A Block-Coupled Finite Volume Methodology for Linear Elasticity and Unstructured Meshes

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SUMMARY

The current article presents a new implicit cell-centred Finite Volume solution methodology for linear elasticity and unstructured meshes. Details are given of the implicit discretisation, including use of a Finite Area method for face tangential gradients and implicit non-orthogonal correction. A number of 2-D and 3-D linear-elastic benchmark test cases are examined using hexahedral, tetrahedral and general polyhedral meshes; solution accuracy and efficiency are compared with that of a segregated procedure and a commercial Finite Element software, where the new method is shown to be faster in all cases.

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1. INTRODUCTION

1 In the realm of Computational Solid Mechanics (CSM), the Finite Element (FE) method is
2 ubiquitous; however, methods such as Finite Difference, Discrete Element, Finite Volume (FV), and
3 so-called Meshfree methods, can provide viable alternatives in many applications. In particular, the
4 FV method has been gradually broadening its applicability beyond Computational Fluid Dynamics
5 and gaining momentum in the field of CSM; this may be primarily attributed to its attractively simple
6 and strongly conservative nature, while also having a close relationship with FE methods. To date,
7 the FV method has been applied to a large range of problems in CSM, appearing in a number of
8 distinct forms characterised by different control volume discretisations: cell-centred [1–25], vertex-
9 centred [26–29], and the so-called parametric formulation [30, 31]. To-date, the cell-centred FV
10 approach has typically employed a segregated solution procedure, where the momentum equation is
11 temporally decoupled into components which are solved sequentially, with outer Picard/Fixed-Point

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iterations providing the coupling. This method is extremely memory efficient but can suffer from poor convergence when the inter-displacement-component coupling is strong. To overcome such inadequacies, the current article presents the development of a block-coupled solution methodology, where inter-component coupling is implicitly included in a block matrix. Independent of the current approach, Das et al. [25] have developed a coupled cell-centred FV solution procedure; the current method shares a similarities with the procedure developed by Das et al. [25], but significantly differs in a number of regards, in particular with discretisation of tangential derivatives, and the treatment of boundary conditions. Details of the differences between the two methods are given later within the Numerical Method section.

The article is constructed as follows: Section 2 outlines the mathematical model, derived from the governing momentum equation and Hookean constitutive relation, where no distinction is made between the initial and deformed configurations. The newly developed implicit cell-centred FV discretisation is presented in Section 3; the control volume face normal derivative terms are discretised using standard central differencing, and the face tangential derivative terms are discretised using the Finite Area method. Details are given of the inclusion of a larger implicit computational molecule within 3-D unstructured polyhedral code, and implementation in open-source C++ library OpenFOAM (foam-extend-3.1). Section 4 presents the application of the method to three benchmark test cases, where the efficiency and accuracy of the method is compared with that of segregated FV approaches, and a commercial FE software.

2. MATHEMATICAL MODEL

Neglecting inertia and body forces for clarity, the conservation of linear momentum for an arbitrary body of volume Ω bounded by surface Γ with unit normal $\mathbf{n}$ is given in integral form as:

$$\int_{\Omega} \nabla \cdot \boldsymbol{\sigma} d\Omega = \oint_{\Gamma} \mathbf{n} \cdot \boldsymbol{\sigma} d\Gamma = 0 \quad (1)$$

where the Cauchy stress tensor $\boldsymbol{\sigma}$ for a linear elastic body is given by Hooke's law:

$$\boldsymbol{\sigma} = \mu \nabla \mathbf{u} + \mu \nabla \mathbf{u}^T + \lambda \text{tr}(\nabla \mathbf{u}) \mathbf{I} \quad (2)$$

The Lamé coefficients μ and λ relating to the Young's modulus of elasticity, E , and the Poisson's ratio, ν , are given respectively as:

$$\mu = \frac{E}{2(1 + \nu)} \quad (3)$$

$$\lambda = \begin{cases} \frac{\nu E}{(1 + \nu)(1 - \nu)} & \text{for plane stress} \\ \frac{\nu E}{(1 + \nu)(1 - 2\nu)} & \text{for plane strain and 3-D} \end{cases} \quad (4)$$

Inclusion of transient effects and body force terms is trivial; the use of more complex constitutive relations is also possible, but may require modifications to the solution procedure for nonlinear materials.

40 The mathematical model is found by substituting the constitutive relation (Eq. 2) into the
 41 governing equation (Eq. 1):

$$\oint_{\Gamma} \mathbf{n} \cdot [\mu \nabla \mathbf{u} + \mu \nabla \mathbf{u}^T + \lambda \text{tr}(\nabla \mathbf{u}) \mathbf{I}] d\Gamma = 0 \quad (5)$$

42 where no distinction is made between the initial and deformed configurations *i.e.* small strains and
 43 small rotations are assumed.

3. NUMERICAL METHOD

44 The mathematical model presented in the preceding section is now discretised in a fully coupled
 45 implicit manner using the cell-centred FV method, providing a discrete approximation of the
 46 previously presented exact integral. The discretisation procedure is separated into two distinct parts:
 47 discretisation of the solution domain and discretisation of the governing equations. If temporal
 48 effects were considered, time would also be discretised into a finite number of time increments,
 49 where the mathematical model is solved in a time-marching manner.

50 3.1. Solution Domain Discretisation

51 The solution domain space is divided into a finite number of convex polyhedral cells bounded by
 52 polygonal faces. The cells do not overlap and fill the space completely. A typical control volume is
 53 shown in Figure 1, with the computational node P located at the cell centroid, the cell volume is Ω_P ,
 54 N is the centroid of a neighbouring control volume, face f has face area vector $\mathbf{\Gamma}_f$, vector $\mathbf{d}_f$ joins P
 55 to N and $\mathbf{r}$ is the positional vector of P . Note that in contrast to standard FE methods, no distinction
 56 is made between different cell volume shapes, as all general polyhedra (*e.g.* tetrahedra, hexahedra,
 57 triangular prism, dodecahedra, *etc.*) are discretised in the same general fashion: this allows greater
 freedom during the often troublesome mesh generation phase.

Figure 1. General polyhedral control volume (adapted from [2, 32])

59 3.2. Equation Discretisation

The standard cell-centred FV discretisation approach for solid mechanics, as previously presented *e.g.* [3, 6, 9], partitions the surface force (diffusion term) into implicit and explicit components; the resulting linear system is then solved in a staggered/segregated manner where outer Picard/Fixed-Point iterations provide the necessary coupling. In contrast, the current method discretises the entire term in a fully implicit manner where only one solution of the final linear equation system is required. To facilitate this, the surface traction ($\mathbf{T} = \mathbf{n} \cdot \boldsymbol{\sigma}$) is decomposed into normal ($\mathbf{T}_n$) and tangential ($\mathbf{T}_t$) components [12]:

$$\begin{aligned}
 \oint_{\Gamma} \mathbf{n} \cdot [\mu \nabla \mathbf{u} + \mu \nabla \mathbf{u}^T + \lambda \text{tr}(\nabla \mathbf{u}) \mathbf{I}] d\Gamma &= \oint_{\Gamma} \mathbf{T} d\Gamma \\
 &= \oint_{\Gamma} \overbrace{[\mathbf{n} \mathbf{n} \cdot \mathbf{T}]}^{\mathbf{T}_n} + \overbrace{(\mathbf{I} - \mathbf{n} \mathbf{n}) \cdot \mathbf{T}}^{\mathbf{T}_t} d\Gamma \\
 &= \oint_{\Gamma} \overbrace{(2\mu + \lambda) \mathbf{n} \cdot \nabla \mathbf{u}_n + \lambda \mathbf{n} \text{tr}(\nabla_t \mathbf{u}_t)}^{\mathbf{T}_n} + \overbrace{\mu \mathbf{n} \cdot \nabla \mathbf{u}_t + \mu \nabla_t u_n}_{\mathbf{T}_t} d\Gamma
 \end{aligned} \tag{6}$$

60 where $\nabla_t = (\mathbf{I} - \mathbf{n} \mathbf{n}) \cdot \nabla$ designates a tangential derivative; quantities in bold font are vectors or
 61 tensors; subscripts n and t represent the normal and tangential components of a vector, respectively.

62 The discretisation of the normal and tangential face-derivates are now given separately.

Normal Derivative Terms The surface integrals may be replaced by a sum over the faces of a control volume, and assuming a linear variation of displacement $\mathbf{u}$ across the control volume, a second-order FV discretisation may be applied. The normal derivative terms ($\mathbf{n} \cdot \nabla$) on face f are discretised as follows:

$$\begin{aligned}
 \oint_{\Gamma} (2\mu + \lambda) \mathbf{n} \cdot \nabla \mathbf{u}_n d\Gamma &\approx \sum_f (2\mu_f + \lambda_f) |\Delta_f| (\mathbf{n}_f \mathbf{n}_f) \cdot \left(\frac{\mathbf{u}^N - \mathbf{u}^P}{|\mathbf{d}_f|} \right) \\
 &\quad + \sum_f (2\mu_f + \lambda_f) (\mathbf{n}_f \mathbf{n}_f) \cdot [\mathbf{k}_f (\nabla_t u_n)_f]
 \end{aligned} \tag{7}$$

63 where subscript f refers to values at control volume faces, and the vector $\Delta_f = \frac{\mathbf{d}_f}{\mathbf{d}_f \cdot \mathbf{\Gamma}_f} |\mathbf{\Gamma}_f|^2$
 64 [33]. The first term on the right-hand side assumes orthogonality of the mesh and discretises
 65 the normal derivative using central differencing. The second term on the right-hand side, which
 66 contains the tangential gradient $\nabla_t u_n$, corrects for any mesh non-orthogonality, where the correction
 67 vector is $\mathbf{k}_f = \mathbf{\Gamma}_f - \Delta_f$. This corresponds to the over-relaxed non-orthogonal correction method
 68 as described by Jasak [33]; however, in contrast to the previous employed iterative deferred/lagged
 69 correction method, the current implementation discretised the corrective tangential derivative term
 70 in a fully implicit manner, as will be described in the subsequent section.

The normal derivative of the tangential component $\mathbf{n} \cdot \nabla \mathbf{u}_t$ is discretised in a similar manner to that of the normal derivative of the normal component $\mathbf{n} \cdot \nabla \mathbf{u}_n$:

$$\oint_{\Gamma} \mu \mathbf{n} \cdot \nabla \mathbf{u}_t \, d\Gamma \approx \sum_f \mu_f |\Delta_f| (\mathbf{I} - \mathbf{n}_f \mathbf{n}_f) \cdot \left(\frac{\mathbf{u}^N - \mathbf{u}^P}{|\mathbf{d}_f|} \right) + \sum_f \mu_f (\mathbf{I} - \mathbf{n}_f \mathbf{n}_f) \cdot [\mathbf{k}_f \cdot (\nabla_t \mathbf{u}_t)_f] \quad (8)$$

71 where the tensor $(\mathbf{n}_f \mathbf{n}_f)$ has been replaced by $(\mathbf{I} - \mathbf{n}_f \mathbf{n}_f)$, referring to the tangential component
72 of displacement.

Tangential Derivative Terms As with the normal derivative terms above, the surface integral over tangential derivative terms is converted to a sum over control volume faces:

$$\oint_{\Gamma} [\mu \nabla_t u_n + \lambda \mathbf{n} \operatorname{tr}(\nabla_t \mathbf{u}_t)] \, d\Gamma = \sum_f [\mu_f (\nabla_t u_n)_f + \lambda_f \mathbf{n}_f \operatorname{tr}(\nabla_t \mathbf{u}_t)_f] |\Gamma_f| \quad (9)$$

The tangential face derivatives, $\nabla_t u_n$ and $\nabla_t \mathbf{u}_t$, are then calculated directly on face f using a face-Gauss/Finite Area (FA) method [34–37]:

$$(\nabla_t u_n)_f = \frac{1}{|\Gamma_f|} \sum_e \mathbf{m}_e (u_n)_e L_e \quad (10)$$

where subscript e refers to an edge of face f , L_e is the length of edge e (see Figure 2), and the summation is performed over all edges enclosing face f . This approach to calculation of tangential face gradients is a generalisation of the method used by Demirdžić et al. [1, 38] on structured meshes. The edge-centre unit bi-normal vector $\mathbf{m}_e$ is calculated as follows:

$$\mathbf{m}_e = \hat{\mathbf{e}} \times \mathbf{n}_f \quad (11)$$

where $\hat{\mathbf{e}}$ is the unit vector parallel with the edge e , and operator $\times$ designates a cross product.

Figure 2. Polygonal control area

The edge-centre displacement components, $(u_n)_e$ and $(u_t)_e$, are approximated as the average of the edge e end-points, assuming a linear variation:

$$(\mathbf{u})_e \approx \frac{1}{2} [(\mathbf{u})_{ep1} + (\mathbf{u})_{ep2}] \quad (12)$$

where the edge end-point displacements, $(\mathbf{u})_{ep1}$ and $(\mathbf{u})_{ep2}$, may be approximated in terms of the neighbouring cell-centre values using a weighted least squares interpolation with linear fit function [13, 34]:

$$\begin{aligned} \mathbf{u}_{epi}(\mathbf{r}_i) &= \mathbf{u}_{i0} + \mathbf{C}_i \cdot (\mathbf{r}_i - \mathbf{r}_{i0}) \\ \mathbf{r}_{i0} &= \frac{\sum_{j=1}^n \omega_j \mathbf{r}_{ij}}{\sum_{j=1}^n \omega_j} \\ \mathbf{u}_{i0} &= \frac{\sum_{j=1}^n \omega_j \mathbf{u}_{ij}}{\sum_{j=1}^n \omega_j} \end{aligned} \quad (13)$$

where subscript j indicates the so-called *point-cell* neighbours (cells that contain the current point) and boundary face centres (boundary faces that contain the current point), and n is the total number of point-cell neighbours around the point; the reference position $\mathbf{r}_{i0}$ and reference field value $\mathbf{u}_{i0}$ are calculated directly as the weighted average of cell-centre and boundary face positions and cell-centre and boundary face field values. The point-cell weights ω_i can be calculated in a number of ways: in the current study an arithmetic average is used, alternatively the weights could be based on the inverse of the distance or its square. $\mathbf{C}_i$ is the unknown least squares coefficient vector (three components):

$$\mathbf{C}_i = [(\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W}] \cdot \mathbf{u}_{\Delta i} \quad (14)$$

74 where $\mathbf{u}_{\Delta i}$ is the vector consisting of the quantity $\mathbf{u}_i - \mathbf{u}_{i0}$ for all cells in the interpolation stencil
 75 of point i , $\mathbf{W}$ is the diagonal matrix consisting of weighting factors for all cells in the interpolation
 76 stencil of point i and $\mathbf{X}$ is the $n \times 3$ matrix whose row j is position vector $\mathbf{r}_{ij} - \mathbf{r}_{i0}$ of the cell
 77 j in the interpolation stencil of the point i . This FA method with least squares cell-centre-to-point
 78 interpolation has been presented previously by Tuković et al. [34] for explicit calculation of face
 79 tangential derivatives; the current articles outlines an implicit implementation of this method.

The discretised form of the tangential derivative of normal component term is:

$$\begin{aligned} \oint_{\Gamma} \mu \nabla_t u_n \, d\Gamma &\approx \sum_f \mu_f \sum_e \mathbf{m}_e \sum_{pc} \frac{1}{2} \omega_{pc} \mathbf{u}_n^{pc} L_e \\ &\approx \sum_f \sum_e \sum_{pc} \frac{1}{2} \mu_f \omega_{pc} L_e \mathbf{m}_e \mathbf{u}_n^{pc} \\ &\approx \sum_f \sum_e \sum_{pc} \frac{1}{2} \mu_f \omega_{pc} L_e (\mathbf{m}_e \mathbf{n}_f) \cdot \mathbf{u}^{pc} \end{aligned} \quad (15)$$

In a similar fashion, the tangential derivative of the displacement tangential component can be discretised, where it is noted that $\mathbf{m}_e \cdot \mathbf{n}_f \equiv \mathbf{0}$ and hence $\mathbf{m}_e \cdot (\mathbf{I} - \mathbf{n}_f \mathbf{n}_f) \equiv \mathbf{m}_e$:

$$\begin{aligned}
 \oint_{\Gamma} \lambda \mathbf{n} \operatorname{tr}(\nabla_t \mathbf{u}_t) \, d\Gamma &\approx \sum_f \lambda_f \mathbf{n}_f \operatorname{tr} \left(\sum_e \mathbf{m}_e \sum_{pc} \frac{1}{2} \omega_{pc} \mathbf{u}_t^{pc} L_e \right) \\
 &\approx \sum_f \sum_e \sum_{pc} \frac{1}{2} \lambda_f \omega_{pc} L_e \mathbf{n}_f \operatorname{tr}(\mathbf{m}_e \mathbf{u}_t^{pc}) \\
 &\approx \sum_f \sum_e \sum_{pc} \frac{1}{2} \lambda_f \omega_{pc} L_e \mathbf{n}_f \operatorname{tr}(\mathbf{m}_e [(\mathbf{I} - \mathbf{n}_f \mathbf{n}_f) \cdot \mathbf{u}^{pc}]) \\
 &\approx \sum_f \sum_e \sum_{pc} \frac{1}{2} \lambda_f \omega_{pc} L_e \mathbf{n}_f \operatorname{tr}(\mathbf{m}_e \mathbf{u}^{pc}) \\
 &\approx \sum_f \sum_e \sum_{pc} \frac{1}{2} \lambda_f \omega_{pc} L_e (\mathbf{m}_e \mathbf{n}_f)^T \cdot \mathbf{u}^{pc}
 \end{aligned} \tag{16}$$

80 where it should be noted that the magnitude of the face area vector Γ_f does not feature in either of
 81 the final discretised tangential terms but instead the edge lengths L_e .

82 The non-orthogonal correction terms that appear in Equations 7 and 8, which contain tangential
 83 derivatives, are discretised in the same manner as Equations 15 and 16. It should be noted that
 84 discretisation is second order in space and strongly conservative. Additionally, the resulting sparse
 85 solution matrix will be symmetric in structure but the coefficients will be asymmetric, potentially
 86 leading to higher memory and computation costs; however, as will be shown in the test cases section,
 87 the resulting method is shown to be efficient in terms of memory and computation time.

88 At this point it is worth mentioning differences with the method developed by Das et al. [25] for
 89 discretisation of face tangential gradients. As described, the current approach calculates tangential
 90 derivatives of displacement directly at control volume faces; in contrast, the approach of Das
 91 et al. [25] calculates tangential derivatives at control volume centres and linearly interpolates
 92 these gradients to the control volume faces. Through interpolation of cell-centre gradients, the
 93 computational molecule includes two levels of neighbour cells (so-called 2^{nd} neighbours) around
 94 a given control volume, whereas in the current approach a smaller computational molecule is
 95 required where neighbours which share a mesh point with the current control volume are included.
 96 In addition to an increase in accuracy, the smaller computational molecule results in a less dense
 97 matrix within the resulting linear system. It should be noted that Das et al. [25] incorrectly refers to
 98 the discretisation procedure as *linearisation* of the stress tensor; under the adopted assumption of
 99 a linear elastic material undergoing small strains and small rotations, the governing momentum
 100 equation is linear in displacement and as such no *linearisation* is necessary. The two terms
 101 containing tangential gradients, $\nabla \cdot (\nabla \mathbf{u})^T$ and $\nabla \cdot \operatorname{tr}(\nabla \mathbf{u}) \mathbf{I}$, introduce inter-component coupling
 102 within the momentum equation but do not introduce any nonlinearity.

103 *Boundary Conditions* Traditionally cell-centred FV methods incorporate boundary condition
 104 equations directly into the governing discretised equation for control volumes adjacent to the
 105 boundary; this method was initially trialled for the current methodology; however, implicit
 106 calculation of tangential gradients along near-boundary faces (those with points on the boundary
 107 but not on the boundary themselves) becomes excessively complicated. Consequently, boundary

conditions are included as additional equations in the current methodology, where boundary face displacements are additional unknowns. This results in one discretised conservation equation for each control volume and one additional discretised boundary condition equation for each boundary face. Although not described in detail, the treatment of boundary conditions by Das et al. [25, 39] differs from the current approach in that boundary face values are not included as additional unknowns. As details of the implementation are not given, it is unclear if the method proposed by Das et al. [25] maintains the discretisation order of accuracy at boundary and near-boundary faces.

The discretisation procedure outlined in the previous section is applied to the faces (internal and boundary) of all mesh control volumes, where boundary-face values are implicitly included just as cell-centre values. This section outlines the implementation of the discrete displacement, traction and symmetry plane boundary condition equations.

Displacement The displacement boundary condition, a Dirichlet condition, may be constant in time or time-varying and fixes the boundary-face centre value of displacement, $\mathbf{u}_b$. The discrete displacement boundary condition vector equation is:

$$\mathbf{I} \cdot \mathbf{u} = \mathbf{U}_b \quad (17)$$

where $\mathbf{u}$ is the boundary-face centre *unknown* displacement, $\mathbf{I}$ is the identity tensor, and $\mathbf{U}_b$ is the user specified boundary-face centre displacement.

Traction The traction boundary condition, a Neumann condition, is a constant in time or time-varying user specified traction; the traction on a boundary face is written as:

$$\mathbf{T}_b |\Gamma_b| = \int_{\Gamma_b} \overbrace{(2\mu + \lambda) \mathbf{n} \cdot \nabla \mathbf{u}_n + \lambda \mathbf{n} \text{tr}(\nabla_t \mathbf{u}_t)}^{T_n} + \overbrace{\mu \mathbf{n} \cdot \nabla \mathbf{u}_t + \mu \nabla_t u_n}^{T_t} d\Gamma \quad (18)$$

where the normal and tangential derivative terms are discretised in the same manner as for internal cells, where the main difference is that the central differencing approximation becomes one-sided; $\mathbf{T}_b$ is the user specified boundary traction. In practice, the negative of this equation is used to ensure that the diagonal coefficients are negative, as is the case for the control volume equations.

Symmetry Plane The symmetry plane condition, a mixed Dirichlet-Neumann condition, specifies by definition a zero normal displacement and a zero normal gradient of tangential displacement:

$$\begin{aligned} \mathbf{u}_n &\equiv \mathbf{0} \\ \mathbf{n} \cdot \nabla \mathbf{u}_t &\equiv \mathbf{0} \end{aligned} \quad (19)$$

where the condition is enforced at the centre of a boundary face. The discretised form of the normal displacement equation is:

$$(\mathbf{n}_b \mathbf{n}_b) \cdot \mathbf{u} = \mathbf{0} \quad (20)$$

where $\mathbf{n}_b$ is the boundary face normal, and $\mathbf{u}$ is the unknown boundary face displacement. The tangential equation becomes:

$$|\Delta_b|(\mathbf{I} - \mathbf{n}_b \mathbf{n}_b) \cdot \left(\frac{\mathbf{u}_b - \mathbf{u}^P}{|\mathbf{d}_b|} \right) + (\mathbf{I} - \mathbf{n}_b \mathbf{n}_b) \cdot [\mathbf{k}_b \cdot (\nabla_t \mathbf{u})_b] = \mathbf{0} \quad (21)$$

where the tangential derivative in the non-orthogonal correction term is calculated at the boundary face and discretised in a similar manner as for internal faces. Equation 20 only refers to the normal component of displacement whereas Equation 21 only refers to the tangential component of displacement; as such, these two vector equations can be summed to produce the final discretised boundary condition vector equation for each boundary face on a symmetry plane.

3.3. Solution Procedure

The final discretised form of the linear momentum equation for each control volume P can be arranged in the form of N_i linear algebraic equations:

$$\mathbf{a}_P^i \cdot \mathbf{u}_P^i + \sum_{n_p} \mathbf{a}_N^i \cdot \mathbf{u}_N^i = \mathbf{b}_P^i \quad (22)$$

where n_p is the number of neighbour control volume and boundary faces in the current implicit molecule, $\mathbf{a}_P^i$ is the central tensor coefficient, $\mathbf{a}_N^i$ are the neighbour tensor coefficients representing interactions with neighbour cell-centred unknowns or boundary-face-centred unknowns, and $\mathbf{b}_P^i$ is the source vector contribution which is zero in all cases here. If included, body forces and inertia terms would contribute to the source vector.

An additional N_b linear equations arise from the discrete boundary conditions, one for each boundary face centre:

$$\mathbf{a}_P^b \cdot \mathbf{u}_P^b + \sum_{n_b} \mathbf{a}_N^b \cdot \mathbf{u}_N^b = \mathbf{b}_P^b \quad (23)$$

where, similar to the control volume equations, $\mathbf{a}_P^b$ is the central tensor coefficient, $\mathbf{a}_N^b$ are the neighbour tensor coefficients, and $\mathbf{b}_P^b$ is the source vector contribution; here the source will only contain contributions from traction boundary conditions and non-zero displacement boundary conditions.

The algebraic linear equations described above (Equations 22 and 23) are then assembled for all control volumes and boundary face centres forming a system of linear equations:

$$[\mathbf{A}] [\phi] = [\mathbf{b}] \quad (24)$$

where $[\mathbf{A}]$ is a sparse $N \times N$ matrix, with $N = N_i + N_b$ being the total number of computational points. The tensorial coefficients $\mathbf{a}_P$ are on the diagonal of matrix $[\mathbf{A}]$ and tensorial coefficients $\mathbf{a}_N$ form the matrix off-diagonal. The solution vector $[\phi]$ contains the unknown cell-centre and boundary-face-centre displacement vectors, and $[\mathbf{b}]$ is the source vector.

Given the nested summations involved in the specification of the matrix coefficients, the calculation of the final matrix coefficients are given here, for clarity, in algorithmic form, where the coefficients stemming from the normal and tangential derivatives are assembled separately. The normal coefficients are assembled as indicated in Algorithm 1.

Algorithm 1 Assembling normal derivate coefficient contributions within the block matrix

```

1: for all internal and boundary faces do:
2:   for both cells straddling the internal face OR boundary face and adjacent cell do
3:      $\text{coeff} \leftarrow (2\mu + \lambda)(\mathbf{n}_f \mathbf{n}_f) \frac{|\Delta|}{|d|} |\Gamma_f| + \mu(I - \mathbf{n}_f \mathbf{n}_f) \frac{|\Delta|}{|d|} |\Gamma_f|$ 
4:      $\mathbf{a}_P \leftarrow \mathbf{a}_P - \text{coeff}.$  ▷ Add contribution to matrix diagonal
5:      $\mathbf{a}_N \leftarrow \mathbf{a}_N + \text{coeff}.$  ▷ Add contribution to matrix off-diagonal
6:   end for
7: end for

```

155 The coefficients arising from the tangential derivatives are assigned using a series of nested loops,
 shown in Algorithm 2.

Algorithm 2 Assembling tangential derivate coefficient contributions within the block matrix

```

1: for all cells do:
2:   for all internal and boundary faces of the current cell do
3:     for all edges of the current face do
4:       for all neighbour cells/boundary-faces of the end-points of current edge do
5:          $\text{coeff} \leftarrow \frac{1}{2} \mu_f \omega_{pc} L_e(\mathbf{m}_e \mathbf{n}_f) + \frac{1}{2} \lambda_f \omega_{pc} L_e(\mathbf{m}_e \mathbf{n}_f)^T$ 
6:         if non-orthogonal correction required then
7:            $\text{coeff} \leftarrow \text{coeff} + \frac{1}{2} \mathbf{n}_f \mathbf{n}_f (2\mu_f + \lambda_f) \omega_{pc} L_e(\mathbf{k}_f \cdot \mathbf{m}_e)$ 
8:            $+ \frac{1}{2} (\mathbf{I} - \mathbf{n}_f \mathbf{n}_f) \mu_f \omega_{pc} L_e(\mathbf{k}_f \cdot \mathbf{m}_e)$ 
9:         end if
10:        if the neighbour cell is the current cell then
11:           $\mathbf{a}_P \leftarrow \mathbf{a}_P + \text{coeff}.$  ▷ Add contribution to matrix diagonal
12:        else
13:           $\mathbf{a}_N \leftarrow \mathbf{a}_N + \text{coeff}.$  ▷ Add contribution to matrix off-diagonal
14:        end if
15:      end for
16:    end for
17:  end for
18: end for

```

156
 157 Algorithms 1 and 2 complete the assembly of the N_i control volume discrete governing equations;
 158 the linear system is finalised once the additional N_b discrete boundary condition equations are added
 159 in a similar manner. In contrast to a segregated solution procedure, the source vector in the current
 160 formulation contains only contributions from the boundary conditions, and can be thought of as the
 161 driving force. If inertial and body force effects were included, they would also contribute to the
 162 source vector.

163 To illustrate the construction of the block matrix coefficients above, the coefficients for an
 164 internal cell in a simple 2-D uniform structured quadrilateral mesh are shown in Figure 3. It is
 165 interesting to note that the normal derivative terms contribute only to the central cell coefficient
 166 and the coefficients of the neighbour cells connected through a face *i.e.* top, left, right and bottom
 167 cells; whereas, the tangential derivative terms contribute exclusively to the far *point-neighbour* cell
 168 coefficients *i.e.* top-left, top-right, bottom-left and bottom-right cells. This is only the case for a
 169 fully uniform mesh; in non-uniform meshes the tangential derivative terms can contribute to all
 170 cells within the computational molecule, where the contributions do not fully cancel out.

$\begin{pmatrix} 0 & -\frac{\mu}{4} \frac{ \Gamma }{ d } \\ -\frac{\lambda}{4} \frac{ \Gamma }{ d } & 0 \end{pmatrix}$	$\begin{pmatrix} \mu \frac{ \Gamma }{ d } & 0 \\ 0 & (2\mu + \lambda) \frac{ \Gamma }{ d } \end{pmatrix}$	$\begin{pmatrix} 0 & \frac{\mu}{4} \frac{ \Gamma }{ d } + \frac{\lambda}{4} \frac{ \Gamma }{ d } \\ \frac{\lambda}{4} \frac{ \Gamma }{ d } + \frac{\mu}{4} \frac{ \Gamma }{ d } & 0 \end{pmatrix}$
Cell P		
$\begin{pmatrix} (2\mu + \lambda) \frac{ \Gamma }{ d } & 0 \\ 0 & \mu \frac{ \Gamma }{ d } \end{pmatrix}$	$\begin{pmatrix} -(4\mu + 2\lambda) \frac{ \Gamma }{ d } & 0 \\ -2\mu \frac{ \Gamma }{ d } & -(4\mu + 2\lambda) \frac{ \Gamma }{ d } \\ 0 & -2\mu \frac{ \Gamma }{ d } \end{pmatrix}$	$\begin{pmatrix} \mu \frac{ \Gamma }{ d } & 0 \\ 0 & (2\mu + \lambda) \frac{ \Gamma }{ d } \end{pmatrix}$
$\begin{pmatrix} 0 & \frac{\mu}{4} \frac{ \Gamma }{ d } + \frac{\lambda}{4} \frac{ \Gamma }{ d } \\ \frac{\lambda}{4} \frac{ \Gamma }{ d } + \frac{\mu}{4} \frac{ \Gamma }{ d } & 0 \end{pmatrix}$	$\begin{pmatrix} \mu \frac{ \Gamma }{ d } & 0 \\ 0 & (2\mu + \lambda) \frac{ \Gamma }{ d } \end{pmatrix}$	$\begin{pmatrix} 0 & -\frac{\mu}{4} \frac{ \Gamma }{ d } - \frac{\lambda}{4} \frac{ \Gamma }{ d } \\ -\frac{\lambda}{4} \frac{ \Gamma }{ d } - \frac{\mu}{4} \frac{ \Gamma }{ d } & 0 \end{pmatrix}$

Figure 3. Block-coupled matrix coefficients for cell P in a simple 2-D structured mesh

As a consequence of the tangential derivative terms contributing solely to the off-diagonal coefficients, the sparse $N \times N$ matrix will not be diagonally dominant, in contrast to the segregated methodology. This lack of matrix diagonal dominance has implications for the choice of linear solver for the linear system of equations: standard preconditioned Conjugate Gradient (CG) methods may not guarantee convergence, and other methods must be considered. In general, there are two choices for the solution of the linear system: direct methods or iterative methods. Candidate direct methods are Gaussian elimination, LU decomposition, or multi-frontal methods, whereas candidate iterative methods are Bi-Conjugate Gradient Stabilised (BiCGStab), or Generalised Minimal Residual (GMRes), where appropriate choice of preconditioner can also greatly affect the efficiency. In general, direct methods are currently the fastest technique to solve small/medium sparse non-diagonally dominant linear systems [40]; however, the memory and calculation costs of direct methods quickly become impractical as the problem size increases. It should be noted that iterative solvers preserve the matrix sparsity pattern during the solution, whereas direct solver procedures result in some level of matrix *fill-in* producing much larger memory footprints. In the current work, both a LU decomposition direct solver and an iterative BiCGStab method with incomplete LU decomposition (ILU) preconditioning have been employed; the ILU preconditioner employs zero fill-in and hence will be referred to as ILU(0). The combination of direct, for small/medium problems, and iterative methods, for medium/large problems, should provide an

189 efficient solution procedure. Although not implemented in the current study, an Algebraic Multi-
 190 Grid (AMG) employing BiCGStab or GMRes should provide considerable speed-ups for larger
 191 problems: this will be the focus of future work.

192 Regardless of linear solver type, the block-coupled solver uses considerably more memory than a
 193 segregated approach: in a 3-D simulation, each entry in the block matrix is a 3×3 tensor; this is in
 194 contrast to the scalar coefficient employed in a segregated approach. Additionally, the larger implicit
 195 molecule required by the coupled approach decreases the sparsity of the matrix in comparison to
 196 the segregated approach. As a result, it would be expected that the memory required by the coupled
 197 approach would be an order of magnitude greater than that of the segregated approach. It should be
 198 kept in mind that the segregated approach was developed when computers possessed prohibitively
 199 small quantities of memory, whereas modern machines, in particular distributed memory super
 200 clusters, have considerably larger memory-to-CPU ratios.

201 Although not the focus of the current study, the extension of the current methodology to
 202 nonlinearity (geometric, material or loading) is worth briefly discussing: the segregated procedure
 203 naturally extends to nonlinearity as inter-component coupling is included in a deferred correction
 204 manner, consequently the inclusion of nonlinear terms requires no modification to the solution
 205 methodology. In contrast, the current coupled methodology would require outer iterations over
 206 the linear system to include nonlinearity. The use of Picard/Fixed-Point iterations would require
 207 the least complexity in terms of implementation; however, the Newton-Raphson method (or
 208 Newton type methods) would be the ideal candidate for an efficient nonlinear algorithm, based
 209 on experiences in nonlinear FE methods.

210 3.4. Notes on Implementation: Sparse Matrix Addressing

211 Within an unstructured mesh code, the storage and addressing of the sparse matrix greatly affects
 212 the efficiency of the implemented procedures. Recently developed block-coupled matrix tools in
 213 OpenFOAM [41] provide many of the tools required for implementation of the current discretisation
 214 and solution procedure, apart from one deficiency: as is the case in typical unstructured cell-centred
 215 FV codes, a compact implicit molecule is employed where only near neighbours cells, connected
 216 through a face, are implicitly coupled within the sparse matrix structure. The discretisation
 217 developed here requires all *point-neighbours* (cells sharing a point with the current cell) to be
 218 included implicitly. Figure 4 compares the standard cell-centred FV implicit molecule with the
 219 required extended molecule; extended molecules for triangular and polygonal meshes are shown in
 220 Appendix A. Consequently, an extended-molecule sparse matrix addressing has been developed to
 221 allow implicit coupled inclusion of *point-neighbour* cell contributions.

222 There are a number of different methods proposed for storage of the sparse matrices
 223 generated from FE/FV discretisations; here, the so-called *Lower-Diagonal-Upper* (LDU) format,
 224 as implemented in OpenFOAM, is employed. The LDU format stores the sparse matrix in three
 225 arrays: the *diagonal* stores the matrix diagonal ($[A]_{ij}$ for $i = j$); the *lower* stores the matrix lower
 226 portion ($[A]_{ij}$ for $i > j$); and the *upper* stores the matrix upper portion ($[A]_{ij}$ for $i < j$). The LDU
 227 format allows implementation of highly efficient iterative linear solvers, as multiplication of the
 228 matrix with the solution vector is straight-forward. Addressing of the off-diagonal arrays (*upper* and
 229 *lower*) is determined by the implicit computational molecule. In the case of the compact molecule,
 230 the length of the off-diagonal arrays is equal to the total number of internal faces in the mesh

231 *i.e.* a given cell with N_{faces} is implicitly coupled to N_{faces} other cells and hence has N_{faces} off-
 232 diagonal coefficients. The mesh face number then determines the addressing of the off-diagonal
 233 coefficients. By considering the internal mesh faces as *implicit bonds*, the method can be modified
 234 to use an extended molecule. For every cell, *implicit bonds* are defined connecting to each neighbour
 235 cell (or neighbour boundary face) within the implicit computational molecule of the current cell.
 236 This new *implicit bonds* connectivity can then be used in an analogous manner to the mesh faces
 237 in the standard approach, thus completely defining the addressing of the extended sparse matrix.
 238 Consequently, no modification is necessary to the implemented OpenFOAM block linear equation
 solvers, as they only require the sparse matrix, the sparse matrix addressing, and the source vector.

Figure 4. Comparison of compact & extended implicit computational molecule

239

240 To further illustrate the differences between the previous sparse matrix addressing format and the
 241 new extended structure, the sparse matrices for a simple 2-D square plate, meshed with 3×3 square
 242 cells, are compared in Figure 5. The **D** entries signify a diagonal coefficient, the **U** entries signify
 243 an upper non-zero off-diagonal coefficient, and the **L** entries signify a lower non-zero off-diagonal
 244 coefficient. It is clear to see that there are three main differences between the previous segregated
 245 compact approach and the new extended approach:

- 246 • The compact approach has N_i unknowns resulting in a $N_i \times N_i$ matrix; the extended approach
 247 has $N = N_i + N_b$ unknowns with a $N \times N$ matrix;
- 248 • Non-zero off-diagonal coefficients are only present for each *face-neighbour* in the compact
 249 approach, whereas for each *point-neighbour* in the extended approach;
- 250 • Each coefficient is a scalar in the segregated approach, whereas each coefficient is a 3×3
 251 tensor in the coupled approach.

252 As a result, the new extended approach clearly has considerably more computer memory
 253 requirements, and when moving to 3-D, the differences increase further; however, it should be kept
 254 in mind that the method is comparable to that of a standard FE block-coupled implementation. This
 255 particularly highlights the level of memory efficiency achieved by segregated approaches. For each
 256 of the test cases examined in the subsequent section, the memory requirements, in addition to the
 257 wall-clock time (entire time taken by the computer to complete the task), are presented.

4. TEST CASES

258 The accuracy and efficiency of the developed block-coupled linear elastic methodology is examined
 259 for three separate representative test cases. The first test case, that of a slender 2-D cantilever

(a) Cell & Boundary Faces Numbering

i	1	2	3	4	5	6	7	8	9
1	D	U				U			
2	L	D	U		U				
3		L	D	U					
4			L	D	U				U
5		L		L	D	U		U	
6	L				L	D	U		
7						L	D	U	
8							L	D	U
9				L				L	D

(b) Standard *compact molecule*

i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21				
1	D	U				U	U				U	U									U	U			
2	L	D	U	U	U	U					U	U	U												
3		L	D	U	U							U	U		U	U									
4			L	L	D	U			U	U					U	U	U								
5	L	L	L	L	D	U	U	U	U	U															
6	L	L				L	D	U	U											U	U	U			
7							L	L	D	U									U	U	U				
8					L	L	L	L	D	U								U	U	U					
9						L	L			L	D						U	U	U	U					
10	L	L									D	U										U			
11	L	L	L								L	D	U												
12			L	L									L	D	U										
13				L	L									L	D	U									
14					L	L									L	D	U								
15						L										L	D	U							
16										L	L						L	D	U						
17											L	L	L					L	D	U					
18												L	L							L	D	U			
19													L	L							L	D	U		
20	L													L	L							L	D	U	
21	L										L												L	D	U

(c) New *extended molecule* with boundary unknownsFigure 5. Sparse matrix addressing comparing diagonal, upper & lower storage for 3×3 quadrilateral 2-D mesh of a plate (adapted from [42])

undergoing bending, has an analytical solution and highlights the efficiency of the developed method in cases where inter-component coupling is strong. The second and third cases, elastic benchmarks as proposed by Demirdžić et al. [3], are 3-D problems requiring relatively fine grids to obtain accurate solutions. For each case, the new coupled procedure is compared with a segregated FV procedure, the Demirdžić et al. [3] benchmark, and a commercial FE software; additionally, the effect of control volume shape is examined, comparing hexahedra, tetrahedra and general polyhedra meshes.

Slender Cantilever in Bending

The test case geometry, shown in Figure 6(a), consists of a rectangular beam 2×0.1 m with a Young's modulus E of 200 GPa and a Poisson's ration ν of 0.3. Five separate systematically refined uniform quadrilateral meshes are considered: 500, 4 500, 12 500 and 50 000 cells; the coarsest mesh is shown in Figure 6(b). The beam is fixed on the left boundary, $U_b = (0 \ 0)$, and a traction of $T_b = (0 \ 1)$ MPa is applied to the right boundary; the top and bottom boundaries are traction-free. Plane strain conditions are assumed.

Figure 6. Slender cantilever beam in bending test case

274 The analytical deflection of the right-end of the beam is given as [43]:

$$\Delta = \frac{PL^3}{3(E/1-\nu^2)I} = 0.01456 \text{ m} \quad (25)$$

275 where $P = 0.1 \text{ MN}$ is the applied load, $L = 2 \text{ m}$ is the length of the beam, and $I = \frac{bh^3}{12} = \frac{0.1^3}{12}$ is
 276 the second moment of area of the beam about its bending axis.

277 Using the difference between the predicted displacement and the analytical solution as a metric,
 278 the accuracy and order of accuracy of the current method may be assessed. Figure 7 compares
 279 the results from the new procedure with those from two segregated FV methods, and commercial
 280 FE software Abaqus (version 6.11-1) [44]. The first segregated FV method (Segregated 1 in
 281 Figure 7) uses internal face tangential gradients interpolated from neighbour cell-centre gradients,
 282 and boundary face tangential gradients extrapolated from the internal domain, as detailed by
 283 Jasak and Weller [6]; the second segregated FV method (Segregated 2 in Figure 7) employs the
 284 same discretisation as the new coupled procedure where the face tangential gradients are directly
 285 calculated using the FA method. The FE solution in Abaqus uses bi-linear shape functions with
 286 reduced-order integration as fully integrated linear elements are known to be erroneously stiff in
 287 bending. Quadratic elements, if used, would be expected to achieve greater accuracy, albeit at a
 288 considerably greater computational cost.

289 Examining Figure 7, it can be seen that the errors for all the methods reduce at an approximately
 290 second order rate, as is expected. Comparing the coupled method to the segregated method with
 291 an equivalent discretisation (Segregated 2), the solutions are almost identical, where the slight
 292 differences are due to the iterative solution tolerance in the segregated method being too loose. In
 293 this case, the new face tangential gradient discretisation (Coupled and Segregated 2) is more accurate
 294 solution than the method where the gradient is interpolated from adjacent cell centres (Segregated
 295 1); furthermore, this face tangential gradient method is more accurate than the FE solution for each
 296 mesh examined. An important point to note is that the FV methods do not suffer erroneous *locking*,
 297 as experienced by standard fully integrated linear FE methods. The meshes examined here have cell

Figure 7. Error in cantilever end-deflection as the mesh spacing is reduced

aspect ratios of unity; although not shown here, it has been found the use of large aspect ratio cells produces a stiffer response than for an equivalent mesh with aspect ratio close to unity, as is the case with the standard FE method. Even in the case of higher aspect ratio meshes, the reduction in error remains second order and the true solution is asymptotically approached.

The models have been solved in double precision using 1 CPU core (2.4 GHz Intel Ivy Bridge cores); the execution times for the newly developed coupled method are compared with those of the segregated FV and FE approaches in Table I. All models have been solved in one quasi-static time-step.

For the coupled approach, the linear system has been solved using a direct sparse LU factorisation method as implemented in open-source C++ library Eigen [45], where an OpenFOAM wrapper class has been written to handle the communication. The segregated FV approaches employ a CG method with incomplete Cholesky preconditioning [46]; for this test case, it was found that the segregated solution required a relatively tight solution tolerance of 10^{-8} to produce equivalent results to the coupled method. The finest meshes were not run for the segregated approaches due to the large expected wall-clock times; it should be noted that a geometric multigrid method (*e.g.* [3]), if used, would be expected to substantially reduce the required time of a segregated method.

Mesh	Coupled		Segregated ¹		Segregated ²		Abaqus	
	Time	Memory	Time	Memory	Time	Memory	Time	Memory
500	0.08	11	58	20	134	24	3	40
4 500	0.5	50	384	27	1 049	41	4	113
12 500	1.4	140	1 387	43	3 171	74	5	197
50 000	6	570	4 737	112	11 583	225	16	881
200 000	36	2 500	-	-	-	-	73	1 800

Table I. Slender cantilever: wall-clock time (in s) and maximum memory usage (in MB).

From Table I, it is clear to see that the developed coupled approach far outperforms the segregated approach showing speedups of over three orders of magnitude. It should be noted that this style of test case is a *worst case scenario* for a segregated approach, due to the dominant inter-component coupling. When compared with the FE procedure, the new approach is at least twice as fast for the examined meshes. Inspecting computer memory requirements, the coupled approach uses at least an order of magnitude more memory than the equivalent segregated approach; as previously discussed this is due to a combination of the extended implicit molecule, the inclusion of boundary face unknowns, and the additional memory requirements of a direct solver due to matrix fill-in. Comparing the coupled and the FE methods, the memory requirements are approximately the same, with the coupled method using slightly less; this is to be expected as the FE solution procedure also uses a block coupled approach with a direct solver.

Out-of-Plane Bending of an Elliptic Plate

This 3-D test case consists of a thick elliptic plate with a centred elliptic hole (Figure 8); a constant pressure of 1 MPa is applied to the upper surface, and the outer surface is fully clamped. The case has been described by the National Agency for Finite Element Methods and Standards (NAFEMS) [47], and in the context of the FV method has been examined and benchmarked in detail by Demirdžić et al. [3]. The assumed mechanical properties are Young's modulus = 210 GPa and Poisson's ratio = 0.3. Due to a double symmetry, only a quarter of the plate is analysed. The thickness of the plate is 0.6 m, and the inner and outer ellipses are given by:

$$\left(\frac{x}{2}\right)^2 + \left(\frac{y}{1}\right)^2 = 1 \quad \text{inner ellipse} \quad (26)$$

$$\left(\frac{x}{3.25}\right)^2 + \left(\frac{y}{2.75}\right)^2 = 1 \quad \text{outer ellipse} \quad (27)$$

Results are calculated on five systematically refined hexahedral meshes (96, 576, 4 608, 36 864 and 294 912 cells); this imitates closely the analysis of Demirdžić et al. [3], allowing fair comparison with their benchmark results. Subsequently, calculations are performed on tetrahedral and polyhedral meshes to examine the effect of employing fully unstructured grids.

The predicted stress distributions of the coupled method on the plane $z = 0.3$ m, σ_{xx} , σ_{yy} , σ_{xz} and σ_{yz} components, are shown in Figures 9(a) and 9(b) side-by-side with those from Demirdžić et al. [3]; qualitatively, a close agreement can be seen with slight mismatches in the alignment of stress contours at the symmetry plane.

The distribution of the local stress component σ_{ss} along the local co-ordinate s is presented for the 5 hexahedral meshes in Figure 10(a), where the local co-ordinate s runs along the upper inner elliptic edge of the plate (see Figure 8). As the mesh is refined, the results can be seen to approach a grid independent solution and the reference solution from Demirdžić et al. [3]. The reference solutions have been generated by fitting cubic splines through the key point values given in Demirdžić et al. [3]. Examining the σ_{ss} stress at $s = 0.0$, as suggested in the NAFEMS benchmark, the percentage discretisation error is shown in Figure 10(b) to reduce at a second order rate with decreasing mesh spacing. The reference solution has been approximated using Richardson extrapolation [48] and the solution from the two finest meshes. As there are no FV computational nodes at the corner point, the stress values are extrapolated from adjacent boundary face-centres and cell-centres. The target

Figure 8. Out-of-plane bending of an elliptic plate

Figure 9. Elliptic plate: stress component distributions on the plane $z = 0.3$ m (right) compared with results from Demirdžić et al. [3] (left)

stress value given in the NAFEMS benchmark cannot be directly used for comparison as the fixed displacement boundary conditions used in the current study mimic those used in Demirdžić et al. [3] and do not correspond exactly to those in the NAFEMS benchmark.

The distribution of the von Mises equivalent stress $\sigma_{eq} = \sqrt{\frac{3}{2}|\boldsymbol{\sigma}'|^2}$, where $\boldsymbol{\sigma}'$ is the deviatoric stress, and displacement components u and v , along $r = \sqrt{x^2 + y^2} = 2.1$ m, $z = 0.3$ m, are shown in Figures 11(a) and 11(b). In each case, the predicted results converge towards the reference solutions. Figures 12(a), 12(b), and 12(c), show the distribution of equivalent stress and displacement components u and v along the line $x = y$, $z = 0.3$ m; the predicted results approach the reference solution in a similar manner to the previous plots.

Table II shows the wall-clock times and memory requirements for each of the runs; for comparison, results are given for the segregated FV methods (Segregated 1 and Segregated 2), and commercial FE software Abaqus. Unlike in the previous 2-D test case where a direct LU

Figure 10. Elliptic plate: σ_{ss} Figure 11. Elliptic plate: distribution of equivalent stress σ_{eq} and displacement components u and v , along $r = \sqrt{x^2 + y^2} = 2.1$ m; $z = 0.3$ m

decomposition solver was employed, here a BiCGStab linear solver with ILU(0) preconditioner has been used for the coupled approach. The BiCGStab solver was found to be more time and memory efficient for 3-D cases than the Eigen library LU decomposition direct solver. A GMRes iterative solver with ILU(0) preconditioner was also trialled, but found to be approximately twice as slow as BiCGStab in all 3-D cases examined. A solution tolerance of 1×10^{-6} has been used in the FV models. From Table II, it can be seen that the new coupled method is faster than the segregated FV methods by a factor of 2.5 to 6 times; as expected, the memory requirements are greater, by approximately 4.5 times in the largest mesh case. Interestingly, when compared to the FE solution, the new coupled method is faster and considerably more memory efficient in all cases; in the finest mesh case the coupled method is almost 6 times faster and uses 8 times less memory. The larger memory requirements of the FE solution may be attributed to the employed direct solver; however, the larger FE wall-clock times are somewhat more surprising, and highlight the efficiency of the new method.

To examine the applicability of the method on truly unstructured meshes, the analysis has been performed on a general polyhedral grid and a tetrahedral grid, each with approximately the same number of cells as the finest hexahedral grid (mesh 5). The polyhedral mesh contains 275 533 cells and has been generated using cfMesh [49], a new open-source cartesian-based meshing software. The tetrahedral mesh contains 295 536 cells and has also been generated using cfMesh; images

Figure 12. Elliptic plate: distribution of equivalent stress and displacement components u and v along $x = y$, $z = 0.3$ m

Mesh	Coupled		Segregated ¹		Segregated ²		Abaqus	
	Time	Memory	Time	Memory	Time	Memory	Time	Memory
72	0.03	7	0.5	6	0.5	6	4	24
576	0.15	13	1	8	2	9	5	31
4 608	1.6	51	6.5	20	14	30	6	107
36 864	11	300	102	80	145	120	34	1 197
294 912	242	2 200	1 474	500	1 990	800	1 375	17 900

Table II. Elliptic plate: wall-clock time (in s) and maximum memory usage (in MB)

of the meshes are shown in Appendix B. The stresses and displacements for the polyhedral and tetrahedral meshes are compared with results from the finest hexahedral solution and Demirdžić et al. [3] benchmark solution in Figure 13. Additionally, solutions are given for comparison using commercial FE software Abaqus where the finest hexahedral mesh has been used. In each case, both the polyhedral and tetrahedral results are seen to be very close to that of the hexahedral solution, the reference solution, and the FE solution. The stress contours in the $z = 0.3$ m x - y plane are shown in Figure 14, comparing with solutions from the finest hexahedral mesh, the Demirdžić et al. [3] benchmark, and the Abaqus solution: all results are seen to agree closely.

Figure 13. Elliptic plate: comparison of predicted results from the new coupled method for hexahedral, polyhedral and tetrahedral meshes, the Demirdžić et al. [3] benchmark, and the Abaqus FE hexahedral mesh solution

389 Narrow T-Section Component Under Tension

390 The final benchmark case, shown in Figure 15(a), consists of a narrow engineering component with a
 391 T cross-section, and has been as proposed by Demirdžić et al. [3] as a benchmark. Due to symmetry,
 392 the solution domain consists of one quarter of the component. A constant negative pressure of
 393 1 MPa is applied to the lower surface and the upper left surface is fully clamped, as illustrated
 394 graphically in Figure 15(a). The Young's modulus is 210 GPa and Poisson's ratio is 0.3. A hole
 395 of radius $R = 5$ mm is located at the expected stress concentration. Four separate systematically
 396 refined hexahedral meshes (624, 4 992, 39 936, and 319 488 cells) are examined, mimicking the
 397 meshes employed by Demirdžić et al. [3]; the coarsest mesh is shown in Figure 15(b).

Figure 14. Elliptic plate: stress component distributions on the plane $z = 0.3$ m (right) for the hexahedral, polyhedral and tetrahedral meshes compared with the Demirdžić et al. [3] benchmark and the Abaqus FE hexahedral mesh solution

398 Figure 16 shows the σ_{xx} and σ_{yy} stress distributions on the plane $z = 0.0$ m for the finest
 399 mesh. When compared with the results of Demirdžić et al. [3], the stress contours are almost
 400 indistinguishable.

401 Follow the proposed benchmark of Demirdžić et al. [3], the equivalent stress and displacement
 402 components are plotted along three separate profiles on the $z = 0$ plane: $r = 1.5R$, $x = 0$ and $y = 0$,
 403 where r and θ are the polar coordinates centred on the hole with $\theta = 0$ at the bottom vertical section.

Figure 15. Narrow T-section component

Figure 16. Narrow T-section component: stress component distributions on the plane $z = 0.0$ m (right) compared with results from Demirdžić et al. [3] (left)

404 The predictions for the four hexahedral meshes are shown in Figures 17, 18 and 19. The results

converge quickly to the the reference solution for each case, except for the displacement component in Figure 19(b); however, the scale here magnifies the discrepancy.

Figure 17. Narrow T-section component: equivalent stress plotted along $z = 0$ plane, $r = 1.5R$

Figure 18. Narrow T-section component: equivalent stress and x displacement component plotted along $z = 0$ plane, $y = 0$

Figure 19. Narrow T-section component: equivalent stress and y displacement component plotted along $z = 0$ plane, $x = 0$

The wall-clock times and memory requirements for each run are given in Table III; once again, for comparison the results are given for the segregated FV methods, and commercial FE software Abaqus. The same linear solvers and tolerances are employed as in the previous 3-D test case.

The results are very similar to those in the previous 3-D test case, where the new coupled method requires approximately a factor of 4 less wall-clock time and a factor of 4 more memory than the segregated FV methods. When compared with the Abaqus FE solution, the new coupled method is once again found to require less time and less memory; for the finest grid, 3 times less wall-clock time, and 5 times less memory, is required.

Mesh	Coupled		Segregated ¹		Segregated ²		Abaqus	
	Time	Memory	Time	Memory	Time	Memory	Time	Memory
624	0.2	15	0.7	8	1.5	10	2	98
4 992	2	58	6	24	10	30	3	102
39 936	29	340	98	88	416	140	33	1 500
319 488	421	2 400	2 220	560	2 647	900	1 236	13 000

Table III. Narrow T-section component: wall-clock time (in s) and maximum memory usage (in MB)

As in the previous test case, results from a polyhedral and tetrahedral mesh are compared with those of the finest hexahedral mesh, the Demirdžić et al. [3] benchmark solution, and the Abaqus FE solution, shown in Figure 20. The polyhedral and tetrahedral meshes have been generated using *cfMesh*, where the polyhedral mesh contains 337 085 cells and the tetrahedral contains 282 415 cells; images of meshes are shown in Appendix B. Figure 21 shows the stress and displacement predictions along the benchmark profiles for the polyhedral and tetrahedral meshes; for comparison, results are given for the finest hexahedral mesh, the Demirdžić et al. [3] benchmark, and FE software Abaqus where the finest hexahedral mesh was used. All predictions are seen to agree closely; the largest discrepancy can be seen in the displacement component v in Figure 20(e); however, this is magnified by the vertical axis scale. Small oscillations are present in the tetrahedral mesh solution, which are visible in the stress distribution images and the stress/displacement plots. Although the origins not clear, these oscillations may be related to the so-called *checker-boarding* issues that can occur with cell-centred FV methods; this will be examined further in future work, and a number of the previously proposed preventative methods will be considered.

5. DISCUSSION & CONCLUSIONS

A new fully implicit block-coupled FV methodology has been presented, including a face tangential derivative approximation based on least squares Finite Area method. The accuracy of the method has been shown through detailed comparison with analytical solutions and numerical benchmarks. For the cases examined, the new method has been found to be faster than the segregated FV methods in every instance, with approximate speed-ups of 5 times. In particular, the coupled method shows speed-ups of three orders of magnitude for the simple 2-D bending cantilever test case. As expected, the new method required approximately 4 times as much memory as the memory efficient segregated methods. When compared with a commercial FE software, the new method has been found to be faster in every case, where for the elliptic plate test case the new coupled method is almost 6 times faster. Examining memory requirements, it was clear that the iterative BiCGStab employed by the new method scaled more favourably than the FE solution direct solver, with a factor of 8 difference

Figure 20. Narrow-T section component: comparison of predicted results from the new coupled method for hexahedral, polyhedral and tetrahedral meshes, and the Abaqus FE hexahedral mesh solution

440 for the largest mesh in elliptic plate test case. It can be concluded that the new method provides
 441 an efficient and accurate alternative to segregated FV methods and standard FE methods for the
 442 analysis of complex 3-D problems in linear elasticity.

Figure 21. Narrow T-section component: stress component distributions on the plane $z = 0.0$ m, σ_{xx} (left) and σ_{yy} (right), comparing the hexahedral, polyhedral, and tetrahedral results with the Demirdžić et al. [3] benchmark and the Abaqus FE hexahedral results

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A. APPENDIX: IMPLICIT COMPUTATIONAL MOLECULE

The extended implicit computational molecule for triangular and general polygonal meshes are shown in Figure 22.

Figure 22. Extended implicit computational molecule for triangular and general polygonal meshes

B. APPENDIX: POLYHEDRAL AND TETRAHEDRAL MESHES

448 The tetrahedral and general polyhedral meshes employed in the elliptic plate test case are shown
 449 in Figure 23. The tetrahedral and general polyhedral meshes employed in the narrow T-section
 component test case are shown in Figure 24.

Figure 23. Elliptic plate: cross-section of the tetrahedral and general polyhedral meshes

450

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Figure 24. Narrow T-section component: front view of the tetrahedral and general polyhedral meshes

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