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Review of “An explicit dynamics framework suited to highly non-smooth interface behaviors”

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Review of version 1

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Please note that the first version submitted to JTCAM is v2 of the hal-04146784 repository

Authors The authors first wish to thank the reviewers for constructive and challenging remarks that will help us to improve the manuscript.

Reviewer 1 (Anonymous)

Reviewer This paper presents a nonsmooth framework to deal with complex interface models accounting for contact, fracture and adhesion recovery. The numerical results demonstrate the ability of the proposed framework to deal with such interface behaviours, including some nonsmooth effects in the response. In my opinion, this paper represents an original and interesting contribution which can deserve publication. However, I have some important remarks about its presentation.

The abstract is vague and does not pinpoint the original contribution of the paper. There is already a huge literature on non-smooth models for contact interfaces and the authors should be more precise on the family of interface models that they want to address.

Authors We tried to improve the abstract, emphasizing the aims and originalities of this paper. Rather than focusing on original interface behaviors, we aim to test the formulations and solving schemes for challenging problems involving highly non-smooth behaviors, beyond classical ideal contact interfaces, for which indeed there have been many contributions (we also tried to improve the bibliography referencing). Note also that the aim was to use models at a macroscopic scale, that may lead to less classical interface behaviors seen as macroscopic homogenized models, that may take into account several mechanisms at lower scale that are not modeled herein. We also tried to clarify this point in the resubmission.

Reviewer In the introduction, an overview of existing interface models in the literature (and their possible embedding in a nonsmooth framework) would be necessary to clarify the novelty of the paper. There is a small discussion on that at the beginning of Section 3, but I think that such information should be already given in the introduction.

Authors References have been added in the introduction and in Section 2, but restricted to phenomenological macroscopic interface models. The beginning of Section 3 has also been reorganized, and partly moved to the introduction as suggested.

- Reviewer** It seems that the first two paragraphs of Section 2 are general considerations not yet related with the contribution of the paper. As a suggestion, the authors may consider moving them to the introduction. This would also help to explain the original contribution of the paper at the level of the introduction.
- Authors** Part of Section 2 have been moved and rephrased in the introduction as suggested.
- Reviewer** Actually, I find the discussion in the second paragraph of Section 2 rather obscure. It could be better supported using references from the literature. Also, the authors talk about “infinite stiffness” but it is not clear if they refer to the stiffness of the bulk of the material or to the stiffness of the interface itself. Is the purpose to highlight the difference between penalty formulation vs exact enforcement of the non-penetration condition? Is the discussion anyhow related to plastic models evoked in the first paragraph of Section 2?
- Authors** For the plastic models, two modifications are proposed: first, another example of phenomenological contact with plasticity has been added, and for each of these two examples, discussion on the physical interpretation, as well as literature references have been added. The infinite stiffness was related to the interface behavior (case referred to as extrinsic model in CZM approaches). It is therefore a model of the interface, that has to be dealt with in the resolution code; in this case, the penalty method is an approximation to help the resolution scheme, but involving some other difficulties (numerical parameter choice, ill-conditioning, critical time step...) Some paragraphs have been added to clarify the approach.
- Reviewer** In Section 2.2, the plastic part of the model is defined by Figure 2. In my opinion, this graphical definition, based on only two loading scenarios, lacks mathematical precision. It would be better to give a mathematical definition first and then illustrate it, e.g., using Figure 2.
- Authors** This has been done. The non-smooth framework with convex cones and subdifferentials has been stated to derive the velocity/impulse behavior. This leads to the depiction of the behavior, then illustrated by the two loading scenarios as suggested.
- Reviewer** In Section 2.2, the motivation and rationale behind the proposed interface model is missing. Why considering a plastic model, generally used to model the behaviour in the bulk, for the interface? Is it supposed to capture local plasticity effects in the neighbourhood of the interface? Is it supposed to capture specific mechanical properties at the interface itself? Was it considered elsewhere in the literature or does it come out of the blue? Or is it only an intermediate preparation step for the more physical model presented in Section 3? Also, it appears that the plastic part of the model is symmetric in traction and compression, with the consequence that the interface can support some traction forces. This fundamentally departs from ideal contact interfaces (Signorini condition) and deserves at least a few comments.
- Authors** The aim is to test different kinds of non-smoothnesses after the recall of ideal contact of section 2.1 which has already been tested in the literature. This has been precised. Depending at which scale the model is stated (in our case a macroscopic model) the behavior of the interface itself can embed plasticity. To be clearer, two different models (defined phenomenologically with two associations of an ideal contact and plastic part (in parallel or serial) are now presented, together with a physical case that may lead to such models (essentially on what happens at a lower scale, i.e. a third body plastic layer that indeed may sustain a traction, and a plasticity developing on micro rugosities for a unilateral contact case, these scales not being described in the macroscopic interface, viewed as a macroscopic homogenized model). The infinite elastic stiffness of the interface and the perfect plasticity of the interface are selected to challenge the algorithm to be able to deal with. Some bibliographic references have been added.
- Reviewer** The relation between the model in Figure 2 and in Figure 3 is not so obvious to me. The shapes of the graphs are visually different. Isn't it just an h-scaling of the vertical axis and a substitution of displacement by velocity on the horizontal axis? This remark is somehow related to the previous one.
- Authors** Indeed, this has been clarified thanks to the previous remark. Former Fig. 2 was some examples

of trajectories in stress vs displacement space (and had a memory effect that is depicted with the arrows) while Fig. 3 is the unique admissible set of states that can be obtained when using a stress (or impulse repartition) vs velocity. The main issue therefore comes from the velocity in place of displacement. With modifications due to the previous remark, the figures are now permuted and the explanation is hopefully improved.

Reviewer In Section 3.1, as in Section 2.2, a mathematical definition of the model should be included. Are there similar models in the literature? If yes, how does the proposed differ from the literature? Please clarify.

Authors Separated behavior mathematical models, i.e. unilateral contact on one hand, cracking interfaces on another one, and adhesion on a third hand, were available. Usually the crack development is regularized using smooth cohesive models with elasticity damage, but to test the ability to solve highly non-smooth case, the limit case of extrinsic perfectly brittle case is considered herein. Mathematical derivations of these separated behaviors are available, and the thermodynamic framework has been adapted to cohesive zone models with possible adhesion in the literature added; but we didn't find some for the limit case embedding the different mechanisms as a whole. Since not so obvious, this part is left as a direct perspective to this work (an issue is the shift between different separated behaviors, usually using a memory function that in this case take only binary values; in the proposed derivation, this is embedded in the value of R_Y parameter: indeed, if $R_Y = 0$, the behavior depicted on current Fig. 10 collapses to the classical contact one). We tried to precise these points.

Reviewer The model includes some conditional statements. Mathematically, such a model may suffer from ill-posedness. Do we have any guarantee about the well-posedness of the proposed formulation? By curiosity (this does not need to be included in the paper), could it be formulated in terms of complementarity conditions or in terms of inclusions, so that it lends itself to a more precise mathematical analysis?

Authors The model of section 3.1 is much more advanced and original, and up to now the perfect mathematical description is not yet available (so is now a perspective) as mentioned previously. It can nevertheless be viewed as a limit case of a contact + elastic with damage evolution such as cohesive zone models, when stiffness is infinite (no elasticity, extrinsic approach) and brittle behavior replaces the damageable one. We nevertheless are confident in the local well-posedness, illustrated in current Fig. 10, where we can see locally the uniqueness of the solution (similarly to current Fig. 4); nevertheless, it is not a mathematical proof as a perspective.

Reviewer In the conclusion, the authors mention that the model may lead to deterministic chaos. I'm not sure if this is really discussed in the body of the paper and/or demonstrated in the numerical results. Do the authors refer here to the problem appearing in case of an initial state with grazing contact? Please clarify the whole paragraph.

Authors Agreed. This has been said but not discussed nor exemplified. The main argument is a dependence on the parameters of the problem. Grazing contact is such a source of deterministic chaos, and we expect that the "grazing" rupture point could be another one. Since not addressed herein, the paragraph has been rewritten to clearly make it appear as a perspective study.

Reviewer 2 (Serge DUMONT)

Reviewer In this manuscript, authors propose explicit dynamics schemes dedicated to highly non-smooth interface behaviors, such as frictional contact, perfect plasticity or fracture. After a detailed presentation of the method, numerical simulations are provided to illustrate the efficiency of the proposed schemes. The manuscript is very interesting, well written and presents new results. It is written very carefully and I found only one small misprint: 3 lines after the beginning of paragraph 3.3, page 12, ... $L_2=0.5$), meshed... (there is no point after the right parenthesis).

Authors Thanks for pointing this typo. It has been fixed.

Reviewer In order to have a better idea of the efficiency of the proposed method, I have only questions on the 3D test case. For example: Is it possible to have an a posteriori verification if the predicted

status of the interaction at each node is effectively the good one after the computation of the velocity $V_{n+3/2}$?

Authors A convergence check has been added. Since dealing with explicit dynamics, the space-time convergence is used, so both the mesh size and the time steps are reduced simultaneously (leading to a constant ratio of time step over critical one). This has been added.

Reviewer Is it possible to have a comparison with other existing method (even for simpler interface models)?

Authors Unfortunately, we didn't build another implicit resolution scheme for these non-smooth problems, that will be harder to program (this is an argument for the explicit approach) and difficult to make converge for a black-box commercial code (without knowing exactly what is used inside as rules of thumb for penalizing, smoothing...) Another explicit scheme could have been built, but this is not trivial again, and would also lead to developments for these kinds of problem. This can nevertheless be a perspective to this work. If we restrain to ideal contact interfaces, this has already been done in the literature, and is out of the scope of this paper.

Review of version 2

Permalink: [hal-04146784v3](https://hal.archives-ouvertes.fr/hal-04146784v3)

Authors Thanks to the new remarks, we hope that we made clearer the aim of this study and the corresponding explanations.

Reviewer 1 (Anonymous)

Reviewer Updated comment on the first 3 remarks of review 1: The description of the originality of the paper is clearer in the new version. Now, I understand that the novelty of the paper is (1) to propose some benchmark problems with non-smooth interface behaviours and (2) to test a particular explicit dynamic solver for these problems. However, this clarification raises new questions about the value of this contribution and the way it is presented in the whole paper.

Authors Sorry if this has not been clear enough again, but the benchmark is not the issue number 1 (though we could think of putting as additional material the input data, mesh, etc... for the 3D case in an AVS UCD ASCII file if this can be useful). Indeed, we wish to say that it could be used as a benchmark (with some reference solutions built numerically as overkilling ones, i.e. by excessive refinements, since analytical solutions are not easy to produce) but this is not addressed herein. Note that previous benchmarks have already been produced in the referenced mentioned paper [Di Stasio et al. 2019] also exemplifying the symplectic aspect, on simpler test cases (Hamiltonian ones). The main issue is herein to be able to formulate the different non-smoothness cases within the framework of the CD-Lagrange scheme, keeping it explicit and matrix-free, and exemplify the feasibility on test cases for different sources of non-smoothness. We tried to make this more explicit.

Reviewer If the paper is intended to present benchmark tests that can be used by the community, I would expect an in-depth presentation of the tests (including some more detailed discussions on well-posedness) and of the results (including some reference solutions, e.g., obtained analytically). Also, it would make sense to include already a comparison of several solvers. Furthermore, the description of the tests should be isolated from the description of the solvers and resolution algorithms. Even though the proposed tests are interesting, in my opinion, the paper does not meet these expectations.

Authors As said before, analytical solutions are possibly complicated and not always easily obtained for the test cases, and the benchmark is only here an on-going possibility. So, benchmarking would be better said: challenges for implementation of these test cases in other solvers. As said before, comparison with other approaches is a direct perspective. Moreover, the tests are not expressed independently of the solver, since the first aim is to design the solver for different cases of non-smoothnesses, and no general algorithmic solver is given that can be applied to every presented test case. Actually we add a clearer sentence saying that the main steps of the algorithm are the same (i.e. the CD-Lagrange framework that is not a novelty for this paper: the

update of the configuration, the free velocity, and after local non-smoothness resolution the computation of the global velocity, and the update of the displacement), but the inner part is the innovative algorithmic issue of this article (the explicit local non-smoothness resolution, depending on the nature of the non-smoothness); this is why the algorithmic part was detailed. Up to our knowledge, this has not been made before with such non-smooth cases and an explicit matrix-free solver.

Reviewer If the idea is to test an existing solver on a number of examples (I think that the paper is actually structured in this direction), then the scientific value is questionable and actually depends on the difficulty of these examples. It would be necessary to show that the proposed examples are really unsolved, i.e., that other non-smooth solvers would fail or would be inefficient. But this is difficult without comparisons. In my opinion, these problems could probably be solved efficiently using Moreau scheme (here, I refer to the original scheme of the 1988 paper “Unilateral contact and dry friction in finite freedom dynamics”). Notice that the position update of this Moreau scheme is also explicit (in the sense that the stiffness matrix should not be inverted), so that its implementation could follow a similar approach as for the proposed CD-Lagrange scheme.

Based on these considerations, it appears essential to include a comparison between the CD-Lagrange scheme and such well-known schemes from literature.

Authors The idea was not to apply a black-box existing solver to different test cases, but to design algorithmic solvers suited to various non-smoothness sources. The framework is the same (symplectic, non-smooth, based on CD-Lagrange), but the algorithmic design may vary, and is progressively adapted along with the test cases. The aim is to provide the CD-Lagrange framework and illustrate the ways different non-smoothness sources can be integrated within this framework. Indeed, this is not yet a standard FE code implementation issue in a commercial code environment, but more an academic advance.

Clearly, the Moreau schemes are the closest to the proposed one, and are probably the most suited for addressing non-smoothness issues. As mentioned, the classical Moreau scheme (with the explicit gap prediction) has been compared for benchmarks in [Di stasio et al. 2019]. Since this comparison (with the discussion on symplecticity) has already been proposed, we left the comparison on the present cases, as well as the benchmarking, as direct perspectives to this work, and stated this in the resubmission. A paragraph and the reference have been added.

Reviewer Updated comment on remarks 4-8: the new version includes additional explanations and mathematical details, and significantly gained clarity. I have no further remarks on these points.

Updated comment on remark 9: if I am not mistaken, this point has been addressed for the first tests, but not for the last ones. This improvement is judged as a sufficient progress, so I’m OK with the correction.

Updated comment on remark 10: the paragraph has been clarified, thanks.

Authors In our mind, we say that the solver is symplectic when, applied to Hamiltonian systems, it produces conservation properties (proved in [Hairer et al 2003], exemplified also in [Di stasio et al. 2019]). We can use it for other cases since it produced good energy preserving and balance equations properties as well... Some mentions of symplecticity have been omitted in the new version, since we agree that this is not the main topic.

Reviewer Additional remarks:

The authors mention at several places that the solver under study is symplectic. To my knowledge, symplecticity is a property only defined for Hamiltonian systems. As the models under study are not Hamiltonian (at least the authors do not present them in this form), this property should not be overemphasized in the paper. In addition, the particular central difference scheme used in this paper is not standard, and therefore it may not inherit all properties (such as symplecticity) of other versions of the central difference scheme. In particular, the formulae of the CD-Lagrange scheme are very different from the formulae of the symplectic central difference scheme studied by Kane, Marsden, Ortiz and West in their paper “Variational integrators and the Newmark algorithm for conservative and dissipative mechanical systems”. At least, the authors should mention in which context a central difference scheme would actually be symplectic and

provide suitable argumentation or references.

Authors The central difference version used herein is the 3-step expression (algorithmically equivalent to the other versions when no non-smooth interfaces are involved) is the one in [Belytschko et al 2014, Hairer et al 2003].

Reviewer The authors use the terms “velocity jump” and “displacement jump” in an inappropriate manner. A jump is in my opinion a sudden change at a particular time instant. Referring to the right and left limits of functions of bounded variations, the velocity jump would be $v^+(t) - v^-(t)$ and the displacement jump would be $u^+(t) - u^-(t)$. Notice that in mechanics, displacements usually remain continuous so that there is no displacement jump. Instead, the authors frequently use the term “jump” to refer to the current value of velocities $v(t)$ and displacements $u(t)$, which is not correct.

Authors Thanks for pointing this. It seems that this is a vocabulary problem: we used the term “jump” for the spatial fields; since a 2D interface model is used, its related kinematic quantities are spatial jump of displacement and spatial jump of velocity across the interface surface. This was not related to the time discontinuities. We changed the expression using “spatial jump” instead.

Reviewer 2 (Serge DUMONT)

Reviewer The manuscript has been significantly improved by the authors. All my questions have been reponed. So, I suggest a publication in JTCAM.

Review of version 3

Permalink: hal-04146784v4

Authors The authors wish also to note that there has been a very interesting discussion by mails with the Journal board, concerning the availability of the source code and data, as well as on providing open-source code. We therefore wish to thank them for that.

Reviewer 1 (Anonymous)

Reviewer The authors have updated the paper to answer my remarks. I still believe that the proposed numerical scheme is very close to Moreau’s method and I would be curious to have more insights about this, but this may be left for perspective. Therefore, I have no further remark on the last submitted version.

Editor’s assessments (Olivier THOMAS)

Editor On the basis of the joint work of the authors and the reviewers, two experts in computational and non-smooth mechanics, the quality of the article was improved until it was found suitable for publication in JTCAM.

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