

A VERTEX BASED DISCRETISATION SCHEME  
APPLIED TO MATERIAL NON-LINEARITY WITHIN A  
MULTI-PHYSICS FINITE VOLUME FRAMEWORK

GARETH ANTHONY TAYLOR <sup>1</sup>

A thesis submitted in partial fulfilment of the  
requirements of the University of Greenwich  
for the degree of Doctor of Philosophy

November 1996

<sup>1</sup>Centre for Numerical Modelling and Process Analysis, School of Computing and Mathematical Sciences, University of Greenwich, London, UK

# Dedications

*For my grandmother,  
Florence Taylor,  
3rd September 1911 – 18th November 1985,*

*and my grandfather,  
George David Taylor,  
17th June 1911 – 4th September 1986.*

# Acknowledgements

Firstly, I acknowledge the people directly associated with this research project. This group includes, primarily, Prof. Mark Cross and Dr. Chris Bailey, who have both provided careful supervision and displayed significant amounts of patience.

This group also includes a considerable number of academic, research and technical staff associated with the School of Computing and Mathematical Sciences at the University of Greenwich. This collection of people have all provided invaluable support to varying degrees, but two people deserve a particular acknowledgement, Nick Croft for his academic contribution and Frank for his technical support.

Secondly, I acknowledge both my parents and my brother for their complete support and also my friends for their entertaining distractions and polite interest.

Finally and maybe most importantly, I acknowledge the Engineering and Physical Sciences Research Council without whose financial support this research may not have been possible.

# Abstract

The objective of this research is the development of novel three dimensional Finite Volume (FV) algorithms for the solution of small strain, quasi-static, Computational Solid Mechanics (CSM) problems involving non-linear material behavior, specifically materials described by an elasto-visco-plastic constitutive relationship and a von-Mises yield criterion. The motivation is to contribute the non-linear CSM capability to an integrated FV framework for the comprehensive solution of the thermo-mechanical behaviour exhibited by the shape casting of metals.

A study of novel two and three dimensional FV algorithms associated with CSM is presented. The algorithms employ a variety of two and three dimensional elements and are compared with the standard Bubnov-Galerkin Finite Element Method, with regard to algorithmic procedure, linear solvers, accuracy and computational cost. A variety of benchmark solid mechanics problems involving elasto-plastic and elasto-visco-plastic material behaviour are studied. These include the plane stress analysis of a perforated tensile strip of aluminium, the plane strain analysis of a hollow metal cylinder and the three dimensional analysis of a hollow metal sphere.

The control volume-unstructured mesh, vertex based, FV algorithm for CSM problems is integrated within a multi-physics FV framework PHYSICA, which includes cell-centred FV procedures for the solution of problems involving simultaneous heat transfer, solidification and fluid flow. The thermo-mechanical coupling is described in detail. A variety of thermo-mechanical benchmark problems involving thermo-elasto-plastic and thermo-elasto-visco-plastic behaviour are studied, these include the quenching and the solidification of an infinite steel plate. Finally, the completely coupled capability of the FV framework PHYSICA is validated against experimental observations obtained from the gravity die casting of a hollow aluminium cylinder.

# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Review of numerical discretisation methods . . . . .	2
1.1.1	Finite Difference Methods (FDM) . . . . .	2
1.1.2	Finite Element Methods (FEM) . . . . .	5
1.1.3	Boundary Element Methods (BEM) . . . . .	7
1.2	Finite Volume Methods . . . . .	8
1.2.1	Cell-centred FVM . . . . .	9
1.2.2	Cell-vertex FVM . . . . .	11
1.2.3	Control Volume-Unstructured Mesh vertex based FVM . . . . .	13
1.3	Overview of the thesis . . . . .	17
<b>2</b>	<b>Material Non-linearity</b>	<b>20</b>
2.1	Classification of Material Non-linearity . . . . .	20
2.1.1	Rate Independent Material Non-linearity . . . . .	21

2.1.1.1	Non-linear Elasticity . . . . .	22
2.1.1.2	Plasticity . . . . .	22
2.1.2	Rate Dependent Material Non-linearity . . . . .	24
2.1.2.1	Visco-elasticity . . . . .	24
2.1.2.2	Visco-plasticity . . . . .	25
2.1.2.3	Creep and Stress Relaxation . . . . .	25
2.2	Mathematical Theory of Plasticity . . . . .	27
2.2.1	Overview of Yield Criteria . . . . .	27
2.2.2	The von-Mises Yield Criterion . . . . .	28
2.2.3	Strain-hardening of Materials . . . . .	30
2.3	Elasto-visco-plasticity . . . . .	32
2.3.1	Linear Elasticity . . . . .	32
2.3.1.1	Tensor Definition . . . . .	33
2.3.1.2	Engineering Definition . . . . .	34
2.3.2	Perzyna Model . . . . .	36
2.3.3	Closure . . . . .	37
<b>3</b>	<b>Numerical Computation</b>	<b>39</b>
3.1	Numerical Discretisation . . . . .	39
3.1.1	Governing Equations . . . . .	40

3.1.2	General Discretisation . . . . .	40
3.1.2.1	Bubnov-Galerkin FEM . . . . .	44
3.1.2.2	Cell-vertex FVM . . . . .	46
3.1.3	Conservative Discretisation . . . . .	48
3.2	Algorithmic techniques . . . . .	50
3.2.1	Standard non-linear approach . . . . .	50
3.2.2	Segregated approach . . . . .	52
3.2.3	Time stepping schemes . . . . .	55
3.2.3.1	Estimation of time step length . . . . .	55
3.2.3.2	Analytical estimation . . . . .	56
3.2.3.3	Empirical estimation . . . . .	56
3.3	Linear solvers . . . . .	57
3.4	Axisymmetric problems . . . . .	57
3.5	Closure . . . . .	59
<b>4</b>	<b>Numerical Analysis</b>	<b>60</b>
4.1	Theoretical analysis of discretisation . . . . .	60
4.1.1	One Dimensional Analysis . . . . .	61
4.1.2	Two Dimensional Analysis . . . . .	65
4.1.2.1	Constant strain triangular elements . . . . .	65

4.1.2.2	Bilinear quadrilateral elements . . . . .	70
4.1.3	Three Dimensional Analysis . . . . .	72
4.1.3.1	Linear Tetrahedral elements . . . . .	75
4.1.3.2	Bilinear Pentahedral elements . . . . .	77
4.1.3.3	Trilinear Hexahedral elements . . . . .	78
4.2	Closure . . . . .	80
<b>5</b>	<b>Mechanical Validation</b>	<b>82</b>
5.1	Test case 1: Uniaxial tensile piece . . . . .	82
5.1.1	Analytical solution . . . . .	83
5.1.2	Numerical solutions . . . . .	84
5.1.3	Algorithm performance . . . . .	87
5.2	Test case 2: Perforated tensile strip . . . . .	88
5.2.1	Reference solution . . . . .	88
5.2.2	Numerical analysis . . . . .	89
5.2.2.1	Reference numerical analyses . . . . .	89
5.2.3	Discussion of numerical results . . . . .	90
5.2.4	Algorithmic performance . . . . .	91
5.2.5	Invariant and integration point scheme . . . . .	92
5.3	Test case 3: Internally pressurised thick cylinder . . . . .	100



5.3.1	Theoretical analysis . . . . .	100
5.3.2	Numerical analysis . . . . .	100
5.3.3	Discussion of numerical results . . . . .	101
5.4	Test case 4: Internally pressurised spherical vessel . . . . .	105
5.4.1	Theoretical analysis . . . . .	105
5.4.2	Numerical analysis . . . . .	106
5.4.3	Discussion of numerical results . . . . .	107
5.4.4	Algorithmic performance . . . . .	109
5.5	Closure . . . . .	118
<b>6</b>	<b>Thermo-mechanical Validation</b>	<b>119</b>
6.1	Conservation equations . . . . .	120
6.2	Thermo-mechanical coupling . . . . .	121
6.2.1	Test case 1: Quenching of a steel slab . . . . .	122
6.2.1.1	Reference solution . . . . .	123
6.2.1.2	Numerical analysis . . . . .	124
6.2.1.3	Discussion of numerical results . . . . .	125
6.2.2	Test case 2: Solidification of a steel slab . . . . .	129
6.2.2.1	Analytical solution . . . . .	129
6.2.2.2	Numerical procedure for solidification . . . . .	132

6.2.2.3	Numerical procedure for liquid regions . . . . .	132
6.2.2.4	Numerical analysis . . . . .	133
6.3	Closure . . . . .	134
<b>7</b>	<b>Applications</b>	<b>135</b>
7.1	Shape casting of metals . . . . .	135
7.1.1	Shape casting processes . . . . .	136
7.1.1.1	Die casting . . . . .	136
7.1.1.2	Sand casting . . . . .	137
7.1.1.3	Investment casting . . . . .	137
7.1.2	Simulation of shape casting processes . . . . .	137
7.1.3	Dual thermo-mechanical coupling . . . . .	138
7.1.3.1	Casting/mould gap formation . . . . .	139
7.2	Gravity die casting of a hollow aluminium cylinder . . . . .	141
7.2.1	Numerical analysis . . . . .	143
7.2.2	Discussion of numerical results . . . . .	146
7.3	Sand casting of an aluminium test bar . . . . .	156
7.3.1	Numerical analysis . . . . .	157
7.3.2	Natural convection . . . . .	159
7.3.3	Discussion of numerical numerical results . . . . .	160

7.3.3.1	Thermal analyses . . . . .	161
7.3.3.2	Thermo-mechanical analyses . . . . .	164
7.4	Closure . . . . .	175
<b>8</b>	<b>Closure</b>	<b>176</b>
8.1	Conclusions . . . . .	176
8.1.1	Elemental comparisons . . . . .	176
8.1.2	Surface tractions . . . . .	177
8.1.3	Thermo-mechanical problems . . . . .	178
8.1.4	Finite volume discretisation . . . . .	178
8.2	Further research . . . . .	178
8.2.1	Contact analysis . . . . .	179
8.2.2	Optimisation . . . . .	179
8.2.3	Solid mechanics . . . . .	179
8.2.4	Shape casting of metals . . . . .	180
<b>A</b>	<b>Standard Formulae</b>	<b>181</b>
A.1	Divergence Theorem (Gauss' Theorem) . . . . .	181
A.2	Green's First Theorem . . . . .	181
A.3	Stokes's Theorem (in the plane) . . . . .	182

A.4	Error Function . . . . .	182
A.5	Kronecker delta . . . . .	182
<b>B</b>	<b>Shape Functions</b>	<b>183</b>
B.1	Constant Strain Triangular Elements . . . . .	183
B.2	Bilinear Quadrilateral Elements . . . . .	183
B.3	Linear Tetrahedral Elements . . . . .	184
B.4	Bilinear Pentahedral Elements . . . . .	184
B.5	Trilinear Hexahedral Elements . . . . .	185
<b>C</b>	<b>Local-global transformation</b>	<b>186</b>
<b>D</b>	<b>Two dimensional approximations</b>	<b>188</b>
D.1	Plane stress . . . . .	188
D.2	Plane strain and Axisymmetry . . . . .	189
D.3	Differential and normal operators . . . . .	189
<b>E</b>	<b>Constraint equations</b>	<b>190</b>

# List of Figures

1.1	Cell-centred FVM applied to a structured mesh . . . . .	10
1.2	FVM applied to an unstructured mesh. (a) Cell-centred and (b) Cell-vertex. . . . .	12
1.3	CV-UM vertex based FVM applied to an unstructured mesh . . . . .	13
1.4	Weighting function $W$ . (a) Cell-vertex FVM and (b) Bubnov-Galerkin FEM and (c) CV-UM vertex based FVM. . . . .	15
2.1	Non-linear stress-strain relationships. (a) Non-linear elasticity and (b) elasto-plasticity. .	22
2.2	Plastic material behaviour. (a) Elastic, perfectly plastic and (b) elastic, linear work-hardening.	23
2.3	Uniaxial strain-time curve at constant stress. . . . .	25
2.4	Yield surface in principal stress space. . . . .	29
3.1	Overlapping control volumes in two dimensions. . . . .	45
3.2	Non-overlapping control volumes in two dimensions. . . . .	47
4.1	One dimensional, two noded element. . . . .	62
4.2	1D (a) shape functions and FEM weighting functions, (b) FVM weighting functions. . .	63

4.3	Two dimensional integration points (a) FVM and (b) FEM. . . . .	66
4.4	CST element. (a) Global, (b) FEM local and (c) FVM local coordinates. . . . .	67
4.5	Elemental contributions to the control volume at node i (a) FEM and (b) FVM. . . . .	68
4.6	Single CST (a) elemental contributions and (b) sides and lengths. . . . .	69
4.7	BLQ element. (a) Global, (b) FEM local and (c) FVM local coordinates. . . . .	71
4.8	Linear tetrahedral element in (a) global coordinates and (b) local coordinates. . . . .	72
4.9	Bilinear pentahedral element in (a) global coordinates and (b) local coordinates. . . . .	73
4.10	Trilinear hexahedral element in (a) global coordinates and (b) local coordinates. . . . .	73
4.11	Three dimensional vertex based control volume. . . . .	74
4.12	LT element Gauss point in local coordinates and associated weighting. . . . .	76
4.13	LT element integration points in local coordinates (a) vertical and (b) horizontally inclined. . . . .	76
4.14	BLP Gauss points in local coordinates. (a) $u = -1/\sqrt{3}$ and (b) $u = 1/\sqrt{3}$ . . . . .	78
4.15	BLP FVM integration points in local coordinates. (a) $u = -\frac{1}{2}$ , (b) $u = \frac{1}{2}$ and (c) $u = 0$ planes. . . . .	79
4.16	TLH Gauss points in local coordinates. (a) $u = 1/\sqrt{3}$ and (b) $u = -1/\sqrt{3}$ . . . . .	80
4.17	TLH FVM integration points in local coordinates. (a) $u$ , (b) $s$ and (c) $t$ planes. . . . .	81
5.1	One dimensional elasto-visco-plastic (a) model and (b) response. . . . .	83
5.2	Uniaxial hardening problem. . . . .	85
5.3	CPU times measured on an Intel 486DX 33Mhz processor. . . . .	87

5.4	Perforated tensile strip . . . . .	89
5.5	Total strain profile of numerical and semi-experimental analyses. . . . .	93
5.6	Stress profile of numerical and semi-experimental analyses. . . . .	93
5.7	Comparison of the total strain for BLQ elements. . . . .	94
5.8	Comparison of the total strain for CST elements. . . . .	94
5.9	Comparison of the stress distribution for BLQ elements. . . . .	95
5.10	Comparison of the stress distribution for CST elements. . . . .	95
5.11	CPU times for BLQ elements on a SPARC 4, 110MHz work station. . . . .	96
5.12	CPU times for CST elements on a SPARC 4, 110MHz work station. . . . .	96
5.13	Comparison with FV integration point method for strain. . . . .	97
5.14	Comparison with FE integration point method for strain. . . . .	97
5.15	Comparison with FV integration point method for stress. . . . .	98
5.16	Comparison with FE integration point method for stress. . . . .	98
5.17	Comparison of integration point methods for strain. . . . .	99
5.18	Comparison of integration point methods for stress. . . . .	99
5.19	Internally pressurized thick cylinder. . . . .	101
5.20	Mesh consisting of BLQ elements. . . . .	103
5.21	Mesh consisting of CST elements. . . . .	103
5.22	Mesh consisting of BLQ elements. . . . .	104

5.23	Mesh consisting of CST elements. . . . .	104
5.24	Plastic region round a spherical cavity, expanded by a uniformly distributed pressure. . .	105
5.25	Meshes employed in the analyses of an internally pressurized spherical vessel. . . . .	107
5.26	Mesh consisting of 1,221 nodes and 950 TLH elements. . . . .	111
5.27	Mesh consisting of 3,165 nodes and 2,646 TLH elements. . . . .	111
5.28	Mesh consisting of 726 nodes and 1,000 BLP elements. . . . .	112
5.29	Mesh consisting of 1,800 nodes and 2,744 BLP elements. . . . .	112
5.30	Mesh consisting of 1,221 nodes and 4,800 LT elements. . . . .	113
5.31	Mesh consisting of 3,165 nodes and 13,328 LT elements. . . . .	113
5.32	CPU times for TLH elements on a SPARC 4, 110MHz. . . . .	114
5.33	FE and FV CPU times for TLH elements on a SPARC 4, 110MHz. . . . .	114
5.34	CPU times for BLP elements on a SPARC 4, 110MHz. . . . .	115
5.35	CPU times for LT elements on a SPARC 4, 110MHz. . . . .	115
5.36	Comparison for FVM with TLH elements. . . . .	116
5.37	Comparison for FEM with TLH elements. . . . .	116
5.38	Comparison for FVM with BLP elements. . . . .	117
5.39	Comparison for FEM with BLP elements. . . . .	117
6.1	Incremental thermo-mechanical coupling within the FV framework. . . . .	122
6.2	Quenching of an infinite steel plate. . . . .	124



6.3	Transient behaviour of stress and plastic strain during quenching. . . . .	126
6.4	Residual stress after quenching (coarse mesh). . . . .	127
6.5	Residual stress after quenching (fine mesh). . . . .	128
6.6	Residual stress after quenching. . . . .	128
6.7	Stress distribution after 10s of solidification. . . . .	131
6.8	Comparison of stress distributions with regard to solidification fronts. . . . .	132
7.1	The die casting/mould interface. . . . .	139
7.2	Experimental design: Top view. . . . .	141
7.3	Experimental design: Side view. . . . .	142
7.4	Mesh employed in the analysis of gravity die casting. . . . .	146
7.5	Temperature profiles in mould and casting. . . . .	147
7.6	Gap formation at mould/cast interface. . . . .	148
7.7	Casting shrinkage and gap formation over time (Mg. $\times 10$ ). . . . .	149
7.8	Temperature profiles in mould and casting. . . . .	150
7.9	Gap formation at mould/cast interface. . . . .	151
7.10	Temperature profiles in the casting. . . . .	152
7.11	Temperature profiles in mould and casting . . . . .	152
7.12	Stress and visco-plastic strain at 500 seconds. . . . .	153
7.13	Stress and visco-plastic strain at 900 seconds. . . . .	153

7.14	Temperature profiles in mould and casting . . . . .	154
7.15	Gap formation. . . . .	154
7.16	Temperature profiles in mould and casting . . . . .	155
7.17	Gap formation. . . . .	155
7.18	Geometry of the sand mould. . . . .	156
7.19	Geometry of aluminium test bar (without sprue). . . . .	157
7.20	Geometry of sprue (top view). . . . .	158
7.21	Geometry of sprue (side view). . . . .	159
7.22	Mesh employed in the analyses of the CTI test bar. . . . .	160
7.23	Cooling rates in the test bar and sand mould. . . . .	161
7.24	Cooling rates for heat transfer without convection (1500 secs.). . . . .	162
7.25	Cooling rates for heat transfer with convection (1500 secs.). . . . .	163
7.26	Cooling rates for heat transfer without convection (300 secs.). . . . .	164
7.27	Cooling rates for heat transfer with convection (300 secs.). . . . .	165
7.28	Cooling rates at various nodal points on the feeder axis. . . . .	166
7.29	Velocity profiles along the diameter of the mid plane of the feeder. . . . .	168
7.30	Temperature profiles along the diameter of the mid plane of the feeder. . . . .	168
7.31	Heat transfer by conduction and convection after 100 seconds. . . . .	169
7.32	Heat transfer by conduction only after 100 seconds. . . . .	169

7.33	Heat transfer by conduction and convection after 300 seconds. . . . .	170
7.34	Heat transfer by conduction only after 300 seconds. . . . .	170
7.35	Resultant liquid velocity through a cross section at 20 seconds. . . . .	171
7.36	Deformation of the test bar after 300 seconds. . . . .	171
7.37	Thermo-mechanical behaviour after 100 seconds, heat transfer with convection. . . . .	172
7.38	Thermo-mechanical behaviour after 100 seconds, heat transfer without convection. . . . .	172
7.39	Thermo-mechanical behaviour after 300 seconds, heat transfer with convection. . . . .	173
7.40	Thermo-mechanical behaviour after 300 seconds, heat transfer without convection. . . . .	173
7.41	Rate dependent thermo-mechanical behaviour after 100 seconds. . . . .	174
7.42	Rate dependent thermo-mechanical behaviour after 300 seconds. . . . .	174

# List of Tables

5.1	Material properties of aluminium alloy 57S. . . . .	84
5.2	Analytical solution of the strain response to an applied stress. . . . .	84
5.3	Numerical results for a plane stress approximation. . . . .	86
5.4	Numerical results for a three dimensional analysis. . . . .	86
5.5	Load increments applied to the perforated tensile strip. . . . .	88
5.6	Material properties of the thick cylinder. . . . .	100
5.7	Load increments applied to the pressurized thick cylinder. . . . .	100
6.1	Material properties associated with the thermal analysis. . . . .	123
6.2	Temperature dependent yield stress. . . . .	123
6.3	Material properties associated with the mechanical analysis. . . . .	123
6.4	Material properties associated with the solidification analysis. . . . .	130
6.5	Material properties associated with the mechanical analysis. . . . .	130
7.1	Relationship between heat transfer coefficient and gap distance. . . . .	143

7.2	Material properties of the aluminium casting alloy. . . . .	144
7.3	Material properties of the mould and core steel. . . . .	145
7.4	Material properties of the insulation. . . . .	145
7.5	Rate dependent material properties. . . . .	148