

VARIATIONAL MECHANICS AND NUMERICAL METHODS FOR STRUCTURAL ANALYSIS

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Abstract

This work focuses on the particular application of the variational principles of Lagrange and Hamilton for structural analysis. Different numerical methods are compared in their computation of the elastic energy through time.

According to variational mechanics, the difference between the stored elastic energy and the applied work should be null on each time step, so by computing this difference we can account for the level of accuracy of each combination of numerical methods. Moreover, in some situations when numerical instabilities are difficult to perceive due to high complexities, this procedure allows for the control and straightforward visualization of them, being an excellent source of hindsight on the behaviour of the analysed system.

The purpose of this dissertation is to present a scheme where the current numerical methods can be benchmarked in a qualitative as well as in a quantitative manner. It is shown how different combinations of methods, even for a simple model, can give very different results, particularly in the field of dynamics, where often also instabilities arise.

The first half of the thesis is a thorough explanation of these concepts and their application in terms of structural analysis. In the second part, a review on the numerical methods in general and of those implemented for our experiments is provided, followed by the experimental results and their interpretation. The model of choice, for simplicity and availability of analytical results is one cantilever column. Bending elastic energy of the column is monitored under transient regimes of different shapes, computing the total action of the system as its integral through time.

1. Introduction

1.1. Targets and interest of our research

Variational mechanics date back as far as the XVIII century, when Leibniz, Euler, Maupertuis and eventually Lagrange devised the calculus of variations and the principle of least action. This methodology of treating physical phenomena is based on the notion that everything in Nature tends to a state of minimal energy⁽¹⁾.

In this work we will be focusing on its particular application in structural analysis, where one deals with “engineering scales” whose dimensions span between 100 times bigger or smaller than those of a human being. This is in contrast with other areas of applied physics like astronomy or molecular dynamics but will be shown how those variational principles still apply and even become powerful tools for the comprehension of the behaviour of our built environment.

Numerical methods, on the other hand, have proliferated since the 1950s alongside with the ever increasing power of computers as a means to simulate physical phenomena. This ceaseless growth in number and terminology has given place to a cumbersome mix of mathematical, physics and computer science often difficult to grasp.

Choosing one simple cantilever beam as our test model, we will utilize and compare different combinations of these methods to compute its elastic energy under transient loading regimes of different shapes. This will render useful in future research in nonlinear analysis of more complex structural systems.

1.2. Variational mechanics

According to the principles of variational mechanics⁽²⁾, the difference between the measured energy and the applied work should be minimal, so by accounting this difference in each time step of our simulations we should be able to infer the degree of accuracy provided by each combination and discuss the reasons that lead to differences in result using the energy as the natural norm for analysing the error⁽³⁾.

1.3. Numerical methods for structural analysis

In a previous work by the authors⁽⁴⁾⁽⁵⁾, it was shown how the vast amount of existing numerical methods can be grouped into three main sets according to the kind of physical phenomena they model and the type of differential equations they discretize: matter integration techniques (Partial Differential Equations), constraint integration techniques (Algebraic Differential Equations) and time integration techniques (Ordinary Differential Equations).

According to this, we will particularize in the following matter integration implementations: Finite Element (FEM), Finite Differences (FDM) and Mass Spring Systems (MSS). For the constraint integration we will be comparing Penalty Method (PM) and Lagrange Multipliers (LM). And for the time integration techniques we will employ Newmark Beta (NB), Houbolt's (HBT), and the Linear Acceleration Method (LAM).

Other combinations are also possible, as the proposed scheme is easily extensible, but for our current purposes it should suffice.

u_{xx} is the axial displacement towards x
 w_{xy} is the axial displacement towards y
 θ_{xy} is the rotation of the section
 ϕ_x is the torsional rotation of the section
 N_x is the axial stress component
 V_y is the shear stress component
 M_z is the moment stress component
 T_x is the torsional stress component
 EA is the axial rigidity
 k_s is a section's shape shear constant
 GA is the shear rigidity
 EI is the flexural rigidity
 GJ is the torsional rigidity
 F_x is the external force towards x
 F_y is the external force towards y
 F_z is the external force towards z
 M_x is the torsional moment

2.3. Elastic strain energy in beams

In elastic materials, the stored potential strain energy can be accounted for as half of the integral over the volume of the internal strains times the internal stresses, whose formula (2):

$$U_{el} = \frac{1}{2} \int_V \{\sigma\}^T \{\varepsilon\} dV \quad (4)$$

where:

$$\{\sigma\}^T = \{\sigma_{xx} \sigma_{yy} \sigma_{zz} \tau_{xy} \tau_{xz} \tau_{yz}\} \quad (5)$$

$$\{\varepsilon\}^T = \{\varepsilon_{xx} \varepsilon_{yy} \varepsilon_{zz} \gamma_{xy} \gamma_{xz} \gamma_{yz}\} \quad (6)$$

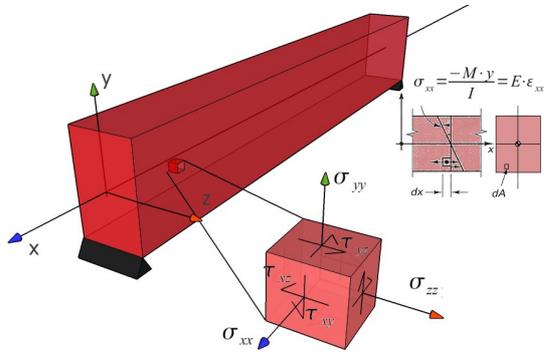


Figure 2.- Stress-strain components in a beam. The directions of the infinitesimal strains and stresses are arranged according to the length of the beam.

In the case of the linearized beam described above, we can then define four kinds of strain energies according to the four main stress components: axial (N), shear (V), bending moment (M) and torsional moment (T). From them, we can develop the analytical formulae for the elastic strain energies within a beam subjected to external loads, referred either to the internal forces or the deformations.

In table 1 below the final formulae for each one of these strain energy components are enunciated. The given expressions can be either a function of the displacements along the beam or of the input forces.

Table 1.- Displacement and force based formulae of elastic strain energy in a beam

	Displacement	Force
Axial	$U_A = \frac{1}{2} \int_0^l EA \left(\frac{du}{dx} \right)^2 dx$	$U_A = \frac{1}{2} \int_0^l \frac{F^2}{EA} dx$
Bending	$U_M = \frac{1}{2} \int_0^l EI \theta^2 dx$	$U_M = \frac{1}{2} \int_0^l \frac{M^2}{EI} dx$
Shear	$U_s = \frac{1}{2} \int_0^l AG \left(\frac{du}{dx} \right)^2 dx$	$U_s = \frac{1}{2} \int_0^l \frac{F^2}{AG} dx$
Torsion	$U_T = \frac{1}{2} \int_0^l GJ \left(\frac{d\phi}{dx} \right)^2 dx$	$U_T = \frac{1}{2} \int_0^l \frac{T^2}{GJ} dx$

For illustrative purposes, the development of the bending strain formula is provided. One of the appeals of the energy approach to structural mechanics is the consistency with which problems can be enunciated.

Bending elastic strain energy:

From the small strain beam theory of Bernoulli-Euler, it is obtained that the strain and stress components are respectively:

$$\varepsilon_{xx} = -w_{xy}''(x) \cdot y = -\kappa_{xy} \cdot y = \frac{\sigma_{xx}}{E} \quad (7)$$

$$\sigma_{xx} = \frac{-M \cdot y}{I} = E \cdot \varepsilon_{xx} \quad (8)$$

That substituted into the incremental form of (4) lead to the relations (force and displacement based, respectively):

$$dU_B = \frac{1}{2 \cdot E} \sigma_{xx}^2 dV = \frac{1}{2} \frac{M^2 \cdot y^2}{E \cdot I^2} dAdl \quad (9)$$

$$dU_B = \frac{E}{2} \varepsilon_{xx}^2 dV = \frac{E}{2} (w''(x) \cdot y)^2 dAdl \quad (10)$$

that integrated under the assumption that the origin of the coordinate system lies on the neutral axis of the beam and the bending moment of inertia is $I = \iint_A y^2 dA$ results in:

$$U_B = \frac{1}{2} \int_l \frac{M^2}{E \cdot I} dl \quad (11)$$

$$U_B = \frac{1}{2} \int_l EI (w''(x))^2 dl \quad (12)$$

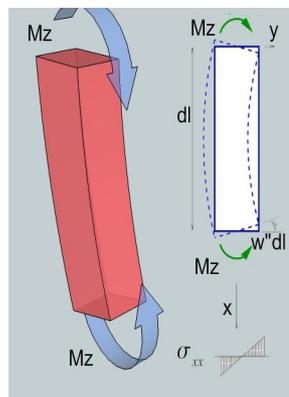


Figure 3- Bending of a column

The remaining formulae from table 1 are obtained in a similar fashion, straight from the constitutive equations (2).

This allows for a coherent manner of treating the different numerical methods of the following chapter, whose formulations are so diverse and in general not possible to benchmark or compare under objective parameters.

3. Numerical methods

For the simulation of structural dynamics three different physical notions 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.

The organization within such scheme serves both the purpose of organizing the overwhelming amount of existing methods in a rational manner as to separate mathematical from physical concepts under the assumption that a numerical method is eventually a sequence of steps.

In previous works by the authors⁽⁴⁾⁽⁵⁾ a qualitative evaluation of numerical methods is offered following the above scheme, whereas in references⁽⁸⁾⁽⁹⁾ and⁽¹⁰⁾ an overview with different levels of detail is offered.

In figure 4 some of the most extended methods are enumerated within their respective group. Initials are given in table 2.

One of the aims of this thesis is to propose a quantitative means for comparison using an energetic norm.

Table 2.- Abbreviations employed for some numerical methods

Abbreviation	Method
FEM	Finite Element Method
FDM	Finite Differences Method
FVM	Finite Volumes Method
MSS	Mass Spring Systems
SPH	Smoothed Particle Hydrodynamics
PU	Partition of Unity
MLS	Mean Least Squares
PM	Penalty Method
LM	Lagrange Multipliers
GC	Generalized Coordinates
UK	Udwadia-Kalaba
IB	Impulse Based
RK	Runge-Kutta
LAM	Linear Acceleration Method
LF	Leapfrog
IE	Implicit Euler
BDF	Backward Difference Formula
NB	Newmark-Beta
HBT	Houbolt

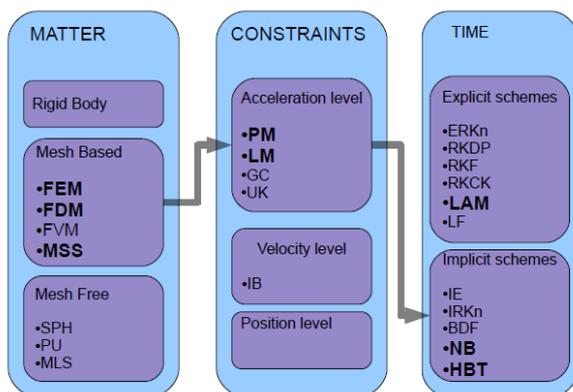


Figure 4.- Schematic of some numerical methods and their associated physical notions. In bold letters those implemented in this thesis. The arrow represents a possible sequence of methods for a dynamics simulation.

3.1. Matter integration

To describe the dynamics of matter we have an infinite number of degrees of freedom because the particles that conform 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, which are applicable to any solid or fluid material, are derived from the constitutive laws of the material.

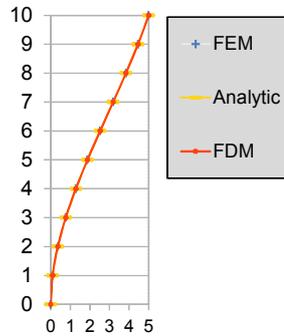


Figure 5.- Deformation polynomial of a cantilever beam under a load in the tip for FDM, FEM, and elasticity theory.

For their solution, two different approaches can be taken in order to control the number of degrees of freedom (i.e. discretize): 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)⁽²⁾.

For the present thesis three mesh based methods with different discretization schemes have been implemented: Finite Element Method (FEM), Finite Differences Method (FDM) and a Mass Spring System (MSS).

For the general computation of nodal displacements and rotations, a framework employing the Direct Stiffness Method (DSM) was prepared⁽¹¹⁾. In our case, where beam elements were used, the analytical solution of Bernoulli-Euler is lumped into local element matrices that are ultimately assembled in a global stiffness matrix⁽²⁾.

For the description of the elastic deformation of the beam, a Hermite interpolation polynomial has been employed for the FEM, obtained from reference⁽²⁾.

FDM establishes the relations between stations along the beam as a sequence of equations that form a linear system easily invertible^{(7),(12)}.

MSS is a bit more complex as it requires a previous discretization of the beam into tetrahedra, but from the point of view of Physics it results clearer as the assumptions are that the nodes are simply connected by bars with a characteristic Young's modulus and area⁽¹³⁾.

Some adjustments had to be made to the position of the masses in the cross section so the inertia of the section would match the value assigned in the polynomial-based methods.

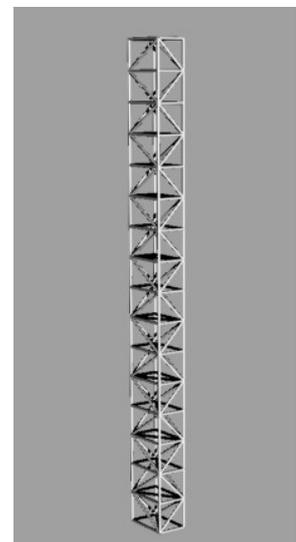


Figure 6.- MSS discretization

The global nodal displacements and rotations computed by means of the DSM were transformed ultimately into local coordinates and served as input variables for each of the three methods above.

3.2. Kinematic constraints integration

When bodies are subject to kinematic constraints, the set of algebraic equations defining the matter have to be satisfied besides from the purely time-related ones. In order to numerically tackle these conditions the equations of motion are rearranged 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 of the equation (13).

In our research we have focused on the acceleration level schemes, particularly developing the code for Lagrange Multipliers (LM) and Penalty Method (PM). In this case, the strategy is to alter the stiffness, damping and mass matrices in such a way that they become invertible (after assembly, the stiffness matrix is symmetrical and singular).

This is achieved by either expanding the matrices, adding extra rows and columns where the degrees of freedom are to be constrained (LM) or by modifying the corresponding values in the diagonal so their inversion gives a number as close to zero as possible (PM).

$$Kg = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \Rightarrow Kg_{ext} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & 1 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

Figure 7.- Lagrange multipliers scheme. The global stiffness matrix is made non singular by symmetrically adding columns and rows where ones are placed in the location of the constrained degrees of freedom.

$$Kg = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \Rightarrow Kg_{sc} = \begin{bmatrix} \infty & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \infty & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \infty & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \infty & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \infty & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \infty \end{bmatrix}$$

Figure 8.- Penalty Method scheme. The singularity of the global stiffness matrix is treated by scaling the diagonal elements of the constrained degrees of freedom with a very large number.

3.3. Time integration

The first possible classification for ODEs solvers distinguishes between explicit, implicit and hybrid methods. This division arises as a consequence of the so called stiff ODEs. The numerical stiffness 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 system (components with large differences in their masses, stiffness and/or damping). However, in many other instances, stiffness is numerically induced due to either the discretization process, the large number of components and equations of motion, or sudden or accumulated violations in the constraint conditions. Explicit methods present this kind of problem. The advantage of implicit methods is that they are usually more stable for solving a stiff equation, meaning also that a larger step size can be used. Nevertheless, extra computations need to be done internally and it requires extra time.

The equation to be integrated in time is:

$$M \cdot \ddot{u}(t) + C \cdot \dot{u}(t) + K \cdot u(t) = F_{ext}(t) \quad (13)$$

From the available different schemes we have chosen Newmark-beta (NB), Linear Acceleration Method (LAM) and Houbolt's (HB) as they are representative of implicit and explicit schemes, being Newmark-beta one of the most extended among structural analysts⁽¹⁴⁾.

4. Experimental results

What follows is the interpretation of the results of our numerical experiments, where several methods were combined in diverse simulations of a cantilever column loaded on its tip.

As reference measure, the analytical value was employed as well as that of the commercial software SAP2000 (R).

4.1. Cantilever beam

The model of choice for our research was a cantilever column under transient loading in its tip. Such structural system is provided with analytical solution for the matter integration while its conceptual simplicity makes it very illustrative, allowing to focus in the comparative issues. This model is extensively utilized for validation in the literature.

Also for the sake of simplicity, we have omitted material and geometrical nonlinearities in our analyses.

The analytical formula for the elastic strain energy of a cantilever beam or column is given by:

$$U(t) = \frac{P(t)^2 L^3}{6EI} \quad (14)$$

Being the values of L, E and I given in table 3, and the load P variable through the time scaled by the input function of choice.

Table 3.- Geometric and mechanic properties of the modelled beam

$$\begin{aligned} L &= 300 \text{ cm} \\ A &= 144 \text{ cm}^2 \\ I &= 7872 \text{ cm}^4 \\ E &= 21000 \text{ KN/cm}^2 \\ G &= 8076,92 \text{ KN/cm}^2 \\ \rho &= 7.892 \cdot 10^{-8} \text{ KN/cm}^3 \end{aligned}$$

4.2. Transient input forces

A load of 10 KN applied to the tip of the column was scaled on each time step with an input signal. Three input signals have been devised to stimulate the loading of our system: a simple sine function, an incremental triangular function and the first two periods of the triangular function with a time step ten times smaller.

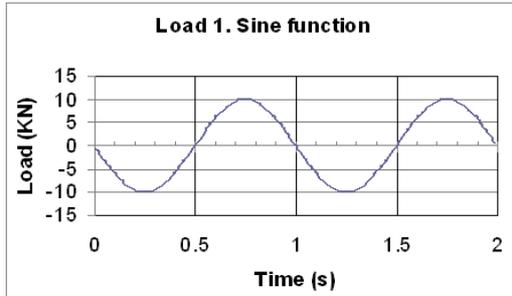


Figure 9.- Sine function. 200 time steps, 2 cycles, 2 seconds. $dt=0.01$ s.

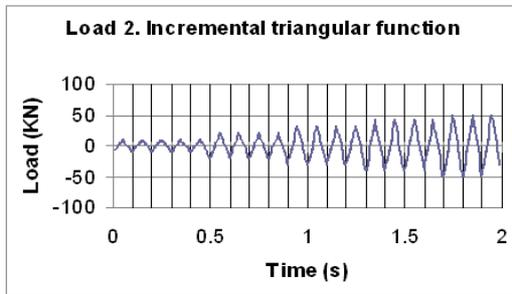


Figure 10.- Incremental triangular function. 200 time steps, four cycles with 5 sub-cycles, 2 seconds, $dt=0.01$ s.

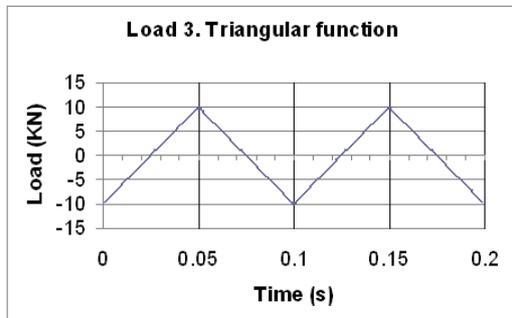


Figure 11.- Triangular function. 200 time steps, two cycles, 0.2 seconds, $dt=0.001$ s.

The sine function, with such a low frequency is seldom encountered in engineering practice but allows for the calibration and tuning of the combined methods given its smoothness and clarity.

The incremental triangular function was constructed to account for earthquake engineering regulations, where sudden changes and peaks are to be simulated.

The purpose of the third signal is to observe the influence of the time step in the results, for which the first two periods of the previous contour were inputted during one tenth of the same time span.

4.3. Numerical results

Given the number of numerical methods implemented, a total of eighteen combinations were possible for each input function, plus the two control curves of the analytical and the SAP2000 results.

For the particular case of SAP2000, the global rigidity matrix Kg provided by the program, was obtained and used with the following formula:

$$U_{elas} = \frac{1}{2} [u]^t [Kg] [u] \quad (15)$$

where u is the global nodal displacement and rotation vector also provided by the program.

Figures 12 and 13 show respectively the time history of the elastic potential energy for the sine and the incremental functions for all the combinations.

In the constraint integration level, the conclusion is that Penalty Method and Lagrange Multipliers provide exactly the same results up to the 12th decimal place.

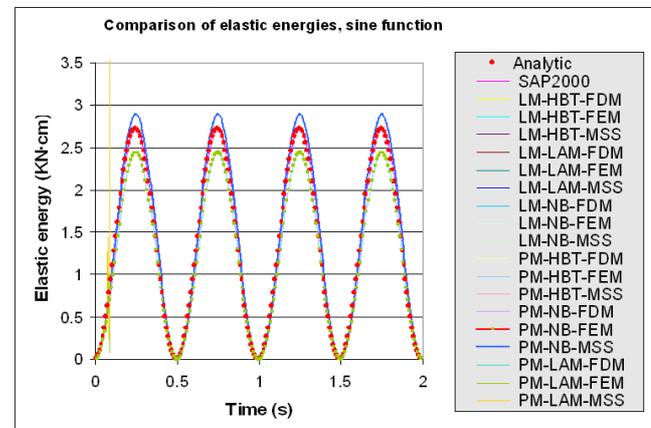


Figure 12.- Computed elastic strain energy for the sine function.

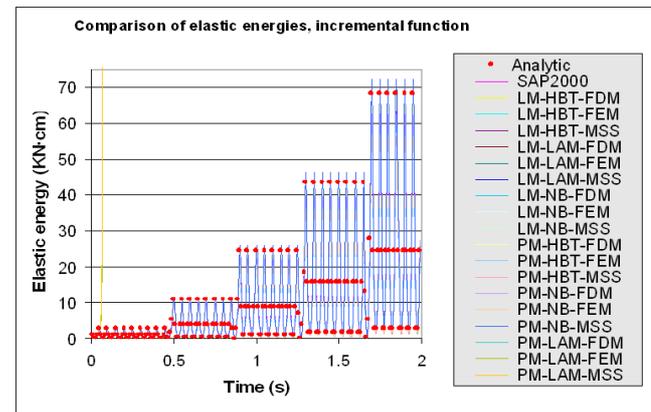


Figure 13.- Computed elastic strain energy for the incremental triangular function.

For the time integration, slight differences were observed in results between Houbolt (HBT) and Newmark-Beta (NB), being the Linear Acceleration Method (LAM) the source of major instabilities from an early stage.

Regarding matter integration, the results were overestimated by the Mass Spring System (MSS), underestimated by the Finite Element Method (FEM) and also underestimated, but to a lesser extent, by the Finite Difference Method (FDM).

Figures 14 and 15 represent the variation through time of the elastic strain energy for the incremental input function in the first 0.2 seconds.

As expected, the higher level of detail in the time stepping gives different results for the computation of the elastic energy, particularly for the case of the LAM, where no better stability was achieved and the results go off from the 6th iteration in either case. The values obtained from NB and HBT (implicit solvers) remain consistent though time, giving only the less fine discretization a coarser shape of the curve. This unstable behaviour in the LAM was expected, as its scheme belongs to the explicit type, very sensitive to stiff problems like the one of our example (the values of the coefficients of the rigidity and mass matrices differ several orders of magnitude from each other).

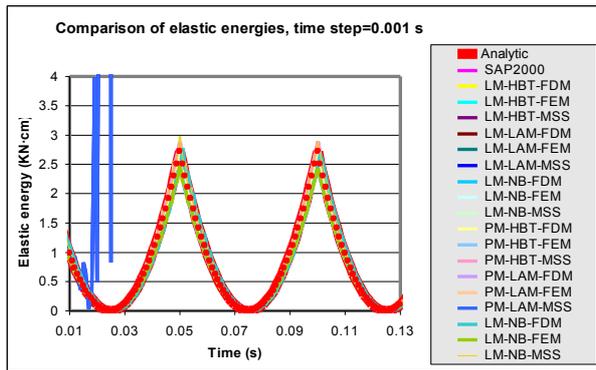


Figure 14.- Computed elastic strain energy for the incremental triangular function, $dt=0.001$ s.

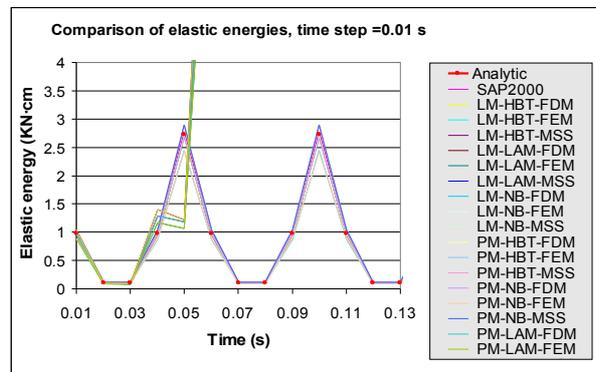


Figure 15.- Computed elastic strain energy for the incremental triangular function, first twenty time steps, $dt=0.01$ s.

The different time step affects however to the computation of the action in this interval, resulting in higher values for the corresponding coarser graph. Figure 16 shows the comparison of such integrated action, whose formula is:

$$A = \int_t U_{elas}(t) dt \quad (16)$$

It can be observed how, for all stable cases, the decrease of one order of magnitude in the time step leads to a reduction of almost 35% in the total value of the computed action. This is an important aspect to be considered given the sensitiveness of the numerical integration of the action to the form of time

discretization. However, the general assumption is that of a consistent time step between the reference input work and the calculated dynamics of the affected system under analysis.

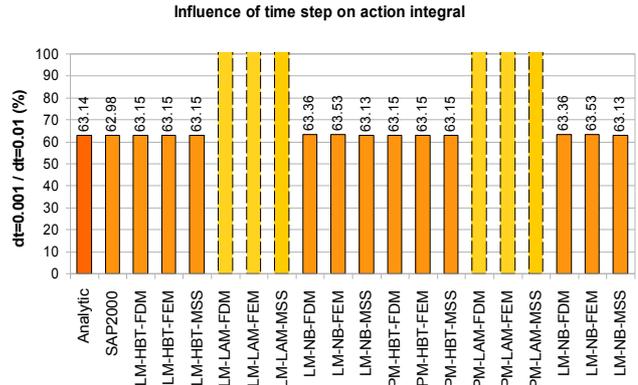


Figure 16.- Computed action for the incremental triangular function. Yellow lines belong to the LAM and are not comparable given their unstable origin. Red line corresponds to the analytical value.

Figure 17 represents the average residual in the computation of the action for all three functions of all eighteen method combinations divided by that of the analytical value. This measure of the deviation from a reference is characteristic of each method and gives very good information not only about the accuracy but also for the stability.

It can be seen how, apart from the combinations where LAM is involved; in general results remain below the 10% of error. The best agreement occurs with the FDM schemes as well as for the SAP2000 computations, where divergence is below 1%. Unexpectedly, MSS give an acceptable level of accuracy, even better than that of the FEM interpolation.

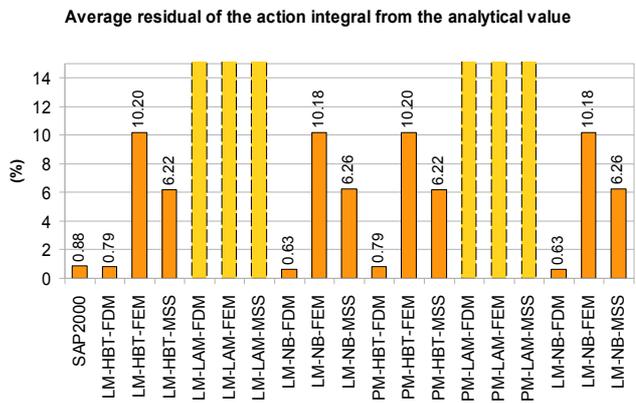


Figure 17.- Average residual of the action divided by the analytical value. Apart from LAM combinations, results remain within 10% of accuracy.

In practical terms, the possibility of a model for which analytical value exists is very uncommon. Nevertheless, in more complex structural models it is possible to replace the given formula by the inputted kinetic energy. It is also worth mentioning that this energy based methods are also applicable out of the linear elastic range, in a similar fashion and with the same degree of consistency.

5. Discussion and future work

A numerical comparison of methods commonly employed in structural mechanics was presented.

It was made on the basis of energy principles and eventually the total action of a system under transient loading has been computed for each possible combination of methods.

It was shown how variational principles and an energetic norm can be employed in the benchmarking and assessment of the accuracy and stability of different implementations.

The scheme provided, tested on a simple example, is easily extensible to more complex systems with more elements. The advantage of this approach is that it allows for the monitoring of the global behaviour by means of one simple scalar, whose value is to be compared against that of an analytical computed from external forces or accelerations.

Also, a conceptual framework for the classification and treatment of numerical methods, grouping them into time, matter and constraint integrators, was used for the systematic analysis of the results.

Future work aims at the application of the same methodology in nonlinear analysis and more complex structures.

The combination with stochastic techniques for the integration of the action and the search of minimal energy states is one of the final targets of the current research.

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7. Key words

Finite Element, Finite Differences, Variational mechanics, Euler-Bernoulli beam