

INFLUENCE OF THE NUMERICAL METHOD ON THE PREDICTED BONE DENSITY DISTRIBUTION IN ELEMENT BASED SIMULATIONS

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Most bone remodeling simulations developed upon the basis of the strain energy density theory make use of Euler method for the numerical integration of density evolution equation. However, it is well known the imprecision of this method. In this work is accomplished a comparison between five numerical methods used for integration of the density evolution equation, namely Euler, Heun, forth order Runge Kutta, second order Adams Bashford uncorrected and corrected using Adams-Moulton. The comparison criteria are the computational time, convergence behavior and final apparent density distribution.

Keywords: bone remodeling, finite element, strain energy density, apparent density, numerical integration

1. Introduction

The natural ability of bones to achieve structural changes according to their mechanical environment, namely bone modeling and/or remodeling, was theoretically investigated by several authors [1-8], resulting different mathematical models of the same problem. The fundamental differences between the mathematical theories rely not on the general formulation, but on the details regarding the mechanical quantities and the mechanisms that locally trigger and control the adaptation process. It was assumed, in this respect, that the bone remodeling driving force may be single mechanical quantities including stress [5], strain [1,2], cumulative damage [6,7] and strain energy density (SED) [8,9] or coupled quantities such as strain with microdamage [10]. From all the specified single quantities, the latter is the most used, probably because the simplicity of implementing it in algorithms due to its scalar nature and to its attribute of incorporating both stresses and strains.

The essence of bone mechanical adaptation models is, in general, a feedback evolution law of bone mass with respect to a homeostatic value of a certain mechanical stimulus which depends on the theory involved. The general form of bone remodeling equation may be written as [11]:

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$$\frac{dM}{dt} = B(S - S_o), \quad (1)$$

where $\frac{dM}{dt}$ is the derivative of a mass dependent function with respect to time, B is a coefficient which controls the remodeling speed, S is the actual mechanical stimulus and S_o is the homeostatic equilibrium value of the mechanical stimulus to which the system seeks to approach. In many studies, the mass change is quantified within the bone tissue apparent density evolution. In some models [8], instead of assuming a single value for the remodeling equilibrium, S_o , of the mechanical stimulus, an interval of equilibrium values, centered in S_o , is defined. Values of the stimulus above this interval cause bone deposition and those under the interval determine bone to resorb away. Considering the SED as mechanical stimulus and imposing the equilibrium interval, the remodeling equation is written as [8]:

$$\frac{dE}{dt} = \begin{cases} B_1[U - (1 + s)U_o], & U > (1 + s)U_o \\ 0, & (1 - s)U_o \leq U \leq (1 + s)U_o \\ B_2[U - (1 - s)U_o], & U < (1 - s)U_o \end{cases}, \quad (2)$$

where U is the actual SED, U_o is the homeostatic SED value and $2s$ measures the length of the equilibrium interval. It is also possible that the resorption and deposition speeds to be different, as coefficients B_1 and B_2 indicate. In the above equation, the mass evolution is replaced with the evolution of Young modulus. Nevertheless, this approach doesn't change the essence of the model, as the Young modulus of bones is correlated with the density using empirical relations of the form [12]:

$$E = a + b\rho^m, \quad (3)$$

where E is the Young modulus of bone material, ρ is a densiometric measure of bone tissue, a , b and m are constants depending on different factors such as the measuring method, the anatomic site or the bone type (compact or spongy) [12].

Euler method is the most simple of all numerical schemes for solving ordinary differential equations (ODEs), but it is not practical as it needs very small integration steps for the accuracy to grow [13]. Nevertheless, in case of bone remodeling simulations, Euler method proved to be preferred. This fact is probably based upon the lack of explicit analytical expression of the stimulus $S=S(t,\rho)$, in equation (1), as it depends on stress-strain field or other mechanical quantities. The problem is usually solved using the finite element method (FEM) which, for given density distributions, allows for numerical estimation of the mechanical stimulus. The mass evolution equation is iteratively coupled with FEM so the values of S are estimated per iteration. In case of using higher order integration schemes, the need to establish intermediate values of S for each

incremental update requires additional FEM calculations. Hence, the time cost is significantly increased. In addition, the implementation is more involved. However, we consider rather important to evaluate whether different integration schemes introduce significant variations in final apparent density distribution.

2. Methods

We have selected from the literature [13-15] the Euler, the Heun and the fourth order Runge-Kutta (RK) as single-step numerical methods and, from the multistep category, the second order Adams Bashford (AB) and second order predictor-corrector Adams Bashford-Adams Moulton (ABAM). We considered the comparison relevant on the basics of the following arguments: Euler method is the most used in bone remodeling simulations due to its simplicity, but is considered as non-practical because its inaccuracy and instability in case of using large integration steps [13]. Heun scheme increases the accuracy of Euler with an acceptable time cost. The RK is usually preferred for its accuracy provided with higher integration steps, based only on the first derivative [13]. The AB was already used in bone remodeling simulations, but in node based approach [16]. It was proved that it keeps the time cost as low as Euler variant, but with improved accuracy. The last scheme was implemented in order to investigate whether improvements to AB density prediction can be attained.

The remodeling process is simulated using an equation of the form (2), but adapted in terms of density evolution, as follows:

$$f(t, \rho) = \frac{d\rho}{dt} = \begin{cases} B \left[\frac{U}{\rho} - (1 + s)k \right], & \frac{U}{\rho} > (1 + s)k \\ 0, & (1 - s)k \leq \frac{U}{\rho} \leq (1 + s)k, \\ B \left[\frac{U}{\rho} - (1 - s)k \right], & \frac{U}{\rho} < (1 - s)k \end{cases} \quad (4)$$

where ρ is the apparent density of bone and k is the equilibrium constant that regulates the process. The values of k and s are determined from the initial conditions which are assumed to correspond to a homeostatic state [10], following:

$$k = \frac{U_o}{\rho_o} \text{ and } s = 0.1 \cdot k. \quad (5)$$

A common way of imposing initial conditions, which is adopted in this work, consists of applying a uniform density distribution equal to half of compact bone density. Hence, we have taken the initial value of apparent density, ρ_o , equal to 0.87 g/cm^3 .

Writing in a more concise form the equation (4) coupled with the initial condition, we have:

$$\begin{cases} f(t, \rho) = \frac{d\rho}{dt} = B[S(t, \rho) - S_o] \\ \rho(t_o) = \rho_o \end{cases} \quad (6)$$

With the notation

$$f_i = f(t_i, \rho_i) = B[S(t_i, \rho_i) - S_o], \quad (7)$$

equations (8), (9), (10) and (11) represent the recurrence relations given by Euler, Heun, RK and AB, respectively, for the density update evaluation described by equation (6):

$$\rho_{i+1} = \rho_i + hf_i, \quad (8)$$

$$\rho_{i+1} = \rho_i + \frac{h}{2} [f_i + f(t_i + h, \rho_i + hf_i)], \quad (9)$$

$$\begin{aligned} \rho_{i+1} &= \rho_i + \frac{1}{6} (K_{1,i} + 2K_{2,i} + 2K_{3,i} + K_{4,i}) \\ K_{1,i} &= hf_i \\ K_{2,i} &= hf\left(t_i + \frac{h}{2}, \rho_i + \frac{K_{1,i}}{2}\right) \\ K_{3,i} &= hf\left(t_i + \frac{h}{2}, \rho_i + \frac{K_{2,i}}{2}\right) \\ K_{4,i} &= hf(t_i + h, \rho_i + K_{3,i}) \end{aligned} \quad (10)$$

$$\begin{cases} \rho_{i+2} = \rho_{i+1} + \frac{h}{2} (3f_{i+1} - f_i) \\ \rho_1 = \rho_o + \frac{h}{5} f_o \end{cases} \quad (11)$$

In the predictor-corrector ABAM variant, the recurrence expressions are:

$$\begin{cases} \rho_1 = \rho_o + \frac{h}{5} f_o \\ \rho_{i+2,pre} = \rho_{i+1} + \frac{h}{2} (3f_{i+1} - f_i) \\ f_{i+2,pre} = f(t_{i+2}, \rho_{i+2,pre}) \\ \rho_{i+2} = \rho_{i+1} + \frac{h}{2} (f_{i+1} + f_{i+2,pre}) \end{cases} \quad (12)$$

The initial values of densities for AB and ABAM were determined using the Euler method in the first increment, but with a diminished step relative to the overall constant value. A five time lower value was chosen.

In order to iteratively simulate the apparent density distribution in bone models, we have written a code which couples Matlab and Ansys programs. The

code comprises two modules, one for carrying out the finite element component of the simulation, making use of Ansys capabilities and the other for numerical solving the remodeling equation, employing Matlab resources. The communication between the two programs and the material update are accomplished according to Martin Groß approach [17]. The implementation is element based [9], which assumes the existence of one sensor per finite element and that the apparent density is constant per element. Figure 1 shows the block diagram of the algorithm.

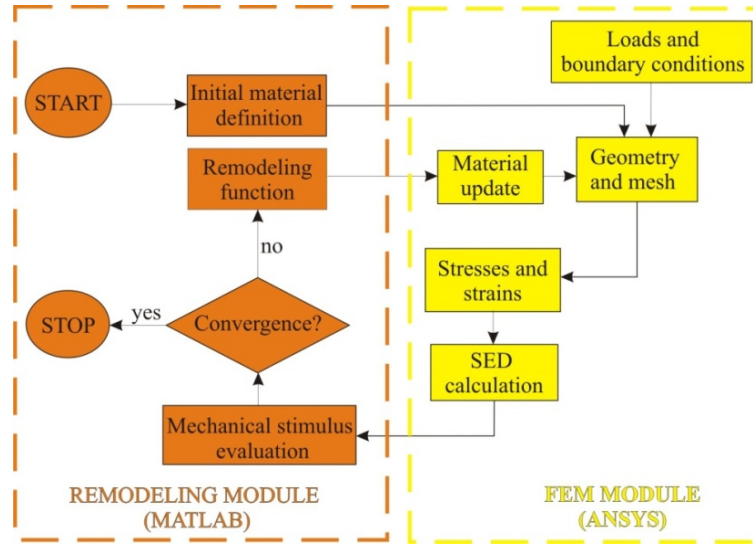


Fig. 1. Block diagram of the remodeling algorithm: the finite element module implemented in ANSYS (right) and the density evolution module implemented in MATLAB (left)

The simulation was performed on the structure presented in figure 2, which is common for employing topology optimization [18]. This approach allows for the qualitative comparison of the density distribution achieved with our code with the one presented in the literature [18]. It is to be mentioned that, although bone remodeling and structural topology optimization are different methods of determining optimum density distribution, they should generate similar topologies. This fact allows a qualitative validation of our models.

In order to evaluate the mechanical stimulus we have developed five Matlab functions, each corresponding to the selected numerical schemes, respectively.

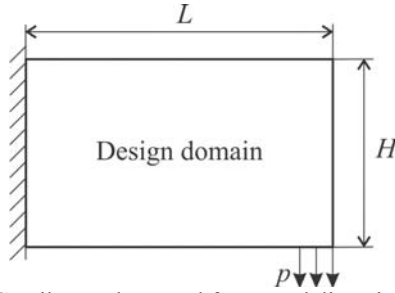


Fig. 2. Cantilever plate used for remodeling simulations

In the simulations presented here, for the cantilever plate from figure 2 we have chosen $L=15 \text{ mm}$, $H=10 \text{ mm}$ and p distributed on several nodes so that the resultant force to be 100 N . Several tests are first performed in order to identify the relevant finite element density and integration step values. It is considered that finer meshes should better approximate the averaged stress-strain field. Hence it is expected for more realistic³ density distributions to reveal in finer meshes. Therefore, we have accomplished our study on two groups of finite element mesh sizes, each with two integration steps. We used squared finite elements with the element edge length of 0.5 mm in the first group and of 0.25 mm in the second, denoted as coarse mesh and fine mesh, respectively. For both groups and for each numerical method, the two integration step values were taken as 0.5 and 0.25.

Ideally, the objective of the simulation would be to attain, in every element, a mechanical stimulus within the homeostatic limits (S_o). This is not the case with the remodeling rule simulated here because the density change is stopped within the elements whose density reach either the superior or the inferior limits. In these elements, the remodeling stimulus is artificially forced to keep a value which is not necessary inside the initial established equilibrium interval. This observation stands for the irrelevance of comparing the uniformity of final stimulus distribution according to each numerical method, as it would be a general objective. The comparison between the predicted densities is only relevant as a global qualitative distribution.

The convergence is controlled using the objective function proposed by Weinnans et. all [9]:

$$\Phi = \frac{1}{NE} \sum_{i=1}^{NE} \left| \frac{U_i}{\rho_i} - S_o \right|, \quad (13)$$

where NE represents the number of finite elements meshing the model, U_i and ρ_i are the SED and the apparent density corresponding to element i . The function Φ

³ The term “realistic” used in this paper is strictly related to the remodeling equation, i.e. to the precision of approximating its solution.

measures the amount of global adaptation towards the value S_o . When no significant change is recorded, in any of the finite elements, the values of ϕ should stabilize. In this respect, the algorithm is stopped when during three consecutive iterations the objective function does not change by more than an imposed tolerance ($10^{-4} \text{ MPa} \cdot \text{g}^{-1} \cdot \text{cm}^3$), i.e.:

$$\Delta\phi_t = |\phi_t - \phi_{t-1}| < 10^{-4}. \quad (14)$$

3. Results and discussions

As shown in figure 3, good resemblance between density distributions is revealed by the five different methods, respectively. One can also notice the qualitative similarity between our results and the ones obtained by Ole Sigmund using a Matlab code for topology optimization [18].

Figure 3 indicates that, if coarse meshes are used, no relevant differences appear between final density distributions whatever the method used. Neither in terms of convergence were not identified any significant aspects that would make the difference, except in the case of AB method which proved to be locally unstable (figures 5a and 5b). Decreasing the integration step is also insignificant. However, when using denser meshes additional density struts appear in the case of multistep methods, as figure 4 reveals. This effect raises the question whether the single-step or multistep methods produce more realistic density distributions. Therefore, we conducted further analysis by deeper refining the finite element mesh. The results in terms of density distribution and convergence behavior are presented in figures 6 and 7, respectively, but only for Euler and AB schemes, because their required computational time is almost the same and significantly lower than the other methods. It is demonstrated that higher mesh refinement introduces similar density struts in both Euler and AB predictions, but has the disadvantage of high computational cost. It is to be observed that AB already predicted similar struts in coarser meshes (figure 4), thus with significant lower computational time. Therefore, it is an argument that accounts for using AB instead of Euler. However, the convergence of AB proved unstable, even in high mesh refinements and small integration steps (figures 5c, 5d and 7). If this detail is important, as in time dependent bone remodeling simulations, a method that shows a smooth convergence should be used.

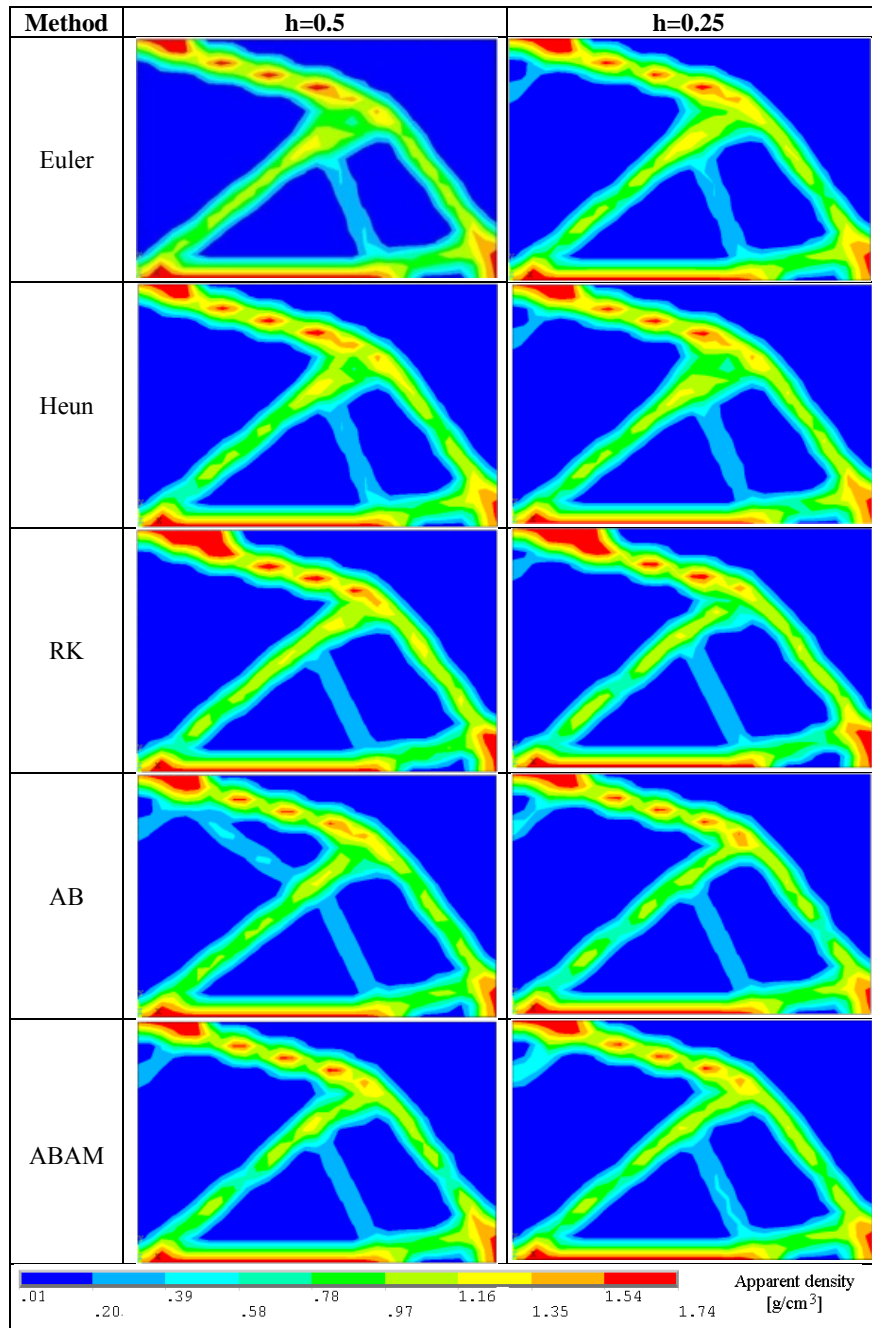


Fig. 3. Final apparent density plots corresponding to each integration scheme in the case of coarse mesh (0.5 mm element edge length)

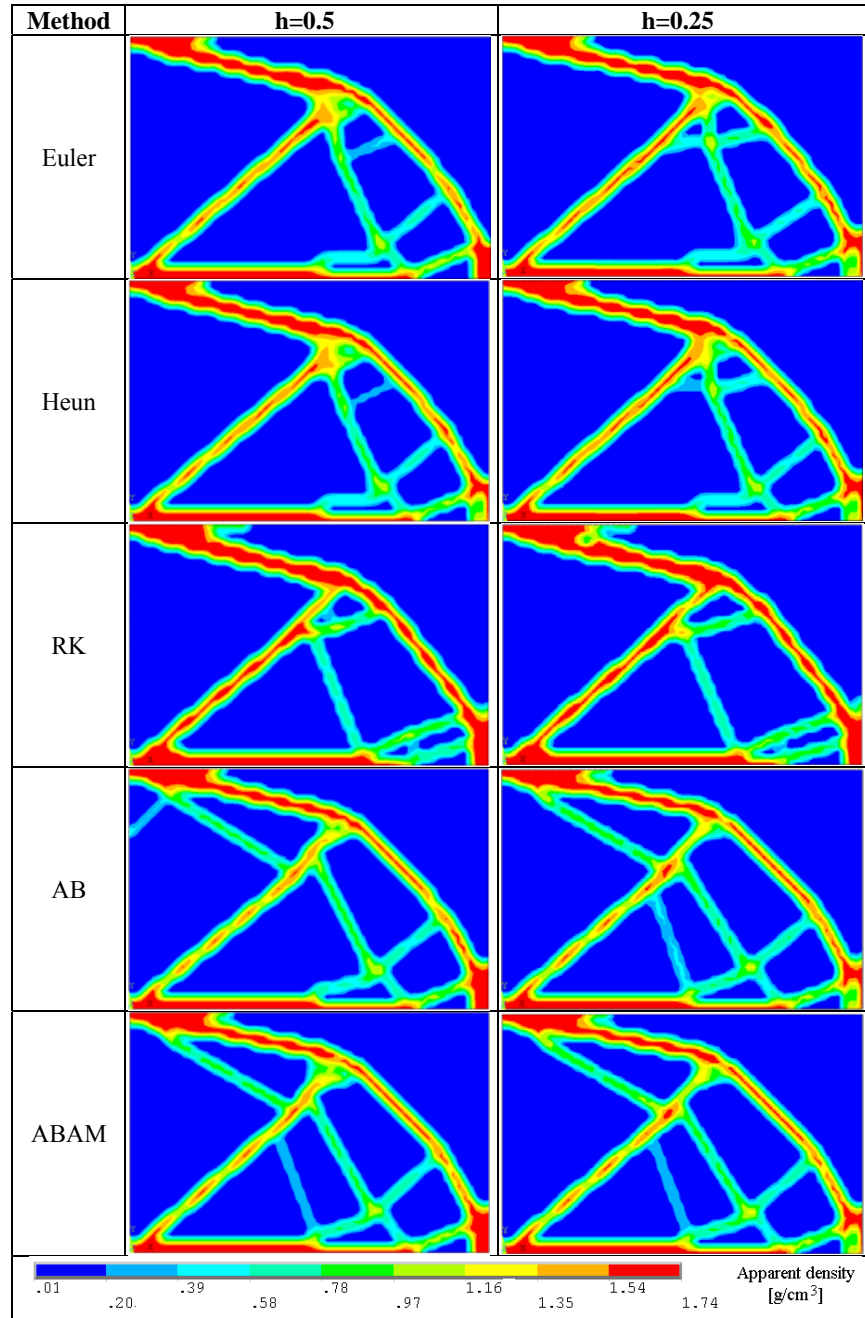


Fig. 4. Final apparent density plots corresponding to each integration scheme in the case of mesh refinement (0.25 mm element edge length)

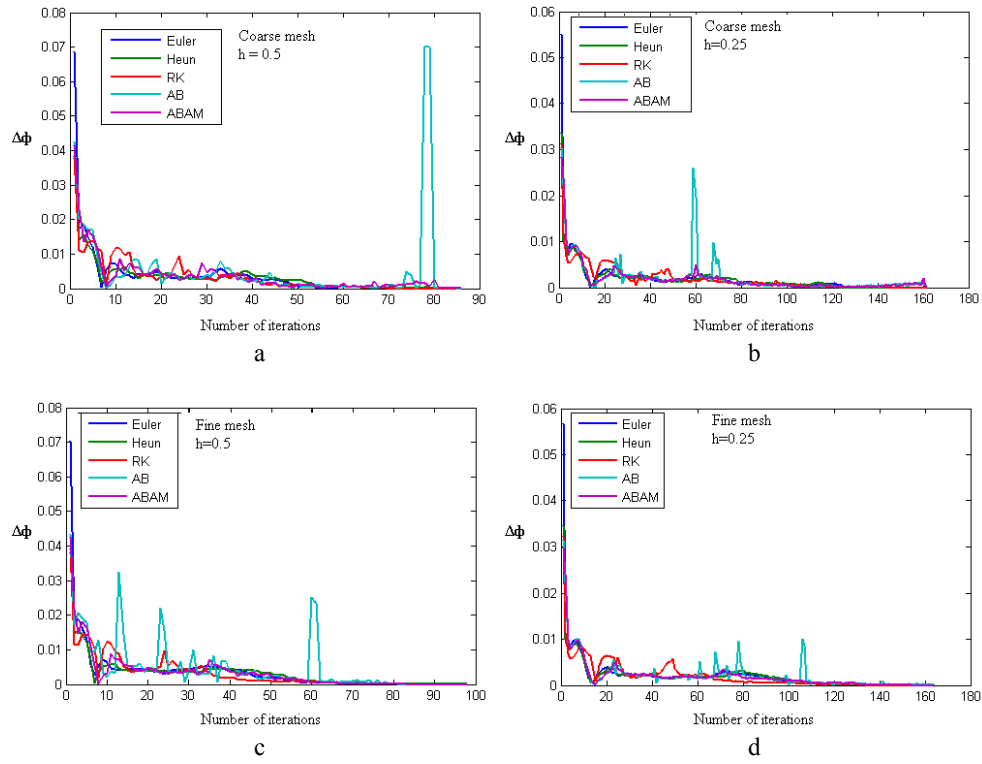


Fig. 5. Convergence plots corresponding to the four initial meshing conditions

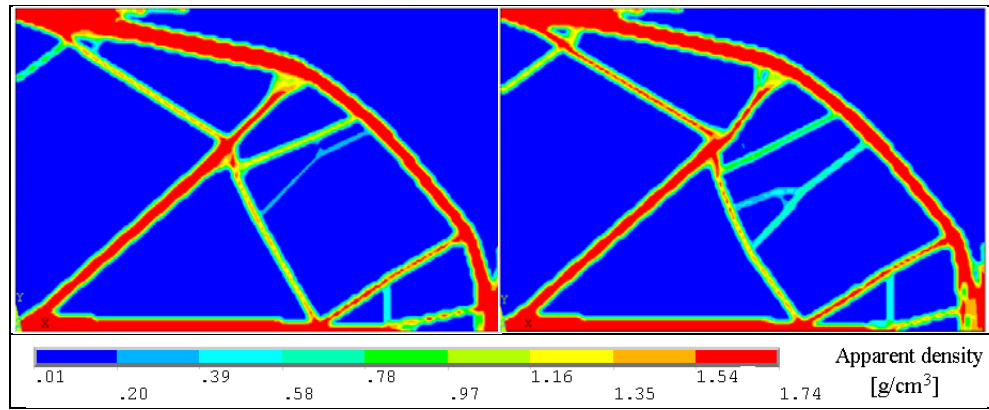


Fig. 6. Final apparent density plots corresponding to Euler (left) and AB (right) integration schemes in the case of high mesh refinement (0.1 mm element edge length) with $h=0.25$

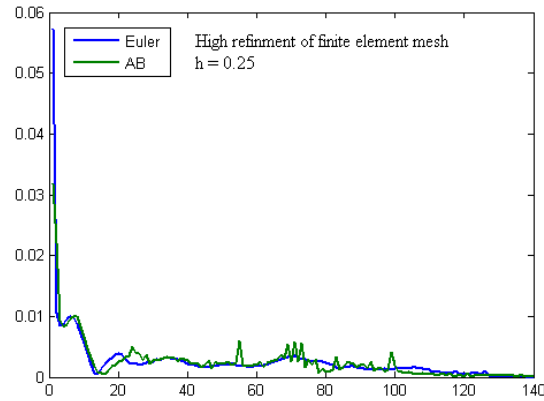


Fig. 7. Convergence plots corresponding to the Euler and AB integration schemes in the case of high mesh refinement (0.1 mm element edge length)

Regarding the other methods studied here (other than Euler and AB), one can observe no important changes neither in terms of predicted density or convergence behavior. Additionally, the time cost is about two times higher in the case of Heun and ABAM and almost four times higher in the case of RK relative to Euler and AB.

4. Conclusions

The comparison presented in this work revealed no significant difference between final apparent density distribution in relatively coarse meshes, but some density struts are found to appear as differences in case of mesh refinement. Because the remodeling problem is mesh dependent, this numerical effect should be taken into account.

Decreasing the convergence tolerance does not imply any supplementary effect. In the case of convergence behavior, all the methods revealed the same evolution, except the AB approach which generated some local instability, irrespective of mesh density.

The use of a certain method is dependent upon the scope of the simulation. For instance, Euler and AB schemes provide similar density distributions but for different mesh sizes. Assuming that mesh refinement ensures more realistic results, the AB method is therefore more appropriate as it reveals the same mesh as Euler but in coarser meshes. This is obviously an advantage in terms of time cost. However, in the case of simulations where time becomes important, the integration step being correlated with the experimental time of remodeling process, the instability of AB would affect the density evolution. In such cases, a scheme that ensures a smooth convergence is more appropriate.

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