Computational Solid Mechanics using a Vertex-based Finite Volume Method

G. A. Taylor, C. Bailey and M. Cross

Centre for Numerical Modelling and Process Analysis University of Greenwich, Woolwich, London SE18 6PF, UK E-mail: g.a.taylor@gre.ac.uk

ABSTRACT A number of research groups are now developing and using finite volume (FV) methods for computational solid mechanics (CSM). These methods are proving to be equivalent and in some cases superior to their finite element (FE) counterparts. In this paper we will describe a vertex-based FV method with arbitrarily structured meshes, for modelling the elasto-plastic deformation of solid materials undergoing small strains in complex geometries. Comparisons with traditional FE methods will be given.

Key Words: Vertex-based, Finite Volume, Solid Mechanics, Elasto-plastic.

1. Introduction

Over the last three decades the FE method has firmly established itself as the pioneering approach for problems in CSM, especially with regard to deformation problems involving non-linear material analysis [OH80, ZT89]. As a contemporary, the FV method has similarly established itself within the field of computational fluid dynamics (CFD) [Pat80, Hir88].

Both classes of methods integrate governing equations over pre-defined control volumes [Pat80, Zie95], which are associated with the elements making up the domain of interest. Additionally, both approaches can be classified as weighted residual methods where they differ with respect to the weighting functions that are adopted [OCZ94].

Over the last decade a number of researchers have applied FV methods to problems in CSM [Tay96]. It is possible to classify these methods into two approaches, cell-centred [DM92, HH95, Whe96, Whe99] and vertex-based [FBCL91, OCZ94, BC95, Tay96]. The first approach is based on traditional FV methods [Pat80] as applied to problems in CFD and suffers from the same difficulties when applied to complex geometries involving arbitrarily structured meshes [DM92, HH95]. The second approach is based on traditional

FE methods [ZT89] and employs shape functions to describe the variation of a variable over an element, and is therefore well suited to complex geometries [FBCL91, OCZ94]. Both approaches apply strict conservation over a control volume and have demonstrated superiority over traditional FE methods with regard to accuracy [Whe96, Tay96], some researchers have attributed this to the local conservation of a variable as enforced by the control volumes employed [FBCL91, BC95] and others have attributed it to the enforced continuity of the derivatives of variables across cell boundaries [Whe96].

The objective of this paper is to describe the application of a vertex-based FV method to problems involving elasto-plastic deformation and provide a detailed comparison with a standard Galerkin FE method.

2. Equilibrium Equations and Boundary Conditions

In matrix form, the incremental equilibrium equations are

$$[L]^T \{ \Delta \sigma \} + \{ b \} = \{ 0 \} \quad \text{in } \Omega, \tag{1}$$

where [L] is the differential operator, $\{\Delta\sigma\}$ is the Cauchy stress, $\{b\}$ is the body force and Ω is is the domain. The boundary conditions on the surface $\Gamma = \Gamma_t \cup \Gamma_u$ of the domain Ω can be defined as [ZT89, OCZ94]

$$[R]^{T} \{ \Delta \sigma \} = \{ t_{p} \} \quad \text{on } \Gamma_{t} \text{ and}$$

$$\{ \Delta u \} = \{ u_{p} \} \quad \text{on } \Gamma_{u},$$

$$(3)$$

$$\{\Delta u\} = \{u_p\} \quad \text{on } \Gamma_u, \tag{3}$$

where $\{t_p\}$ are the prescribed tractions on the boundary Γ_t , $\{u_p\}$ are the prescribed displacements on the boundary Γ_u and [R] is the outward normal operator [OCZ94, Tay96].

3. Constitutive Relationship

In matrix form, the stress is related to the elastic strain incrementally as follows; $\{\Delta\sigma\} = [D]\{\Delta\epsilon_e\}$, where [D] is the elasticity matrix. For the deformation of metals, the von-Mises yield criterion is employed and the elastic strain is given by $\{\Delta \epsilon_e\} = \{\Delta \epsilon\} - \{\Delta \epsilon_{vp}\}$, where $\{\Delta \epsilon\}$ and $\{\Delta \epsilon_{vp}\}$ are the total and visco-plastic strain, respectively. The visco-plastic strain rate is given by the Perzyna model [Per66]

$$\frac{d}{dt}\{\epsilon_{vp}\} = \gamma \left\langle \frac{\sigma_{eq}}{\sigma_y} - 1 \right\rangle^{\frac{1}{N}} \frac{3}{2\sigma_{eq}}\{s\}, \tag{4}$$

where σ_{eq} , σ_y , γ , N and s are the equivalent stress, yield stress, fluidity, strain rate sensitivity parameter and deviatoric stress, respectively. The $\langle x \rangle$ operator is defined as follows;

$$\langle x \rangle = \begin{cases} 0 & \text{when } x \leq 0 \text{ and } \\ x & \text{when } x > 0. \end{cases}$$

The total infinitesimal strain is $\{\Delta \epsilon\} = [L]\{\Delta u\}$, where $\{\Delta u\}$ is the incremental displacement.

4. Vertex-based Discretisation

Employing the constitutive relationship of the previous section in equations (1) and (2), and assuming the boundary conditions as described by equation (3) are directly satisfied by the vector $\{\Delta u\}$, the method of weighted residuals can be applied to the equations to obtain the following weak form of the equilibrium equation [ZT89];

$$- \int_{\Omega} [LW]^T ([D][L] \{\Delta u\} - [D] \{\Delta \epsilon_{vp}\}) d\Omega + \int_{\Omega} [W]^T \{b\} d\Omega + \int_{\Gamma_u} [RW]^T ([D][L] \{\Delta u\} - [D] \{\Delta \epsilon_{vp}\}) d\Gamma + \int_{\Gamma_t} [W]^T \{t_p\} d\Gamma = \{0\}.$$
 (5)

where [W] is a diagonal matrix of arbitrary weighting functions.

At this point the unknown displacement can be approximated as [ZT89]

$$\{\Delta u\} \simeq \{\Delta \hat{u}\} = \sum_{j=1}^{n} [N]_{j} \{\Delta \bar{u}\}_{j} = \sum_{j=1}^{n} [I] N_{j} \{\Delta \bar{u}\}_{j},$$
 (6)

where $\{\Delta \bar{u}\}_j$ is the unknown displacement at the vertex j, N_j is the shape function associated with the unknown displacement and [I] is the identity matrix. The displacement approximation can be introduced into equation (5) if the arbitrary weighting functions [W] are replaced by a finite set of prescribed functions $[W] = \sum_{i=1}^{n} [W]_i$, for each vertex i [ZT89, OCZ94],

$$- \int_{\Omega} [LW]_{i}^{T}([D][L]\{\Delta \hat{u}\} - [D]\{\Delta \epsilon_{vp}\}) d\Omega + \int_{\Omega} [W]_{i}^{T}\{b\} d\Omega + \int_{\Gamma_{u}} [RW]_{i}^{T}([D][L]\{\Delta \hat{u}\} - [D]\{\Delta \epsilon_{vp}\}) d\Gamma + \int_{\Gamma_{t}} [W]_{i}^{T}\{t_{p}\} d\Gamma = \{0\}$$
for $i = 1, n.$ (7)

Equation (7) can be expressed as an incremental linear system of equations of the form $[K]\{\Delta \bar{u}\}-\{f\}=\{0\}$, where [K] is the global stiffness matrix, $\{\Delta \bar{u}\}$ is the global displacement approximation and $\{f\}$ is the global equivalent force vector and can be formed from the summation of the following contributions;

$$[K]_{ij} = \int_{\Omega_i} [LW]_i^T [D] [LN]_j \, d\Omega - \int_{\Gamma_{u_i}} [RW]_i^T [D] [LN]_j \, d\Gamma \quad \text{and} \quad (8)$$

$$\{f\}_i = \int_{\Omega_i} [W]_i^T \{b\} \, d\Omega + \int_{\Omega_i} [LW]_i^T [D] \{\Delta \epsilon_{vp}\} \, d\Omega$$

$$+ \int_{\Gamma_{t_i}} [W]_i^T \mathbf{t}_p \, d\Gamma - \int_{\Gamma_{u_i}} [RW]_i^T [D] \{\Delta \epsilon_{vp}\} \, d\Gamma, \quad (9)$$

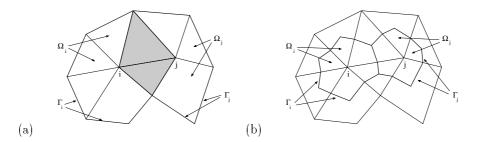


Figure 1: 2D control volumes, (a) overlapping FE and (b) non-overlapping FV.

where Ω_i is the control volume associated with the vertex i and $\Gamma_i = \Gamma_{u_i} \cup \Gamma_{t_i}$ is the boundary of the control volume.

4.1. Standard Galerkin FE Method

In the standard Galerkin FE method the weighting function associated with a vertex is equal to the shape function of the unknown associated with that vertex [ZT89, Hir88, OCZ94], $[W]_i = [N]_i$. The shape functions describe the variation of an unknown over an element and there can be a number of elements associated with each vertex. Hence, it is apparent that control volumes described by weighting functions of this form will always overlap. This is illustrated in Figure 1(a) for a simple two dimensional case of two adjacent nodes i and j, where the control volumes Ω_i and Ω_j have contributions from all the elements associated with their respective vertices i and j.

Hence, for the standard Galerkin FE method the contributions as described by equations (8) and (9) are

$$[K]_{ij} = \int_{\Omega_i} [B]_i^T [D] [B]_j \, \mathrm{d}\Omega \quad \text{and}$$
 (10)

$$\{f\}_{i} = \int_{\Omega_{i}} [N]_{i}^{T} \{b\} d\Omega + \int_{\Omega_{i}} [B]_{i}^{T} [D] \{\Delta \epsilon_{vp}\} d\Omega + \int_{\Gamma_{t_{i}}} [N]_{i}^{T} \{t_{p}\} d\Gamma, (11)$$

where $[B]_i = [LN]_i$.

It is important to note that if the boundary of the control volume, such as that described by Γ_i in Figure 1(a), coincides with the external boundary of the domain, the shape functions are not necessarily zero along that part of the boundary. Thus, if a flux is prescribed such as a traction this will not necessarily disappear and may contribute to the equivalent force vector as described in equation (11). Additionally, the symmetrical nature of the stiffness matrix as indicated by equation (10) should be noted. The Galerkin approach is

accepted as the optimum technique for treating physical situations described by self-adjoint differential equations, particularly those in solid mechanics, as the inherent symmetrical nature is preserved by the choice of weighting functions [ZT89, OCZ94].

4.2. Vertex-based FV Method

In the vertex-based FV method the weighting functions associated with a vertex are equal to unity within the control volume, $[W]_i = [I]$, and zero elsewhere. This definition is equivalent to that for the subdomain collocation method as defined in the standard texts [Hir88, ZT89]. Though it is important to note that weighting functions defined in this manner permit a variety of possibilities with regard to the control volume definition [OCZ94]. This is because the weighting functions are not restricted to to a direct association with the cell or element as in the Galerkin case. This is an important consideration and requires the recognition of the vertex-based FV method as a discretisation technique in its own right [Hir88].

For the vertex-based FV method the contributions as described by equations (8) and (9) are

$$[K]_{ij} = -\int_{\Gamma_{ui}} [R]_i^T [D][B]_j \, \mathrm{d}\Gamma \quad \text{and}$$
 (12)

$$\{f\}_i = \int_{\Omega_i} \{b\} d\Omega - \int_{\Gamma_{u_i}} [R]_i^T [D] \{\Delta \epsilon_{vp}\} d\Gamma + \int_{\Gamma_{t_i}} \{t_p\} d\Gamma. \quad (13)$$

It is important to note that the traction boundary conditions can be applied directly as another surface integral, but in the previous Galerkin approach an additional surface element is generally included on the domain boundary. A non-overlapping control volume definition suitable for a vertex-based FV method is illustrated in two and three dimensions in Figures 1(b) and 2(a), respectively. The Figures illustrate the assembling of vertex-based control volumes from their required sub-control volumes [Tay96]. Additionally, the asymmetric nature of the contributions to the overall stiffness matrix as described by equation (12) does not ensure that symmetry will always be preserved. For this reason FV methods were initially argued as being inferior, but in the light of recent research where different control volume definitions have been proposed, the extent of this inferiority has come into question [OCZ94, Zie95, BC95].

5. Results and Conclusions

In this section the vertex-based FV method is applied to a three dimensional validation problem and compared with the standard Galerkin FE method. The non-linear solution procedure adopted in for both these methods is based upon

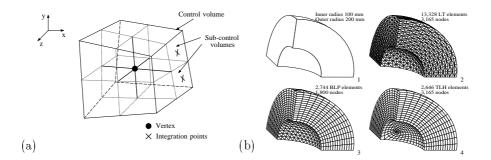


Figure 2: (a) 3D assembly of FV sub-control volumes and (b) spherical vessel.

that of Zienkiewicz and Cormeau [ZC74, Tay96]. Both methods utilised an explicit technique with regard to time stepping of the Perzyna equation (4). It is important to note that the FV solution procedure only differs from that of the FE in contributions to the global equivalent force vector and the global stiffness matrix. Hence, allowing an accurate comparison of the two methods [Tay96]. The methods are compared with regard to accuracy and computational cost. They are also analysed for a variety of meshes with different element assemblies.

5.1. Test case: Internally pressurised spherical vessel

For this validation problem a thick walled spherical vessel, consisting of an elastic–perfectly plastic material, undergoes an instantaneously applied internal pressure load. The pressure load is 30 dNmm⁻², the Youngs modulus and Poisson ratio required to define the elasticity matrix are 21,000 dNmm⁻² and 0.3, respectively, and the yield stress is 24 dNmm⁻². This problem is rate independent and the final solution is equivalent to that of an elasto-plastic analysis [ZC74]. A closed form radial solution is available [Hil50].

Numerically the problem can be modelled in three dimensional Cartesian coordinates, with the displacement components fixed to zero in the relative symmetry planes. The spherical vessel is then reduced to an octant as illustrated in Figure 2(b)¹. Examples of meshes consisting of linear tetrahedral (LT), bilinear pentahedral (BLP) and trilinear hexahedral (TLH) elements are illustrated in Figures 2(b)², 2(b)³ and 2(b)⁴, respectively.

Firstly, the problem was analysed with a series of meshes consisting of TLH elements. The hoop stress profiles, along the radii, as obtained from one of the numerical analyses are plotted and compared against the reference solution in Figure 3(a). The profiles illustrate the stress in the plastic and elastic regions, and the radial extent of the plastic region according to the analytical solution. The close agreement of the two methods is illustrated. However, it

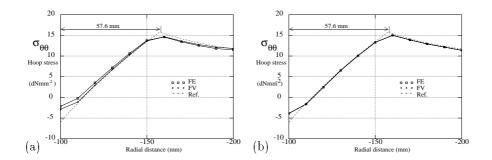


Figure 3: (a) 950 TLH and (b) 4,800 LT elements.

is important to note the closer agreement between the reference solution and the FV method when a coarse mesh is employed. These observations may be associated with the higher order, trilinear nature of the elements employed in the three dimensional analysis at this stage. With regard to the FV method, the implementation of pressure loads (tractions) will involve bilinear face elements for TLH elements. Hence, when considering the application of pressure loads for the two methods as described in equations (11) and (13), the contributions are different due to the individual weighting technique associated with each method. Furthermore, the weighting technique employed for the FV method may be more complementary, when applied generally, as all the terms are integrated conservatively at a local level. Conversely, for the FE method the weighting is not locally conservative which may introduce errors when pressure loads are employed. These conclusions are tentative and rely on the interpretation of the present observations, but they agree with the findings of other researchers [Whe96] and strongly suggest that further research of the FV method is worthwhile.

Secondly, the problem was analysed with a series of meshes consisting of BLP elements and there was much closer agreement between the methods [Tay96]. This is attributable to the lower order, bilinear nature of the element concerned and the linear nature of the triangular faces over which the pressure loads were applied. As illustrated in Figure 2(b)³ the BLP elements are orientated so the pressure load was prescribed over a triangular face. This was an outcome of the automatic mesh generator employed [Fem] and it is possible to further study the element when pressures are applied to the bilinear, quadrilateral faces, though it was not studied in that research.

Thirdly, the problem was analysed with a series of meshes consisting of LT elements. The hoop stress profiles from one of the analyses are plotted in Figure 3(b). There is complete agreement between the methods with regard to LT elements as the global stiffness matrices and global force vectors constructed by the two methods are identical. This is a consequence of the linear nature of

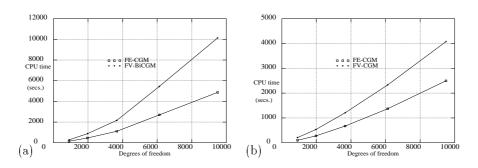


Figure 4: (a) CPU times on a SPARC 4, 110MHz.

both the element concerned and the triangular faces over which the pressure is applied. It is possible to demonstrate this equivalence analytically [Tay96] by extending to three dimensions, a two dimensional analysis which has been applied to elastic problems involving linear triangular elements [OCZ94].

Finally, the methods were compared with regard to computational cost. Considering LT elements, as the matrices are identical and symmetric a conjugate gradient method (CGM) is applicable in both cases. As illustrated in Figure 4(b), the FV method (FV-CGM) requires more CPU time than the FE method (FE-CGM) even when the same linear solver is employed. This is expected as the FV method visits six integration points, while the FE method visits a single Gauss point when adding contributions to the linear system of equations [Tay96].

Considering TLH elements, the geometrical nature of this validation problem prohibits an orthogonally assembled mesh. Hence, for the FV method a bi-conjugate gradient method (Bi-CGM) is required due to the asymmetric nature of the coefficient matrix obtained [Tay96]. Conversely, for the FE method a CGM is sufficient as the matrix obtained is symmetric. These requirements agree with the discussions in the previous section. As illustrated in Figure 4(a), the FV method (FV-BiCGM) requires approximately twice the CPU time as the FE method (FE-CGM). This is also expected due to the computational requirements of the two different linear solvers employed. Also for TLH elements, the FV method visits twelve integration points per element, while the FE method visits eight Gauss points per element.

Hence, it can finally be concluded that any improvement in accuracy obtained by employing the vertex-based FV method must be offset against the extra computational cost required.

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