Computational aspects of generalized continua based on moving least square approximations

Sebastian Skatulla

Thesis submitted to the University of Adelaide for the degree of Doctor of Philosophy

September, 2006

School of Mechanical Engineering The University of Adelaide

Abstract

In recent years, current engineering technology lead to a renewed interest in generalized continuum theories. In particular, generalized continua are able to address fundamental physical phenomena which are related to the underlying microstructure of the material. Specifically scale-effects are of special interest.

In this work a generalized deformation formulation is developed which allows to incorporate material information from the microscopic and the macroscopic space into an unified constitutive model. The approach is based on a theory developed by Sansour (1998) which was originated in theoretical considerations of Ericksen and Truesdell (1957) and later on Eringen and his co-workers (Eringen 1999). The basic idea is to construct a generalized continuum consisting of macro- and micro-continuum and subsequently to compose the generalized deformation by a macro- and micro-component. This procedure results in a generalized problem formulation. Furthermore, new strain measures as well as corresponding field equations can be identified. Here, it is assumed that the deformation field can only be varied within the macro-continuum so that the balance equations are established for the macro-space. The constitutive law is defined at the microscopic level and the geometrical specification of the micro-continuum is the only material input which goes beyond those needed in a classical description.

A special detail of this approach is that it involves first order strain gradients which are expressed by second order derivatives of the displacement field. It allows to address relative motion between micro- and macro-space without adding extra degrees of freedom. In order to model this formulation this work makes use of a meshfree method based on moving least squares (MLS) which is able to provide the required higher order continuity (Lancaster and Salkauskas 1981).

Examples of meshfree methods are the diffuse element method (Nayroles, Touzot, and Villon 1992), the element-free Galerkin method (Belytschko, Lu and Gu 1994), the reproducing kernel particle method (Liu and Chen, 1995), the partition of unity method (Melenk and Babuska 1997) and the hp-cloud method (Duarte and Oden 1996), just to name a few. It was demonstrated that these kind of methods can deal especially well with problems which are characterized by large deformation or changing domain geometry. The potential in modelling formulations involving higher order derivatives has not been widely recognized yet, with the exception of a few one- respectively two-dimensional case studies (Tang et al., 2003).

This work now aims to illustrate the excellent applicability of the proposed generalized deformation formulation in combination with MLS by modelling elastic and plastic problems which are proven to exhibit size-scale effects (Yang and Lakes 1981; Fleck et al. 1994; Aifantis 1999; Lam et al. 2003). Furthermore, a large-scale case study on underground excavation design reveals the potential and adaptivity of this theory with respect to heterogeneous material such as rock.

Statement of originality

This work contains no material which has been accepted to the award of any other degree
or diploma in any university or other tertiary institution and, to the best of my knowledge
and belief, contains no material previously published or written by another person, except
where due reference has been made in the text.

I give consent to this copy of my thesis,		•		University	${\bf Library,}$	being
made available in all forms of media, now	or he	reafter kno	own.			
Student's Signature				Da	ate	

Acknowledgements

Prof. Carlo Sansour encouraged me to take up an academic career and gave me the opportunity to study at the University of Adelaide. During my Master as well as my PhD studies he provided me with continuous guidance and advice on the directions this thesis should pursue. His sharp editorial eye and constructive criticism helped me to do my very best in writing this thesis. Furthermore, I very much appreciated his support and friendship which I found to be invaluable. In particular, he introduced me to the magical world of Tango Argentino.

Dr. Suzanne Hunt never lost belief in me. Her support was decisive to receive the extension of my scholarship which made it possible for me to successfully finish my PhD-studies.

Prof. Peter Behrenbruch, I also want to thank for his support, encouragement and interest he took on my research.

Prof. Colin Hansen helped me to adapt and feel comfortable in the School of Mechanical Engineering after having left the Australian School of Petroleum. He always had good advice for me and supported my leave to the University of Nottingham to finish my thesis there.

Dr. Bassam Dally who accepted my supervision, when I became a student in the School of Mechanical Engineering. I valued his interest in my research progress.

My charming partner Aphrodite for her emotional support, patience and understanding putting up with me during the last stages of my PhD-studies.

Contents

	List	of figures	X
	List	of tables	ζ.
	Nota	ation and list of symbols	I.
1	Intr	roduction	1
	1.1	Background	1
	1.2	Thesis motivation, aim and objectives	.(
	1.3	Layout of the thesis	
2	Fou	ndations of continuum mechanics 1	Ę
	2.1	Kinematics and geometry	ļ
	2.2	Stress measures	.8
	2.3	Balance Laws of Continuum Mechanics	. (
		2.3.1 Conservation of mass	. (
		2.3.2 Linear momentum principle	?(
		2.3.3 Angular momentum principle) 2
3	Mes	shfree methods 2	4
	3.1	Meshfree approximation based on MLS	34
		3.1.1 Moving Least Square Method	24
		3.1.2 Weight function	3(
		3.1.3 Basis polynomial	35
	3.2	MLS-approximation characteristics	37
	3.3	Details of a MLS implementation	j(
		3.3.1 Numerical integration	. 1

II Contents

		3.3.2 Enforcement of essential boundary conditions	53
4	Cla	ssical Green strain tensor-based formulation	60
	4.1	A modified variational principle	60
	4.2	A stabilized modified variational principle	62
	4.3	Numerical examples	64
		4.3.1 Study on essential boundary condition enforcement	64
		4.3.2 Shell deformation examples	69
5	Cos	serat continuum	74
	5.1	Overview	74
	5.2	Strain measures of the Cosserat continuum	74
	5.3	Variation of the rotation group	76
	5.4	The weak form and its corresponding equilibrium equations	77
	5.5	Multiplicative updating of the rotation field	80
	5.6	Enforcement of displacement boundary conditions	83
	5.7	Numerical examples	83
6	Ger	neralized Continua	90
	6.1	Generalized deformation	90
	6.2	Generalized continuum based on a triade of normal vectors \mathbf{n}_{α}	93
		6.2.1 Generalized Cauchy-Green deformation tensor	94
	6.3	Generalized continuum involving the macroscopic basis vectors \mathbf{g}_{α}	96
		6.3.1 Generalized Cauchy-Green deformation tensor	97
		6.3.2 A generalized variational formulation and its corresponding equilibrium equations	98
		6.3.3 Numerical examples	102
	6.4	Generalized micropolar continuum involving the macro-scopic rotation tensor ${\bf R}$	118
		6.4.1 Generalized micropolar strain measures	119
		6.4.2 The generalized variational formulation and its corresponding equilibrium equations	120
		6.4.3 Numerical examples	123

Contents

7	Exp tive	periments in mixed and modified formulations with higher order deriva es	- 127
	7.1	Overview	127
	7.2	Variational principle with independent displacement and stress field	128
		7.2.1 First version	128
		7.2.2 Second version	129
		7.2.3 Numerical applicability	130
	7.3	Variational principle with independent displacement, rotation and stress field	133
	7.4	Modified variational principle inspired by the <i>Hu-Washizu</i> functional	135
		7.4.1 Variational formulation	135
		7.4.2 Numerical experiments	137
	7.5	Integral form of the equilibrium equations	140
	7.6	Summary	141
8	Con	nclusion	142
9	Fut	ure work	145
\mathbf{A}	Cus	stomizing a spline with a specific continuity	146
В	Par	allelization	150
\mathbf{C}	\mathbf{Iter}	ative stabilization parameter determination algorithm	158
D	Son	ne definitions and relations of tensor calculus	160
Bi	bliog	graphy	163

List of Figures

3.1	domain covering	30
3.2	cubic spline $\Phi = w(x) w(y) \dots \dots \dots \dots \dots \dots \dots \dots \dots$	32
3.3	first order derivative of the cubic spline $\Phi_{,y}=rac{1}{\varrho}ww_{,y}(y)\ldots\ldots\ldots\ldots$	32
3.4	second order derivative of the cubic spline $\Phi_{,xy}=rac{1}{arrho^2}w_{,x}(x)w_{,y}(y)\ldots\ldots$	32
3.5	second order derivative of the cubic spline $\Phi_{,xx}=rac{1}{arrho^2}w(x)w_{,yy}(y)$	32
3.6	quartic spline $\Phi = w(x) w(y)$	33
3.7	first order derivative of the quartic spline $\Phi_{,y}=rac{1}{\varrho}w(x)w_{,y}(y)$	33
3.8	second order derivative of the quartic spline $\Phi_{,xy}=rac{1}{arrho^2}w_{,x}(x)w_{,y}(y)$	33
3.9	second order derivative of the quartic spline $\Phi_{,yy}=rac{1}{arrho^2}w(x)w_{,yy}(y)$	33
3.10	Gaussian spline $\Phi = w(x) w(y) \dots \dots \dots \dots \dots \dots \dots$	34
3.11	first order derivative of the Gaussian spline $\Phi_{,y}=rac{1}{\varrho}w(x)w_{,y}(y)$	34
3.12	second order derivative of the Gaussian spline $\Phi_{,xy}=rac{1}{arrho^2}w_{,x}(x)w_{,y}(y)$	34
3.13	second order derivative of the Gaussian spline $\Phi_{,yy}=rac{1}{arrho^2}w(x)w_{,yy}(y)$	34
3.14	shape function distribution for a zero order basis polynomial $\varrho=0.51$	37
3.15	shape function distribution for a first order basis polynomial $\varrho=1.01$	37
3.16	shape function distribution for a second order basis polynomial $\varrho=2.01$	38
3.17	first order shape function derivative distribution for a second order basis polynomial $\varrho=2.01$	38
3.18	second order shape function derivative distribution for a second order basis polynomial $\varrho=2.01\ldots\ldots\ldots\ldots$	38
3.19	shape function distribution for a third order basis polynomial $\varrho=3.01$	38
3.20	first order shape function derivative distribution for a third order basis polynomial $\rho = 3.01 \dots \dots \dots \dots \dots \dots \dots$	39

List of Figures V

3.21	second order shape function derivative distribution for a third order basis polynomial $\varrho=3.01\ldots\ldots\ldots\ldots$
3.22	shape function using a first order basis polynomial and a constant weight function for different ϱ
3.23	shape function using a first order basis polynomial and the C^3 weight function for different ϱ
3.24	first order shape function derivative using a first order basis polynomial and a constant weight function for different ϱ
3.25	first order shape function derivative using a first order basis polynomial and the C^3 weight function for different ϱ
3.26	shape function using a second order basis polynomial and a constant weight function for different ϱ
3.27	first order shape function derivative using a second order basis polynomial and a constant weight function for different ϱ
3.28	second order shape function derivative using a second order basis polynomial and a constant weight function for different ϱ
3.29	shape function using a third order basis polynomial and a constant weight function for different ϱ
3.30	first order shape function derivative using a third order basis polynomial and a constant weight function for different ϱ
3.31	second order shape function derivative using a third order basis polynomial and a constant weight function for different ϱ
3.32	shape function distribution for a zero order basis polynomial $\varrho=1.51$
3.33	first order shape function derivative distribution for a zero order basis polynomial $\varrho=1.51$
3.34	second order shape function derivative distribution for a zero order basis polynomial $\varrho=1.51$
3.35	shape function distribution for a first order basis polynomial $\varrho=1.75$
3.36	first order shape function derivative distribution for a first order basis polynomial $\varrho=1.75$
3.37	second order shape function derivative distribution for a first order basis polynomial $\varrho=1.75$
3.38	function based on a tenth-order polynomial
3.39	first order derivative of the function based on tenth-order polynomial
3.40	second order derivative of the function based on a tenth-order polynomial

VI List of Figures

3.41	nomial for various ϱ
3.42	MLS -approximation of the first order derivative of a tenth-order polynomial using a zero order basis polynomial for various ϱ
3.43	MLS-approximation of the second order derivative using a tenth-order polynomial using a zero order basis polynomial for various ϱ
3.44	MLS -approximation of a tenth-order polynomial using a first order basis polynomial for various ϱ
3.45	MLS-approximation of the first order derivative of a tenth-order polynomial using a first order basis polynomial for various ϱ
3.46	MLS -approximation of the second order derivative of a tenth-order polynomial using a first order basis polynomial for various ϱ
3.47	MLS -approximation of a tenth-order polynomial using a second order basis polynomial for various ϱ
3.48	MLS-approximation of the first order derivative of a tenth-order polynomial using a second order basis polynomial for various ϱ
3.49	MLS-approximation of the second order derivative using a tenth-order polynomial using a second order basis polynomial for various ϱ
3.50	MLS -approximation of a tenth-order polynomial using a third order basis polynomial for various ϱ
3.51	MLS-approximation of the first order derivative of a tenth-order polynomial using a third order basis polynomial for various ϱ
3.52	MLS -approximation of the second order derivative of a tenth-order polynomial using a third order basis polynomial for various ϱ
3.53	MLS-approximation of a tenth-order polynomial using a first order basis polynomial for various spline weight functions with $\varrho=2.51\ldots\ldots$
3.54	MLS-approximation of the first order derivative of a tenth-order polynomial using a first order basis polynomial for various spline weight functions with $\varrho=2.51$
3.55	MLS-approximation of the second order derivative using a tenth-order polynomial using a first order basis polynomial for various spline weight functions with $\varrho=2.51$
3.56	MLS-approximation of a tenth-order polynomial using a second order basis polynomial for various spline weight functions with $\varrho=3.01\ldots\ldots$
3.57	MLS-approximation of the first order derivative of a tenth-order polynomial using a second order basis polynomial for various spline weight functions with $\varrho=3.01$

List of Figures VII

3.58	MLS-approximation of the second order derivative using a tenth-order polynomial using a second order basis polynomial for various spline weight functions with $\varrho=3.01$
3.59	MLS-approximation of a tenth-order polynomial using a third order basis polynomial for various spline weight functions with $\varrho=3.51\ldots\ldots$ 49
3.60	MLS-approximation of the first order derivative of a tenth-order polynomial using a third order basis polynomial for various spline weight functions with $\varrho=3.51\ldots\ldots\ldots\ldots\ldots$
3.61	MLS-approximation of the second order derivative of a tenth-order polynomial using a third order basis polynomial for various spline weight functions with $\varrho=3.51$
4.1	problem definition
4.2	boundary enforcement
4.3	displacement diagram
4.4	deformed configuration at loading parameter $p = 30$
4.5	deformed configuration at loading parameter $p = 50$
4.6	problem definition
4.7	displacement diagram
4.8	deformed configuration at loading parameter 13.5×10^4
4.9	deformed configuration at loading parameter 69.0×10^4 67
4.10	problem definition
4.11	displacement diagram of the midpoint deflection - linear material 67
4.12	displacement diagram of the midpoint deflection - non-linear material 67
4.13	problem definition
4.14	displacement diagram
4.15	deformed configuration at loading parameter 8.78
4.16	deformed configuration at loading parameter 53.95
4.17	problem definition
4.18	displacement diagram
4.19	deformed configuration at loading parameter $0.015 \times 10^6 \dots 71$
4.20	deformed configuration at loading parameter $0.189 \times 10^6 \dots 71$
4.21	$problem\ definition\ \dots\ \dots\ \dots\ \dots\ 72$

VIII List of Figures

4.22	displacement diagram	72
4.23	deformed configuration at loading parameter 0.008×10^6	72
4.24	deformed configuration at loading parameter $0.439 \times 10^6 \dots \dots$	72
5.1	problem configuration	84
5.2	load displacement with diagram $l=21\mum$ and $\nu=0.3$	84
5.3	load displacement diagram with $l=25\mum$ and $\nu=0$	85
5.4	load displacement diagram with $l=25\mum$ and $\nu=0.3$	85
5.5	problem configuration	86
5.6	displacement diagram with displacement boundary conditions	86
5.7	displacement diagram with displacement boundary conditions	87
5.8	$displacement\ diagram\ with\ displacement\ and\ rotation\ boundary\ conditions\ .\ .$	87
5.9	$displacement\ diagram\ with\ displacement\ and\ rotation\ boundary\ conditions\ .\ .$	87
5.10	problem configuration	88
5.11	diagram: normalized torsion vs. cross-section size	88
5.12	diagram: normalized torsion vs. twist	89
6.1	load deflection diagram with $l_3=42\mum$ and $\nu=0.3$	103
6.2	load deflection diagram with $l_1=l_2=l_3=42~\mu$ m and $\nu=0.3~\dots~\dots~$	103
6.3	load deflection diagram with $l_3=42\mum$ and $\nu=0$	104
6.4	load deflection diagram with $l_1=l_2=l_3=42~\mu$ m and $\nu=0~\dots$	104
6.5	load-deflection diagram	105
6.6	load-deflection diagram	105
6.7	problem configuration	106
6.8	diagram: normalized torsion vs. cross-section size	106
6.9	diagram: normalized torsion vs. twist	106
6.10	problem definition	108
6.11	$maximum\ principal\ stress\ plotted\ along\ a\ line\ between\ point\ A\ and\ point\ B\ \ .$	108
6.12	$\ minimum\ principal\ stress\ plotted\ along\ a\ line\ between\ point\ A\ and\ point\ B .$	108
6.13	shear stress plotted along a line between point A and point B	108
6.14	absolute value of displacement vector - classical solution [m]	109

List of Figures IX

6.15	$absolute \ value \ of \ displacement \ vector \ - \ generalized \ solution \ with \ a \ two-dimensional \ micro-continuum \ [m] \ . \ . \ . \ . \ . \ . \ . \ . \ . \ $	109
6.16	max principal stress - classical solution [MPa]	109
6.17	$\begin{array}{llllllllllllllllllllllllllllllllllll$	109
6.18	min principal stress - classical solution [MPa]	110
6.19	$\begin{array}{llllllllllllllllllllllllllllllllllll$	110
6.20	plane shear stress - classical solution [MPa]	110
6.21	$\begin{array}{llllllllllllllllllllllllllllllllllll$	110
6.22	problem definition	111
6.23	maximum principal stress plotted along a line between point A and point B .	111
6.24	$\ minimum\ principal\ stress\ plotted\ along\ a\ line\ between\ point\ A\ and\ point\ B\ .$	111
6.25	shear stress plotted along a line between point A and point B	111
6.26	$absolute \ value \ of \ displacement \ vector \ - \ classical \ solution \ [m] . \ . \ . \ . \ . \ .$	112
6.27	$absolute \ value \ of \ displacement \ vector \ - \ generalized \ solution \ with \ a \ two-dimensional \ micro-continuum \ [m] \ \dots \ \dots \ \dots \ \dots \ \dots \ \dots$	112
6.28	max principal stress - classical solution [MPa]	112
6.29	$\begin{array}{llllllllllllllllllllllllllllllllllll$	112
6.30	min principal stress - classical solution [MPa]	113
6.31	$\begin{array}{llllllllllllllllllllllllllllllllllll$	113
6.32	plane shear stress - classical solution [MPa]	113
6.33	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	113
6.34	$absolute \ value \ of \ displacement \ vector \ - \ generalized \ solution \ with \ a \ one-dimensional \ micro-continuum \ [m] \ \dots \ \dots \ \dots \ \dots \ \dots \ \dots \ \dots$	114
6.35	$\begin{array}{llllllllllllllllllllllllllllllllllll$	114
6.36	min principal stress - generalized solutions with a one-dimensional micro- continuum [MPa]	114

X List of Figures

0.37	continuum [MPa]	11
6.38	problem definition	11
6.39	load displacement diagram with $l_1 = 4.2 \times 10^{-2}$	11
6.40	load deflection diagram with $l_1 = 4.2 \times 10^{-2}$	11
6.41	load displacement diagram with $l_2 = 4.2 \times 10^{-2}$	11
6.42	load deflection diagram with $l_2 = 4.2 \times 10^{-2}$	11
6.43	deformed configuration at loading parameter $q=3.3$ with $l_1=4.2\times 10^{-2}$	11
6.44	deformed configuration at loading parameter $q=3.3$ with $l_2=4.2\times 10^{-2}$	11
6.45	problem definition	12
6.46	deformed configuration at loading parameter $83.41mN/mm^2$ with $l_1=21\mum$	12
6.47	deformed configuration at loading parameter $83.41mN/mm^2$ with $l_2=21\mum$	12
6.48	deformed configuration at loading parameter 231.83 mN/mm ² with $l_1=21~\mu$ m and $l_2=21~\mu$ m	12
6.49	load displacement diagram with $l_1=21\mum$	12
6.50	load deflection diagram with $l_1=21\mum$	12
6.51	load displacement diagram with $l_2=21\mum$	12
6.52	load deflection diagram with $l_2=21\mum$	12
6.53	load displacement diagram with $l_1=21\mum$ and $l_2=21\mum$	12
6.54	load deflection diagram with $l_1=21\mum$ and $l_2=21\mum$	12
7.1	problem configuration	13
7.2	problem configuration	13
7.3	$deformed\ configuration\ \dots\dots\dots\dots\dots\dots\dots\dots\dots$	13
7.4	$deformed\ configuration\ \dots\dots\dots\dots\dots\dots\dots\dots$	13
A.1	C^3 quartic spline $\Phi = w w \dots \dots \dots \dots \dots \dots \dots$	1
A.2	first order derivative of the C^3 quartic spline $\Phi_{,y} = \frac{1}{\varrho} w w_{,y} \dots \dots$	14
	second order derivative of the C^3 quartic spline $\Phi_{,xy} = \frac{1}{\varrho^2} w_{,x} w_{,y} \dots \dots$	
	second order derivative of the C^3 quartic spline $\Phi_{,yy} = \frac{1}{\varrho^2} w w_{,yy}$	
B.1	particles support across the partition boundary	15

List of Tables

3.1	$particle\ support$	distribution	for	$various \ arrho$																		4	6
-----	---------------------	--------------	-----	-------------------	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	---	---

Notation and list of symbols

In the following the general scheme of notation and list of frequently used symbols are assembled:

Further notations are explained as they appear in the thesis. The used operations and relations of tensor calculus are specified in App. D.