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Report on the thesis submitted by Ricardo Jorge Fonseca Birjukov Canelas to obtain a PhD degree in Civil Engineering

1. Introduction

The present report concerns the thesis submitted by Ricardo Jorge Fonseca Birjukov Canelas to obtain a PhD degree in Civil Engineering entitled *Numerical modeling of fully coupled solid-fluid flows*.

The present work is devoted to the solution of flows of solid-fluid mixtures. Although the principles of Continuum Mechanics are well known and understood, their practical application to this particular problem is still a huge challenge due the difficulty in capturing the response in the relevant temporal and spatial scales.

The discretization presented in this work resorts the Smoothed Particle Hydrodynamics (SPH) and the Distributed Contact Discrete Element Method (DCDEM). The study of the contact in between solid-fluid and solid-solid is detailed and fully developed. Special attention is devoted to the implementation using Graphics Processing Unit (GPU).

Validation of the developed code is made not only by running a series of benchmark tests but also by comparing with original experimental data. Finally, three practical examples are presented. These are all original and extremely difficult to tackle.

2. Analysis of the document

In chapter one an overview of the modeling of solid-fluid flows is presented. The review is concise and concentrated on SPH. It would be informative to exhibit other alternatives that were conceived to approach the same problem, like the Particle Finite Element Method, see Idelsohn *et al.* (2004) and Oñate *et al.* (2008).

Chapter two briefly reviews the governing equations of the fluids and contact between solids. It is recognized the effort to be concise, although both of the topics would benefit with a more detailed discussion. The problem statement is independent of the specific discretization employed to solve the resulting system of differential equations. Thus, all the boundary and initial conditions should be clearly written, see note on next section.

The fundamental tool for the spatial discretization is presented on chapter three. It would be informative to the reader to present works from other authors besides Monaghan and his co-workers in the introduction of SPH as, *e.g.*, Liu and Liu (2003). The major properties of the SPH approximation are exposed, followed by its discretization and application to the governing equations of the fluid problem. Attention is also given to the explicit modeling of turbulence, the introduction of the equation of state and the boundary conditions. The rigid body discretizations is accompanied by a detailed description of the forces that two rigid bodies undergo when contact occurs.

The implementation using High Performance Computing is described in chapter four. It is to praise the candidate's courage in going down paths that are not very common in civil engineering. The programming in Compute Unified Device Architecture (CUDA) and the use of parallel computing are decisive factors for the success of the implementation.

In chapter five a series of validation tests are presented.

The Hagen-Poiseuille Flow and the Couette Flow tests are classical in SPH bibliography. The graphics presented in figures 5.1 and 5.2 do not allow a clear understanding of the convergence of the solutions. The most appropriate measure would be the *rates of convergence* of some error norm of the solution with a discretization parameter. This is, by no means, a problem of the present work. On the contrary, it a common way of presenting the results by the SPH community, see (Liu, 2003, section 4.6) or (Liu, 2003, section 9.3.4.1).

It is very interesting in the "Free stream consistency" example to notice that the adopted discretization allows the simulation of constant and linear velocity practically without any perturbation along the time. This test proves the robustness of the method.

The example "Experimental Validation: Dam-break with moving obstacles" is remarkable because it shows that the candidate does not limit itself to reproduce benchmark tests, but also proposes new tests, which were verified on an original experimental campaign.

The results presented in chapter five verify the correctness of the model and its implementation. Disappointing is the fact that no information is provided about the computational time required to perform the analysis. Interestingly, this information is displayed in one of the articles recently published by the candidate (Crespo *et al.*, 2015, figura 3), in spite of referring to other examples which are not contained in this thesis.

In chapter six applications of the developed method to three practical situations are presented: coastal geomorphology, Sines port and a Debris flow. The examples are well chosen, illustrating the ability of the code under very different situations. The correctness of the found solutions cannot be verified, although they all make physical sense.

The illustrations presented along the whole document and particularly in the present chapter are outstanding. Unfortunately no information is provided on how the output is made. It was noticed however that the colormap presented in figures 6.6 and 6.7 is similar to the default one employed by ParaView (Ahrens *et al.*, 2005).

It was felt some lack of information on how the initial particle distribution is generated.

Conclusions and future developments are presented in chapter seven.

3. Suggestions

In this section some suggestions for improving the quality of the final document are provided.

Along the document the units of measurement are in *italic*, instead of the conventional upright[1], *e.g.*, N m should be employed instead of *N m*.

The functions designations should be upright. Hence, in page 12 the trace of a second-order tensor is $\mathrm{tr}(\boldsymbol{D})$ instead of $tr(\boldsymbol{D})$.

References to equations should be written inside parenthesis.

Although a list of abbreviations is provided, these should also be introduced in the text.

The direct notation is employed along the document. Although useful due to the absence of indexes and readiness for computer implementation, careful should be taken when manipulating expressions using it. Two examples of its misuse are:

(i) In page 9, equations (2.8) and (2.10) exhibit the terms $\nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u})$ and $\boldsymbol{u}\boldsymbol{u} \cdot \nabla \rho$, respectively. Notice that two vectors admit operations like $\boldsymbol{u} \cdot \boldsymbol{u}$, $\boldsymbol{u} \times \boldsymbol{u}$ and $\boldsymbol{u} \otimes \boldsymbol{u}$, but $\boldsymbol{u}\boldsymbol{u}$ is undefined.

(ii) In page 11, equation (2.22), it is not intended to compute the divergence of the vector $\boldsymbol{u}$, but its gradient. Hence, $\nabla \boldsymbol{u}$ should be employed instead of $\nabla \cdot \boldsymbol{u}$. Moreover, the transpose of a vector is not defined (notice the diference between a vector, which is a first-order tensor, and a column-matrix). In order to express the transpose of the second-order tensor arising from the application of the gradient operator over vector $\boldsymbol{u}$ use $(\nabla \boldsymbol{u})^T$. Hence, equation (2.22) may be written as $\ldots \mu \left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right) = \ldots$

In page 11 the positions vectors and velocities are designated by (x, y) and (u, v) in figure 2.1 and equation (2.20) and (2.21). However, in equation (2.22) indicial notation is used, designating the mentioned quantities by (x_1, x_2) and (u_1, u_2). It is advisable to use solely the later notation. In page 54 the velocity vector components are again denoted by u and w.

In page 8 the boundary of Ω is designated by $\partial\Omega$. In page 12 this designation is changed to $\delta\Omega$.

The kinematic boundary conditions, which are simply $\boldsymbol{u} = \overline{\boldsymbol{u}}$, where $\overline{\boldsymbol{u}}$ is the prescribed velocity vector along the kinematic boundary, should be stated in page 12. Initial conditions should also be presented. The presented static boundary conditions merely involve the specification of the stress tensor on the static boundary or at the interface fluid-solid. This is inappropriate, as the boundary conditions (i) should depend on the orientation of the boundary and (ii) should only constraint the *traction vector*, see *e.g.* Donea and Huerta (2003, page 270, equation (6.7)).

In equation (2.27) a ∂ is missing in the denominator.

In page 17 the title "Lagrange Interpolation and the SPH Method" is misleading. In numerical analysis "Lagrange Interpolation" refers to an interpolation technique, which is the basis of the Lagrangian family of finite elements, see Hughes (2000, page 127, section "Higher-order elements; Lagrange polynomials"). In the present context the term "Lagrange" is related to the description of the kinematics. The term "Interpolation" seems unnecessary.

The sentence in page 19

> Assuming symmetrical invariance $(\overline{\Omega}_0 = \Omega_0)$, then the integral is equal to its opposite and condition, true only if both integrals are null, rendering condition 3.6 satisfied.

should be improved.

[1]The conventional rule was used at times, like in page 36.

In the second member of equation (3.29) the denominator has an error, as the square of a vector is undefined. Probably the author means $\|\boldsymbol{r}_{ij}\|^2$ instead of $\boldsymbol{r}_{ij}^2$. The same error occurs in page 26, see equations (3.34) and (3.35).

In page 25 it is referred "... $\boldsymbol{u} = k$ field". A vector cannot be equal to a scalar.

In page 26 the velocity field is denoted by $\boldsymbol{v}$. Until this point, this vector was denoted by $\boldsymbol{u}$.

In page 26, in equations (3.35) and (3.36) the sum on the right-hand-side is extended to all j particles. Hence the left hand side should not have a reference to j index. This problem occurs also in equation (3.41).

In page 33, equation (3.51), it is not defined what is $|I|$. Probably is the number of particles that constitute the body. The absolute value of an integer number does not seem to be an appropriate notation.

4. Overall assessment

This work comprises the proposed objectives. In order to accomplish them the candidate had to profoundly study and research several areas: fluid mechanics, contact mechanics and SPH. Moreover, the implementation was made in non-standard environments, resorting GPU and MPI. The original model was validated in a series of problems. The applications range from benchmark tests to real engineering problems. One of the tests was experimentally validated.

The final document is concise and well written, being the cited bibliography extensive but appropriate.

The developed work was presented in five conferences, being two papers published in top journals of the area. One more paper is presently submitted.

It is my belief that the present thesis should be accepted for public defence in its present form.

Lisboa, Wednesday 24th June, 2015

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UNIVERSITY OF AGDER

EVALUATION REPORT

PhD Thesis: Numerical modeling of fully coupled solid-fluid flows

Candidate: Ricardo Jorge Fonseca Birjukov Canelas

The thesis is focused on numerical modeling flows of solid-fluid mixtures flows with a unified discretization, which allows tackling several engineering applications where traditional numerical approaches are difficult to implement. The work includes a complex, large, and in some extent novel, numerical model implementation, involving international partners with recognized expertise in the field of SPH. Although the thesis is mainly dedicated to numerical issues, the author also performed quite complex laboratorial work, involving technologies like particle tracking and PIV, in order to have data to validate the conceptual and numerical approaches.

The objectives of this work are quite clear and the conclusions fulfil them completely. The document is concise and clear, and the structure of the thesis follows closely an adequate research methodology. The analysis is made rigorously and the conceptual and numerical hypotheses are checked through comparison of new experiments or existing data. The results allowed achieving a new state-of-the-art numerical model able to cope with the complex fluid-solid interactions in a wide range of applications.

The research was published in 2 papers in ISI journals, in 5 international conference papers and 1 paper was also submitted to ISI journal (although it is still in the reviewing stage, its scientific content allows to expect that it will be approved in the near future).

The rich and ambitious research work developed by the candidate naturally raises some issues that deserve discussion and will allow a fruitful and interesting public defence.

In an attached document, some small remarks/corrections are suggested, which the candidate can easily include in a final version.

Resuming, the thesis contributes with new knowledge for the research field and is in accordance with highest international academic standards for this type of degree. Therefore, the thesis should be accepted/approved for public defence as it is.

Grimstad, 23/06/2015

João Bento Leal
Professor
Faculty of Engineering and Science

UNIVERSITY OF AGDER

REMARKS/CORRECTIONS:

- Chapters should begin in odd pages (for example, Chapter 3 begins in p. 16). Check all chapters and pay attention to page numbering change in eventual cross-references.
- The "List of Symbols" is incomplete (examples: Ω, Ω_0, q, Φ in chapters 2 and 3) and should be shorted alphabetically. The definition of ∇ operator should be given, since there seems to be scalar ∇ and a vector $\boldsymbol{\nabla}$ (this last seems to correspond to the most common definition).
- There is an inconsistency on the verbal tense. For example, in the 1st paragraph in p. 18, the present perfect tense is used "...Morris et al. (1997) have performed...", in the same paragraph the present tense is used "Dehnen and Aly (2012) calculate...", in the last paragraph in p. 25, the simple past tense is used "...Violeau (2012) used...". Please review all text (verbal tense) when referring to previous studies; I suggest using the simple past tense.
- p. 18, 1st paragraph, a space is missing in "models(Monahan, 2005)".
- Give the definitions (eventually as footnotes) for some properties like "central-symmetrically invariant" and "compact support" (see p. 19).
- h appearing in eq. 3.10 should be defined in the text.
- p. 19, before eq. 3.14, "and renders Equation 3.13" should be "and Equation 3.13 renders".
- Eq. 3.16, the first RHS term should be $A(r)$ and not $A(r')$. In the second and third RHS terms a vector (dot) product seems to be missing, otherwise the results would not be a scalar.
- p. 22, after eq. 3.22, revise "... *Dp* can be set used...".
- p. 27, before eq. 3.37, instead of "...the motion equations governing of the resolved scales..." I suggest "...the governing motion equations of the resolved scales...".
- p. 28, after eq. 3.40, the value of constant C_S should be given.
- p. 28, before eq. 3.43, what represents symbol "P"? It is not defined and is not in the "List of Symbols".
- p. 28, after eq. 3.43, what represents "$\max_i$"?
- p. 28, before eq. 3.44, replace "linealized" by "linearized".
- p. 34, Fig. 3.9 (also Fig. 5.22), what material is "A1203/A1"?
- p. 36, eq. 3.62 and following paragraph, what represents subscripts "I" and "J", is it a typing error and they should be "i" and "j"?
- p. 48, last sentence, instead of "For a initially at rest fluid..." I suggest "For a fluid initially at rest...".
- Section 5.1.3, the objective of the dam break flow test was not clearly explain as it was for the Hagen-Poiseuille and Couette flows. I think that also the length of the computational domain should be given.
- p. 52, before eq. 5.3, instead of "...an adimentional..." I suggest using "...a dimensionless...".
- p. 54, replace "...verical..." by "...vertical...".
- The format of units is inconsistent throughout the document. For example, both "m" and "*m*" are used for meter (example: pp. 51 and 55). I suggest not using italic format for units and leaving a space between the numbers and the units. Check all text.
- p. 55, Fig. 5.11 (also Fig. 5.12), what represent the black and red arrows?
- Section 5.2.2.A, the conditions of the problem/simulation are not presented. A cylinder is mentioned but it is hard to devise the set-up.
- p. 57, 2nd sentence, "The used...in a viscous fluid". Please revise the English; I think some commas are needed.

Jo~ Ly

- p. 57, penultimate paragraph, "*DP*" should be "*Dp*".
- p. 59, end of 1st paragraph, a dot "." Is missing at the end.
- p. 62, last sentence, "Domínguez et al. (2013)" is somehow out of context in the sentence.
- p. 64, last sentence, verify the reference "...(Capel, Fitzgibbon,..., Capel et al.)...".
- p. 66, before the title of section 5.2.4.B, revise English "...to correctly transition from static...".
- Section 5.2.5 could be included in section 5.2.4A, maintaining the link between sections and test cases.
- p. 67, after Fig. 5.27, revise the English "The overall agreement is positive...".
- p. 70, after the title of section 5.2.5, "The PIV results suffer since..." it seems that something is missing after suffer.
- p. 71, last sentence, the value of Ritter's solution should be given.
- p. 73, after the title of section 6.1, may be it would be wise to specify what "high-energy sedimentary deposits" mean.
- p. 84, last paragraph, I suggest replacing "...and is now in the fluid." by "...and are now in the fluid.".
- Section 6.3, the value of *d*50 is never given.
- p. 86, 1st paragraph, consider replacing "ensure" in "...The flow characteristics ensure...".
- p. 87, eqs. 6.2 and 6.3, I think it is confusing to call the laboratorial model (prototype) and the numerical set-up (model). Usually, the prototype is the real scale and the model relates to the laboratorial physical model.
- p. 89, last sentence, replace "Table 6.4 and 6.30..." by "Table 6.4 and Figure 6.30...".
- p. 90, 2nd paragraph, revise the English of "...the experimental procedure initial conditions...".
- p. 99, 3rd reference, should be "Soares-Frazão". Similar problem occurs at Lemieux et al. 2008.
- In some of the references in the "Bibliography" a number or the month appears inside brackets along with the year (for example: Colagrossi et al. 2011).
- The last author in Crespo et al. 2011 is not right.