

Efficient Harmonic Simulation of a Trabecular Bone Finite Element Model by means of Model Reduction

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Abstract

Three-dimensional serial reconstruction techniques allow us to develop very detailed micro-finite element (micro-FE) model of bones that can very accurately represent the porous bone micro-architecture. However, such models are of very high dimension and, at present, simulation is limited to a linear elastic analysis only. In the present paper, we suggest to use model reduction in order to enable harmonic simulation for micro-FE models. We take two bone models of dimensions 130 000 and 900 000 and report results for implicit moment matching based via the Arnoldi process. We demonstrate that for the first model a low-dimensional subspace of dimension 10 allows us to accurately describe frequency response up to 190 Hz. For the second model, a low-dimensional subspace of dimension 25 is enough to accurately describe frequency response up to 30 Hz. We show that the time to perform model reduction and then to simulate the low-dimensional model is orders of magnitude less than that needed for harmonic simulation of the original model.

Introduction

Fig. 1 sketches the micro finite element analysis [1]. Micro computer tomography (CT) is employed to make 3D high-resolution images (~50 microns) of a bone. Then the 3D reconstruction is directly transformed into an equally shaped micro finite element model by simply converting all bone voxels to equally sized 8-node brick elements. This results in finite element (FE) models with a very large number of elements (~ 1 - 10 million elements per cm³) and special iterative solvers are usually required to solve such high dimensional problems. This allows us to simulate, for example, compression tests, and in this way it is possible to calculate the stiffness of a bone specimen while fully accounting for its micro-architecture.

Such models can be used, for example to study differences in bone tissue loading between healthy and osteoporotic human bones during quasi static loading [2]. The main disadvantage of this approach is its huge computational requirements because of the high dimensionality of the models (on the order of 100 millions nodes). This led to the fact that such a computational analysis is limited to a static solution.

There is increasing evidence, however, that bone responds in particular to dynamic loads [3]. It has been shown that the application of high-frequency, very low magnitude strains to a bone can prevent bone loss due to osteoporosis and can even result in increased bone strength in bones that are already osteoporotic. In order to better understand this phenomenon, it is necessary to determine the strain as sensed by the bone cells due to this loading. This would be possible with the micro-FE analysis, but then such an analysis need to be a dynamic one.

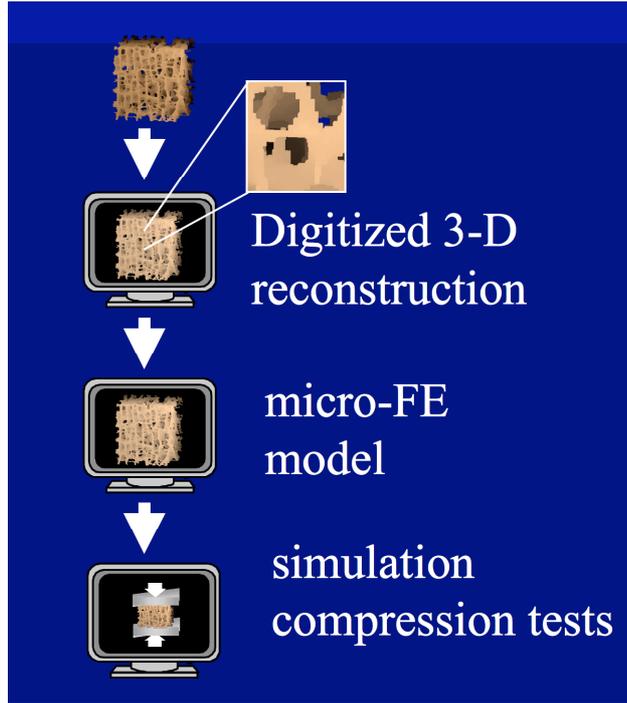


Fig. 1. Micro finite element analysis.

In the present study, it is investigated if a new technique called model order reduction can make the dynamic analysis feasible. Model order reduction is a relatively new area of mathematics that aims at finding a low-dimensional approximation for the high-dimensional system of ordinary differential equations. It has been used successfully over the last few years in different engineering disciplines like electrical engineering, structural mechanics, heat transfer, acoustics and electromagnetics [4].

We start by a short overview of how model order reduction can speed up harmonic simulation. Then we present results of harmonic analysis with the use of model reduction for the two micro-FE models representing bone specimens, one model with 42 528 and one with 305 066 nodes (number of equations is three times more).

Harmonic Simulation by Means of Model Order Reduction

After the discretization in space of a mechanical model, one obtains a system of ordinary differential equations of the second order as follows

$$M \frac{d^2 x(t)}{dt^2} + E \frac{dx(t)}{dt} + Kx(t) = Fu(t) \quad (1)$$

where M , E , and K are the mass, damping and stiffness matrices accordingly, F is the load vector and x is the vector of unknown displacements. Harmonic simulation of (1) includes solution of a system of linear equations

$$\{M(i2\pi f)^2 + Ei2\pi f + K\}X(f) = F \quad (2)$$

in the given range of frequencies, f . Computational time for harmonic simulation is close to that of the stationary solution multiplied by the number of required frequencies. Provided it is necessary to evaluate the harmonic response at 100 frequencies, simulation time is roughly 100 times more than the time required for the stationary solution.

The idea of model reduction (see the review [4] for more detail) is that a trajectory of the high-dimensional state vector x in Eq (1) actually belongs to a low-dimensional subspace:

$$x \approx Vz \quad (3)$$

where the matrix V has a few columns describing the generalized coordinates and the low-dimensional vector z contains amplitudes of these coordinates. Provided that the subspace V is known, the original dynamic system can be projected on it. For example, harmonic simulation requires solution of a low-dimensional system of linear equations as follows.

$$\left\{ V^T M V (i2\pi f)^2 + V^T E V i2\pi f + V^T K V \right\} Z(f) = V^T F \quad (4)$$

Because of low dimensionality, harmonic simulation of the reduced system (solution of Eq 4) is much faster than that of the original system (solution of Eq 2).

The most efficient way to compute a reasonably accurate low-dimensional subspace V is implicit moment matching via the Arnoldi process [4]. For dynamic systems with proportional damping and an expansion point of zero, it is equivalent to the computation of the Krylov subspace

$$V = \text{span}\left(\mathfrak{K}\{K^{-1}M, K^{-1}F\}\right) = \text{span}(b, Ab, A^2b, A^3b, \dots) \quad (5)$$

coupled with internal orthogonalization, where $b = K^{-1}F$ and $A = K^{-1}M$ [5]. This is an iterative process where it is necessary to evaluate a matrix-vector product $K^{-1}Mu_i$ during each iteration step. However, the inverse of the stiffness matrix is never evaluated explicitly. Rather the product $K^{-1}v_i$ is estimated as a solution of the system of linear equations

$$Kx_i = v_i. \quad (6)$$

The use of direct solvers allows us to factorize the stiffness matrix once (Cholesky factorization) before the iteration process and then employ back substitution to solve Eq (6) during the iteration step. Computational experiments [6] have shown that

- 30 generalized coordinates are enough to accurately capture dynamic behavior for many mechanical models;
- Modern direct solvers are competitive up to 500 000 degrees of freedom on computers with 4 Gb RAM;
- In this case, computational time to evaluate the low-dimensional subspace is comparable with that of stationary solution.

Trabecular Bone Case Studies

Fig. 2 shows two solid bone models employed in the present work. Numerical characteristics are given in Table 1. The first model referred later on as "small" is made with low resolution and, as a result, is rather stiff. The second model referred later on as "big" is made with high resolution and it represents the trabecular bone structure much more accurately.

The number of equation in (1) is about 130 000 for the first model and about 900 000 for the second model. Damping has been neglected. The mor4ansys computational engine [6] has been used to perform the computations. For symmetric positive definite matrices, the multifrontal solver from the TAUCS library [7] has been used and otherwise that from the UMFPACK library [8]. Calculations has been performed on 450 MHz Sun Ultra-80 with 4 Gb of RAM.

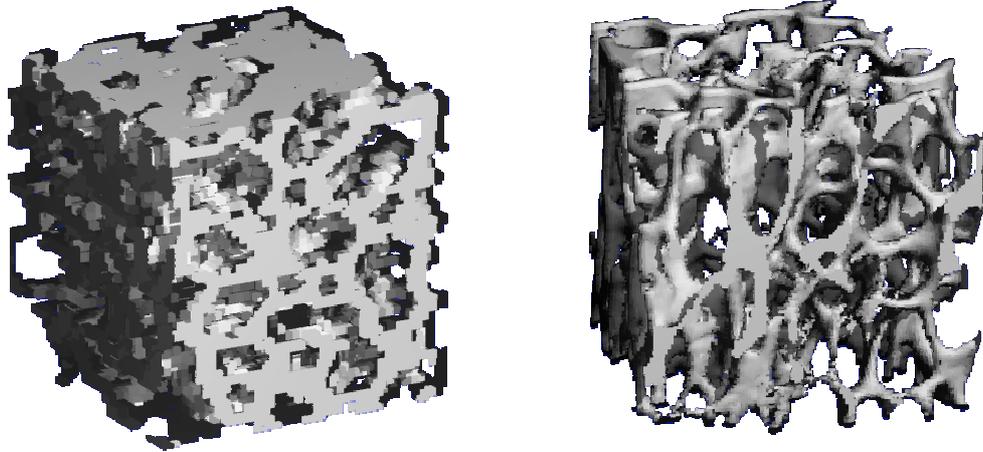


Fig. 2. Bone samples. Low resolution ("small") on the left, high resolution ("big") on the right.

Table 1. Description of case studies (timing is for 450 MHz Sun Ultra-80 with 4 Gb of RAM)

	"small"	"big"
dimensions	4.8 mm	4.5 mm
element size	120 microns	36 microns
number of elements	20098	192539
number of nodes	42508	305066
number of DoFs	127224	914898
nnz in half of M	1185888	9702186
nnz in half of K	3430140	28191660
Cholesky factor of K	$\approx 4.30e+07$ nnz, ≈ 400 Mb	$\approx 2.77e+08$ nnz, ≈ 3 Gb
Cholesky factorization of K	TAUCS in-core: 145 s	TAUCS out-of-core: 1072 s
time to generate 30 vectors	103 s	wall time $500 \times 30 = 15000$ s
full harmonic simulation	UMFPACK: 650 s x 60 frequencies = 39000 s	n/a

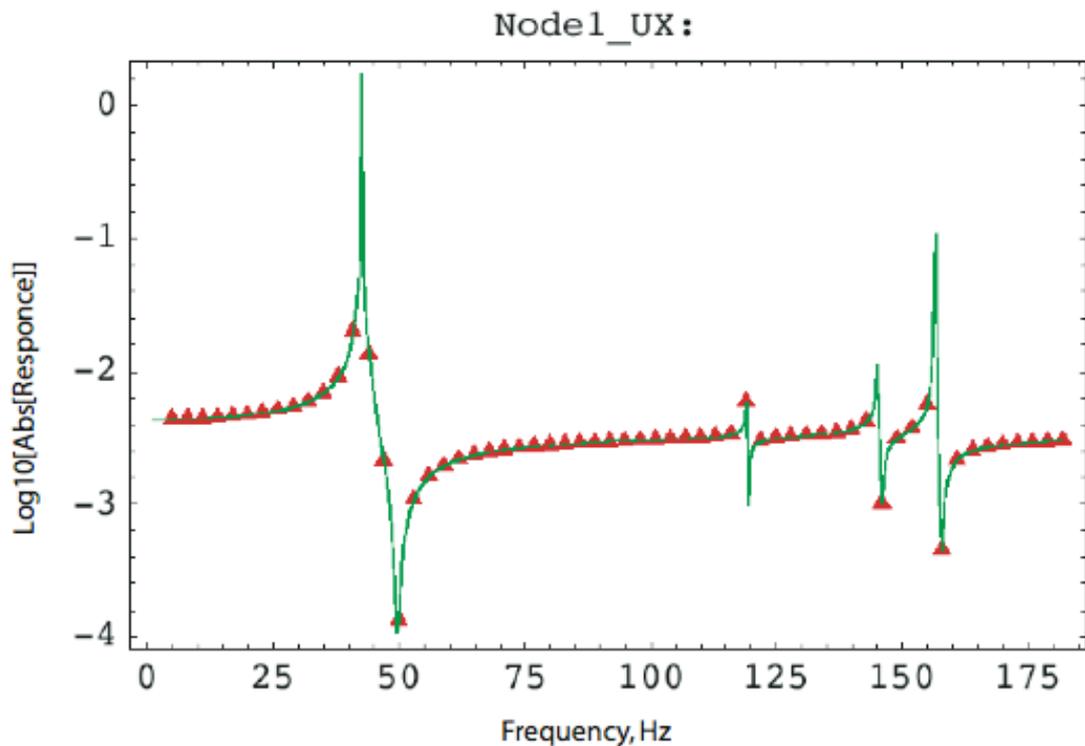


Fig. 3. Harmonic response for the "small" model. Red triangles are for the original high dimensional model (127224 equation), green line is for the reduced model of dimension 10.

In the case of the "small" model the size of the stiffness matrix factor was about 400 Mb and it was possible to use the in-core multifrontal algorithm from the TAUCS library. As a result, time to generate 30 vectors for the Krylov subspace (5) via the Arnoldi process was comparable with that to factorize the matrix. The total model reduction time was about two times of stationary solution with the accordance to observations in [6].

At the same time, harmonic response for the reduced model of dimension 10 matches perfectly that of the original model (see Fig. 3). We needed to use UMFPACK to compute the harmonic response of the original model as the final matrix in the system of linear equations in (2) is indefinite. The UMFPACK solver is designed for general non-symmetric matrices and its time for the stationary solution is four times more that that of TAUCS. However, even if we reduce the time for the full-scale harmonic simulation by a factor of four, it is still much longer then the model reduction time plus simulation of the reduced model. Needless to say that harmonic simulation of a model of dimension 10 takes just small part of a second. It is worthy of noting that the number of frequencies to evaluate harmonic response should be more than 60 and in this case simulation time for the original high-dimensional model increases accordingly.

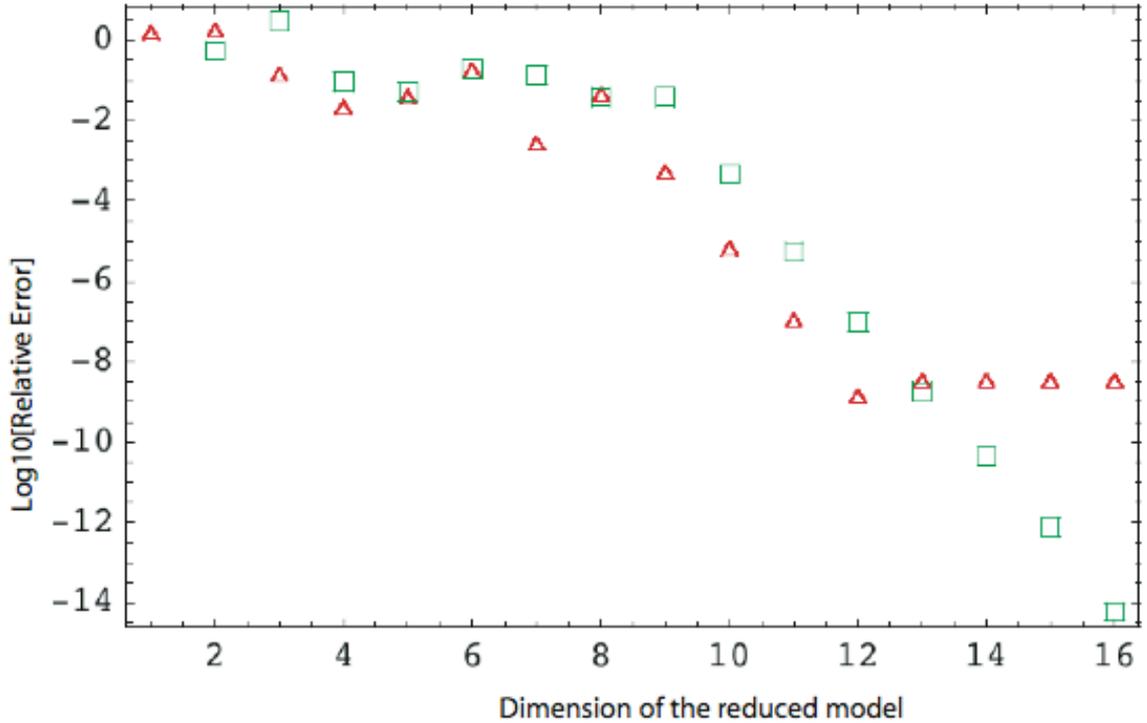


Fig. 4. Relative error for harmonic response at 182 Hz for the "small" model. Red triangles are for the true relative error, $\text{Abs}[\text{Full} - \text{Reduced}]/\text{Abs}[\text{Full}]$, green boxes are for the error indicator, $\text{Abs}[G_{n+1} - G_n]/\text{Abs}[G_{n+1}]$.

A natural question for model reduction is when to stop generating vectors in (5). Moment matching is based on the expansion of the transfer function around a chosen point. In our case, the expansion point is zero and thus the transfer function of a reduced model at zero is exactly the same as for the original model. Hence, a reasonable strategy to choose the dimension of a reduced model is to take the maximum frequency of interest and compare the transfer function at that frequency with the original model.

Fig. 4 shows the convergence of the relative error at 182 Hz for the "small" model. We see that the difference between the reduced and full models as a function of the dimension of the reduced model decreases rapidly after 8 vectors has been generated (red triangles). This explains our choice for the dimension equal 10 in Fig. 3.

The evaluation of the transfer function for the original model is expensive. In Ref [9], it has been shown that an error indicator could be employed instead. The error indicator is defined as the difference between the transfer functions of a reduced model with dimensions n and $n+1$. This is shown by green boxes in Fig. 4. We see that behavior of the error indicator is pretty close to the true error.

In the case of the "big" model, the factor size was already about 3 Gb. It was impossible to keep it and other matrices in the memory. Therefore, the only option was to use the out-of-core multifrontal algorithm from the TAUCS library. In this case, factoring time was by itself acceptable but a back substitution step took about 50% of the factoring time. It should be noted that the back substitution time was reported as "wall" time, the processor time being about 4 times less. In any case, there will be considerable saving in simulation time in respect to the original model.

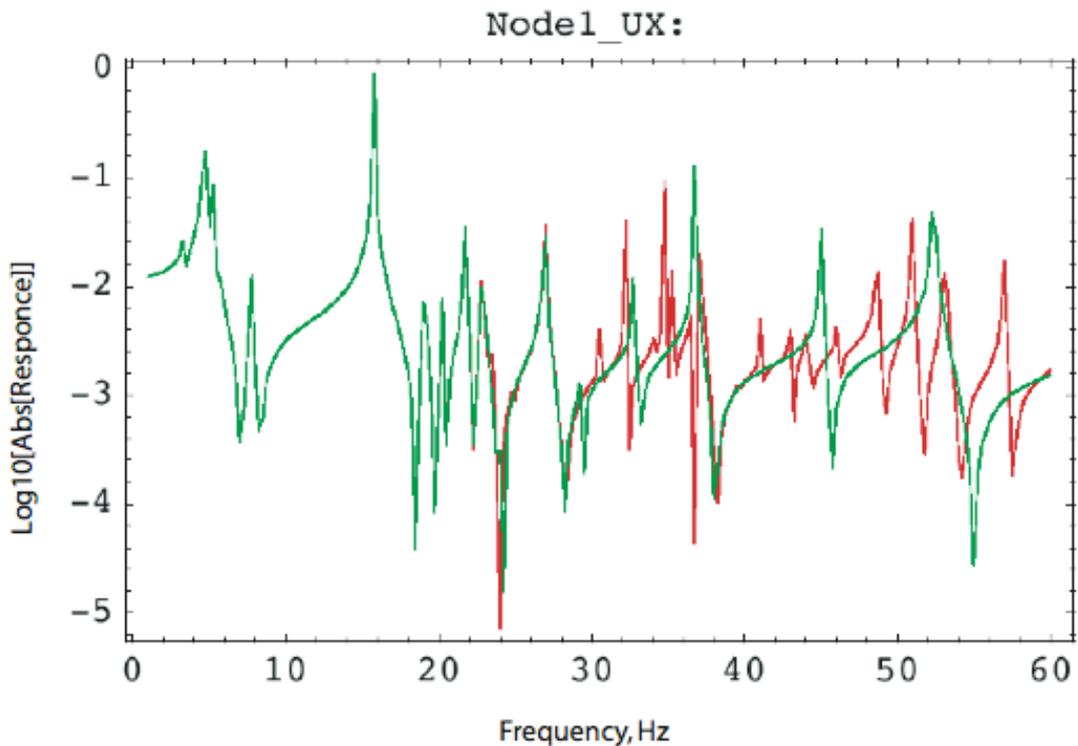


Fig. 5. Harmonic response for the "big" model. Green line is for the reduced model of dimension 25, red line is for the reduced model of dimension 50.

We could not make harmonic simulation for the original "big" model as UMFPACK does not support out-of-core. In Fig. 5, the harmonic response of the two reduced models with dimensions of 25 and 50 is shown. We see that up to about 30 Hz the results are the same. This means that there is no doubt that the behavior of the original model is described accurately up to this frequency (see also Fig. 6). After 30 Hz, the results for the reduced model with dimension of 50 (red line) is clearly more accurate. However, the error indicator at 60 Hz (see Fig. 6) says that even this reduced model may not be accurate up to 60 Hz.

Conclusion

We have demonstrated that model reduction is an efficient means to speed up harmonic simulation. With 4 Gb of memory and modern direct solvers, one can apply the model reduction algorithm to finite element models with up to 1 000 000 degrees of freedom. At the same time, this seems to be a limit for the hardware employed in our study. Parallel computing with a modern mainframe is required to scale the software to treat models with 100 000 000 degrees of freedom.

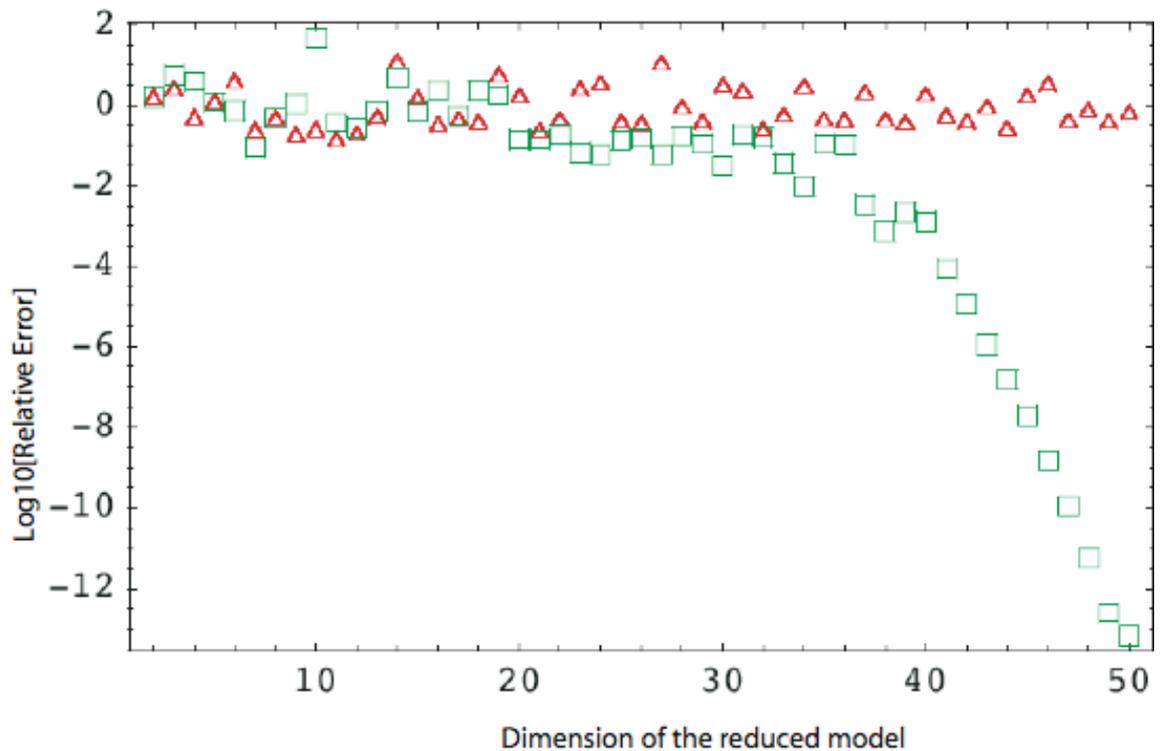


Fig. 6. Relative error for harmonic response for the "big" model. Red triangles are for the error indicator at 60 Hz, green boxes are for the error indicator at 30 Hz.

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