

A Non-smooth Newton Method for Multibody Dynamics

K. Erleben* and R. Ortiz†

*University of Copenhagen, Denmark

†Tulane University, USA

Abstract. In this paper we deal with the simulation of rigid bodies. Rigid body dynamics have become very important for simulating rigid body motion in interactive applications, such as computer games or virtual reality. We present a novel way of computing contact forces using a Newton method. The contact problem is reformulated as a system of non-linear and non-smooth equations, and we solve this system using a non-smooth version of Newton's method. One of the main contribution of this paper is the reformulation of the complementarity problems, used to model impacts, as a system of equations that can be solved using traditional methods.

Keywords: Complementarity Problem, Non-smooth, Non-linear, Newton Method

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A NEW REFORMULATION AND ITERATIVE METHOD

Constraint based simulation of multibody dynamics can be classified into two groups of algorithms: minimal coordinate methods, which tend to be recursive in nature [1], and maximal coordinate methods. The focus of this paper is on complementarity formulations, which is a type of maximal coordinate method. Complementarity formulations come in two flavors: Acceleration-based formulations and velocity-based formulations [2]. Acceleration-based formulations cannot handle collisions, and one must stop at the point of collision and switch to a impulse-momentum law. Further, acceleration-based formulations suffer from indeterminacy and inconsistency. Although mostly overlooked in the computer graphics literature, the velocity-based formulation suffers from none of these drawbacks.

In the field of interactive physics it is popular to use iterative methods based on splitting methods [3]. Examples are found in rigid body simulators such as Open Dynamics Engine. One such method is the projected Gauss-Seidel method. Gauss-Seidel solvers have previously been applied for multibody dynamics [4] although in a blocked version. These types of iterative methods are attractive due to their simplicity and are easily accelerated on modern hardware. However, the methods are based on a traditional linear complementarity problem formulation and offer at best linear convergence. This has motivated us to investigate the complementarity problem formulation and a new iterative method. Newton's method has been popular since the invention of calculus. Fast local convergence rates and simplicity makes it attractive for this type of application. The parallelization of the internal processes in the method may make it very attractive to implement on modern hardware.

A NON-SMOOTH AND NON-LINEAR APPROACH

The multibody dynamics problem can be stated as a complementarity equation and these can be reformulated into a non-smooth equation similar to the generalized minimum map of [5]. However, due to friction bounds our version has variable linear bounds whereas the generalized minimum map reformulation has constant bounds. The frictional impact model can be written in a discretized form as, see [6]:

$$\begin{aligned} J^T M(q)^{-1} J \Delta t \lambda + J^T (\bar{b} + R) &= y_+ - y_- \\ 0 \leq \lambda - l(\lambda) \perp y_+ &\geq 0 \\ 0 \leq u(\lambda) - \lambda \perp y_- &\geq 0. \end{aligned}$$

Where J is the kinematic Jacobian, $M(q)$ is a generalized mass matrix, λ contain normal and tangential forces, Δt is the time step, and vector $J^T (\bar{b} + R)$ contains external and gyroscopic forces. The functions $l(\lambda)$ and $u(\lambda)$ are linear functions of λ and represent frictional bounds. Note that y_+ and y_- represent positive and negative components of $J^T M(q)^{-1} J \Delta t \lambda + J^T (\bar{b} + R)$ respectively.

Let $A = J^T M(q)^{-1} J$, $x = \Delta t \lambda$ and $b = J^T (\bar{b} + R)$, then we can rewrite the discretized model as:

$$Ax + b = y_+ - y_- \quad (1a)$$

$$0 \leq x - l(x) \perp y_+ \geq 0 \quad (1b)$$

$$0 \leq u(x) - x \perp y_- \geq 0. \quad (1c)$$

The matrix A is sparse and symmetric positive semi-definite because $M^{-1}(q)$ is block diagonal and positive definite. Observe that Δt is positive and multiplying $\lambda - l(\lambda)$ or $u(\lambda) - \lambda$ by a positive number does not change the complementarity constraint.

Notice that we can rewrite every component of (1) as

$$(Ax + b)_i = (y_+)_i - (y_-)_i \quad (2a)$$

$$\min(x_i - l(x)_i, (y_+)_i) = 0 \quad (2b)$$

$$\min(u(x)_i - x_i, (y_-)_i) = 0. \quad (2c)$$

Now we rewrite this in to a non-smooth system of equations by observing that if $(y_-)_i > 0$, then we have $(y_+)_i = 0$ and from (2b) $x_i - l(x)_i \geq 0$, thus

$$\min(x_i - l(x)_i, (y_+)_i - (y_-)_i) = -(y_-)_i.$$

Note that if $(y_-)_i = 0$ we get $x_i - l(x)_i = 0$ and the above equation is trivially satisfied. Substitute this into (2c) to get

$$\min(u(x)_i - x_i, -\min(x_i - l(x)_i, (Ax + b)_i)) = 0 \quad (3)$$

or equivalently

$$\max(x_i - u(x)_i, \min(x_i - l(x)_i, (Ax + b)_i)) = 0. \quad (4)$$

We can now define the *complementarity equations* as

$$H(x) = \max(x - u(x), \min(x - l(x), Ax + b)) = 0. \quad (5)$$

Here $\max(\cdot, \cdot)$ and $\min(\cdot, \cdot)$ are taken over each component of the vectors. Observe that the non-smooth function $H(x)$ is continuous but non-differentiable. This means that the classical derivative is not defined for some points in the domain of H .

The idea is to use a modified version of the classical Newton method with line-search to solve the non-smooth equation (5). We can achieve this by generalizing the concept of derivative. We start by noticing that the non-smooth function $H_i(x)$ is a *selection function* of the affine functions, $x_i - l(x)$, $(Ax + b)_i$, and $x_i - u(x)$. Further, each H_i is Lipschitz continuous and each of the components are also Lipschitz, thus the non-smooth function $H(x)$ must be Lipschitz.

We use a *B-derivative* (B stands for Bouligand) [7], to calculate a descent direction for the natural merit function $\theta(x) = \frac{1}{2} H(x)^T H(x)$. Using this B-derivative we formulate a linear subproblem whose solution will always provide a descent trajectory in the line-search Newton method. In fact, the biggest computational task for solving the non-smooth and non-linear system (5) is the solution of a large linear system of equations. This is similar to what Billups does to solve his non smooth system in [5] and we repeat this same technique in this work. One critical difference between Billups work and ours is that he uses a smoothed version of the minimum map (5). The main drawback of his approach is that sparsity of the matrix A is lost, increasing the computational work.

Define the generalized Newton equation as

$$H(x) + BH(x, dx) = 0 \quad (6)$$

where $BH(x, dx)$ is the B-derivative of $H(x)$ in the direction dx . Each Newton iteration is finished by doing a correction of the previous iterate:

$$x^{k+1} = x^k + \tau dx, \quad (7)$$

where τ is the step length. Due to the connection of the non-smooth Newton method with the classical Newton method, global convergence is unlikely if we start in an arbitrary starting point x^0 . To remedy this we perform an Armijo back-tracking line search on our merit function. Convergence proofs are found in [8].

Now we proceed to compute the B-derivative. For this particular case of multibody dynamics, we use a friction pyramid (we could extend this straightforwardly to a n -sided cone) approximation of Coulomb Friction law. Given the vector index i , then we have

$$r = i \bmod 3 = \begin{cases} 0 & \text{if } i \text{ is normal force} \\ 1 & \text{if } i \text{ is first tangential force} \\ 2 & \text{if } i \text{ is second tangential force} \end{cases} \quad (8)$$

We can rewrite the B-differential $BH_{ij} = \frac{\partial H_i}{\partial x_j}$ compactly by using a Kronecker-delta and defining μ_i to be zero if i is a normal force index and non-zero for friction directions. The result is

$$\frac{\partial H_i}{\partial x_j} = \begin{cases} \delta_{ij} + \mu_i \delta_{i-r,j} & \text{if } y_i > x_i - l_i \\ a_{ij} & \text{if } x_i - l_i > y_i > x_i - u_i \\ \delta_{ij} - \mu_i \delta_{i-r,j} & \text{if } x_i - u_i > y_i \end{cases} \quad (9)$$

We define three index sets corresponding to our choice of active selection functions:

$$\mathcal{L} = \{i | y_i > x_i - l_i\}, \quad \mathcal{A} = \{i | x_i - l_i \geq y_i \geq x_i - u_i\}, \quad \text{and} \quad \mathcal{U} = \{i | x_i - u_i > y_i\} \quad (10)$$

Let us define the auxiliary index set $\mathcal{J} = \mathcal{L} \cup \mathcal{U}$. Next we use a permutation of the indexes such that all variables with $i \in \mathcal{J}$ are shifted to the end of the B-differential. Hereby we have creating the imaginary partitioning of the B-differential:

$$BH' = \begin{bmatrix} A_{\mathcal{A}\mathcal{A}} & A_{\mathcal{A}\mathcal{J}} \\ C & D \end{bmatrix} \quad (11)$$

Note this convenient block structure with $A_{\mathcal{A}\mathcal{A}}$ being a principal submatrix of A . The matrices D and C have a very special structure. In particular D can be inverted by changing the sign of the off-diagonal entries.

If we use the blocked partitioning of our B-differential from (11) then the corresponding permuted version of the Shur system of the Newton equation (6) is

$$\begin{bmatrix} S & 0 \\ D^{-1}C & I \end{bmatrix} \begin{bmatrix} dx_{\mathcal{A}} \\ dx_{\mathcal{J}} \end{bmatrix} = - \begin{bmatrix} H_{\mathcal{A}}(x^k) - A_{\mathcal{A}\mathcal{J}} D^{-1} H_{\mathcal{J}}(x^k) \\ D^{-1} H_{\mathcal{J}}(x^k) \end{bmatrix},$$

where $S = A_{\mathcal{A}\mathcal{A}} - A_{\mathcal{A}\mathcal{J}} D^{-1} C$ is the Schur complement of (11). Our problem is reduced to a potentially smaller linear systems in $dx_{\mathcal{A}}$. Once we solve for $dx_{\mathcal{A}}$ we then can obtain $dx_{\mathcal{J}}$ by direct substitution. Since the original matrix A is positive semi-definite, there is little we can say about the Schur complement other than it may also be singular. This poses a big challenge for linear iterative solvers used to solve the Newton equation, and for this reason we use singular value decomposition (SVD) to solve this system.

NUMERICAL BEHAVIOR AND FUTURE WORK

We have generated random symmetric positive definite systems of increasing problem size. For each problem size we run 100 test cases. In all test cases we have set the absolute tolerance to 10^{-6} and an upper iteration maximum of 100. The tests were performed on a Dell M90 Precision Laptop, having Centrino Duo CPU and 2 GB of RAM.

Since the projected Gauss-Seidel is cheap computationally, although not very accurate, we use it to obtain a good initial iterate to warm-start the Newton method. For our test cases we used a fixed count of 4 projected Gauss-Seidel iterations to find a good initial iterate. The results are shown in Tables 1 and 2. The size column is the total number of variables. The Newton solver was tested on 13 real cases obtained from a multibody simulator. These problems ranged in sizes from 3 to 250 variables and were generated from simulations of simple joints with motors and limits, stacks of boxes and rag-dolls. Ten of the 13 cases reached absolute convergence, two presented stagnation, and for one case the back-tracking failed. All the converged cases reached termination before the 5th iteration. We think that the reason for this bad behavior is because over-determination of contact forces which is reflected in the large null-space of the matrix A .

The Convergence column in Table 1 indicates the number of cases in which absolute convergence was attained. Stagnation indicates the maximum component-wise difference between the current and previous iterate was below a

TABLE 1. Test results of using projected Gauss-Seidel to warm-start non-smooth Newton method on both synthetic data and real multibody dynamics problems.

Size	Convergence	Stagnated	Back-tracking failed
12	100	0	0
24	100	0	0
48	98	0	2
96	95	0	5
192	82	0	18
384	70	0	30

TABLE 2. Timing and iteration results of using projected Gauss-Seidel to warm-start non-smooth Newton method on both synthetic data and real multibody dynamics problems. Recall that the first 4 iterations are those of the projected Gauss-Seidel method.

Size	Min (secs)	Avg (secs)	Max (secs)	Min (#)	Avg (#)	Max (#)
12	0.000006	0.000112	0.000389	0	5.14	9
24	0.000104	0.000286	0.000950	5	6.19	12
48	0.000227	0.000793	0.002232	5	7.26	12
96	0.000955	0.003472	0.010998	6	9.99	20
192	0.004041	0.014365	0.039365	7	12.72	24
384	0.016313	0.077198	0.248553	6	16.37	30

specified threshold (set to 10^{-5}). Notice that the number of cases in which we observe convergence decreases and the back-tracking failures increase as the number of variables increase. For us this is surprising since we expected global convergence from a back-tracking approach. We should mention that trust-region methods are another alternative to the back-tracking method we have not tried.

In this paper we presented a reformulation of the non-linear complementarity problem for multibody dynamics. We have developed a non-smooth Newton method to solve the resulting reformulation. Warm-starting with a solution from a projected Gauss-Seidel method worked very well. Knowing how to solve the Newton equation, it may also be interesting to develop a trust region Newton method instead of using a line-search method.

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