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Abaques Numériques: Visualisation et Post-Traitement de Solutions à Variable Séparée. Application au Temps Réel Non Linéaire

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Résumé — Today many solution strategies use internally some separation of variables to represent all the quantities (fields, linear operators...). This type of representation, in many cases, enables us to reduce drastically the amount of data to manipulate and store. But, the exploration and the post-treatment of this type of solutions is not an easy task. Mainly, because all the available software are not capable of taking into account the "separated" structure of the solutions. In this paper, we present a series of tools for the efficient storage and post-treatment of solutions in separated representation. Three application are presented : 1) the post-processing of a multidimensional solution of a mechanical problem, and the generation of the Pareto front of an associated optimisation problem, 2) the simulation in “real time” of a non linear deformable body, and an associated control problem. 3) practical application to the on-site help in the decision making process using lightweight device.

1 Introduction

The PGD (Proper General Decomposition) method [1] applied to multidimensional problems uses some kind of separation of variable to represent all the quantities of the problem to solve. In most cases, the quantities are represented as a finite sum of product of functions. For example, one possible separation is :

$$u(\mathbf{x}_1, \cdots, \mathbf{x}_{dim}) = \sum_{m=1}^{modes} f_1^m(\mathbf{x}_1) \times \cdots \times f_{dim}^m(\mathbf{x}_{dim}) \tag{1}$$

This decomposition of the field u, called canonical decomposition, is not unique. Others decompositions are possibles, like Tucker or H-Tucker [2] can be used. In this paper we focus our work on canonical decompositions only.

1.1 Multidimensional problems and PGD

The PGD method can be seen as a separation of variables strategy for finding a separated representation of an unknown field, knowing only the operator of the differential equation and the right hand side term. The solution of a problem using the PGD method is done in two steps. First, we decompose all the quantities (geometry, fields, operators...) of the problem in a separated form (similar to equation 1). Then, the strategy in its simplest form consists in the sequential calculation of the different terms of the sum (called "mode"). This stage in the strategy is called the enrichment step. The calculation of one mode is a non linear problem addressed by a classic fixed point algorithm. The main advantage of this approach is that inside the fixed point iteration only low dimensionality problems must be solved (dimension of the coordinate space $\mathbf{x}_i$). This enables us to solve multidimensional problems at very low cost.

The PGD method is capable of solving multidimensional problems in a very efficient way. This enables us to consider very challenging simulations. For example including parameters (like material properties, boundary conditions, geometrical parameters) as extra coordinates in the original problem. By post-processing these multidimensional solutions we are able to generate *virtual charts* or *computational vademecum*, that can be used to solve associated engineering design problems [3].

Some examples are :

1. finding the optimal parameters for a process,
2. identification of material properties,
3. real time simulation-based control,
4. on-site help in the decision making process using lightweight devices.

All these examples can benefit from the previously constructed *computational vademecum* in different ways. A very important point is that the sensitivity of the solution with respect to a coordinate can be calculated directly, e.g. :

$$\frac{\partial u(\mathbf{x}_1,\cdots,\mathbf{x}_{dim})}{\partial \mathbf{x}_{dim}} = \sum_{m=1}^{modes} f_1^m(\mathbf{x}_1)\times\cdots\times\frac{\partial f_{dim}^m(\mathbf{x}_{dim})}{\partial \mathbf{x}_{dim}} \tag{2}$$

1.2 Exploration of a "Virtual Chart"

The multidimensional solutions generated by the PGD method are very rich. But they must be kept in separated representation if we want to have a minimal memory footprint during exploration, because the full reconstruction of the solution is plagued by the curse of dimensionality.

With the aim of storing these solution a new file format, called PXDMF, was developed. It is based on the popular XDMF format (eXtensible Data Model and Format) [1], from which it inherits all the advantages like the compressed binary storage.

The 3D visualization of a separated variable solution needs the reconstruction of the multidimensional solution in a smaller dimension space. This is done by fixing some dimensions in order to always reconstruct solutions in lower dimension spaces. To make this task easier a plug-in was developed for the open source software ParaView [4] This module is able to reconstruct the solution on the fly, and to calculate automatically the sensitivity of the fields with respect to the fixed coordinates.

2 The PXDMF File Format

In general, the PGD method makes use of some kind of discretization of the spaces $\mathbf{x}_j$ (finite elements, finite difference…). So storing a solution in separated representation means that we have to store the spaces discretizations and all the functions $f_j^m(\mathbf{x}_j)$. This means that we have to store *dim* space discretizations, and *modes* fields in each discretized space (meshes and nodal values, in the case of FEM).

The main idea was to use an already existing format, the requirements were ; portability, robustness, and simplicity and of course the ability to store more than one mesh. The popular XDMF format (eXtensible Data Model and Format), fulfils all the requirements. In addition the XDMF format can handle binary and compressed data.

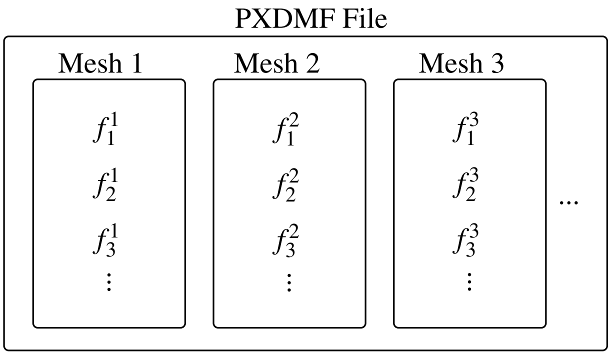


Fig. 1 – PXDMF internal Structure

A key advantage is that the files are written using the XML language (Extensible Markup Language) [2] to describe the data, making it human readable. In the case of large data, compressed binary files can be

[1] www.xdmf.org

[2] http://www.w3.org/TR/REC-xml/

used for a more efficient storage. The complete description of the PXDMF file format can be found in our site[5].

3 The ParaView PXDMF Tools Plugin

As said before, the evaluation of the solution at a point needs the evaluation of the functions f_j^m. To facilitate the reconstruction and the exploration, a series of tools was developed. These tools were in the form of a plugin for the visualization software ParaView.

The name of the plugin is PXDMFReader and the current version is 1.5.2. The plugin contains a reader, capable of reading PXDMF files and a series of filters and python routines. After loading the plugin in ParaView, a new file format is available in the `open` menu, and a new menu bar is available.

The plug-in (in binary format) is available on the site. Videos for the installation and examples are available on the web site[5].

3.1 The PXDMF Reader

The PXDMF Reader adds support to ParaView for reading separated representation data-sets stored in PXDMF file format. The PXDMF Reader was developed to reconstruct solutions stored in separated representation in a very user-friendly way. Once the solution is reconstructed, the data can be treated with all the techniques available in ParaView.

The properties of the reader are (Figure 3) :

Point Data and Cell Data : The Point (Cell) field to be loaded. If the number of Point (Cell) data modes are less than 100, then individual modes can be selected. This is used mainly for debugging purposes.

Visualization Space : The user can select the dimension(s) to put in the Visualization Space. Note : the Visualization Space can be different from the physical space of the problem. For example, an arbitrary parametric dimension can be selected and mapped to any dimension of the Vizualisation Space (Figure 2).

Visualization Time : The user can select a one-dimensional dimension to put in the Visualization Time. Again the Visualization Time can be different from the temporal dimension of the problem. Any unidimensional dimension can be in the Visualization Time (Figure 2).

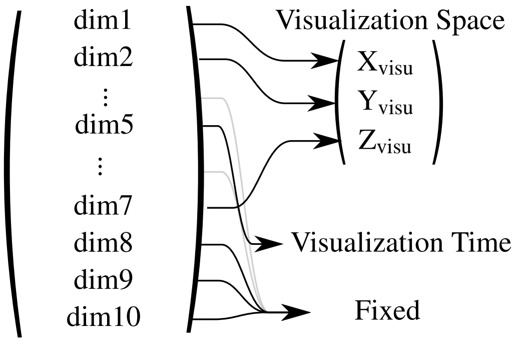


Fig. 2 – Mapping from the problem space to the Visualizaton Space and Time

Use Interpolation : This activate the use of the interpolation generated by the mesh. So the field can be computed at any point in the space. For example, between two point in a temporal dimension. If this check-box is not checked the closest point is used for the reconstruction.

Compute Derivatives : Compute Derivatives requires "Use Interpolation" to be enabled. When this option is enabled, the sensibility of the Point fields are automatically calculated with respect to the Fixed Dimensions and to the Temporal Dimension.

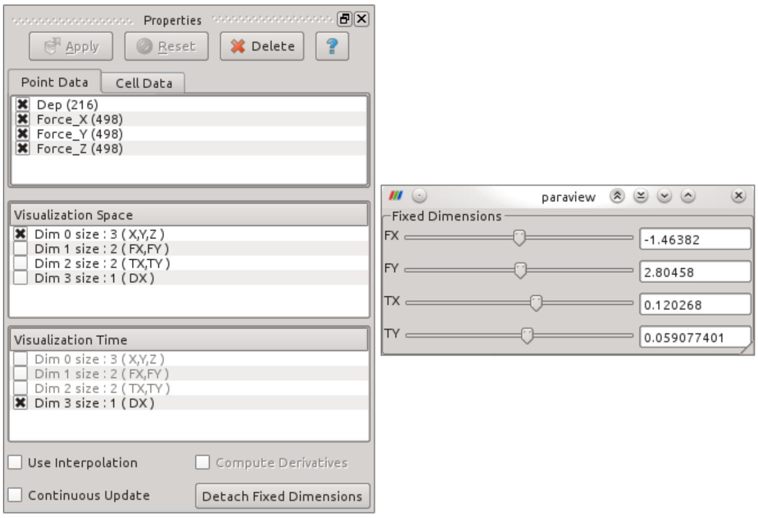
Continuous Update : This option enables us to bypass the need of clicking on the Apply button every time that we change a Fixed dimension. So the solution is updated in real-time (be careful not to use this option with very big data-sets).

Detach Fixed Dimensions : This button enables us to detach the Fixed Dimensions sliders so they can be changed easily.

Fixed Dimensions : All the dimension not in the Visualization Space neither in the Visualization Time.

Figure 3, shows the same dialog in a "Detach Fixed Dimension" mode with the first dimension ("Dim 0 size : 3 (X,Y,Z)") in the Visualization Space, and the fourth dimension ("Dim 3 size : 1 (DX)") in the Visualization Time. The two mapped spaces are automatically removed from the "Fixed Dimension" dialog.

The information about the names (and the units) of the dimensions used in the Visualization Space is passed to the generated solution, so if the user activates the option "Show cube axes" correct labels are generated.



☒ Dep (216)
☒ Force_X (498)
☒ Force_Y (498)
☒ Force_Z (498)

Visualization Space
☒ Dim 0 size : 3 (X,Y,Z)
☐ Dim 1 size : 2 (FX,FY)
☐ Dim 2 size : 2 (TX,TY)
☐ Dim 3 size : 1 (DX)

Visualization Time
☐ Dim 0 size : 3 (X,Y,Z)
☐ Dim 1 size : 2 (FX,FY)
☐ Dim 2 size : 2 (TX,TY)
☒ Dim 3 size : 1 (DX)

☐ Use Interpolation ☐ Compute Derivatives
☐ Continuous Update
Detach Fixed Dimensions

Fixed Dimensions
FX -1.46382
FY 2.80458
TX 0.120268
TY 0.059077401

Fig. 3 – Properties Dialog with X,Y,Z in the Visualization Space, DX in the Visualization Time and with Detached Fixed Dimensions

4 The Filters

Four filters are available in the plugin. The aim of these filter is to make easier some operations related with the separated representation of the solutions.

A new toolbar and a new sub-menu (Figure 4) inside the filter menu are available.

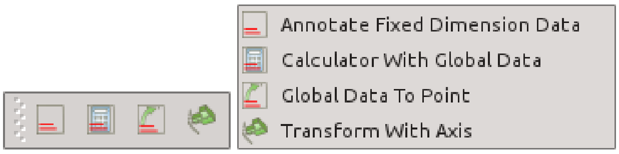


Fig. 4 – (Left) The PXDMF toolbar, (Right) The PXDMF menu on the Filter menu of ParaView

4.1 Annotate Fixed Dimension Data Filter

This filter enable one to annotate all the Fixed Dimension data including the Visualization Time dimension.The format of the annotation can be changed in the properties of the filter using C style format.The `%f` correspond to the format of the value and the `%s` correspond to the format of the unit (if present).

4.2 Calculator With Global Data Filter

The "Calculator With Global Data" filter computes a new data array or new point coordinates as a function of existing scalar or vector arrays. This filter is based on the original Calculator Filter available in ParaView. But adds the possibility of using global data (Fixed Dimension and Visualization Time) in the formula.

4.3 Global Data To Point Filter

The "Global Data To Point" filter creates a new point from the Global Data (Fixed dimension and Visualization Time). This filter is very useful for solution with parametric dimensions based on the physical space (e.g. position of a force, position of a crack).

4.4 Transform With Axis Filter

The "Transform With Axis" filter allows us to specify the position, size and orientation of a data sets. This filter is based on the original Transform Filter available in ParaView. Additionally this filter will move/scale/rotate the axis information. So when "Show cube axes" is enabled the axis are correctly named and correctly moved/scaled/rotated.

The "On Axes Also" option apples the transform filter on the axis of the data-set also.

This filter is very useful in the case of data with very different scales. For example, in the case of parametric data with very different units (Young modulus in one axis, and Poisson ratio in the other axis). The Young modulus normally is in the order of 10 GPa, and the Poisson ration is in the order of 1.

4.5 Python Routines

ParaView has a python console. This console allows the user to control most of the visualization using command lines. To make the control of the PXDMF Reader easier, some extra function are present in the plugin.

The class ReaderSync enables the user to synchronize and control several PXDMFReader at the same time. Additionally, extra functions are present to ease the manipulation of the camera.

note : Render() must be called to redraw the scene

5 Applications

5.1 Post-treatment and Pareto front

A first example is the post-treatment of a multidimensional solution of a mechanical problem, and the generation of the Pareto front of an associated optimisation problem. We consider a parametric model related to the elasticity problem in which parameters describing the material and the geometry are considered as extra-coordinates. A basic simple (but three-dimensional) problem was treated. In addition to the three-dimensional physical space, we add three new coordinates, one related to the Young's modulus E, one to the Poisson's ratio ν and one to the geometrical parameter e depicted in Figure 5. The boundary conditions are the followings : distributed surface force on the light-grey surface (red arrows), and displacement equal to zero on the dark-grey surface (left part of the left hole).

The simulation was done using the PGD method, to obtain a multidimensional solution containing the solution for any combination of material and geometrical parameters. More details about the PGD method applied to this example can be found in [3].

This problem was solved for $E \in [100, 250000]$MPa, $\nu \in [0, 0.45]$ and $e \in [1, 5]$, using the following decomposition.

$$\mathbf{u}(x,y,z,E,\nu,e) = \sum_{i=1}^{25} f_{xy}^{i}(x,y) \cdot f_{z}^{i}(z) \cdot f_{E}^{i}(E) \cdot f_{\nu}^{i}(\nu) \cdot f_{e}^{i}(e) \tag{3}$$

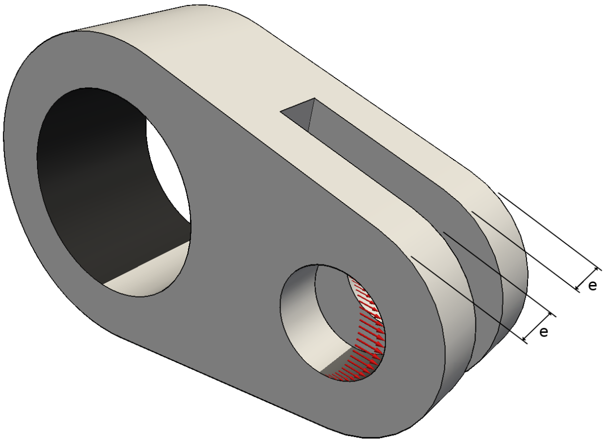


Fig. 5 – Physical space parametrized by the parameter *e*

The main motivation behind this kind of problem, is to optimize the parameter *e* as a function of the material properties. For example, for a series of given material families we can find the optimal thickness of the piece to ensure an elastic behaviour and the weight for the given thickness.

Figure 6 shows the optimal value of *e* for every material in the library. One important point is that the lightest piece does not correspond to the lowest value of *e*.

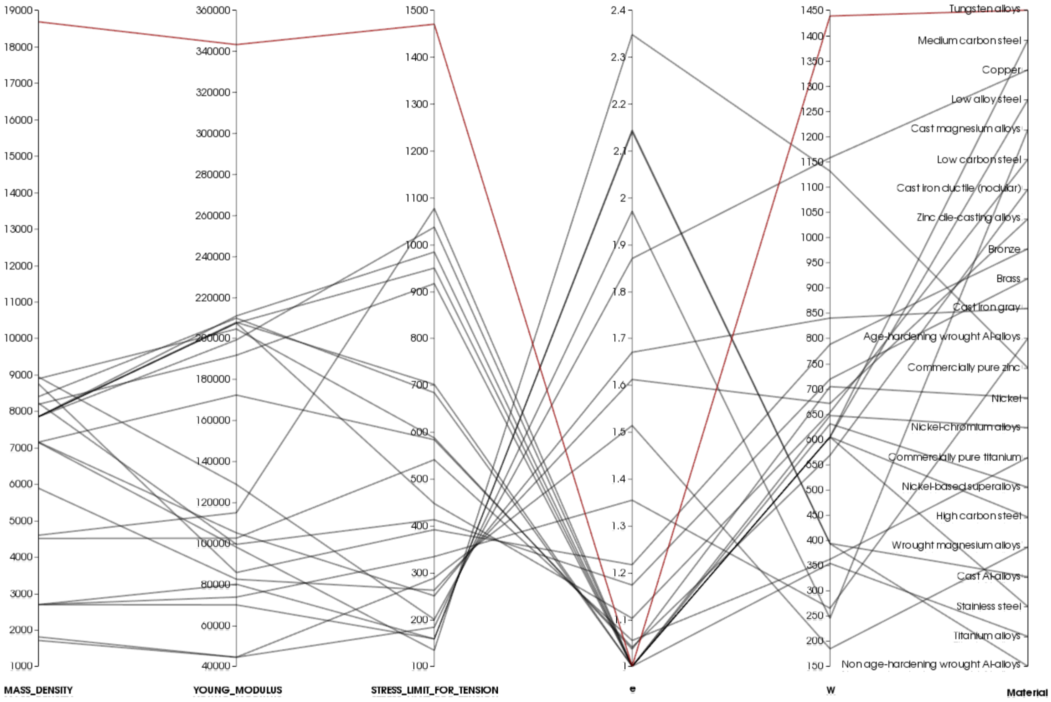


Fig. 6 – Parameters, optimal value of *e* and weight for ever material in the data base

The algorithm used for the optimisation was written in python using the tools presented in the previous sections.

5.2 Real time simulation of a deformable body

Real time simulation is one of the most challenging scenarios for simulation-based engineering sciences. The term *real time* strongly depends on the particular application, but surgery simulation is among the most demanding ones. Haptic surgery simulators compute the response of biological soft tissues and give it back to the peripherals at, at least, 25 Hz of feedback rate if visual realism is needed, and notably 500Hz-1kHz if haptic response is desired.

In this example, we pre-calculate using the PGD the response of a liver, to a force distribution applied on its surface. This force is parametrised by the position (p_x, p_y), the orientation $(\theta_x, \theta_y \in [-\pi/4, \pi/4])$ and the amplitude $(a \in [0,1])$. Additionally, we consider an extra coordinate to tune the stiffness of an embedded tumour $(e \in [0,5])$ (e represent the rigidity factor with respect to the healthy liver tissue).

The solution was written using the following decomposition :

$$\mathbf{u}(x,y,z,p_x,p_y,\theta_x,\theta_y,e,a) = \sum_{i=1}^{182} X_i(x,y,z) \cdot P_i(p_x,p_y) \cdot \Theta(\theta_x,\theta_y) \cdot E(e) \cdot A(a) \tag{4}$$

Figure 7 schematically shows the haptic device and the virtual (simulated) solid.

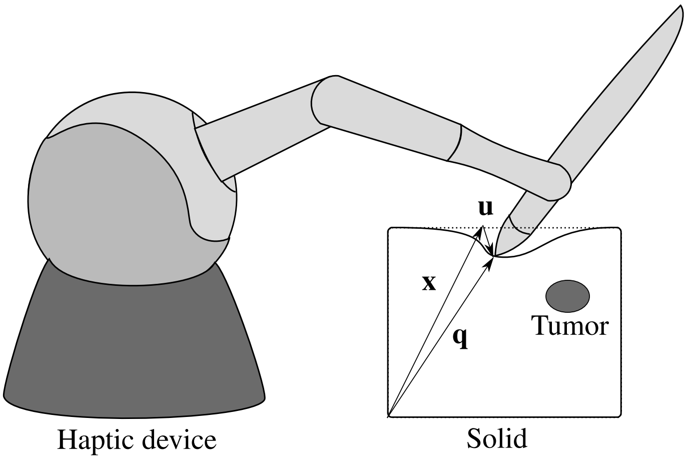


Fig. 7 – Haptic and cinematic relations

Is important to notice that the position of the force must be evaluated in the deformed configuration for realistic sensations. This means that the equation $\mathbf{q} = \mathbf{x} + \mathbf{u}$ must be satisfied for all times. Where $\mathbf{q}$ correspond to the position of the haptic device, $\mathbf{x}$ the position of the force in the reference configuration and $\mathbf{u}$ the displacement of point $\mathbf{x}$.

This non-linear equation must be solved in real time (at 1kHz rate). As said before the sensitivity of the field ($\mathbf{u}$) can be calculated directly using the equation (4). This enables us to use a Newton-Raphson algorithm for the resolution. After some tests we conclude that we need only one Newton-Raphson iteration at each haptic frame, since the algorithm is restarted 850 times per seconds with a initial guess that is very close to the solution.

Figure 8 shows a user manipulating the haptic arm at a visual frame rate of 20Hz and haptic frame rate of 850Hz.

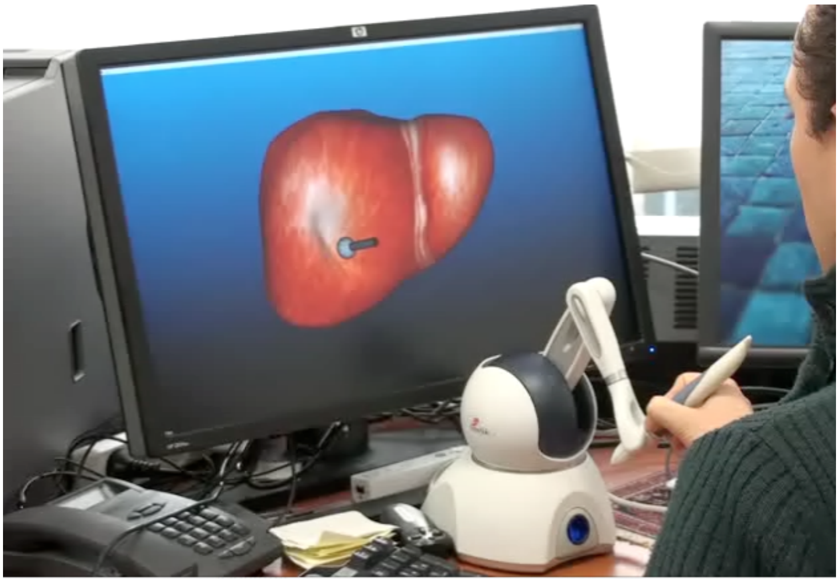


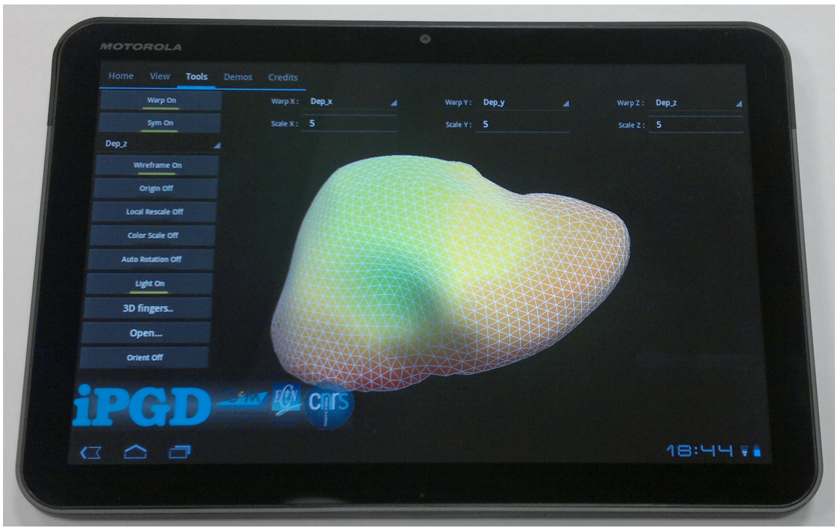
Fig. 8 – Liver palpation simulation at 850Hz haptic frame rate

5.3 Application using a lightweight device

In most cases the computed solution can be stored in such a compact form that it is compatible with handheld devices like smartphones and tablets. For Android-operated devices, an application has been developed (iPGD, freely downloadable form [5]) that can open and post-process separated representation solutions.

The user can fix some dimensions and the application is able to reconstruct the solution and generate a visual representation (1D, 2D or 3D). These solutions can be post-processed for the calculation of associated quantities of interest.

Figure 9 shows the visualisation of a solution on a Motorola Xoom Tablet.



Warp X : Dep_x
Scale X : 5
Warp Y : Dep_y
Scale Y : 5
Warp Z : Dep_z
Scale Z : 5

Fig. 9 – Visualisation of a multidimensional solution on a tablet

6 Conclusions

The PGD-based off-line/on-line approach opens numerous possibilities in the context of simulation based engineering for simulating, optimizing or controlling materials, processes and systems. The multidimensional structure of these *virtual charts* or *computational vademecum* demands innovative tools to circumvent the curse of dimensionality.

Références

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