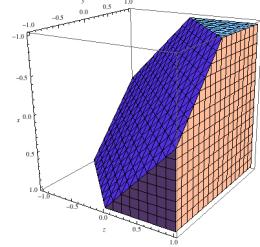


EQUIVALENT POLYNOMIALS LIBRARY

APPLICATION NOTE

By: Giulio Ventura – Politecnico di Torino
Library version: 1.1
Document version: 1.1
Website: www.equivalent-polynomials.net
Email: info@equivalent-polynomials.net



1. PREFACE

The Equivalent Polynomial Library is derived from the two papers:

1. Ventura G., On the elimination of quadrature subcells for discontinuous functions in the extended finite-element method. *International Journal for Numerical Methods in Engineering* 66 (2006) 761–795.
2. Ventura G., Benvenuti E., Equivalent polynomials for quadrature in heaviside function enriched elements, *International Journal for Numerical Methods in Engineering* 102 (2015) 688–710.

where the reader can find the theoretical background behind this library. *Users of this Library are kindly asked to cite these two papers in all their publications where the library has been used even if their publications does not directly address the problem of quadrature in Heaviside enriched formulations. Software houses are kindly asked to report these references in their manuals and online helps.*

The Library includes the FORTRAN Library files, an application example file calling the Library (main.f90) and the BibTeX file of the two above references.

The Library has been developed with reference to continuum mechanics problems. However, its methodology can be used in all fields of application of finite elements. Please feel free to contact me for custom development agreements of this Library.

Comments to this Application Note and Library usage are welcome.

2. NOTATION

In the present document x, y, z are the coordinates in the *parent local reference* of the element, with $x, y, z \in [-1, +1]$ for hexahedral elements (and quadrilaterals in 2D) and $x, y, z \in [0, +1]$ or tetrahedral elements (and triangles in 2D).

The discontinuity plane is assumed given in the parent reference system by the equation

$$a x + b y + c z + d = 0 \quad \text{in the 3D case}$$

$$a x + b y + c = 0 \quad \text{in the 2D case}$$

In the element the signed distance function is then defined by the equation (the 2D case is omitted for brevity)

$$\varphi = a x + b y + c z + d$$

Two cases will be considered, the standard XFEM/GFEM formulation, where the Heaviside function usually assumes the values +1 and -1 on the two sides of the discontinuity and the phantom node approach, where it is convenient to use the standard Heaviside function for “splitting” the element into its “positive” and “negative” part. To distinguish the two cases the Heaviside function will have a subscript indicating the jump in the Heaviside function.

Therefore, it will be:

$$H_2(\varphi) = \begin{cases} +1 & \varphi > 0 \\ -1 & \varphi \leq 0 \end{cases} \quad \text{for standard XFEM/GFEM formulations}$$

$$H_1(\varphi) = \begin{cases} +1 & \varphi > 0 \\ 0 & \varphi \leq 0 \end{cases} \quad \text{for phantom node formulations}$$

Let \mathbf{k}_e be the finite element matrix integrand to be evaluated and Ω_e the element (quadrature) domain. The finite element matrix will be given by

$$\mathbf{K}_e = \int_{\Omega_e} \mathbf{k}_e \, d\Omega$$

where some terms in \mathbf{k}_e will contain the discontinuous Heaviside function H_2 in the XFEM/GFEM case.

The Library has been developed considering $H = H_1$. However, it can be used also in the case $H = H_2$ as detailed in the following.

2.1. PHANTOM NODE APPROACH

In the phantom node approach, the element matrices related to the “positive” and “negative” part are evaluated as

$$\mathbf{K}_e^{(+)} = \int_{\Omega_e^{(+)}} \mathbf{k}_e \, d\Omega \quad \text{with } \Omega_e^{(+)} = \{x, y, z \in \Omega_e : \varphi > 0\}$$

$$\mathbf{K}_e^{(-)} = \int_{\Omega_e^{(-)}} \mathbf{k}_e \, d\Omega \quad \text{with } \Omega_e^{(-)} = \{x, y, z \in \Omega_e : \varphi < 0\}$$

this is equivalent to write

$$\mathbf{K}_e^{(+)} = \int_{\Omega_e} H_1(+\varphi) \mathbf{k}_e \, d\Omega$$

$$\mathbf{K}_e^{(-)} = \int_{\Omega_e} H_1(-\varphi) \mathbf{k}_e \, d\Omega$$

where the introduction of the Heaviside function allows to extend the integration to the entire element domain.

The above integrals (both in the XFEM/GFEM case and in the phantom node approach) cannot be evaluated by Gaussian quadrature because of the discontinuity of the integrands. However, as detailed in the reference papers reported above, this problem may be circumvented replacing the Heaviside function H_1 with its equivalent polynomial P_H . Note that this

replacement will double the polynomial degree of the integrand (P_H has the same polynomial degree as \mathbf{k}_e) and this must be accounted for by selecting the proper Gaussian quadrature rule.

Therefore, in the phantom node approach, the element matrices for the positive and negative part will be given by (note the integration in the entire element domain):

$$\mathbf{K}_e^{(+)} = \int_{\Omega_e} P_H(+\varphi) \mathbf{k}_e \, d\Omega$$

$$\mathbf{K}_e^{(-)} = \int_{\Omega_e} P_H(-\varphi) \mathbf{k}_e \, d\Omega$$

2.2. XFEM/GFEM APPROACH

When using XFEM/GFEM formulations the element matrix integrand can be always transformed as follows (see the above references for details):

$$\mathbf{k}_e = \mathbf{k}_e^P + H_2 \mathbf{k}_e^H$$

where \mathbf{k}_e^P and \mathbf{k}_e^H are polynomial functions (the effect of the Jacobian is neglected, see the References). In the above expression it has been taken into account the fact that the derivatives of H_2 are zeros, the even powers of H_2 are identically 1 and the odd powers of H_2 are equal to H_2 .

Therefore, the element stiffness is given by:

$$\mathbf{K}_e = \int_{\Omega_e} \mathbf{k}_e^P \, d\Omega + \int_{\Omega_e} H_2 \mathbf{k}_e^H \, d\Omega$$

The first addend has polynomial integrand and is Gauss integrable. The second is made polynomial by introducing the equivalent polynomial P_H as follows

$$\mathbf{K}_e = \int_{\Omega_e} \mathbf{k}_e^P \, d\Omega + \int_{\Omega_e} P_H(\varphi) \mathbf{k}_e^H \, d\Omega - \int_{\Omega_e} P_H(-\varphi) \mathbf{k}_e^H \, d\Omega$$

where the second addend on the r.h.s computes the integral in $\Omega_e^{(+)}$, where $H_2 = +1$, and the third computes the integral in $\Omega_e^{(-)}$, where $H_2 = -1$.

The above three addends are necessary since the Library has been constructed for the Heaviside function H_1 , not H_2 as needed by XFEM/GFEM standard formulations. An optimized library for XFEM/GFEM can be built, but the present choice allows the provided Library to be used for XFEM/GFEM and phantom node formulations at the same time.

3. LIBRARY USAGE

In the following a pseudocode is given for using the library in your computational code. This is given as an application example. A double loop over quadrature points is observed, one computing the result for the subdomain of the element where $\varphi > 0$ and the second for the subdomain where $\varphi < 0$. Note however that, by definition of equivalent polynomial, the quadrature domain and quadrature points are *always* referred to the *entire element*. In 2D applications the discontinuity plane coefficient d and the z coordinate are unused.

3.1. PHANTOM NODE APPROACH

```
Begin loop over finite elements e
    Determine discontinuity plane coefficients a,b,c,d
    Set element type etype
    /* compute equivalent polynomial coefficients */
    Call Heqpol_coefficients(a,b,c,d,eqcv,etype)
    Begin loop over Gauss points
        Set the Gauss point coordinates x,y,z
        /* evaluate equivalent polynomial at the Gauss point */
        PH = HEqPol(x,y,z,eqcv,etype)
        ke = ke + your code for element matrix calculation
    End loop over Gauss points
    Element assembly stage
    /* compute equivalent polynomial coefficients */
    Call Heqpol_coefficients(-a,-b,-c,-d,eqcv,etype)
    Begin loop over Gauss points
        Set the Gauss point coordinates x,y,z
        /* evaluate equivalent polynomial at the Gauss point */
        PH = HEqPol(x,y,z,eqcv,etype)
        ke = ke + your code for element matrix calculation
    End loop over Gauss points
    Element assembly stage
End loop over finite elements
```

3.2. XFEM/GFEM FORMULATION

```
Begin loop over finite elements e
    Determine discontinuity plane coefficients a,b,c,d
    Set element type etype
    /* compute equivalent polynomial coefficients */
    Call Heqpol_coefficients(a,b,c,d,eqcv,etype)
    Begin loop over Gauss points
        Set the Gauss point coordinates x,y,z
        /* evaluate equivalent polynomial at the Gauss point */
        PH = HEqPol(x,y,z,eqcv,etype)
        ke = ke + your code for element matrix calculation
    End loop over Gauss points
    /* compute equivalent polynomial coefficients */
    Call Heqpol_coefficients(-a,-b,-c,-d,eqcv,etype)
    Begin loop over Gauss points
        Set the Gauss point coordinates x,y,z
        /* evaluate equivalent polynomial at the Gauss point */
        PH = - HEqPol(x,y,z,eqcv,etype)
        ke = ke + your code for element matrix calculation
    End loop over Gauss points
    Element assembly stage
End loop over finite elements
```

4. MONOMIAL BASES AND TESTING PROCEDURE

In the following Table the monomial terms of the equivalent polynomial are given for the elements implemented in the Library. This is useful for determining proper quadrature rules.

Element description	etype	Monomial basis
2D linear triangle	20	{1}
2D bilinear quadrilateral	21	{1, x, x ² , y, xy, y ² }
3D linear triangle	30	{1}
3D trilinear hexahedron	31	{x, x ² , y, xy, x ² y, y ² , xy ² , x ² y ² , z, xz, x ² z, yz, xyz, x ² yz, y ² z, xy ² z, z ² , xz ² , x ² z ² , yz ² , xyz ² , y ² z ² }

In general, the monomial term has the form $x^i y^j z^k$ with $i, j, k \in \mathbb{N}$. By definition of equivalent polynomial it is, for any i, j, k in the above Table:

$$\int_{\Omega_e} x^i y^j z^k P_H(\varphi) d\Omega = \int_{\Omega_e^{(+)}} x^i y^j z^k d\Omega$$

$$\int_{\Omega_e} x^i y^j z^k P_H(-\varphi) d\Omega = \int_{\Omega_e^{(-)}} x^i y^j z^k d\Omega$$

This property can be used for testing purposes, as the volumes and the moments of the two subdomains $\Omega_e^{(+)}$ and $\Omega_e^{(-)}$ can be computed. This testing procedure is implemented in the file `main.f90`.

The terms contained in the monomial basis Table above are the ones appearing in the integrand \mathbf{k}_e for continuum mechanics problems. Custom libraries can be developed for different fields of application as specified in the Preface of this Application Note.

5. APPLICATION REMARKS

There is only one tunable parameter in the Library that is the tolerance tol for vanishing plane coefficients. As default, a coefficient is assumed zero if its absolute value is smaller than $tol \max(|a|, |b|, |c|)$ in the 3D case and $tol \max(|a|, |b|)$ in the 2D case. The coefficient tol is set by default to 10^{-4} .

6. LIBRARY FILES

File	Description
<code>eqpol.f90</code>	Equivalent Polynomial Library file
<code>main.f90</code>	Library usage example file
<code>hex_ph_23_a.f90, hex_ph_23_ab.f90, hex_ph_23_abc.f90, hex_ph_23_ac.f90, hex_ph_23_b.f90, hex_ph_23_bc.f90, hex_ph_23_c.f90</code>	Coefficients for hexahedrons (used by include statements)
<code>quad_ph_6_a.f90, quad_ph_6_ab.f90, quad_ph_6_b.f90</code>	Coefficients for quadrilaterals (used by include statements)