High-Order Elements in Position Based Dynamics (Supplementary material)

Bastien Saillant* $\,\cdot\,$ Florence Zara $\,\cdot\,$ Guillaume Damiand $\,\cdot\,$ Fabrice Jaillet

1 Finite Element's Shape functions

In this section, we recall the shape functions used for the elements presented in this article, *i.e.* considering P1, P2, P3 tetrahedra, hexahedron Q1, pyramid and prism. These shape functions N_i are defined in their reference element (for $i \in \{0, ..., n\}$ with *n* the number of nodes of the considered element). Their partial derivatives have then been calculated using Sympy.

Linear tetrahedra (P1)

$$\begin{split} N_0(r) &= 1 - r_x - r_y - r_z \\ N_1(r) &= r_x \quad N_3(r) = r_y \quad N_4(r) = r_z \end{split}$$

Quadratic tetrahedra (P2)

$$\begin{split} N_0(r) &= (1 - r_x - r_y - r_z)(2(1 - r_x - r_y - r_z) - 1) \\ N_1(r) &= r_x(2r_x - 1) \\ N_2(r) &= r_y(2r_z - 1) \\ N_3(r) &= r_z(2r_z - 1) \\ N_4(r) &= 4r_x(1 - r_x - r_y - r_z) \\ N_5(r) &= 4r_xr_y \\ N_6(r) &= 4r_y(1 - r_x - r_y - r_z) \\ N_7(r) &= 4r_z(1 - r_x - r_y - r_z) \\ N_8(r) &= 4r_xr_z \\ N_9(r) &= 4r_yr_z \end{split}$$

Cubic tetrahedra (P3)

 $\begin{aligned} &a = (1 - r_x - r_y - r_z) \\ &N_0(r) = \frac{1}{2}(3a - 1)(3a - 2)a \\ &N_1(r) = \frac{1}{2}(3r_x - 1)(3r_x - 2)r_x \\ &N_2(r) = \frac{1}{2}(3r_y - 1)(3r_y - 2)r_y \\ &N_3(r) = \frac{1}{2}(3r_z - 1)(3r_z - 2)r_z \end{aligned}$

B. Saillant

E-mail: bastien.saillant@liris.cnrs.fr, INSA Lyon, UCBL, CNRS, LIRIS, UMR5205, F-69622 Villeurbanne

F. Zara

E-mail: florence.zara@liris.cnrs.fr, UCBL, CNRS, INSA Lyon, LIRIS, UMR5205, F-69622 Villeurbanne

F. Jaillet

E-mail: fabrice.jaillet@liris.cnrs.fr, IUT Lyon 1, UCBL, CNRS, INSA Lyon, LIRIS, UMR5205, F-69622 Villeurbanne

G. Damiand

E-mail: guillaume.damiand@liris.cnrs.fr, CNRS, INSA Lyon, UCBL, LIRIS, UMR5205, F-69622 Villeurbanne

$$\begin{split} N_4(r) &= \frac{9}{2}(ar_x)(3a-1)\\ N_5(r) &= \frac{9}{2}(ar_x)(3r_x-1)\\ N_6(r) &= \frac{9}{2}(r_xr_y)(3r_y-1)\\ N_7(r) &= \frac{9}{2}(r_xr_y)(3r_y-1)\\ N_8(r) &= \frac{9}{2}(ar_y)(3r_y-1)\\ N_9(r) &= \frac{9}{2}(ar_y)(3a-1)\\ N_{10}(r) &= \frac{9}{2}(ar_z)(3a-1)\\ N_{11}(r) &= \frac{9}{2}(ar_z)(3r_z-1)\\ N_{12}(r) &= \frac{9}{2}(r_xr_z)(3r_z-1)\\ N_{13}(r) &= \frac{9}{2}(r_yr_z)(3r_z-1)\\ N_{14}(r) &= \frac{9}{2}(r_yr_z)(3r_z-1)\\ N_{15}(r) &= \frac{9}{2}(r_yr_z)(3r_z-1)\\ N_{16}(r) &= 27a(r_xr_z)\\ N_{17}(r) &= 27(r_xr_yr_z)\\ N_{18}(r) &= 27a(r_yr_z)\\ N_{19}(r) &= 27a(r_xr_y)\\ \end{split}$$

Hexahedra (Q1)

$$\begin{split} N_0(r) &= \frac{1}{8}(1-r_x)(1-r_y)(1-r_z)\\ N_1(r) &= \frac{1}{8}(1+r_x)(1-r_y)(1-r_z)\\ N_2(r) &= \frac{1}{8}(1+r_x)(1+r_y)(1-r_z)\\ N_3(r) &= \frac{1}{8}(1-r_x)(1+r_y)(1-r_z)\\ N_4(r) &= \frac{1}{8}(1-r_x)(1-r_y)(1+r_z)\\ N_5(r) &= \frac{1}{8}(1+r_x)(1-r_y)(1+r_z)\\ N_6(r) &= \frac{1}{8}(1+r_x)(1+r_y)(1+r_z)\\ N_7(r) &= \frac{1}{8}(1-r_x)(1+r_y)(1+r_z) \end{split}$$

Pyramid

$$\begin{split} N_0(r) &= (-r_x + r_y + r_z - 1)(-r_x - r_y + r_z - 1)(4 - 4r_z)^{-1} \\ N_1(r) &= (-r_x - r_y + r_z - 1)(r_x - r_y + r_z - 1)(4 - 4r_z)^{-1} \\ N_2(r) &= (r_x + r_y + r_z - 1)(r_x - r_y + r_z - 1)(4 - 4r_z)^{-1} \\ N_3(r) &= (r_x + r_y + r_z - 1)(-r_x + r_y + r_z - 1)(4 - 4r_z)^{-1} \\ N_4(r) &= r_z \end{split}$$

Prism

$$\begin{split} N_0(r) &= \frac{1}{2}(1-r_x-r_y)(1-r_z) \\ N_1(r) &= \frac{1}{2}r_x(1-r_z) \end{split}$$

$$N_2(r) = \frac{1}{2}r_y(1 - r_z)$$

$$N_3(r) = \frac{1}{2}r_x(1 + r_z)$$

$$N_4(r) = \frac{1}{2}r_y(1 + r_z)$$

2 Isoparametric linear tetrahedron

Lets' now focus on the linear tetrahedron (P1) which is composed of 4 nodes $i \in \{0, 1, 2, 3\}$. As see previously, its shape functions N_i are defined in the reference element by:

$$N_0(r) = 1 - r_x - r_y - r_z.$$

 $N_1(r) = r_x, \ N_2(r) = r_y, \ N_3(r) = r_z$

The partial derivative with respect to the reference position is thus defined by:

$$\frac{\partial N(r)}{\partial r} = \left(\begin{array}{cc} \frac{\partial N_0(r)}{\partial r} & \frac{\partial N_1(r)}{\partial r} & \frac{\partial N_2(r)}{\partial r} \end{array}\right) = \begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}.$$

Considering initial position X and deformed position x, the Jacobian is defined by:

$$J(X,r) = \sum_{i=0}^{n=3} X_i \frac{\partial N_i(r)}{\partial r}^T = (X_1 - X_0, X_2 - X_0, X_3 - X_0)$$

$$J(x,r) = \sum_{i=0}^{n=3} x_i \frac{\partial N_i(r)}{\partial r}^T \\ = (x_1 - x_0, x_2 - x_0, x_3 - x_0)$$

In the FEM formulation proposed by Bender & Macklin [1,2] these Jacobians are called D_m and D_s . Note that the partial derivative of the shape function gives a constant matrix. Consequently, we don't need to define the coordinates of the quadrature point, and we only need a single evaluation for complete quadrature. In this case, the weight of the quadrature is equal to the volume of the tetrahedron at rest (denoted V_0), with $V_0 = w_0 \det(J(X, r_0)), w_0 = 1/6$, where w_0 corresponds to the weight of the quadrature point. This gives us the following energy gradient:

$$\nabla U = \sum_{i=0}^{n=3} V_i \mathbb{P}(x, r_i) J(X, r_i)^{-T} \frac{\partial N(r_i)}{\partial r}$$
$$= V_0 \mathbb{P}(x) J(X, r_0)^{-T} \frac{\partial N(r_0)}{\partial r},$$

where \mathbb{P} corresponds to the First Piola-Kirchhof stress tensor, V_i are quadrature's volume terms. Then, using the properties of the shape functions according to which the sum of their weights is always equal to one, we can deduce that a force is the negative sum of the others. This allows us to delete one row (the first in this case) from the partial derivative matrix, giving us the identity matrix. This is simplified as follows:

$$\left(\frac{\partial \nabla U}{\partial x_1}, \frac{\partial \nabla U}{\partial x_2}, \frac{\partial \nabla U}{\partial x_3}\right) = V_0 \mathbb{P}(x) J(X, r_0)^{-T}$$
$$\frac{\partial \nabla U}{\partial x_0} = -\frac{\partial \nabla U}{\partial x_1} - \frac{\partial \nabla U}{\partial x_2} - \frac{\partial \nabla U}{\partial x_3}.$$

We finally obtain the energy gradient presented by Bender [1].

3 Comparison with PolyFEM

Some of our experiments have been reproduced that shows some of the failure cases of linear element but compared this time with a reference generated using Polyfem. This open source library provides a state-ofthe-art pipeline for finite element simulation. Our reference meshes are the same as the one used in our paper. The experiments were carried out for linear (P1), quadratic (P2) and cubic (P3) tetrahedra. We use a Saint-Venant material which defined in our paper and Polyfem. We reproduced the tension (Fig. 1), torsion (Fig. 2) and bending test (Fig. 3 and Table 3). All experiment have the same poisson coefficient ($\nu = 0.35$), density ($\rho = 1000$). We do 1 iteration and 50 sub-step with the XPBD solver. The young modulus is E =1MPa for torsion and stretch tests, and E = 3MPafor the bending test.

Overall, the difference between elements is less striking. In particular, in the tension and rotation tests, it is difficult to see a difference between the element types as they all match the reference solution closely. However, in the bending experiment we observe that high order elements still give an accurate result with a coarse mesh where linear elements require a dense mesh to achieve the same accuracy.

Beam	#vertices	#elements	time (ms)	<i>e</i> (m)
	425	1,280	43.6	$1.5e^{-1}$
P_1	2,417	$10,\!240$	363	$5.1e^{-2}$
	$16,\!625$	81,920	$3,\!116$	$9.4e^{-3}$
P_2	393	160	20.9	$3.1e^{-3}$
P_3	573	80	28.1	$1.2e^{-2}$

Table 1: Bending test. Displacement error of the middle point at the end of each beam compared to the reference solution obtained for a beam composed of Q_1 elements.



Fig. 1: Tension test performed on P_1 , P_2 and P_3 biased beams having 637 vertices using a Poisson ratio ν set to 0.35. With a low Poisson ratio, elements acheive a similar result than the reference.



Fig. 2: Torsion test. Visualization of the cross-section of biased and unbiased beams colored according to the displacement. P_1 slightly deviate from the silhouette of the reference (in red). In both cas, they are a rough approximation of the reference. High-order meshes closely matched the reference for biased or unbiased meshes.

References

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Fig. 3: Top view of the beams considered in the unreformed state colored by the displacement induced by the bending test. A good solution must have all colors aligned with the reference obtained for a beam having 16,384 Q_1 elements. The greatest offset was for the beam composed of 1,280 P_1 elements. With 64 times more element, linear tetrahedron reach the same accuracy that cubic element.