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A HIGH-ACCURACY APPROACH TO FINITE ELEMENT ANALYSIS USING THE HEXA 27-NODE ELEMENT*

Pedro V. Marcal

MPACT, Corp.
5297 Oak Bend Lane, Suite 105
Oak Park, CA 91377
pedrovmarcal@gmail.com

Jeffrey T. Fong

National Institute of Standards & Technology
100 Bureau Drive
Gaithersburg, MD 20899
fong@nist.gov

Robert Rainsberger

XYZ Scientific Applications, Inc.,
2255 Morello Avenue, Suite 220
Pleasant Hill, CA 94523
rains@ruegrid.com

Li Ma

National Institute of Standards & Technology
100 Bureau Drive
Gaithersburg, MD 20899
lima@nist.gov

ABSTRACT

In most finite-element-analysis codes, accuracy is achieved through the use of the hexahedron hexa-20 elements (a node at each of the 8 corners and 12 edges of a brick element). Unfortunately, without an additional node in the center of each of the element's 6 faces, nor in the center of the hexa, the hexa-20 elements are not fully quadratic such that its truncation error remains at $h^2(0)$, the same as the error of a hexa-8 element formulation

To achieve an accuracy with a truncation error of $h^3(0)$, we need the fully-quadratic hexa-27 formulation. A competitor of the hexa-27 element in the early days was the so-called serendipity cubic hexa-32 solid elements (see Ahmad, Irons, and Zienkiewicz, Int. J. Numer. Methods in Eng., 2:419-451 (1970) [1]). The hexa-32 elements, unfortunately, also suffer from the same lack of accuracy syndrome as the hexa-20's.

In this paper, we investigate the accuracy of various elements described in the literature including the fully quadratic hexa-27 elements to a shell problem of interest to the pressure vessels and piping community, viz. the shell-element-based analysis of a barrel vault. Significance of the highly accurate hexa-27 formulation and a comparison of its results with similar solutions using ABAQUS hexa-8, and hexa-20 elements, are presented and discussed. Guidelines are proposed for selection of better elements.

Keywords: finite element method, MPACT, ABAQUS, element selection, tetras, hexas, truncation errors, numerical methods.

1. INTRODUCTION

In most finite-element-analysis codes, accuracy is achieved through the use of the hexahedron hexa-20 elements (a node at each of the 8 corners and 12 edges of a brick element). Unfortunately, without an additional node in the center of each of the element's 6 faces, nor in the center of the hexa, the hexa-20 elements are not fully quadratic such that its truncation error remains at $h^2(0)$, the same as the error of a hexa-8 element formulation (see Zienkiewicz and Taylor [2]).

To achieve an accuracy with a truncation error of $h^3(0)$, we need the fully-quadratic hexa-27 formulation. A competitor of the hexa-27 element in the early days was the so-called 'serendipity' cubic hexa-32 solid elements (see Ahmad, Irons, and Zienkiewicz [1]). The hexa-32 elements, unfortunately, also suffer from the same lack of accuracy syndrome as the hexa-20's.

In a 3-part series of papers, of which this paper is Part I, we investigate the applicability of the fully quadratic hexa-27 elements to a problem of interest to the pressure vessels and piping community, the shell-element based analysis of a barrel vault.

For engineering applications, the lack of uncertainty estimates is generally tolerated when the FEM simulation results show convergence as a function of the mesh density, since decisions are made with code-prescribed safety factors and engineering judgment. However, for advanced

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engineering and scientific applications, where input parameters are not well characterized and the fundamental governing equations are sometimes not even known, the lack of uncertainty quantification (UQ) in FEM simulations falls short for making the FEM a credible tool for scientific investigation without a mandatory process of verification (for mathematical and computational correctness) and validation (against experiments or field measurements of a full-scale structure or component).

To address this challenge, we develop a 3-part series of papers, of which this paper is the first part, or, Part I:

Part I (Marcal, Fong, Rainsberger, and Ma [3]) This paper: In the first part, we address the selection of Element Type by applying the theory of truncation errors to prove that the 27-node element, Hexa-27, is superior to any of the other commonly-used elements, namely, Tetra-04, Hexa-08, and Hexa-20, because the truncation error of Hexa-27 is $h^3(0)$, and that of the others, $h^2(0)$.

Part II (Fong, Filliben, Heckert, Marcal, Rainsberger, and Ma [4]): In this part, we address the source of error due to Mesh Density by developing a 2-step method, first to estimate the uncertainty of a converging series of finite-element-mesh-density-parametric solutions of a specific quantity (e.g., a stress component) using a nonlinear least square fit [6] of a 4-parameter logistic function [7, 8], and then to extrapolate the results of that quantity to an extremely fine mesh density approaching the infinite degrees of freedom. Assuming the chosen quantity increases with mesh density, the estimated upper asymptote of the logistic function serves as the “best” estimate of that chosen quantity. Throughout this paper, we use a public domain statistical analysis software package named “DATAPLOT” [9] to code the nonlinear least squareS (NL-LSQ) fit and plot the results.

Part III (Rainsberger,Fong,Marcal[5]): in the third part, we develop a super-parametric method to address not only errors due to Model Parameters by parametrizing the geometry, material properties, and boundary conditions using a FEM pre-processor named TrueGrid [10], but also the other four sources by parametrizing the solution platform (Source-1), the element type (Source-2), the mesh density (Source-3), and, to a limited extent, the mesh quality (Source-4).

Most of the discussions on accuracy of the finite element method start with the completeness of the element representation using the adaptation of the Pascal Triangle [2], which in turn links back to errors of approximation by truncation of the terms in a binomial expansion. Here we explain the expansion in two dimensions using the Pascal Triangle.

The expansion for a square (may be iso-parametric) is given by all the terms included by the diamond pattern as shown in Fig.1.

So for a quadratic square we have the following formula:

$$u = [1, x, xy, y, x^2, x^2y, x^2y^2, xy^2, y^2] \{a\} + h^3(0) \quad (1)$$

where u is a single degree of freedom in an element, $\{a\}$ are nine undetermined coefficients, and $h^3(0)$ is the order of the

truncation error. The corresponding element in 2D is the 9-node quadrilateral

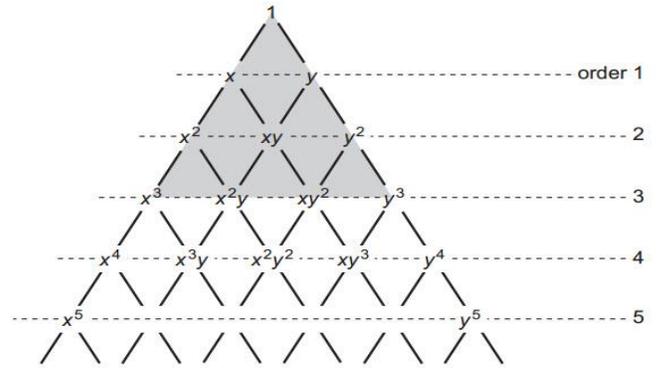


Fig 1 THE PASCAL TRIANGLE OF THE ORDER OF TRUNCATION ERRORS (AFTER [2], FIG. 5.5)

The order of the truncation error can be read off from the Pascal Triangle as the lowest order that is not included in the Pascal Diamond for the square elements and by the triangle for simplex elements. By this we can write a similar expression for the quadratic triangle as

$$u = [1, x, xy, y, x^2, y^2] \{a\} + h^2(0) \quad (2)$$

where $\{a\}$ are six undetermined coefficients, and $h^2(0)$ is the order of the truncation error, e.g. the truncated terms x^2y , x^2y^2 , xy^2 in (1) have been left out.

As shown by Zienkiewicz and Taylor [9], the so-called ‘serendipity’ elements are among the most popular of elements. In the two dimensional case these elements are obtained by dropping the x^2y^2 term so that the eight undetermined coefficients $\{a\}$ result in a truncation error of $h^2(0)$ compared to that of $h^3(0)$ for the full nine terms. The corresponding element does not have the center node.

The Pascal Triangle can be generalized to the third dimension by considering a third axis for z . Then the terms to be included or excluded are obtained by multiplying the terms in the third axis by the respective triangle or diamond for the first two axes as shown by the Fig. 1. All terms are obtained by cyclic permutation. As an example, we consider the case for the quadratic serendipity element in three directions. Here the excluded seven terms are

$$x^2y^2, y^2z^2, z^2x^2, x^2y^2z, xy^2z^2, x^2yz^2, x^2y^2z^2 \quad (3)$$

This is for the 20-node hexa element with a truncation error of $h^2(0)$.

This may be compared to the full expansion quadratic element resulting in a 27-node hexa with a truncation error of $h^2(0)$. This element has three layers of nine nodes each with the middle layer at the mid-plane. Though the value of the truncation errors are problem dependent, we can conclude qualitatively that the serendipity elements are a poor trade off

because they result in a lower order of truncation error for the sake of approximately dropping a quarter of the terms in the case of the 20-node hexa. This approximation adopted for convenience and reduction of computing in the early FEA days is now so widely accepted that many analysts are surprised by its poor performance.

In the displacement method of the finite element analysis (FEA), we calculate the element stiffness and assemble these into a master stiffness. By the principle of virtual work, for an elastic body and using the usual finite element notation, we have for an elemental cube $dx \times dy \times dz$

$$\begin{aligned} & \{du\}^T ([B] [N])^T [D] [B] [N] \{u\} \\ & + (d(h^n(0))/dxi)^T [D] d(h^n(0))/dxi \\ & = \{du\}^T \{P\} + h^n(0) \{P\} \end{aligned} \quad (4)$$

where T indicates transpose of a vector or matrix,

[N] is the displacement to undetermined coefficient matrix,

[B] is the displacement to strain transformation matrix,

[D] is the strain to stress transformation matrix,

n is the truncation order of the error, and

$d(h^n(0))/dxi$ is the differentiation of the error term w.r.t. the three axis directions.

The inclusion of the error terms indicates the existence of the error even at convergence. It also shows that there are two types of error in the normal case, with both error terms contributing to the error in an integral sense. However in the case of strain singularities the differential local term dominates. This was noted by Zienkiewicz and Taylor [2] in their study of super-convergence. The error terms indicate that they are element dependent and with the orders as discussed previously.

The early work on modeling shells with solid elements was encouraging [1]. However, when it came to modeling thin shells, some doubt was cast on the ability of the solid elements to do so. There were three reasons given for this. The first one was the apparently superior performance of the shell element formulation advanced in [1]. The second, based on the cubic solid elements used, was that this would lead to large computing times. The third was the worry that the thin shells would lead to numerical problems with the use of the solid elements, albeit unsubstantiated. The writers have been using the hexa 27 element for shell problems and have not come across any problems.

2. CASE STUDY 1: THE STRESS ANALYSIS OF A BARREL VAULT USING SHELL ELEMENTS

In our first test case, we consider the problem of the barrel-vault, a much studied shell problem [1, 11, 12]. Because of symmetry, we only need to consider a quarter of the shell. The shell has no edge beam and is supported by a diaphragm at its ends. The shell properties are: Young's Modulus = 3.0×10^6 psi, and Poisson Ratio = 0. The shell mass density is 90

lbs/ft². The shell has a radius to thickness ratio of 100, and can be considered a thin shell. The shell is shown in Fig. 2.

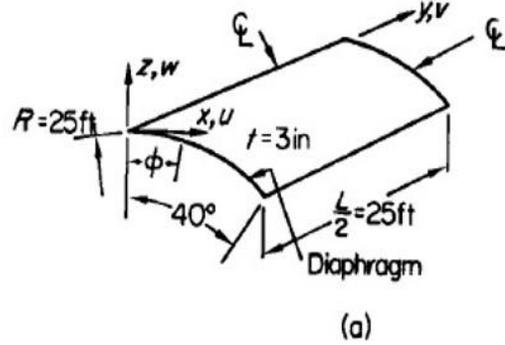


Fig 2 GEOMETRY OF A BARREL VAULT

The vertical displacement on the mid-plane from [1] is shown below in Fig. 3.

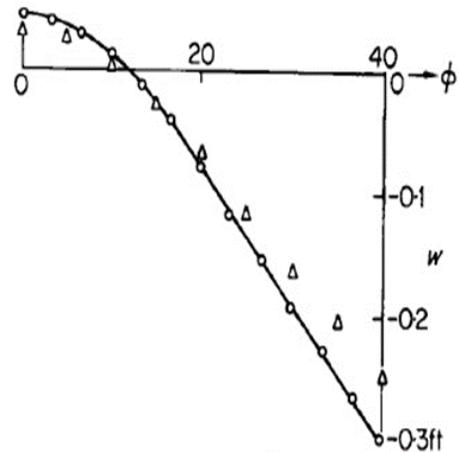


Fig 3 VERTICAL DISPLACEMENT OF MID-PLANE (after [1])

The results for hexa 6 X 6 sits exactly over the results shown here for the 6 X 4 in [6]. The important dimension for both elements being in the mid-plane. The following table shows the variation of the maximum displacement with respect to the number of subdivisions along the mid-plane, given as the second dimension.

The analysis also included the estimation of the buckling load at the end of the incremental analysis. This buckling is indicated with a negative multiplier which indicates that the shell is more susceptible to a negative weight generated perhaps by wind forces rather than by its weight [12]. We concluded our study of this case by reducing using a 6 X 6 mesh to show that the same results as the 9 X 6 mesh could be obtained with a 6 X 6 mesh, since in general, one could not tell the preference of one dimension versus the other. Finally we reduced the shell thickness to 0.25 in. resulting in a radius to shell thickness ratio of 1200, which may be considered as a very thin shell. This is typical of the shell used in our study of the micro-lattices.

Now the maximum vertical displacement is -16.4 ins. And the buckling multiplier becomes -0.21 respectively. A much weaker shell in resisting buckling.

TABLE 1. EFFECT OF MESH SIZE ON RESULTS SECOND DIMENSION IS ALONG THE MID-PLANE.

Shell Subdivision	2 X 2	6 X 4	9 X 6
Vertical Disp. In mid-plane, in.	-0.98	-3.03	-3.54
Buckling multiplier	-13.56	-5.77	-4.53

3. CASE STUDY 2: VARIATION OF ELEMENT TYPES FOR ABAQUS AND IMPACT

In this section we start off the discussion of accuracy in [2] for the much studied barrel vault problem presented above. Their study is shown in Fig. 4.

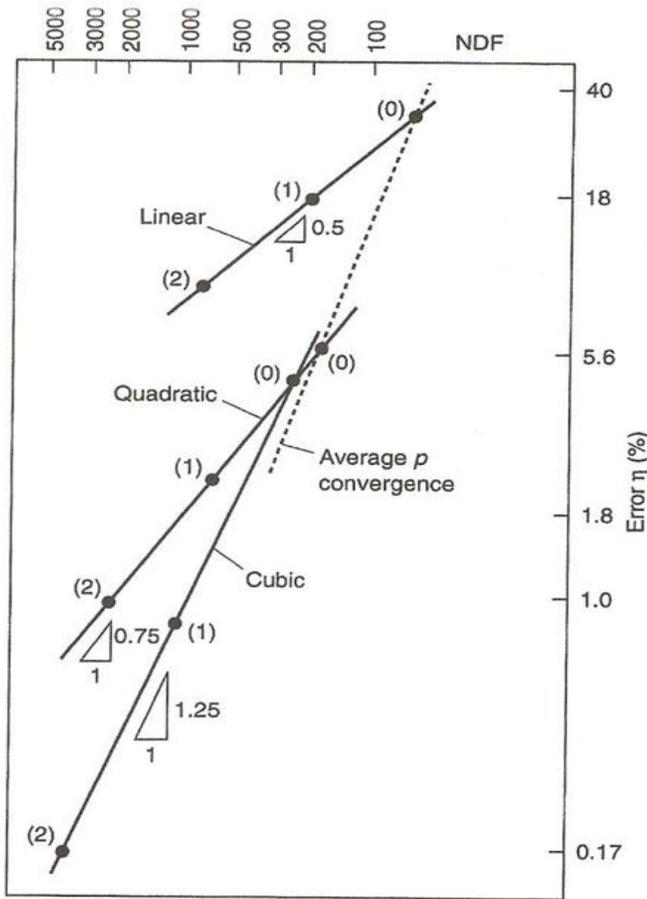


Fig 4 CONVERGENCE STUDY WITH SERENDIPITY ELEMENTS

This diagram shows the normalized % error (normalize=previous value/current value) plotted against the dof. Bearing in mind that the results were obtained in a time when computing time was at a premium, two criticism can be raised. The first is that it assumed a linear log-log function as a

relation between the two values. Because the prevailing view was that all elements would converge to the same answer, no attempt was made to obtain converged values.

In our three part series we introduce the use of a logistic function. This allows us to vary the number of dof for 5 points and use the logistic fit to extrapolate to an estimate of the value at an infinite number of dof. (We define this as the converged value). Fig. 5 shows such a plot for an ABAQUS set of results for the Hexa8 element type.

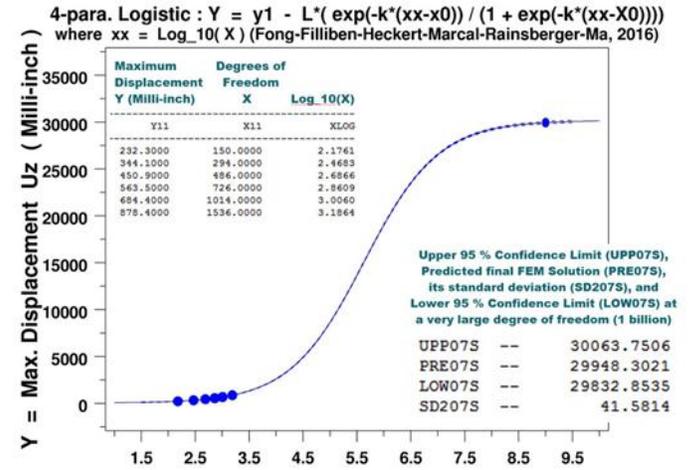


Fig 5 LOGISTIC FIT FOR MAX. DISPLACEMENT Y

This method is described more fully in the Part 3 of our series of papers. The results are shown here to illustrate the good answers that can be achieved with a reasonable size mesh, circa 100,000 max.. All our other results in this paper will be based on this method of obtaining the converged values.

Now we will present a series of results for ABAQUS [13] using the tetra-4, Hexa8 and hexa-20 respectively.

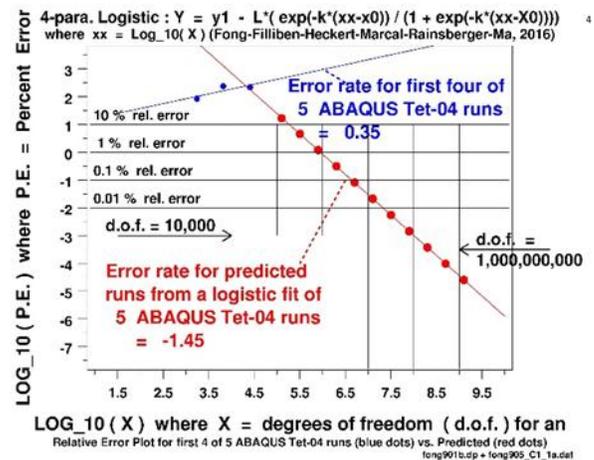


Fig 6 ERROR VS DOF FORTET-4

In the above plot, we show the error rate for the first four of 5 tet-4 runs as a least square fit. Finally each best estimate of the displacement is given after the equal '=' sign. Note that the logistic function produces a much better answer. The linear error rate due to the logistic function is shown by the fitted red points.

Each red point represents the dof that corresponds to the largest displacement projected by the logistic fit. Though results are shown for very small errors ($\ll 0.001\%$) and large dof ($> 1.e+9$), we do so to study general trends. The real values for various typical log values are included in our diagrams to help the reader relate to practical values.

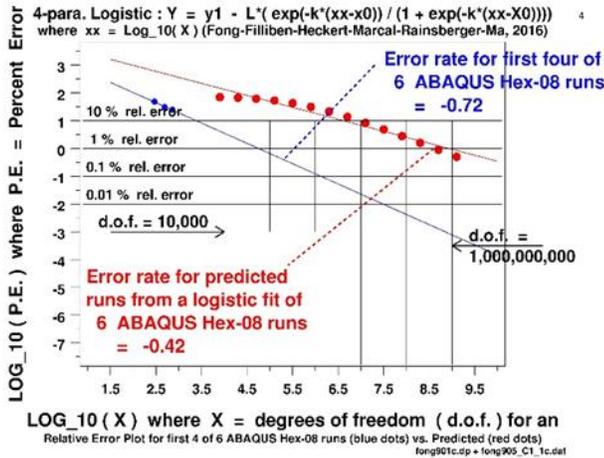


Fig 7 ERROR VS DOF FOR HEXA-8

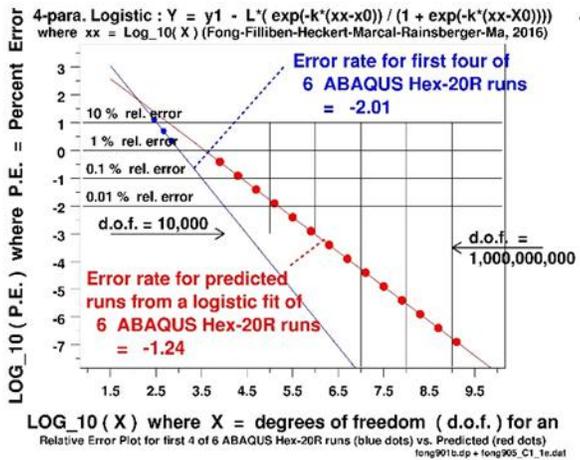


Fig 8 ERROR VS DOF FOR HEXA-20

We now show plots for the MPACT program for tet-4, tet-10, hexa-8 and hexa-27 respectively.

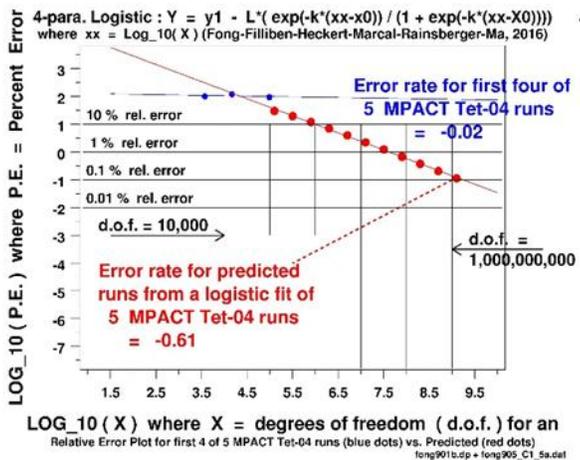


Fig 9 ERROR VS DOF FOR TET-4 (MPACT)

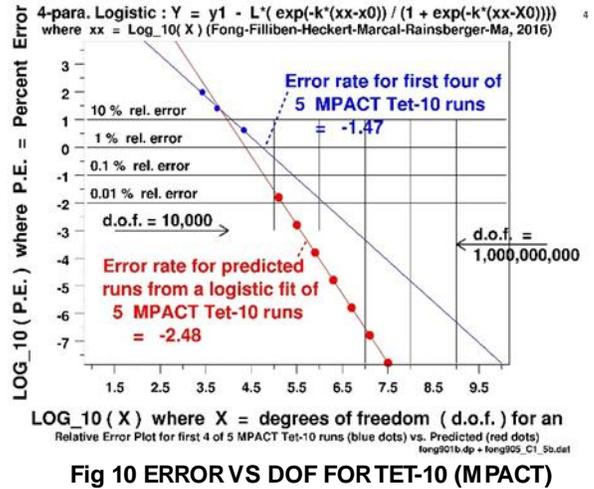


Fig 10 ERROR VS DOF FOR TET-10 (MPACT)

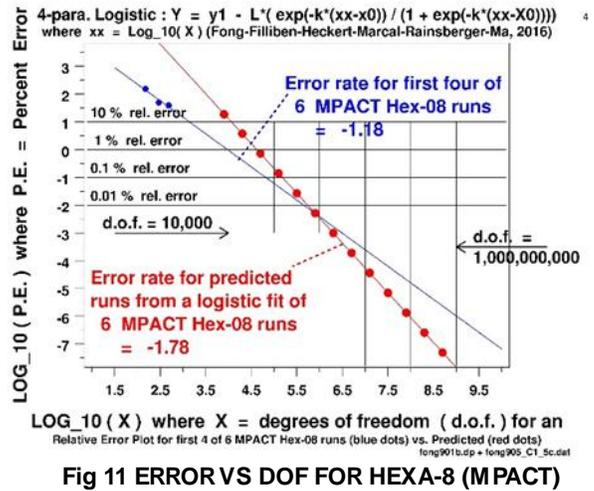


Fig 11 ERROR VS DOF FOR HEXA-8 (MPACT)

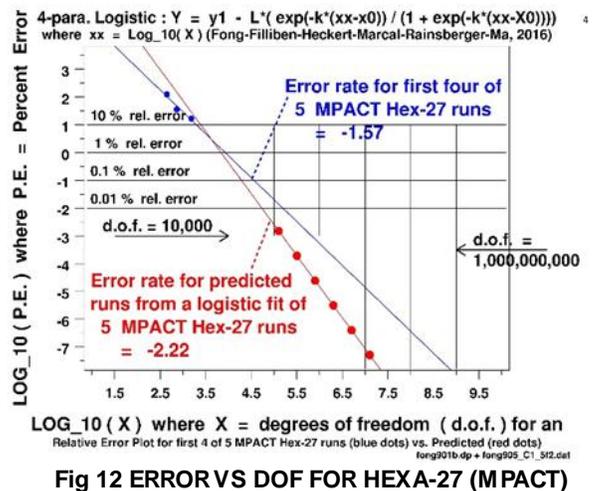


Fig 12 ERROR VS DOF FOR HEXA-27 (MPACT)

The converged Max. displacements predicted by each of the element types by each of the programs is shown in the following table.

TABLE 2. SUMMARY OF MAX. DISPLACEMENTS

	Error rate from first 3_runs	Fitted_Data
C1_1_Abaqus		
C1_1a_Barrel_5ATet04	+0.35	-1.46
C1_1c_Barrel_6AH08	-0.72	-0.42 (Question)
C1_1e_Barrel_5AH20R	-2.01	-1.24
C1_5_MPact		
C1_5a_Barrel_5MTet04	-0.02	-0.61
C1_5b_Barrel_5MTet10	-1.47	-2.48
C1_5c_Barrel_6MH08	-1.18	-1.78
C1_5f2_Barrel_5MH27	-1.57	-2.22

4. DISCUSSION OF RESULTS

We will first examine the MPACT results because they exhibit a consistent pattern. The results show two slopes for the error rate, viz. an initial rate that is negative that turns into one that is even more negative as the total dof is increased.. The tet-10 and the hexa-27 slopes go from -1 to -2 approx. while the hexa-8 goes from -0.66 to -1.7. The increase in the slope is a desirable rate for element types because they indicate an accelerating trend consistent with convergence. In addition, both the tet-10 and hexa-27 elements exhibit early transition to the higher rate at dof of 10,000 and 7,000 respectively. This may be interpreted as these element types require less dof to calculate convergence.

Turning to the ABAQUS results, we note that the tet-4 is the only element that exhibits the desirable characteristics shown by the MPACT elements. The tet-4 results lie between the MPACT tet-4 and the tet-10 results. The ABAQUS hexa-8 and hexa-20 elements show a decrease in the slope of the error rate with increase in the dof. This is a negative property implying decrease of the convergence rate with increase in the total dof used. Finally, none of the ABAQUS elements produce the Max. Displacements given by the MPACT elements. The final value is assumed to be that of the hexa-27 with a value of -2.22. This assumption is justified because this element has the highest order truncation error.

5. CONCLUSIONS

We have demonstrated an effective method based on a fit of the Logistic curve for estimating the converged value of a finite element analysis.

1. By a study of the error rates of convergence, ie error reduction per increase of total dof. We have observed that linear initial rates (log-log) transform into larger linear rates with increase of total dof. We have tentatively concluded that the MPACT elements exhibit the desirable increase in rates of convergence with increase in the total dof used.

2. Another desirable property of an element type is the early transition of the error rate to its final value. This results in reduced computation to achieve a converged solution.

3. The ABAQUS element types do not exhibit any of the desirable traits found here. As a result, they produced poor results for the max. displacement of the barrel vault shell problem.

6. REFERENCES

- [1] Ahmad, S., Irons, B. M., and Zienkiewicz, O. C., "Analysis of Thick and Thin Shell Structures by Curved Finite Elements", *Int. J. for Numerical Methods in Engineering*, Vol. 2, 419-451 (1970).
- [2] Zienkiewicz, O. C., and Taylor, R. L., *The Finite Element Method*, 5th ed., Vol. 1: The Basis, Sections 8.3 and 8.4, pp. 168-172. Butterworth-Heinemann (2000).
- [3] P.V. Marcal, J.T. Fong, R. Rainsberger, L. Ma, *Finite Element Analysis of a Pipe Elbow Weldment Creep- Fracture Problem Using an Extremely Accurate 27-node Tri-Quadratic Shell and Solid Element Formulation*, Proc. ASME PVP-2016, Vancouver, Canada, 2016.
- [4] R. Rainsberger, J.T. Fong, P.V. Marcal, *A super-parametric approach to estimating accuracy and uncertainty of the finite element method*, Proc. ASME PVP-2016, Vancouver, Canada, 2016.
- [5] J.T. Fong, J.J. Filliben, N.A. Heckert, P.V. Marcal, R. Rainsberger, L. Ma, *Uncertainty Quantification of Stresses in a Cracked Pipe Elbow Weldment using a Logistic Function Fit, a Nonlinear Least Square Algorithm, and a Super-Parametric Method*, Proc. ASME PVP-2016, Vancouver, Canada, 2016.
- [6] N.R. Draper, H. Smith, *Applied Regression Analysis*, Chapters 1-3, pp. 1-103, and Chapter 10, pp. 263-304. Wiley, 1966.
- [7] M. Evans, N. Hastings, B. Peacock, *Statistical Distributions*, third ed., pp. 124-128. Wiley, 2000.
- [8] N. Balakrishnan, *Handbook of the Logistic Distribution*. Marcel Dekker, New York, 1992.
- [9] J.J. Filliben, N.A. Heckert, *Dataplot: A Statistical Data Analysis Software System*, National Institute of Standards & Technology, Gaithersburg, MD 20899, U.S.A., <http://www.itl.nist.gov/div898/software/dataplot.html>, 2002.
- [10] R. Rainsberger, *TrueGrid User's Manual: A Guide and a Reference*, Volumes I, II, and III, Version 3.0.0. Published by XYZ Scientific Applications, Inc., Pleasant Hill, CA 94523, U.S.A., www.truegrid.com/pub/TGMAN300.1.pdf, 2014.
- [11] Marcal, P. V., *MPACT User Manual*, Mpack Corp., Oak Park, CA (2001).
- [12] Pfaffinger, D. D., Dupuis, G. A., and Marcal, P. V., "Effective Use of the Incremental Stiffness Matrices in Nonlinear Geometric Analysis", *Proc. IUTAM Symposium on High Speed Computing of Elastic Structures*, Liege, Belgium, August 1970. (see also Marc User Manual for description of the quadrilateral shell element).

[13] Anon., Abaqus/CAE User's Guide, and Abaqus Analysis User's Guide, version 6.13. Dassault Systemes Simulia Corp., Providence, RI, U.S.A., <http://www.3ds.com/products-services/simulia/support/documentation/>, 2015

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