

The unsymmetric finite element formulation and variational incorrectness

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Abstract. The unsymmetric finite element formulation has been proposed recently to improve predictions from distorted finite elements. Studies have also shown that this special formulation using parametric functions for the test functions and metric functions for the trial functions works surprisingly well because the former satisfy the continuity conditions while the latter ensure that the stress representation during finite element computation can retrieve in a best-fit manner, the actual variation of stress in the metric space. However, a question that remained was whether the unsymmetric formulation was variationally correct. Here we determine that it is not, using the simplest possible element to amplify the principles.

Keywords: mesh distortion; unsymmetric formulation; best-fit paradigm; parametric-metric element; projection theorem; three-node bar element.

1. Introduction

Distorted finite elements are known to be much less accurate than finite elements of regular shape, e.g., a quadrilateral element as compared to a rectangular element (Stricklin *et al.* 1977, Backlund 1978, Gifford 1979, Arnold *et al.* 2002). Isoparametric plane stress elements (8-node and 9-node based on the serendipity and Lagrangian shape functions) performed extremely well for regular meshes based on elements of square or rectangular geometry but this degraded rapidly when the elements were distorted. These are all based on standard symmetric finite element formulations where identical trial and test functions are used.

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Rajendran and co-workers (Rajendran and Liew 2003, Ooi *et al.* 2004, Rajendran and Subramanian 2004) explored the novel use of unsymmetric formulations characterized by the use of two separate sets of shape functions, viz., the so-called *compatibility* (or *continuity*) enforcing shape functions and the so-called *completeness* enforcing shape functions. The former are chosen to satisfy exactly the minimum inter- as well as intra-element displacement continuity requirements, while the latter are chosen to satisfy all the (linear and higher order) completeness requirements so as to reproduce exactly a quadratic displacement field. Numerical results from test problems reveal that the new plane stress element (Rajendran and Liew 2003) is capable of reproducing exactly a complete quadratic displacement field under all types of admissible mesh distortions only if the *continuity* enforcing shape functions are based on *isoparametric* functions and are actually the *test* functions while the *completeness* enforcing shape functions are based on *metric* forms and are now the *trial* functions. The physical insight into why the test functions should be *continuity* enforcing and why this is ensured if *isoparametric* functions are adopted is easy to understand (Rajendran and Subramanian 2004).

Prathap and co-workers (1993) have proposed that variationally correct (i.e., no variational crimes are committed) finite element computation automatically seeks out stresses in a best-fit manner (the computed stresses are a best-approximation of the actual stresses) at the element level. This is stated mathematically as a projection theorem (Strang and Fix 1973) or as an orthogonality condition (Babuska and Stroubolis 2001) at the global level. Recently (Prathap and Mukherjee 2003, 2004) it has been shown that the best-fit nature is valid at the global level because it is indeed valid at the element level, the global best-fit emerges holistically out of the local best-fits. Prathap *et al.* (2005) also showed that the reason why the unsymmetric parametric-metric formulation has the greatest mesh distortion immunity is because the stress representation is managed in the metric space and this is what is expected of the best-fit paradigm of finite element computation.

One issue that has not been addressed so far is whether the unsymmetric formulation is variationally correct. It is easy to appreciate that where symmetric formulations are used, e.g., the PP formulation or the MM formulation where both the trial and test functions are based consistently on using the parametric functions (P-functions) throughout or the metric functions (M-functions) throughout, the energy is defined by symmetric matrices, and that the virtual work condition is exactly satisfied. Here, we return to the virtual work statements to determine that the PM formulation, even though it is practically a very useful device to meet the continuity requirements and the best-fit stress recovery requirements in a distorted element, is not variationally correct. The simplest possible element, the three-noded bar element, is used to amplify the principles.

2. The weak form or virtual work statement of the standard symmetric FEM formulation

Following the nomenclature used in Strang and Fix (1973), we write the weak form in terms of the energy inner product for the exact solution for the displacements u to the problem.

$$a(u, u) = (f, u) \quad (1)$$

$$a(u, u^h) = (f, u^h) \quad (2)$$

where $a(u, u)$ is the bilinear symmetric functional and (f, u) is the integral $\int u f dV$ over the system domain V . Note that this statement is made over the global domain and is not meaningful at the element domain unless the element boundary conditions are also introduced in the form of prescribed element boundary displacements or boundary stress resultants or reactions.

The first two virtual work statements refer to the exact solution of the elastostatic problem. In Eq. (1), the trial function and test function are taken as u and the virtual work argument establishes that Eq. (1) is truly satisfied only when u is the exact solution at the point of equilibrium. In Eq. (2), we take note of the fact that the test function u^h (the Ritz or finite element solution) need not be the exact displacement function for the virtual work principle to be true. For convenience, we take this to be the discrete finite element displacement field, as long as it is admissible (that is, satisfies all the geometric boundary conditions).

It is in the next equation that we take the final step towards discretisation. By using u^h for both the trial and test function (i.e., the standard symmetric FEM formulation), we get the actual finite element equations, with the right hand side leading to the consistent load vector and the left hand side representing the stiffness matrix.

$$a(u^h, u^h) = (f, u^h) \quad (3)$$

This equation will now reflect the error due to the finite element discretisation. We are now in a position to see how the error $e = u - u^h$ can be assessed. Comparing Eqs. (2) and (3) and noting that the energy inner product is bi-linear, we can arrive at

$$a(u, u^h) = a(u^h, u^h)$$

and from this we obtain the projection theorem

$$a(u - u^h, u^h) = 0 \quad (4)$$

The finite element solution is therefore seen to be a best-fit or best approximation solution at the global level when the standard symmetric formulation is used.

3. What happens when we use \hat{u} as the M-function and \bar{u} as the P-function in the unsymmetric formulation?

In the unsymmetric formulation, we examine the possibility of using separate trial and test functions. Rajendran *et al.* (Rajendran and Liew 2003, Ooi *et al.* 2004, Rajendran and Subramanian 2004) propose two possible candidates for the basis functions. We can use the isoparametric interpolation functions (here denoted by \bar{u} as the P-function finite element spaces instead of u^h) or the metric interpolation functions (here denoted by \hat{u} as the M-function finite element spaces instead of u^h).

The exact virtual work statement represented by Eq. (2) earlier can now be re-stated alternatively as

$$a(u, \bar{u}) = (f, \bar{u}) \quad (5)$$

$$a(u, \hat{u}) = (f, \hat{u}) \quad (6)$$

In Eqs. (5) and (6), the virtual work equations are still exactly satisfied.

The approximate PP finite element formulation is now governed by

$$a(\bar{u}, \bar{u}) = (f, \bar{u}) \quad (7)$$

Similarly, the approximate MM finite element formulation is governed by

$$a(\hat{u}, \hat{u}) = (f, \hat{u}) \quad (8)$$

We see immediately, following the same argument that deduced Eq. (4) from Eqs. (2) and (3), that from Eqs. (5) and (7) and Eqs. (6) and (8) respectively

$$a(u - \bar{u}, \bar{u}) = 0 \quad (9)$$

$$a(u - \hat{u}, \hat{u}) = 0 \quad (10)$$

This ensures that the symmetric formulations, namely the PP and MM versions are both variationally correct, and produce best-fit results.

We now investigate what happens in the approximate PM formulation. This is governed by

$$a(\hat{u}, \bar{u}) = (f, \bar{u}) \quad (11)$$

The appropriate comparison now is between Eq. (11) and Eq. (7) and this leads to the interesting orthogonality condition that

$$a(\bar{u} - \hat{u}, \bar{u}) = 0 \quad (12)$$

In other words, the PM formulation is not an exact best-fit of the exact solution u and to that degree is variationally incorrect. Indeed, the orthogonality we are assured of in Eq. (12) is that the stress from the PM formulation will be orthogonal to the stress from the PP formulation. We will use this later in the error analysis section.

4. The 3-noded bar element using parametric and metric functions

Fig. 1 shows the 3-noded bar element of length L with nodes at x_1 , x_2 and x_3 . We assume that the node x_2 is not at the centre of the bar so that the distortion parameter $\eta = x_2 - L/2$. The parametric

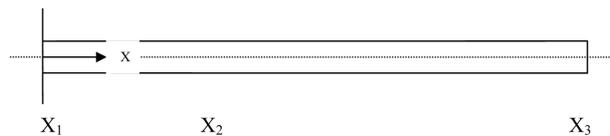


Fig. 1 The 3-noded bar element with nodes at x_1 , x_2 and x_3

(better known as isoparametric) formulation requires the interpolation of the x coordinate using $x = N_i x_i$ and the displacement field $u = N_i u_i$ where N_i are the quadratic interpolation parametric functions and x_i are the nodal coordinates and u_i is the nodal displacement vector.

If g is the natural coordinate so that x_1 is at $g = -1$, x_2 is at $g = 0$ and x_3 is at $g = 1$, then x and u are interpolated by

$$x = g(g-1)/2x_1 + (1-g^2)x_2 + g(g+1)/2x_3 \quad (13a)$$

$$u = g(g-1)/2u_1 + (1-g^2)u_2 + g(g+1)/2u_3 \quad (13b)$$

Although a quadratic interpolation is assumed for the displacement field, we note that when node x_2 is not at the centre of the bar so that the distortion parameter \circ is non-zero, the strain $\varepsilon = du/dx$ is no longer a linear function of x .

Indeed we have

$$\varepsilon = du/dx = [(u_3 - u_1)/2 + g(u_1 + u_3 - 2u_2)]/[(x_3 - x_1)/2 + g(x_1 + x_3 - 2x_2)] \quad (14)$$

where the denominator represents the Jacobian governing the transformation from x to g spaces. If x_2 is not exactly mid-way between x_1 and x_3 , J is no longer a constant and it is this that accounts for the inaccuracy of the distorted element (Prathap *et al.* 2005). Rajendran and co-workers (Rajendran and Liew 2003, Ooi *et al.* 2004, Rajendran and Subramanian 2004) proposed that distortion immunity is obtained if the interpolation for the real strain/stress is derived from trial functions in the metric, i.e., x space. The metric part of the formulation now uses $u = M_i u_i$, where M_i are the metric functions. It is a simple exercise to derive these functions (Rajendran and Subramanian 2004).

5. Formulation of PP, PM and MM versions of the 3-noded bar element

Rajendran and co-workers have given a very elaborate account of the formulation of the unsymmetric problem (Rajendran and Liew 2003, Ooi *et al.* 2004, Rajendran and Subramanian 2004). For the sake of completeness, this is summarized as shown below. The parametric shape functions are defined as

$$N_1 = g(g-1)/2, \quad N_2 = (1-g^2) \quad \text{and} \quad N_3 = g(g+1)/2 \quad (15)$$

From this, the strain displacement matrices can be written as

$$\mathbf{B}_p = [N_{1,g}, N_{2,g}, N_{3,g}]/x_{,g} \quad (16)$$

The metric functions M_i can be easily derived (Rajendran and Subramanian 2004) and the corresponding strain displacement matrices are

$$\mathbf{B}_m = [M_{1,x}, M_{2,x}, M_{3,x}] \quad (17)$$

The stiffness matrices for the PP, MM and PM elements are then

$$\mathbf{K}_{pp} = \int (\mathbf{B}_p)^T \mathbf{D} \mathbf{B}_p dx \quad (18)$$

$$\mathbf{K}_{mm} = \int (\mathbf{B}_m)^T \mathbf{D} \mathbf{B}_m dx \quad (19)$$

and

$$\mathbf{K}_{pm} = \int (\mathbf{B}_p)^T \mathbf{D} \mathbf{B}_m dx \quad (20)$$

The consistent load vector for the PP and PM cases is identical and is given by

$$\mathbf{f}_{pp} = \mathbf{f}_{pm} = \int (\mathbf{N})^T \mathbf{b} dx \quad (21)$$

while that for the MM case is

$$\mathbf{f}_{mm} = \int (\mathbf{M})^T \mathbf{b} dx \quad (22)$$

where \mathbf{b} is the body force.

6. A numerical experiment with the 3-noded bar element

We take up a single element test where the bar is fixed at $x_1 = 0$ and free at $x_3 = 1$. The length of the bar is therefore $L = 1$. The Young's modulus is taken as $E = 1$, area of cross-section $A = 1$, and a concentrated load $P = 1$ is assumed to be applied at node N_2 . The units are assumed to be consistent so that we have $\sigma = \varepsilon = 1.0$ for $x < x_2$ and $\sigma = \varepsilon = 0$ for $x > x_2$.

Three elements are developed for the purpose of the present investigation. The PP element, is the standard symmetric formulation using the parametric interpolations for both trial and test functions. The MM element uses metric interpolations for both test and trial functions thus resulting again in a symmetric formulation, while the PM element uses parametric interpolations for the test functions and metric interpolations for the trial functions and this is an unsymmetric formulation. The matrix algebra corresponding to these versions of the element has been outlined above. The PP and PM element formulations use a 2 pt. order of numerical integration for the stiffness matrix while the MM element requires a 3 pt. order of numerical integration. The 2 pt. rule is generally favoured for the PP element in the literature as this produces the best results. Indeed this is so as it is the optimal rule that corresponds to the best-fit nature of stress recovery. We shall see later that because of this the stresses are optimal at the Gauss points corresponding to the 2 pt. rule whatever the distortion.

Table 1 displays the results from a single-element mesh using the PM and MM models described above of the test case when the distortion term \cap is varied. Immediately, we notice that the displacements u_3 from the two FEM models, and for whatever value of distortion, are exact!

Table 1 Displacements u_2 and u_3 for a single-element test of fixed-free bar with concentrated load of $P = 1$ at node N_2 as location x_2 is moved by \cap

Disp.	$\cap = 0$			$\cap = -0.05$			$\cap = -0.15$		
	MM	PM	Exact	MM	PM	Exact	MM	PM	Exact
u_2	0.4375	0.4375	0.500	0.3863	0.3881	0.450	0.2778	0.2931	0.350
u_3	0.500	0.500	0.500	0.450	0.450	0.450	0.350	0.350	0.350

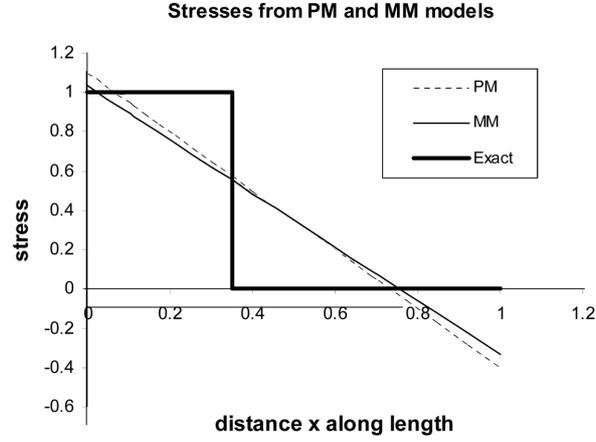


Fig. 2 Stresses from PM and MM models compared with exact stress when concentrated load is placed at $x_2 = 0.35$

However, this is not true of the displacement u_2 for all the cases displayed in Table 1. This is in fact a consequence of the best-fit paradigm.

Fig. 2 shows the variation of stresses computed from the displacements from the PM and MM models as compared to the exact stress in the bar when the concentrated load is placed at $x_2 = 0.35$ ($\cap = -0.15$). Both PM and MM, due to the use of the M-trial functions, give a linear variation. It can be very easily checked that the stress from MM (shown by the thin solid line) is an exact best-fit of the actual stress variation (thick solid line) whereas the stress from PM (thin broken line) is in error. By exact best-fit we mean that the projection theorem (Eq. (4) or (10)), which is a consequence of the virtual work principle, is exactly satisfied. In an approximate sense, this can be interpreted as the minimization of the least squares error of the stresses (or strains) over the element domain. We shall make the predictions relevant to this in the next section so that a more definitive closure between predictions and computations is achieved.

7. Closure between predictions and computations

What has been observed phenomenologically (in this case, computed by the finite element model) must be reconciled with predictions independently arrived at from first principles.

The exact stress/strain is defined in metric space as $\sigma = \varepsilon = 1.0$ for $x < x_2$ and $\sigma = \varepsilon = 0$ for $x > x_2$. This is shown as the thick solid line in Fig. 2. Note that $x_2 = 0.5 + \cap$. We also know that the stress from the PM and MM models, which are derived from quadratic functions in the metric space will be linear. Let us denote by σ_{pm} and σ_{mm} the stresses computed from the PM and MM models. We shall also denote by $\sigma' = a + bx$, the stress which is a best fit to σ . It is a very easy exercise to show that a consequence of σ' being a best-fit to σ following the projection theorem (Eq. (10)) is the relationship

$$\sigma' = a + bx = (1.25 + \cap - 3\cap^2) - (1.5 - 6\cap^2)x \quad (23)$$

when the concentrated load is placed at $x_2 = 0.5 + \cap$.

We know that at the Gauss points $g_i = \Gamma/3$, the values of x_i are

$$x_a = (0.5 + \cap) - 0.5/3 - \cap/3 \quad (25a)$$

$$x_b = (0.5 + \cap) + 0.5/3 - \cap/3 \quad (25b)$$

Let us now propose that the stress σ^* can be interpolated in the linear fashion in x as

$$\sigma^* = a + bx \quad (26)$$

We see from Table 3, that at the Gauss points $g_i = \Gamma/3$, the stresses σ_{pm} are exactly 0.93301 and 0.06699 and that this is independent of the distortion parameter \cap . We now presume that this can be used to constrain σ^* in Eq. (26) and determine the constants a and b . Indeed in doing so we get

$$a + bx_a = 0.93301 \quad (27a)$$

$$a + bx_b = 0.06699 \quad (27b)$$

from which we get $a = (1.25 + \cap)$ and $b = -(1.5)$ and we have now predicted from these simple first principles that

$$\sigma^* = (1.25 + \cap) - (1.5)x \quad (28)$$

These predictions are now incorporated into Table 3. The scientific closure is now complete! The PM formulation yields stresses which are a best fit to the stresses from the PP formulation and not to the actual stresses and this is variationally incorrect.

8. Variational correctness, orthogonality and best fit of an unsymmetric formulation like the PM formulation

The three issues, namely variational correctness, orthogonality and the best-fit paradigm are intermingled in a curious way. Immediately, we can ask about the significance of terms like variational correctness, orthogonality and what is meant by the best-fit nature of finite element computation. This has never been an issue when symmetric formulations based on the conventional Galerkin method are used. If no other variationally incorrect procedures are introduced (e.g., reduced integration, use of non-conforming basis functions, etc.) then the orthogonality condition implies the best-fit of the computed stresses to the stresses from the exact solution as seen from Eq. (4) above. However, we also saw above that when an unsymmetric formulation like the PM approach is adopted, this is no longer clear cut. Thus a closer examination of the issues is in order.

Rajendran (2005) pointed out that the unsymmetric formulation is in conformity with the virtual work principle, as seen from Eq. (11). However Eq. (12) seems to indicate that even if this is interpreted as being variationally correct, the orthogonality that ensues from this ensures only a best-fit of the computed PM stress to the computed PP stress, as we established above when we closely examined the scientific closure of the predictions.

We can review this as follows:

For unsymmetric formulations (say, PM) the virtual work statement is written as shown in Eq. (11). Comparing Eqs. (11) with Eqs. (5) and (7), the possible orthogonality conditions for the PM formulation are

$$a(u - \hat{u}, \bar{u}) = 0 \quad (29)$$

$$a(\bar{u} - \hat{u}, \bar{u}) = 0 \quad (30)$$

Both Eqs. (29) and (30) emerge from the virtual work principle and seemingly satisfy the orthogonality condition. This can be verified after the actual computations are performed, as has been confirmed by Rajendran (2005). However, from Eq. (29), one cannot conclude that \hat{u} is a best fit to either u or \bar{u} . Fortunately, from Eq. (30), one can actually conclude that \hat{u} is a best fit to \bar{u} . So here, a dilemma presents itself: whether to equate this best fit possibility to variational correctness, or to equate orthogonality to variational correctness, as both definitions appear possible. What we are proposing here is that the latter is a more meaningful and useful statement. The engineer is often concerned about whether the stress he has computed is a best-fit of the actual state of stress in the exact solution of the problem.

Jafarali (2005), in a personal communication, suggested a graphical way to represent the orthogonality conditions reflected in Eq. (30). Fig. 3 is a geometric representation of the PP finite element computation from the best-fit and the function space point of view. Fig. 4 is the equivalent geometric representation of the MM finite element computation from the same considerations. The PP and MM surfaces are easy to identify as the trial and test functions are identical and belong to the same sub-space. The PM formulation is now a tricky one to represent in this manner. Following Jafarali (2005), the geometric representation of the PP, MM and the PM finite element computation from the best-fit and the function space point of view is shown in Fig. 5. With the PM formulation, we have to negotiate two subspaces. The virtual strain (test function) is in the P space while the real stress (trial function) is in the M space. The orthogonality is usually expressed between the error, e.g., $(u - \bar{u})$ and the approximation (\bar{u}) . The exact solution then becomes $(u) = (\bar{u}) + (u - \bar{u})$. In

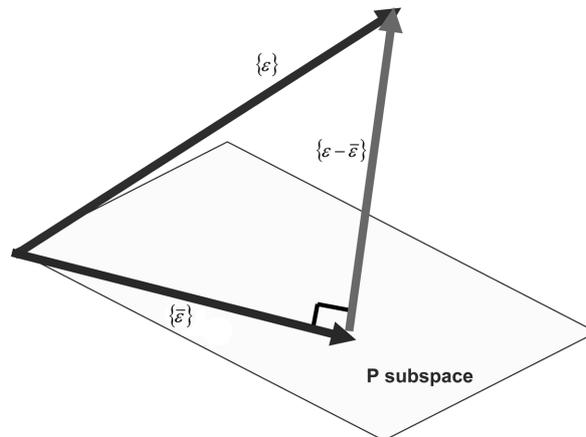


Fig. 3 The geometric representation of the PP finite element computation from the best-fit and the function space point of view

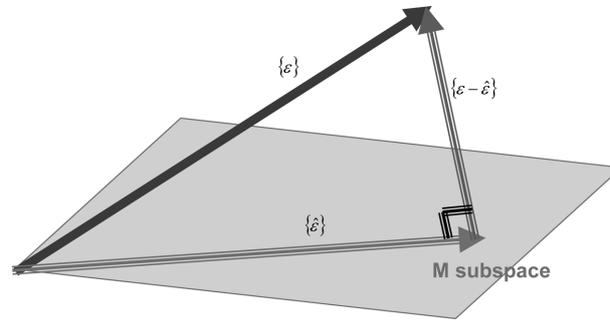


Fig. 4 The geometric representation of the MM finite element computation from the best-fit and the function space point of view

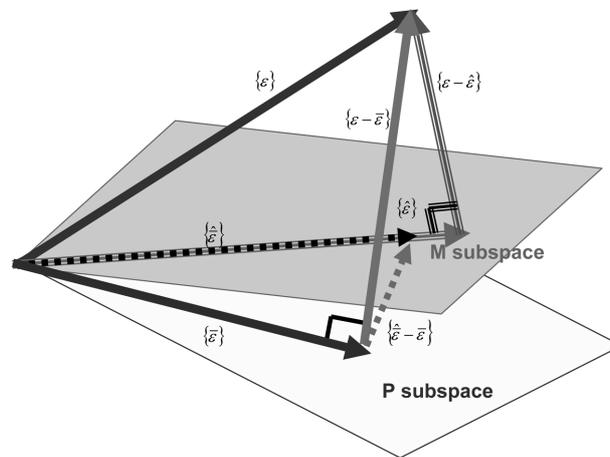


Fig. 5 The geometric representation of the PP, MM and the PM finite element computation from the best-fit and the function space point of view

both the PP and MM formulations, the approximate solution is a “shadow” of the exact solution projected on to the respective sub-space of the approximate function space. But in the PM case, this is not straight forward. The error, shown in Fig. 5 as the blue-green dotted arrow, is now orthogonal to (\bar{u}) , in other words, we are computing the “shadow” (e_{PM}) which will produce another “shadow” (e_{PP}).

9. Conclusions

The novel unsymmetric finite element formulation using parametric functions for the test functions and metric functions for the trial function works surprisingly well (Rajendran and Liew 2003, Ooi *et al.* 2004, Rajendran and Subramanian 2004). It was shown by Prathap *et al.* (2005) that this is enabled only because the use of parametric functions for the test functions helps satisfy the continuity conditions across element edges while the use of metric functions for the trial functions ensures that the stress representation during finite element computation can retrieve in a best-fit manner, the actual variation of stress in the metric space, when elements are distorted. In

this paper, we have seen that this unsymmetric formulation, although very effective, is strictly not variationally correct. When it comes to a distorted mesh, especially in 2D and 3D modelling (Rajendran and Liew 2003, Ooi *et al.* 2004, Rajendran and Subramanian 2004), one has to choose between satisfying the continuity condition on the edges of adjoining element and the variational correctness of the correspondence between the actual stress and the approximate stress. Some compromise has to be made.

Again, this paper confirms that in finite element modelling, the best-fit paradigm gives an accurate picture of how strains and stresses are computed, even when there is distortion in the element leading to a non-uniform mapping from the parametric to metric space. We could also succeed in using the best-fit paradigm to predict independently from first principles, the stresses that the unsymmetric PM formulation will produce in an actual finite element computation.

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