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Error Estimates for h-Adaptive Finite Element Analysis

by

Marilyn Ann Johnston
B. Eng. (Mechanical)

A thesis submitted to the Faculty
of Graduate Studies and Research
in partial fulfilment of the
requirements for the degree of

Master of Engineering

Department of
Mechanical and Aerospace Engineering
Ottawa-Carleton Institute for Mechanical and Aerospace Engineering
Carleton University
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**Error Estimates for h-Adaptive Finite
Element Analysis**

submitted by

M. A. Johnston, B.Eng.
in partial fulfilment of the requirements
for the degree of Master of Engineering

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July 1994

Abstract

The development of adaptive mesh-management algorithms enables a finite element solution to be improved by modifying the mesh according to given criteria. This development requires the use of a quality control measure to drive the adaptive procedures. Error estimates measure the error in the finite element solution, and provide necessary information to modify the mesh, and obtain an improved solution.

A generic *a posteriori* error estimate is developed to interact between the finite element analysis and the adaptive mesh-management software. The error estimate is independent of the nature of the problem. It can drive the adaptive procedures by computing errors in any scalar quantity such as temperature, displacement, effective stress, phase fraction and effective plastic strain fields. The error estimate provides both a local and a global error prediction.

The error estimate software is tested with four preliminary testcases. The analytical solutions for these tests are computed so the true error in the finite element solution can be calculated for comparison. In all testcases the error estimations are consistent with the true errors and, as expected, refining the mesh is shown to decrease element and global errors.

A second stage of verification considers more complex, practical engineering problems, for which analytical solutions do not exist. Here, errors for a thick-walled pressure vessel and a single-pass weld are calculated. The error predictions correspond to expected values and the error estimate software is judged to be useful, sufficiently accurate and reliable.

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Nomenclature

a	radius of plastic deformation
C^0	the function is continuous, the first derivative is not
COUNT	counter
D	material property matrix
e	difference between true solution and finite element solution
en	energy norm
E	element error
E_{gt}	global error
FEAG	global array of nodal gradients
g	true gradient
$\hat{g}$	gradient obtained from finite element analysis
gl	global
GPARRAY	Gauss point gradient data
i	counter
j	j^{th} element
J	Jacobian matrix
k	thermal conductivity
L_2	L_2 or mean square norm
LNODS	global list of nodes
m	counter
n	Gauss point
N	shape functions
NSUB	number of subelements

P	weighted least squares projection matrix
P_i	internal pressure
PRMVAR	primary variable
Q	flux
r	radial coordinate
r_i	inner radius
r_o	outer radius
SMTHNG	array of local smoothed nodal gradients
SUBGP	Gauss point subelement gradient data
T	true temperature
T_i	temperature at inner surface
T_o	temperature at outer surface
T_∞	surrounding temperature
$\hat{T}$	temperature obtained from FEA
TMPSM	temporary array of smoothed nodal gradients
TRUEG	array of global smoothed Gauss point gradients
TYPXYZ	subelement orientation
u	true displacement
$\hat{u}$	displacement obtained from finite element analysis
W	Gauss point weight
$\ x\ _e$	norm of x for each element
$\ x\ _{en}$	energy norm of x
$\ x\ _{gl}$	global norm of x
$\ x\ _{L_2}$	L_2 norm of x
XDIV	subelement division in x -direction
YDIV	subelement division in y -direction

ZDIV	subelement division in z -direction
ϵ_{pl}	plastic strain
σ_1	first principal stress
σ_2	second principal stress
σ_3	third principal stress
σ_{eff}	effective stress
σ_h	hydrostatic stress
σ_l	longitudinal stress
σ_r	radial stress
σ_t	tangential stress
σ_y	yield stress
ξ	local coordinate
η	Zienkiewicz and Zhu error estimate
Ω	domain of the analysis

Chapter 1

Introduction

The finite element (FE) method is a vital tool for the analysis of structural, solid, fluid, and material mechanics. An important issue for researchers today, is to determine the errors involved and to make a judgement of the quality of the obtained solution. In the past, commercial computer codes incorporated few, if any, quality control measures into their solution procedures. The quality of the solution was therefore judged by the user, based primarily on his or her own experience. Current research has shown that there are numerous procedures for estimating the error in the FE analysis and therefore improving the solutions.

There are two fundamental and important questions facing users of modern computational methods. First, how good are the answers, and second, how can one obtain the best possible answer for a fixed computational effort, for example limited financial or human resources?

The solution to these questions as stated by Oden *et al.*^[1] is to develop procedures which use the evolving computed solution to determine estimates in local errors in various norms, over each element and at each time step. This is followed by adaptive procedures which continually change the structure of the mesh so as to keep local errors within a specified limit. These adaptive procedures might be necessary to follow temporal changes, such as a moving heat source, or when elements in a mesh have become severely distorted. The latter might occur, for example, in an analysis of a forging process.

When problem solving, analysts are frequently faced with several different concerns. In one case, the analyst may be interested in a global quantity such as forming pressure, in another, the extent of the plastic zone may be of interest. Ductile rupture might require accurate predictions of the effective plastic strain, or the stress triaxiality factor, σ_h/σ_{eff} . Predictions of principal stress may be a concern for fracture analysis. In each case, the analyst needs to have some prediction of the accuracy of the solution. An error estimate capable of examining many different quantities, would provide this prediction.

Error estimates are intended to provide solutions to the following three questions:

1. How good is the overall solution?
2. How good is the local solution at critical points of interest? The areas of interest could include, for example, a crack tip or a heat-affected zone.
3. Where should the mesh be refined or coarsened?

A solution to the first question is necessary as a general measure of the quality of the solution. Questions 2 and 3 are essential for adaptive methods. Both are local measures of solution accuracy and can be useful even if the overall solution is considered incorrect. For example, if elements with the largest estimated error correspond to those with the largest true error, the prediction can still show where to refine the mesh, regardless of the overall solution.

When the computed error is higher than a specified limit for a given adaptive analysis, the estimated element errors are used to guide the mesh refinement. After the mesh has been redefined according to some desired or given error distribution, the local properties are mapped from the old mesh to the new mesh before the solution process can resume^{[2][3]}.

Once the error of the element is obtained the FE mesh can be adaptively altered using one of three approaches. The first approach involves p-refinement^{[4][5]} and/or h-refinement^{[6][7][8][9]}. P-refinement is the procedure of increasing the order of the polynomial approximation within an element. H-refinement consists of

subdividing the element into smaller elements. The second approach, classified as moving finite element methods or r-methods^[10], deforms the function space by moving the nodes. Finally an entirely new mesh can be created through a rezoning or remeshing process^{[11][12][13]}.

H-refinement and h-coarsening are used in the present research project^{[14][15]}. H-refinement is simple and intuitively understood^[16]. H-coarsening is a natural extension. When the solution is rough or irregular; i.e., the gradient is discontinuous, h-refinement is thought to be more efficient than p-refinement^[17]. Discontinuous gradients are often found at elasto-plastic boundaries and in the vicinity of local effects. To reduce the computational costs which arise from maintaining a fully refined mesh, h-coarsening may be implemented if required^[17].

The numerous errors involved in the finite element solution include modelling errors, discretization errors, and manipulation errors^[18]. Modelling errors could arise due to the choice of continuum model for the problem, for example, three-dimensions (3D) simplified to two-dimensions (2D) or one-dimension (1D), or because of uncertain input data such as geometry or load. Discretization errors are a result of the geometric approximation of the domain, choice of element mesh, element approximation, and numerical integration. Finally, manipulation errors include errors in input data, truncation errors, and round-off errors. The primary concern of this research is to determine the discretization errors resulting from the choice of element mesh.

An optimal mesh is often defined as, one in which the error is equally distributed over all the elements^[12]. There are two reasons why FE programmers strive toward an optimal mesh. First, if the exact solution has a singularity, then the rate of convergence is governed by this singularity as the mesh is refined. The singularity effect on the rate of convergence is eliminated with an optimal mesh^[18]. This makes it possible to achieve a prescribed accuracy with the least number of degrees of freedom. Secondly, the degree of error can be improved as the mesh is refined toward the optimal configuration^[18].

Although an optimal mesh would be ideal, each iteration of an adaptive anal-

ysis involves a FE analysis and therefore increases the computational costs. Thus it is important to seek a reasonably optimal mesh and achieve the accuracy requirements as quickly and efficiently as possible.

Error estimates measure the error in the solution and provide information required to modify the mesh and obtain an improved solution. There are two types of error estimators, *a priori*, and *a posteriori*. *A priori* error estimates are frequently used for very simple problems but are rarely available for more complex analysis. *A posteriori* estimates use the information obtained during the solution process to determine errors in both the local and global sense^[17]. Of the three main types of *a posteriori* error estimates, Babuška and Rheinboldt^[20] developed the residual type, Zienkiewicz and Zhu^[21] the post-processing type and Eriksson and Johnson^[22] the interpolation type. Zienkiewicz and Zhu's error estimate appears to be the most widely used method^[18]. It is shown to be simple, reliable and accurate for most engineering problems, provided an appropriate post-processing technique is used^{[16][21][23][24][25][26][27]}. A brief description of remeshing techniques, the three common forms of *a posteriori* error estimates, along with the duality method developed by Mashaie^[19], are outlined in the following sections.

1.1 Remeshing Techniques

Although remeshing techniques are not generally applicable to the current research which uses h-adaptive procedures, it is important to acknowledge developments made in error estimation for remeshing methods^{[11][12]}. In these methods the entire mesh is rezoned when the error becomes too large. Cheng *et al.*^[11] developed a criterion to indicate when remeshing should be performed for stress problems. Cheng believes that physically, the error represents the difference in deformation among the elements and thus serves as an indicator of element distortion. Once the maximum accumulated error among all the elements reaches a prescribed level; perhaps 10%, a new, less distorted mesh is created on the deformed configuration. Habraken *et al.*^[12] developed a similar error estimate by assuming that remeshing

should be done when the errors due to spacial discretization become too large.

1.2 Residual Methods

There are two forms of residual methods, the first being the element residual method, and the second the subdomain residual method. In the element residual method the difference between the finite element solution and the differential equation is computed over each element. An error estimation is made by utilizing residuals from the governing differential equations. For stress problems, residuals determined from the equilibrium equations and the jump in the normal derivative of the solutions along element boundaries are used. For this method the error as well as the finite element solution are substituted in the weak form of the problem statement; e.g., a Galerkin formulation. The weak statement is an integral over the domain and is equivalent to satisfying the governing equations and the natural boundary conditions. Interpolating functions of higher order than those used to compute the solution are then used to estimate the error. Babuška and Rheinboldt developed this method for both linear and nonlinear problems and produced the results in 1978^[20]. The error indicators were determined for each element in a local sense, therefore eliminating global computations.

From 1982 to 1986 Zienkiewicz^[28] also developed techniques based on the element residual method. The error measures are computed from the residuals in the equations of equilibrium, measured in the energy norm due to the introduction of one additional degree of freedom in the finite element solution. The error in the system will asymptotically diminish as the number of degrees of freedom increases. Both Wiberg^[18] and Mashaie^[19] feel that although this method is widely used, the error estimations based on residual calculations are not reliable since they do not indicate the true error in the solution. The validation of finite element results by this method is slow and very expensive^[19]. Furthermore, unless the differential equation is known, the error can not be computed for different variables as required.

The second residual method, the subdomain method, uses a patch of sur-

rounding elements to find the error for a given element. It is a very complicated mathematical procedure in which the error estimates are expressed in the energy norm and are different for coarse and fine meshes. Mashaie^[19] believes that the complexity of the subdomain-residual method reduces the viability of this error estimator.

1.3 Interpolation Method

The interpolation method involves approximating the second order derivatives of the primary variable in the problem. To do this, the difference between the gradients in the element and those of its neighbors is calculated. The gradients are normalized using the element size. The local error is the maximum error value of the surrounding elements.

In FE analysis it is often important to determine accurate estimates of the derivatives of the local variable. For example, in stress analysis the primary unknowns are the displacements, however it is frequently necessary to determine the strains and stresses which are computed from the derivatives of displacements. It is well known that the stresses at the boundaries are discontinuous so it is important to determine the location in the element that will give the most accurate estimate of the derivatives. These points are called the superconvergent points^[18]. Frequently, the use of superconvergent points is implemented to improve the estimates of the second order derivatives^{[29][30][31]}.

To implement this method it is necessary to determine a constant, which depends on the geometry of the domain and varies as the problem changes. This constant is generally difficult to compute. Also, this method assumes that there is a bound on the second order derivative, however this assumption does not hold when concentrated loads are considered^[18]. Furthermore, sufficient accuracy in this error estimation has not been consistently observed^[27].

1.4 Postprocessing Method

There are numerous postprocessing methods used in practice today. One of the most popular postprocessing methods is that of Zienkiewicz and Zhu^[21]. This technique has been implemented in heat transfer and fluid flow problems^[16], stress analysis^[21] including plate flexure and general thick plate theory, including shear deformations^[24], and plastic flow of metals and polymers^[25].

To determine the error estimate, Zienkiewicz and Zhu^[21] compare the FE solution to a postprocessed solution. Zienkiewicz and Zhu^[21] showed that globally smoothed values of stresses which represent a higher order approximation to the original stresses obtained from the finite element analysis, can be used instead of the exact value to calculate the error norm. A nodal averaging or projection process is used in which it is assumed that the continuous stress field is interpolated by the same function as the displacement. This process is easily implemented in any code because, generally, the continuous stress field and the FE stress field have already been evaluated. This error estimate allows the global energy norm error to be determined and also gives a good evaluation of local errors. This method is computationally simple, and by coupling the error estimate with an automatic mesh generator many difficulties associated with integrating a fully adaptive structure with an existing code can be bypassed^[23].

The method developed by Zienkiewicz and Zhu^[21] was used by Lewis *et al.*^[16] for heat transfer where a globally smoothed value of the temperature gradients is calculated. The smoothing is done by the least squares method using basis functions of the same order as those used for the temperature. They require that all the elements of the final mesh must contain an approximately equal error^[16]. The research of Lewis *et al.*^[16] also included developing an error estimate and adaptive procedure for steady-state flow problems. They suggest using an adaptive procedure governed by the Navier-Stokes equations that is based on an energy norm. The error norm is defined much the same as in the heat diffusion problem using velocity gradients rather than temperature gradients.

Another example of the use of Zienkiewicz and Zhu's^[21] postprocessing method is the work of Yunus *et al.*^[27]. This error estimate combines the Zienkiewicz and Zhu^[21] estimator with a continuous stress field approach. It is effective, efficient, and is applicable to all the plate and shell elements developed using either classical plate and shell or continuum mechanics theories^[27].

Other postprocessing error estimators have been developed by Donzelli *et al.*^[30] and Shephard *et al.*^[31]. The adaptive analysis of Donzelli *et al.*^[30] is based on an error indicator which is the L_2 norm of the difference between the finite element solution and a projected finite element solution. They show a projector-based error indicator scheme which successfully combines with finite element analysis of soft hydrated tissues to produce adequate results.

Shephard *et al.*^[31] also use stress projectors to evaluate the error estimate. The stress projectors are defined to yield C^0 continuous values over the domain of the problem. Shephard *et al.* show that the use of projectors to define a continuous field is more useful than the discontinuous finite element results.

In general, the postprocessing method is simple and can be implemented in any finite element code^[21]. The drawback to this method is that it fails to produce a bound for the error incurred in the finite element solution. The stress fields are not exact nor do they belong to the function space of statically admissible stress fields. A stress field which is not statically admissible does not satisfy the equations of equilibrium within an element. Furthermore, Johnson and Hansbo^[32] feel that because this method is based on superconvergent points, the results may be valid for uniform or nearly uniform meshes, however they may not cover the cases of unstructured meshes.

This method appears to be more reliable than the element residual method but theoretical analysis shows none of the above methods is totally reliable^[19] because they do not generate error bounds. The ability to generate upper and lower error bounds is one of the positive aspects of the duality method.

1.4.1 Duality Method

Sometimes considered as a separate error estimation method, the duality method also implements some postprocessing. This method involves two postprocessed evaluations of the FE results to determine first, the kinematically admissible stress field (KAS) and second, the statically admissible stress field (SAS). The KAS satisfies the constitutive and compatibility equations exactly but not the equilibrium equation exactly. The SAS satisfies the equilibrium and constitutive equations exactly but not the compatibility equation. Mashaie^[19] estimates local error measures for elliptic boundary value problems using this principle of duality and shows that the kinematic and statically admissible stress fields can determine upper and lower bounds on the energy of the exact solution of the problem. This robust method is useful, however mathematically very complex and somewhat limited in its applications.

1.5 Summary

The error estimation method implemented in the present research will involve some form of the postprocessing error measure. It has been shown^{[16][21][30]} that the postprocessing method is applicable in a variety of situations; such as, stress, heat transfer and fluid flow problems. Further, it is believed to be computationally simple^[21], accurate^[23] and reliable^[24].

Chapter 2

Development of a Generic Error Estimate

An error estimate is required for the current research program using h-adaptive mesh management^{[3][14][15]}. The intention is to drive the adaptive procedures through the use of any number of primary variables including temperature, displacement, hardness, phase fraction and effective plastic strain. A number of desirable characteristics of an error estimate have been identified^{[18][19]}. In general, it is felt that error estimates or error measures for h-adaptive procedures should:

1. be physically and mathematically meaningful;
2. be independent of the nature of the problem;
3. be accurate;
4. be reliable;
5. be acceptable as both the number of elements, and the size of elements vary;
6. have monotonic convergence;
7. have a low computational cost and
8. be simple to code.

There are two additional requirements which should be addressed. First, the error estimate should not be sensitive to scale; e.g., converting from ksi to MPa or, in the case of physical dimensions from in. to mm. The multiplication of a variable by a constant value is considered to be a change in scale. Second, the error

estimate should not be sensitive to reference values: e.g., converting from $^{\circ}\text{C}$ to K or rigid body motions. The addition or subtraction of a constant is considered to be a reference change. These requirements do not appear to be mentioned explicitly in the literature, although they may be inherently satisfied in some error estimates.

In the case of Zienkiewicz and Zhu^[21] and several others based on the Zienkiewicz and Zhu's error estimate, both of these situations are a concern. First, in the case of displacements (eq. 2.1), where e is a function of the exact displacement, u , and the FE solution, $\hat{u}$, or indeed any other primary variables such as stress, σ , or temperature, T (eq. 2.2).

$$e_u = u - \hat{u}, \quad e_\sigma = \sigma - \hat{\sigma} \quad [21] \quad (2.1)$$

$$e_T = T - \hat{T} \quad [16] \quad (2.2)$$

The error is defined through the use of either the energy norm (eq. 2.3), or the L_2 norm (eq. 2.4).

$$\|e\|_{en} = \left(\int_{\Omega} [e_\sigma]^T D^{-1} [e_\sigma] d\Omega \right)^{1/2} \quad [21] \quad (2.3)$$

$$\|e\|_{L_2} = \left(\int_{\Omega} [e_u]^T [e_u] d\Omega \right)^{1/2} \quad [21] \quad (2.4)$$

Clearly, a change of scale from ksi to MPa, or a change in dimensions from in. to mm will alter the estimated error. Users not familiar with this fact may encounter serious difficulties resulting in unreliable error predictions. The problem is eliminated in this case by normalizing the error with respect to another value. For example, in the well-known Zienkiewicz and Zhu^[21] error estimate for stress analysis, the normalization eliminates the sensitivity to a scale change.

$$\eta = \frac{\|e\|}{\|u\|} \times 100\% \quad (2.5)$$

Equation 2.5 is, however, susceptible to changes in reference value. Any FE analysis should be able to capture a uniform field such as uniform temperatures or uniform hydrostatic stress, with no error regardless of how coarse the mesh is. Therefore, an error estimate should also be insensitive to a change in a uniform field. This is equivalent to merely changing the reference point for the scale used to represent the variable. For instance, a large rigid body displacement superimposed on the elastic displacements would reduce η , by increasing $\|u\|$. In a thermal analysis, changing $^{\circ}C$ to K would cause a similar effect.

2.1 Proposed Error Estimate

This research uses both refinement and coarsening h-adaptive procedures, for 8- to 26-node elements^{[14][15]}. The 8- to 26-node hexahedron behaves very much like the familiar 8-node linear brick. Constraints associated with grading are embedded in the element's basis functions to guarantee interelement compatibility. In a thermal-elasto-plastic analysis these elements produce temperature or displacement fields which are linear functions of the three Cartesian coordinates.

Clearly, a given mesh produces a piecewise linear approximation to the temperature or displacement fields. If this is a good approximation then the temperature or displacement fields should be smooth. If this is a poor approximation then the FE solution will provide only a least square best fit of the true answer in the linear subspace.

The elements chosen guarantee a specific level of continuity in the solution; for example, linear elements are C^0 continuous. They guarantee that while the temperatures or displacements are continuous the gradients of these variables are not. Therefore, if the gradient is discontinuous then there is an associated error caused by the imposition of a constant gradient. For linear elements the error is associated with the gradients which are discontinuous at interelement boundaries. For this reason, the error estimate should be based on the gradients in the solution rather than on the primary variable.

McDill's mesh-management algorithm requires an error estimate to drive the adaptive function throughout a FE analysis. Coupled thermal/mechanical/microstructural analysis involves the prediction of temperature, stress, displacement and microstructural fields present in a body. It is necessary that the mesh adequately capture all desired fields. Several variables such as, phase fraction, void growth and plastic strain, have no partial differential equations describing how they vary in a body. Consequently, upper and lower error bounds, along with residual methods, can not be computed. It is still desired, however, to have smooth fields for all quantities in the analysis.

It is necessary that the error estimate determine whether the given mesh is an adequate representation for different fields in the problem. It is hoped that the use of a generic error estimate will eliminate the need for different standards to be applied in different types of analysis. In many current error estimates, different variables; for example, temperature and displacement, are said to have acceptable error yet the acceptable values of the errors are different.

It is proposed that the discontinuity of the gradients could be incorporated in an error measure for the adaptive mesh management. Intuitively a mesh would be refined where large differences in the gradients exist between elements. Gradients, or derivatives of the primary variable, are widely used in the estimation of error. Interpolation methods use differences in gradients to determine a second order derivative. Zienkiewicz and Zhu's^[21] postprocessing version for stresses uses derivatives in the sense that strain, and therefore the stress, is related to the gradient of the displacement. Lewis^[16] uses the gradient of temperature for the purposes of heat transfer analysis. An L_2 norm of the gradient is proposed since several different fields are of concern, and an L_2 norm is appropriate in that it does not require the use of material properties^[18].

The local error, e , for the proposed method, is considered to be the difference between the local FE gradient and the exact gradient. Consider, for example, the case of thermal analysis,

$$e_n = (g_n) - (\hat{g}_n) \quad (2.7)$$

where, n is the Gauss point being considered: g is the exact gradient and $\hat{g}$ is the FE approximation of the gradient in T .

For a 1D case,

$$\hat{g}_n = \frac{\partial \hat{T}}{\partial x} = \left[\frac{\partial N_1}{\partial x} \quad \frac{\partial N_2}{\partial x} \quad \dots \quad \frac{\partial N_n}{\partial x} \right] \begin{bmatrix} \hat{T}_1 \\ \hat{T}_2 \\ \vdots \\ \hat{T}_n \end{bmatrix} \quad (2.8)$$

$$\frac{\partial N_i}{\partial x} = J^{-1} \left[\frac{\partial N_i}{\partial \xi} \right], \quad J = \frac{\partial x}{\partial \xi} \quad (2.9a, b)$$

and

$$x(\xi) = \sum_{i=1}^n N_i(\xi) x_i \quad (2.9c)$$

where i varies from 1 to the number of nodes in the element.

The L_2 norm of the error for the j^{th} element is,

$$\|e\|_j = \left[\int_{\Omega} [e]^T [e] d\Omega \right]^{1/2} = \left[\sum_{i=1}^n [e_i]^T [e_i] \det J_i(\xi) W_i \right]^{1/2} \quad (2.10)$$

The L_2 norm of the smoothed gradient can found in a similar manner, however for both local and global errors, the sum of all elements will be used. This will provide an estimation of the element contribution to the global error.

$$\|g\| = \left[\int_{\Omega} [g]^T [g] d\Omega \right]^{1/2} = \left[\sum_{i=1}^j \left(\sum_{m=1}^n [g_m]^T [g_m] \det J_m(\xi) W_m \right) \right]^{1/2} \quad (2.11)$$

where, j is the number of elements and n is the Gauss point for the j^{th} element.

The ratio of equations 2.10 and 2.11 will provide an estimated local element error.

One of the fundamental assumptions in postprocessing error estimation is that an appropriately smoothed field can be used in place of the exact solution^{[16][21][23]}. This assumption will be implemented in the proposed method. Averaging the gradients of the primary variable will produce a smoothed field which is assumed to approximate the exact solution^{[16][21]}. In the proposed method, the gradients are projected from the Gauss points to the nodes. The contributions from the neighbouring elements are averaged to produce a smoothed gradient field at the nodes. This smoothed field is then interpolated back to the Gauss points. Once the gradients at the Gauss points from the FEA and the smoothed gradients are determined, the element and global errors can be computed.

Error methods which compare a computed smooth solution to the FE solution provide only a measurement of the roughness of the solution. All such error estimates use the implicit assumption that the solution is good when the solution is smooth. Generally, this is true. However, in the case of a very coarse mesh that gives an inaccurate, uniform solution, the error estimates would predict no error. It is important, therefore, that any analyst using an error estimate based on a smoothed solution be aware of this concern.

In some cases, singularities in the solution cause large discontinuities in the gradients. Even repeated refinement would never result in a completely smoothed solution. In this case, the error measure would overestimate the true error and continually predict localized refinement. This estimate would, however, be conservative.

To avoid difficulty with the summation of element level errors, local errors will be computed based on a level of error which is associated with an adequate representation of the field. Each element will be judged on its contribution to the global error.

$$E_j = \frac{\|e\|_j}{\|g\|} = \frac{\left[\sum_{i=1}^n [e_i]^T [e_i] \det J_i(\xi) W_i \right]^{1/2}}{\left[\sum_{i=1}^j \left(\sum_{m=1}^n [g_m]^T [g_m] \det J_m(\xi) W_m \right) \right]^{1/2}} \quad (2.12)$$

$$E_{gl} = \frac{\|e\|_{gl}}{\|g\|} = \frac{\sum \|e\|_1}{\|g\|}$$

$$E_{gl} = \frac{\left[\int_{\Omega} [e]^T [e] d\Omega_{gl} \right]^{1/2}}{\left[\int_{\Omega} [g]^T [g] d\Omega_{gl} \right]^{1/2}} = \frac{\left[\sum_{i=1}^J \left(\sum_{m=1}^n [e_m]^T [e_m] \det J_m(\xi) W_m \right) \right]^{1/2}}{\left[\sum_{i=1}^J \left(\sum_{m=1}^n [g_m]^T [g_m] \det J_m(\xi) W_m \right) \right]^{1/2}} \quad (2.13)$$

It is important to note that the proposed error estimate is not influenced by scale or reference changes. Both local and global estimates are normalized by a quantity with the same units as the numerator, thus eliminating scale changes. If the error estimate was a function of a primary variable, such as temperature, the estimate would be affected by reference changes. Reference changes are the addition or subtraction of a constant, as shown in equation 2.14.

$$E_j = \frac{\|\hat{T} + T_o\|_j}{\|T + T_o\|} \quad (2.14)$$

where: $T_o = \text{constant}$

The proposed estimate uses the gradient, or derivative of the primary variable. The derivative of the constant is clearly zero, and consequently, the estimate is not affected by the reference change.

It will be necessary, in multi-increment problems, to monitor the change in the denominator of equation 2.12. For example, transient thermal conduction problems often involve the nonuniform addition of energy to a body which creates thermal gradients and heat flow. As time passes, and heat flow evens out, the temperatures in the body eventually reach a uniform distribution and gradients no longer exist. If the L_2 norm of the smoothed gradients gets very small, the element error will tend toward infinity. This is not an appropriate representation of the actual error. In fact, the field may be constant, therefore the gradients small, and the FE solution would be accurate. In this case, if the L_2 norm decreases from the previous increment, the previous value of $\|g\|$ will be used.

Hand-calculations for 1D and 2D heat transfer examples are shown in Appendix A. These examples show all steps required to compute both the element

and global error.

The following is pseudocode developed for the error estimation.

Initialize arrays

* Begin first loop over the elements in the mesh

Do Label 2 for j elements 1 to j

 Read in element topology and primary variable

 Get element orientation

Do Label 1 for i Gauss points 1 to i

 Evaluate FE gradients at the Gauss points, $\hat{g}_i$

Label 1: Continue

 Store FE gradients at the Gauss points for second loop

 Project gradients from the Gauss points to the nodes, $\hat{g}$

 Compute a running average of $\hat{g}$ at node n to give a smoothed value of g_n

Label 2: Continue

* Begin the second loop over the elements in the mesh

Do Label 3 for j elements 1 to j

 Interpolate g_n to Gauss points, use same basis functions as primary variable

 Compute the Jacobian matrix

 Compute $\|e\|_{L_2}$ for element j

 Compute $\|g\|_{L_2}$ for element j

 Sum $\|g\|_{L_2}$ for all elements

Label 3: Continue

* Begin the third loop over the elements in the mesh

Do Label 4 for j elements 1 to j

 Compute element error, E_j

Label 4: Continue

Compute global error, E_{gt}

A proposed method for an error estimate has been determined for the current research program. This error measure will drive the adaptive procedures through the use of any number of primary variables including temperature, displacement, hardness, phase fraction and effective plastic strain. The error estimate will incorporate measures to eliminate scale and reference effects. The development of the proposed algorithm into working software is presented in the following chapter.

Chapter 3

Development of the Error Estimate Code

The requirements of a generic error estimator and the foundation for the proposed method were established in the previous chapter. These concepts have been converted into functional software which produces error estimates at both the local and global levels.

The error estimate produced by the software is independent of the nature of the problem. The only requirements are the input of mesh topology and, depending on the problem, the value of the primary variable at the nodes. The primary variables can be, for example, temperature, displacement, hardness, phase fraction or effective plastic strain. This information may be obtained from the FEA.

The main program for the developed software is `ERROR.F`. This routine acquires the appropriate information from the FEA. It then establishes the element orientation such as the position and number of subelements. The main routine then calls a subroutine `GETGRAD.F`, to evaluate the gradient of the primary variable at the Gauss points. Once the gradients are determined, `ERROR.F` calls the necessary routines to project the Gauss point gradients to the nodes, average the gradients at the nodes, interpolate the averaged gradients to the Gauss points and calculate the element and global errors. `ERROR.F` consists of three main loops, all over the number of elements in the mesh. The first loop projects the Gauss point gradients to the nodes and then averages the nodal values. The second loop interpolates the

averaged gradients to the Gauss points and calculates the L_2 norms for the element and global errors. Although both loops are over the number of elements, all the averaging must be done first because the neighboring elements contribute to the averaged gradient at each node. The third loop takes the L_2 norm of the difference between the smoothed and FE gradients and normalizes it by the sum of the L_2 norm of the smoothed gradient. This produces the local element error.

ERROR.F also computes the true error for several test cases where the exact analytical solution can be found. A comparison of the true error and that predicted by ERRCAL will allow the proposed method to be assessed.

3.1 Element and Subelement Orientation

The first step in the main program, ERROR.F, is to determine the topology of the elements and the primary variable at the nodes. This information is obtained from the FEA. For computations which occur later in the program, it is necessary to determine the existence and position, of any midedge and midface nodes. This is done by calling GETGP.F. GETGP.F determines the number of Gauss points in each element, and how the element should be divided into subelements.

The 8- to 26-node grading brick elements can have one, two, four, or eight subelements. The number of subelements is determined by the placement of the midedge and midsurface nodes. The eight possible subelement orientations are shown in Figure 3.1. Although elements can have 8 to 26 nodes, all subelements must have 8 nodes when projection takes place. The nodes that are created to satisfy the condition of 8 nodes per subelement are referred to as psuedo-nodes or temporary nodes. These nodes do not exist in the element topology but have been created specifically for this purpose. Determining the orientation of the subelements is followed by reading in the value of the primary variable at the nodes. The initial

a) Orient=1

b) Orient=2

c) Orient=3

b) Orient=4

e) Orient=5

f) Orient=6

h) Orient=7

Figure 3.1 - Subelement Orientation

section of the main program is shown below.

Procedure: ERROR.F

```

Do Label 1 for j elements 1 to j
  Read element topology
  Determine subelement orientation, NSUB, XDIV, YDIV, ZDIV GETGP.F
  Read primary variable information, PRMVAR
Label 1: Continue

```

3.2 Evaluation of Gradients

The subroutine GETGRAD.F calculates the gradients at the Gauss points which are later used in the prediction of the error estimate. This subroutine is called once for every element in the mesh. An array, GPARAY, stores the gradient information, element by element. This information is used at the end of the main program. A second array of the gradient information is projected to the nodes in the subroutine PROJG.F. This subroutine computes the projected gradients so that they can be averaged and a smooth gradient field can be obtained.

Procedure: GETGRAD.F

```

Read in primary variable information at the nodes. PRMVAR
Do Label 1 for dimensions 1 to 3
  Evaluate the gradients at the Gauss points, GETGRAD.F
  Store gradient information, GPARAY
Label 1: Continue

```

3.3 Projection

The subroutine PROJG.F is responsible for projecting the gradients at the Gauss points to the nodes. This routine is called by the main program, ERROR.F, once for each subelement. It is passed the subelement gradients at the 8 Gauss points, SUBGP, and the subelement orientation.

For each direction, GRDNOD.F, is called to calculate the gradients at the nodes. The least squares projection matrix^[35], P , is used to project the gradients from the Gauss points to the nodes. The P matrix is obtained from previously written code^[36], PDATA.F. The projection matrix can handle the projection of

8 Gauss point values to 8 nodes. If the subelement has psuedo-nodes then the information is stored in this temporary nodal position. The nodal gradients of the subelement are then passed back to GRDNOD.F. Based on the subelement orientation, the local nodal gradients can then be assigned to the global array, FEAG. The values at the psuedo-nodes are not assigned to the global array because these nodes do not exist in the mesh.

Procedure: PROJG.F

Read in local subelement gradients at Gauss points, SUBGP

Read in subelement orientation, NSUB, XDIV, YDIV, ZDIV

Do Label 1 for dimension 1 to 3

 Get weighted least squares projection matrix P, PDATA.F

 Project Gauss point gradients to nodes GRDNOD.F

 Use orientation to assign the global nodal gradients, FEAG

Label 1: Continue

3.4 Averaging Nodal Gradients

Once the gradients at the nodes, FEAG, are known, a running average is calculated for the elements with common nodes. This will produce smoothed gradient values at the nodes. These smoothed gradients provide an approximation to the exact, or true solution at the nodes^[21].

The averaging subroutine, AVGRAD.F, is called once for every subelement in the mesh. It is passed the global array of gradients at the nodes, the subelement orientation and a counter for each node in the mesh. The counter, COUNT, keeps track of how many additions are made to each node so that the appropriate gradient in each direction is calculated. It should be noted that any contributions to nodes created for the purpose of projection are not averaged. These nodes are not considered to be 'real' nodes, rather, temporary local nodes which do not belong to the original mesh.

The global list of nodes, LNODS, and the orientation and order of the subelement, TYPXYZ, determine which nodes in the element are the psuedo-nodes. These nodes are not used in the running average in the subelement. The averaged gradients are then stored in the smoothed nodal gradient array, SMTHNG.

Procedure: AVGRAD.F

Read in global subelement gradients at Gauss points, FEAG

Read in subelement orientation, NSUB, XDIV, YDIV, ZDIV

Do Label 1 for nodes 1 to 8

 Do Label 2 for dimensions 1 to 3

 Calculate running average for real nodes

 Store averaged gradient, SMTHNG

 Increment counter, COUNT

 Label 2: Continue

Label 1: Continue

3.5 Interpolation

The second main loop over the elements in program ERROR.F, begins once the averaging is complete. The smoothed gradients at the nodes are now interpolated to the Gauss points so that the error of the element can be determined. The subroutine, INTERP.F, is called once for every element in the mesh. The subelement information is still required, but only to determine the position of the Gauss points. The interpolation itself can be done for elements with midedge or midface nodes.

The subroutine INTERP.F makes use of existing code from ASGARD^[36], a large multipurpose 3-D thermal-elasto-plastic FEA code. The code determines subelement coordinates, Gaussian integration information, basis functions and derivatives.

The interpolation is done using the element topology and the local smoothed nodal gradients. INTERP.F calls subroutine SUBDOM.F to compute the number of subdomains in the element and the Gauss point weights. This information is necessary when integrating over the domain of the element. After collecting the Gauss point data, by calling GAUSPT.F, INTERP.F calls BASIS.F to assemble the basis function array and compute the derivatives of the basis functions for later use in the calculation of the Jacobian matrix. Finally, the interpolation is performed and the smoothed gradients at the Gauss points are returned in the array, TRUEG. At this point interpolation of the FE nodal values takes place, FEVAR. These values will be used to evaluate the true analytical error.

Analytical solutions to several test cases are calculated through a call to the subroutine ANLYT.F. This subroutine computes the true solution at the Gauss points which is then used to calculate the true error in the solution. The true error is defined as the difference between the true solution and the FE solution.

Procedure: INTERP.F

Read in smoothed nodal gradient, **TMPSM**
 Subdomain orientation, **SUBDOM.F**
 Gauss point data, **GAUSPT.F**
Do Label 2 for gp Gauss points 1 to gp
 Basis function array, $N_i(\xi, \eta, \zeta)$ and derivatives of basis functions, **BASIS.F**
 Do Label 1 for j dimensions 1 to j
 Solve for n nodes $g_{gpj} = \sum_{i=1}^n N_i(\xi, \eta, \zeta) g_i$,
 Store gradient at Gauss point gp, **TRUEG**
 Label 1 Continue
 Solve for n nodes $FEVAR_{gp} = \sum_{i=1}^n N_i(\xi, \eta, \zeta) TMPVAR_i$
 Compute the analytical solution at Gauss point gp
Label 2 Continue

3.6 Error Calculation

The error calculation is computed at the end of the main program, **ERROR.F**. The error computation itself involves solving two integrals over the domain of the element. Both error norms are computed at the end of the second loop over the elements. First, the norm of the difference between the smoothed and FE gradients and second, the norm of the smoothed gradients. The norm of the smoothed gradients is summed over all the elements and used as the denominator in the element error prediction.

At this point a check is done to see if the current test case is a multi-increment problem. If so, the norm of the smoothed gradients from the previous increment is read in and compared to the current value. If the current value is less than the previous then the previous value is used.

The element error calculation is done in the third loop over the elements. For example, from Chapter 2, the element and global errors are computed as follows,

$$E_j = \frac{\left[\int_{\Omega} [e]^T [e] d\Omega \right]^{1/2}}{\left[\int_{\Omega} [g]^T [g] d\Omega \right]^{1/2}} = \frac{\left[\sum_{i=1}^n [e_i]^T [e_i] \det J_i(\xi) W_i \right]^{1/2}}{\left[\sum_{i=1}^J \left(\sum_{m=1}^n [g_m]^T [g_m] \det J_m(\xi) W_m \right) \right]^{1/2}} \quad (3.1)$$

$$E_{gl} = \frac{\left[\int_{\Omega} [e]^T [e] d\Omega_{gl} \right]^{1/2}}{\left[\int_{\Omega} [g]^T [g] d\Omega_{gl} \right]^{1/2}} = \frac{\left[\sum_{i=1}^J \left(\sum_{m=1}^n [e_m]^T [e_m] \det J_m(\xi) W_m \right) \right]^{1/2}}{\left[\sum_{i=1}^J \left(\sum_{m=1}^n [g_m]^T [g_m] \det J_m(\xi) W_m \right) \right]^{1/2}} \quad (3.2)$$

To solve these equations it is necessary to call JACOB3D.F^[36] to compute the Jacobian transformation matrix. This is the product of the derivatives of the basis functions and the nodal coordinates. This code calculates the determinant of the Jacobian matrix. Once the L_2 norms are computed the element and global errors can easily be determined. The true error is also computed for testcases with a known analytical solution. The L_2 norms for the true error are, the difference between the exact solution and the solution of the FEA, and second, the norm of the exact solution itself.

Procedure: ERROR.F

Do Label 3 for i elements 1 to i

Retrieve smoothed gradient at the Gauss points, TRUEG

Retrieve gradient at the Gauss points from the FEA, GPFEAG

Retrieve exact solution of the primary variable at the Gauss points, PRMVAR

Retrieve FE solution of the primary variable at the Gauss points, FEAVAR

Do Label 2 for j Gauss points 1 to j

Do Label 1 for dimensions 1 to 3

Compute L_2 norm of difference between smoothed and FE gradient (numerator)

Compute L_2 norm of smoothed gradient (denominator)

Compute L_2 norm of difference between exact and FE solutions (numerator)

Compute L_2 norm of exact solution (denominator)

Label 1: Continue

Label 2 Continue

Store the numerators

Sum the denominators

Label 3 Continue

If incremental problem, compare current and previous denominators

Do Label 4 for i elements 1 to i

Compute element error

Compute true element error

Label 4 Continue

Compute global error

Compute true global error

Chapter 4

Verification

The purpose of this project is to produce *a posteriori* error estimates at both local and global levels for h-adaptive mesh management. The error values produced will drive the adaptive procedures to refine or coarsen the mesh where necessary. This process will improve both the quality and efficiency of the FE solution. It is of fundamental importance to verify ERRCALC, the error estimate software. As an initial check, problems with known analytical solutions were modelled.

Subroutines based on the analytical solutions were added to the code so that the true error in the FE solution could be computed and compared to the error estimates produced by ERRCALC. The true error is based on the difference between the analytical solution and the FE solution at the Gauss points. An L_2 norm is used to evaluate the true error in the FEA. The preliminary testcases provided an estimate of how well, and in which situations, the error estimation method functions best.

In the initial stages of verification, four different cases were considered, each testing a different aspect of the software. The first step for each test is to obtain the FE solution from ASGARD. Depending on the testcase, variables such as temperature or displacements, at the nodes, were extracted from the FE solution and used as input for ERRCALC. ERRCALC also requires the mesh topology and nodal coordinates as input.

The four testcases are different in nature and are described below. For convenience, short form titles are used to identify the cases.

1. Column - prescribed temperatures at the ends of a column, giving a linear temperature field;
2. Patch Test - McNeal-Harder patch testcase with prescribed displacements and severely distorted elements giving a uniform strain field;
3. Cylinder - quarter of a thick cylinder, with prescribed temperatures at the inner and outer surfaces;
4. Boussinesq - prescribed heat source on a semi-infinite body resulting in a $\frac{1}{r}$ singularity effect in the temperature field.

4.1 Column

The 3D column of elements has prescribed temperatures on the top surface and bottom. This testcase produces a linear temperature field. The FE code is able to predict the solution very accurately and, as such, the element errors should be minimal.

The dimensions of the column are 2.5 m x 2.5 m x 10 m. Two meshes were tested. In the first, only 8-node bricks were used. In the second, graded elements resulted in the addition of midedge and midface nodes. The geometry and applied boundary conditions were the same for both meshes tested. Steady-state conditions were modelled. The thermal conductivity was $1 \frac{W}{m^{\circ}C}$. Prescribed temperatures of $0^{\circ}C$ and $300^{\circ}C$ were assigned to the bottom and top surfaces respectively.

The analytical solution for this simple problem is found by the following interpolation:

$$T = \left(\frac{T_t - T_b}{z_t - z_b} \right) \times z \quad (4.1)$$

where:

T is the temperature at any z -coordinate in the mesh.

T_b is the temperature on the bottom surface;

T_t is the temperature on the top surface:

z is the position of interest;

z_b is the z -coordinate for the bottom surface;

z_t is the z -coordinate for the top surface.

Errors for the linear field were found for the mesh with the 8-node elements and for the graded mesh.

Column - 4 Elements

The first mesh consisted of 4, 8-node elements, as shown in Figure 4.1. Eight of 20 nodes were assigned prescribed temperatures. The eight nodes are located on the top and bottom surface of the column.

Figure 4.1 - Element Mesh for Column Test (4 Elements)

Figure 4.2 shows a linear plot of temperature versus z -coordinate for the FE

results and the analytical solution.

Figure 4.2 - Temperature vs. z-coordinate for Column Test

The FE results show excellent correspondence to the analytical solution. The true element errors and estimated errors were found to be negligible; i.e., less than 10^{-14} . The same results were found for the true and estimated global errors.

Column - 11 Elements

The purpose of the second mesh is to show that the developed software can handle graded elements. Graded elements have more than 8 nodes and the FE solution and ERRCALC software must integrate over subelements. It is important that the error estimation code be able to properly project and average the Gauss point data when subelements are involved.

As shown in Figure 4.3, the 4-element mesh was refined one level in all directions so that the bottom-most element was divided into 8 elements. This created 1 midface and 4 midedge nodes on the adjoining element.

Figure 4.3 - Element Mesh for Column Test (11 Elements)

Again, the estimated element and global errors, as well as the true element and global errors were negligible; i.e., less than 10^{-14} . The ERRCALC software properly predicted the estimated errors for both 8-node and graded elements for this linear field. It was noted that both the true and estimated, element and global errors, decreased as the mesh was refined.

4.2 Patch Test

Element distortion was not considered in the previous test. The Patch test, by McNeal and Harder^[37], was selected because all the elements are severely distorted and it is important that the ERRCALC software be able to handle distorted meshes.

Figure 4.4 shows the McNeal and Harder patch test consisting of a cube of 7 elements with 8 nodes each. Here, the dimensions of the cube were 1 m / 1 m × 1 m. The test used a Young's Modulus of 1.00 MPa and a Poisson's ratio of 0.25.

Prescribed displacements generate a uniform tensile hydrostatic stress field in the cube. Below are the applied displacements:

$$u = 0.001(2x + y + z)/2$$

$$v = 0.001(x + 2y + z)/2$$

$$w = 0.001(x + y + 2z)/2 \quad (4.2)$$

where:

u, v, w are the nodal displacements in the x -, y - and z -directions;

x, y, z are the nodal coordinates.

Figure 4.4 - Element Mesh for the Patch Test

This test produces uniform strain at all Gauss points in the mesh. The FEA is able to correctly predict the displacements throughout the mesh, and consequently

the element and global errors for displacement should be very small. Table 4.1 shows the element and global errors for this mesh based on the nodal displacements in the axial, y -direction.

Table 4.1 Element Errors in y -displacement for Patch Test

Element	Error	True Error
1	$1.1589e - 5$	$1.6575e - 6$
2	$2.4390e - 5$	$3.7234e - 6$
3	$7.8073e - 6$	$1.8970e - 6$
4	$2.1221e - 6$	$4.1559e - 6$
5	$9.3743e - 6$	$8.3058e - 7$
6	$2.4651e - 5$	$3.6270e - 6$
7	$3.8014e - 6$	$2.3913e - 6$
<i>Global Error</i>	$4.4164e - 5$	$7.5523e - 6$

As expected the estimated errors are negligible and correspond well to the true errors in the FE solution.

4.3 Cylinder

The Cylinder testcase was chosen because it displays a logarithmic temperature distribution. One-quarter of an infinitely long, thick cylinder with prescribed temperatures at the inner and outer surfaces was modelled. The cylindrical geometry produces a steady-state temperature distribution determined from Holman^[38]:

$$T = T_i - \left(\frac{(T_i - T_o) \times \ln(\frac{r}{r_i})}{\ln(\frac{r_o}{r_i})} \right) \quad (4.3)$$

where:

r is the radial coordinate of interest;

r_i is the inner radius;

r_o is the outer radius;

T is the temperature at radius r ;

T_i is the temperature at the inner surface;

T_o is the temperature at the outer surface.

The geometry and applied boundary conditions remained the same for all meshes considered. The following properties and dimensions were used:

r_i 100 m;
 r_o 4600 m;
 T_i 100°C;
 T_o 0°C.

The plot of temperature versus radial distance from the center of the cylinder is shown in Figure 4.5. The logarithmic temperature distribution is clearly shown in this plot.

Figure 4.5 - Temperature vs. Radial Distance for the Cylinder Test

Three cases were modelled. The applied boundary conditions limit the heat

flow to the radial direction. Accordingly, the meshes were refined using RPL_SELECT^[40] so that there was no refinement longitudinally. Refinement was limited to the x - and y -directions. Element errors for each mesh are reported first. Global errors follow.

Cylinder - 24 Elements

The mesh, shown in Figure 4.6, consisted of 24, 8-node elements with prescribed temperatures applied to 20 of the 70 nodes. Prescribed temperatures were applied to 20 nodes on the inner and outer surfaces of the cylinder. Elements 1 through 6 are labelled for convenience.

Figure 4.6 - Element Mesh for the Cylinder Test

Table 4.2 shows typical values of the element errors, in this case, for those elements along a common radial segment. Clearly, where the curvature in the temperature distribution is the greatest, the element errors are correspondingly large. Throughout the mesh, the predicted element errors are shown to correspond with the true errors.

Table 4.2 Element Errors in Temperature for Cylinder (24 Elements)

Element	Radial Distance (m)	Error	True Error
1	475.4	0.0815	0.0577
2	1234.2	0.0882	0.0485
3	1995.2	0.0336	0.0374
4	2756.5	0.0224	0.0264
5	3517.9	0.0175	0.0154
6	4279.5	0.0186	0.0058

Cylinder - 96 Elements

The second mesh for this case had 96 elements. The previous mesh was refined one level in the x - and y -directions. Prescribed temperatures were applied to 36 nodes on the inner and outer surface. The increased number of degrees of freedom allowed the FEA to more closely predict the solution and as expected, the element errors have decreased from the previous mesh. Table 4.3 shows the element errors for those elements along the same radial segment as the first case.

Table 4.3 Element Errors in Temperature for Cylinder (96 Elements)

Element	Radial Distance (m)	Error	True Error
1	287.7	0.0429	0.0123
2	663.8	0.0468	0.0109
3	1040.2	0.0174	0.0101
4	1416.6	0.0108	0.0090
5	1793.0	0.0078	0.0081
6	2169.5	0.0062	0.0070
7	2546.0	0.0053	0.0059
8	2922.4	0.0047	0.0048
9	3293.9	0.0042	0.0037
10	3675.4	0.0038	0.0026
11	4051.8	0.0035	0.0016
12	4428.3	0.0045	0.0007

In most cases the true error is found to be smaller than the predicted error. The true error in the FE solution is a function of the difference between the analytical solution and the FE solution at the Gauss points. This is obtained by interpolating the nodal data from the FE analysis to the Gauss points. If the FE solution is very close to the analytical solution, the error will be small. The applied boundary conditions cause several nodes to be prescribed to the analytical solution. At these nodes, there is no difference between the FE and analytical solution, and therefore, no error.

Cylinder - 384 Elements

The final mesh for this case had 384 elements. The previous, 96-element mesh, was refined one level in the x - and y -directions giving 384, 8-node elements. Prescribed temperatures were applied to the inner and outer surfaces of the cylinder, affecting 68 of the 895 nodes. The FEA can accurately predict the solution for this case, and consequently, the element errors have decreased. Table 4.4 shows the element errors for those elements along the same radial segment as the previous two cases. Every second element is shown for convenience.

The predicted and true global errors for all meshes are shown below in Table 4.5. Clearly, refining the mesh causes a decrease in both the local and global errors. The true errors are again smaller than the predicted errors. In general, the ERRCALC software appears to give a conservative, upper bound, prediction of the errors.

Table 4.4 Element Errors in Temperature for Cylinder (384 Elements)

Element	Radial Distance (m)	Error	True Error
1	193.8	0.0206	0.0023
3	569.1	0.0092	0.0019
5	944.5	0.0041	0.0018
7	1208.2	0.0025	0.0016
9	1695.2	0.0018	0.0014
11	2070.6	0.0015	0.0012
13	2446.0	0.0012	0.0010
15	2821.3	0.0011	0.0008
17	3196.7	0.0009	0.0006
19	3572.1	0.0009	0.0005
21	3947.4	0.0008	0.0003
23	4322.8	0.0009	0.0001

Table 4.5 Global Errors in Temperature for Cylinder (All Meshes)

Mesh Type	Global Error	True Global Error
24 <i>elements</i>	0.2578	0.1794
96 <i>elements</i>	0.1869	0.0733
384 <i>elements</i>	0.1259	0.0252

4.4 Boussinesq

Many situations in FEA involve singularities. It is important that the ER-RCALC software be able to handle such complex situations. One Boussinesq testcase^[39] is that of a point load on a semi-infinite body has a $\frac{1}{r}$ singularity in the temperature distribution. Further, the radial thermal gradient has a $\frac{1}{r^2}$ singularity. When the radius, r , is zero the temperature is infinite. As will be seen, FE solutions which must produce a finite value for the temperature behave poorly in situations where the analytical solution predicts an infinite value. At steady-state,

the analytical solution for this problem is^[39]:

$$T = \frac{Q}{2 \times \pi \times k \times r} + T_{\infty} \quad (4.4)$$

where:

k is the thermal conductivity, $\frac{W}{m^{\circ}C}$;

Q is the applied flux, W ;

r is the radial distance from the heat source, m;

T_{∞} is the surrounding temperature, $^{\circ}C$.

Figure 4.7 shows the singularity when temperature is plotted against radial distance from the source.

Figure 4.7 - Temperature vs. Radial Distance From Source for the Boussinesq Test

A quadrant of the semi-infinite body was modelled with 8, 64 and 512 elements

and had dimensions of $1.0 \text{ m} \times 1.0 \text{ m} \times 1.0 \text{ m}$. Temperatures on the three planes at $x=1 \text{ m}$, $y=1 \text{ m}$ and $z=1 \text{ m}$ were prescribed to the analytical solution which was evaluated using a simple program developed for that purpose. The planes at $x=0 \text{ m}$ and $y=0 \text{ m}$ were planes of symmetry. The plane at $z=0 \text{ m}$ was a free surface. The heat source, Q , applied in the positive z -direction at the origin was 15 W ; T_{∞} was 20°C and the thermal conductivity, k was $1 \frac{\text{W}}{\text{m}^{\circ}\text{C}}$.

Four testcases were considered. The first two used uniform meshes. The others were graded versions of the first case. Element level and global errors were determined in each case.

Boussinesq - 4 x 4 x 4 Uniform

The first mesh had a uniform distribution of 8-node elements with 61 of the 125 nodes assigned prescribed temperatures. The nodes assigned prescribed temperatures were on the external surfaces; $x=1 \text{ m}$, $y=1 \text{ m}$ and $z=1 \text{ m}$.

Table 4.6 shows the error for the elements on the diagonal where, $x = y = z$. The radial distance from the heat source to the centroid of the element and the true error are also shown.

**Table 4.6 Element Errors in Temperature for Boussinesq
(4 x 4 x 4 Uniform)**

Element	Radial Distance (m)	Error	True Error
1	0.2165	0.2887	0.0173
2	0.6495	0.0081	0.0014
3	1.0825	0.0014	0.0003
4	1.5155	0.0021	0.0000

The element errors correspond to those predicted by the true solution except in the element where the heat source is located. Once again the predicted errors are shown to be larger than the true errors.

Boussinesq - 8 x 8 x 8

The second mesh had 8 elements per edge; i.e., a uniform distribution of 512 elements. As in the first mesh there were no graded elements. Prescribed temperatures were applied to 217 of the 729 nodes. Good agreement is again observed between the predicted error and the true error in the FEA results except in the corner element. The error for the corner element with the heat source remained larger than all other elements in the mesh. All element errors decreased from the first mesh, showing that refinement causes a decrease in element errors. Table 4.7 shows the element errors for this mesh.

**Table 4.7 Element Errors in Temperature for Boussinesq
(8 x 8 x 8 Uniform)**

Element	Radial Distance (m)	Error	True Error
1	0.1083	0.2851	0.0122
2	0.3248	0.0080	0.0009
3	0.5413	0.0014	0.0002
4	0.7578	0.0003	0.0000
5	0.9743	0.0001	0.0000
6	1.1908	0.0000	0.0000
7	1.4073	0.0000	0.0000
8	1.6238	0.0000	0.0000

Boussinesq - Graded

The third mesh is shown in Figure 4.8. The element containing the heat source in the 4 x 4 x 4 mesh was refined once in each direction to create 8 additional elements some with midedge and midface nodes. The total number of elements is 71. Due to the boundary conditions, 61 of 144 nodes were prescribed to the analytical temperature.

Figure 4.8 - Graded Element Mesh for the Boussinesq Test

This mesh provided a second opportunity to observe the projection of Gauss point data in a graded mesh and ensure that it was being computed correctly for subelements. It also showed the effect of refinement on the element error for this particular testcase.

Table 4.8 shows the element errors for the 5 elements on the quadrant diagonal.

Table 4.8 Element Errors in Temperature for Boussinesq (Graded)

Element	Radial Distance (m)	Error	True Error
1	0.1083	0.2842	0.0115
2	0.3248	0.0088	0.0002
3	0.6495	0.0052	0.0008
4	1.0825	0.0009	0.0003
5	1.5155	0.0001	0.0000

Again, in general, the predicted element errors are similar to the true error in the FE solution. As in the other cases, the element with the heat source has a much greater error than the true error. It should be noted that the error for the element with the heat source corresponds to the error in the 8x8x8 case, where the element is the same size.

Both the true and estimated error for this element decreased from the 4x4x4 case, however not by a significant amount. This result shows that the error estimate, because it is based on the gradient of the temperature, may be influenced by the singularity at the heat source. Further testing and analysis of this localized effect was necessary to conclude why the error is so high in this element.

Boussinesq - Second Refinement

The corner element where the point heat source is applied was refined again to produce the final mesh. The element was refined in all directions giving 78 elements with 61 out of 163 nodes prescribed. The results for the 6 elements on the diagonal are reported in Table 4.9.

**Table 4.9 Element Errors in Temperature for Boussinesq
(Graded Twice)**

Element	Radial Distance (m)	Error	True Error
1	0.0541	0.2826	0.0079
2	0.1624	0.0087	0.0004
3	0.3248	0.0063	0.0002
4	0.6495	0.0036	0.0007
5	1.0825	0.0006	0.0003
6	1.5155	0.0001	0.0000

As with the first three meshes, the element with the heat source has a large error compared to the true error. Continual refining of the corner element does not seem to significantly effect the element error value. However, in the surrounding

elements, the local error decreased by significant amounts. For instance, element 2 was created when the corner element in the previous mesh was refined. The size of element 1 and 2 in the current mesh is the same. The important difference between element 1 and 2 is the presence of the heat source. The error in element 2 is approximately 27% less than the error for element 1. This indicates that the singularity may be increasing at the same rate as the volume of the element at the heat source is decreasing, resulting in a poor solution at the element nearest the source, regardless of its size. This is expected, as the analytical solution for the temperature is infinity at the source.

The estimated and true global errors, for all meshes, are shown in Table 4.10. The estimated global error is significantly higher than the true global error, with the element nearest the heat source being the primary contributor to the global error. However, as the mesh is refined the estimated global error follows a similar decreasing trend as the true global error.

**Table 4.10 Global Errors in Temperature for Boussinesq
(All Meshes)**

Mesh Type	Global Error	True Global Error
<i>4x4x4 – 64 elements</i>	0.4250	0.0260
<i>4x4x4 (1 level of rfn.) – 71 elements</i>	0.4217	0.0185
<i>4x4x4 (2 levels of rfn.) – 78 elements</i>	0.4213	0.0135
<i>8x8x8 – 512 elements</i>	0.4199	0.0184

4.5 Preliminary Assessment

The four preliminary testcases used to verify the ERRCALC software were very simple in nature. The errors resulting from prescribed temperatures on a column and a thick-walled cylinder, prescribed displacements on a cube and a prescribed heat source on an infinite body, were computed.

In each case the FEA was able to closely predict the analytical solution. Con-

sequently, element errors for all but one of the testcases remained relatively low, even when the gradient of the solution was very large. For instance, the largest element error in the thick-walled cylinder test was found to be approximately 8%.

However, the Boussinesq testcase showed that the estimated element error is affected by singularities. In this particular case, the element closest to the source showed only a very small decrease in element error after repeated refinement. Even though repeated refinement causes the volume of the element to decrease, the gradient is increasing by $\frac{1}{r^2}$. The error estimate measures the difference in gradient from one element to the next. This test shows that if the analytical solution goes to infinity, it is impossible for refinement to produce a smooth gradient at the singularity.

The preliminary tests showed the error estimate can determine whether a given mesh is an adequate representation for both temperature and displacement fields. The error estimate is not affected by scale or reference changes. ERRCALC is also capable of handling graded meshes and distorted elements. The element errors for these preliminary test cases were shown to be consistent with the true errors. As each mesh was refined both element and global errors decreased. The use of this generic error estimator in different fields, such as effective plastic strain and effective stress is shown in the following chapter.

Chapter 5

Practical Engineering Problems

The second stage of verification considers more complex, practical engineering problems. The common question of, "how good are the answers?", needs to be addressed for nonlinear problems where an analytical solution does not exist. The error estimator implemented in the present research will allow the use of adaptive procedures to modify the mesh, and consequently, drive the FEA toward an improved solution.

The developed software was tested on three problems for which analytical solutions are not known. The first two, of the three tests, examined the analysis for a cylindrical pressure vessel. The third problem was a thermal analysis of a submerged arc weld. The three testcases are described below:

1. Pressurized Cylinder - quarter of a thick-walled cylinder with prescribed internal pressure, error estimate based on effective stress (σ_{eff}).
2. Pressurized Cylinder - quarter of a thick-walled cylinder with prescribed internal pressure, error estimate based on effective plastic strain (ϵ_{pl}).
3. Arc Weld - thermal analysis of a weld on a thin slice of an HY-80 plate, error estimate based on the temperature distribution.

5.1 Pressurized Cylinder (σ_{eff})

A thick-walled cylindrical pressure vessel is a good example of a three-dimensional

stress situation in that there are radial and hoop stresses and generally, axial stress. This problem is of considerable practical importance in the analysis of pressure vessels and gun barrels. It is often desirable to have compressive hoop stresses at the bore of the cylinder. This will result in a greater allowable internal pressure for the vessel. A method for creating compressive hoop stresses is known as autofrettage. Internal pressure is applied to the cylinder causing plastic deformation at the bore. The hoop stress decreases in magnitude from the inner to outer surfaces leaving part of the cylinder in the elastic range and plastically deforming the inner surface. After releasing the internal pressure, the cylinder cannot return to its original state due to the deformation at the inner section of the vessel. The material that was in the plastic range will be subjected to compressive hoop stresses and the elastic outer material subjected to tensile hoop stresses.

As with the Cylinder test, one-quarter of an infinitely long thick cylinder with prescribed internal pressure was modelled. The inner and outer radii were 100 m and 200 m respectively. The boundary conditions remained the same for all meshes tested. The applied internal pressure was incrementally increased from 75 MPa to 226 MPa and then released for the final step of the analysis. The maximum pressure caused a plastic deformation one-third of the way through the thickness of the cylinder. A 2% force norm was applied for the convergence criteria. The analysis considered an ideal elastic-plastic material. The test used a Young's modulus of 204 GPa, a Poisson's ratio of 0.3 and a yield stress of 400 MPa.

The analytical solution for the stress distribution is given by the following set of equations. For radii where the material behaves elastically, equations 5.1 to 5.3 hold^[41]. Once plasticity begins, equations 5.4 to 5.6 are used^[42]. The cylinder ends are free to move, consequently, the stress in the longitudinal direction is negligible.

$$\sigma_t = \frac{P_i r_i^2 (r_o^2 + r^2)}{r^2 (r_o^2 - r_i^2)} \quad (5.1)$$

$$\sigma_r = \frac{-P_i r_i^2 (r_o^2 - r^2)}{r^2 (r_o^2 - r_i^2)} \quad (5.2)$$

$$\sigma_t = 0 \quad (5.3)$$

$$\sigma_t = \sigma_y \left(1 - \ln \frac{a}{r}\right) - \frac{\sigma_y}{2r_o^2} (r_o^2 - a^2) \quad (5.4)$$

$$\sigma_r = -\sigma_y \ln \frac{a}{r} - \frac{\sigma_y}{2r_o^2} (r_o^2 - a^2) \quad (5.5)$$

$$\sigma_t = 0 \quad (5.6)$$

where:

a is the radius of the plastic deformation boundary;

P_i is the internal pressure;

r is the current radius;

r_i, r_o are the internal and external cylinder radii;

σ_t is the longitudinal component of stress;

σ_r is the radial component of stress;

σ_t is the tangential component of stress;

σ_y is the yield stress.

It is important to note that equations 5.4 and 5.5 were derived^[42] using the assumption of the Tresca yield criteria. However, the FEA uses the Von Mises yield criteria. An analytical solution assuming the Von Mises yield criteria did not appear to be available in the literature. There will therefore, be significant differences between the analytical and FE solutions which are caused by this discrepancy. An error based on the difference between the FEA and the analytical solution is computed and is called the reference error. Strictly speaking this is not the true error in the FE solution, but is presented for the purposes of comparison.

The effective stress was used as the criterion to establish the error estimates. Effective stress, also known as Equivalent or Von Mises stress, is given by equation

5.7.

$$\sigma_{eff} = \left[\frac{1}{2} ((\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2) \right]^{\frac{1}{2}} \quad (5.7)$$

where:

$\sigma_1 - \sigma_3$ are principal stresses;

σ_{eff} is the effective stress.

Three cases were modelled. The applied boundary conditions give a radially symmetric stress field. The meshes were refined only in the radial and tangential directions. The element errors for each mesh are reported first. Global errors for all meshes will follow.

Three increments for each mesh are reported. The internal pressure for the first increment was 75 MPa. The entire cylinder remained elastic for this increment. The FEA prediction for the elastic case gives very low errors. The ninth increment had an internal pressure of 226 MPa which plastically deformed the cylinder to about one-third of the radius. In the final increment, the tenth, the internal pressure was reduced to 0 MPa. The errors resulting from the residual stresses were found for this increment.

Pressurized Cylinder (σ_{eff}) - 24 Elements

The mesh consisted of 24, 8-node elements with internal pressure applied to the innermost surfaces of 4 of the 24 elements. Figure 5.1 shows the mesh for this testcase.

Figure 5.1 - Element Mesh for the Pressurized Cylinder Test

Figures 5.2, 5.3 and 5.4 show the analytical and the FE solutions of the effective stress for 3 of the 10 increments. As shown, the FE solution for the elastic case corresponds to the analytical solution. However, when plasticity occurs, the difference between solutions using Tresca and Von Mises yield criteria becomes obvious. Although generally similar in magnitude and distribution significant differences are evident.

Figure 5.2 - Effective Stress vs. Radial Distance for $P_i = 75$ MPa

Figure 5.3 - Effective Stress vs. Radial Distance for $P_i = 226$ MPa

Figure 5.4 - Effective Stress vs. Radial Distance for $P_i = 0$ MPa

Errors for the elements labelled in Figure 5.1 are shown below, in Tables 5.1 through 5.3.

Table 5.1 Element Errors in σ_{eff} for Elastic Pressurized Cylinder (24 Elements, $P_i=75$ MPa)

Element	Radial Distance (m)	Error	True Error
1	110.0	0.0345	0.0171
2	126.9	0.0359	0.0050
3	143.9	0.0291	0.0049
4	160.8	0.0194	0.0047
5	177.7	0.0159	0.0047
6	194.6	0.0189	0.0049

As expected, element errors are low for the elastic steps. The largest errors appear at the bore of the cylinder where the stress field is changing most rapidly. All predicted errors are in agreement with true errors in the FE solution.

Elements on the inner surface of the cylinder, such as element 1, are affected by the applied boundary conditions. Four of the 8 nodes in element 1 are prescribed to the internal pressure. During the smoothing process, the values at these nodes remain unchanged. Thus the error estimate is slightly lower at the surface. It is likely that the applied boundary conditions cause the calculated gradients in this element to be smaller, and consequently the error is less than the second element on the same radial segment.

Table 5.2 Element Errors in σ_{eff} for Elasto-plastic Pressurized Cylinder (24 Elements, $P_i=226$ MPa)

Element	Radial Distance (m)	Error	Reference Error
1	110.0	0.0836	0.0311
2	126.9	0.0983	0.0160
3	143.9	0.0336	0.0275
4	160.8	0.0282	0.0247
5	177.7	0.0230	0.0224
6	194.6	0.0272	0.00205

Because the internal pressure causes plastic deformation at the bore of the cylinder, elements 1 and 2 show a significant increase in element errors. Elements 3 through 6, remain elastic and show similar elemental errors to those in Table 5.1.

Table 5.3 Element Errors in σ_{eff} for Elasto-plastic Pressurized Cylinder (24 Elements, $P_i=0$ MPa)

Element	Radial Distance (m)	Error	Reference Error
1	110.0	0.1782	0.2351
2	126.9	0.1657	0.0537
3	143.9	0.0057	0.1102
4	160.8	0.0038	0.0985
5	177.7	0.0029	0.0878
6	194.6	0.0032	0.0876

As shown in Table 5.2 and 5.3 errors for elements which plastically deformed

($r < 133.33$ m) are greater than those in the elastic region. Further, the errors decrease as the radius increases. It should be noted that, because of the difference in yield criteria, the predicted and true errors should not be directly compared, but are shown for reference.

Pressurized Cylinder (σ_{eff}) - 96 Elements

The second mesh tested had 96 elements. The previous mesh was refined one level in the radial and tangential directions giving 96, 8-node elements. Internal pressure was applied to the innermost surfaces of 8 elements. The increased number of degrees of freedom allows the FEA to more closely predict the solution and as expected, the element errors have decreased from the previous mesh. Tables 5.4 to 5.6 show the element errors for those elements along the same radial segment as in the 24-element case.

Table 5.4 Element Errors in σ_{eff} for Elastic Pressurized Cylinder (96 Elements, $P_i=75$ MPa)

Element	Radial Distance (m)	Error	True Error
1	104.6	0.0092	0.0034
2	112.9	0.0144	0.0005
3	121.3	0.0111	0.0005
4	129.7	0.0084	0.0006
5	138.0	0.0068	0.0006
6	146.4	0.0055	0.0007
7	154.8	0.0045	0.0007
8	163.1	0.0038	0.0007
9	171.5	0.0032	0.0007
10	179.8	0.0026	0.0007
11	188.2	0.0035	0.0007
12	196.6	0.0053	0.0006

**Table 5.5 Element Errors in σ_{eff} for Elasto-plastic Pressurized Cylinder
(96 Elements, $P_i=226$ MPa)**

Element	Radial Distance (m)	Error	Reference Error
1	104.6	0.0026	0.0158
2	112.9	0.0395	0.0166
3	121.3	0.0348	0.0122
4	129.7	0.0225	0.0047
5	138.0	0.0108	0.0112
6	146.4	0.0082	0.0106
7	154.8	0.0067	0.0099
8	163.1	0.0055	0.0093
9	171.5	0.0046	0.0088
10	179.8	0.0038	0.0083
11	188.2	0.0052	0.0080
12	196.6	0.0078	0.0088

**Table 5.6 Element Errors in σ_{eff} for Elasto-plastic Pressurized Cylinder
(96 Elements, $P_i=0$ MPa)**

Element	Radial Distance (m)	Error	Reference Error
1	104.6	0.0269	0.1139
2	112.9	0.0716	0.0809
3	121.3	0.0899	0.0329
4	129.7	0.0183	0.0220
5	138.0	0.0024	0.0556
6	146.4	0.0009	0.0525
7	154.8	0.0007	0.0492
8	163.1	0.0005	0.0464
9	171.5	0.0004	0.0439
10	179.8	0.0003	0.0417
11	188.2	0.0005	0.0400
12	196.6	0.0007	0.0449

Pressurized Cylinder (σ_{eff}) - 384 elements

The final mesh for this testcase had 384 elements. This mesh was created by refining the previous 96-element mesh in the radial and tangential directions. Internal pressure was prescribed to the innermost surfaces of 16 of the 384 elements. Element errors have again decreased due to the increased number of degrees of freedom. Tables 5.7 to 5.9 show the element errors for those elements along the same radial segments as the previous two cases. For convenience, every second element is shown.

Table 5.7 Element Errors in σ_{eff} for Elastic Pressurized Cylinder (384 Elements, $P_i=75$ MPa)

Element	Radial Distance (m)	Error	True Error
1	102.2	0.0045	0.0007
3	110.5	0.0035	0.0001
5	118.9	0.0024	0.0001
7	127.2	0.0018	0.0002
9	135.5	0.0014	0.0002
11	143.9	0.0011	0.0002
13	152.2	0.0009	0.0002
15	160.6	0.0008	0.0002
17	168.9	0.0007	0.0002
19	177.3	0.0006	0.0002
21	185.6	0.0004	0.0002
23	193.9	0.0014	0.0002

**Table 5.8 Element Errors in σ_{eff} for Elasto-plastic Pressurized Cylinder
(384 Elements, $P_i=226$ MPa)**

Element	Radial Distance (m)	Error	Reference Error
1	102.2	0.0000	0.0078
3	110.5	0.0000	0.0080
5	118.9	0.0195	0.0076
7	127.2	0.0027	0.0015
9	135.5	0.0023	0.0054
11	143.9	0.0018	0.0051
13	152.2	0.0014	0.0048
15	160.6	0.0012	0.0045
17	168.9	0.0010	0.0042
19	177.3	0.0008	0.0040
21	185.6	0.0007	0.0038
23	193.9	0.0021	0.0042

**Table 5.9 Element Errors in σ_{eff} for Elasto-plastic Pressurized Cylinder
(384 Elements, $P_i=0$ MPa)**

Element	Radial Distance (m)	Error	Reference Error
1	102.2	0.0082	0.0538
3	110.5	0.0174	0.0466
5	118.9	0.0545	0.0218
7	127.2	0.0010	0.0039
9	135.5	0.0003	0.0276
11	143.9	0.0002	0.0260
13	152.2	0.0001	0.0244
15	160.6	0.0001	0.0230
17	168.9	0.0000	0.0218
19	177.3	0.0000	0.0207
21	185.6	0.0000	0.0199
23	193.9	0.0002	0.0210

The predicted true and global errors for all meshes are shown below in Table 5.10. Refining the mesh decreases both the local and global errors.

Table 5.10 Global Errors in σ_{eff} for Pressurized Cylinder (All Meshes)

Mesh Type	Global Error	Reference Global Error
<i>24 elements (75 MPa)</i>	0.1455	0.0397
<i>96 elements (75 MPa)</i>	0.0817	0.0135
<i>384 elements (75 MPa)</i>	0.0493	0.0046
<i>24 elements (226 MPa)</i>	0.2911	0.1182
<i>96 elements (226 MPa)</i>	0.1786	0.1107
<i>384 elements (226 MPa)</i>	0.1268	0.1087
<i>24 elements (0 MPa)</i>	0.4943	0.6211
<i>96 elements (0 MPa)</i>	0.3565	0.5770
<i>384 elements (0 MPa)</i>	0.2899	0.5657

Both the estimated and true global errors decrease as the mesh is refined. In general, the estimated local and global errors are greater than the true error. However, in cases where the difference in yield criterion is the main source of difference between the FEA and the analytical solution, the true error is greater.

5.2 Pressurized Cylinder (ϵ_{pl})

The cylindrical pressure vessel described in Section 5.1 was used again in this test. The geometry and boundary conditions for the problem remained the

same and the same three FE meshes were used. Plastic strain, instead of effective stress, was used as the criterion for the error estimates. Data for plastic strain were obtained from the ninth increment of the test where the internal pressure was 226 MPa.

Engineers are often interested in the plastic yield boundary, where large deformations can cause instantaneous and permanent material changes. Plastic deformation is relevant in many problems such as structural design and the deformation of metals in forming processes. The effective plastic strain is related to ductile rupture for instance. Further, it is often necessary in practice to pick out what appear to be the important variables and analyse their significance. For this reason, effective plastic strain was used as the error criterion for this problem.

Errors for elements along a common radial segment for the 3 meshes are shown in Table 5.11 to Table 5.13. The element errors for each mesh are reported first. Global errors for all meshes will follow.

**Table 5.11 Element Errors in ϵ_{pl} for Pressurized Cylinder
(24 Elements)**

Element	Radial Distance (m)	Error
1	110.0	0.1300
2	126.9	0.1015
3	143.9	0.0527
4	160.8	0.0000
5	177.7	0.0000
6	194.6	0.0000

**Table 5.12 Element Errors in ϵ_{pl} for Pressurized Cylinder
(96 Elements)**

Element	Radial Distance (m)	Error
1	104.6	0.0194
2	112.9	0.0648
3	121.3	0.0498
4	129.7	0.0293
5	138.0	0.0001
6	146.4	0.0000
7	154.8	0.0000
8	163.1	0.0000
9	171.5	0.0000
10	179.9	0.0000
11	188.2	0.0000
12	196.6	0.0000

**Table 5.13 Element Errors in ϵ_{pl} for Pressurized Cylinder
(384 Elements)**

Element	Radial Distance (m)	Error
1	102.2	0.0092
2	110.5	0.0056
3	118.9	0.0185
4	127.2	0.0018
5	135.5	0.0000
6	143.9	0.0000
7	152.2	0.0000
8	160.6	0.0000
9	168.9	0.0000
10	177.3	0.0000
11	185.6	0.0000
12	193.9	0.0000

The largest errors appear at the bore of the cylinder where the stress field is changing most rapidly. As the number of degrees of freedom increase, element errors decrease. Table 5.14 shows the global error for each mesh.

Table 5.14 Global Errors in ϵ_{pl} for Pressurized Cylinder (All Meshes)

Mesh Type	Global Error
<i>24 elements</i>	0.3469
<i>96 elements</i>	0.2451
<i>384 elements</i>	0.1336

5.3 Arc Weld

The Arc Weld test is a thermal analysis of a submerged arc weld on a thin slice of an HY-80 plate. This analysis allowed the ERRCALC software to be tested using a complex temperature field. As the heat source moved across the plate, the temporal changes would require the mesh to refine and coarsen accordingly. As the source moves, the ERRCALC software should indicate the necessary mesh changes.

The dimensions of the plate were 552 mm $\times$ 216 mm $\times$ 1 mm and the weld conditions were 32 V, 475 A, 6.14 mm/s with a welding efficiency of 93%^[43]. An elliptical heat source 20 mm long, 20 mm wide and 7 mm deep was used. The weld was active for the first 8 of 94 time steps, or increments.

The error estimates are based on the temperature distribution for increments 3, 4 and 5. The temperature at any radial distance from the source, varies with time. Inside the weld pool, temperatures are approximately uniform. Just outside the weld pool, there is a sharp increase in thermal gradients. As the weld pool radius increases, the sharp decrease in temperature moves further from the source. The temperature distributions for increments 3 to 5 are shown in Figure 5.5.

Figure 5.5 - Temperature vs. Radial Distance from the Source

Two cases were modelled. A very coarse 36-element 3D mesh was used to model the plate in the first case. Boundary conditions reduced the problem to that of a 2D slice. This reduces the computational time necessary for the solution while having only a negligible effect on the solution accuracy^[43].

The first mesh was then refined one level in all directions to produce the second mesh. The applied boundary conditions remained the same for both testcases. All external surfaces were initially prescribed to 20°C. Element errors for each mesh are reported first. Global errors follow.

Arc Weld - 36 Elements

The mesh consisted of 36, 8-node elements. Figure 5.6 shows the mesh for this testcase with the weld path and direction indicated. The weld started at node 9 and ended at node 10.

Figure 5.6 - Element Mesh for the Arc Weld (36 Elements)

Table 5.15 shows typical values for the element errors, in this case, for the first 6 elements in the y -direction starting at the corner with the source. As the weld pool boundary moves into the plate, the errors for the elements on the boundary increase.

**Table 5.15 Element Errors in Temperature for Arc Weld
(36 Elements)**

Element	Radius (mm)	Error (inc.3)	Error (inc.4)	Error (inc.5)
1	2.016	0.1519	0.0654	0.0256
2	4.070	0.1130	0.1184	0.0475
3	6.447	0.1076	0.1188	0.1000
4	8.892	0.0592	0.0732	0.1696
5	11.98	0.0422	0.0791	0.1159
6	15.70	0.0201	0.0217	0.0283

The largest errors are not necessarily found at the source centre, but are found where the slope of the temperature curve changes most rapidly. This corresponds to a location in the vicinity of the weld pool boundary and determines the elements where refinement will best improve the solution. At the weld pool boundary, the thermal gradients change rapidly. These differences are caused by the higher thermal conductivity assumed for the molten metal, and the fact that the weld energy

is being deposited in the molten pool.

Arc Weld - 288 Elements

The second mesh for this testcase had 288 elements. Figure 5.7 shows the mesh for this testcase. The increased number of degrees of freedom allows the FEA to more closely predict the actual temperature field in the plate. Consequently the element errors decreased. Table 5.16 shows the errors for those elements along the same section of plate as the first case.

Figure 5.7 - Element Mesh for the Arc Weld (288 elements)

**Table 5.16 Element Errors in Temperature for Arc Weld
(288 Elements)**

Element	Radius (mm)	Error (inc.3)	Error (inc.4)	Error (inc.5)
1	1.008	0.0112	0.0088	0.0085
2	2.035	0.0111	0.0082	0.0080
3	3.223	0.0188	0.0072	0.0068
4	4.446	0.0350	0.0068	0.0056
5	5.680	0.0444	0.0308	0.0054
6	6.920	0.0175	0.0343	0.0306
7	8.163	0.0127	0.0222	0.0350
8	9.408	0.0088	0.0183	0.0248
9	10.97	0.0093	0.0141	0.0271
10	12.84	0.0063	0.0072	0.0113
11	14.71	0.0015	0.0032	0.0041
12	16.58	0.0013	0.0016	0.0020

The predicted global errors for increments 3 to 5 for both meshes are shown in Table 5.17. Refining the mesh resulted in a decrease in global error ranging between 37% and 46%. Clearly, refining the mesh causes a decrease in both the local and global errors.

**Table 5.17 Global Errors in Temperature for Arc Weld
(All Meshes)**

Mesh Type	Gl. Error (inc.3)	Gl. Error (inc.4)	Gl. Error (inc.5)
<i>36 elements</i>	0.3760	0.3597	0.4277
<i>288 elements</i>	0.2025	0.2267	0.2471

5.4 Assessment

A pressurized thick-walled cylinder and a submerged arc weld were tested using the ERRCALC software. Analytical solutions for these practical engineering problems do not exist. In such cases, the quality of the error prediction is judged by the user.

Effective stress was used as the criterion for error prediction in the first test-case. In those steps with an elastic stress state, the FE solution was very good, and consequently the element and global errors were low. For increments with plasticity, the errors increased, especially where the gradient of the stress field was greatest. In the final increment, the autofrettage caused residual stresses. The largest stresses were located at the bore of the cylinder. Here, the element errors were considerably larger than in the remaining section of the cylinder. As the mesh was refined from 24, to 96, and finally, to 384 elements, the element and global errors decreased for all increments.

Effective plastic strain was used as the criterion for the second test on the cylinder. The errors were largest near the bore of the cylinder, where the plastic strain gradients were greatest. As expected, both element and global errors decreased as the mesh was refined.

The Arc Weld error results were particularly encouraging. The criterion for

the error estimates was based on the temperature distribution. During welding, the thermal gradients change most rapidly at the boundary of the weld pool and the plate. This position is where the FEA will have the most difficulty predicting the solution. Correspondingly, it was at the weld pool boundary that ERRCALC predicted the largest element errors. Even at the weld pool boundary, refinement reduced element errors from approximately 15% to 1%.

5.5 Discussion

The ERRCALC software was tested on several cases where the analytical solution is known, and also on three practical engineering problems. The error estimate predicted element and global errors by measuring the smoothness of the FE solution. If the solution is not smooth, the errors increase. Even if the nodal values are equal to the correct values, the error estimate will still measure the second derivative, or curvature, of the solution. Therefore, by definition, the error measure will overestimate the error.

The results from all the testcases show that refining the mesh will improve the FE solution and decrease the errors. However, if the curvature is large and the gradients change rapidly, it may be necessary to have an extremely fine mesh to approach the condition where the gradients are nearly constant from element to element. In some cases, with localized effects, refinement is only necessary in specific locations to obtain a quick, efficient and accurate FE solution.

Chapter 6

Conclusions and Future Work

6.1 Conclusions

1) An *a posteriori* error estimate for h-adaptive FEA has been developed. The estimate measures the error in the FE solution and provides information required to modify the mesh and obtain an improved solution. The error estimate is not sensitive to scale or reference changes. It is also capable of accomodating uniform or graded meshes.

2) The developed software provides both local and global estimates of the errors. The error measure is based on the difference between a smooth gradient field and the FE field. The smooth gradient field is assumed to approximate the exact solution.

3) The error estimate is independent of the nature of the problem. It is driven by input of any number of primary variables including temperature, displacement, effective plastic stress, hardness, phase fraction and effective plastic strain.

4) The error estimator was tested on four problems for which the analytical solutions are known. Three additional tests on practical engineering problems were conducted. In general, estimated errors for problems for which an analytical solution was available were in agreement with the true errors in the FE solution. Estimated errors from the practical engineering problems were judged to behave appropriately and to have reasonable values.

5) It is recommended that ERRCALC. be fully integrated with ASGARD^[36] and RPLMSH3D^[40]. The developed software will readily accept ASGARD output, compute the element errors and drive the adaptive procedures.

6.2 Future Work

At this point, ERRCALC, takes the FE output and calculates an element error that can be used as input for RPLMSH3D to modify the mesh. It is recommended that the ERRCALC software be fully integrated with ASGARD^[36] and RPLMSH3D^[40] so as to fully automate the FEA. Integration will consist mainly of developing an interface to read and write the data in an appropriate manner. The data transfer code DATTRAN^[3], should also be integrated. DATTRAN transfers nodal data between the old and the new mesh in the adaptive mesh-management cycle.

Consideration will need to be given to the implication of the applied boundary conditions. Elements on boundaries may have error values lower than the surrounding elements. Users will have to use their judgement. For example, if the surrounding elements need to be refined, the elements on the boundaries may also need to be refined.

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Appendix A: Error Estimate Validation

This appendix shows the hand-calculations required for an error estimate at both the element and global levels. The estimation is based on the information gained from a FE analysis. Two heat transfer examples will be considered. In these examples it is assumed that the FE analysis produces temperatures, $\hat{T}$ at the nodes. The error estimation code will calculate the gradients at the Gauss points from the temperatures at the nodes.

A.1 : One-Dimensional Heat Transfer Example

In this example one-dimensional elements will be used for simplicity. The problem, as seen in Figure A.1, consists of three equal-sized elements with the temperatures shown at the nodes, and the Gauss points marked with an x.

The basis functions for a 1D element are:

$$N_1 = \frac{1}{2}(1 - \xi)$$

$$N_2 = \frac{1}{2}(1 + \xi)$$

where, ξ is the coordinate of the point being considered. The locations of the Gauss points are:

$$\xi_a = -0.57735$$

$$\xi_b = 0.57735$$

The temperatures at the nodes in the given mesh are:

$$\hat{T}_1 = 20$$

$$\hat{T}_2 = 2.0$$

$$\hat{T}_3 = 30$$

$$\hat{T}_4 = 22$$

FE mesh showing nodal temperatures

Figure A.1 Mesh used in Error Estimate Verification

A.1.1 Gradients at the Gauss Points, $\hat{g}_{gp}$

The gradients at the Gauss points, in general, are equal to the derivatives of the basis functions multiplied by the the primary variable at the nodes. The matrix containing the derivatives of the basis functions will be referred to, in future references, as the B matrix. This matrix is also known as the temperature gradient interpolation matrix¹.

The equation used to evaluate the gradients for this 1D heat transfer example is:

$$\hat{g}_{gp} = \frac{\partial \hat{T}}{\partial x} = \left[\frac{\partial N_1}{\partial x} \quad \frac{\partial N_2}{\partial x} \right] \begin{bmatrix} \hat{T}_1 \\ \hat{T}_2 \\ \vdots \\ \hat{T}_n \end{bmatrix} \quad (A.1.1 - 1)$$

The components of the B matrix are defined as,

¹ Bathe, K.J., *Finite Element Procedures in Engineering Analysis*, Prentice Hall, N.J., 407-414 (1982).

$$\frac{\partial N_i}{\partial x} = J^{-1} \left[\frac{\partial N_i}{\partial \xi} \right] \quad (A.1.1 - 2)$$

The Jacobian matrix, J , is found by.

$$J = \frac{\partial x}{\partial \xi} \quad (A.1.1 - 3)$$

where,

$$x(\xi) = \sum_{i=1}^n N_i(\xi) x_i \quad (A.1.1 - 4)$$

The variables in the above equations are defined as:

$\hat{g}_{gp}$ are the gradients at the Gauss points obtained from the FE solution;

n is the number of nodes in the element;

N_i are the basis functions for the 1D element;

$\hat{T}_i$ are the temperatures at the nodes obtained from the FE solution;

x_i is a global coordinate;

ξ is a local coordinate.

It is now possible to substitute the known parameters for this problem into the above equations.

$$x(\xi) = N_1 x_1 + N_2 x_2 = \frac{1}{2}(1 - \xi)x_1 + \frac{1}{2}(1 + \xi)x_2 = \frac{x_1}{2} - \frac{x_1}{2}\xi + \frac{x_2}{2} + \frac{x_2}{2}\xi$$

$$J = \frac{\partial x}{\partial \xi} = -\frac{x_1}{2} + \frac{x_2}{2} \quad \text{and} \quad J^{-1} = \frac{2}{x_2 - x_1}$$

For this example all elements are 1 unit in length, so $x_2 - x_1 = 1$, therefore,

$$J = \frac{1}{2} \quad \text{and} \quad J^{-1} = 2$$

It is now necessary to solve for the derivatives of the basis functions,

$$\frac{\partial N_1}{\partial \xi} = -\frac{1}{2}$$

$$\frac{\partial N_2}{\partial \xi} = \frac{1}{2}$$

The components of the B matrix are:

$$\frac{\partial N_1}{\partial x} = 2 \times \left(-\frac{1}{2}\right) = -1$$

$$\frac{\partial N_2}{\partial x} = 2 \times \frac{1}{2} = 1$$

Finally, the temperature gradients at the Gauss points are:

$$\hat{g}_{1a} = \begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} 20 \\ 2.0 \end{bmatrix} = -18$$

$$\hat{g}_{1b} = \begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} 20 \\ 2.0 \end{bmatrix} = -18$$

$$\hat{g}_{2a} = \begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 30 \end{bmatrix} = 28$$

$$\hat{g}_{2b} = \begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 30 \end{bmatrix} = 28$$

$$\hat{g}_{3a} = \begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} 30 \\ 22 \end{bmatrix} = -8.0$$

$$\hat{g}_{3b} = \begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} 30 \\ 22 \end{bmatrix} = -8.0$$

A.1.2 Project $\hat{g}_{gp}$ to the Nodes

To project the gradients at the Gauss points to the nodes in 1D, a simple linear extrapolation can be used. For example:

$$\frac{(\hat{g}_{1a} - \hat{g}_{1b})}{(-0.57735 - 0.57735)} = \frac{(\hat{g}_{1,from1} - \hat{g}_{1a})}{(-1 - (-0.57735))}$$

Clearly, for this 1D example, where the gradients at the Gauss points for each element are the same, the gradients at the nodes will also be the same.

$$\hat{g}_{1,from1} = -18$$

$$\hat{g}_{2,from1} = -18$$

$$\hat{g}_{2,from2} = 28$$

$$\hat{g}_{3,from2} = 28$$

$$\hat{g}_{3,from3} = -8.0$$

$$\hat{g}_{4,from3} = -8.0$$

A.1.3 Obtain a Smoothed Temperature Field, g

By averaging $\hat{g}_{gp}$ at the nodes, it is possible to obtain an estimate of the exact temperature field. This will give a smoothed temperature field g .

$$g_1 = -18$$

$$g_2 = \frac{(-18+28)}{2} = 5.0$$

$$g_3 = \frac{(28+(-8))}{2} = 10$$

$$g_4 = -8.0$$

A.1.4 Interpolation

The smoothed temperature field, g , is then interpolated to the Gauss points. It is assumed that the gradients can be interpolated by the same basis functions as the primary variable. The equation describing interpolation is,

$$g_{gp} = \sum_{i=1}^n N_i(\xi) g_i \quad (A.5 - 1)$$

where:

g_i are the gradients at the nodes;

g_{gp} is the gradient value at the Gauss point;

n is the number of basis functions;

N_i are the basis functions of the element.

For this problem, the basis functions evaluated at the Gauss points are:

$$N_1(-0.57735) = 0.7885$$

$$N_1(0.57735) = 0.2115$$

$$N_2(-0.57735) = 0.2115$$

$$N_2(0.57735) = 0.7885$$

The gradients at the Gauss points are therefore:

$$g_{1a} = (0.7885)(-18) + (0.2115)(5.0) = -13.136$$

$$g_{1b} = (0.2115)(-18) + (0.7885)(5.0) = 0.136$$

$$g_{2a} = (0.7885)(5.0) + (0.2115)(10) = 6.058$$

$$g_{2b} = (0.2115)(5.0) + (0.7885)(10) = 8.943$$

$$g_{3a} = (0.7885)(10) + (0.2115)(-8.0) = 6.193$$

$$g_{3b} = (0.2115)(10) + (0.7885)(-8.0) = -4.193$$

A.1.5 Compute the Error at the Gauss Points

The Gauss point error is the difference between the smoothed gradient, g_{gp} , and the FE gradient, $\hat{g}_{gp}$.

$$e_{1a} = g_{1a} - \hat{g}_{1a} = (-13.136) - (-18) = 4.864$$

$$e_{1b} = (0.136) - (-18) = 18.136$$

$$e_{2a} = (6.058) - (28) = -21.942$$

$$e_{2b} = (8.934) - (28) = -19.057$$

$$e_{3a} = (6.193) - (-8) = 14.193$$

$$e_{3b} = (-4.193) - (-8) = 3.807$$

A.1.6 Compute L_2 Norms

The norms used in the proposed method are the L_2 norm of the Gauss point errors and the L_2 norm of the smoothed gradients at the Gauss points.

$$\|e\|_j = \left[\int_{\Omega} [e]^T [e] d\Omega \right]^{1/2} = \left[\sum_{i=1}^n [e_i]^T [e_i] \det J_i(\xi) W_i \right]^{1/2}$$

$$\|g\| = \left[\int_{\Omega} [g]^T [g] d\Omega \right]^{1/2} = \left[\sum_{i=1}^j \left(\sum_{k=1}^n [g_k]^T [g_k] \det J_k(\xi) W_k \right) \right]^{1/2}$$

where W is the weight for the chosen integration scheme.

For simplicity, the calculations of these norms will only be shown for the first element.

$$\|e\|_1 = \left[[4.864][4.864]\left(\frac{1}{2}\right)(1) + [18.136][18.136]\left(\frac{1}{2}\right)(1) \right]^{1/2}$$

$$\|e\|_1 = 13.277$$

$$\|e\|_2 = 20.550$$

$$\|e\|_3 = 10.391$$

$$\|g\|_1 = \left[[-13.136][-13.136]\left(\frac{1}{2}\right)(1) + [0.136][0.136]\left(\frac{1}{2}\right)(1) \right]$$

$$\|g\|_1 = 86.453$$

$$\|g\|_2 = 58.339$$

$$\|g\|_3 = 27.963$$

$$\|g\| = \left[86.453 + 58.339 + 27.963 \right]^{1/2} = 13.144$$

A.1.7 Compute the Element Errors

It is now possible to compute the error involved with each element in the mesh, E_j .

$$E_j = \frac{\|e\|_j}{\|g\|}$$

$$E_1 = \frac{(13.277)}{(13.144)} = 1.010$$

$$E_2 = \frac{(20.550)}{(13.144)} = 1.563$$

$$E_3 = \frac{(10.391)}{(13.144)} = 0.791$$

A.1.8 Compute the Global Error

The global error is defined as:

$$E_{gl} = \frac{\left[\int_{\Omega} [e]^T [e] d\Omega_{gl} \right]^{1/2}}{\left[\int_{\Omega} [g]^T [g] d\Omega_{gl} \right]^{1/2}} = \frac{\left[\sum_{i=1}^I \left(\sum_{k=1}^n [e_k]^T [e_k] \det J_k(\xi) W_k \right) \right]^{1/2}}{\left[\sum_{i=1}^m \left(\sum_{k=1}^n [g_k]^T [g_k] \det J_k(\xi) W_k \right) \right]^{1/2}} \quad (2.13)$$

For this example problem the global error was computed to be:

$$E_{gl} = 2.023$$

A.2 : Two-Dimensional Heat Transfer Example

Two-dimensional elements will be used in this example, to show that the proposed error estimator is valid for multi-dimension problems. The problem, as seen in Figure A.2, consists of three equal-sized elements with the temperatures shown at the nodes, and the Gauss points marked with an x.

The basis functions for a 2-D element are:

$$N_1 = \frac{1}{4}(1 + \xi)(1 + \eta)$$

$$N_2 = \frac{1}{4}(1 - \xi)(1 + \eta)$$

$$N_3 = \frac{1}{4}(1 - \xi)(1 - \eta)$$

$$N_4 = \frac{1}{4}(1 + \xi)(1 - \eta)$$

where, ξ and η are the coordinates of the point being considered. The locations of the Gauss points are:

$$\xi_a = -0.57735, -0.57735$$

$$\xi_b = -0.57735, 0.57735$$

$$\xi_c = 0.57735, -0.57735$$

$$\xi_d = 0.57735, 0.57735$$

The temperatures at the nodes in the given mesh are:

$$\hat{T}_1 = 16$$

$$\hat{T}_2 = 20$$

$$\hat{T}_3 = 17$$

$$\hat{T}_4 = 15$$

$$\hat{T}_5 = 30$$

$$\hat{T}_6 = 33$$

$$\hat{T}_7 = 8$$

$$\hat{T}_8 = 4$$

Figure A.2 Mesh used in Error Estimate Verification

A.2.1 Gradients at the Gauss Points, $\hat{g}_{gp}$

The gradients at the Gauss points, in general, are equal to the B matrix multiplied by the the primary variable at the nodes. The equation used to evaluate the gradients for this 2D heat transfer example is,

$$\begin{bmatrix} \hat{g}_{gp_x} \\ \hat{g}_{gp_y} \end{bmatrix} = \begin{bmatrix} \frac{\partial \hat{T}}{\partial x} \\ \frac{\partial \hat{T}}{\partial y} \end{bmatrix} = \begin{bmatrix} \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \frac{\partial N_3}{\partial x} & \frac{\partial N_4}{\partial x} \\ \frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \frac{\partial N_3}{\partial y} & \frac{\partial N_4}{\partial y} \end{bmatrix} \begin{bmatrix} \hat{T}_1 \\ \hat{T}_2 \\ \vdots \\ \hat{T}_n \end{bmatrix} \quad (\text{A.2.1} - 1)$$

The components of the B matrix are defined as,

$$\begin{bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \end{bmatrix} = J^{-1} \begin{bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \end{bmatrix} \quad (\text{A.2.1} - 2)$$

The Jacobian matrix, J, is found by

$$J = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix} \quad (\text{A.2.1} - 3)$$

2 of/de 2

PM-1 3½"x4" PHOTOGRAPHIC MICROCOPY TARGET
NBS 1010a ANSI/ISO #2 EQUIVALENT

where,

$$x(\xi, \eta) = \sum_{i=1}^n N_i(\xi) x_i \quad \text{and} \quad y(\xi, \eta) = \sum_{i=1}^n N_i(\xi) y_i \quad (A.2.1 - 4, 5)$$

The variables in the above equations are defined as:

$\hat{g}_{gp}$ are the gradients at the Gauss points obtained from the FE solution;

n is the number of basis functions;

N_i are the basis functions for the 2D element;

$\hat{T}_i$ are the temperatures at the nodes obtained from the FE solution;

x_i, y_i are global coordinates;

ξ, η are local coordinates.

It is now possible to substitute the known parameters for this problem into the above equations.

$$x(\xi, \eta) = \frac{1}{4}(1 + \xi)(1 + \eta)x_1 + \frac{1}{4}(1 - \xi)(1 + \eta)x_2 + \frac{1}{4}(1 - \xi)(1 - \eta)x_3 + \frac{1}{4}(1 + \xi)(1 - \eta)x_4$$

Now, $x_1 = x_4$ and $x_2 = x_3$, so,

$$x(\xi, \eta) = \frac{x_1}{2} + \frac{x_1}{2}\xi + \frac{x_2}{2} - \frac{x_2}{2}\xi$$

For this example all elements are 1 unit in length, so $x_2 - x_1 = 1$, therefore,

$$\frac{\partial x}{\partial \xi} = \frac{x_1}{2} - \frac{x_2}{2} = \frac{1}{2}$$

$$\frac{\partial x}{\partial \eta} = 0$$

By the same method the partial derivatives for y can be found,

$$\frac{\partial y}{\partial \xi} = 0$$

$$\frac{\partial y}{\partial \eta} = \frac{y_1}{2} - \frac{y_3}{2} = \frac{1}{2}$$

These values are then substituted to derive the Jacobian.

$$J = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \quad \text{and} \quad J^{-1} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

The derivatives of the basis functions with respect to the global coordinates can now be found. For example;

$$\begin{bmatrix} \frac{\partial N_1}{\partial x} \\ \frac{\partial N_1}{\partial y} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} \frac{1}{4} + \frac{\eta}{4} \\ \frac{1}{4} + \frac{\xi}{4} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} + \frac{\eta}{2} \\ \frac{1}{2} + \frac{\xi}{2} \end{bmatrix}$$

The components of the B matrix can now be found and consequently, the gradients at the Gauss points can be derived. For simplicity, this calculation will only be shown explicitly for Gauss point a, element 1.

$$\begin{bmatrix} \hat{g}_{p_x} \\ \hat{g}_{p_y} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} + \frac{\eta}{2} & -\frac{1}{2} - \frac{\eta}{2} & -\frac{1}{2} + \frac{\eta}{2} & \frac{1}{2} - \frac{\eta}{2} \\ \frac{1}{2} + \frac{\xi}{2} & \frac{1}{2} - \frac{\xi}{2} & -\frac{1}{2} + \frac{\xi}{2} & -\frac{1}{2} - \frac{\xi}{2} \end{bmatrix} \begin{bmatrix} \hat{T}_1 \\ \hat{T}_2 \\ \hat{T}_3 \\ \hat{T}_4 \end{bmatrix}$$

Gauss point 1a is located at (-0.57735, -0.57735). By substituting these coordinates for ξ and η the following B matrix is found,

$$\begin{bmatrix} \hat{g}_{1a_x} \\ \hat{g}_{1a_y} \end{bmatrix} = \begin{bmatrix} 0.2113 & -0.2113 & -0.7887 & 0.7887 \\ 0.2113 & 0.7887 & -0.7887 & -0.2113 \end{bmatrix} \begin{bmatrix} 16 \\ 20 \\ 17 \\ 15 \end{bmatrix}$$

$$\begin{bmatrix} \hat{g}_{1a_x} \\ \hat{g}_{1a_y} \end{bmatrix} = \begin{bmatrix} -2.4226 \\ 2.5774 \end{bmatrix} \quad \begin{bmatrix} \hat{g}_{1b_x} \\ \hat{g}_{1b_y} \end{bmatrix} = \begin{bmatrix} -3.5774 \\ 2.5774 \end{bmatrix}$$

$$\begin{bmatrix} \hat{g}_{1c_x} \\ \hat{g}_{1c_y} \end{bmatrix} = \begin{bmatrix} -2.4226 \\ 1.4226 \end{bmatrix} \quad \begin{bmatrix} \hat{g}_{1d_x} \\ \hat{g}_{1d_y} \end{bmatrix} = \begin{bmatrix} -3.5774 \\ 1.4226 \end{bmatrix}$$

$$\begin{bmatrix} \hat{g}_{2a_x} \\ \hat{g}_{2a_y} \end{bmatrix} = \begin{bmatrix} 17.1548 \\ 0.1548 \end{bmatrix} \quad \begin{bmatrix} \hat{g}_{2b_x} \\ \hat{g}_{2b_y} \end{bmatrix} = \begin{bmatrix} 14.8452 \\ 0.1548 \end{bmatrix}$$

$$\begin{bmatrix} \hat{g}_{2c_x} \\ \hat{g}_{2c_y} \end{bmatrix} = \begin{bmatrix} 17.1548 \\ -2.1548 \end{bmatrix} \quad \begin{bmatrix} \hat{g}_{2d_x} \\ \hat{g}_{2d_y} \end{bmatrix} = \begin{bmatrix} 14.8452 \\ -2.1548 \end{bmatrix}$$

$$\begin{bmatrix} \hat{g}_{3a_x} \\ \hat{g}_{3a_y} \end{bmatrix} = \begin{bmatrix} -27.5209 \\ -1.5209 \end{bmatrix} \quad \begin{bmatrix} \hat{g}_{3b_x} \\ \hat{g}_{3b_y} \end{bmatrix} = \begin{bmatrix} -23.4791 \\ -1.5209 \end{bmatrix}$$

$$\begin{bmatrix} \hat{g}_{3c_x} \\ \hat{g}_{3c_y} \end{bmatrix} = \begin{bmatrix} -27.5209 \\ 2.5209 \end{bmatrix} \quad \begin{bmatrix} \hat{g}_{3d_x} \\ \hat{g}_{3d_y} \end{bmatrix} = \begin{bmatrix} -23.4791 \\ 2.5209 \end{bmatrix}$$

A.2.2 Project $\hat{g}_{gp}$ to the Nodes

To project the Gauss point gradients to the nodes in 2D, a weighted least square bilinear projection matrix² is used. For example,

$$\begin{bmatrix} \hat{g}_{1x} \\ \hat{g}_{2x} \\ \hat{g}_{3x} \\ \hat{g}_{4x} \end{bmatrix} = [\mathbf{P}] \begin{bmatrix} \hat{g}_{1ax} \\ \hat{g}_{1bx} \\ \hat{g}_{1cx} \\ \hat{g}_{1dx} \end{bmatrix}$$

where the P matrix is:

$$[\mathbf{P}] = \begin{bmatrix} 0.13397 & -0.50000 & -0.50000 & 1.86603 \\ -0.50000 & 1.86603 & 0.13397 & -0.50000 \\ 1.86603 & -0.50000 & -0.50000 & 0.13397 \\ -0.50000 & 0.13397 & 1.86603 & -0.50000 \end{bmatrix}$$

Each node will have a gradient in both the x and y directions. The nodes which are connected to more than one element will have gradients from each of the respective elements.

$$\begin{array}{lcl} \begin{bmatrix} \hat{g}_{1x} \\ \hat{g}_{2x} \\ \hat{g}_{3x} \\ \hat{g}_{4x} \end{bmatrix}_{from1} & = & \begin{bmatrix} -4.0001 \\ -4.0001 \\ -1.9999 \\ -1.9999 \end{bmatrix} & \begin{bmatrix} \hat{g}_{1y} \\ \hat{g}_{2y} \\ \hat{g}_{3y} \\ \hat{g}_{4y} \end{bmatrix}_{from1} & = & \begin{bmatrix} 0.9999 \\ 3.0001 \\ 3.0001 \\ 0.9999 \end{bmatrix} \\ \begin{bmatrix} \hat{g}_{5x} \\ \hat{g}_{1x} \\ \hat{g}_{4x} \\ \hat{g}_{6x} \end{bmatrix}_{from2} & = & \begin{bmatrix} 13.9998 \\ 13.9998 \\ 18.0002 \\ 18.0002 \end{bmatrix} & \begin{bmatrix} \hat{g}_{5y} \\ \hat{g}_{1y} \\ \hat{g}_{4y} \\ \hat{g}_{6y} \end{bmatrix}_{from2} & = & \begin{bmatrix} -3.0002 \\ 1.0002 \\ 1.0002 \\ -3.0002 \end{bmatrix} \\ \begin{bmatrix} \hat{g}_{7x} \\ \hat{g}_{5x} \\ \hat{g}_{6x} \\ \hat{g}_{8x} \end{bmatrix}_{from3} & = & \begin{bmatrix} -21.9997 \\ -21.9997 \\ -29.0003 \\ -29.0003 \end{bmatrix} & \begin{bmatrix} \hat{g}_{7y} \\ \hat{g}_{5y} \\ \hat{g}_{6y} \\ \hat{g}_{8y} \end{bmatrix}_{from3} & = & \begin{bmatrix} 4.0003 \\ -3.0003 \\ -3.0003 \\ 4.0003 \end{bmatrix} \end{array}$$

² Patel, B., *Thermo-Elasto-Plastic Finite Element Analysis of Deformations and Residual Stresses Due to Welds*, Ph.D. Thesis, Carleton University, Ottawa (1985).

A.2.3 Obtain a Smoothed Temperature Field, g

By averaging $\hat{g}_{gp}$ at the nodes, it is possible to obtain an estimate of the exact temperature field. This will give a smoothed temperature field g .

$$\begin{aligned} g_{1x} &= \frac{(-4.0001+13.9998)}{2} = 4.9999 \\ g_{2x} &= -4.0001 \\ g_{3x} &= -1.9999 \\ g_{4x} &= \frac{(-1.9999+18.0002)}{2} = 8.0002 \\ g_{5x} &= \frac{(13.9998+-21.9997)}{2} = -4.0000 \\ g_{6x} &= \frac{(18.0002+-29.0003)}{2} = -5.5001 \\ g_{7x} &= -21.9997 \\ g_{8x} &= -29.0003 \end{aligned}$$

$$\begin{aligned} g_{1y} &= \frac{(0.9999+1.0002)}{2} = 1.0001 \\ g_{2y} &= 3.0001 \\ g_{3y} &= 3.0001 \\ g_{4y} &= \frac{(0.9999+1.0002)}{2} = 1.0001 \\ g_{5y} &= \frac{(-3.0002+-3.0003)}{2} = -3.0003 \\ g_{6y} &= \frac{(-3.0002+-3.0003)}{2} = -3.0003 \\ g_{7y} &= 4.0003 \\ g_{8y} &= 4.0003 \end{aligned}$$

A.2.4 Interpolation

The smoothed temperature field, g , is then interpolated to the Gauss points. It is assumed that the gradients can be interpolated by the same basis functions as the primary variable. The equation describing interpolation is,

$$g_{gp} = \sum_{i=1}^n N_i(\xi) g_i \quad (A.5 - 1)$$

where:

g_i are the gradients at the nodes;

g_{gp} is the gradient value at the Gauss point;

n is the number of basis functions;

N_i are the basis functions of the element.

For this problem, the basis functions evaluated at the Gauss points are:

$N_1(-0.57735, -0.57735) = 0.0447$	$N_1(0.57735, -0.57735) = 0.1668$
$N_1(-0.57735, 0.57735) = 0.1668$	$N_1(0.57735, 0.57735) = 0.6217$
$N_2(-0.57735, -0.57735) = 0.1668$	$N_2(0.57735, -0.57735) = 0.0447$
$N_2(-0.57735, 0.57735) = 0.6217$	$N_2(0.57735, 0.57735) = 0.1668$
$N_3(-0.57735, -0.57735) = 0.6217$	$N_3(0.57735, -0.57735) = 0.1668$
$N_3(-0.57735, 0.57735) = 0.1668$	$N_3(0.57735, 0.57735) = 0.0447$
$N_4(-0.57735, -0.57735) = 0.1668$	$N_4(0.57735, -0.57735) = 0.6217$
$N_4(-0.57735, 0.57735) = 0.0447$	$N_4(0.57735, 0.57735) = 0.1668$

The interpolation of element 1, Gauss point a, in the x direction is shown as an example:

$$g_{1a_x} = (0.0447)(4.9999) + (0.1668)(-4.0001) + (0.6217)(-1.9999) + (0.1668)(8.0002)$$

$g_{1a_x} = -0.3527$	$g_{2a_x} = 4.7114$	$g_{3a_x} = -9.9072$
$g_{1a_y} = 2.5770$	$g_{2a_y} = 0.1540$	$g_{3a_y} = -1.5195$
$g_{1b_x} = -1.6288$	$g_{2b_x} = 3.5299$	$g_{3b_x} = -8.3701$
$g_{1b_y} = 2.5770$	$g_{2b_y} = 0.1540$	$g_{3b_y} = -1.5195$
$g_{1c_x} = 5.2952$	$g_{2c_x} = -2.529$	$g_{3c_x} = 13.2635$
$g_{1c_y} = 1.4230$	$g_{2c_y} = -2.154$	$g_{3c_y} = 2.51950$
$g_{1d_x} = 3.6836$	$g_{2d_x} = -2.213$	$g_{3d_x} = -19.428$
$g_{1d_y} = 1.4230$	$g_{2d_y} = -2.154$	$g_{3d_y} = 2.51950$

A.2.5 Compute the Error at the Gauss Points

The Gauss point error is the difference between the smoothed gradient, g_{gp} , and the FE gradient, $\hat{g}_{gp}$.

$$[e]_{1a} = \begin{bmatrix} g_{1a_x} - \hat{g}_{1a_x} \\ g_{1a_y} - \hat{g}_{1a_y} \end{bmatrix} = \begin{bmatrix} (-0.3527) - (-2.4226) \\ (2.5770) - (2.5774) \end{bmatrix}$$

$[e]_{1a} = \begin{bmatrix} 2.0699 \\ 0.0001 \end{bmatrix}$	$[e]_{1b} = \begin{bmatrix} 1.9486 \\ 0.0001 \end{bmatrix}$	$[e]_{1c} = \begin{bmatrix} 7.7178 \\ 0.0004 \end{bmatrix}$	$[e]_{1d} = \begin{bmatrix} 7.2637 \\ 0.0004 \end{bmatrix}$
$[e]_{2a} = \begin{bmatrix} 2.0699 \\ 0.0000 \end{bmatrix}$	$[e]_{2b} = \begin{bmatrix} 1.9486 \\ 0.0000 \end{bmatrix}$	$[e]_{2c} = \begin{bmatrix} 2.0699 \\ 0.0001 \end{bmatrix}$	$[e]_{2d} = \begin{bmatrix} 1.9486 \\ 0.0001 \end{bmatrix}$
$[e]_{3a} = \begin{bmatrix} 2.0699 \\ 0.0014 \end{bmatrix}$	$[e]_{3b} = \begin{bmatrix} 1.9486 \\ 0.0014 \end{bmatrix}$	$[e]_{3c} = \begin{bmatrix} 2.0699 \\ 0.0014 \end{bmatrix}$	$[e]_{3d} = \begin{bmatrix} 1.9486 \\ 0.0014 \end{bmatrix}$

A.2.6 Compute L_2 Norms

The norms to be used in the proposed method are the L_2 norm of the Gauss point errors and the L_2 norm of the smoothed gradients at the Gauss points.

$$\|e\|_2 = \left[\int_{\Omega} [e]^T [e] d\Omega \right]^{1/2} = \left[\sum_{i=1}^n [e_i]^T [e_i] \det J_i(\xi) W_i \right]^{1/2}$$

$$\|g\|_2 = \left[\int_{\Omega} [g]^T [g] d\Omega \right]^{1/2} = \left[\sum_{i=1}^j \left(\sum_{k=1}^n [g_k]^T [g_k] \det J_k(\xi) W_k \right) \right]^{1/2}$$

For simplicity, the calculations of these norms will only be done for the first element. For this example the contributions from the y direction are negligible.

$$\begin{aligned} \|e\|_1 &= \left[[2.0699 \quad 0.0001] \begin{bmatrix} 2.0699 \\ 0.0001 \end{bmatrix} \left(\frac{1}{4}\right)(1) + [1.9486 \quad 0.0001] \begin{bmatrix} 1.9486 \\ 0.0001 \end{bmatrix} \left(\frac{1}{4}\right)(1) + \right. \\ &\quad \left. [7.7178 \quad 0.0004] \begin{bmatrix} 7.7178 \\ 0.0004 \end{bmatrix} \left(\frac{1}{4}\right)(1) + [7.2637 \quad 0.0004] \begin{bmatrix} 7.2637 \\ 0.0004 \end{bmatrix} \left(\frac{1}{4}\right)(1) \right]^{1/2} \\ \|e\|_1 &= 5.4865 \\ \|e\|_2 &= 15.5023 \\ \|e\|_3 &= 23.5494 \end{aligned}$$

The norm of the smoothed gradients at the Gauss points clearly has contributions from both the x and y directions.

$$\begin{aligned} \|g\|_1 &= \left[[-0.3527 \quad 2.5770] \begin{bmatrix} -0.3527 \\ 2.5770 \end{bmatrix} \left(\frac{1}{4}\right)(1) + [-1.6288 \quad 2.5770] \begin{bmatrix} -1.6288 \\ 2.5770 \end{bmatrix} \left(\frac{1}{4}\right)(1) + \right. \\ &\quad \left. [5.2952 \quad 1.4230] \begin{bmatrix} 5.2952 \\ 1.4230 \end{bmatrix} \left(\frac{1}{4}\right)(1) + [3.6863 \quad 1.4230] \begin{bmatrix} 3.6863 \\ 1.4230 \end{bmatrix} \left(\frac{1}{4}\right)(1) \right] \\ \|g\|_1 &= 15.4339 \\ \|g\|_2 &= 13.8183 \\ \|g\|_3 &= 184.7207 \\ \|g\| &= \left[15.4339 + 13.8183 + 184.7207 \right]^{1/2} = 14.6278 \end{aligned}$$

A.2.7 Compute the Element Errors

It is now possible to compute the error involved with each element in the mesh. E_j , where:

$$E_j = \frac{\|e\|_j}{\|g\|}$$

$$E_1 = \frac{(5.4865)}{(14.6278)} = 0.3751$$

$$E_2 = \frac{(15.5023)}{(14.6278)} = 1.0598$$

$$E_3 = \frac{(23.5494)}{(14.6278)} = 1.6099$$

A.2.8 Compute the Global Error

The global error is defined as:

$$E_{gl} = \frac{\left[\int_{\Omega} [e]^T [e] d\Omega_{gl} \right]^{1/2}}{\left[\int_{\Omega} [g]^T [g] d\Omega_{gl} \right]^{1/2}} = \frac{\left[\sum_{i=1}^j (\sum_{k=1}^n [e_k]^T [e_k] \det J_k(\xi) W_k) \right]^{1/2}}{\left[\sum_{i=1}^m (\sum_{k=1}^n [g_k]^T [g_k] \det J_k(\xi) W_k) \right]^{1/2}}$$

For this example problem the global error was computed to be:

$$E_{gl} = 1.9636$$

END

0 | 2 + 0 6 + 9 | 5

FIN