

Interdisciplinary Approach to Numerical Methods for Structural Dynamics

¹Rabindranath Andújar, Jaume Roset and ²Vojko Kilar

¹Universitat Politècnica de Catalunya, Department of Applied Physics,
Jordi Girona, 1-3. 08034 Barcelona, Spain

²University of Ljubljana, Faculty of Architecture, Zoisova 12, SI-1000 Ljubljana, Slovenia

Abstract: Structural dynamics is a rather complex field of research that concerns to a broad range of disciplines, from structural engineering to graphics animation, robotics or aeronautics. A primary consequence of this is an overwhelming amount of literature on the topic, apparently disconnected, as each author focuses on his / her particular field. To complicate things further, the daunting list of numerical methods severely blurs the scope of the researcher, making it very difficult to understand what their purpose is in each case and even if these are applicable to the analysis of structural behavior. This paper presents a reference framework where researchers and developers from diverse disciplines can assess the main methods currently used in structural dynamics simulation. A direct correlation is made between methods to solve Ordinary, Partial and Algebraic Differential Equations and their physical counterparts Time, Matter and Constraints. It is also discussed their application in different industries.

Key words: Multi Body Dynamics • Structural Dynamics • Finite Element Method • Time Integration • Matter Integration • Constraint Integration

INTRODUCTION

Previous surveys exist where a rigorous mathematical background is provided. However, they present a certain excess of specialization towards their natural disciplines, so for example [1, 2] have a marked bias towards Robotics while [3, 4] are excellent reviews for the Computer Graphics community and [4, 5] belong to the structural engineering expertise. The present paper aims to facilitate a holistic and more unified view on the subject of structural dynamics and the numerical methods employed to simulate them. For the sake of simplicity formulations have been considered unnecessary and only practical matters are discussed.

The analysis of structural dynamic behavior is a topic of specialized research in many modern disciplines: Civil Engineering, Aeronautics, Automotive, Robotics, Medicine, Biomechanics, Molecular Dynamics and Graphics Animation are some of the industries currently developing applications that allow for the simulation of the dynamics of structures and related literature about it. From a scientific point of view, it must be regarded as a great success and should be considered as positive that

so many multidisciplinary points of view focus on this matter. However, it means also that the intrinsic complexity of the subject increases somehow chaotically as each author contributes with his particular approach. Furthermore, the already daunting list of numerical methods for the solution of dynamics problems grows by means of mixed concepts making it very difficult to understand what they really do. It is common to encounter in the literature how methods for the approximation of standard algebraic problems present “physical” properties or that some method to solve partial differential equations is enunciated as “explicit” referring to the ordinary differential equations also involved in the solution.

The following chapter presents a general reference framework where researchers and developers from diverse disciplines can assess, according to its performance, the main methods currently used for structural simulation. It is divided into three concepts: time, matter and constraints, as they respectively correspond to very well defined mathematical areas: Ordinary Differential Equations (ODEs), Partial Differential Equations (PDEs) and Differential-Algebraic Equations (DAEs).

Corresponding Author: Assoc. Prof. Dr. Vojko Kilar, University of Ljubljana, Faculty of Architecture,
Zoisova 12 1000 Ljubljana, Slovenia. Tel: +386 12 000 720 (office),
Fax: +386 14 257 414.

The last part discusses these methods as they are utilized in the main industrial environments, and provides some explanatory approach as to how and why they have evolved in that particular manner.

MATERIAL AND METHODS

For the simulation of structural dynamics three different physical concepts need to be integrated: time, matter and kinematic constraints. Each one of these notions involves the simultaneous solution of Ordinary Differential Equations (ODEs), Partial Differential Equations (PDEs) and Differential-Algebraic Equations (DAEs), respectively.

When performing numerical simulations the main concerns are the accuracy of the solution, the stability of the simulation and the efficiency of the calculation. The first subject arises from the fact that computational precision is finite whereas the physical/mathematical models are continuous, hence only approximations to the behavior can be obtained. By stable is meant that small errors due to either arithmetic inaccuracies or to the approximate nature of the derivative expressions will not accumulate and grow as one proceeds. Efficiency involves the speed of computation and the occupied memory, which are also very sensitive to the design of the algorithms. There is a fourth item to take into consideration of almost equivalent importance which is the ease of implementation of the algorithms that lead to the numerical results. High algorithmic complexity leads to difficulties not only in tracking the possible errors but also in the human comprehension of the simulated phenomenon.

Numerical Methods for Ordinary Differential Equations (Time Integration): The most comprehensive classification for ODEs solvers distinguishes between explicit, implicit and hybrid methods. This division arises as a consequence of the so called numerical stiffness. This phenomenon forces the size of the adopted time step to be so small that the time to convergence never arrives, or otherwise adopt time steps so large that the simulation becomes unstable. Stiffness can be produced by the physical characteristics of the multi-body system (components with large differences in their masses, stiffness and/or damping), the discretization process, the large number of components and equations of motion, or sudden or accumulated violations in the constraint conditions.

Another classification is possible according to the order of the derivative employed in the equation of motion. By this means a method is characterized as first, second, third or higher orders accordingly. The higher the order the more accurate the result would be, though it limits the span of possible time steps due to instabilities. The third possibility is that of the method being Single or Multi-Step. Single-step methods refer to only one previous calculated value and its derivative to determine the current value. Multi-step methods attempt to gain efficiency by keeping and using the information from previous steps rather than discarding it. Consequently, multi-step methods refer to several previous points and derivative values. In the case of linear multi-step methods, a linear combination of the previous points and derivative values is used.

Explicit Methods: Explicit methods use the differential equation at time t to predict a solution at time $t+dt$. In structural dynamics, where stiff equations often arise, the required time step is very small to avoid instabilities. Explicit methods are hence conditionally stable with respect to the time step size.

Forward/Explicit Euler Method (EE): This method works considering that from any point on a curve, it is possible to find an approximation of a nearby point on the curve by moving a short distance along a line tangent to the curve [7].

Explicit Runge-Kutta Methods (ERKn): The original formulation is that of a single step solver. In general this is adequate for non stiff problems and provides an acceptable level of accuracy. Lower order formulations provide lower accuracy, being the 4th order the most commonly utilized [8].

Explicit Euler's method (EE) can be also considered a 1st order Runge-Kutta. Dormand-Prince method (RKDP), Fehlberg method (RKF) and Cash-Karp method (RKCK) are variations on this method, implying higher orders and also interpolation within the integration to make them more efficient.

Explicit Runge-Kutta Methods (ERKn): ABM methodology employs multiple previously recorded steps to achieve a solution, hence being more efficient. Initial values need to be provided and are usually obtained from a Runge-Kutta scheme. It also presents an acceptable level of accuracy depending on the chosen step size and

is meant to solve non stiff systems. Shampine-Gordon method (SG) is based on this methodology, using interpolation to resolve efficiency problems [9].

Leapfrog/Velocity Verlet Method (LF): Leapfrog integration is equivalent to calculating positions and velocities at interleaved time points, interleaved in such a way that they 'leapfrog' over each other. For example, the position is known at integer time steps and the velocity is known at integer plus half time steps [9].

Implicit Methods: For implicit methods the strategy consists on satisfying the differential equation at time t once the solution at time $t-dt$ is available. This requires the solution of a set of linear equations at each time step, but allows for larger time steps and gives further stability or even unconditionally stable schemes [10].

Backward/Implicit Euler Method (IE): Backward Euler chooses the step, k , so that the derivative at the new time and position is consistent with k . Doing this requires solving this equation for k , which amounts to a root finding problem if $f(x)$ is nonlinear. The forward Euler step is a common place to start the root finding iteration [7].

Implicit Runge-Kutta methods (IRKn): Implicit Runge-Kutta methods are usually more stable than any explicit method of the same family. The simplest example of an implicit Runge-Kutta method is the backward Euler method enumerated above.

Crank-Nicholson method (CN), also known as the trapezoid method is another example of implicit Runge-Kutta methods [11].

Gear's/Backward Differentiation Formula Method (BDF): BDFs are formulas that give an approximation to a derivative of a variable in terms of its function values and earlier times (hence the "backward" in the name). They are derived by forming the k -th degree interpolating polynomial approximating the function using the values up to the k -th value, differentiating it, and evaluating it. Despite of being multi step, this is a generally less efficient method than RK4 of ABM [12].

Chung-Hulbert method (CH): This algorithm is devised for structural dynamics calculations where high frequency dissipation is needed. It uses a set of parameters to enable treating physical damping explicitly without reducing the accuracy [13].

Newmark-Beta Method (NB): The Newmark-Beta method is a particular one of several time-step methods originally proposed by Newmark in 1959. It is commonly used for the solution of linear and non-linear equations and uses a numerical parameter designated as Beta. It is devised specifically for structural analysis. Newmark's algorithms are unconditionally stable for linear problems, but only conditionally stable for non linear problems [15]. The Hilbert-Hughes-Taylor method (HHT) is a generalization of the Newmark-Beta method. With the HHT method it is possible to introduce numerical dissipation without degrading the order of accuracy.

Numerical Methods for Differential-Algebraic Equations (Kinematic Constraints integration): When bodies are subject to kinematic constraints, further equations have to be satisfied. These constraints come either in the taste of contacts between different bodies or as joints in particular chain configurations (planar constraints, cylindrical, spherical, rectangular, revolute or screw joints, etc). In order to numerically tackle these conditions the equations of motion are rearranged in literature to obtain different schema from which construct stable, accurate and faster formulations. The possibilities are to do it either in the acceleration level, the velocity level or in the position level. Other approaches are currently subject to study but given their conceptual level of complexity their application is still limited to research areas [17].

Acceleration Level Schema: This is the most common, "classic" approach utilized to solve the constraint equations. The methods using this approach are considered Constraint Based. By means of this, at the beginning of each time step the internal forces (elastic, viscous or pressure) and the external ones (gravity, collisions, etc) are computed and accumulated. Then, by means of Newton's second law, they are transformed into accelerations and then velocities and positions are updated for each integration time step. Given the tendency to numerical drift shown by these approaches, stabilization techniques are generally accessories to them, being Baumgarte's the most popular one [16].

Penalty method (PM): This method adds a force to a multi-body system if a constraint is not satisfied. The magnitude and direction of this force depends on the constraint violation. Its level of accuracy depends directly on how close the value of the penalty factor approximates infinite [17].

Lagrange Multipliers (LM): The Lagrange multipliers are numerical artifacts (additional algebraic variables) that enforce constraint conditions between the elements. It allows for the solution of the dynamic problem at the expense of solving for an augmented set of $(n+m)$ unknowns [17, 18].

Generalized Coordinates/Reduced Coordinates Method (GC): A reduced-coordinate formulation provides a more accurate simulation. Holonomic (redundant) constraints reduce the degrees of freedom of a multi-body system permanently. This property is used by reduced-coordinate methods [19].

Udwadia-Kalaba Formulation (UK): This method represents a more compact and general form of solving the DAEs by means of the Moore-Penrose generalized inverse matrix. It is based on Gauss' Principle of Minimum Constraint, which establishes that the explicit equations of motion be expressed as the solution of a quadratic minimization problem subjected to constraints, but at the acceleration level [20].

Velocity Level Schema: Originated by the necessity of efficiently handle the collision constraints, these methods utilize the notion of impulse as a fast acting force, hence they are more commonly known as Impulse Based methods.

Impulse Based Methods (IB): The approach has several advantages, including simplicity, robustness, parallelizability, and an ability to efficiently simulate classes of systems that are difficult to simulate using constraint based methods. The accuracy of impulse based simulation has been experimentally tested and is sufficient for many applications [19, 20]. Currently under very active development, results particularly popular among the Computer Graphics community given their remarkable speed and stability.

Numerical Methods for Partial Differential Equations (Matter Integration): To describe the dynamics of matter we have an infinite number of degrees of freedom because the particles that compose it can have arbitrary displacements with respect to each other. Such systems are described using partial differential equations where time and spatial coordinates are related. These general partial differential equations (PDE), which are applicable to any solid or fluid material, are derived from the constitutive laws of the material. For their solution, three

different approaches are classically taken in order to control the number of degrees of freedom (i.e. discretize): by means of rigid body models, by creating a mesh where the material displacements are limited (mesh based methods) or establishing the equations in the form of potential functions so that they compose a system of particles that regulate each other (mesh free methods) [21]. Other approaches still under experimental development also serve for the solution of PDE [22-24], but will not be addressed here given their conceptual complexity.

Rigid Body Models (RBM): This is the simplest approach to modeling the continuum and implies that no PDEs are integrated. Rigid bodies, in contrast to particles, occupy space and have geometrical properties (center of mass, moments of inertia, etc.). These properties characterize motion in six degrees of freedom (translation in three directions plus rotation in three directions).

Mesh based Methods: In this group of methods, the governing equations of continuum mechanics appear in two main tastes: Lagrangian description and Eulerian description. In the Lagrangian description, which is made in the material domain, the material quantities mass, energy and momentum move along with the mesh cells. When the material deforms, the mesh deforms accordingly [20]. This description results efficient for computational solid mechanics problems, where small deformations occur, but is very difficult to apply when the mesh is heavily distorted. It is typically represented by the Finite Element Method (FEM). In the Eulerian scheme, the shape and volume of the mesh cell remain unchanged along the whole simulation. The main exponent of the Eulerian description is the Finite Difference Method (FDM).

There is still a third possibility by means of which it is intended to combine the advantages of each description above so as to strengthen their advantages and to avoid their disadvantages. It has given place to Arbitrary Lagrange Eulerian and Coupled Eulerian Lagrange, but given their complexity will not be covered here.

Finite Element Method (FEM): For FEM analysis the body is divided into elements. Assuming that these elements are small enough one can use low-order polynomials to describe the set of vectors that describe the change of the element from one configuration to another (its displacement field). This provides a very rich set of powerful tools that, however, presents some well known

limitations, such as a dependence on nicely formed meshes that consumes a substantial quantity of manpower, a considerable loss of accuracy when handling large deformations, great difficulties to represent fragmentation and interfaces between bodies of different material properties [25-28].

Finite Differences Methods (FDM): For this method it is important that a uniform grid is applied over the region to reduce the errors by the differencing method. Finite Differencing methods are thus less reliable for irregular shaped bodies than finite element methods [3].

Finite Volume Method (FVM): The finite volume method is a discretization method well suited for the numerical simulation of various types of conservation laws (elliptic, parabolic or hyperbolic, for instance); it has been extensively used in several engineering fields, such as fluid mechanics, heat and mass transfer or petroleum engineering [3].

Mass-spring Systems (MSS): In most particle systems, the forces derived from tension energy are equivalent to spring forces. Since particle systems already represent a discretization in space, only a system of ordinary differential equations has to be solved. The trajectory of each particle with mass m at position x is computed by Newton's equation of motion [29].

Mesh Free Methods: The key idea of the mesh free methods is to provide accurate and stable numerical solutions for integral equations or PDEs with all kinds of possible boundary conditions with a set of arbitrarily distributed nodes (or particles) without using any mesh that provides the connectivity of these nodes or particles [25-28].

Smoothed Particle Hydrodynamics (SPH): In the SPH method, the state of a system is represented by a set of particles which possess individual material properties and change according to the governing conservation equations. SPH was developed for hydrodynamics problems in the form of PDEs of field variables such as velocity, density, energy, etc. [25].

Partition of Unity (PU): Mesh free methods can also be based on partitions of unity. A partition of unity is a paradigm in which a domain is covered by overlapping patches [30].

Moving Least Squares (MLS): An alternative but related approach to developing a mesh-less approximation is to use a moving least square (MLS) technique. Moving Least Squares serves for the reconstruction of continuous functions from sets of unorganized point samples. It is based on the Least Squares regression techniques, which are statistical modeling methods [26].

DISCUSSION

Numerical Methods Summary: Tables 1 to 3 present in a condensed manner the methods enunciated above (abbreviations can be found in bold letters in the previous section). These tables intend to facilitate an approximated evaluation and comparison over the four most relevant aspects regarding numerical methods: accuracy, stability, efficiency and ease of implementation. Their values range between one and three for the sake of generality.

It is important to notice that there is not an easy manner to objectively compare numerical methods, hence that most authors focus on particular applications for particular methods. Conclusions obtained from these works are commonly too specific for our purposes.

Table 1: ODE methods / Time integration comparison

Scheme	Method	Accuracy	Stability	Efficiency	Ease of implementation
Explicit	EE	*	**	***	***
	ERKn	**	**	**	***
	RKDP	**	***	***	**
	RKF	**	***	***	**
	RKCK	**	**	***	**
	ABM	**	**	***	**
	SG	**	**	***	*
	LF	**	**	***	***
Implicit	IE	**	**	**	**
	IRKn	**	**	**	*
	CN	***	***	**	*
	BDF	***	***	**	*
	CH	***	***	***	*
	NB	**	**	**	**
	HHT	**	**	**	*

Table 2: DAE methods / Constraint integration comparison

Scheme	Method	Accuracy	Stability	Efficiency	Ease of implementation
Acceleration	PM	*	*	***	***
	LM	**	**	*	***
	GC	**	**	**	**
	UK	***	***	**	*
Velocity	IB	**	***	**	***
Position	PBD	**	**	**	***

Table 3: PDE methods / Matter integration comparison

Scheme	Method	Accuracy	Stability	Efficiency	Ease of implementation
Rigid Body	RB	*	***	***	***
Mesh based	FEM	***	***	**	**
	FDM	**	***	**	**
	FBM	**	***	**	**
	MSS	***	***	**	**
Mesh free	SPH	***	***	*	**
	PU	***	***	*	*
	MLS	**	***	*	*

Table 4: Relation of different fields, integration concepts and sample specialized implementations

Field of Original Application / Industrial Background	ODE	DAE	PDE	Implementation Name
Mechatronics/Robotics	SG / ERK3 / ERK4 / ERK5	GC	FEM	SPACAR
	ERKF2 / ERKF3 / ERKF4 / ERKF5 / RKDP / ABM / BDF	GC / LM	RBM	Sim Mechanics
Aerospatial	CN / IE / BDF	LM	FVM	MBDyn
Automotive	ERK2	LM	RBM	SimCreator
	BDF / ABM / ERK4	IB / LM	FEM	Universal Mechanism
Games / Graphics / Animation	EE	IB	RBM	ODE
	ERK4	IB / LM	RBM	IBDS
	EE	IB	RBM / MSS	Havok Physics
Multiphysics	ERK5 / IRK4	LM	FVM / FEM	OpenFOAM
	BDF / ERK4 / ERK5 / IE	LM	FEM	COMSOL
Medical / Biomechanics	EE / ERK2 / ERK4 / IE	PM / IB	MSS / FEM / RBM / SPH	SOFA (Simulation Open Framework Architecture)
Structural Engineering	NB / HHT / IRK / CH	GC	FEM	SAP2000
	NB / IE / HHT / IRK2	PM	FEM	DIANA
	Explicit unspecified	LM / PM	FEM / FVM / SPH	EUROPLEXUS
	ERK4 / ERK5 / CN / NB	LM / PM	FEM / FVM / SPH	ANSYS
	NB / HHT	GC / PM / LM	FEM	ABAQUS FEA

In terms of accuracy and stability ODE solvers depend directly on the time-step parameter and the order of the derivative. Paradoxically however, the more one increases the accuracy of the simulation the lower becomes its stability field. For DAE methods, the accuracy is directly affected by the previous choice of ODE parameters (time-step primarily). Besides, as they operate in the formulation level, for each of them exists a particular set of parameters. For instance the Penalty Method gains accuracy the more its penalty parameter approaches infinity. This value is obviously limited by the computer capabilities. Impulse Based methods require an extra iterative subprocess whose convergence is limited as to the type of problem to be solved. When it comes to PDE solvers, the main factor that affects accuracy is the density of the mesh in mesh based methods, and the density of interpolation points in the mesh free schema.

But also the form of the characterizing functions and polynomials should be finely tuned according to different problems. Adjustment of these parameters depends highly on the choice of the analyst at the time of modeling, not so much in the method itself.

In terms of efficiency in ODE methodologies there are obvious advantages for explicit schemes as they do not require extra computations. DAE methods generally involve extra algebraic sub steps, which are determinant in their computational cost, but they are not always applicable to every type of problem. PDE methods have their most simplistic approach in the form of rigid bodies, where no differentiation nor operation is made, being the mesh free methods the least efficient as state computations have to be made over the whole population of approximating points on each time step.

The ease of implementation for each method is not only reflected in the number of sub algorithms contained but also in the conceptual background, intuitiveness of their inherent principles and availability of information on how they work. In general ODE methods are broadly available and extended, but given their generality it can result difficult to discriminate when to apply them for particular problems. DAE methods are often entangled within the very formulation of ODE methods in some applications, and their mathematical approach and explanation results often awkward and counterintuitive. PDE methods range from the easiest Finite Difference to the very complex formulations of Finite Elements and Smoothed Particle Hydrodynamics.

Industry Tendencies: Table 4 enumerates some different scientific and engineering fields. By means of a sample of random available packages (either commercial or open source), and exposing the numerical methods in them implemented, it is shown how these industries are related to the integration concepts described in the previous chapter.

It can be appreciated how mechatronics, robotics and aerospace oriented packages, where a high level of accuracy and stability is compulsory, facilitate analysts a wide range of time solvers, whether implicit and explicit, and rely on the more “classical” acceleration based methods for enforcing the constraints. The integration of continuum mechanics ranges from the simplistic Rigid Body Models, utilized in robotics, to the Finite Volume Method that allows for easier implementation of flow-solid interactions.

Automotive simulators and game engines, where real time experience and computer efficiency are the main concerns, make a wider use of explicit time integrators (lower accuracies), the faster impulse-based methods to compute the constraints and show a dominating presence of the simpler Rigid Body Models. Also in the automotive field safety simulations and prototyping are made, hence the use of implementations with more sophisticated methods such as FEM.

Multiphysics packages, by means of which highly complex interactions are analyzed (thermal, dynamic, electrical, etc) utilize mostly FEM given its versatility in PDE solution. General purpose time integrators either implicit and explicit are present, given the broad scope of these applications.

When it comes to health environments, where the level of detail is focused on complex tissue-like materials, the span of choices regarding matter integrators grows

considerably. Given the need for real time interactivity in surgical simulations, the span of ODE integrators is fairly broad, along with the faster impulse based constraint solvers. Human limbs are approximated by means of Rigid Bodies for the study of the behavior of articulations.

For the Structural Engineering field it is shown the dominance of FEM and the application of very specialized time integrators. It is remarkable how computational cost is not regarded so much as accuracy and numerical stability, as the choice of these integrators along with the more canonical constraint enforcing methods can prove. Also the tendency towards analyzing fluid-structure interactions appears in the form of FVM and SPH methods.

Conclusions and Future Work: A qualitative comparison of numerical methods employed in structural dynamics and simulation has been provided. Also a concise yet illustrative overview was provided. The purpose of this overview is to facilitate the transition for those who already have an interest in the matter but find it hard to tackle it given the scatter in literature currently existing. It is also aimed to give some scope and to put together common subjects which, although available to every researcher during the formation period, seem too abstract and inapplicable. Despite the daunting amount of literature available, it was not found by the authors any organized scheme in terms of tangible concepts such as time, matter and constraints.

Future research should be focused on objective experimental benchmarking. Given the complex interactions that arise when integrating nonlinearities in the equations of motion the choice of a proper comparative framework must be made carefully.

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