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

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Abstract

matrix calculation methods including a newly developed Complex Taylor Series Expansion (CTSE)-based "complex-step" method alongside established methods: forward-difference, central-difference and automatic differentiation. Tangent-stiffness matrix is a term from computational mechanics which here refers to the Jacobian matrix as used in first-order Newton-Raphson methods for the solution of non-linear algebraic systems of equations developed to describe physical or theoretical systems studied in math, science, engineering and business. To perform the comparative study, the above tangent-stiffness calculation methods were applied in a massively parallel computational peridynamics code developed at Sandia National Labs, called *Peridigm*. In the comparative study, for each datum for each run, complex-step was multiple orders of magnitude more accurate the finite-difference methods, according to a common comparison made to the automatic-differentiation method datum. However, for the implementation contemporary to the study, complex-step was also the slowest method among the four for each datum for each run. A mathematical definition of *Michael:* ~~the methods~~complex-step and and automatic differentiation, description of the computer implementations and justification of the comparative study precede results for clarity. The intended audience of this paper includes researchers, professionals and students, *Michael:* ~~therefore conceptually explicit language appealing to multiple levels of understanding is used~~therefor readers are directed to selected background sources in the text for well-known concepts while less familiar concepts are derived

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in-paper with an attempt made to lay steps out plainly for those in disparate fields or who are new to their studies.

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2. Introduction

In order to maintain the quadratic convergence properties of the first-order Newton's method in quasi-static nonlinear analysis of solid structures it is crucial to obtain accurate, algorithmically consistent tangent-stiffness matrices. For an extremely small class of nonlinear material models, these consistent tangent-stiffness operators can be derived analytically; however, most often in practice, they are found through numerical approximation of derivatives.

A goal of this comparative study, was to develop and evaluate a new, accurate, and practical method for calculating tangent-stiffness matrices against established methods. This new method is based on a complex number Taylor series expansion and refered to as CTSE or the "complex-step" method. The distinction of 'accurate' is defined by comparison of the new method to popular finite differencing techniques used for computing tangent-stiffness matrices and with the exact algorithmically consistent derivatives computed with *automatic differentiation*.

It was thought that in addition to comparative information regarding the new method, comparisons of exclusively finite-difference, central-difference and automatic differentiation could prove valuable for developers or analysts not necessarily considering complex-step but needing data to help decide whether or not to invest in automatic-differentiation vs. finite-difference. A comparison and discrimination of the methods was to be achieved through application and the measurement of results in-situ. The results would largely be treated as deterministic consequences of method choice. There was not an attempt made to mathematically prove the suitability of one method over another of the methods. The study was retrospective, as explained in section SECTION of the instant paper.

The scope of the application component of the study was limited to the Linear Peridynamic Solid material model implemented in the computational peridynamics code, *Peridigm*. Identifying a specific application provided a practical framework for implementing the new method and solving engineering problems to generate the data needed to compare the methods. In particular, *Peridigm* was chosen cause it combined several helpful characteristics: The reliance on Newton's method and tangent-stiffness matrices for solving quasi-static implicit problems, prior inclusion of finite-difference, central-difference and automatic-differentiation based methods needed for comparison to a new method that would be developed, and being largely based in the Ansi standard version of the popular C++ programming language.

The aim of this paper is to introduce new information, but also to compile prior art to serve as a general reference for solving non-linear systems. *Michael:*~~The former is mainly intended for an audience of experienced researchers and professionals who are seeking novel tools, the later is intended for an audience of undergraduate to graduate level students who would benefit from a source detailing basic methodology. According to this aim, concepts are presented in multiple levels of detail to accommodate both a broad and deep audience.~~ After giving background on the *Michael:*possibly less familiar differentiation techniques underlying the methods to be discussed here, presented in this paper is: a description of tangent-stiffness matrices and how to use them to solve non-linear systems, detailed directions for producing tangent-stiffness matrices with each the methods identified above *Michael:*~~preceded by background as it becomes necessary~~, a description and justification of a new method, called 'complex-step' for calculating tangent-stiffness matrices, a description of implementing complex-step in the software package used in the comparative study, a description of the parameters of the comparative study conducted to rank the methods, a presentation and analysis of the results of the comparative study, and conclusions and thoughts on potential future work. Finally, the reader is referred to the corresponding author's website for c++ source-code and data necessary to reproduce the results presented here. Additionally included on the website is a C+ template library with classes for solving non-linear systems using the techniques dicussed here, as well as two validation and verification example problemsi which show how to use the library.

2.1. Differentiation Techniques

This subsection contains background information on the differentiation techniques underlying the tangent-stiffness matrix calculation methods compared in the study. Since first-order finite difference techniques are considered well known, they are not described where. Instead the reader is referred to [1, Chap. 4.1.3].

2.1.1. Basis of New Method, 'Complex Step', in CTSE

Michael: [TODO: cite lyness and moler, complete section]

During a literature review in preparation of material distinct from the instant paper, one of the instant authors identified a work presenting an application of the prior work of applied mathematicians Lyness and Moler to the numerical approximations of the first derivatives of real functions. First called Complex Taylor Series Expansion (CTSE) in (Lyness and Moler) and later by [2], where Dr. Millwater is one of the instant authors, the use of the term and its acronym are adopted out of deference to their originators. Lyness and Moler described CTSE based on approximating the Taylor Series Expansion of a function F, where $F : R^1 \to R^1$ about a complex point and solving for the first derivative. The application of Lyness and Moler's work demonstrated by Squire and Trap showed that there was empirical evidence that a CTSE based numerical derivative formula could resist the accuracy reducing phenomenon of subtractive cancellation in circumstances where central-difference and forward-difference were demonstrated to succumb to subtractive-cancellation.

Michael:

~~The types of first-order finite-difference that will be discussed are forward-difference and central difference. CTSE and these finite-difference techniques are similar in that they have been developed by algebraically solving approximated Taylor series expansions for first derivative terms.~~

2.1.3. Differentiation Technique: Automatic-differentiation

Automatic-differentiation or 'AD' is a computerized method for computing exact derivatives based the chain-rule from calculus. AD takes advantage of the fact that any mathematical function executed on a computer, no matter how complicated, is a "composition of simple operations" (add, multiply, power, transcendental and the like) each having known analytical derivatives

[3]. For reference, the AD implementation used in the study is the "Sacado" package from the "Trilinos" library developed out of Sandia National Labs [4].

The way an AD system works is by first evaluating the innermost function of the composition, then presenting that function's output as input to the next level function until all levels are complete, in a way no different from how a normal computer program or human would evaluate composition functions. AD departs in that as each nested function is evaluated, the function's partial derivative with respect to the designated variables of the given input is also calculated. This is possible because the elementary math functions are hard-coded into the AD source-code along with their analytical derivatives, and linked by special instructions, so that when the elementary math functions are called upon for computation, their partial derivatives may be computed and stored in a sequence. The AD system then multiples the final sequence of partial derivatives together to produce the exact equivalent to taking a partial derivative of the corresponding composition function made up of the elementary functions with respect to a designated variable at a particular value. It is obviously, but bears mentioning, that the AD system could simply store one value for partial derivatives, modifying it as appropriate for every function evaluation rather than keeping a sequence. In the literature, the AD scheme described here is called 'forward automatic-differentiation'. For brevity, only forward AD will be covered since it is pertinent to the study, however the reader is referred to the introduction section of [5] and its references list for further information on AD, particularly [6] which is foundational.

To make the above description complete, this subsection concludes with an example forward AD process, with an emphasis on how general purpose information known to the computer is specialized with additional information from the problem and used to carry out AD:

1. Take an example composition function $f(x) = (sin(cos(x)))^2$

2. Suppose we want to know $\frac{df}{dx} |_{x_0}$ where x_0 is a particular value of x.

   (a) Given that:

      i. $S \in R^1$
      ii. $X \in S$

iii. $g, h, k \in H : S \to S$
iv. $\forall s \in S : g(s) = s^2,\ h(s) = sin(s),\ k(s) = cos(s)$
v. $\forall x \in X : f(x) = g(h(k(x)))$

(b) Given that the computer is programmed with some mathematical definitions:

i. A. $u, v, w \in H : R^3 \to R^1$

B. $s, a, b, x \in R^1$

ii. particular values can be identified:
$s = s_0, .., s_n, ...s_\infty \mid n = [0, \infty)$
and similarly for the other variables a, b, x

iii. functions u, v, w and their partial derivatives w.r.t s are defined such that:

for a, b, s equal to a_n, b_n, s_n:

$u \mid_{a_n,b_n,s_n} = a_n \cdot s_n^{b_n}$	$\frac{\partial u}{\partial s} \mid_{a_n,b_n,s_n} = a_n \cdot b_n \cdot s_n^{b_n - 1}$
$v \mid_{a_n,b_n,s_n} = a_n \cdot sin(b_n \cdot s_n)$	$\frac{\partial v}{\partial s} \mid_{a_n,b_n,s_n} = a_n \cdot b_n \cdot cos(b_n \cdot s_n)$
$w \mid_{a_n,b_n,s_n} = a_n \cdot cos(b_n \cdot s_n)$	$\frac{\partial w}{\partial s} \mid_{a_n,b_n,s_n} = -a_n \cdot b_n \cdot sin(b_n \cdot s_n)$

(c) Given that it is possible to describe $f(x) = (sin(cos(x)))^2$ in terms the computer understands by inputting $f(x)$ such that the computer stores an equivalent statement $f(x) = u(a, b, s) \mid_{arguments}$, iff the arguments of u, v, w are chosen such that u, v, w approximate g, h, k as follows:

Function	a	b	s	Approximates Function
u	1	2	v	g
v	1	1	w	h
w	1	1	x	k

3. It follows from 2(a)v that we can evaluate $\frac{d}{dx} f(x) \mid_{x_0}$ with the chain rule:

$$\frac{d}{dx} f(x) = \frac{d}{dx} \cdot g(h(k(x))) \mid_{x_0}$$
$$\frac{d}{dx} f(x) = \frac{dg}{dh} \cdot \frac{dh}{dk} \cdot \frac{dk}{dx} \mid_{x_0}$$

From the rest of 2a it follows that we can approximate $\frac{d}{dx} f(x) \mid_{x_0}$ by specializing the computer's general forms of u, v, w according to 2c, with parameters a, b chosen for each function and held as constant, and evaluating, such that the total derivative our original function w.r.t x where $x = x_0$ is approximated by the partial derivative of our equivalent statement, $f(x) = u(a, b, s) \mid_{arguments}$, w.r.t s where $s = x_0$.

For completeness we write out the computer's steps to evaluate 3 under the conditions of 2c with a particular value of $s = x_0$, in equation format:

$$\frac{\partial}{\partial x} f(x) \mid_{x_0} = \frac{\partial u}{\partial v} \mid_{1,2,v|_{1,1,w|_{1,1,x_0}}} \cdot \frac{\partial v}{\partial w} \mid_{1,1,w|_{1,1,x_0}} \cdot \frac{\partial w}{\partial s} \mid_{1,1,x_0} \cdot \frac{ds}{dx}$$

Repeating above in tabular format:

Current Evaluation	s Value	Partial Derivative
$w(a, b, s) \mid_{1,1,s}$	x_0	$\frac{\partial w}{\partial s} \mid_{1,1,x_0}$
$v(a, b, s) \mid_{1,1,s}$	$w(a, b, s) \mid_{1,1,x_0}$	$\frac{\partial v}{\partial w} \mid_{1,1,w\mid_{1,1,x_0}} \cdot \frac{\partial w}{\partial s} \mid_{1,1,x_0}$
$u(a, b, s) \mid_{1,2,s}$	$v(a, b, s) \mid_{1,1,w(a,b,s)\mid_{1,1,x_0}}$	$\frac{\partial u}{\partial v} \mid_{1,2,v\mid_{1,1,w\mid_{1,1,x_0}}} \cdot \frac{\partial v}{\partial w} \mid_{1,1,w\mid_{1,1,x_0}} \cdot \frac{\partial w}{\partial s} \mid_{1,1,x_0} \cdot 1$

Because the computer knew the analytical forms of the partial derivatives of each of u, v, w beforehand, all it needed to do was:

1. to evaluate each of u, v, w according to 2c, in order from $w \to v \to u$,
2. to remember the values for x_0 and the output of each function evaluation besides u,
3. then to use x_0 and the output of the function evaluations as input for the corresponding partial derivative function evaluations, and
4. store the individual partials.

Lastly, to compute the partial derivative of the entire composition function, the computer multiplies the individual partials together in observance of the chain-rule.

Some things to note about AD are that no approximation of derivatives is being made because the analytical forms of the partials of the elementary math functions are defined alongside them. Accuracy of AD is then limited by the precision of the AD system's definition of the elementary math functions and their partials.

2.2. Tangent-stiffness Matrices

This subsection gives a working definition of a tangent-stiffness matrix and background on a Newton-Raphson method which uses a tangent-stiffness matrix to help solve nonlinear systems of equations, similarly to the the solution method used by the software package used in the study.

2.2.1. What is a Tangent-stiffness Matrix

It is important to identify what a tangent-stiffness matrix is and what it is used for to help show the motivation for the work discussed here. It is helpful to begin with the thought that a tangent-stiffness matrix is a type of slope for vector valued functions of vector variables at a single point in the space of the vector valued variable. A tangent-stiffness matrix is similar to the "m" in the scalar function $y = mx + b$, except that y and x are vectors while m is a matrix.

In detail, a tangent-stiffness matrix (or operator) can be described as a collection of the first order partial derivatives of a vector valued function w.r.t each degree of freedom of the vector valued function for a given value of the vector variable. The tangent-stiffness matrix comprises a linear operator that can be used to transform a difference in the vector variable into a difference in the value of the vector valued function via an inner product between the tangent-stiffness matrix and the vector variable. As an example in a solid mechanics system, suppose some dependent variables represented force components of force vectors at nodes of discretization, and independent variables represented displacement components for those same nodes. Suppose that as is possible in peridynamic nodes each dependent variable is a function of all of the independent variables. For this situation, the tangent-stiffness matrix would be the first derivatives of every force component variable with respect to every displacement component variable, with the rows ordering the force components and the columns ordering the displacement components.

How is a tangent-stiffness matrix computed? The mathematical formula for a tangent stiffness matrix can be expressed in indicial notation as:

$$\frac{\partial F_i}{\partial X_j} \,|_{X_0,...,X_n} \tag{1}$$

Where F_i is the i'th component of the vector valued function, X_j is the j'th component of the vector variable, and a particular value of the vector variable is chosen $X_0, ..., X_n$. One then evaluates the expression for each combination i, j corresponding to an element at $row, column$ in the tangent-stiffness matrix. By inspection, the elements of a tangent-stiffness matrix can be estimated using the CTSE, AD and finite-difference techniques for functions $F : R^1 \rightarrow R^1$, since taking partial derivatives entails holding all but a single independent variable of the function constant, and each component of a vector valued function can be evaluated independently of the other components.

2.2.2. Calculating Tangent-stiffness Matrices with Each Method

For reference, expressions for calculating tangent stiffness matrices with CTSE, AD, central-difference and forward-difference will be shown and explained.

When the using the forward-difference technique the formula for calculating a tangent-stiffness matrix is:

$$K_{ij} = \frac{\partial F_i^{int}(x + \delta e_j) - F_i^{int}(x)}{\delta} \tag{2}$$

Where K_{ij} is the index notation representation of an element of the tangent-stiffness matrix at row i, column j. The expression says that the partial derivative of the i'th component of F w.r.t the j'th component of x is equal to the quotient of the partial difference of two terms and a denomenator. The first of the 'two terms' is F_i evaluated at x where the j'th component of x has been perturbed by an very small amount in the direction of the positive x_j axis. The second of the 'two terms' is F_I evaluated at an unperturbed x. The denominator is the magnitude of perturbation called "probe distance" ADDAGIO MANUAL REF

When using the central-difference technique the formula for calculating a tangent-stiffness matrix is:

$$K_{ij} = \frac{\partial F_i^{int}(x + \delta e_j) - F_i^{int}(x - \delta e_j)}{2\delta} \tag{3}$$

The distiction between the central difference-method and the forward-difference method tangent-stiffness calculation formula is that the partial difference is now between two perturbed function evaluations, rather than between an unperturbed and perturbed function evaluation as in forward-difference. Additionally, the minuend involves a perturbation of x in the direction opposite to the direction of the j'th component of x.

When using the comple-step technique, which is based on CTSE, the formula for calculating a tangent-stiffness matrix is:

$$K_{ij} = \frac{imag(F_i^{int}(x + \delta e_j^{imag}))}{\delta} \tag{4}$$

Where our model F is treated as function of complex variables and x is treated as a vector of complex values. The expressions says that the real valued partial derivative of the i'th component of F w.r.t the j'th component of x is equal to the imaginary component of F_i evaluated at x where x is perturbed by a very small amount in the direciton of the imaginary axis corresponding to the j'th component of x all divided by the magnitude of the perturbation. There is no partial notation because a partial difference is not taken.

When using automatic-differentiation to calculate a tangent-stiffness matrix, one only needs to follow the definition of the tangent-stiffness matrix and issue the correct commands to the AD system. The formula is just as expected:

$$K_{ij} = \frac{\partial F_i^{int}}{\partial x_j} \tag{5}$$

2.2.3. Solve a Nonlinear System with a Tangent-stiffness Matrix

Michael: ~~An accurate tangent stiffness matrix is a main part of the Newton Raphson method for iteratively solving non-linear systems for equilibrium solutions. The method is derived by a linearisation using Taylor expansion of the vector valued function modelling the system in a way reminiscent of how forward difference is derived from the Taylor expansion of a scalar valued function. Here the two derivations are shown side by side: The difference between the two is that in the forward difference derivation, it is assumed that the derivative term is unknown and can be determined from knowing change in location, while in the Newton-Raphson derivation, it is assumed that the change in location is unknown and can be determined from knowing the value of the derivative term. Additionally we could derive a version of Newton Raphson for CTSE directly: The Newton Raphson method is applied in the following manner: It is clear to see how if the tangent-stiffness matrix used in the Newton Raphson method is inaccurate, predicted changes in location will be inaccurate. However, non linear functions don't have constant slopes by definition, meaning that a perfectly accurate tangent stiffness matrix at the current guess location is not a guarantee of a one step solution path to the solution location since slope changes over the interval guess to updated guess.~~ The reader is referred to a succinct explanation of the Newton Raphson method, which shows the role of a tangent-stiffness matrix or Jacobian in that solution method [7, chap. 13].

3. Methods and Materials

3.1. Material: Perdynamics Code

The following subsubsections identify the program modified to run the simulations for the comparative study and explain what modifications were necessary.

3.1.1. Perdigm *and Peridynamics*

3.1.2. Implementing Complex-Step in Peridigm

Complex step was implemented in *Perdigm* as follows. First a way of persistently allocating memory needed to store imaginary values for nodal position and dilatation was determined. Persistent memory allocation is a very basic way to improve performance in general for a computer program. The way memory was allocated for similar vector and scalar variables used by the prior existing forward difference method was copied and new 'field spec' variables were added into the 'elastic' material model to store imaginary position coordinates and imaginary dilatation. Model evaluation computer code methods that were used in the course of applying the forward difference method were copied, renamed and re-written to follow the CTSE formula, which mainly involved changing the datatype of intermediate variables which were method-local and dynamically casting process-local variables to complex compatible datatypes. Additional modifications were for the purpose of collecting experimental data and are not part of complex-step itself. The mathematical difference between the original forward-difference and complex-step code was covered in 2.2.1. The source code for implementing complex-step in *Perdigim* can be found on the corresponding author's website. Because *Peridigm* was written by computer scientists, many advanced techniques in C++, such as multiple virtual inheritance, pointer arithmetic and distributed data structures were used in the basic code and by necessity in the modified code. To see complex-step in a more narrow context, it is advised that readers also take a look at the examples of complex-step provided on the corresponding author's website.

3.2. The Comparative Study

The methods were compared by running two sets of test problems where each method would solve a problem concurrently. Each test problem simulated a $4 by .25 by .25$ meter block of metal undergoing tension along the axis parallel to the long dimension of the block. The test problems were set up in *Perdigm* as qausistatic equillibrium problems, where the displacement boundary conditions used to apply tension were applied gradually, in 'load steps', and an equilibrium solution for each load step was achieved before applying the next load step. The material properties of the model were set at $8.0E-9 metric tonne/mm^3$ density, $1.515E4 MPa$ bulk modulus, and $7.813E4 Mpa$ shear modulus. The peridynamic horizon used in a test problem was three times the node spacing for the corrisponding model mesh. This number was chosen out of experience to insure that every node could have at least one nonlocal connection along the diagonal of the initial node grid.

A series of nine of these test problems were run, with the mesh discretization used in the model finer and finer with every test in the series. The aim of increasing the mesh complexity was to see if possible differences between the methods in terms of accuracy and speed would be affected. This series would comprise the single core runs. The specific parameters of these tests can be found in *Peridigm* input xml files included in the archive for this paper which can be found in the corresponding author's website. These xml files allow users with appropriately modified versions of *Peridigm* to reproduce the results found in this paper.

Another series of four test problems were run, however this time the number of cores used to solve the problem was varied from test to test rather than the mesh refinement. While mesh refinement was not varied from test to test, it was set at a somewhat high $1E6$ perdidynamic nodes of discretization. This allowed the simulation computer to be challenged sufficiently that the effect of varying the number of cores used could be more clearly seen. The specific parameters of these tests can be found in *Perdigm* input xml files also included in the archive for this paper on the corresponding author's website.

What was recorded during the test runs as experimental data is the subject the following subsubsection. It is organized to explain "what", "why" and "how" in that order.

3.2.1. Justification: Goals, Assumptions, and Metrics

A goal of the study was to rank complex-step against forward-difference and central difference on the basis of accuracy. AD was ommited from the comparison because it served as the standard of accuracy for the other methods in the absence of appropriate analaytical forms for the Jacobian associated with the nonlinear system solved in the study. The assumption that AD is accurate enough to serve as a standard is supported by AD's implementation as a computerized chain rule as explained in 2.1.3.

Because it makes no sense to compare tangent-stiffness matrices from different problems, load steps, or from different iterations, it was necessary to solve one load step and conclude each iteration within that load step by updating displacement guess only from the the results of the AD method, and to subsequently feed all four methods the same updated guess the following iteration. This decision precluded a comparison of convergence rate, since if the methods were allowed to solve a problem at their individual pace, differences in accuracy would produce differences in guess updates and therefor the number and nature of iterations perfomed. Different guesses from iterations started with different previous guesses could not be data for a valid comparison of tangent-stiffness accuracy between methods. However a separate convergence rate comparison study could be done given some modifications to the materials for the study described in this paper, and of course, the resources to perform that study. Additionally, having each of the methods physically operate in the same process, single or parallel, allowed the comparison of tangent-stiffness matrices as loaded from random access memory rather than from the hard-disk. Loading from RAM gives the benefit of vastly greater speed and the simpler programming compared to some other solution speculatively involving dynamic file management on files which for one of the components of the study would be on the order of $1XE10$ bytes for which "vastly" is not hyperbole. However, the price of running the methods together in the same process and avoiding the use of the hard-disk was that at least two tangent-stiffness matrices had to be stored in RAM during simulation, which meant that special high-memory compute nodes were needed for the $1E6$ peridynamic element problem series.

The other goal was to rank the four methods, that is including AD, on the basis of speed. Instead of convergence rate being measured, speed of iteration was measured because it could be so done at the same time as accuracy was being measured given a single tangent-stiffness calculation. It was assumed that the order that each method was evaluated was unimportant, that evaluating each method sucessively within each solver iteration did not affect their performance individually and that speed of computation did not change with time. These assumptions allowed the test program to run the same problem with each of the methods at effectively the same time and generate an equal volume of data from each method. It was also assumed that the Jacobian matrix calculation time for each of the methods did not vary based on what values the independent variables held, as they do from iteration to iteration as the guessed equilibrium solution is updated. This assumption allowed calculation time measurements to be averaged over all iterations within a solution attempt. The purpose of averaging calculation time measurements was to informally address the extraneous variables of evaluation order and computer system load due to other user's processes or processes not associated with the study. It begs the question that if it is assumed that the value of independent variables had no effect on iteration speed, than why couldn't each of the method have been run independently so that convergence data were recorded, so long as system being solved was the same? The answer is that this would have made accuracy comparisons invalid if measured concurrently with convergence rate, while it would cost additional time and resources if convergence rate were measured in serparate runs. Instead, while not part of the study, the example programs available on the corresponding author's website allow the reader to make a comparison of the methods for themselves on the basis of accuracy and convergence rate for two example nonlinear systems. In the examples, notice how convergence rate decreases when the step size selected for forward-difference or complex-step is set to larger numbers such that accuracy relative to AD is decreased. While likely not the best possible implementations of these methods, they each were coded with the same skill level such that a comparison of their relative strengths is reasonable from the standpoint of intuition.

Once the selection of what to measure, why to measured it, and if it could be measured was determined, the task was to find a way to take measurements that satisfied our goals. The goals of collecting accuracy and speed measurements were achieved by developing and implementing metrics within the simulation program used in the study. The metric used to measure the accuracy of a tangent-stiffness matrix was the Frobenius norm of the element-wise difference between the tangent-stiffness matrix produced by the method being evaluated and the tangent-stiffness matrix produced by the AD based method, given that both methods were set upon the same problem. The lower the value of this metric, the closer the other method's Jacobian was to the AD Jacobian, and therefore the more accurate the method was. The expression for the accuracy metric:

$$D = \sqrt{\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}(J_{AD}(i,j) - J_M(i,j))^2} \tag{6}$$

Where D is distance, n is the number of degrees of freedom, J_{AD} is the Jacobian matrix produced by the AD based method, M stands for other *M*ethod, and the root of the summed squared element-wise differences between the matrices is taken. The metric used to compare the speed of the methods was the time in seconds taken to resume execution in the calling method after instructing the implementation of the method being evaluated to run and complete itself. Another basis of comparison used in the study, but not quite a metric, called computational efficiency is based on the ratio of calculation time to number of Jacobian matrix elements.

3.2.2. Materials: Computers, Other Software

Mesh generation for the test problems run in the study was done using the software package *Cubit* developed at REFERENCE. For the test series in which peridynamic node density was varied, journal scripts compatible with *Cubit* were used. The rule used to select the arangement of nodes within the borders designated by simulated material block's dimensions was to manually choose a node spacing, fit the maximum whole number of nodes in a regular grid within the block, and then check whether or not this number of nodes matched the number of nodes desired for a particular test. The same process was used for the multicore series. An example journal script can be found on the corresponding author's website. For future work, it may be beneficial to automate and randomize this process for statistic reasons and for time efficiency.

The test problems were run the *Stampede* HPC cluster computer housed at *TACC* (Texas Advanced Computing Center) based out of UT Austin. The single core test series was run using the normal queue compute nodes, while the multicore test series was run using one to four "large memory" nodes each having one terrabyte of local RAM. This large amount of memory was required for reasons explained in 3.2.1.

3.2.3. Methods: Reduction of Data

The output produced by *Perdigm* including the additional accuracy and speed measurements it was modified to provide was redirected from the console to text files by the resource manager, *SLURM* (Simple Linux User Resource Manager). Directories and filenames were chosen so that data would be easy to sort by individual test run. Extraneous information was manually deleted from copies versions of the output text files so that they would be regular enough to be easily read by scripts written in *Python.* These scripts averaged accuracy or speed data for a test corresponding to a particular peridynamic node density over all iterations for that run, and then plotted this averaged data as if it were a function of peridynamic node density as it varied from test to test in the series. Similarly, for the multicore tests, data was averaged and plotted in much the same way, but as a funciton of number of cores used to solve the problem rather than as a function peridynamic node density which was held constant. These data reduction and plotting scripts can be found on the corresponding autor's website.

Since samples were not repeated, because there was not resources for it, confidence intervals were not calculated. However, if results of iterations within the same test problem were considered samples of the same thing, then a confidence interval could be calculated. This assumption was made for the purpose of plotting reporting average values, but a confidence interval was not calculated. But, a cursory review of data showed no range overlap among the methods for accuracy or speed data from any test run of either series.

4. Results and Discussion

Averaged Results, Entire Test Matrix			
Cores	Jacobian Els.	Calc. Time (s)	Accuracy Diff. (MPa)
		CS, CD, FD, AD	CS, CD, FD
1	1.99E6	3.5, 2.7, 1.7, 1.6	1.92E-10, 1.21E-4, .137
1	4.25E6	6.2, 4.9, 3.2, 2.9	2.28E-10, 9.94E-4, .148
1	7.79E6	11.2, 8.9, 5.7, 5.2	2.38E-10, 1.59E-4, .145
1	1.54E7	26.7, 21.0, 13.4, 12.2	2.33E-10, 4.61E-4, .12
1	2.00E7	28.1, 22.2, 14.4, 13.1	2.76E-10, 1.05E-3, .145
1	3.14E7	47.6, 37.7, 24.2, 21.9	2.64E-10, 1.65E-3, .133
1	4.01E7	55.6, 44.1, 28.4, 25.9	3.03E-10, 1.92E-3, .148
1	8.39E7	138.9, 109.6, 70.2, 64.0	3.63E-10, 1.64E-3, .123
1	1.65E8	277.3, 218.1, 139.4, 126.5	3.26E-10, 2.18E-3, .128
32	1.67E10	336.1, 277.7, 200.6, 233.1	6.21E-10, 1.52E-2, .176
64	1.67E10	169.9, 140.7, 102.0, 119.7	6.20E-10, 1.50E-2, .177
96	1.67E10	114.7, 95.0, 69.1, 79.7	6.18E-10, 1.50E-2, .177
128	1.67E10	86.4, 71.8, 52.4, 58.8	6.16E-10, 1.47E-2, .177

4.1. Speed Data

4.2. Accuracy Data

4.3. Efficiency Data

5. Conclusions and Further Work

5.1. Thoughts on Results

5.2. Thoughts on Perdigm

After the bulk of the study had been conducted, it was determined that the implementations of forward-difference, central-difference and by inherited code complex-step, in *Peridigm* were not optimal. Each of these implementations included extensive looping over noncontiguous addresses in memory and unnecessary re-calculation of constant values. Unpublished preliminary results show that when calculations for the quantity 'zeta' are re-used and only perturbed and previously pertubed functions of independent variables are recomputed throughout the course of a Jacobian evaluation, complex-step performs at the speed of forward-difference. Because of this it is speculated that forward-difference and central-difference could be modified in nearly the same way to perform more quickly than AD. An enhanced performance implementation of forward-difference will eventually be made available on the corresponding author's website.

5.3. Final Thoughts on Complex-Step

Complex-step was shown to be highly accurate by the standards of this study, but as it is implemented in *Peridigm* may not be any better than AD, and it is almost certainly slower for a naive implementations. When looking to the future of *Peridigm*, Complex-step holds the advantage of relying on byte-copiable datatypes, while AD requires a complicated serialization and deserialization in order to function as byte-copiable. This is fine for copying in between MPI processes, but deserialization on an accelerator or GPU is very difficult, as this would require compiling a version of the AD library being used that were compatible with the accelerator or GPU being used. What this means is that if *Peridigm* were to be reformulated to take advantage of accelerators like GPU's or similar, which is likely, given their performance and power efficiency advantages over traditional host CPU's, complex-step would become more attractive.

Appendix A. Extra

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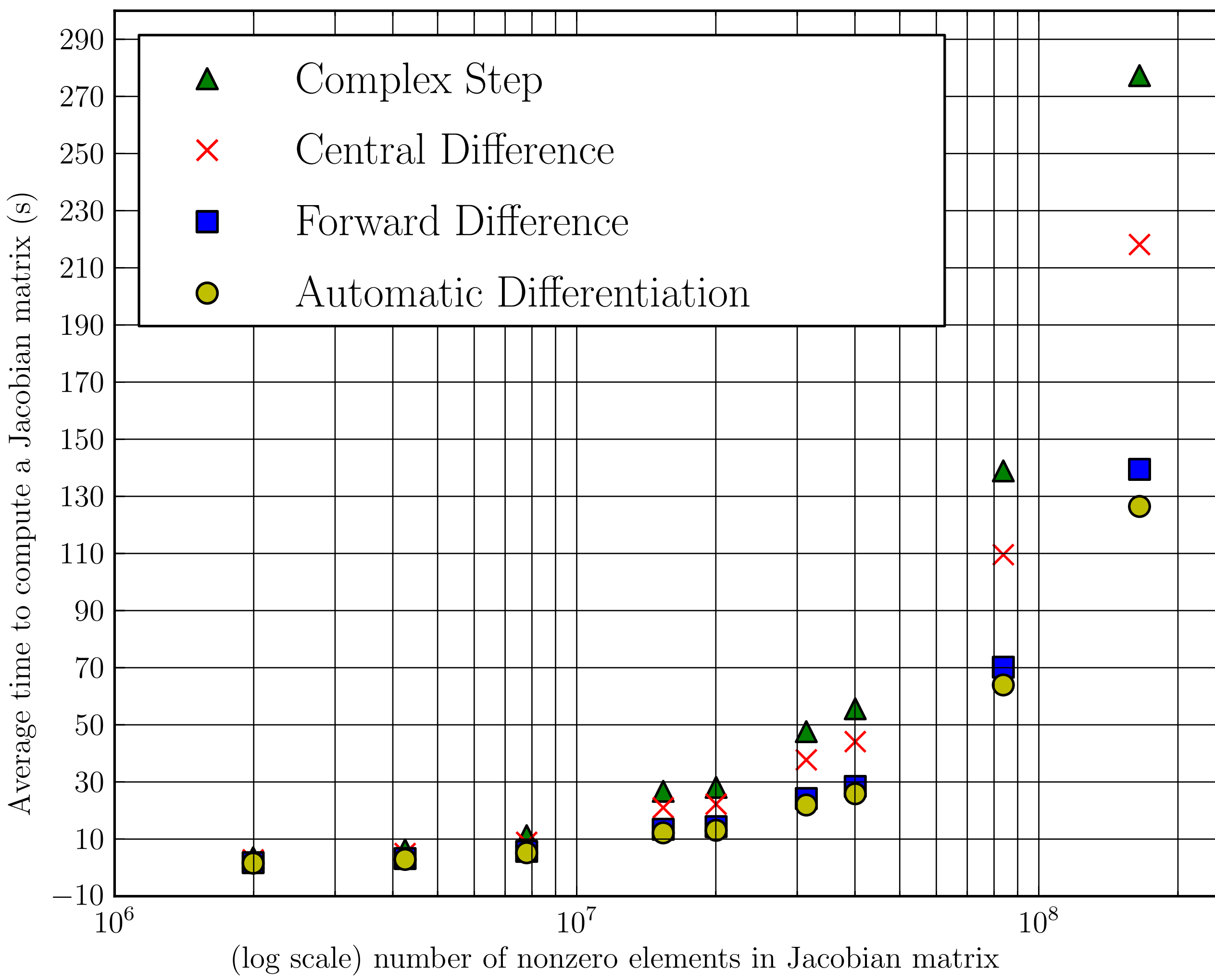
Complex Step
Central Difference
Forward Difference
Automatic Differentiation
Average time to compute a Jacobian matrix (s)
(log scale) number of nonzero elements in Jacobian matrix
290
270
250
230
210
190
170
150
130
110
90
70
50
30
10
−10
10^6
10^7
10^8