Computer Methods in Applied Mechanics and Engineering (CMAME)
Referee Report

Title: "A comparison of different methods for calculating tangent-stiffness matrices in a massively parallel computational peridynamics code"

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A. Summary

This manuscript presents comparisons between different numerical differentiation methods for the computation of entries of tangent-stiffness matrices, used in Newton's method for quasi-static nonlinear analysis of solid structures. The methods include: automatic differentiation (AD), forward finite difference (FD), centered finite difference (CD) and complex-step (CS). The authors perform the comparisons within the computational peridynamics code *Peridigm*, where the authors implemented the CS method. Numerical results include comparisons of computational times between all the methods, as well as comparisons of accuracy between FD, CD, and CS, relative to AD. The results show that AD is the fastest method in serial and FD in parallel, whereas CS is the slowest method. However, the accuracy of CS is several orders of magnitude higher than the finite difference methods (FD and CD). Consequently, although AD seems to be the best method in terms of combined speed and accuracy, the results suggest that CS may represent a viable alternative for cases where AD implementations are not practical.

B. Evaluation

This manuscript focuses on the CS method. This method and its comparison to other finite-difference methods have been previously presented in the literature. For example, the CS method has been described in [1], with a comparison between FD and CS. Applications of the CS method to compute tangent matrices appear in [2, 3], with comparisons between FD, CD, and CS. In addition, the CS method has been used for sensitivity analysis in [5, 6], and in [4], a detailed description of the CS method and comparisons to FD, CD, and AD are presented. Further uses of the complex-step method appear in [7, 8, 9], and extensions of the CS method are discussed in [10, 11].

However, this manuscript presents some aspects of the CS method which seem novel. These are:

1. comparisons between FD, CD, CS, and AD in terms of computational time,
2. implementation of the CS method in parallel,
3. implementation of the CS method within Peridigm.

In particular, the implementation in Peridigm is of strong interest to researchers working with the peridynamic theory of solid mechanics.

I believe this manuscript is of value to both the computational mechanics community in general, and the peridynamic community in particular. I suggest it to be considered for publication in the Computer Methods in Applied Mechanics and Engineering journal, after the issues described below have been properly addressed.

C. Information to the authors

I. Larger issues

1. Some parts of the manuscript suggest that the authors introduced a new method, i.e., the complex-step (CS) method. For example, in the introduction, they say "A goal of this study was to develop and evaluate a new, accurate, and practical method ..." Another example appears in page 3, where the authors say "The aim of this paper is not only to introduce the new complex-step method in the context of evaluating tangent-stiffness matrices ..". However, the CS method has already appeared in many publications since 1998 [1]. Please revise the way you refer to the CS method along the manuscript.
2. The work presented focuses on a parallel computational peridynamic code, and uses peridynamic models for mechanics. However, no detailed explanation of the equations involved is presented. Although the tangent-stiffness calculations are not specialized to Peridigm, the authors should include a short section introducing the peridynamic theory and the specific constitutive model used, i.e., the elastic peridynamic solid. You may add this to the already included very brief description of peridynamics in page 9 (lines 15-26). This will also help to explain the concept of the peridynamic horizon in page 10.
3. The manuscript seems to be written in a language more familiar to computer scientists. I would encourage the authors to revise certain parts of the manuscript to be presented in a language more familiar to the computational mechanics community.
4. In Section 1.1.1, please include a more comprehensive literature review for the CS method, including further references (some of them are listed below). In particular, specify what aspects of the CS method have been investigated in each reference. Then, you need to clearly mention your contribution within the CS method, in contrast to the other references (some comments in this regard appear in the manuscript in page 8).
5. The comparisons of the different algorithms are only performed with respect to the construction of tangent-stiffness matrices. In particular, the authors always use the solution of AD at each time step to compute the entries of the tangent-stiffness matrices, even for the FD, CD, and CS methods. However, the authors need to demonstrate the performance of the CS method, in comparison to the other ones, with respect to the solution of real, ideally non-linear problems. In other words, how the solutions compare in terms of accuracy and speed between the methods when solving given problems? Please include two examples of interest. The authors suggest that two examples involving non-linear systems are already included in the paper repository.
   The authors say in the Conclusion: "While the results showed that CS produced more accurate tangent-stiffness matrices than CD and FD under the parameters of the tests, it was not determined whether or not this is a clear advantage of CS over FD in terms of accuracy of final predicted displacements and speed of convergence." This needs to be studied and results in this regard added to this manuscript.

II. Smaller issues

1. Pg. 2: In line 14, explain what does the term "algorithmically consistent" mean.
2. Pg. 2: In line 36, what do you mean by "discrimination"?
3. Pg. 2: In line 37, explain what do you mean by "in-situ instrumentation".
4. Pg. 3: In lines 19-29, specify the sections where each part of the manuscript is included.

5. Pg. 3: You may consider including the exact web address of the *paper repository*.
6. Pg. 3: Please include the forward and centered finite difference expressions for easier comparison with (2); include the truncation error as well. You do not have to derive these expressions though.
7. Pg. 4: In Eq. (1), " $\frac{\partial f^2}{\partial x^2}$ " should be " $\frac{\partial^2 f}{\partial x^2}$ "; similarly, for the third derivative.
8. Pg. 4: You may consider writing Eq. (2) with the truncation error, i.e.,

$$\frac{\partial f(x)}{\partial x} = \frac{\mathrm{Im}(f(x+ih))}{h} + \mathcal{O}(h^2). \tag{2}$$

   In this case, one replaces "$\approx$" by "$=$".
9. Pg. 6: In lines 9-11, please add references to the "Poisson problem" and to the "mathematical optimization".
10. Pg. 7: Should Eqs. (4), (5), and (6) use "$\approx$" instead of "$=$"?
11. Pg. 7: In line 28, note that $\vec{u}$ is not the current configuration, but the displacement field. Please revise the sentence.
12. Pg. 7: Please provide an expression for F_i^{int} in the model used.
13. Pg. 9: In line 26, please add the reference [12] below to "coupling to molecular simulations [29]."
14. Pg. 10: Please add an illustration of the block undergoing tension in Section 2.2, for clarity. Also, clarify the displacement boundary conditions; are they applied in a volumetric layer?
15. Pg. 10: In line 40, you mentioned a bandwidth of 7. This seems to be clear in 1D. Does this hold in higher dimensions? Please clarify.
16. Pg. 10: In lines 47-49, you say "The specific parameters ... can be found ... in the paper repository." It seems a good idea to have the paper repository with files that a user can eventually use. However, the content of the paper should be independent of the repository. Please include a table with the parameters used. Similarly, in page 11 (lines 11-13).
17. Pg. 14: In line 55, is there any conclusion you can draw from the power law index 1.0×10^{-6}?
18. Pgs. 14-: Please clarify the value of the meshsize used on each of the experiments.
19. Pg. 16: Would it be possible to rescale Fig. 2, so that the dependence of the time on the number of cores will look indeed linear?
20. Pg. 16: In lines 54-56, you say "It should be pointed out that compared to the ℓ^2-norms of any of the TS matrices by themselves, the magnitude of the accuracy metric ... is relatively small." Please include in the manuscript the explicit information on the relative error. It seems that you already have such information in the paper repository.
21. Pg. 17: Include the values of the probe distances h used for each method.
22. Pg. 17: In lines 53-54, you say "Accuracy trends matched those for the single core tests." Indeed, comparing Figs. 3 and 4, the results for FD seem to be quite the same in serial and in parallel. For CS the accuracy seems higher in serial. For CD, the accuracy is also higher in serial and, in serial, it has a fluctuating behavior. Can you comment on these observations?
23. Pgs. 17-18: What are the units of K? If F^{int} in Eq. (4) etc. is internal force, then K should have units of `force/length`. However, in Figs. 3 and 4 you use the unit of MPa, which is `force/length`^{2}. Please clarify.
24. Pg. 19: Are the units of the vertical axis in Fig. 5 "seconds", as in Figs. 1 and 2? Please indicate that. Also, is the label of the vertical axis in Fig. 6 correct?

25. Pg. 20: In lines 32-35, clarify what “byte-copyable” mean and why is that important.
26. Pg. 21: Please include a section title for the references.
27. Pg. 24: In line 23, you may add the truncation error $\mathcal{O}(h^2)$ to the expression. Otherwise, you may need to replace the “$=$” sign by the “$\approx$” sign. However, adding the error term would make more clear the limiting expression when $h \to 0$. Also, replace the comma by a period.
28. Pg. 24: Why do we need S and X in Appendix B?
29. Pgs. 25-26: Are the functions in the second column of the table in 2(c) (page 25) approximations? Why do you label the column “Approximates Function”? Similarly, in line 16 (page 26) you say “approximated by the partial derivative”; is it an approximation?
30. Pg. 26: Please clarify whether storage is needed in automatic differentiation. For example, do we need to store w, v, and u?

III. Typos/editing suggestions

1. Pg. 1: In line 43, remove “the” in “all the of the code”.
2. Pg. 1: In line 46, replace “numeric differentiation” by “numerical differentiation”.
3. Pg. 2: In line 25, the sentence “The distinction of “accurate” is defined by ...” is awkward. Please revise it.
4. Pg. 2: In lines 32 and 48, “finite-difference” should be “forward-difference”.
5. Pg. 2: In lines 33, I believe “aide” should be “aid”.
6. Pg. 3: In line 12, I would replace “such as required” by “such as those required”.
7. Pg. 3: In line 22, replace “with each the methods” by “with each of the methods”.
8. Pg. 3: In line 25, replace “implementing complex-step” by “implementing the complex-step method”.
9. Pg. 3: I would replace the title of Section 1.1, “Differentiation Techniques” by “Differentiation techniques” for consistency, i.e., only capitalize the first letter of the first word. Similarly, for the rest of the section titles.
10. Pg. 4: In line 10, “be be made complex” should be “be made complex”.
11. Pg. 4: In Eq. (1), replace comma by period.
12. Pg. 4: In line 22, you have an extra white space in “$\mathcal{O}\text{␣}(h^2)$”.
13. Pg. 4: I would check the proper use of hyphens along the manuscript. For example, in the title of Section 1.1.2, I would replace “Automatic-differentiation” by “Automatic differentiation” (i.e., no hyphen).
14. Pg. 4: In line 42, replace “based the chain-rule” by “based on the chain rule”.
15. Pg. 4: In lines 45-46, “(add, multiply, power, transcendental and the like)” should probably be “(addition, multiplication, exponentiation, and the like)” or similar.
16. Pg. 4: In line 47, I would replace “used in the study” by “used in this study”. Similarly, in other instances of the manuscript.
17. Pg. 5: In line 39, you may replace “the partials” by “the partial derivatives”. Similarly in page 26.
18. Pg. 5: I would replace the title of Section 1.2 “Tangent-stiffness” by “Tangent-stiffness matrix”. Similarly, in line 50.
19. Pg. 6: In line 14, “quasi-Newton’s method’s” should probably be “quasi-Newton methods”.
20. Pg. 6: In line 18, “about about a particular” should be “about a particular”.
21. Pg. 6: In line 51, you may replace “argument to F” by “argument of F”.
22. Pg. 7: In line 11, you may replace “single independent vector component of the function” by “single independent vector component of the argument of the function”.

23. Pg. 7: In line 24, replace “Where K_{ij} is” by “where K_{ij} is”.
24. Pg. 7: In line 40, replace “in literature [19]” by “in the literature [19]”.
25. Pg. 8: Remove the period at the end of the titles of Sections 2 and 2.1, for consistency. Similarly, for the rest of the manuscript. Also, use italic font for “Peridigm” in the title of §2.1.
26. Pg. 9: In line 29, replace “*Perdigm*” by “*Peridigm*”. Similarly in page 13 (line 44).
27. Pg. 9: In line 37, replace “be simply be declared” by “be simply declared”.
28. Pg. 9: In line 55, I would replace “computational scientists” by “computer scientists”.
29. Pg. 10: In line 30, I would replace “The purpose of applying the load” by “Applying the load”.
30. Pg. 13: I would add a comma at the end of Eq. (8), and replace “Where D is distance” by “where D is distance” in line 14.
31. Pg. 13: In line 15, replace “based method, M is” by “based method, and M is”.
32. Pg. 13: In line 31, replace “correspond to” by “corresponds to”.
33. Pg. 14: In lines 19-21, you have twice the word “nonzero” in “number of nonzero tangent-stiffness (TS) non-zero matrix elements”.
34. Pg. 14: In lines 22, I would replace “The units for accuracy are derived equation (8) and the units used to define bulk material properties, mentioned in Section 2.2.” by “The accuracy measure is given by equation (8) and the choice of elastic moduli is mentioned in Section 2.2.”
35. Pg. 15: In line 54, it seems that “yet still fall” should be “yet still falls”.
36. Pg. 17: In line 45 you say “h, cannot be too small,”. I understand that you mean that you can take h as small as possible. However, the way written may have the opposite connotation. I would revise it for clarity.
37. Pg. 18: In lines 35-36, replace “the number nonzero” by “the number of nonzero”.
38. Pg. 18: In line 39, replace “the the number of nonzero” by “the number of nonzero”.
39. Pg. 18: In line 50, I would replace “experimental results,” by “computational experiments,”. Otherwise, it may give the impression of physical experiments.
40. Pg. 20: In line 13, is the use of the word “order” in “number of iterations taken order to measure” correct?
41. Pg. 20: In lines 26-27, replace “complex-step all of the methods” by “complex-step in all of the methods”.
42. Pg. 20: In line 50, you may either replace “to implement; It only” by “to implement; it only”; or replace the semicolon by a period.
43. Pgs. 21-23: You may capitalize the first letters on the journal names in your references [9, 20]
44. Pg. 22: In your reference [10], you may replace “fréchet” by “Fréchet”.
45. Pg. 23: Update your reference [21] (see the reference [3] in this report). Also, update your reference [27].
46. Pg. 24: In line 18, replace the comma by a period.
47. Pg. 24: I would replace the comma by a period in line 28, and replace “using L’Hôpital’s rule” by “Using l’Hôpital’s rule” in line 31.
48. Pg. 24: I would replace the comma by a period in line 34, and replace “of course, as $h \to 0$” by “As $h \to 0$” in line 37.
49. Pg. 24: I would replace the title of Appendix B “AD Example” by “Automatic differentiation example”.
50. Pg. 24: In line 45, you may replace “$sin(cos(x))$” by “$\sin(\cos(x))$”. For that, use `\sin` instead of `sin`, etc. (similarly in the bottom of the page and in page 25). Also, add a period at the end of the expression.

51. Pg. 25: In line 55, you may remove the "$\cdot$" symbol in "$\frac{d}{dx} \cdot g(h(k(x)))$".
52. Pgs. 25 and 26: I would number the table in 2(c) (page 25). Let's assume the number is "2". Then, in line 13 (page 26), I would replace "chosen for each function and held as constant" by "chosen for each function as in Table 2 and held constant".
53. Pg. 26: In line 24, add a period at the end of the expression.

References

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