhere, nor is it set to any value.
- On page 31: At the end of the paragraph in Section 2.5, I expect some references.

- On page 36: The sentence "The parabolic PDE describes heat transfer is given." The sentence sounds like that: no other equation satisfies this, and only this one exists. I would be more cautious in these statements.
- On page 36: Again, here is the variable t presented as time. There is a need for greater clarity in these statements.
- On page 36: For Equation (3.5), you talk about the rod once and the bar twice. What is the difference?
- On page 37: The reference to Equation (3.13) in the text that follows needs to be revised.
- On page 39: Section 3.3.1 is not a section but a subsection.
- On page 40: It says "nth-order" before it says n to th order. How is this correct?
- On page 40: The phrase "The higher the power of h ..." does not seem right and should be rewritten.
- On page 42, Equation (3.43): This is valid only if the matrix A is regular. Are you guaranteed to have a regular matrix?
- On page 43: Is it not possible to mark the variables DX1 to DX4 differently than this?
- On pages 45 and 47: The division you have for "Forward difference formulas" and "Backward difference formulas" only applies to equidistant division but not in general.
- On page 46, Equation (3.66): Why are the variables y_(k+3) and y_(k+4) presented here when the variables x with the appropriate index should be here instead?
- On page 49: You have stated that "O=" but missing what. What value should be here?
- On page 49: The value of 4.2e-17 is at the limit of computer precision, and it is pretty strict for absolute error.
- On page 50: There is no legend in Figures 3.4 and 3.5 to describe the curves.
- On page 51: If you use any variables in the equations, they should have a single letter, not a cluster of letters. It is misleading.
- On page 52: There are captions in Figures 3.7 and 3.8 that should not be there and should be in the figure caption. Also, the caption of Figure 3.7 says O=40, and the caption of Figure 3.8 says n=60. What is the message?
- On page 52: If there are more than two items listed, there should be a comma before the conjunction “and”.
- On page 56: Variable j starts with what index?
- On page 56, Equation (3.86): Why is here an index i when there should only be an index j?
- On page 56, Equation (3.89): Same case as above.
- On page 56, Figure 3.9: Does it always have to be an equidistant division? Can it not be a general division?
- On page 56, Equation (3.90): This will not hold for j = 1. It would help if you include other conditions in.
- On page 57, Equation (3.91): The indices n, i, x, j are not explained. In addition, some have been used as variables before, and this needs to be clarified.
- On page 57, Equation (3.83): What does the star mean? The star variable is not explained.
- On page 58, Equation (3.86): Again, it does not add up if j equals 1.
- On page 59: At the end of the page, t is given to n. This looks like the variable t scaled to n, but that does not fit with what is behind the equation. If t is the index of the variable t, wouldn't it be more appropriate to write the indices as subscripts?

- On page 60: Why are the subscripts and superscripts for j and n interchanged in Equations (3.102) and (3.103)?
- On page 62: The text states that Figure 3.12 shows the Verner Runge-Kutta method, but the legend and caption show the Fehlberg method. Are these methods equivalent?
- On page 71: Defining variables using whole words and underscores is not good. I know it is done in programming, but it has no business in equations.
- On page 72, Figure 4.1: If it is supposed to be a circle, why can't you see the circle but the ellipse?
- On page 73: Is the experiment setting something up, or is the experiment more likely to be set to ...?
- On page 79: Is it really supposed to refer to Equation 4.13, which is only in the next chapter?
- There are more similar comments in the rest of the text.

7. Final evaluation

I find this dissertation on a timely topic, coupled with the student's above-average publication activity, to be commendable. I recommend the thesis for defense, and upon successful defense, I recommend granting the Ph.D. degree.