NONRECURSIVE FORMULATIONS OF MULTIBODY DYNAMICS AND CONCURRENT MULTIPROCESSING

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ABSTRACT

Since the late 1980's, research in recursive formulations of multibody dynamics has flourished. Historically, much of this research can be traced to applications of low dimensionality in mechanism and vehicle dynamics. Indeed, there is little doubt that recursive order N methods are the method of choice for this class of systems. This approach has the advantage that a minimal number of coordinates are utilized, parallelism can be induced for certain system topologies, and the method is of order N computational cost for systems of N rigid bodies.

Despite the fact that many authors have dismissed redundant coordinate formulations as being of order N^3, and hence less attractive than recursive formulations, we present recent research that demonstrates that at least three distinct classes of redundant, nonrecursive multibody formulations consistently achieve order N computational cost for systems of rigid and/or flexible bodies. These formulations are the

(i) preconditioned range space formulation,
(ii) penalty methods, and
(iii) augmented Lagrangian methods

for nonlinear multibody dynamics. The first method can be traced to its foundation in equality constrained quadratic optimization, while the last two methods have been studied extensively in the context of coercive variational boundary value problems in computational mechanics. Until recently, however, they have not be investigated in the contrext of multibody simulation, and present theoretical questions unique to nonlinear dynamics. All of these nonrecursive methods have additional advantages with respect to recursive order N methods: (1) The formalisms retain the highly desirable order N computational cost, (2) the techniques are amenable to concurrent simulation strategies, (3) the approaches do not depend upon system topology to induce concurrency, (4) and the methods can be derived to balance the computational load automatically on concurrent multiprocessors. In addition to the presentation of the fundamental formulations, this paper presents new theoretical results regarding the rate of convergence of order N constraint stabilization schemes associated with the newly introduced class of methods.

Introduction

It is well known that the nonlinear equations governing the motion of complex multibody systems give rise to differential-algebraic equations that present unique and interesting problems in their solution [Gear, Petzold]. The mathematical study of differential-algebraic equationsis justifiably a field of research unto itself. However, in multibody applications, it appears that most researchers prefer to eliminate the troublesome multipliers, and deal exclusively with the problems associated with the solution of sets of ordinary differential equations. The point in the analysis at which the multipliers are eliminated has become one criteria for distinguishing among the various formulations. During the last 1970's and early 1980's, numerous publications appeared in which the constraint multipliers are eliminated at computation time by numerically constructing a basis for the instantaneous nullspace of the constraint Jacobian. Some representative work from this class includes [Singh, Wampler, Wehage, Amirouche,...], and are referred to as the nullspace methods. These algorithms have been so named due to their similarity to the nullspace methods in quadratic, equality constrained optimizations [Gill]. Despite their elegance, numerical calculation of the nullspace basis and its use to eliminate the multipliers leads to a dense system coefficient matrix. This matrix is of order (N-M) X (N-M) where N is the number of redundant coordinates and M is the number of constraints. Consequently, the nullspace methods are of $O(N-M)^3$ at each time step.

As opposed to techniques that eliminate the multipliers numerically at computation time, a number of authors have derived elegant techniques for eliminating the constraints a priori; that is during the derivation of the equations. The works [Rodriguez, June 1987; Rodriguez, 1987] are representative of this class. These methods have a number of distinct and well-known advantages over the cubic order nullspace methods:

(i) They employ a minimal coordinate set.
(ii) They attain an O(N) computational cost for systems of rigid bodies.
(iii) They can be employed in concurrent architectures for classes of problems.

These methods have come to be known as the order N or recursive methods of formulating multibody dynamics.

Despite their numerous advantages, there are several aspects of the recursive order N methods that can cause difficulties for classes of problems. Foremost among these problems is that concurrency in the recursive methods is induced, at present, by assigning topologically independent branches of the structure to computationally independent processors. One need only consider the problem of modelling a tethered satellite system to realize that not all structures exhibit such structural parallelism. Furthermore, most systems exhibit low levels of inherent structural parallelism appropriate for the concurrent implementation of recursive order N methods as in [Bae]. Typical space structures such as the space station or the CSI Evolutionary model at NASA Langley have only on the order of 6-12 "independent branches." Gross underutilization of moderately parallel architectures, with 16 to 128 processors, can result when mapping the recursive algorithm onto such a computer. Finally, computational load balancing of the problem among processors in most implementation is carried out by hand, which can be a tedious and time consuming task.

Nonrecursive Formulations

This paper surveys the results of several recent approaches presented in [Kurdila 1,2,3] and described in detail in the dissertation by [Menon]. Collectively, the authors refer to these methods as nonrecursive formulations of multibody dynamics. In point of fact, the nonrecursive formulations described in this paper represent a synthesis of a family of formulations and constraint stabilization procedures that are closely related. These methods can be employed simultaneously, independently, or in combination selected by an analyst to meet accuracy and computational speed requirements in a highly predictable manner. This class includes

(i) The PCG/Range Space Method : As with the nullspace method, this approach can be traced historically to equality constrained quadratic optimization [Gill]. Analysis of the application of the approach to multibody simulation has been carried out recently in [Kurdila] and [Menon] using an iterative technique, and earlier noniterative versions appear in [Placek] and [Wittenburg]. The primary advantage of the range space method is that is is the most numerically efficient of the three methods presented in this paper.

(ii) The Penalty Method : Of course, the penalty method has been studied in detail in application to optimization [Luenberger] and coercive variational boundary value problems [Oden]. Still, it has only recently been studied in detail in the context of nonlinear multibody simulation [Bayo, Park, Kurdila]. An advantage of this approach is that explicit bounds on the constraint violation can be achieved in terms of the penalty parameter, even in the nonlinear case. [Kurdila] One disadvantage of the method that has been noted in the literature [Kurdila] , [Bayo] is that prohibitively large values of the penalty parameter are required to achieve the analytical guarantees of accuracy, but result in numerical ill-conditioning.

(iii) The Augmented Lagrangian Method : As in the case of the penalty method, the augmented Lagrangian formulations have been studied extensively for use in the solution of variational boundary value problems [Glowinski]. Again, as in the case of the penalty method, this approach has only recently been studied within the field of nonlinear multibody dynamics [Bayo]. Empirical evidence in [Bayo1,2] suggests that the method is superior to the penalty method from a computational viewpoint in that required accuracy can be achieved without large penalty parameters. The analytical study of Augmented Lagrangian formulations of nonlinear multibody dynamics remains an open and interesting field of research.

To derive the equations employed in this paper, one must first consider the exact governing system of differential-algebraic equations

$$M(q)\ddot{q} = f(q, \dot{q}, t) + C^T\lambda$$
$$\Phi(q, t) = 0 \qquad (1)$$

and differentiated form of the constraints

$$\left[\frac{\partial \Phi}{\partial q}\right]\dot{q} + \Phi_t = 0 \tag{2}$$

$$C(q, t) \equiv \left[\frac{\partial \Phi}{\partial q}\right] \tag{3}$$

In these equations, q are the generalized coordinates selected for the problem at hand, and $\Phi(q)$ are the functional relations defining the holonomic constraints acting on the system.While the interested reader is referred to [Menon] for the details of their derivation, the equations governing the simulation of multibody systems considered in this paper can be written

$$\lambda_0 = 0 \tag{4}$$

or

$$(CM^{-1}C^T)\lambda_0 = -CM^{-1}f - \dot{C}\dot{q} - \dot{\Phi}_t \tag{5}$$

$$M(q)\ddot{q}_n = f(q, \dot{q}, t) - C^T\frac{1}{\varepsilon}(\ddot{\Phi}_n + 2\xi\omega\dot{\Phi} + \omega^2\Phi) - C^T\lambda_n \tag{6}$$

$$\lambda_{n+1} = \lambda_n + \frac{1}{\varepsilon}(\ddot{\Phi}_n + 2\xi\omega\dot{\Phi} + \omega^2\Phi) \tag{7}$$

The terms λ are unknown Lagrange multipliers, λ_{n+1} are iterative corrections the the multipliers, and $\ddot{\Phi}_n$ are iterative values of the constraint equations. The relationship of the above system to the aforementioned range space, penalty and Augmented Lagrangian formulations can be summarized as follows:

(i) By employing equation (5) to initiate the integration procedure and letting

$$\frac{1}{\varepsilon} = 0 \tag{8}$$

the above equations reduce to the range space equations, and provide the most computationally efficient version of the above set of equations when a judiciously selected preconditioned conjugate gradient method is employed.

(ii) By employing only equation (6), and by setting

$$\lambda_n \equiv \lambda_{n+1} \equiv 0 \tag{9}$$

the equations above reduce to the inertial penalty method introduced in [Bayo] and studied in further detail in [Kurdila]. This form of the governing equations provides some guarantees on accuracy, but is more expensive computationally.

(iii) By using equation (4) for the initialization procedure, and choosing equations (6) and (7) iteratively, these equations reduce to the augmented Lagrangian approach introduce in [Bayo] and studied further in [Kurdila] and [Menon]. While this version of the governing equations are the most computationally expensive, they also provide the most control over the accuracy attained in the simulation.

At this point it should be noted that both the penalty and augmented Lagrangian methods can be viewed as stabilizaton procedures for the range space method. In the following discussion, the range space formulation will be referred to as the "baseline method". In fact, it will be demonstrated later that this is a useful interpretation and leads to hybrid simulation methods that combine the computational efficiency of the range space method and the accuracty of the penalty or augmented Lagrangian methods.

In the following sections it will be emphasized that the simulation of transient response of multibody systems using various versions of the nonrecursive formulation above has many advantages:

(i) The method achieves an order N computational cost while employing a redundant formulation.

(ii) Consequently, the often complicated relative reference frame kinematics of the recursive methods can be avoided.

(iii) The method is amenable to concurrent implementation on a wide variety of forthcoming parallel architectures.

(iv) The technique is essentially automatically, computationally load balancing

(v) The approach does not depend upon system topology to induce parallelism, and does not result in gross underutilization of available processors.

Order N Computational Cost of the Baseline Algorithm

The order N computational cost of the baseline algorithm when the governing equations are selected to be simplified versions of equations (5) and (6)

$$\begin{aligned} (CM^{-1}C^T)\lambda &= -CM^{-1}f - \dot{C}\dot{q} - \dot{\Phi}_t \\ M(q)\ddot{q} &= f(q,\dot{q},t) - C^T\lambda \end{aligned} \tag{10}$$

, otherwise denoted as the preconditioned range space formulation in [Kurdila] and [Menon], is well documented. While the details of the convergence properties of the algorithm exceed the scope of this paper the reader is referred to [Menon] for a complete discussion. In summary, the computational performance of the algorithm can be attributed to

(i) the derivation of a rapidly convergent block Jacobi preconditioner based on the directed connectivity graph of the multibody system,

(ii) the exploitation of the block-diagonal structure of the system coefficient matrices in the formulation, and

(iii) the parallel implementation of the algorithm based upon subdomain decomposition techniques that are only weakly coupled to the system topology.

Results extracted from [Kurdila] and [Menon] in figures (1) through (4) illustrate results typical of the preconditioned conjugate gradient / range space formulation.

Accuracy and Order N Performance with Constraint Stabilization

The motivation for deriving additional variants of the preconditioned conjugate gradient / range space formulation arises from the well-known need for stabilization in redundant formulations as well as the documented conditioning problems that can occur in the range space method of optimization [Gill]. Essentially, the accuracy of the simulation relies on the condition number of the constraint metric

$$CM^{-1}C^T \tag{11}$$

appearing in equation (5) and (10). As noted in [Gill], this condition number is bounded above by

$$\kappa(CM^{-1}C^T) \leq \kappa^2(C)\,\kappa(M) \tag{12}$$

and may become large when the constraints become nearly redundant. However, inasmuch as great efforts have been made to ensure the order N computational cost of the baseline formulation, it has been a central goal in this work to derive stabilization methods that retain the order N com-

Figure (1) : Order N Timing Results for Z- Truss Prototype Model

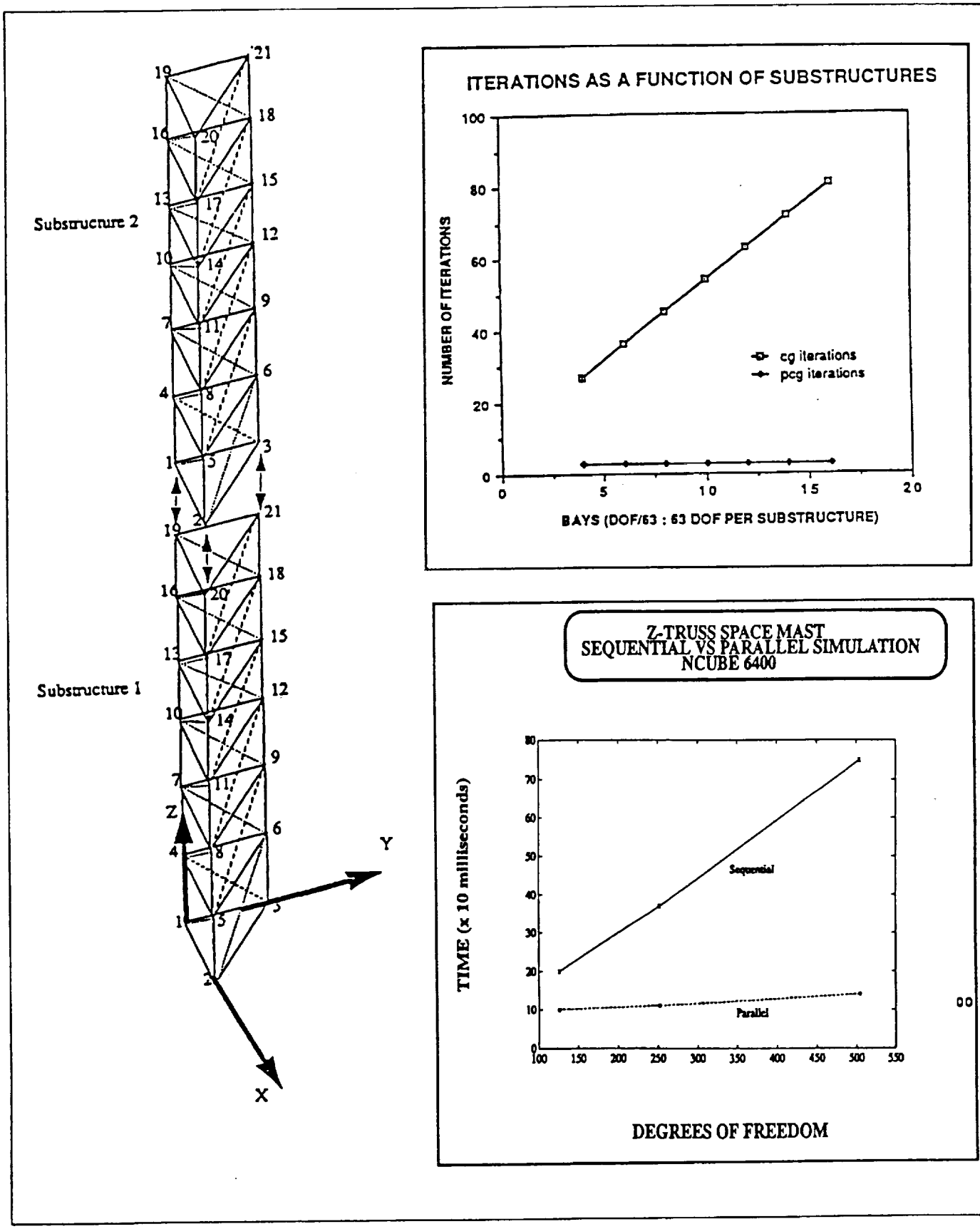
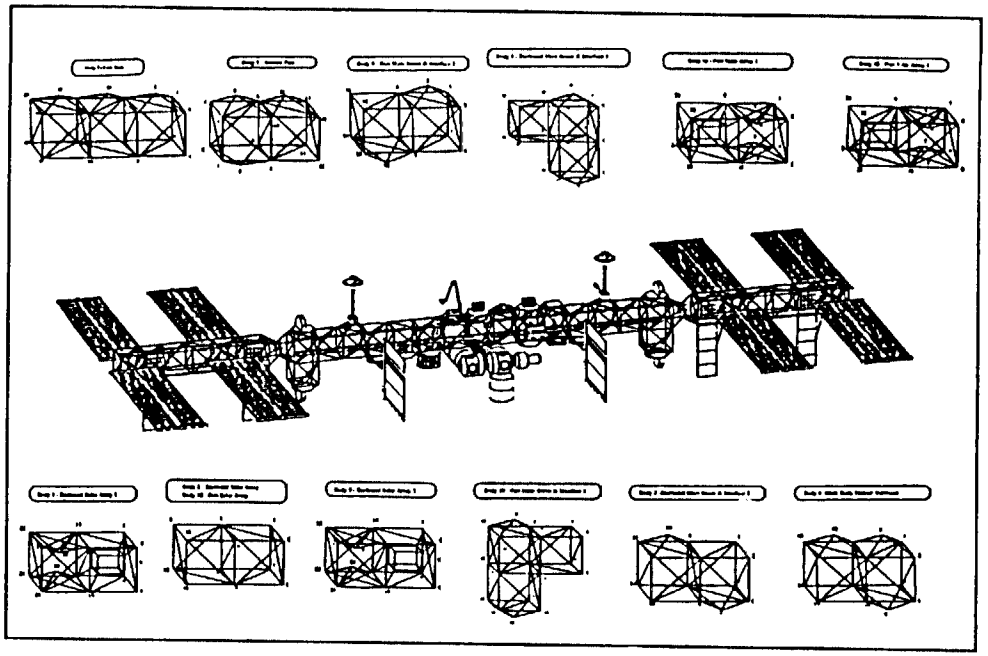


Figure (2) : Order N Timing Results for Space Station Prototype Model



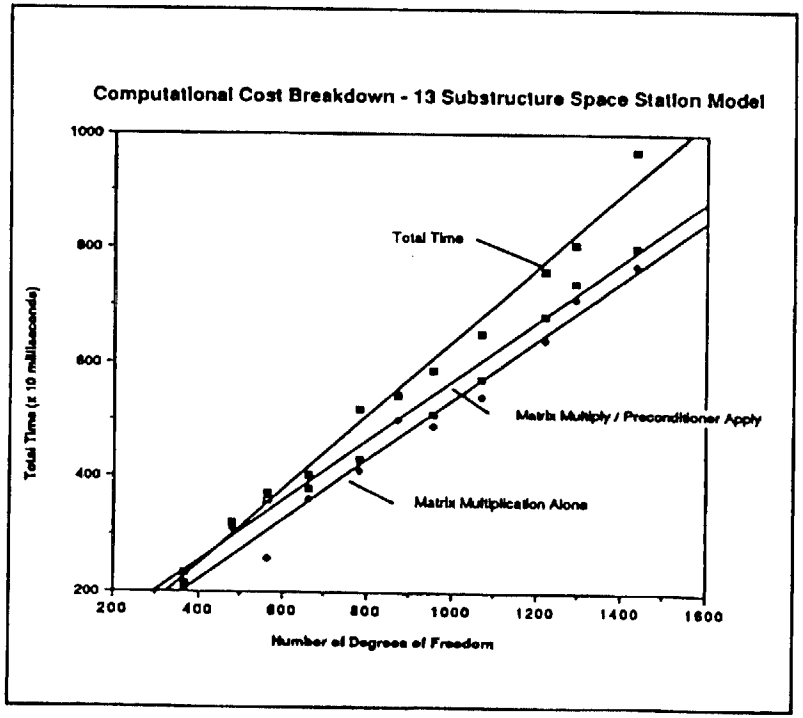
1434 DEGREES OF FREEDOM

300 CONSTRAINTS

72 TO 150 DOF/SUBSTRUCTURE

ORDER N PERFORMANCE

ENERGY RATE MATCHING INTEGRATION



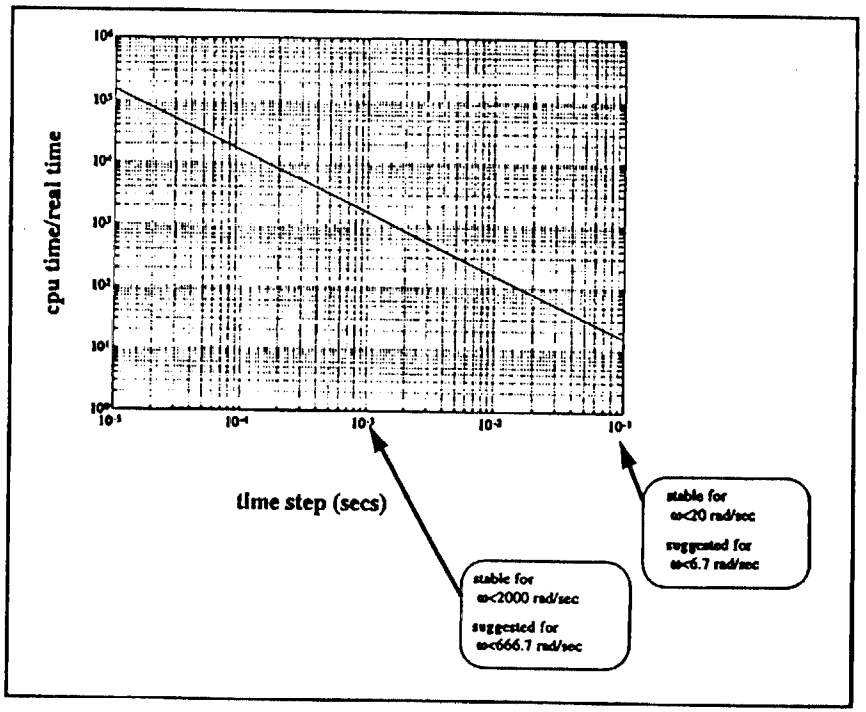


Figure (3) : Order N Timing Results for CSI Evolutionary

13 SUBSTRUCTURES

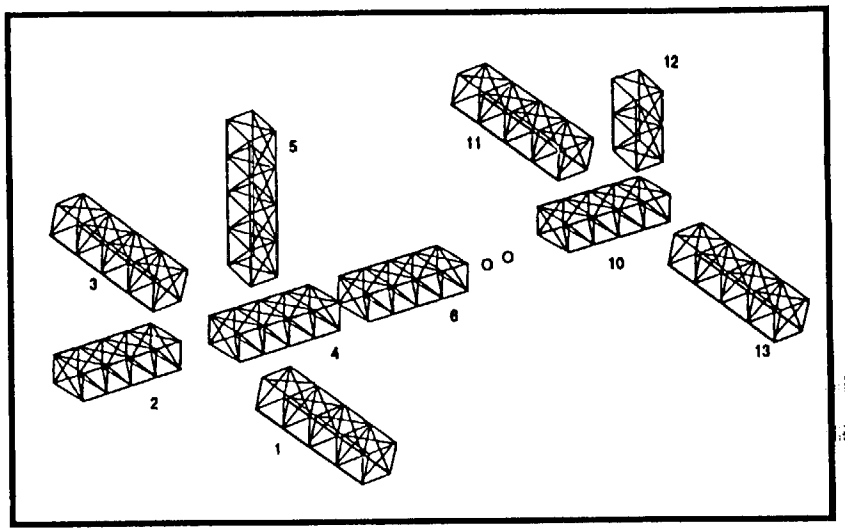
1656 DEGREES OF FREEDOM

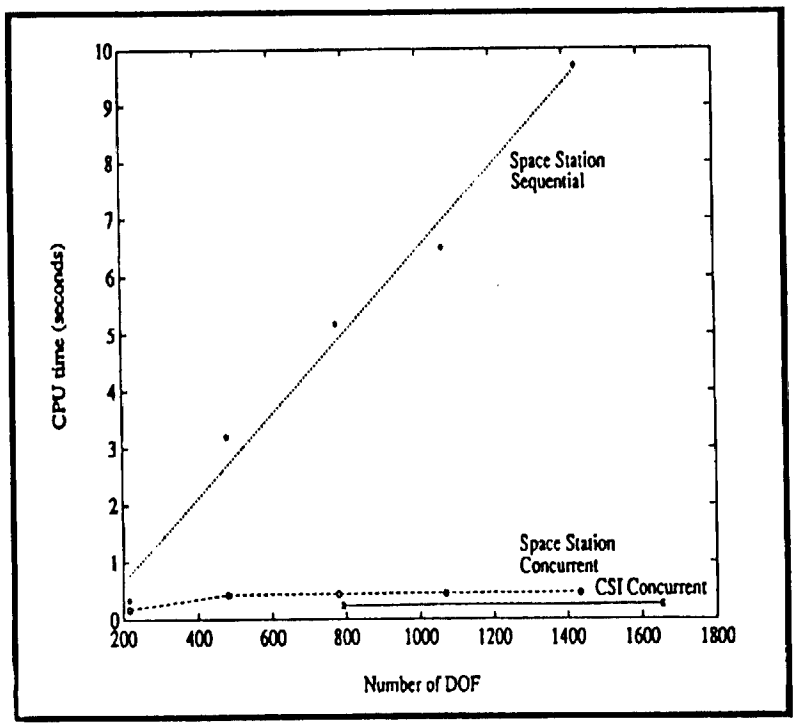
144 CONSTRAINTS

72 TO 132 DOF/SUBSTRUCTURE

ORDER N PERFORMANCE

ENERGY RATE MATCHING INTEGRATION





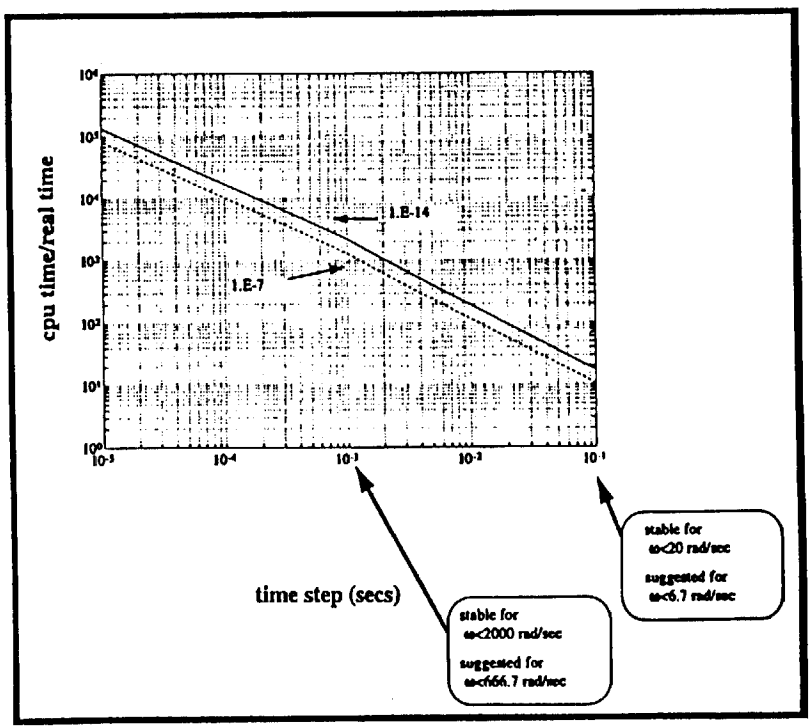


Figure (4) : Order N Timing Results for Nonlinear Tracking Prototype Model

NONRECURSIVE FORMULATION

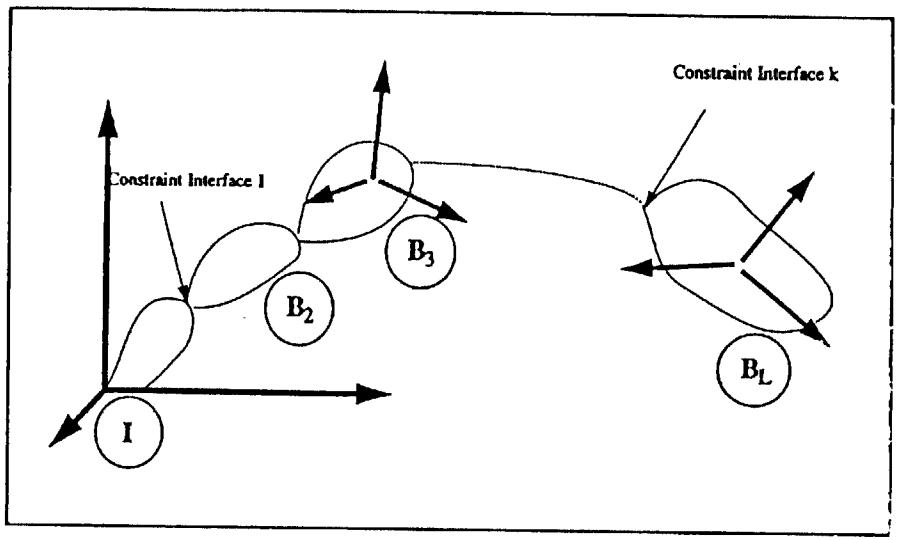
SYMBOLIC CONTRAINT JACOBIAN

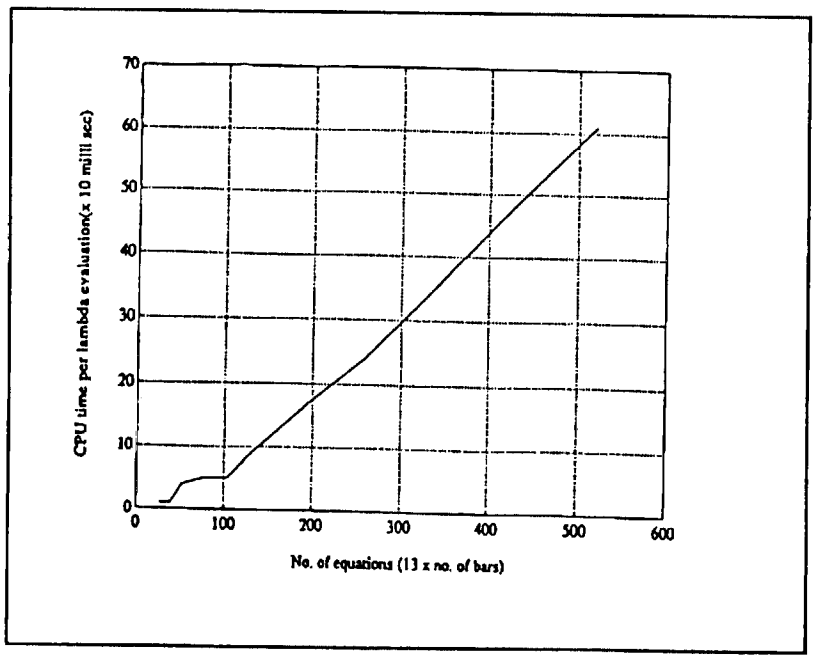
ORDER N PERFORMANCE

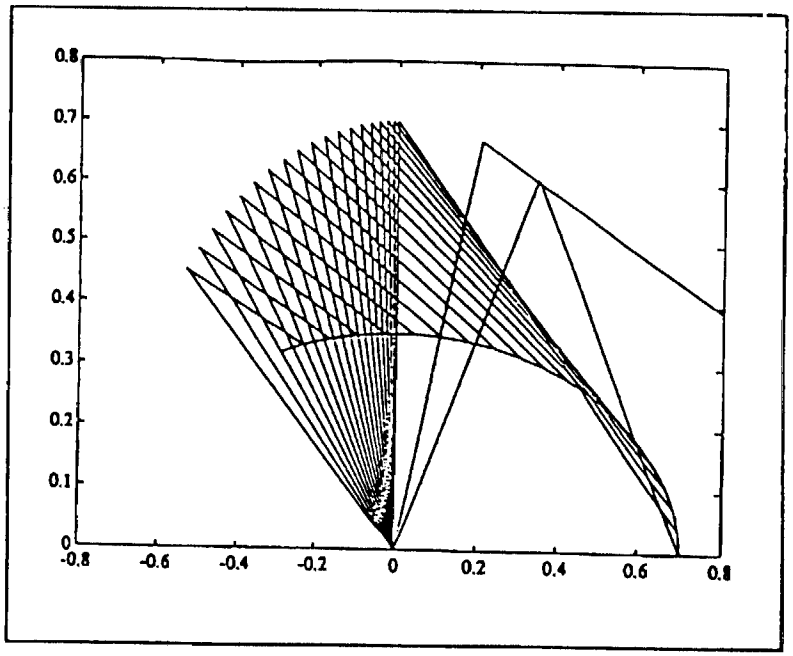
1 TO 40 RIGID BODIES

520 DEGREES OF FREEDOM

HAMILTONIAN TRACKING LAW







putational cost.

This goal has in fact been achieved and is depicted in figures (5) and (6). In figure (5), the timing results for a benchmark linear structural problem as a function of the number of degrees of freedom is depicted. Two critical observations should be made upon inspection of this graph

(i) All variants of the class of nonrecursive algorithms under investigation exhibit an order N compuational cost.

(ii) The baseline preconditioned conjugate gradient / range space algorithm is the most efficient simulation.

(iii) The computational cost of the nonrecursive methods with stabilization increases with the number of iterative corrections per time step. Hence, the penalty stabilization is more expensive thant the preconditioned conjugate gradient / ranges space method. But, the augmented Lagrangian formulation is more computationally expensive than the penalty method. In fact, the slope of the performance curve simply rotates counterclockwise as the number of fixed iterations per time step increases.

In view of the measures of accuracy depicted in figures (7) and (8), it is not surprising that the iterative corrections of the augmented Lagrangian are more costly. It is precisely the addition of the stabilization methods that yields the desired improvement in accuracy. As shown in [Kurdila], for certain classes of multibody systems the constraint violation can be bounded by

$$\left\| \dot{\Phi}_{\varepsilon} \right\|^2 + \left\| \Phi_{\varepsilon} \right\|^2 \leq \frac{2E(0)}{min\left(\sigma^2_{min}(\alpha), \sigma^2_{min}(\beta)\right)}$$

As noted earlier, a major criticism of achieving stringent tolerances using this bound is that large penalty factors must be used in the simulation which can lead to poor conditioning in practice. This result has been extended rigorously to the augmented Lagrangian stabilization methods in [Bustimante] and [Menon] in the form of the equation

$$\left| \ddot{\Phi} + 2\xi\omega\dot{\Phi} + \omega^2\Phi \right|_{i+1} \leq \frac{\varepsilon}{\upsilon} \left| \ddot{\Phi} + 2\xi\omega\dot{\Phi} + \omega^2\Phi \right|_i$$

and is depicted graphically in figure (7). Furthermore, empirical results suggest the stronger result that

$$\left| \dot{\Phi}(t)^2 + \omega^2\Phi(t)^2 \right|_{i+k} \leq \left(\frac{\varepsilon}{\upsilon}\right)^{2k} \left| \dot{\Phi}(t)^2 + \omega^2\Phi(t)^2 \right|_i$$

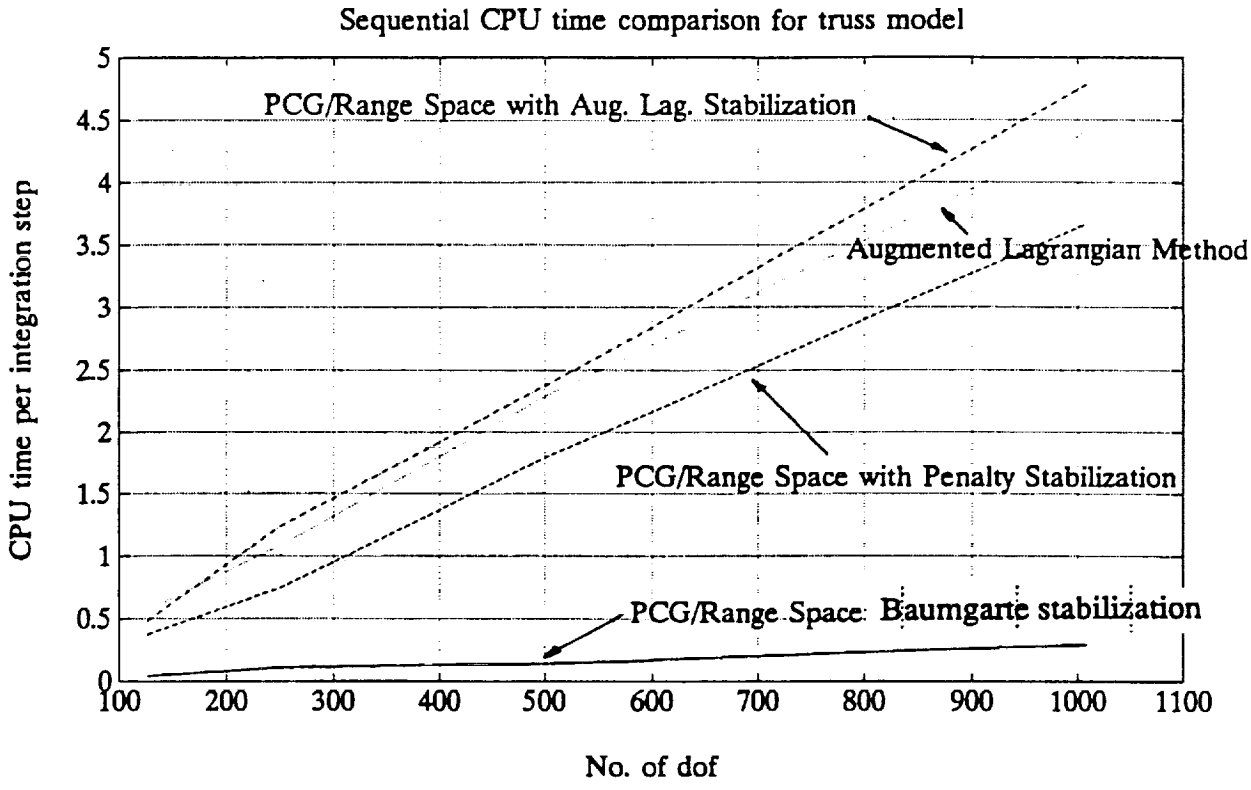
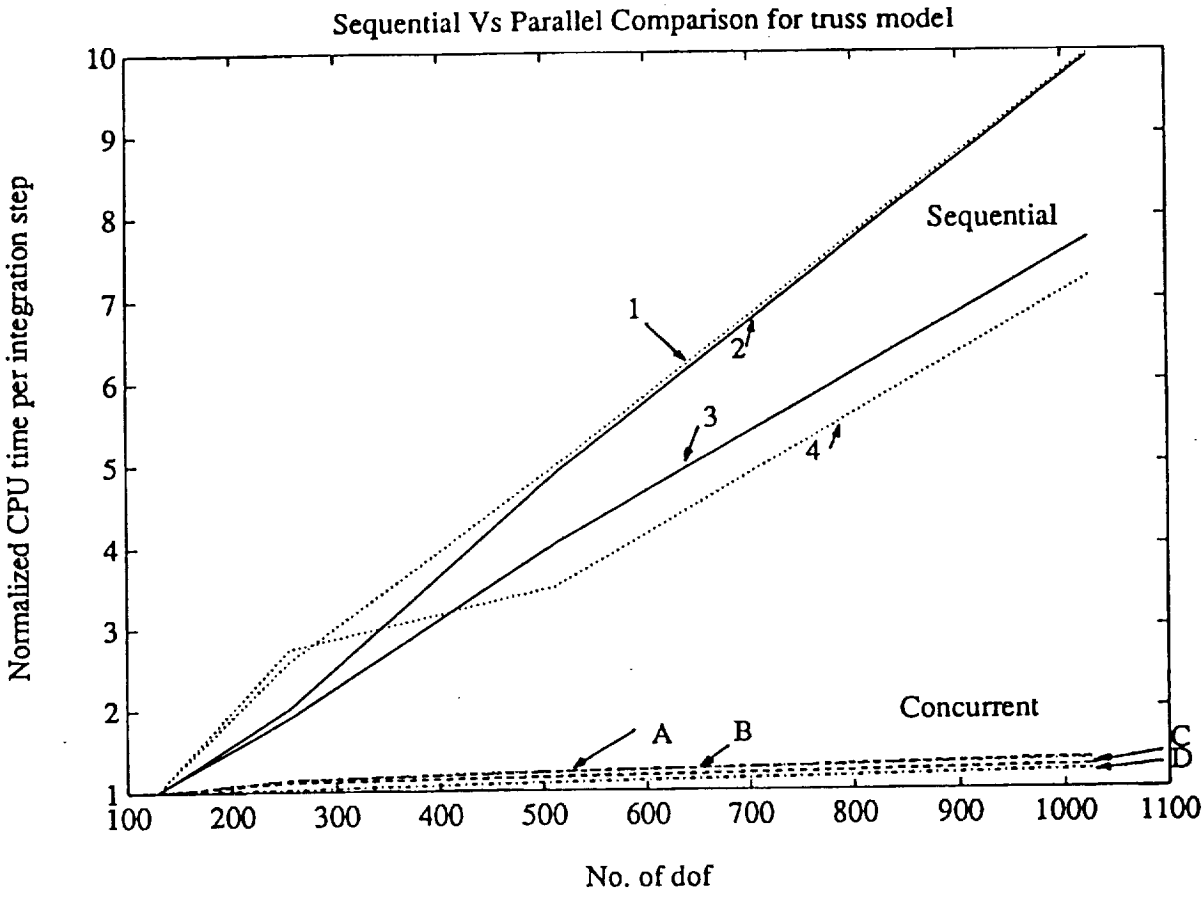


Figure (5) : Order N Computational Cost for Nonrecursive Formulation Class



LEGEND: PCG with Augmented Lagrangian, 1 and A
Augmented Lagrangian Solution, 2 and B
PCG with Penalty, 3 and C
PCG with Baumgarte's, 4 and D

Figure (6) : Normalized Order N Computational Cost for Nonrecursive Formulation Class

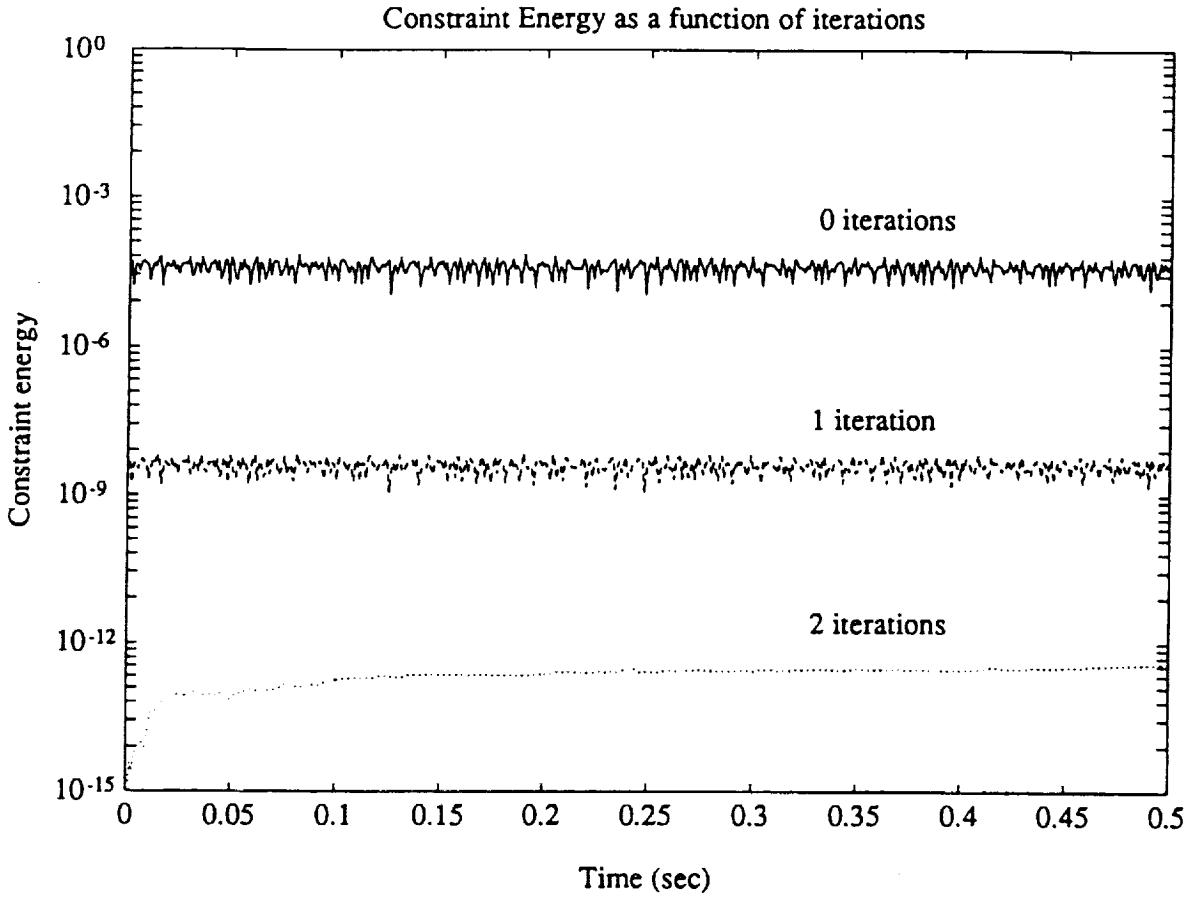


Figure (7) : Constraint Violation and Correction Steps

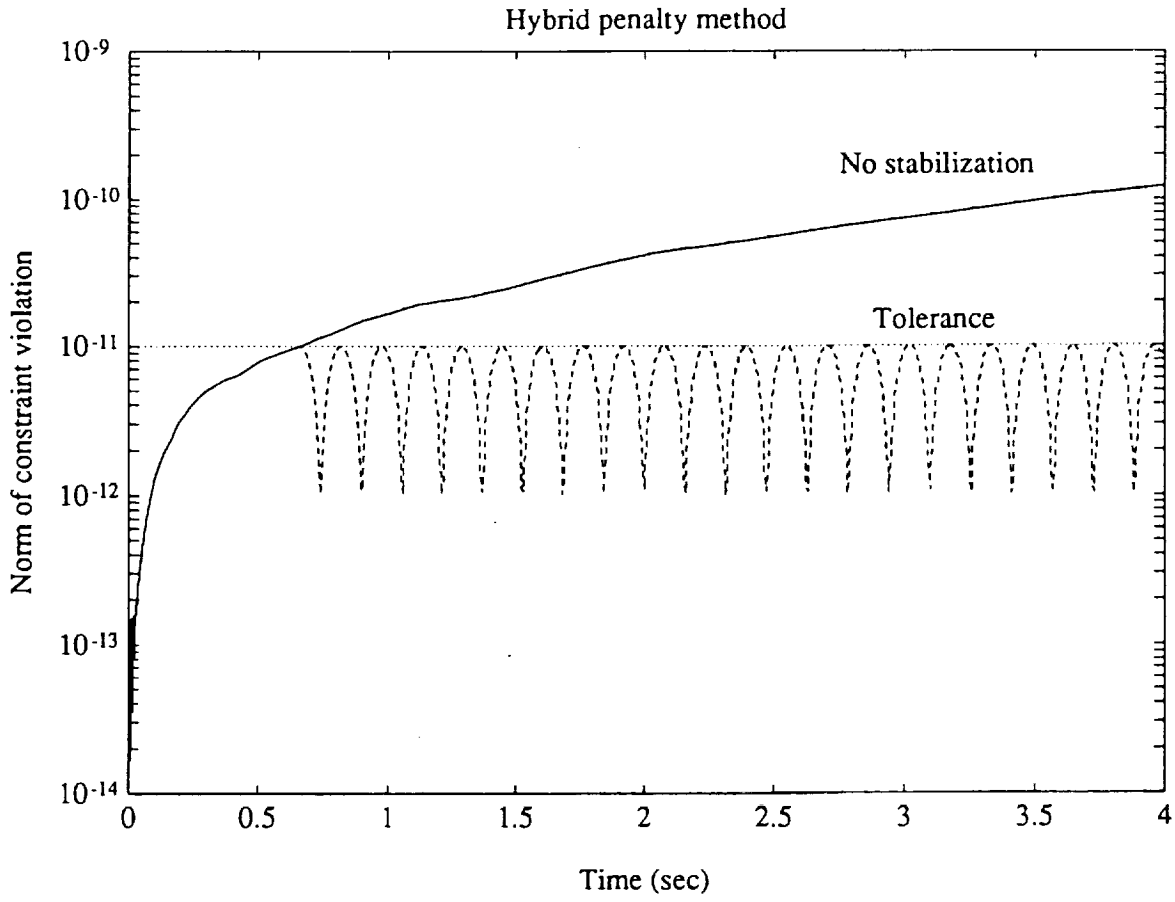


Figure (8) : Hybrid Range Space Simulation and Augmented Lagrangian Stabilization

Simply put, the "energy of constraint violation shrinks by a factor of e for each iteration" employed in the augmented Lagrangian formulation.

Thus, figures (5) and (7), illustrate the fundamental tradeoff between execution time and accuracy. Another natural consequence of this tradeoff is the design of hybrid methods such as depicted in figure (8). In these methods, the preconditioned conjugate gradient / range space method is empolyed until a specific pre-selected tolerance is met, at which point the augmented Lagrangian method is employed until another more stringent tolerance is reached. In this fashion, the computational efficiency of the range space method is retained as long as possible, at which point the iterative augmented Lagrangian method is used to guarantee the desired accuracy.

Conclusions

This paper has presented a class of nonrecursive formulations of multibody dynamics, all of which exhibit an order N computational cost. The methods are complementary to the existing class of recursive order N methods in that they seem most appropriate for large dimensional models without inherent structural parallelism. Figures (9) and (10) graphically summarize the contribution of this paper. Figure (9) shows that as of 1988 only one order N method had been derived. Figure (10) depicts the state of affairs currently, and shows that at least three distinct approaches can achieve order N computational cost, as well as numerous combinations of these algorithms.

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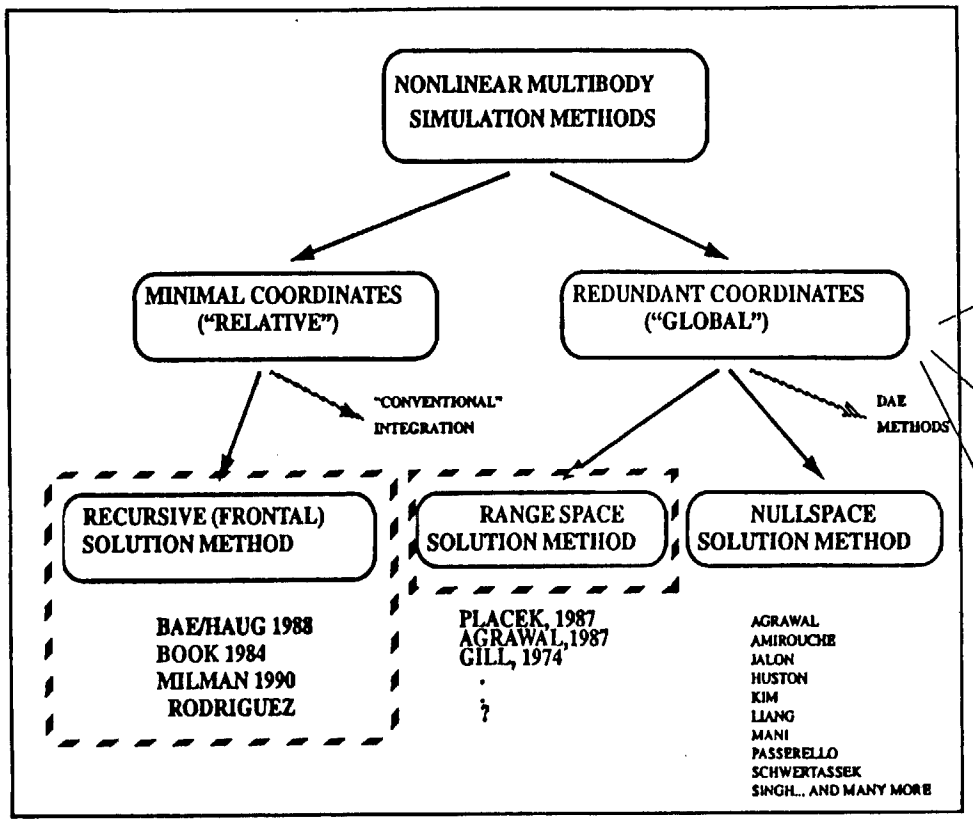

Figure (9) : Order N Methods, <=1988

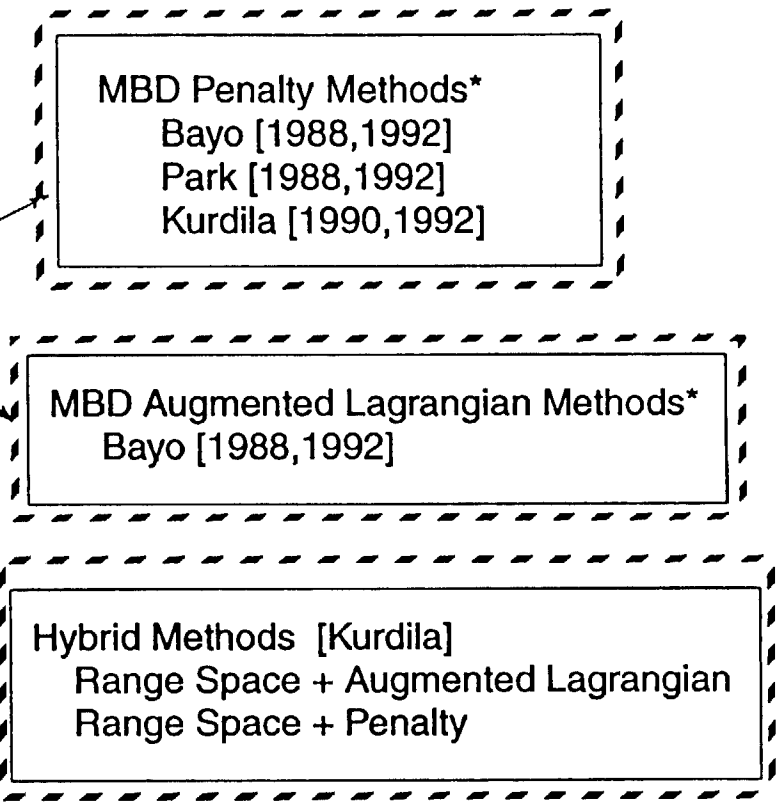

Figure (10) : Order N Methods, <= 1992

* DENOTES THE FACT THAT PENALTY AND AUGMENTED LAGRANGIAN METHODS HAVE A LONG HISTORY IN OPTIMIZATION, COMPUTATIONAL MECHANICS...

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