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**Three-dimensional Fold Geometry and Folding:
Deformation Scale and Spectral Curvature
Computational Methods**



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David Nathan

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School of Earth Sciences

Supervisors:

Prof. Eun-Jung Holden (Coordinating)

Dr. Daniel Wedge

Dr. Mario Zelic

Abstract

Geological structural analysis requires the description of rock volumes and the identification of their spatial extent with respect to their deformation history. Thus, the development of terminology and geometric descriptions of structures that are commensurate with the deformation process are essential. The interaction of geological structures at multiple scales though can also results in three-dimensional geometries that appear more complex. For continuous structures (i.e., folds and ductile shear zones), the use of scale-dependent geometric descriptors such as thickness variation or shear band width/displacement rather than orientation measurements that are scale-independent, can often be used as the basis for kinematic and dynamic analysis but are not always utilised in a consistent manner to constrain geometry in modelling.

This thesis comprises a body of work that investigates the multi-scale geometric characterisation of three-dimensional geological surfaces using manifold harmonics together with the development of methods for deformation statistics. This provides for a better understanding of three-dimensional finite strain as it relates to geodynamic models of multi-layer viscous folding and contact surface curvature. Geometric multi-scale curvature methods are developed and applied specifically to the interpretation of a progressively deformed multi-layer fold system. These types of fold systems will often have complex non-cylindrical geometries of varying scale and congruity, which are rheologically controlled by the layer-parallel contrast in competency. The fold system model is developed for a poly-clinal regional syncline in the south-eastern Hamersley province of Western Australia using field measurements of bedding orientation and bedding contact trace points from outcrop. These measurements are subsequently interpolated using an implicit modelling approach. The analysis demonstrates how the asymmetry in the fold intensity between the northern and southern limb, can be understood as a result of buckling from hinge-lockup as the synclinal hinge progressively rotates.

A multi-layer viscous buckling numerical model is then developed to demonstrate how the manifold statistics of a set of passive finite strain markers can be used to test models of heterogeneous deformation zone development and three-dimensional finite strain partitions. A finite difference numerical model on a staggered grid is used to solve the three-dimensional thermo-mechanical equations of motion. Four models are examined with a variety of velocity boundary conditions to simulate different tectonic settings including: (1) a thick-skinned compressional/pure shear model with free slip base, (2) a thin-skinned compressional/pure shear model with no slip base, (3) a strike-slip/simple shear model, and (4) a combined transpressional/pure and simple shear model. These deformation regions are partitioned and compared using their kinematic vorticity and strain ellipsoid spheroid shape. The topology of these deformation regions is then analysed to highlight dilational and contractional pathways. This provides important insights into how curvature together with field observations of strain can be utilised to understand the three-dimensional geometry

of strain pathways, which subsequently can be used to narrow the spatial extent of targets that occur due to structure-enhanced permeability and other localised features coupled with ductile flow.

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The mountains melt like wax (*ductile*) before the LORD,
before the Lord of all the earth
— *Psalms 97.5*

Mountains are to the rest of the body of the earth, what violent muscular action is to the body of man. The muscles and tendons of its anatomy are, in the mountain, brought out with force and convulsive energy, full of expression, passion, and strength.

— *John Ruskin, Modern Painters, Of Mountain Beauty (1860)*

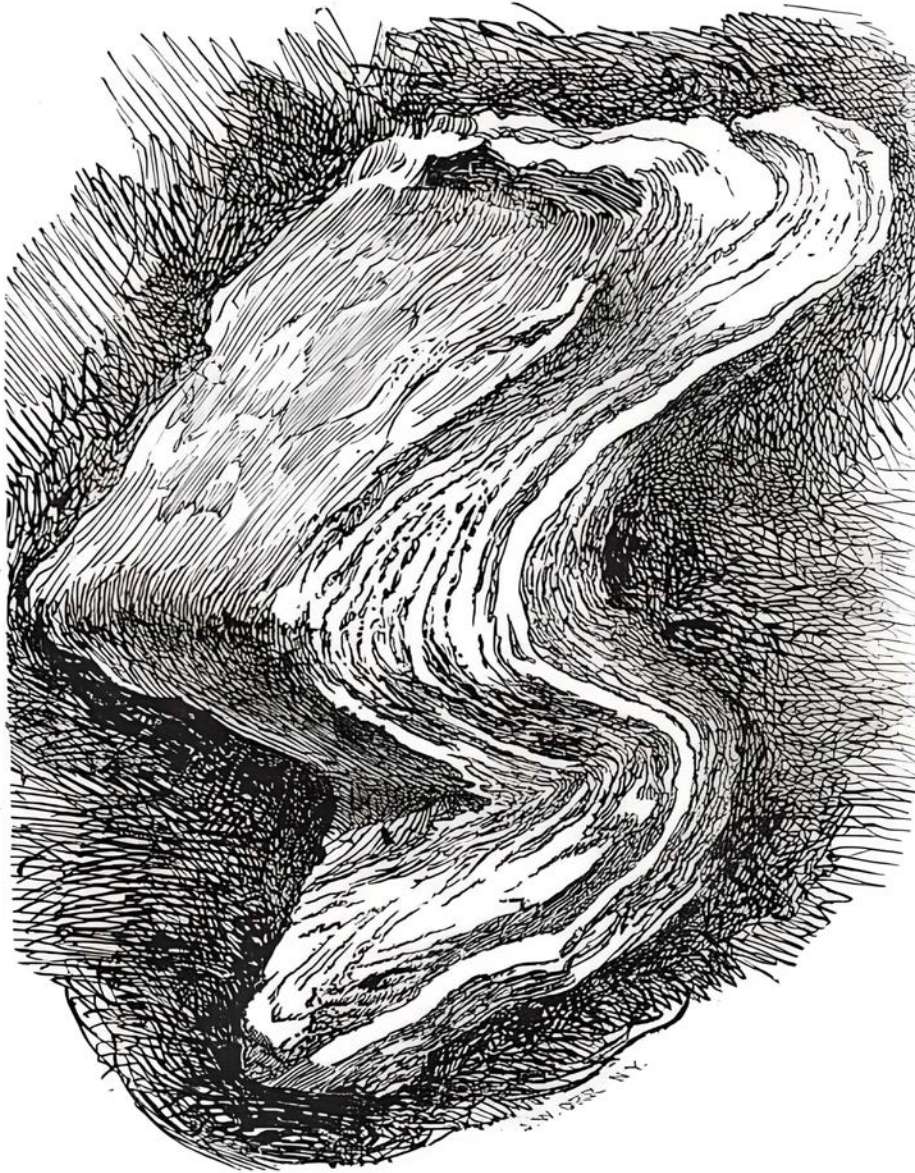


Figure 1: A piece of the gneiss of the Montanvert, near the Châlets of Blaitière dessous. — *Of Mountain Beauty*, John Ruskin (https://www.gutenberg.org/files/31623/31623-h/31623-h.htm#FnAnchor_46).

Declaration of Authorship

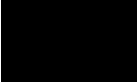
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 Date: 02/05/2022

Student signature:  Date: 04/05/2022

I, Eun-Jung Holden certify that the student's statements regarding their contribution to each of the works listed above are correct.

As all co-authors' signatures could not be obtained, I hereby authorise inclusion of the co-authored work in the thesis.

Coordinating supervisor signature:  Date: 02/05/2022

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Chapter 1

Introduction

1.1 Fold Geometry and Folding

Folds are one of the most common types of geological structures found in nature and occur in many different environments and tectonic settings [67]. The size of folds can also vary significantly from the micro-scale to the lithospheric-scale [72], and in the case of layer-parallel shortening of stratified rock, can also occur across scales [7; 63]. This relationship between different scales of folding provides important constraints in exploration for predicting hydrocarbon traps [53] and mineralization [4; 21], as well as geological modelling, resource development, and engineering problems such as the stability of open pits or underground excavations [38; 76] and groundwater flow [43]. Thus, descriptions of these features as they relate to the scales of deformation are essential for interpretation and three-dimensional modelling.

The description of structures can be inhibited though by uncertainty in how they are formed. When considering how the geometry of folds can produce uncertainty, Carreras and Druguet [10] provide a helpful overview of *intrinsic factors*, which are related to more localised/rheological complexity, and *extrinsic factors*, which are more global factors related to the deformation flow field and temporal evolution (Figure 1.1). While intrinsic factors have often been the focus of much fold research through analogue modelling and plane strain assumptions [37], the coupling of extrinsic factors with the intrinsic often results in larger scale geometric uncertainty. Even though recent advances in X-ray computed tomography present the ability to directly observe 3D finite strain [70], 3D thermo-mechanical numerical modelling is widely available and allows the direct interrogation of a flow field for finite strain analysis.

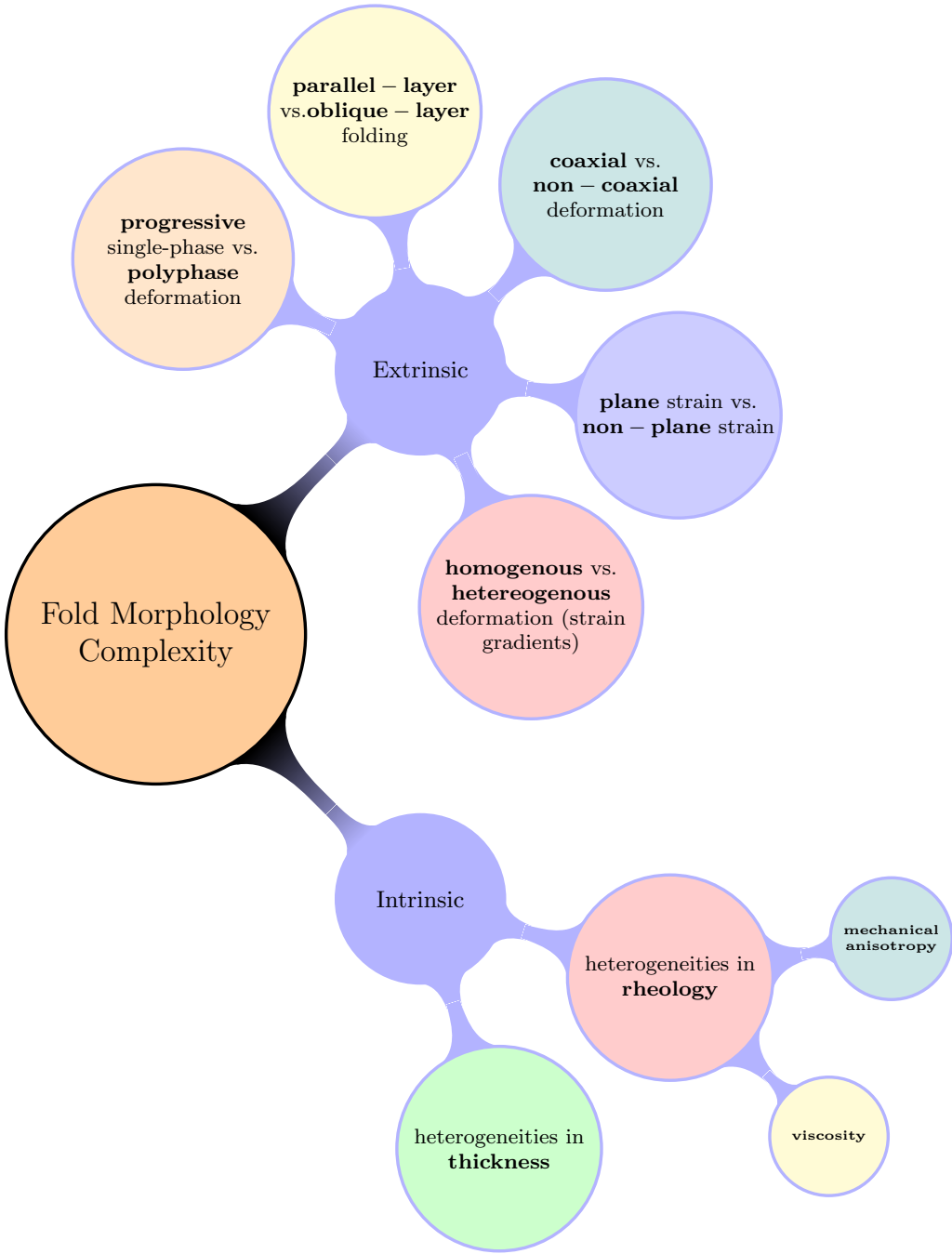


Figure 1.1: Factors related to the complexity of fold morphology based on Carreras and Druguet [10].

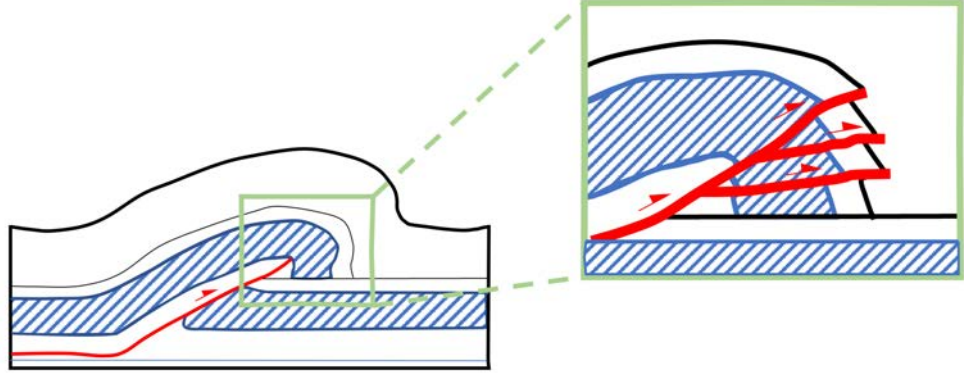


Figure 1.2: Example of the scale-dependent nature of ductile deformation styles illustrated by a fault-bend fold where the front-limb of the anticline at a larger scale is observed as a ductile structure while at a smaller scale is observed to be multiple small-displacement thrust faults. These thrust faults can be interpreted to have developed to accommodate the forward shear of the front limb in the late stages of folding [54].

1.2 Scale

While these factors will result in uncertainty in subsurface geometry, they often can be mitigated by considering observations at multiple scales. Hence, collecting and correlating data across scales is standard practice in field geology [19; 49]. The practice of observing structures and indicators at a small scale to constrain crustal scale processes is an active area of research and important tool in tectonic studies [57; 89]. In particular, continuous geological structures, such as folds and shear zones, can preserve geometric characteristics across scales, i.e. the orientation of hinge lines and fold axial surfaces [23], but it is also important to consider the scale of observation, particularly when it is used as the basis for understanding deformation. The value of comparing scale-dependent geometric descriptions, rather than scale-independent measures such as orientation, is illustrated in Figure 1.2. This shows where the distinction between brittle and ductile deformation mechanisms is ambiguous based on the structure at the larger scale. But when we observe the asymmetry, hinge curvature and thickness variation along the fault-bend fold, we can interpret that the forelimb geometry is a result of late stage folding rather than syn-kinematic buckling or imbrication.

Another important consideration for the multi-scale development of structures is the nature and growth of different types of instabilities [9; 14; 15; 59; 60; 68]. The nature of strain localisation is a result of non-equilibrium dynamics [9] and results in strain partitioning (Figure 1.3b and Figure 1.3c). While localisation is often approached through material softening/hardening [34] and/or thermal instability [32], for rocks with strong mechanical anisotropy, banded perturbations under non-coaxial flow produce localised superposed structures too [9; 15]. In terms of the development of curvature along contrasting viscosity layers we consider this a property of geometric scale and isothermal perturbation. Thus I assume purely geometric instabilities within a fluid dynamic evolution in this thesis. The behaviour of localised deformation can then be constrained to geometric perturbations,

rather than thermal instabilities which can otherwise be formulated in terms of energy bifurcations that produce localised phenomena [59].

1.3 3D Fold Geometry and Modelling

The consideration of scale and ductile structure though has important and practical implications in understanding subsurface geology and find industry relevance in geological resource modelling. The application of 3D geological models for resource estimation and engineering risk management requires that it being continually updated when new data becomes available [87]. Objective measures of qualifying a model as being structurally complex to constrain sources of uncertainty then become important when assessing the relative merits between models. For example, this could be when comparing the model feasibility of introducing detachment folds or out-of-syncline faults [18]. Approaches to measuring structural complexity in 3D geological models though currently use connectivity and topology as the only geometric elements [58]. This does not incorporate elements such as surface curvature which are important for the structural complexity that arise from fold scale [48; 71].

The description of fold geometries commonly assumes either a cylindrical or conical model [88]. These models are advantageous since the orientations of folds can be fully described by their fold axis direction and hinge plunge, and are able to be analysed using β and α diagrams [84]. Nonetheless, the assumption of cylindricity can give a false impression of the geometry for non-cylindrical folding [64]. In particular, every fold can be considered as non-cylindrical at some scale since it cannot extend infinitely along its axis [25; 88]. Examples of this are shown in Figure 1.3.

The multi-scale feature of fold systems has long been observed and the practice of using the style and attitudes of minor folds (or parasitic folds) to constrain the geometry of major folds is common in geological mapping and structural analysis and interpretation [61]. Moreover, the development of the analytical theory of viscous folding [7; 62] has allowed the study of fold systems to be applied across many scales from the microscale to the lithospheric and continental [37; 72]. The behaviour of natural fold systems though is complex and can result in localized non-periodic folding where the relationship between scales is chaotic and difficult to decompose [33; 56]. This presents challenges when integrating multi-scale observations since fold geometries constructed from orientation measurements of structural features will often have some scale-dependence [78]. Moreover, the precise relationship between fold scales in parasitic folding can only be calculated analytically if a viscosity ratio is large enough that a fold train will behave as an effective thicker layer so that larger wavelengths will develop [83]. This also requires specific rheological assumptions about when and where buckling instabilities may emerge as a result of changes in ambient temperature or layer thickness during the folding process [27], or the degree of matrix anisotropy [42]. The number and degree of these assumptions makes the inverse modelling and prediction of fold scales prohibitively difficult for most applications. Moreover, the ambiguity of *extrinsic* factors in the regional deformation that often effects localised folding



(a) Non-cylindrical multi-layer fold system of metasediments and quartz from Bremer Bay, Albany-Fraser shear zone. The metasediments shows similar folding [65] characterised by thickening of the hinge areas and thinning of the limbs.



(b) Strain partitioning in 3D within folded gneiss from Bremer Bay, Albany-Fraser shear zone. The gneiss is characterised by devolvement of foliation which is tightly to isoclinally folded.



(c) Strain partitioning due to rheological heterogeneity/mechanical anisotropy in banded iron formation from Meekatharra area, Yilgarn Craton, Western Australia (Quinns District).

Figure 1.3: Field example of a non-cylindrical fold system and strain partitioning from the Albany-Fraser shear zone and the Meekatharra area, Yilgarn Craton. Courtesy of Chris Gonzalez and Mario Zelic.

through strain partitioning means the use systematic use of fold geometry challenging to interpret rheology in field studies [11; 30; 35].

The study of non-cylindrical geological surfaces and superposed structures that result from tectonic, sedimentary, or geomorphological processes has meant that scale-based descriptions using wavelength and amplitude have been developed and applied [31; 65; 81]. However, the complex nature of multiscale tectonic structures that result from progressive and multiphase deformation [10; 24; 26] means that common geometric fold classification schemes cannot be applied for characterizing across scales [2; 29; 82].

An alternative description of folded surfaces that can describe non-cylindrical geometrics and are able to directly characterize multi-scale surface features have come from curvature analysis [45; 46; 69]. While different approaches to calculating surface curvature have been proposed [6; 46], the differential coordinates (dx , dy , dz) used for calculations will often use a regular grid or offset nodes. These use calculations of the principal curvatures along with the Gaussian and mean curvature (see Figure 2.5 for illustration) to describe geological surfaces [45]. This importantly is only cylindrical when the Gaussian curvature is 0. These curvature measures are often applied to 3D data such as 3D subsurface seismic horizons or outcrops using photogrammetry or lidar data [1; 80]. Moreover, these curvature measures have kinematic implications in terms of flexural folding and isometric bending [45; 90]. They can also be used as criteria for targeting in the exploration of sedimentary-hosted stratiform mineral deposits [50] and fracturing in hydrocarbon traps [3].

It is important to note that surface curvature is not a quantitative calculation of strain since it does not take into account either the strain distribution within layers, nor the strain parallel to a surface [5; 20; 28]. This means that while curvature analysis as an indicator for predicting deformation is generally accepted it cannot always be used to estimate fracture densities [5; 12], or for strain indications for small fault-dip in fault-related folding [41]. Nevertheless, at the scale of seismic resolution, curvature is often an effective way to highlight small-displacement faults [80]. The application of curvature analysis for regional geological modelling has been used for uncertainty quantification of geometries [44] but

not in deformation modelling.

Early approaches to the scale analysis of folds used harmonic series, specifically Fourier analysis to characterise fold shapes by wavelength and amplitude [36; 67; 75]. This scale analysis is only applied for folds with defined axial planes and so is only possible for cylindrical folds in two-dimensions. Conversely, some multi-scale 3D curvature approaches for extracting structures include 2D Fourier and wavelet decomposition [6; 79; 81], wavelet scale space analysis [81], low-pass filters [6], and variable grid offsets when calculating curvature [77; 80; 90].

The curvature properties of geological surface can be calculated differently when applied to geological modelling and triangulated meshes by applying advances in discrete differential geometry from the fields of geometry processing and mathematics [16]. A fundamental approach in this field is the discretization of the Laplacian by using differential coordinate properties that allow kinematic equations to be numerically solved for deformation. In geometry processing and deformation modelling for arbitrary meshes, the discretization of the Laplacian has developed to allow fast real-time deformation for geometry modelling [8]. The formulation of the discretization uses finite element/finite volumes methods by considering a mesh surface as consisting of 3D elements with appropriate differential coordinates, which then allows the reconstruction of surfaces by scale in a similar manner to linear stability analysis [85]. Thus, a measure of structural complexity can be derived as variability in curvature across scales.

I present a case-study of a structural model for a regional syncline in the eastern Hamersley province (Figure 5.1) to demonstrate how surface complexity can be calculated using harmonic curvature analysis. Given 1:5000 surface mapping and observed surface bedding measurements, a model is developed to generate an implicit geological model using universal Co-Kriging [17]. The surface of the base contact interpolated from the lithology block model is then extracted by taking an isocontour of the scalar field. An isotropic triangular remeshing scheme is then applied to generate a mesh of sufficient quality in terms of triangle aspect ratio for curvature analysis [40]. This surface is then used as the basis from which the discrete Laplacian matrices are calculated [51]. Eigenspaces for the resulting Laplacian curvature, related to the mean curvature normal, for a study area are interpreted for the syncline to demonstrate some of the possible folding deformation mechanisms observed, and anomalous/uncertain curvature regions that can be further used, for example in targeting and drill hole planning.

The validity of the geometric measures that are developed are compared using three-dimensional geodynamic computational modelling of viscous folding. Often times criticisms of numerical models are that the experiments are too complex or that the variables to understand geological processes have too large a range of values. My aim here is to connect the structural observations of the region as well as the geometrical multi-scale curvature analysis in a holistic view that incorporates 3D mechanics, which is otherwise unused together in the literature. This allows me to test how interacting 3D folding can either confirm hypothesis in an area with regards to deformation history. An application of this

may be in understanding the mechanics of general features existing in saddle reef deposits [74; 86].

In this thesis I develop the first results of 3D curvature analysis from geodynamic numerical modelling with respect to global velocity boundary conditions. While Fernandez and Kaus [22] apply curvature analysis to their surface topography evolution, the mechanical stratigraphy used is specific to salt-detachment tectonics of the Zagros Fold-Thrust-Belt. Instead, I consider how a mixture of different velocity boundary conditions which can be considered as global plate velocities may have different effects on localised curvature on confined competent layers within a sequence.

Moreover, I present the first comparison of geological curvature and 3D finite strain development during deformation. While other studies have considered the relationship between curvature and strain, limitations such as assume flexural slip restoration [73] or use 2D strain markers on the curved surface [41] rather than 3D. This is critical when relating mesoscopic field observations to macroscopic curvature structures.

I introduce the novel application of computational methods to analyse the scale-dependence of strain partitioning using supervoxel methods. Strain partitioning has a significant impact for interpreting kinematics in the field [35; 47]. While strain partitioning is traditionally applied to micro-structure deformation mechanisms such as distinguishing between cataclasis and crystal plasticity [66], there are few field studies that validate macroscopic strain partitioning with the microscopic, a notable exception being the study of Mitra [52] which validates the classic study of Cloos [13]. Moreover, the degree of partitioning within the deformation is often more pronounced when rocks are rheologically heterogeneous and/or mechanically anisotropic [11]. By using the methods I have developed in this thesis, the ability of quantitatively demonstrating how regional scale deformation effects the degree of strain partitioning is shown for the first time.

1.4 Thesis Objectives

A major objective of this thesis is the development of multi-scale methods that can be applied to understanding ductile deformation styles. This is approached from both a purely geometric formulation as well as continuum mechanics. These methods attempt to bridge a gap between fold geometry kinematics and computational geodynamics. This is particularly addressed in terms of 3D geometry and how the developed structural analysis methods have implications for geological modelling.

Lastly, a suite of analytical computer programs have been developed that can be used to investigate thesis problems within exploration and scientific frameworks. The geometry processing algorithms including manifold harmonic transform and principal curvature were implemented using the open-source library `libigl`¹ [39] and MATLAB. The finite strain and deformation scale processing were all implemented in MATLAB. The reading of the geodynamic model output and saving of the processed meshes used the `meshio`² library.

¹<https://github.com/libigl/libigl/>

²<https://github.com/nschloe/meshio>

1.5 Thesis Structure

The main objective of developing multi-scale curvature measures as it relates to ductile deformation is summarised in the following sections. The chapters of the thesis are derived from one publication and further work that is related to it. The chapters *Geometric Scale*, *Case Study: Padtherung Syncline* and part of *Numerical Modelling* are based on the publication, while *Deformation Scale* and majority of *Numerical Modelling* are separate.

1.5.1 Chapter 2 - *Geometric Scale*

In this chapter, I present an overview of fold geometry terminology and concepts as it relates to curvature, and develop the technique of multi-scale curvature. This involves the mathematical approach to triangulated meshes and how the discretization of the Laplacian operator efficiently computed.

1.5.2 Chapter 3 - *Deformation Scale*

Background of deformation concepts used in structural geology and numerical modelling of mechanics are outlined in this chapter. I then develop some of the computational methods used for deformation statistics that can be applied to flow fields, including positive-definite manifolds statistics and supervoxel segmentation based on kinematic vorticity and finite strain ellipsoid shape.

1.5.3 Chapter 4 - *Numerical Modelling*

The results for the 3D synthetic geometric scale and mechanical numerical model are presented this chapter. This demonstrates how structural complexity using multi-scale curvature and the cosine distance sum is concentrated across fold limbs rather than hinges where the principal curvatures are maximal. Moreover, the supervoxel method applied to finite deformation demonstrates the numerical properties of strain partitioning when comparing pure shear/compression and transpression.

1.5.4 Chapter 5 - *Case Study: Padtherung Syncline*

The development of a 3D implicit model is presented for a regional syncline in the Eastern Hamersley province, Western Australia. This 3D model is basis for the application of the multi-scale curvature method. The background geology is presented and the mapping data used is described. Moreover, a kinematic model of progressive hinge rotation and lock-up is confirmed by the curvature analysis.

1.6 Statement of candidature

1.6.1 Summary declaration

I, David Nathan, certify that:

This thesis has been substantially accomplished during enrolment in this degree. This thesis does not contain material which has been submitted for the award of any other degree or diploma in my name, in any university or other tertiary institution. In the future, no part of this thesis will be used in a submission in my name, for any other degree or diploma in any university or other tertiary institution without the prior approval of The University of Western Australia and where applicable, any partner institution responsible for the joint-award of this degree. This thesis does not contain any material previously published or written by another person, except where due reference has been made in the text. This thesis does not violate or infringe any copyright, trademark, patent, or other rights whatsoever of any person.

This thesis contains published work and/or work prepared for publication, some of which has been co-authored.

Signature: Date: 04/05/2022

1.6.2 Bibliographical details of publications and abstracts arising from this thesis

Publications

- D. Nathan, M. Zelic, E.-J. Holden, and D. Wedge. Deformation scale using harmonic curvature analysis: A case study from the Hamersley Province. *Journal of Structural Geology*, 146:104302, May 2021. ISSN 0191-8141. doi: 10.1016/j.jsg.2021.104302

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Chapter 2

Geometric Scale

2.1 Introduction

The development of terminology and measures of folds has coincided with the understanding of the kinematic processes that produce them [11; 29; 31]. In this chapter a review of the definitions of fold geometry and curvature is presented, followed by the theory of multi-scale curvature that is developed and applied to geological surfaces in subsequent chapters.

2.2 Definitions

2.2.1 Fold Geometry

The scope of potential structures that can be included under the description of geological fold is quite broad since it implies a process of deformation so that the terminology around their geometry and orientation has changed overtime [11]. In that sense, it is more straightforward to define *folding*, which is the deformation of planes, surfaces, or aligned linear elements into curvilinear or curvilinear configurations [17]. Hence, the preferred definition used in this thesis is from [29] which combines the two so that folds are defined as:

"curvilinear structures that form by transformation of any tectonic or primary foliation into curved geometries through a non-linear transformation".

The geometric description of folds as they relate to kinematics is therefore key and forms an important motivation for the application of surface curvature measures [1]. I outline some fold geometry definitions that are illustrated in Figure 2.2 relevant to our methods and present examples of folds from the Hamersley province, Western Australia in Figure 2.1.

The *hinge curve* on a folded surface is made up of the points of maximum curvature. A single fold can have more than one hinge and the hinge curve may or may not be linear Figure 2.3. A cylindrical fold is one where the hinge curve is linear and is called the *fold axis*. A surface is defined as a *ruled surface* when every point that lies on the surface has a line passing through it that lies on the surface too. These lines are called the *generators* of

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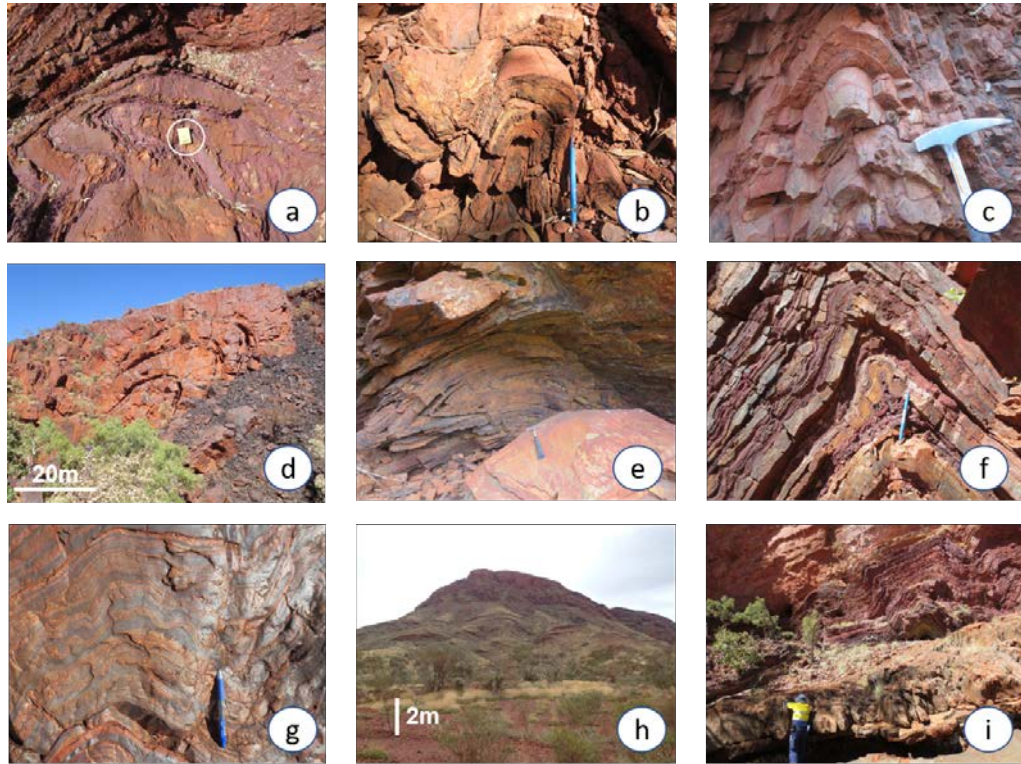


Figure 2.1: Examples from Hamersley Province, Western Australia of (a) non-cylindrical, (b) cylindrical and (c) conical fold. (d) Typical occurrence of Ophthalmia fold, north vergent; East Hamersley Province. (e) Example of fold interference pattern or apparent fold interference structures as a result of progressive deformation during Ophthalmia Orogeny. Cathedral Gorge, Eastern Hamersley Province. (f-h) Folding style in the Hamersley Province, Pilbara, Western Australia is related to the rheology, layer/layer packages thickness, competency and viscosity contrast. Examples from West Hamersley Province. (i) Detachment fault within the Wittenoom Formation: Folded chert, BIF and shale in the fault hangingwall, non-folded dolomite and sandstone in the fault footwall, West Hamersley Province.

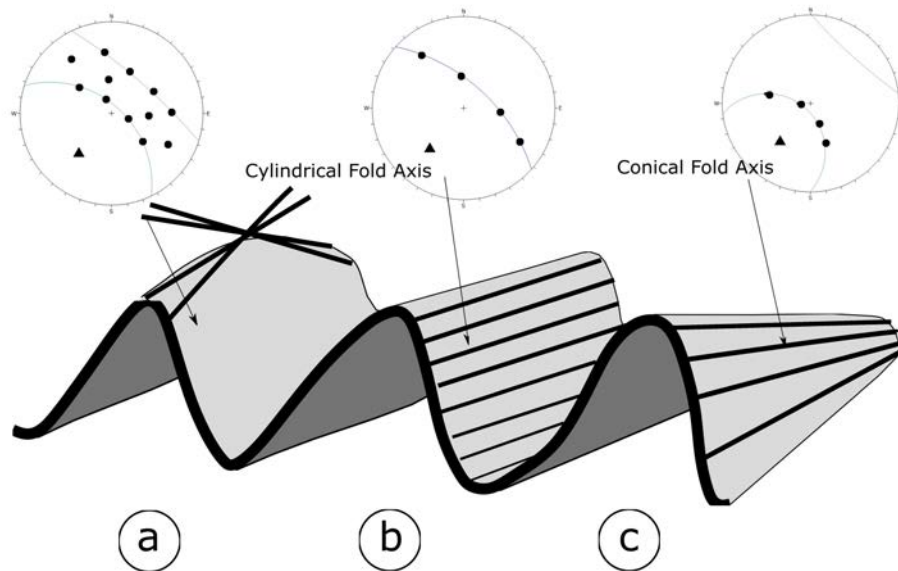


Figure 2.2: Examples of (a) non-cylindrical, (b) cylindrical and (c) conical fold. Cylindrical and conical folds are ruled surfaces while non-cylindrical folds are not. Circles represent bedding poles while triangles are fold axis.

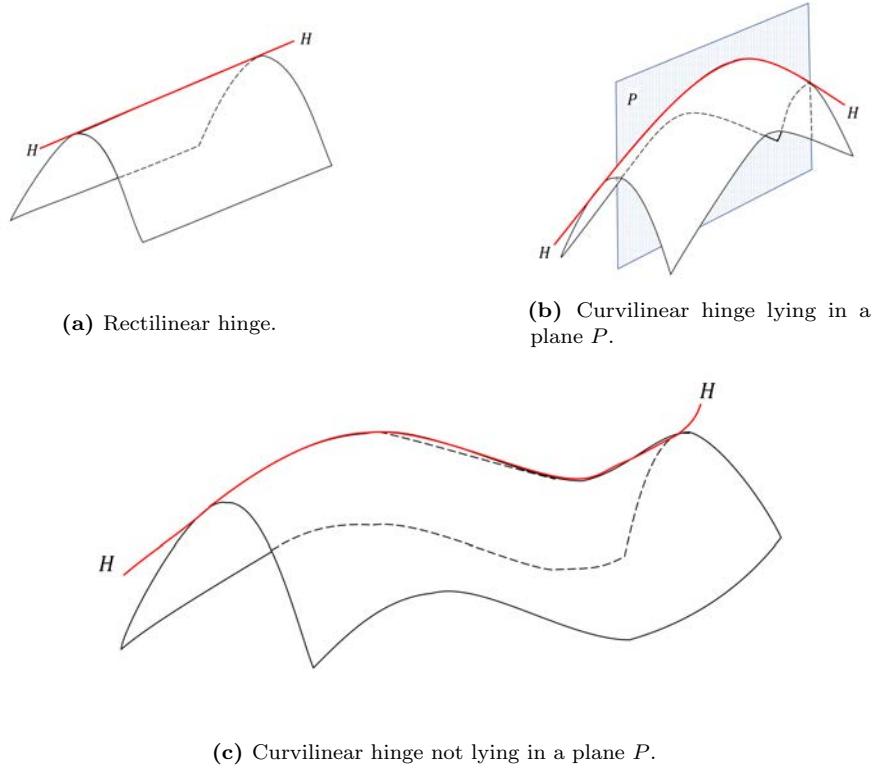


Figure 2.3: Hinges H of folds based on Turner and Weiss [35].

the surface. A fold axis can be considered as a generator of a cylindrical fold, since the line can move parallel across the surface of the fold. If no single generator line exists for the surface, the fold is considered non-cylindrical.

While the hinge curve is defined physically across a fold and thus has a specific orientation and location, importantly, the fold axis is defined geometrically, so that it does not necessarily have a specific location on a folded surface. A *conical fold* is a noncylindrical fold where the generator lines along the surface converge to a point. The orientation of the line passing through this point is used to define the fold axis of a conical fold [37].

The geometry of folds have thus been classified according to the planarity of the axial surface and the cylindricity of the folded surface Figure 2.4.

2.2.2 Surface Curvature

For a given point on a folded surface, we can also define the *normal curvature* $\kappa_n(\varphi)$ for a specific direction φ , by considering the curve γ defined as the intersection of the surface with the plane that is the linear span of $\mathbf{t}$ in the given direction. When this is evaluated in all directions, it can be shown that there are two extreme values which are called the *principal curvatures* $\mathbf{p}_u$ and $\mathbf{p}_v$ [4]. These correspond to the *maximum curvature* κ_1 and the *minimum curvature* κ_2 . If $\kappa_1 \neq \kappa_2$, then there are two principal directions that correspond to the principal curvatures, otherwise the point is considered locally spherical or planar [4].

Other measures of surface curvature that can be considered are the *mean curvature*

2. GEOMETRIC SCALE

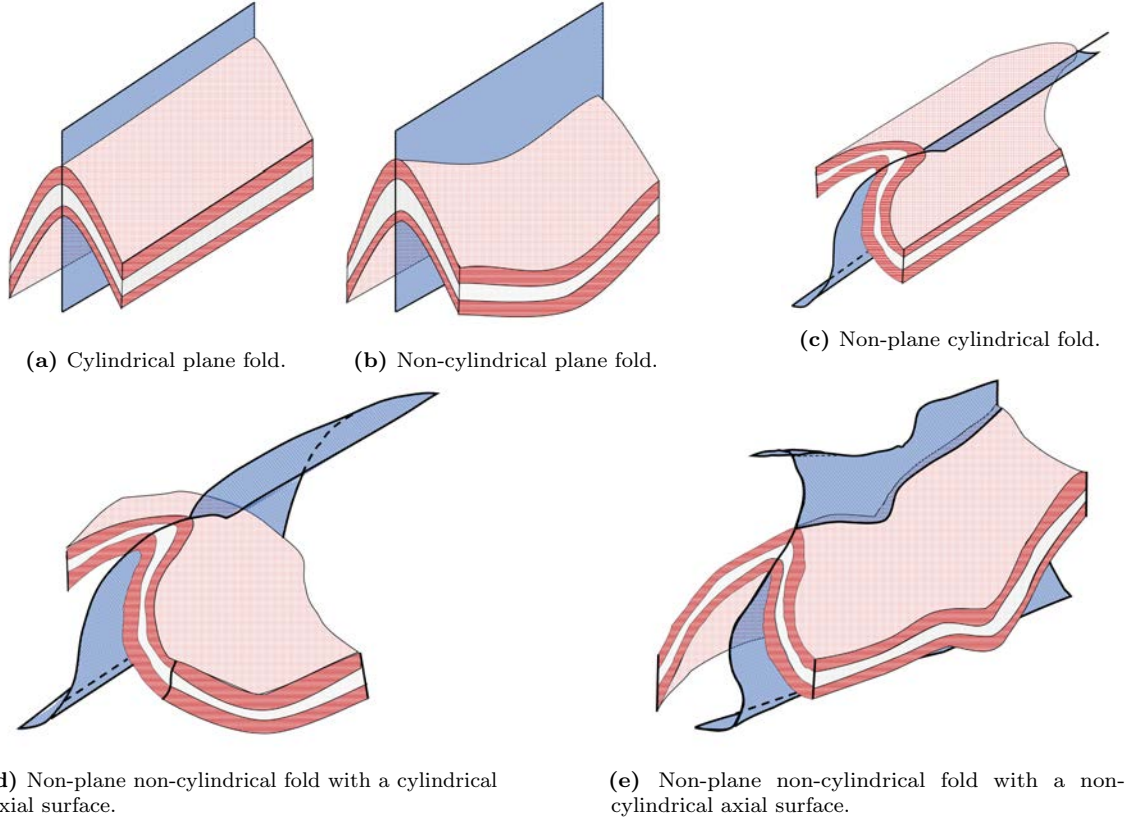


Figure 2.4: Fold descriptions based on the cylindricity of the surface and the planarity of the axial surface. Based on Turner and Weiss [35].

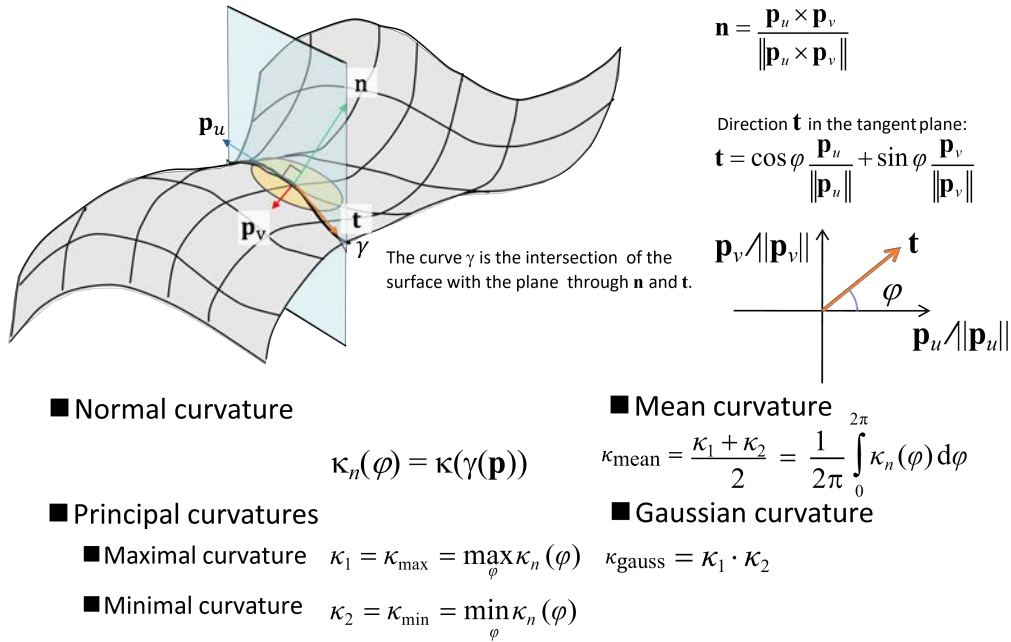


Figure 2.5: The definition and derivation of different surface curvature measures. Here $\mathbf{n}$ is the surface normal at a particular point, $\mathbf{t}$ is the tangent to the surface, $\mathbf{p}_u$ is the maximum principal curvature direction, and $\mathbf{p}_v$ is the minimum principal curvature direction.

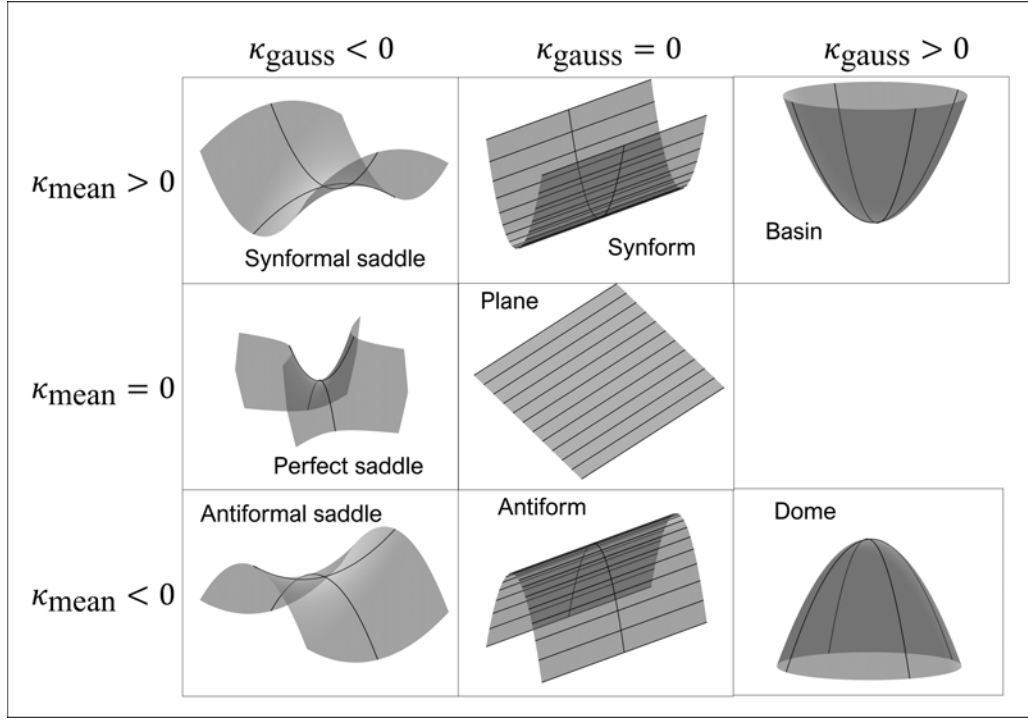


Figure 2.6: Geological curvature classification based on Gaussian κ_{gauss} and Mean κ_{mean} curvature [28].

κ_{mean} and *Gaussian curvature* κ_{gauss} [30]. The mean curvature is defined as the average of the two principal curvatures and so can be considered as the magnitude of curvature locally. Gaussian curvature is defined as the product of the two principal curvatures so that points can be considered as locally saddle-shaped ($\kappa_{\text{gauss}} < 0$) or locally dome/basin shaped ($\kappa_{\text{gauss}} > 0$) [30]. These two measures have been used to classify the curvature of points on folded surfaces which is termed *geological curvature* [23; 28].

2.3 Methods

Approaches used in geostatistics for structural modelling are first introduced as a geometric approach to produce surfaces of geological interfaces. I then introduce the manifold harmonic curvature analysis method by first outlining the Laplacian operator's connection to surface curvature, then presenting the spectral properties of the mesh Laplacian as 1D contour smoothing. Lastly, the cotangent mesh Laplacian is outlined.

2.3.1 Implicit Geological Modelling

The recent advances in geological interpolation algorithms [3; 6; 13; 14; 24] has meant that the development of realistic 3D geological models algorithms is routine practice in resource and geology [16]. These algorithms are often described as implicit methods which treats geological surfaces as equipotential contours within a scalar field, which is visualized in Figure 2.7 [3; 7; 18]. Implicit model methods can be very useful for structural modelling as they can directly enforce geometric validity criteria for a conformable sequence of surfaces

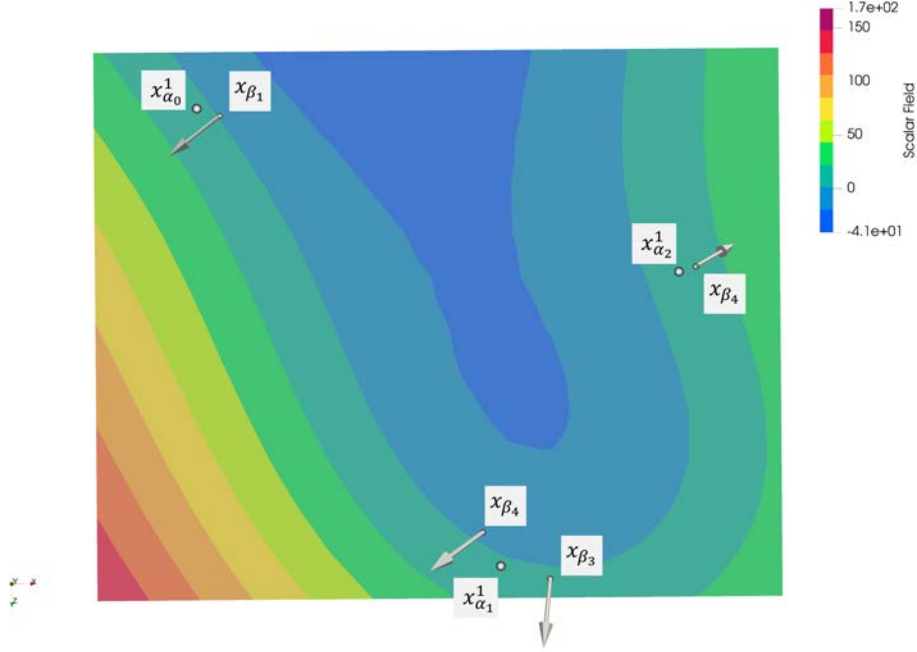


Figure 2.7: An example of a scalar field interpolation, using three layer interface points x_{α} and four orientation x_{β} [14]. The isocontours connect the interface points and the scalar field is perpendicular to the orientation points.

[16], as well as foliation and axial surface fields [18; 19; 25]. The representation of the scalar field and the interpolation can be separated into two approaches: (1) polynomial trend approaches and (2) discrete interpolation approaches. Polynomial trend approaches model the trend using the orientation data field and model the residual using either a co-Kriging system between the orientation field and interface field [7; 10] or by using a set of radial basis function weights [9; 14]. Discrete implicit methods instead represent surfaces as isocontours of a piecewise linear scalar field that is interpolated within a coarse 3D element that can be progressively refined [5; 6; 12].

2.3.2 Manifold Harmonics

Manifold Harmonics and Fold Scale

A common technique of analysing fold geometries is Fourier analysis, which approximates shapes as the sum of sine and cosine functions [15; 32]. These analysis though are limited to the 2D analysis of the fold curvature, which led to surface curvature attributes for describing fold curvature in three-dimensions [23; 28]. While classifications based on curvature provide a means to quantify fold geometry without the any assumption of cylindricity, they do not naturally quantify the periodicity of surfaces within a fold system and therefore the scale.

Surface Curvature from Laplacian While there are many geometric properties that are related to curvature, the Laplacian quantity when applied to a surface is an efficient and convenient measure. The *Laplacian operator* (Δ) is a second-order differential operator

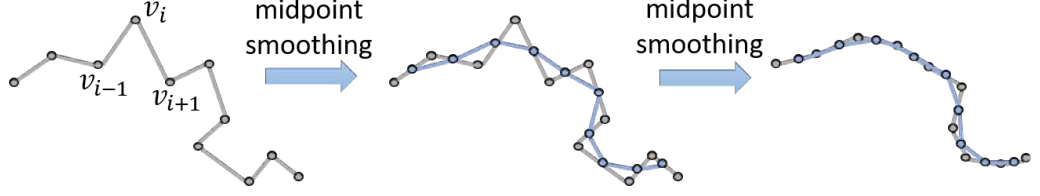


Figure 2.8: Contour smoothing is similar to the applications of the Laplacian operator in 1D in terms of curvature behaviour. This demonstrates midpoint smoothing for a contour.

that is defined as the divergence of the gradient, (∇) . In Euclidean space this evaluates to the sum of second partial derivatives

$$\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}, \quad (2.1)$$

For a scalar function $f(x, y, z)$. The differential operator often arises in physics for the heat diffusion equations and fluid flow where the functions f that satisfy Laplace's equation, $\Delta f = 0$, are defined as *harmonics* [4]. The *Laplace-Beltrami operator* ($\Delta_{\mathcal{S}}$) extends the concept of the Laplacian operator to functions that are defined on a manifold surface $\mathcal{S}$ [4]. Importantly, when applied to the coordinate function $\mathbf{x}$ of a surface, the Laplace-Beltrami operator evaluates to the *mean curvature normal*:

$$\Delta_{\mathcal{S}} = -2\kappa_{\text{mean}}\mathbf{n}, \quad (2.2)$$

where κ_{mean} is the mean curvature defined as the average of the two principal curvature, and $\mathbf{n}$ is the normal vector.

Combinatorial Mesh Laplacian The Laplacian also arises in the area of spectral graph theory where the diameter and connectivity of a graph $G = (V, E)$, with vertices V and edges E , is derived from the eigenvalues of the *graph Laplacian* [8]. The graph Laplacian is useful for geometry processing because it can be thought of as a combinatorial version of the Laplace-Beltrami [27], i.e. a discrete Laplacian whose spectral properties are only defined by the graph's connectivity.

Instead of introducing the harmonic and scale properties of the combinatorial mesh Laplacian via graphs, we can instead treat the scale analysis in terms of frequency by considering the problem of contour smoothing. For a more thorough description of spectral mesh processing the authors suggest consulting Botsch et al. [2], and Lévy and Zhang [22].

If we consider a contour $f = \mathbf{x} = (v_1, v_2, \dots, v_n)^T$, where each vertex is $\mathbf{x}_i = v_i = (x_i, y_i)$. We can then smooth the contour by calculating the midpoint between each vertex twice (apart from the boundary vertices) to give a *local average* such that,

$$\hat{\mathbf{x}}_i = \frac{1}{2} \left[\frac{1}{2} (v_{i-1} + v_i) \right] + \frac{1}{2} \left[\frac{1}{2} (v_i + v_{i+1}) \right] = \frac{1}{4}v_{i-1} + \frac{1}{2}v_i + \frac{1}{4}v_{i+1}. \quad (2.3)$$

The 1D Laplacian operator is also then defined as

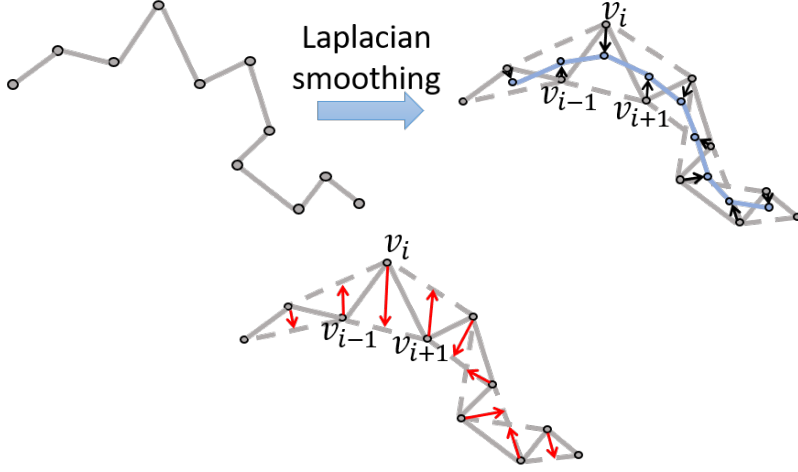


Figure 2.9: One step of Laplacian smoothing is equivalent to two steps of midpoint smoothing. The 1D Laplacian vectors in this case are represented by the red arrows.

$$\begin{aligned}
 \Delta f(v_i) &= L(\mathbf{x}_i) = \frac{1}{2}(v_{i-1} - v_i) + \frac{1}{2}(v_{i+1} - v_i) \\
 &= \frac{(x_{i-1} - x_i) + (x_{i+1} - x_i)}{2} + \frac{(y_{i-1} - y_i) + (y_{i+1} - y_i)}{2} \\
 &= \frac{d^2 f}{dx^2} + \frac{d^2 f}{dy^2}
 \end{aligned} \tag{2.4}$$

—so that in one step we can offset the contour vertices in the direction of the 1D Laplacian vectors (the red arrows in Figure 2.9) by a factor of $\frac{1}{2}$, so that two steps of midpoint and one step of Laplacian smoothing operations are equivalent.

If we now consider the sequence of vertices $\mathbf{x}$ as a closed contour, we can interpret the signal as a discrete time n -periodic signal that can be smoothed iteratively by $\hat{\mathbf{x}}_i^{(t+1)} \leftarrow \mathbf{x}_i^{(t)} + \frac{1}{2} L(\mathbf{x}_i^{(t)})$. To inspect the spectral properties of the 1D Laplacian, we now consider only the x -component of the contour as a $n \times 1$ coordinate vector X .

Since the contour is n -periodic, we can express the discrete 1D Laplacian as an $n \times n$ matrix L such that

$$\nabla(X) = LX = \begin{bmatrix} 1 & -\frac{1}{2} & 0 & \dots & \dots & 0 & -\frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & 0 & -\frac{1}{2} & 1 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \dots & \dots & 0 & -\frac{1}{2} & 1 \end{bmatrix} X. \tag{2.5}$$

The new Laplacian smoothed contour $\hat{X}$ can then be expressed as

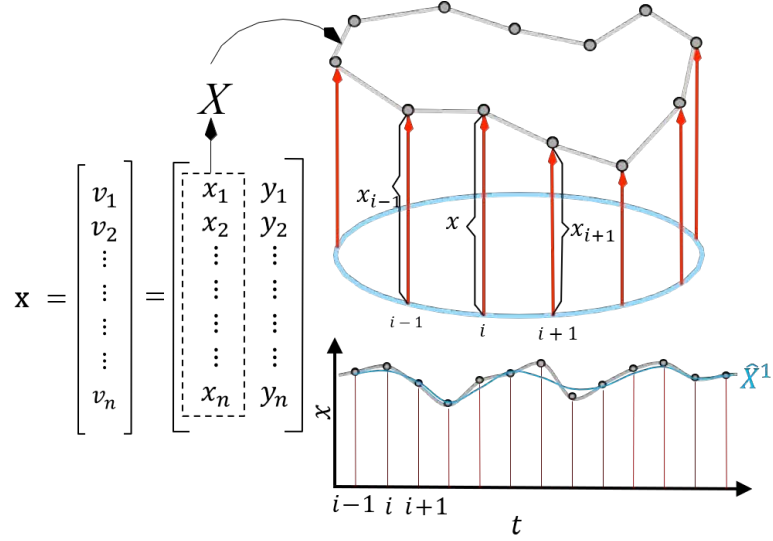


Figure 2.10: If we consider a closed contour, the x-component of the contour coordinate vector can be viewed as a 1D periodic signal. The 1D Laplacian operator can then be expressed as a circulant matrix.

$$\hat{X} = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \\ \vdots \\ \hat{x}_{n-1} \\ \hat{x}_n \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{4} & 0 & \dots & \dots & 0 & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} & 0 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & 0 & \dots & \dots & 0 & \frac{1}{4} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = (I - \frac{1}{2}L)X \quad (2.6)$$

The important property of the matrix L is that it is symmetric which implies that it has a set of real eigenvalues $\{\lambda_1, \dots, \lambda_n\}$ and real orthogonal eigenvectors $E = \{\mathbf{e}_1, \dots, \mathbf{e}_n\}$, where each $\mathbf{e}_i$ is a $n \times 1$ vector and E is a matrix is a $n \times n$ matrix whose columns are $\mathbf{e}_i$. Thus any vector of length n can be expressed as a linear sum of E , in particular the coordinate vector X can be expressed as

$$X = \sum_i^n \mathbf{e}_i \tilde{x}_i = \begin{bmatrix} E_{11} \\ E_{21} \\ \vdots \\ E_{n1} \end{bmatrix} \tilde{x}_1 + \dots + \begin{bmatrix} E_{1n} \\ E_{2n} \\ \vdots \\ E_{nn} \end{bmatrix} \tilde{x}_n = \begin{bmatrix} E_{11} & \dots & E_{1n} \\ E_{21} & \dots & E_{2n} \\ \vdots & \vdots & \vdots \\ E_{n1} & \dots & E_{nn} \end{bmatrix} \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \\ \vdots \\ \tilde{x}_n \end{bmatrix} = E\tilde{X}. \quad (2.7)$$

We use the above expression as the definition of the *spectral transform* of a mesh so that we can map the vertices of a mesh from the *spatial domain* to the *frequency domain* as $E^T X \rightarrow \tilde{X}$, and vice versa as $E\tilde{X} \rightarrow X$. Another observation is that each row of L is also a circular shift of the previous row. This property demonstrates that L is a circulant matrix and is important since the linear combination of its eigenvectors can then be shown to be equivalent to the Discrete Fourier Transform [33].

A property from spectral graph theory that has applications in scale analysis is the *Fiedler vector* $\mathbf{e}_F$ of the graph Laplacian, which corresponds to the smallest nonzero

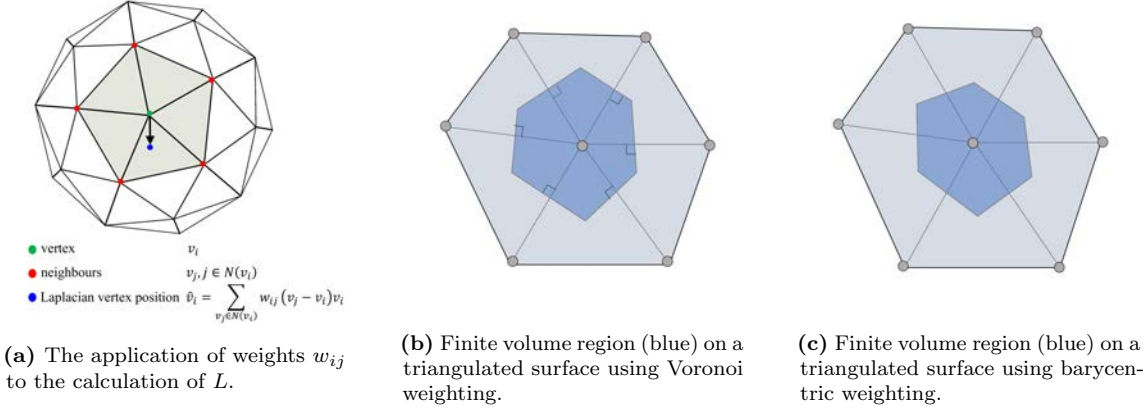


Figure 2.11: A smooth surface can be approximated by a manifold polygonal mesh by a local averaging of differential properties.

eigenvalue λ_2 [27]. The vector gives a 1-dimensional embedding of the graph or mesh that respects the Laplacian between the nodes or vertices [21]. The eigenvalue λ_2 thus measures the largest wavelength that spans the entire mesh.

Geometric Mesh Laplacian An important assumption in the above contour example is that the neighbouring points to the vertex v_i have an equal influence and so the operator is only defined by the connectivity between the points. This results in a factor of $\frac{1}{2}$ in Equation 2.4 and subsequently in the discrete 1D Laplacian matrix. This is important when we consider meshes since accurate discretization will often require irregular sampling of points from a continuous surface or when we are interested in the eigenvalues of the Laplacian, since the eigenvalues of the combinatorial Laplacian are not unique [27]. Mesh Laplacians that incorporate not only the connectivity between vertices but instead also approximate a smooth surface are called geometric mesh Laplacians [27] and are considered more accurate for geometric processing tasks such as curvature analysis. I introduce weighted-spatial averages for geometric mesh Laplacians (see Figure 2.11) and then introduce the cotangent Laplacian Figure 2.12.

For a manifold polygonal mesh we can make the assumption that it can be interpreted as a piecewise linear approximations of smooth surfaces. The goal is then to compute approximations of the differential properties of this underlying surface directly from the mesh data. If we consider instead a discrete surface signal f defined on a regular polyhedra, we can define the discrete Laplacian as a weighted average for v_i :

$$\Delta_S f(v_i) = \sum_{v_j \in N(v_i)} w_{ij} (v_j - v_i), \quad (2.8)$$

where w_{ij} are positive weights that sum to 1 for each i , and $N(v_i)$ is the local neighbourhood of a vertex v_i . There are several ways of calculating the edge weight w_{ij} , the simplest, introduced by [34], being the uniform edge weight. This is calculated as the inverse of the number of neighbourhood vertices ($\frac{1}{|N(v_i)|}$).

A different weighting scheme that has useful differential properties is the cotangent of

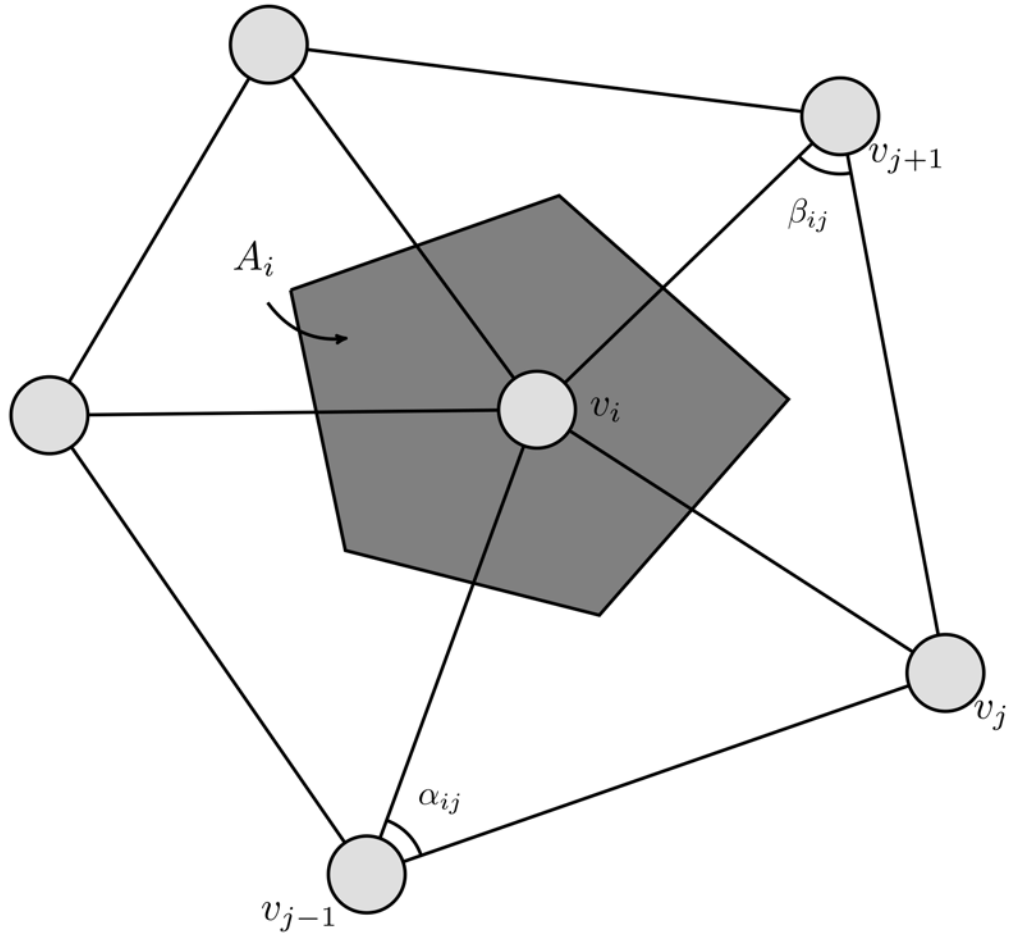


Figure 2.12: The angles α_{ij}, β_{ij} and the (dark grey) barycentric area A_i used to discretize the *Laplace-Beltrami* operator at a vertex v_i . Figure based on Botsch et al. [2].

the internal angles of a neighbouring vertex Figure 2.12. In contrast to the uniform edge weight Figure 2.8, the cotangent Laplacian includes introducing a per-vertex weight w_i :

$$\Delta_S f(v_i) = w_i \sum_{v_j \in N(v_i)} w_{ij} (v_j - v_i) \quad . \quad (2.9)$$

The per-vertex weight w_i acts as a spatial average A_i for vertex v_i for which there are number of ways of computing. Two common methods for calculating A_i are to either use the barycentric points of adjacent triangle of the vertex v_i or to use the Voronoi cell circumcenter point of adjacent triangles (see Figure 2.11). The edge weights introduced by [26], uses the cotangent weights of the opposing internal angles of the edge between v_i and v_j (see Figure 2.12). Thus, the weights in Figure 2.9 are calculated as:

$$w_i = \frac{1}{A_i}, w_{ij} = \frac{1}{2} (\cot \alpha_{ij} + \cot \beta_{ij}) \quad . \quad (2.10)$$

Thus, the cotangent Laplacian for a mesh with n vertices is a matrix L with entries

$$L_{ij} = \begin{cases} \cot\alpha_{ij} + \cot\beta_{ij}, & j \in N(i) \\ 0, & j \notin N(i) \\ -\sum_{k \neq i} L_{ik}, & i = j \end{cases}, \quad (2.11)$$

where $N(i)$ are the neighbouring vertices to vertex i and α_{ij}, β_{ij} are the angles opposite to the edge between vertices ij . These angles behave in such a way that if we treated the triangulated mesh not as a surface but instead made up of volumes or elements, then the differential coordinates on the surface could be fully derived from the cotangent angles [26].

To calculate the eigenscales of the mesh we then multiply the Laplacian matrix by the per-vertex area. This is called the mass-matrix M and is a diagonal $n \times n$ matrix where the diagonals correspond to A_i . When this is multiplied with the cotangent Laplacian it can be considered as a discretization of the Laplace-Beltrami matrix ($L_{\mathcal{S}}$) for a mesh surface $\mathcal{S}$. The generalized eigenproblem can then be solved as

$$L_{\mathcal{S}}\mathbf{v}_i = \phi_i\mathbf{v}_i. \quad (2.12)$$

Where $L_{\mathcal{S}}$ is the Laplace-Beltrami matrix, $\mathbf{v}_i$ is an eigenvector and ϕ_i is an eigenvalue. Moreover, since the only non-zero entries of $L_{\mathcal{S}}$ correspond connected vertices, efficient algorithms for finding eigenvalues and eigenvectors in sparse matrices can be used [20]. The smallest eigenvalue corresponds to the lowest spatial frequency on the manifold surface which is the inverse of the wavelength of the shape. The eigenvector $\mathbf{v}_i$ for a given harmonic i contains the amplitude at each vertex for i . This amplitude it should be noted is defined on the manifold surface so that it is not directly measured for the absolute vertex coordinate values. We can then transform the eigenvectors into the canonical basis by multiplying them by M^{-1} . This can be considered as analogous to the frequency-space used in Fourier analysis so that we can specify how many eigenvectors to use in the inverse transform to regenerate the mesh at larger harmonic. This transform is commonly referred to as the Manifold Harmonic Transform [36].

2.3.3 Surface Complexity

To derive a measure of the surface complexity, I calculate the variability of the mesh across harmonic scales. This requires reconstructing the mesh at successively smaller wavelengths and calculating the face normal vector for each triangle. I use the cosine distance to quantify the difference in orientation between face normals. This is calculated as $1 - \cos\theta$ where θ is the angle between the two vectors. The sum of the pairwise cosine distances across all harmonic scales for each triangular face is then used as the measure of surface complexity.

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Chapter 3

Deformation Scale

3.1 Introduction

The study of deformation within computational geodynamics requires certain assumptions for numerical models, depending on the processes under investigation. This is particularly important when comparing numerical deformation results to the observations of structural geology. Within structural geology, many of these assumptions are encompassed under *finite strain theory*, and was significantly developed through the work of Ramsay [21].

When considering the validity of numerical approaches in modelling folds, another helpful definition used by Nabavi and Fossen [19] is that a fold can be defined as:

"the result of a folding history dominated by growth dominated by permanent ductile deformation, during which material continuity and cohesion is largely maintained at the scale of observation".

3.2 Definitions

3.2.1 General Deformation

An idealised homogeneous finite deformation in three-dimensions can be summarised by the deformation matrix [25].

$$\mathbf{D} = \begin{bmatrix} k_1 & \Gamma_{xy} & \Gamma_{xz} \\ 0 & k_2 & \Gamma_{yz} \\ 0 & 0 & k_3 \end{bmatrix} \quad (3.1)$$

Here, k_1, k_2, k_3 represent extensions in the x, y and z axes, respectively, and the off-diagonal terms represent shear deformation. The deformation in Equation 3.1 is made of simultaneous thrusting in the x -direction (Γ_{xz}), thrusting in the y -direction (Γ_{yz}), and a wrenching in the x -direction (Γ_{xy}).

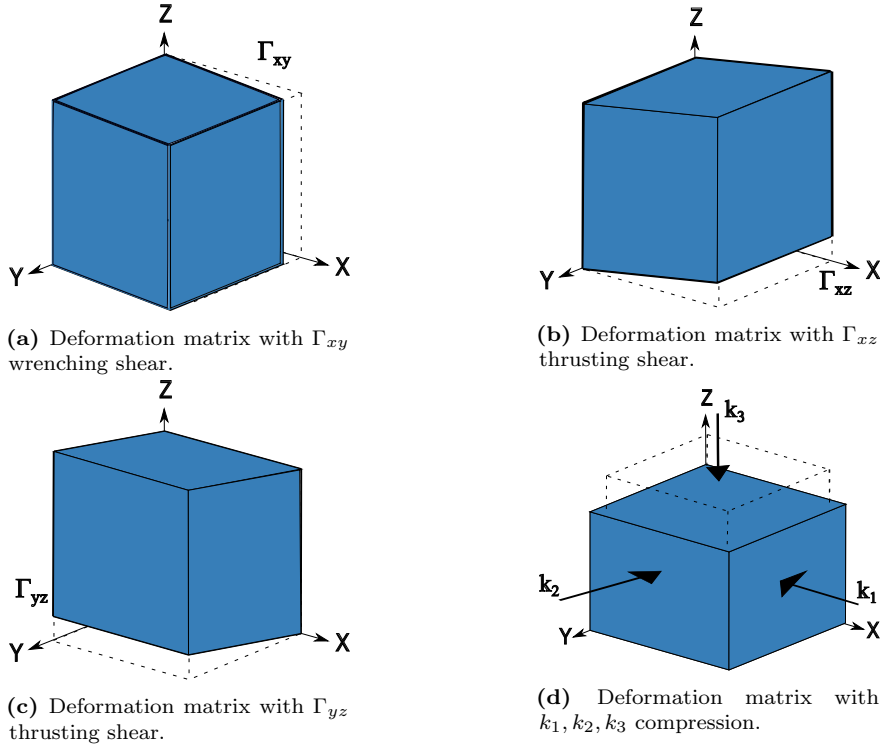


Figure 3.1: Examples of deformation matrices for shear strain rates Γ_{ij} and longitudinal compression k_i

Pure and Simple Shear

As far as finite strain theory, the development was applied to the understanding of ooids [6] or reference fossil deformation [13]. Hence, the development of terminology that is limited to plane strain: pure and simple shear (Figure 3.3). An important distinction between the shear deformation is whether they preserve initially parallel linear elements as parallel throughout deformation. Hence, pure shear, where parallel lines are preserved, is also described as irrotational deformation and simple shear as rotational deformation [18].

Strain Ellipsoid

In three-dimensions and during homogenous deformation, we can consider how the particles lying on the surface of an undeformed sphere will lie on an ellipsoid when deformed. This is then called the *strain ellipsoid* [18].

The three lengths of the principal strain axes that span the planes of symmetry of the ellipsoid are the *principal stretches* ($X > Y > Z$). The vectors that describe the shape and orientation of the strain ellipsoid are named $\mathbf{e}_1, \mathbf{e}_2$ and $\mathbf{e}_3$, where $\mathbf{e}_1$ is the longest and $\mathbf{e}_3$ the shortest. If we place a coordinate system with axes x, y and z along the principal strain axes X, Y and Z , we can write the equation for the strain ellipsoid as:

$$\frac{x^2}{\lambda_1} + \frac{y^2}{\lambda_2} + \frac{z^2}{\lambda_3} = 1 \quad (3.2)$$

Moreover, λ_1, λ_2 and λ_3 are the eigenvalues of the symmetric matrix $\mathbf{D}\mathbf{D}^T$ and $\mathbf{e}_1, \mathbf{e}_2$ and $\mathbf{e}_3$ are the eigenvectors, where $\mathbf{D}$ is the finite deformation matrix (Equation 3.1). An

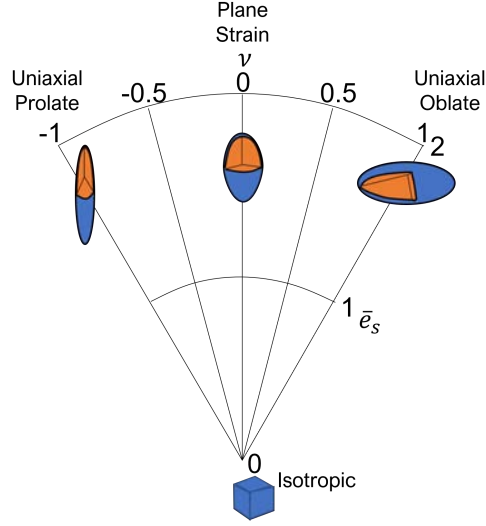


Figure 3.2: The Nadai-Hsu diagram for strain, where ν is Lode's ratio (Equation 4.3) and $\bar{e}_s$ (Equation 4.2a) is the natural octahedral unit shear.

important property of the principal strain axes is that lines that are parallel with them are orthogonal, and were also orthogonal when undeformed [10].

To distinguish between different amounts and shapes of strain we can visualize a strain ellipsoid using the Nadai-Hsu diagram (Figure 4.4). Here we use the natural octahedral unit shear $\bar{e}_s$ which is directly related to the mechanical work that is performed during the deformation history [10]. It is defined as:

$$\bar{e}_s = \frac{\sqrt{3}}{2} \bar{\gamma}_{\text{oct}}, \quad (3.3a)$$

$$\bar{\gamma}_{\text{oct}} = \frac{2}{3} \sqrt{(\bar{e}_1 - \bar{e}_2)^2 + (\bar{e}_2 - \bar{e}_3)^2 + (\bar{e}_3 - \bar{e}_1)^2}. \quad (3.3b)$$

where $\bar{e}_s$ are the natural principal strains. The natural octahedral unit shear $\bar{e}_s$ is then plotted against the Lode parameter (ν) defined as:

$$\nu = \frac{2\bar{e}_2 - \bar{e}_1 - \bar{e}_3}{\bar{e}_1 - \bar{e}_3} \quad (3.4)$$

3.2.2 Continuum Mechanics

Continuum Mechanics theory allows the prediction of material behaviour during the application of mechanical forces and is therefore a powerful tool for the study of geological deformation. Nonetheless, some of the necessary assumptions are that materials form continuous bodies without any discontinuous or abrupt changes in property [14]. The governing equations of the material behaviour can then be derived for a closed physical systems by applying the principles of the *conservation of mass*, the *conservation of momentum* and their *constitutive* relationships.

Continuity equation If we consider a fixed-point (*Eulerian*) in three-dimensions, the continuity equation, that ensures that mass is conserved, is defined as:

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{v}) = \frac{\partial \rho}{\partial t} + \frac{\partial \rho v_x}{\partial x} + \frac{\partial \rho v_y}{\partial y} + \frac{\partial \rho v_z}{\partial z} = 0, \quad (3.5)$$

where $\frac{\partial}{\partial t}$ is the Eulerian time derivative; ρ is the local density, which characterizes the amount of mass per unit volume kg/m^3 ; $\vec{v}$ is local velocity m/s , $\text{div}()$, is the divergence operator, x, y, z are Cartesian coordinates and v_x, v_y, v_z are components parallel to the respective coordinate axes of the velocity vector $\vec{v}$. The equivalent equation for a moving-point or material-point (*Lagrangian*) in three-dimensions is defined as:

$$\frac{D\rho}{Dt} + \rho \text{div}(\vec{v}) = 0 \quad (3.6)$$

where instead, $\frac{D}{Dt}$ is the Lagrangian time derivative.

The difference in Eulerian and Lagrangian derivation can be considered in terms of how to represent the change in density over time. If we note that using the product rule, we can write $\text{div}(\rho \vec{v}) = \rho \text{div}(\vec{v}) + \vec{v} \text{grad}(\rho)$, then by using Equation 3.5 and Equation 3.6 the relationship between Eulerian ($\frac{\partial \rho}{\partial t}$) and Lagrangian ($\frac{D\rho}{Dt}$) time derivatives of density becomes:

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \vec{v} \text{grad}(\rho) = \frac{\partial \rho}{\partial t} + \vec{v} \left(\frac{\partial \rho}{\partial x}, \frac{\partial \rho}{\partial y}, \frac{\partial \rho}{\partial z} \right) \quad (3.7)$$

where $\text{grad}()$ is the *gradient* which is a vector function of a scalar field.

Incompressibility It is common in geodynamics to assume the condition of incompressibility, i.e. the material density does not change over time:

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \vec{v} \text{grad}(\rho) = 0 \quad (3.8)$$

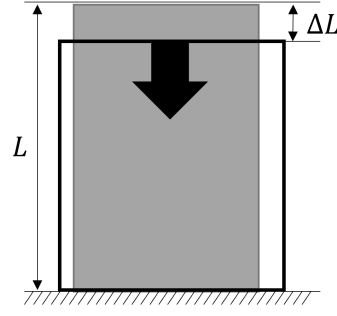
When we combine Equation 3.8 with the product rule of $\text{div}(\rho \vec{v})$ and Equation 3.6, we then find that for both Eulerian and Lagrangian formulation the continuity equation simplifies to:

$$\text{div}(\vec{v}) = 0. \quad (3.9)$$

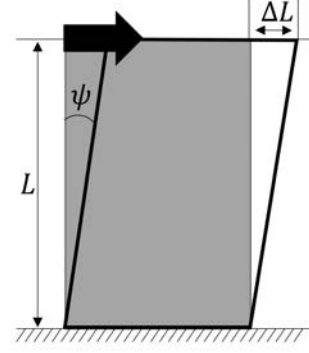
Momentum equation The conservation of momentum is described by the momentum equation, which for a continuous medium in a gravity field is defined as:

$$\text{Eulerian : } \frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i = \rho \left(\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} \right), \quad (3.10a)$$

$$\text{Lagrangian : } \frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i = \rho \frac{Dv_i}{Dt} \quad (3.10b)$$



(a) Axial Strain definition where the elongation (or longitudinal strain) is defined as $e = \frac{\Delta L}{L}$. This is an example of *pure shear*.



(b) Shear Strain definition such that $\gamma = \frac{\Delta L}{L} = \tan \psi$, where ψ is the angular shear. This is an example of *simple shear*.

Figure 3.3: Examples of axial and shear strain, based on Gerya [12]. While in both cases the strain is calculated as $= \frac{\Delta L}{L}$, angles between parallel lines are preserved across deformation only during Figure 3.3a, while they rotate in Figure 3.3b by an angle of ψ [10]. This implies that L will need to be measured orthogonal to the direction of displacement in Figure 3.3b. These two cases can be considered examples of *pure* and *simple* shear respectively.

Constitutive equation When considering viscous flow, it is often more convenient to consider the strain-rate $\dot{e}$ rather than strain e . In three-dimensions, the strain-rate tensor, i.e. the time derivative of the strain tensor, is defined as:

$$\dot{\epsilon}_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right). \quad (3.11)$$

The strain-rate tensor $\dot{\epsilon}$ can also be separated into isotropic normal strain components $\dot{\epsilon}_{kk}$ and deviatoric strain components $\dot{\epsilon}'_{ij}$ that are defined as:

$$\dot{\epsilon}_{kk} = \dot{\epsilon}_{xx} + \dot{\epsilon}_{yy} + \dot{\epsilon}_{zz}, \quad (3.12a)$$

$$\dot{\epsilon}'_{ij} = \dot{\epsilon}_{ij} - \delta_{ij} \frac{1}{3} \dot{\epsilon}_{kk} \quad (3.12b)$$

where δ_{ij} is the Kronecker delta function.

The constitutive relationship defines how stress and strain are related for a specific material. Hence, for a linear viscous material undergoing steady-state creep, the constitutive relationship can be described by Newton's law of viscous friction, given by:

$$\tau_{ij} = 2\eta\dot{\epsilon}'_{ij} + \delta_{ij}\eta_{bulk}\dot{\epsilon}_{kk}. \quad (3.13)$$

where η and η_{bulk} are the shear viscosity and bulk viscosity, $\dot{\epsilon}_{kk}$ are the normal strain rate components (Equation 3.12a), $\dot{\epsilon}'_{ij}$ is the deviatoric strain rate (Equation 3.12b), and δ_{ij} is the Kronecker delta function [11]. The bulk viscosity η_{bulk} is also sometimes referred to as the *volume viscosity* since it expresses the internal friction that resists shear-less compression or expansion of a fluid. It is thus closely related to volumetric strain. When we consider an incompressible fluid though, i.e. $\dot{\epsilon}_{kk} = 0$ so that $\dot{\epsilon}'_{ij} = \dot{\epsilon}_{ij}$, the incompressible

law of viscous friction simplifies to

$$\tau_{ij} = 2\eta\dot{\epsilon}_{ij}. \quad (3.14)$$

3.2.3 Viscous Creep

The permanent deformation of a crystalline rock under an applied stress occurs through a process called *solid-state creep*. When this permanent deformation results in the continuous change of passive markers, it is called plastic flow and when abrupt and discontinuous is called brittle flow. The two major types of creep are known as *diffusion creep* and *dislocation creep*.

Diffusion creep is often dominant at relatively smaller differential stresses (σ_d) and is a result atoms moving from their stable positions due to thermally activated processes [15]. The mass transfer can occur from within grains (*Herring-Nabarro creep*) or along grain-boundaries (*Coble creep*). The transition between Coble and Nabarro-Herring creep is mainly influenced by temperature; the transitions of Nabarro-Herring creep to dislocation creep, and dislocation creep to brittle failure are mainly an effect of shear stress. The transition from Coble creep to dislocation creep is influenced by both temperature and shear stress. Temperature and strain rate have conflicting influence, as mentioned above, and this allows extrapolation of experimental data to geological strain rates. Notice that with increasing grain size, the dislocation creep field increases in size and the diffusion creep fields shrink. The constitutive equation forms a linear (Newtonian) relationship between strain-rate ($\dot{\epsilon}$) and differential stress (σ_d) such that:

$$\dot{\epsilon} = A_{\text{diff}}(\sigma_d)\exp(-E^*/RT). \quad (3.15)$$

where E^* is the activation energy, R is the gas constant, T is temperature and A_{diff} is an experimentally derived constant [10; 15]. While the constant A_{diff} will often be insensitive to the applied stress, it is dependent on grain-size, as well as pressure, temperature, and oxygen and water fugacity [12].

Dislocation creep will be more dominant at higher temperatures and applied stresses, and results from the migration of imperfections, or dislocations, in a crystalline lattice. The energy required to overcome the bonds around a dislocation highly depend on the type of dislocation, i.e. much less energy is required to move an edge dislocation compared to a screw dislocation. Moreover, the density of dislocations increases with applied stress so that the constitutive equation forms a non-linear (non-Newtonian) relationship between strain-rate ($\dot{\epsilon}$) and differential stress (σ_d):

$$\dot{\epsilon} = A_{\text{disl}}(\sigma_d)^n\exp(-E^*/RT). \quad (3.16)$$

where E^* is the activation energy, R is the gas constant, T is temperature, A_{disl} is an experimentally derived constant and n is the stress exponent [10; 15]. For the constant A_{disl} it independent of stress and grain-size, but is still dependent on pressure, temperature,

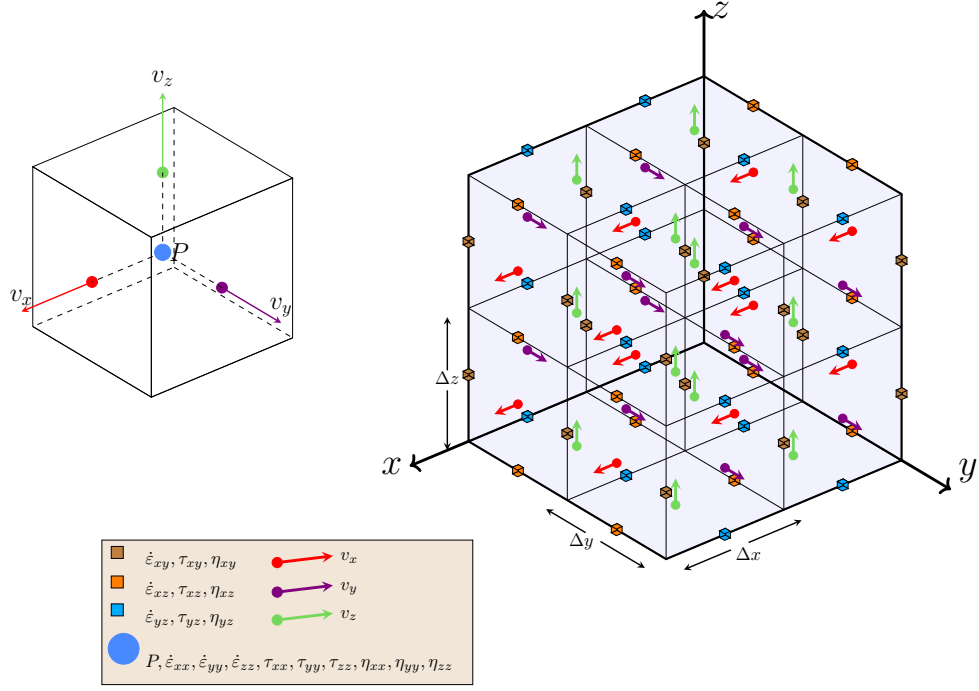


Figure 3.4: The full-staggered finite-difference grid used in LaMEM for solving the mechanical equations. Here P is pressure, $\dot{\epsilon}_{ij}$ is the strain-rate, τ_{ij} is the deviatoric stress, η_{ij} is the viscosity, and v_i is the velocity.

and oxygen and water fugacity [12].

The effective viscous flow law that combines the two can then be defined as:

$$\dot{\epsilon} = A_D h^m (\sigma_d)^n \exp\left(-\frac{E_a + V_a P}{RT}\right). \quad (3.17)$$

where P is the pressure, T is the temperature, R is the gas-constant, h is the grain-size. The remaining constants are all experimentally derived including n the stress exponent, m the grain size exponent, E_a and V_a the energy and volume activation respectively, and A_D a proportionality material constant [12]. For example, if we consider a constant strain-rate deformation experiment where we need to fit to the second-invariant strain-rate ($\dot{\epsilon}_{\text{II}}$), we can then formulate the effective viscosity in terms of $\dot{\epsilon}_{\text{II}}$ as:

$$\eta_{\text{eff}} = \frac{1}{2^{(n-1)/n} 3^{(n+1)/(2n)}} \times \frac{1}{(A_D)^{1/n} h^{m/n} (\dot{\epsilon}_{\text{II}})^{(n-1)/n}} \exp\left(\frac{E_a + V_a P}{nRT}\right). \quad (3.18)$$

3.2.4 Numerical Approach

Finite Difference Staggered Grid (FDSTAG)

To solve the equations of momentum and continuity, I use a finite-difference fully staggered grid (Figure 3.4). This approach is widely used in computational geodynamics [12], and is implemented in the open-source code Lithosphere and Mantle Evolution Model (LaMEM) [16].

Boundary Conditions

There are two types of boundary conditions: *Dirichlet boundary conditions* and *Neumann boundary conditions*. The Dirichlet boundary conditions specify values along the boundary of a model, while Neumann conditions specify values for derivative of the solution along the boundary. I compare a variety of free slip and no slip boundary conditions in LaMEM and outline numerically what this means here.

free slip free slip conditions require that the normal component of the velocity component on boundary is zero. This implies zero shear strain rates and shear stresses along the boundary. For example, for the vertical boundary orthogonal to the x axis, the free slip condition is formulated as follows

$$v_x = 0, \quad (3.19)$$

$$\frac{\partial v_y}{\partial x} - \frac{\partial v_z}{\partial x} = 0, \quad (3.20)$$

no slip no slip conditions requires all velocity components on the boundary to be zero.

$$v_x = v_y = v_z = 0, \quad (3.21)$$

Moreover, the application of different boundary conditions can be used to simulate different tectonic processes [9].

Marker-in-Cell/Particle-in-Cell for Variable Viscosity

The Marker-in-Cell method for variable viscosity has proved a robust and numerically stable approach to solving fluid mechanics problems with significant competency contrast [8]. The important aspect in terms of rheology is the harmonic averaging of viscosities in the advection of the markers.

3.2.5 Finite Strain

We can compute the *finite strain tensor* from the *finite deformation gradient tensor* $\mathbf{F}$ [2; 4]. We define the deformation gradient tensor $\mathbf{F}$ as:

$$d\mathbf{x} = \mathbf{F} \cdot d\mathbf{X} \quad \text{or} \quad dx_i = F_{ij}dX_j \quad \text{where} \quad F_{ij} = \frac{\partial x_i}{\partial X_j} \quad (3.22)$$

where $\cdot$ is the *Gibbs dyadic notation*. We accumulate and store $\mathbf{F}$ on the numerical markers. To obtain the finite deformation gradient tensor we first compute the components of the *incremental deformation gradient tensor* $\Delta\mathbf{F}$ for every time step from the velocity field as:

$$\Delta\mathbf{F} = \mathbf{I} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \Delta t \quad (3.23)$$

where $\mathbf{I}$ is the second order identity tensor, v the velocity vector, x the spatial coordinate vector, and Δt the time step. The second term in Equation 3.23 is also called the *displacement gradient tensor*.

If we consider a coordinate map $x = x(X, t)$ where the current coordinates x are a function of the original coordinates X and time, we can use the chain rule on a time step:

$$\frac{\partial x_{n+1}}{\partial X} = \frac{\partial x_{n+1}}{\partial x_n} \frac{\partial x_n}{\partial X} \quad (3.24)$$

From Equation 3.24, the deformation gradient tensor $\mathbf{F}$ is updated from the previous time step in a multiplicative manner:

$$\mathbf{F}_{n+1} = \Delta \mathbf{F} \mathbf{F}_n \quad (3.25)$$

To derive the principal strain axes and principal strains, we must also consider the polar decomposition of the deformation gradient, which is:

$$\mathbf{F} = \mathbf{V} \mathbf{R} \quad (3.26)$$

where $\mathbf{R}$ is an orthogonal tensor representing rigid body rotation, and $\mathbf{V}$ is a symmetric positive definite tensor representing finite strain in the current configuration, which is called the *left stretch tensor*. The polar decomposition can be performed by computing the spectral representation of the left Cauchy–Green deformation tensor $\mathbf{B}$ as follows:

$$\mathbf{B} = \mathbf{F} \mathbf{F}^T = \mathbf{V}^2 = \sum_{i=1}^3 \lambda_i^2 \mathbf{n}_i \otimes \mathbf{n}_i \quad (3.27)$$

Here, λ_i and $\mathbf{n}_i$ are the eigenvalues and eigenvectors of the left stretch tensors $\mathbf{V}$. The *eigenvalues represent principal strains*, and the *eigenvectors represent the directions of the principal strain axes*.

Velocity Gradient Tensor ($\mathbf{L}$)

While the deformation gradient tensor has a clear relationship to strain, it is often more convenient to use the velocity gradient tensor $\mathbf{L}$ [20], defined as:

$$\mathbf{L} = \mathbf{v} \otimes \nabla_{\mathbf{y}} \equiv L_{ij} = \frac{\partial v_i}{\partial y_j} \quad (3.28)$$

The velocity gradient can also be expressed by the deformation gradient and its time derivative as:

$$\mathbf{v} \otimes \nabla_{\mathbf{y}} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} \frac{\partial v_i}{\partial y_j} = \dot{F}_{ik} \cdot F_{kj}^{-1} \quad (3.29)$$

The velocity gradient tensor can then be separated into the sum of two tensor components:

$$\mathbf{L} = \mathbf{S} + \mathbf{R} \quad (3.30)$$

where $\mathbf{S}$ is the stretching tensor and $\mathbf{R}$ is the rotation tensor.

Strain Ellipsoid Shape (J)

The characterise the shape of the finite strain ellipsoid, the ratios of X/Y and Y/Z have been used to distinguish between oblate and prolate shapes. Alternatively, a single value [3] can be also be derived such that:

$$j = \frac{X/Y - 1}{Y/Z - 1} \quad (3.31)$$

This separates shapes into prolate ($j > 1$) and oblate ($j < 1$) shapes.

Kinematic Vorticity ($\mathbf{W}_k$)

Vorticity analysis, which measures the internal rotation (vorticity) and the external accumulation of strain, has become an essential part of deformation studies in structural geology [5; 27]. Nonetheless, the use of kinematic vorticity (W_k) has limitations for interpreting finite strain and shear direction, since it is importantly an instantaneous measure [26].

The vorticity vector ($\mathbf{w}$) is defined as the curl of the velocity field ($\mathbf{v}$) and is thus related to angular velocity (ω) such that:

$$\mathbf{w} = 2\omega = \text{curl}\mathbf{v} \quad (3.32)$$

The vorticity tensor $\mathbf{W}$ can be derived from the velocity gradient tensor $\mathbf{L}$ as:

$$\mathbf{W} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T) \quad (3.33)$$

The kinematic vorticity W_k can be derived from the instantaneous stretching axis [10] as:

$$W_k = \frac{\mathbf{w}}{\sqrt{2(s_x^2 + s_y^2 + s_z^2)}} \quad (3.34)$$

where s_n are the principal strain rates, i.e. the strain rates along the instantaneous stretching axis, i.e. the eigenvectors of the stretching matrix $\mathbf{S}$.

Alternatively, it can be directly derived from the velocity gradient tensor $\mathbf{L}$ and stretching tensor $\mathbf{S}$ [18] as:

$$W_k = |\mathbf{S}|/|\mathbf{L}| \quad (3.35)$$

3.3 Methods

3.3.1 Passive Finite Strain Marker

I accumulate the finite strain on a set of passive markers in a similar manner to Le Pourhiet et al. [17]; Spitz et al. [23]. This requires bilinearly interpolating the velocity field within

the numerical grid and calculating the velocity gradient tensor. The finite gradient tensor is then incrementally updated for the given time lapse.

3.3.2 Finite Deformation Tensor (F) convolution

To show the change in deformation scale, I also implement a finite deformation averaging based on Riemannian metric and PSD manifold statistics [7]. This requires that log matrix of the tensor is calculated before being averaged. To develop the average deformation of the volume, I apply a convolution operation to calculate the manifold average, and compare these results to the full resolution passive finite strain markers.

3.3.3 Superpixel method of segmentation/regionalization

Furthermore, I assess the three-dimensional strain partitioning and deformation zonation of the volume, by applying the superpixel segmentation to the volume [1; 24]. The technique is used often in image processing where rather than processing individual pixel values, it is advantageous to group pixels before using more computational intensive analysis. To ensure that nearby pixels are grouped, the colour or intensity proximity is normalised with the spatial proximity, and then clustered to produce N superpixels. In our case, the kinematic vorticity W_k and strain ellipsoid shape $\log J$ is used in place of colour or intensity.

To calculate the superpixels the normalised distance metric D' is needed to be calculated. The finite strain distance is given as $d_{fs} = \sqrt{(f_j - f_i)^2}$, while the spatial distance is $d_s = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$. The normalised distance requires two normalisation values N_{fs} and N_s such that

$$D' = \sqrt{\left(\frac{d_{fs}}{N_{fs}}\right)^2 + \left(\frac{d_s}{N_s}\right)^2} \quad (3.36)$$

The value of N_s is simply the sampling interval so that for N pixels and K superpixels, $N_s = \sqrt{N/K}$. For N_{fs} though, the approach of the simple linear iterative clustering (SLIC) algorithm [1] is used, where it is set to a constant m . This value can also be iteratively refined to make sure the cluster centres have maximal separation [24].

3.3.4 Region meshing and topological analysis

Once the superpixel segmentation is generated, a median filter is applied to ensure coherent regions and the marching cubes contouring algorithm is applied to create a mesh of each volume. Moreover, a mesh boolean intersection operation is applied between each region to calculate the contact surface area between each region to consider the strain topology. Each region is also tetrahedralized [22] and clipped by the folded surface mesh so visualize the strain regions along the contact surface.

3.3.5 κ_{gauss} multi-scale segmentation

The methods from Figure 2.3.2 are also implemented, and a k-means clustering is applied for a given range of scales. This then shows how different values of κ_{gauss} for each curvature region are distributed across the scales.

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Chapter 4

Numerical Modelling

4.1 Introduction

To demonstrate how surface harmonic curvature can be used to constrain interpretation of ductile deformation two numerical models are developed. The first model developed is a synthetic test surface that demonstrates how the cosine distance sum relates to the geometry of a surface. The fold superposition of two different angles and wavelengths is created using the method of Ramsay and Lisle [22]. The second model consists of a three-dimensional thermo-mechanical numerical model that uses multi-layer viscous rheologies using the fully-staggered finite-difference code Lithosphere and Mantle Evolution Model or LaMEM¹ [12]. The model is based on a three-dimensional geometry setup similar to the five-layer model used in Ramberg [20] and Treagus and Fletcher [25]. White-noise perturbations for a thin stiff layer and sinusoidal perturbations for the thick stiff layer are used which are commonly applied in the comparison of analytical and numerical fold growth [1; 7].

4.2 Methods

4.2.1 Geometric Synthetic Test Surface

To demonstrate how structural surface complexity can be interpreted, a simple model of similar fold superpositions with geometries similar to the Padtherung folding are applied [22]. Folds are idealised by the displacement equation:

$$\begin{aligned}x' &= x \\y' &= Cy \\z' &= Bz + AB\sin y\end{aligned}\tag{4.1}$$

where (x, y, z) is the initial position and (x', y', z') are the deformed coordinates. The vertical axial surface of the similar fold is parallel to the xz -plane with amplitude AB and wavelength $2C\pi$. This model assumes passive shear folding, where A is the shear amplitude

¹<https://bitbucket.org/bkaus/lamem/>

	A_1	B_1	C_1	A_2	B_2	C_2
Model 1	3	1	1	$3/2$	2	$1/2$
Model 2	3	1	1	3	1	1
Model 3	3	1	1	$9/2$	$2/3$	$3/2$

Table 4.1: Parameters used for the superposed fold model. Note that fold amplitude is AB and wavelength $2C\pi$.

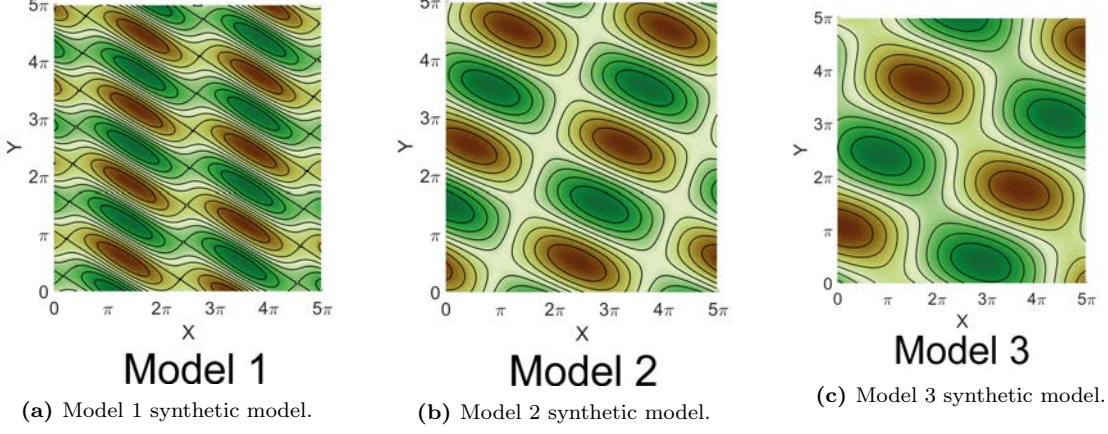


Figure 4.1: Synthetic Interface model with height contour intervals of 2. From left-to-right the figures correspond to Model 1, Model 2 and Model 3 using a variety of parameters (Table 4.1).

at the hinge zone, with B and C , controlling the magnitude of the principal directions of the homogeneous strain.

The F_1 folding is applied using parameters A_1, B_1, C_1 then rotated about the x -axis through an angle of ω_x to change the dip, then rotated by an angle ω_z about the vertical z -axis to change the dip direction. The second fold F_2 is then applied using parameters A_2, B_2, C_2 . Three models are developed with oblique strain $\omega_x = 0$ and $\omega_z = 45^\circ$ to represent the $D2$ and $D3$ folds. The F_1 folds are identical across the three models while the F_2 folds have increasing fold wavelengths with the same amplitude (see Table 4.1). The homogeneous strain parameters are also set using $C = 1/B$ so that there is no volume change. The three models with height contour intervals of 2 are visualised in Figure 4.1.

The different A_2 provide increasing shear amplitude across the F_2 hinge zone. Since the B_2, C_2 values correspond to the principal strain axes ($\mathbf{e}_1, \mathbf{e}_3$) in the z and x direction, the different values also describe a progression where the homogeneous strain directions are $\mathbf{e}_1 > \mathbf{e}_3$, $\mathbf{e}_1 = \mathbf{e}_3$, and $\mathbf{e}_1 < \mathbf{e}_3$.

4.2.2 Geodynamic Mechanical Model

The mechanical models are computed using LaMEM using an extent of $25(\text{km}) \times 15(\text{km}) \times 5(\text{km})$ and resolution of $128 \times 128 \times 128$ in the X, Y and Z respectively (see Table 4.2). The per element marker resolution is $3 \times 3 \times 3$ which defines the background matrix, thick stiff layer, or thin stiff layer material. The thick stiff layer to background matrix viscosity ratio is 20 with a thickness of 1000m, while the thin stiff layer viscosity to background matrix ratio is 200 with a thickness of 100m. Assuming Newtonian viscosities, the Biot-Ramberg

Parameter	Unit	Value
Extent	$X(\text{km}) \times Y(\text{km}) \times Z(\text{km})$	$25 \times 15 \times 5$
Grid Resolution	num elements $x \times$ num elements $y \times$ num elements z	$128 \times 128 \times 128$
Per Element Marker Resolution	num markers $x \times$ num markers $y \times$ num markers z	$3 \times 3 \times 3$
Thin Stiff Layer Thickness	$T_{\text{thin}}(\text{m})$	100
Thin Stiff Layer Viscosity	$\eta_{\text{thin}}(\text{Pa} \cdot \text{s})$	2×10^{16}
Thin Stiff Layer Interface Perturbations	white noise $A_{\text{thin}}(\text{m})$	4
Thin Stiff Layer Dominant Wavelength	$\lambda_{d\text{thin}}(\text{m})$	2022
Thick Stiff Layer Thickness	$T_{\text{thick}}(\text{m})$	1000
Thick Stiff Layer Viscosity	$\eta_{\text{thick}}(\text{Pa} \cdot \text{s})$	2×10^{15}
Thick Stiff Layer Interface Perturbations	sinusoidal $[\lambda_{\text{thick}}, A_{\text{thick}}](\text{m}, \text{m})$	$[15000, 20]$
Thick Stiff Dominant Wavelength	$\lambda_{d\text{thick}}(\text{m})$	9386
Background Matrix Viscosity	$\eta_{\text{background}}(\text{Pa} \cdot \text{s})$	1×10^{14}
Temperature	Celsius($^{\circ}$)	300

Table 4.2: The geodynamic model parameters used in LaMEM for all models. This include geometry and viscosity models but not the velocity boundary conditions.

Model	$\dot{\epsilon}_{xx}$	$\dot{\epsilon}_{xy}$	Boundary Slip Conditions					
			Left	Right	Front	Back	Bottom	Top
Compressional	$-1 \times 10^{-15} \text{s}^{-1}$	none	no	no	free	free	free	free
Pure Shear with free-slip base	$-1 \times 10^{-15} \text{s}^{-1}$	none	no	no	free	free	no	free
Compressional	$-1 \times 10^{-15} \text{s}^{-1}$	none	no	no	free	free	no	free
Pure Shear with no-slip base	$-1 \times 10^{-15} \text{s}^{-1}$	none	no	no	free	free	no	free
Strike-Slip Simple Shear	none	$-1 \times 10^{-15} \text{s}^{-1}$	no	no	free	free	free	free
Transpressional combined Pure and Simple Shear	$-1 \times 10^{-15} \text{s}^{-1}$	$-5 \times 10^{-16} \text{s}^{-1}$	no	no	free	free	free	free

Table 4.3: The geodynamic model velocity boundary conditions parameters used in LaMEM.

dominant wavelength λ_d can then be calculated as $\lambda_d = 2\pi T(\eta_L/6\eta_M)^{1/3}$ where T is the layer thickness, η_L is the layer viscosity and η_M is the matrix viscosity [6]. This results in dominant wavelength of 2.0km for the thin stiff layer and 9.4km for the thick stiff layer.

To test how curvature and finite strain scale to the deformation flow field, a set of four different velocity boundary conditions are applied to simulate different tectonic settings (see Table 4.3). These are specified as a constant strain-rate in LaMEM. The method of implementing a pure shear strain-rate velocity boundary condition is visualized in Figure 4.2, while the implementation of a simple shear boundary condition is visualized in Figure 4.3.

A post-processing script is then developed to calculate the finite strain and extract the contact mesh for the thin stiff layer. The finite strain is calculated as a passive marker and with the velocity gradient tensor ($\mathbf{L}$) bi-linearly interpolated. To test the degree of strain partitioning, the supervoxel segmentation method is applied to the deformation field for the different geodynamic models across the thin stiff layer folding. This is applied using either the criteria of kinematic vorticity (W_k) or the strain ellipsoid shape ($\log J$) to

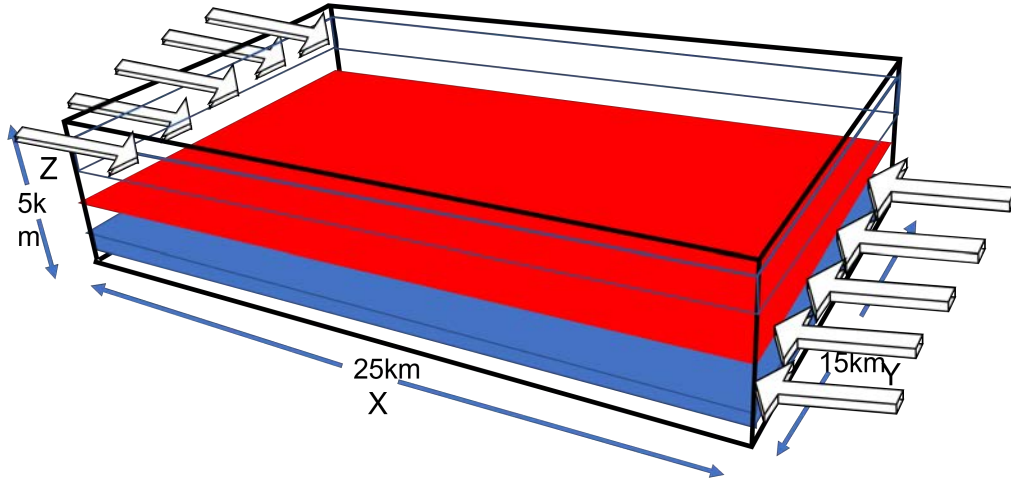


Figure 4.2: The model setup for the Compression/Pure Shear three-dimensional mechanical model. A constant $\dot{\epsilon}_{xx} = -1 \times 10^{-15} \text{s}^{-1}$ velocity boundary condition is used. Free slip boundary conditions are used for the front and back ($Y = \text{minimum } y$ and $Y = \text{maximum } y$), while no slip conditions are used for the left and right ($X = \text{minimum } x$ and $X = \text{maximum } x$). The top boundary is free slip with the bottom boundaries varied between no slip and free slip conditions. The blue layers correspond to thick stiff layers, while the red layers correspond to the very stiff thin layers (see Table 4.2)

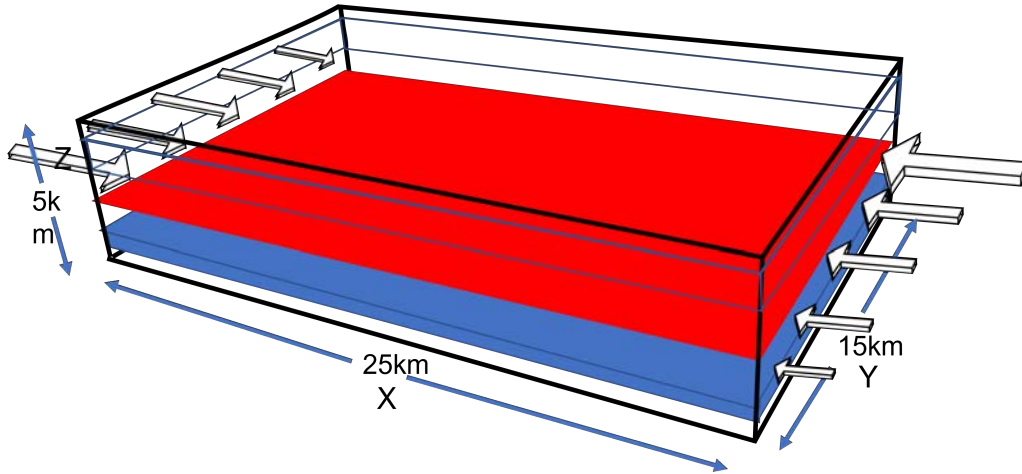


Figure 4.3: The model setup for the Strike-Slip/Simple Shear three-dimensional mechanical model. A constant $\dot{\epsilon}_{xy} = -1 \times 10^{-15} \text{s}^{-1}$ velocity boundary condition is used. Free slip boundary conditions are used for the front and back ($Y = \text{minimum } y$ and $Y = \text{maximum } y$), while no slip conditions are used for the left and right ($X = \text{minimum } x$ and $X = \text{maximum } x$). The top boundary is free slip while the bottom is no slip. Note the change in magnitude of the velocity along the left and right sides for the implementation of simple shear strain rates. The blue layers correspond to thick stiff layers, while the red layers correspond to the very stiff thin layers (see Table 4.2).

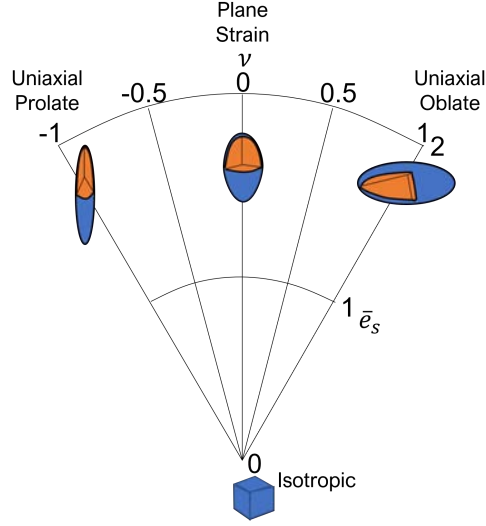


Figure 4.4: The Nadai-Hsu diagram for strain, where ν is Lode's ratio (Equation 4.3) and $\bar{e}_s$ (Equation 4.2a) is the natural octahedral unit shear.

inform how the the interpretation in the field of vorticity should be coupled with cleavage and lineations. Finite strain characteristics are then visualized in Nadai-Hsu diagrams and a stereonet of the major principal strain axis orientation. The Nadai-Hsu diagram (Figure 4.4) plots the degree of strain by the natural octahedral unit shear along its radial axis and how prolate or oblate the finite strain ellipsoid is along its circumference. Here the natural octahedral unit shear $\bar{e}_s$ is defined as:

$$\bar{e}_s = \frac{\sqrt{3}}{2} \bar{\gamma}_{\text{oct}}, \quad (4.2a)$$

$$\bar{\gamma}_{\text{oct}} = \frac{2}{3} \sqrt{(\bar{e}_1 - \bar{e}_2)^2 + (\bar{e}_2 - \bar{e}_3)^2 + (\bar{e}_3 - \bar{e}_1)^2}. \quad (4.2b)$$

where $\bar{e}_s$ are the natural principal strains. The natural octahedral unit shear $\bar{e}_s$ is then plotted against the Lode parameter (ν) defined as:

$$\nu = \frac{2\bar{e}_2 - \bar{e}_1 - \bar{e}_3}{\bar{e}_1 - \bar{e}_3} \quad (4.3)$$

The topology of the regions are then highlighted using the contact surface area between regions. This combined with finite strain characteristics gives an automated method of how strain partitioned domains are configured and also a visualization of the complexity or degree of partitioning. The network analysis could also be used an indication of how fluid-mass transfer could behave for a given tectonic setting [16; 17]. Moreover, the distribution of (W_k) and $(\log J)$ within each region is visualised using a swarm chart. These measures are related to deformation scale by using the convolution operation. The smallest distance between the centroid of the regions between the full resolution and larger scale averaged model are used to name the averaged model regions so that they can be compared to each other. The nature of multi-scale curvature is then compared against this deformation by

using a K -means segmentation of the Gaussian curvature (κ_{gauss}). How this multi-scale curvature can be specified to different scales, is then demonstrated by applying the K -means segmentation to subset of smaller wavelengths too.

4.3 Results

4.3.1 Geometric Synthetic Test Surface

The results for the surface structural complexity are calculated using a set of the 500 largest eigenvalues and summing the pairwise cosine distance for each triangulated face across the reconstructed mesh. The surface complexity across the three models shows the lowest cosine distance sums in the saddle regions. The intermediate F_2 wavelength model (middle Figure 4.5) shows the hinge zone of the domes having a lower cosine distance sum, while the largest F_2 wavelength model (right Figure 4.5) shows the high cosine distance sum concentrating around the limbs of folds.

In terms of the harmonic scale of each model, 10 contours of the Fiedler vector $\mathbf{e}_F$ together with the eigenvalue λ_2 are shown in Figure 4.6. The eigenvalue scales range from 4.8π to 0.11π . The direction of the eigenvector contours gives the ordering of the vertices which preserves the Laplacian weighting relationships. The narrow XY spacing of the contours in Model 1 conforms with the smaller $\mathbf{C}_2$ (Table 4.1) value and the larger eigenvalue since there is a higher frequency superposition. The trend towards a lower frequency superposition in Model 3 shows how the larger $\mathbf{e}_3$ produces contours that vary in width according to flow direction.

The maximum (κ_{max}) and minimum (κ_{min}) principal curvature are also computed to demonstrate how they are different from our cosine distance sum [18]. The κ_{max} and κ_{min} magnitude values can be seen to correspond well to hinge zones, while the cosine distance sum extreme values correspond to limb zones Figure 4.7.

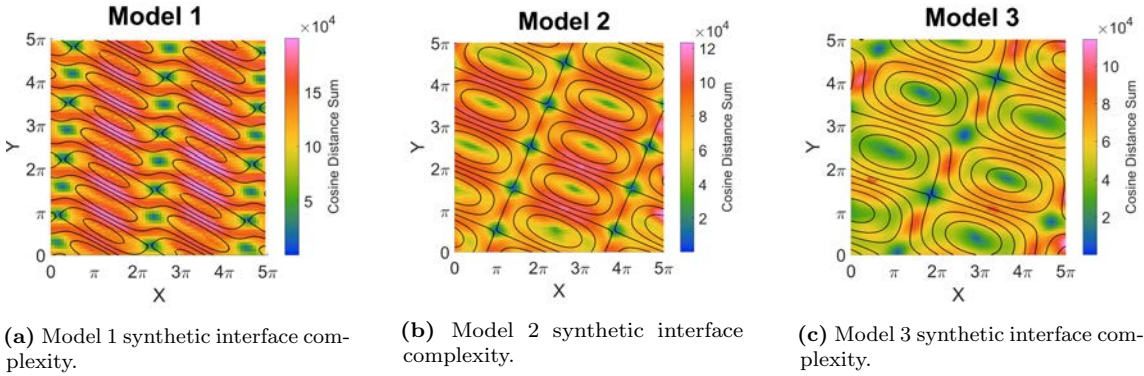


Figure 4.5: Synthetic Interface Complexity using the cosine distance sum with height contour intervals of 2. Note that fold limbs have greatest orientation variability across scales, while hinge zones have least.

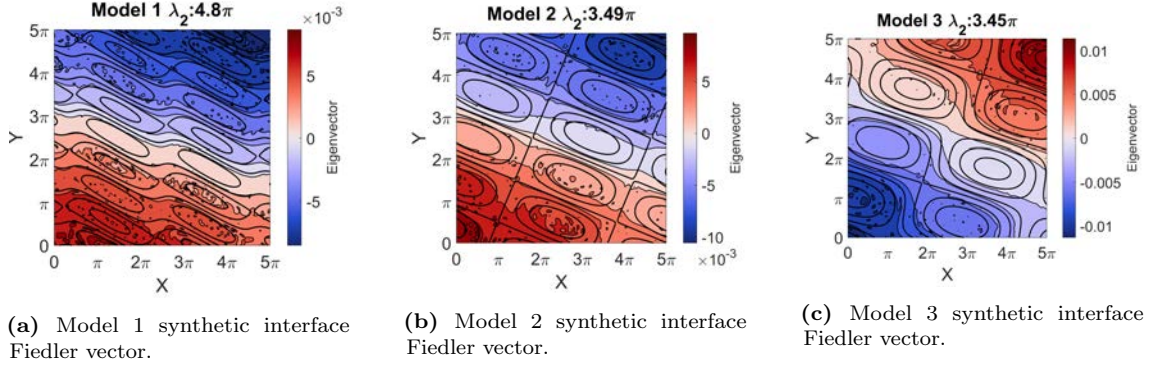


Figure 4.6: Eigenvector contours for the three models for the second largest eigenvalue (Fiedler vector) Section 2.3.2.

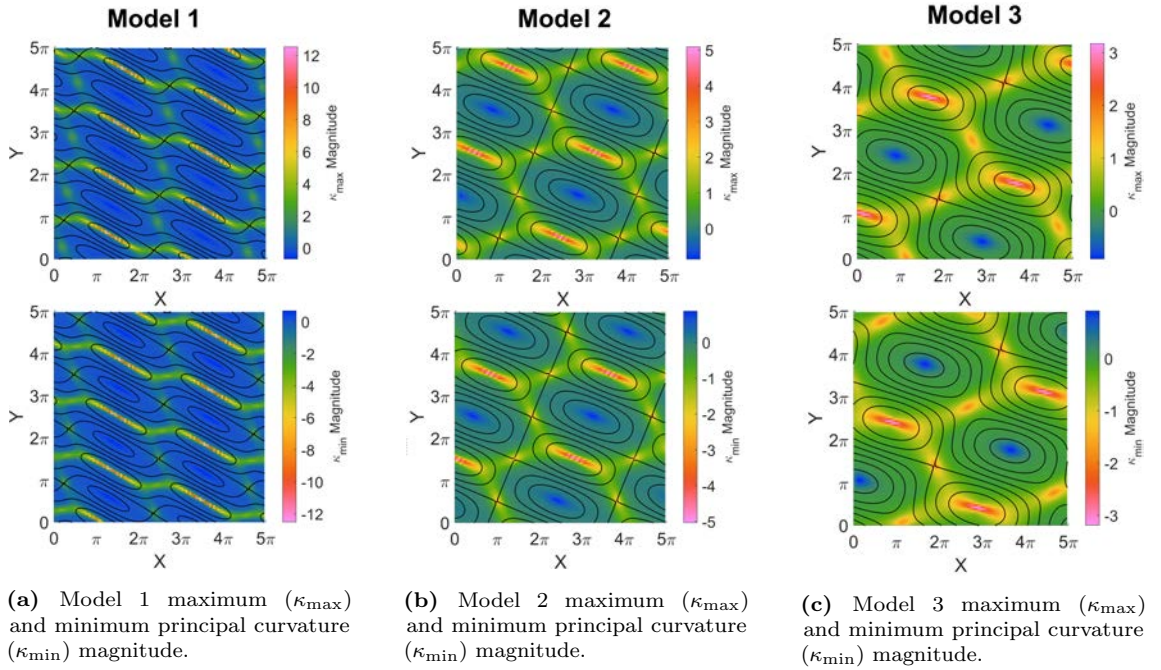


Figure 4.7: The magnitude of the (top row) maximum ($\kappa_{\max}$) and (bottom row) minimum principal curvature ($\kappa_{\min}$). Note how hinge zones are highlighted.

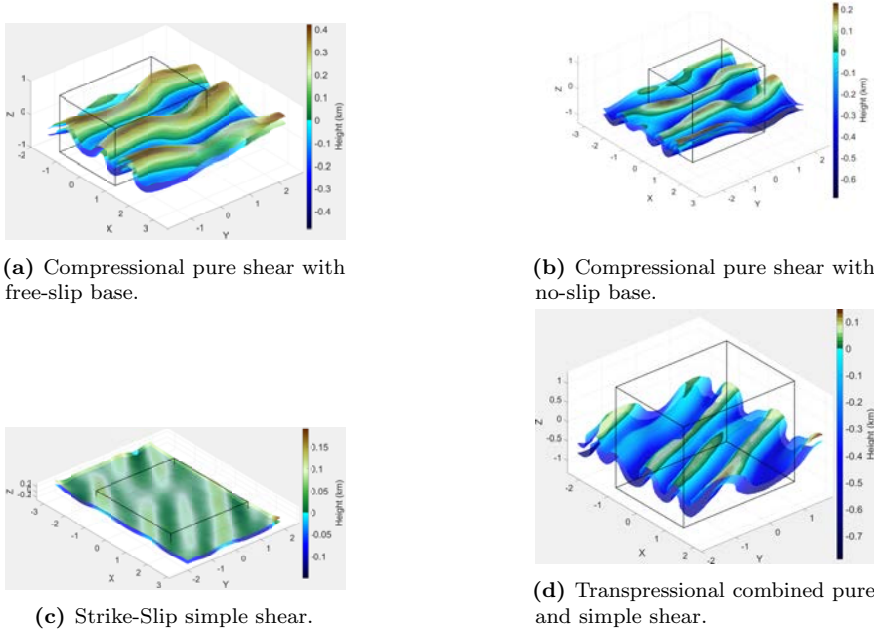


Figure 4.8: LaMEM models (see Table 4.3) after 15.1562Myr. Black outlines are finite strain passive marker extent. Note that Figure 4.8b is more folded than Figure 4.8a, and that both Figure 4.8c and Figure 4.8d have oblique folds.

4.3.2 Geodynamic Three-dimensional Mechanical Model

The models were run for 20 Myrs and each ran for approximately 24 hours on an Intel i9-10900KF desktop. The results for the four models in Table 4.3 after 15.1562Myr is visualized in Figure 4.8. The free-slip base in Figure 4.8a is observed to be less folded compared to the no-slip base in Figure 4.8b, which is consistent with the motivation that a no-slip base may act as a detachment. The strike-slip case in Figure 4.8c has much less fold growth in the Z direction compared to the other models, but the oblique orientation of the axis is consistent with shear zone fold development [3; 6]. The results for the strain partitioning in the Pure Compression free-slip model are presented in detail and compared against the Transpression model, since these models have the most pronounced amount of hinge rotation and closely resemble a poly-clinal structure. For completeness, the strain partitioning and curvature segmentation figures for the Simple Shear Strike-Slip (Appendix C), the Pure Compression no-slip base (Appendix B), and Pure Compression free-slip base (Appendix A), Transpression (Appendix D) figures not discussed here are included as appendices.

4.3.3 Compressional Pure Shear with free-slip base

There are two anticlines that are outlined Figures 4.9b and 4.15b. One anticline (Clusters 13, 8 and 11 in Figure 4.9b and Clusters 12 and 13 in Figure 4.15b) is more symmetric and has a higher strain that is flattening Figure 4.11a. The other anticline (Clusters 15 and 13 in Figure 4.9b and Clusters 16 and 15 in Figure 4.15b) has a more periclinal structure and rotated hinge region. This has lower overall strain that is constrictional Figure 4.11a.

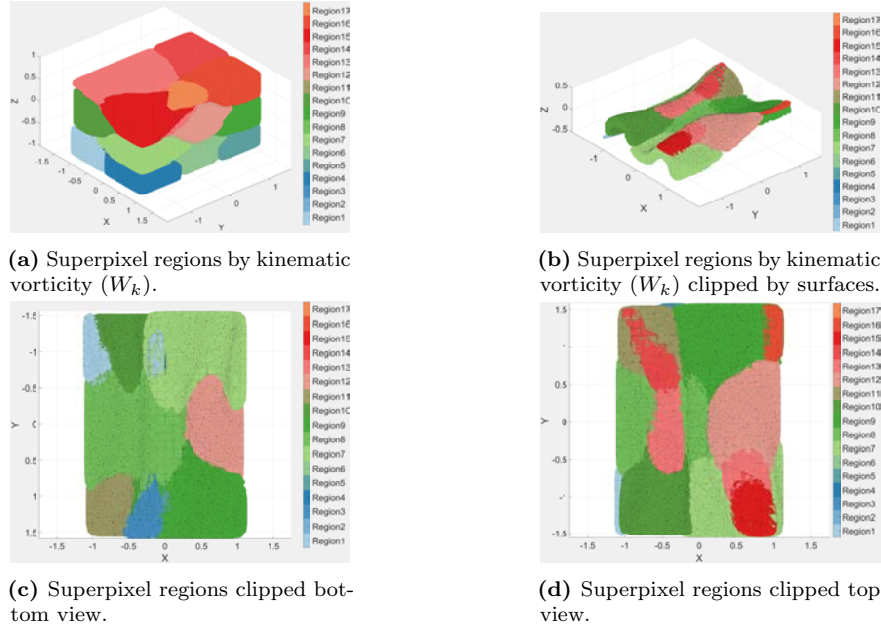


Figure 4.9: Compression pure shear with free-slip base boundary condition after 15.1562Myr. Superpixel region results using kinematic vorticity (W_k) at full marker resolution. Two anticlinal ridges develop: one more symmetric (regions 10, 13, 14) and one more asymmetric (regions 12, 13, 15).

When comparing the W_k to the $\log J$ Figure 4.15b the asymmetry of the rightmost anticline can be observed to be better demonstrated by the $\log J$ segmentation.

Moreover, between Figure 4.9c and Figure 4.15c, the segmentation based on $\log J$ more closely separates the synclinal region than the W_k segmentation. The rotation of the hinge in the right-most anticline in Figure 4.15d is also more accurately separated rather than in Figure 4.9d. Moreover, the curvature of the upper contact surface in Figure 4.10c also reflects the hinge-rotation and corresponds to the $\log J$ better too. This is consistent with the instantaneous nature of W_k as a measure of strain partitioning since the progressive rotation of structure will accumulate through finite strain and thus more representative through $\log J$.

In comparing Figure 4.10d to Figure 4.13d, the region around $(X = -0.5, Y = -0.5)$, it can be observed that the cluster $K = 3$ is larger in the smaller eigenvalue set. This is along the anti-clinal ridge and demonstrates multi-scale curvature behaving as expected.

To compare the full and average resolution superpixel regions, a single region's shape and extent is compared in Figure 4.16 and Figure 4.17. When using kinematic vorticity W_k as the criteria for partitioning, the region extent is relatively stable when compared to partitioning based on $\log J$.

4.3.4 Transpressional combined Pure and Simple Shear

The variability in Nadai-Hsu strain and PSA1 orientation within in the transpression model shows how potentially more likely dilatational jogs would form along hinge-parallel structures Figure 4.20a and Figure 4.20b. Moreover by comparing Figures 4.21 and 4.23 with Figures 4.12 and 4.14, the cluster centres for the transpressive surface curvature

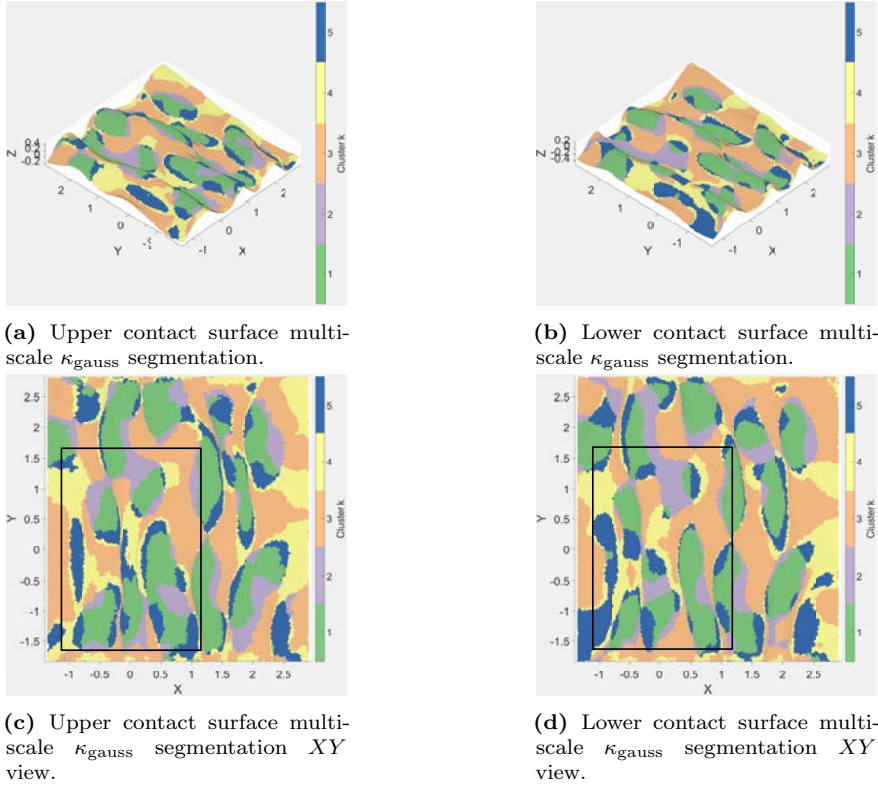
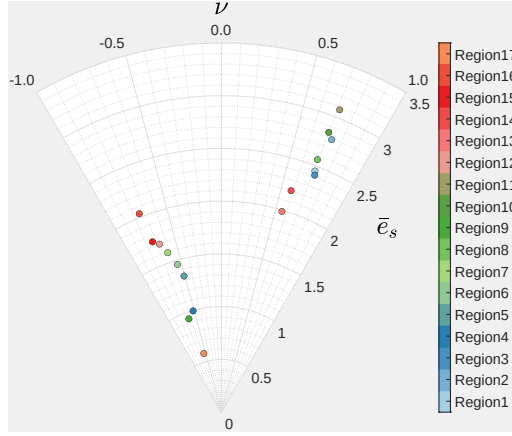


Figure 4.10: Compression pure shear with free-slip base boundary condition after 15.1562Myr. Multi-scale Gaussian(κ_{gauss}) curvature segmentation. The range of eigenvalues that form the basis is **min** $\lambda_2 = 1.77$ km to **max** $\lambda_{150} = 0.13$ km, with $K = 5$ clusters.

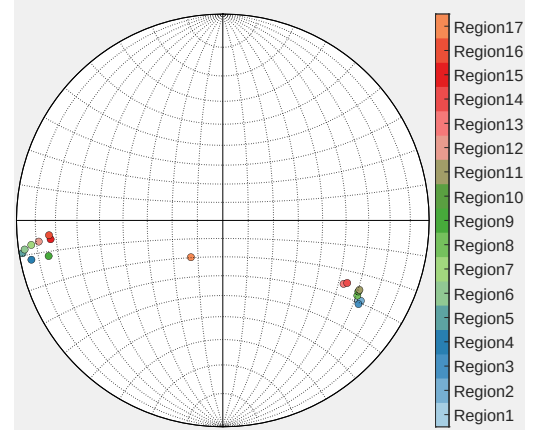
appear to have greater variability across scales. This is important since when compared to the Pure Compression case, multi-scale curvature appears to have distinct characteristics between them even though it is a purely geometric measure. Moreover, when comparing the curvature segmentation regions upper and lower contact of the Pure Compression free-slip model (Figure 4.10 and Figure 4.13), the transpression model does not have as clear correspondence between upper and lower surfaces (Figure 4.19 and Figure 4.22). The curvature segmentation between the two sets of eigenvalues in Figure 4.19 and Figure 4.22 show that in the transpressive case how sensitive the curvature is scale compared to the compressive.

Moreover, the benefit of using the strain ellipsoid shape $\log J$ over the kinematic vorticity W_k is even more significant for the transpressional case as demonstrated by Figure 4.18 and Figure 4.24. The strain ellipsoid shape $\log J$ regions from the bottom contact in Figure 4.24c partition along the anticlinal region 5 and the synclinal region 4, while W_k doesn't distinguish between these in Figure 4.18c. It should be noted that both partitions separate along the fold axis in the East-West direction, which would be the case for the different coaxial regions across a hinge rotation.

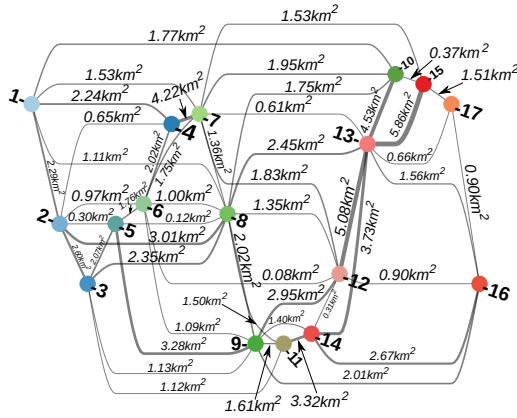
The larger scale averaged $\log J$ partitioning in Figure 4.25 shows separation along the hinges. Moreover, the path between regions 2a and 2b to 5a and 5b follows parallel to the hinges in Figure 4.25c and Figure 4.25d. By considering the topology of Figure 4.26c, regions 3 and 6 are potential dilational stepovers given how shallowly dipping the PSA1



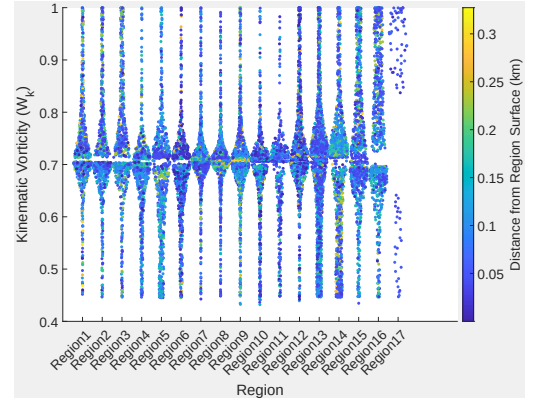
(a) Nadai-Hsu finite strain for kinematic vorticity (W_k) regions.



(b) Orientation of the major principal strain axis for kinematic vorticity (W_k) regions.



(c) Topology by contact surface area for kinematic vorticity (W_k) regions.



(d) Swarm chart for kinematic vorticity of the passive markers in each region .

Figure 4.11: Compression pure shear with free-slip base boundary condition after 15.1562Myr. Strain region analysis for kinematic vorticity(W_k) at full marker resolution (Figure 4.9).

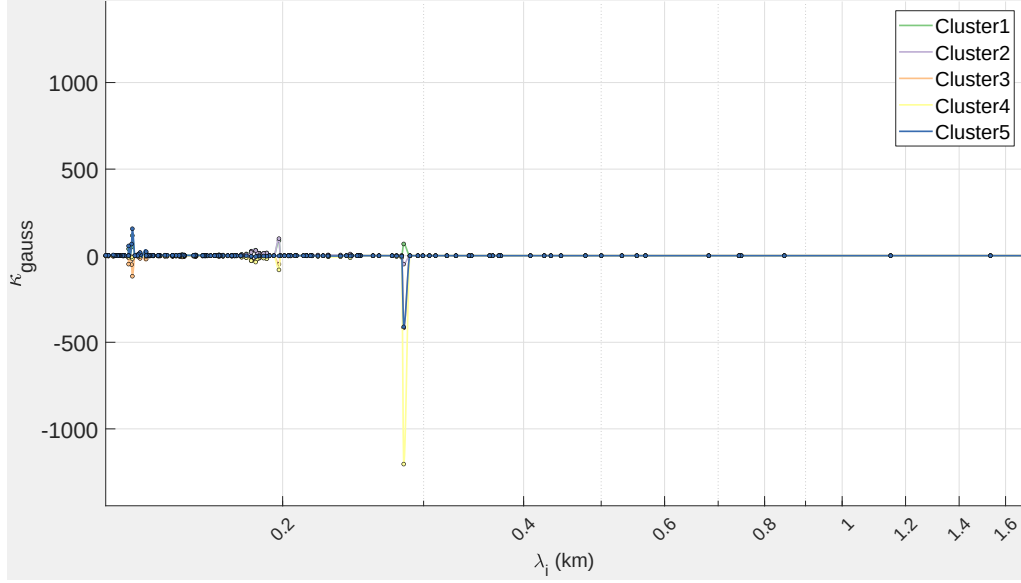
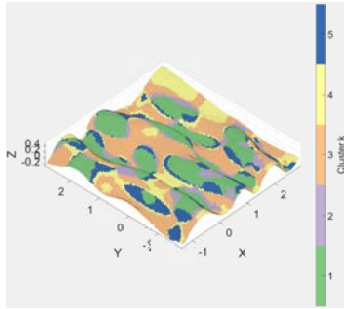
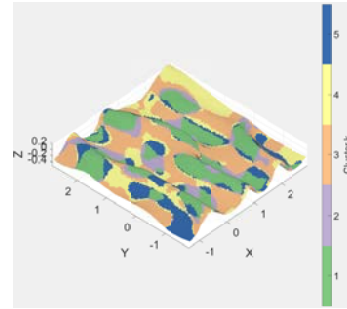


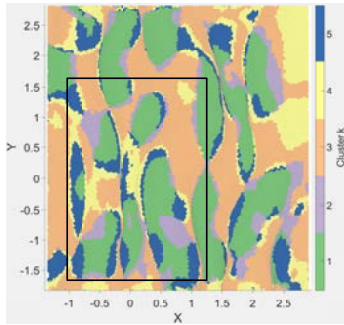
Figure 4.12: The cluster centres of the Gaussian(κ_{gauss}) curvature segmentation for the Compression pure shear with free-slip base boundary condition model(Figure 4.10). Each cluster is a $148 = (150 - 2)$ dimensional vector where each dimension corresponds to a κ_{gauss} value. Note that $\kappa_{\text{gauss}} < 0$ values imply that locally the shape is saddle-shaped and $\kappa_{\text{gauss}} > 0$ values imply the shape is locally dome/basin (Figure 2.6).



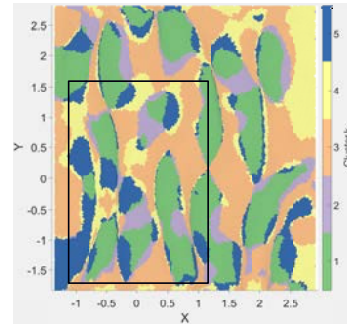
(a) Upper contact surface multi-scale κ_{gauss} segmentation.



(b) Lower contact surface multi-scale κ_{gauss} segmentation.



(c) Upper contact surface multi-scale κ_{gauss} segmentation XY view.



(d) Lower contact surface multi-scale κ_{gauss} segmentation XY view.

Figure 4.13: Compression pure shear with free-slip base boundary condition after 15.1562Myr. Multi-scale Gaussian(κ_{gauss}) curvature segmentation. The range of eigenvalues that form the basis is **min** $\lambda_{61} = 0.21$ km to **max** $\lambda_{150} = 0.13$ km, with $K = 5$ clusters.

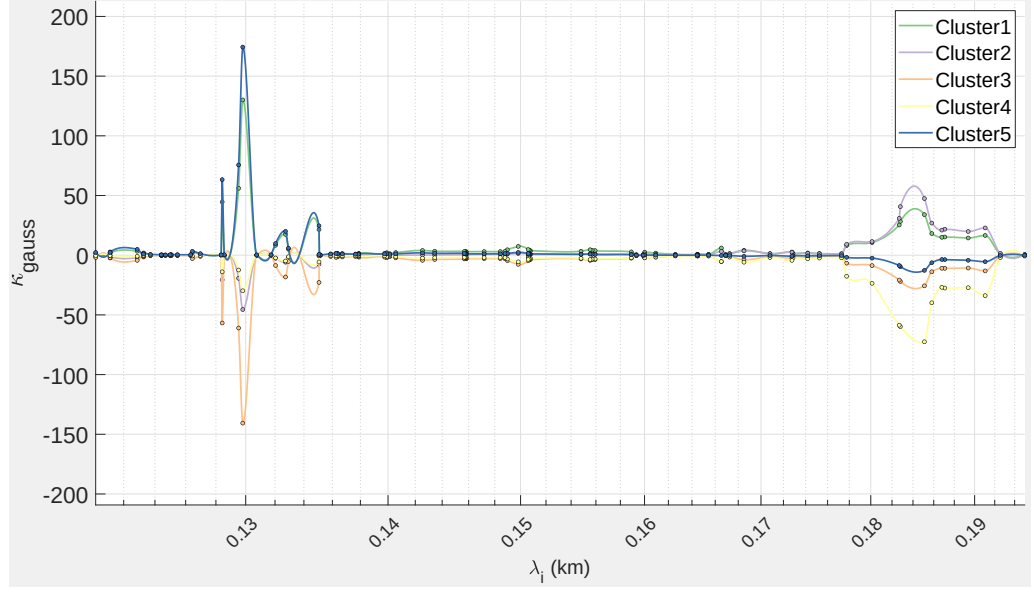
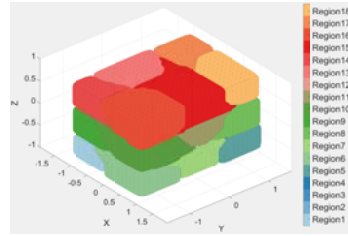
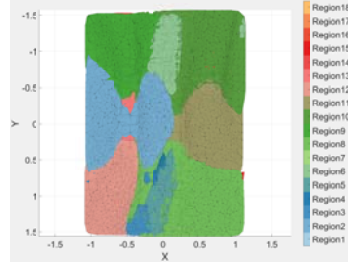


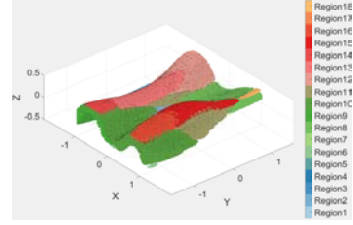
Figure 4.14: The cluster centres of the Gaussian(κ_{gauss}) curvature segmentation for the Compression pure shear with free-slip base boundary condition model (Figure 4.13). Each cluster is a $89 = (150 - 61)$ dimensional vector where each dimension corresponds to a κ_{gauss} value. Note that $\kappa_{\text{gauss}} < 0$ values imply that locally the shape is saddle-shaped and $\kappa_{\text{gauss}} > 0$ values imply the shape is locally dome/basin (Figure 2.6).



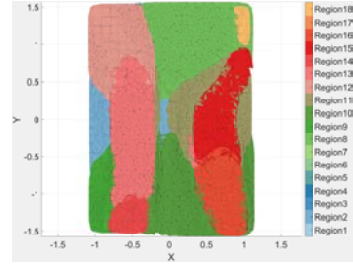
(a) Superpixel regions by strain ellipsoid shape ($\log J$).



(c) Superpixel regions clipped bottom view.

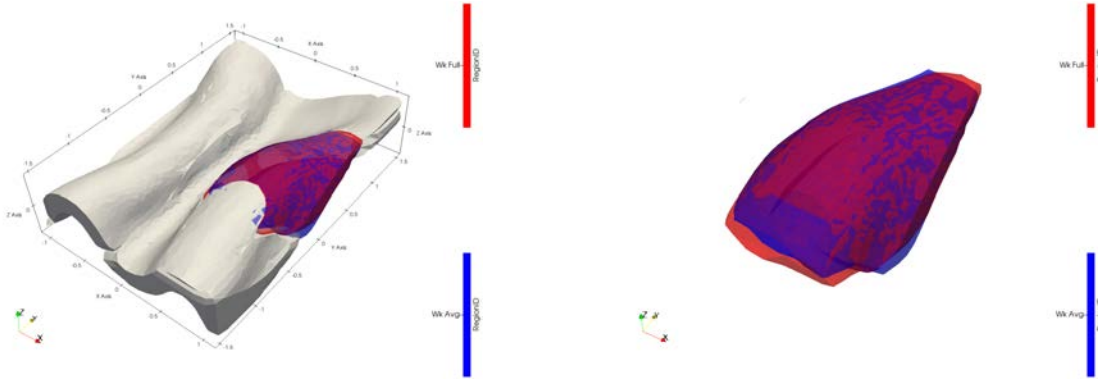


(b) Superpixel regions by strain ellipsoid shape ($\log J$) clipped by surfaces.



(d) Superpixel regions clipped top view.

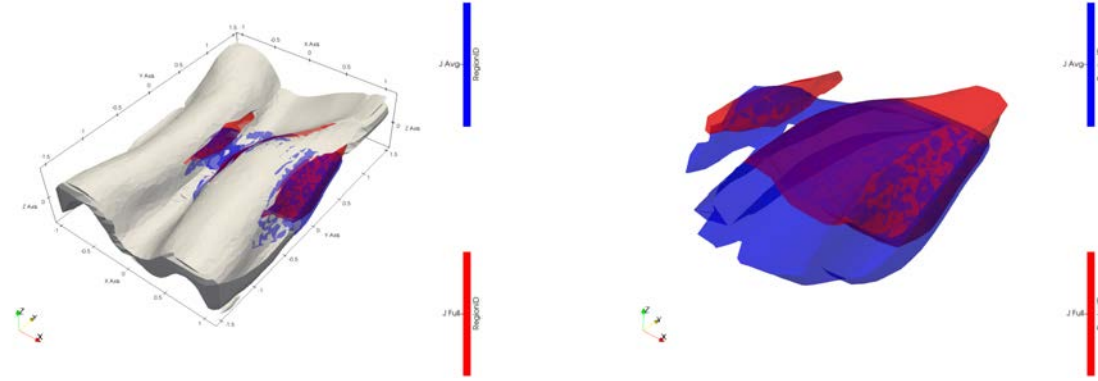
Figure 4.15: Compression pure shear with free-slip base boundary condition after 15.1562Myr. Superpixel region results using strain ellipsoid shape ($\log J$) at full marker resolution. Two anticlinal ridges develop: one more symmetric (regions 12, 13, 14) and one more asymmetric (regions 13, 15, 16). The rotation of the hinge region is more partitioned here (region 15) than in Figure 4.9.



(a) Figure 4.9d and Figure A.1d superpixel region 12 wide view.

(b) Figure 4.9d and Figure A.1d superpixel region 12 zoom view.

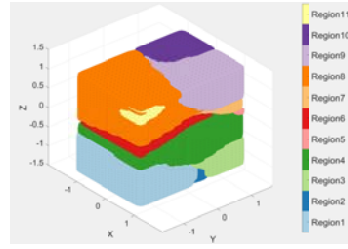
Figure 4.16: Comparison of full and average resolution for superpixel region 12 using W_k . Note that the extents and shape are similar between the two resolution scales.



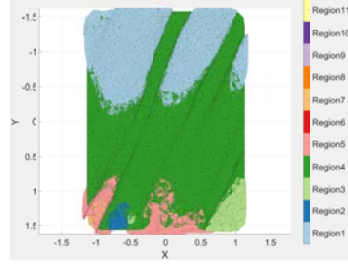
(a) Figure 4.15d and Figure A.4d superpixel region 11 wide view.

(b) Figure 4.15d and Figure A.4d superpixel region 11 zoom view.

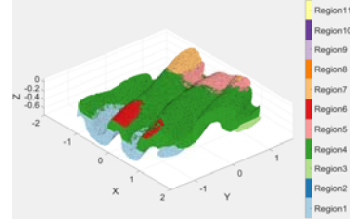
Figure 4.17: Comparison of full and average resolution for superpixel region 11 using $\log J$. Note that the full resolution (smaller scale) separates across the syncline while the average is connected. Moreover, the average resolution (larger scale) has a larger extent and is less elongate than the full.



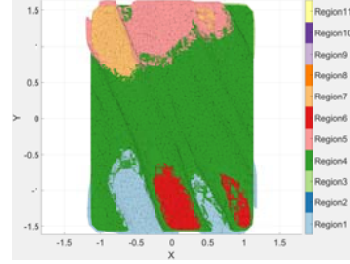
(a) Superpixel regions by kinematic vorticity(W_k).



(c) Superpixel regions clipped bottom view.

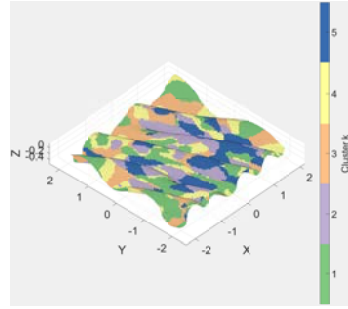


(b) Superpixel regions by kinematic vorticity(W_k) clipped by surfaces.

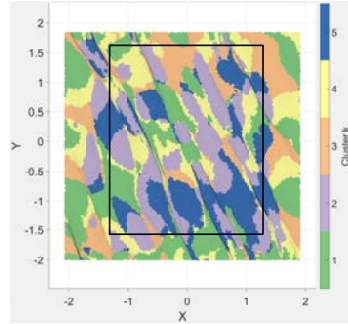


(d) Superpixel regions clipped top view.

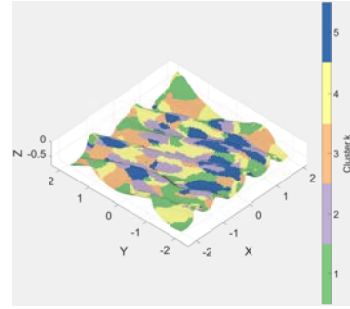
Figure 4.18: Transpressional with both pure and simple shear boundary condition after 15.1562Myr. Superpixel region results using kinematic vorticity(W_k) at full marker resolution.



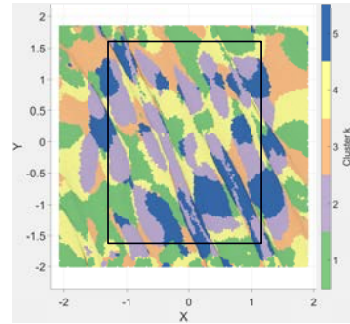
(a) Upper contact surface multi-scale κ_{gauss} segmentation.



(c) Upper contact surface multi-scale κ_{gauss} segmentation XY view.



(b) Lower contact surface multi-scale κ_{gauss} segmentation.



(d) Lower contact surface multi-scale κ_{gauss} segmentation XY view.

Figure 4.19: Transpressional with both pure and simple shear boundary condition after 15.1562Myr. Multi-scale Gaussian(κ_{gauss}) curvature segmentation. The range of eigenvalues that form the basis is $\min \lambda_2 = 1.77 \text{ km}$ to $\max \lambda_{150} = 0.13 \text{ km}$, with $K = 5$ clusters.

4. NUMERICAL MODELLING

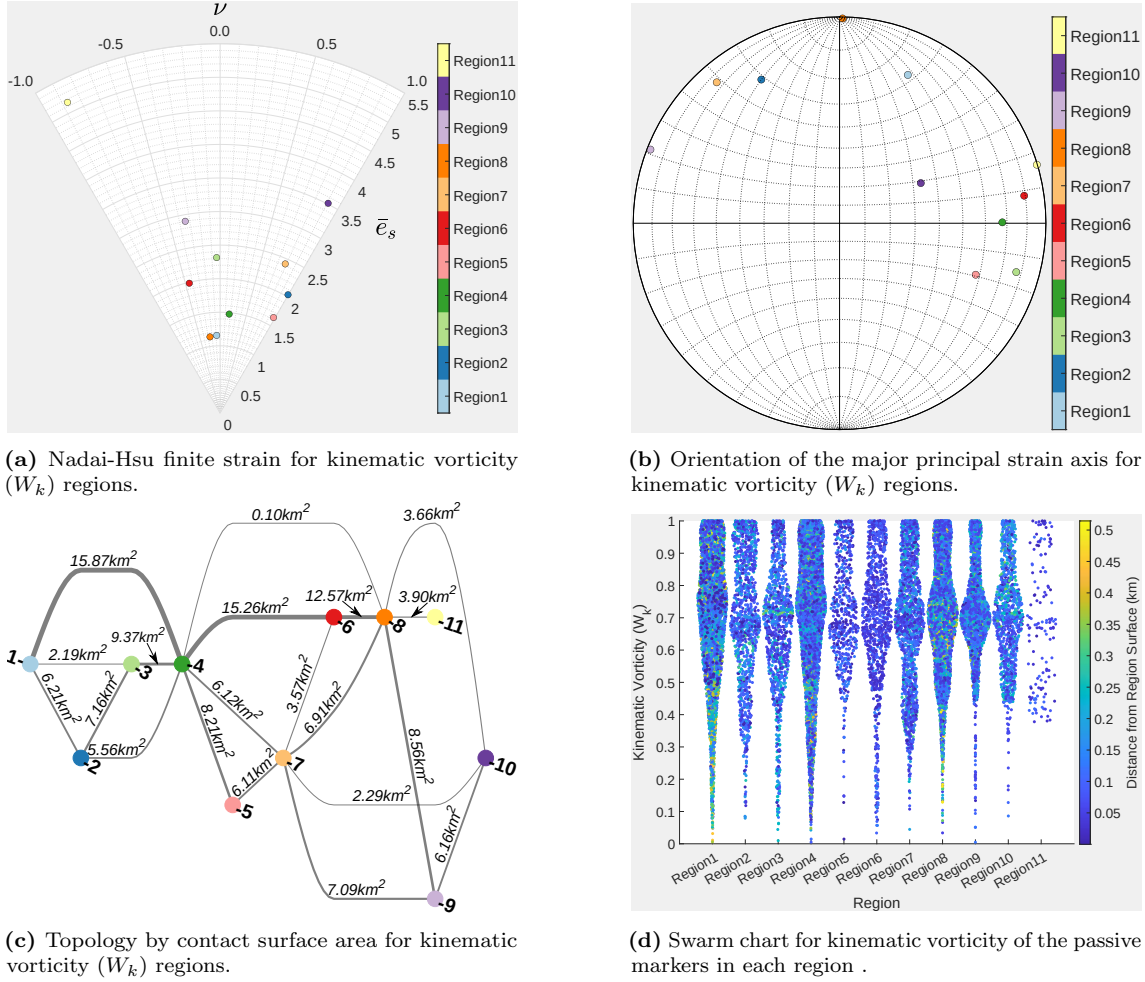


Figure 4.20: Transpressional with both pure and simple shear boundary condition after 15.1562Myr. Strain region analysis for kinematic vorticity (W_k) at full marker resolution (4.18).

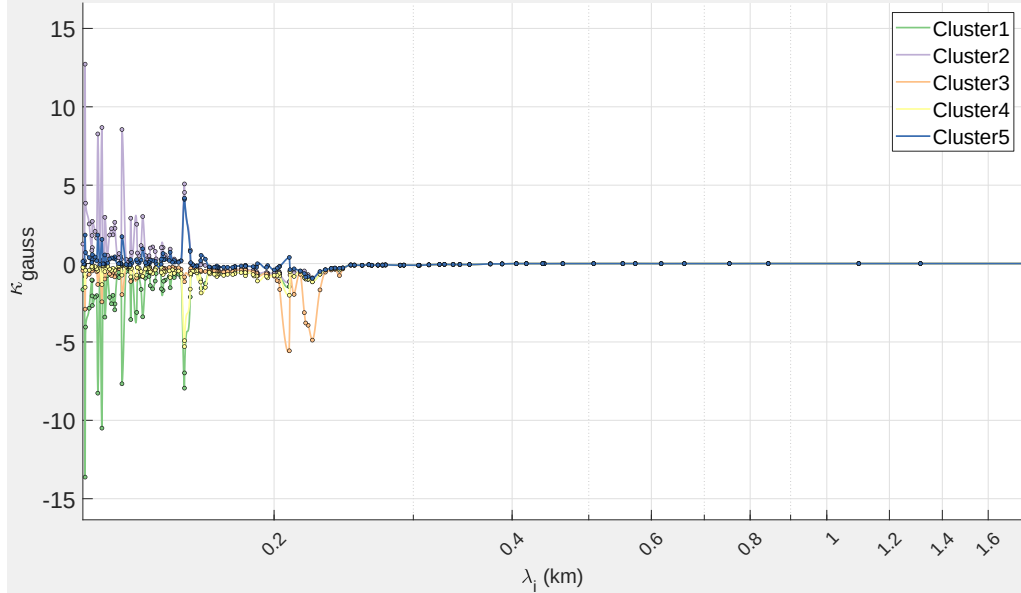


Figure 4.21: The cluster centres of the Gaussian (κ_{gauss}) curvature segmentation for the transpression pure and simple shear boundary condition model(4.19). Each cluster is a 148 = (150 - 2) dimensional vector where each dimension corresponds to a κ_{gauss} value. Note that $\kappa_{\text{gauss}} < 0$ values imply that locally the shape is saddle-shaped and $\kappa_{\text{gauss}} > 0$ values imply the shape is locally dome/basin (2.6).

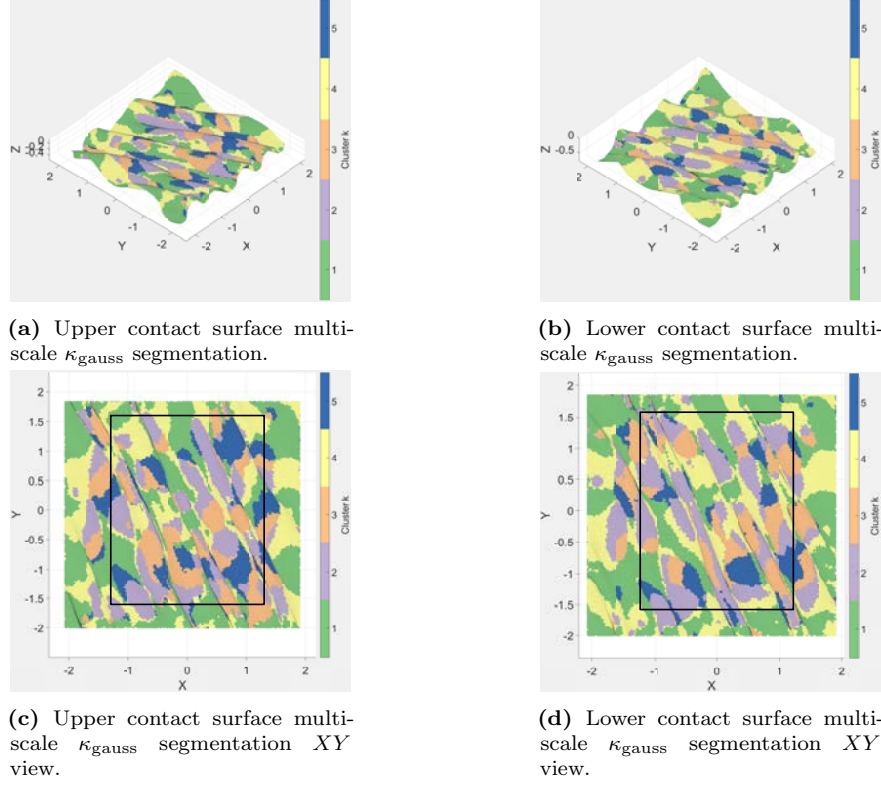


Figure 4.22: Transpressional with both pure and simple shear boundary condition after 15.1562Myr. Multi-scale Gaussian(κ_{gauss}) curvature segmentation. The range of eigenvalues that form the basis is $\min \lambda_{61} = 0.21$ km to $\max \lambda_{150} = 0.13$ km, with $K = 5$ clusters.

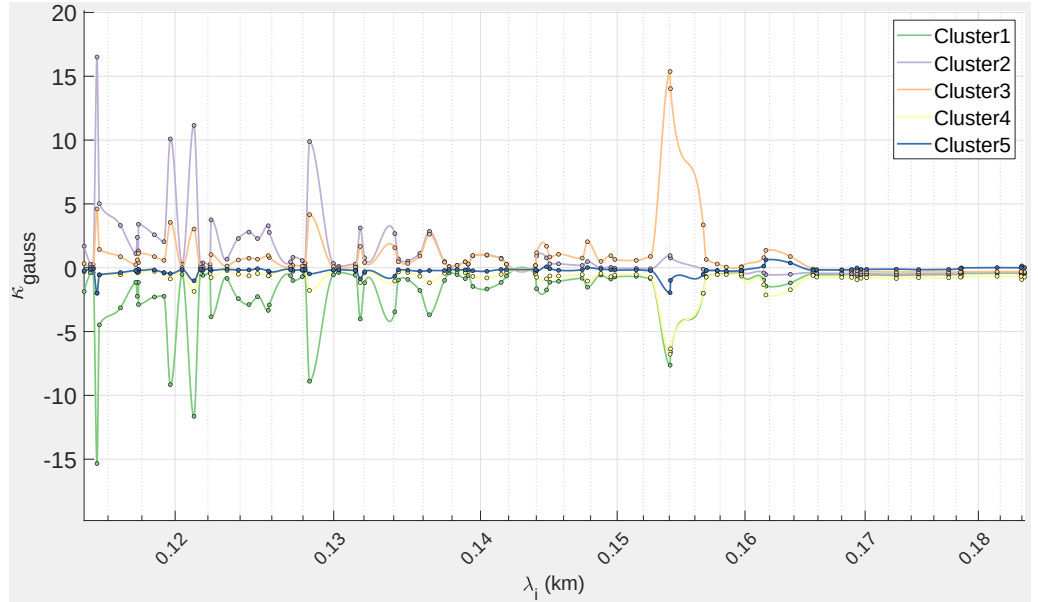
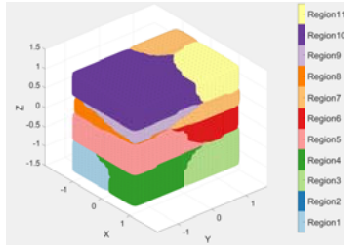
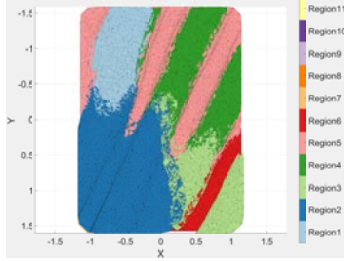


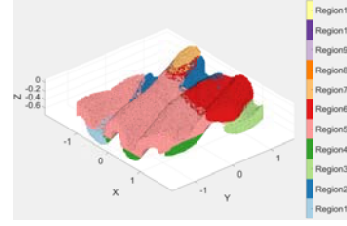
Figure 4.23: The cluster centres of the Gaussian(κ_{gauss}) curvature segmentation for the transpression pure and simple shear boundary condition model (4.22). Each cluster is a $89 = (150 - 61)$ dimensional vector where each dimension corresponds to a κ_{gauss} value. Note that $\kappa_{\text{gauss}} < 0$ values imply that locally the shape is saddle-shaped and $\kappa_{\text{gauss}} > 0$ values imply the shape is locally dome/basin (2.6).



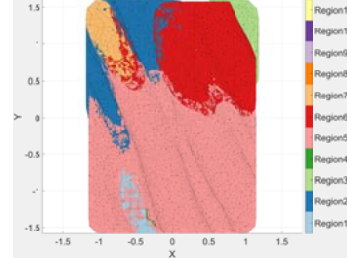
(a) Superpixel regions by strain ellipsoid shape ($\log J$).



(c) Superpixel regions clipped bottom view.



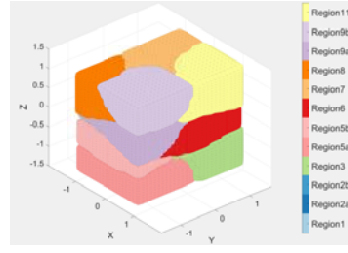
(b) Superpixel regions by strain ellipsoid shape ($\log J$) clipped by surfaces.



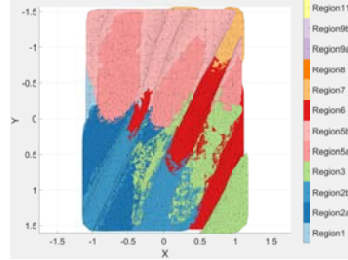
(d) Superpixel regions clipped top view.

Figure 4.24: Transpressional with both pure and simple shear boundary condition after 15.1562Myr. Superpixel region results using strain ellipsoid shape ($\log J$) at full marker resolution.

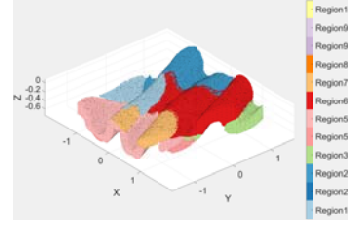
axis is relative to $2a/2b$ and $5a/5b$ PSA1 axis.



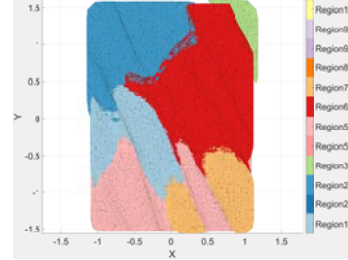
(a) Superpixel regions by strain ellipsoid shape ($\log J$).



(c) Superpixel regions clipped bottom view.

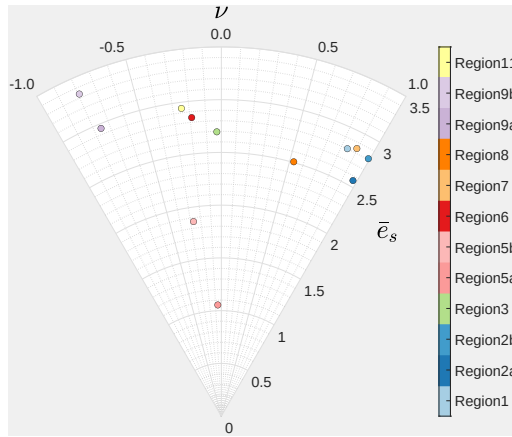


(b) Superpixel regions by strain ellipsoid shape ($\log J$) clipped by surfaces.

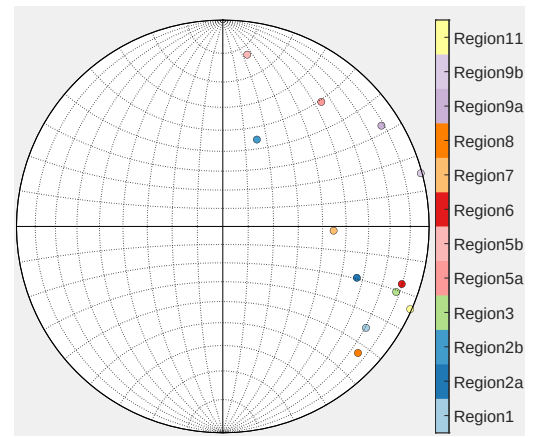


(d) Superpixel regions clipped top view.

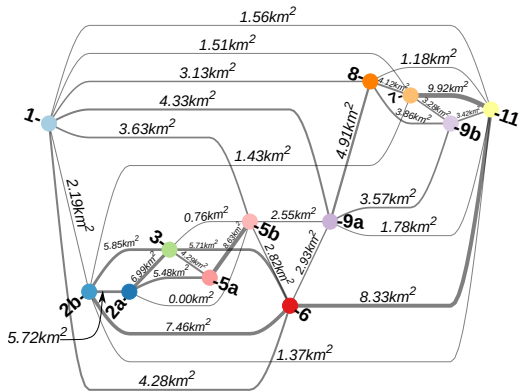
Figure 4.25: Transpressional with both pure and simple shear boundary condition after 15.1562Myr. Superpixel region results using strain ellipsoid shape ($\log J$) using a tensor convolution of size (5, 5, 5).



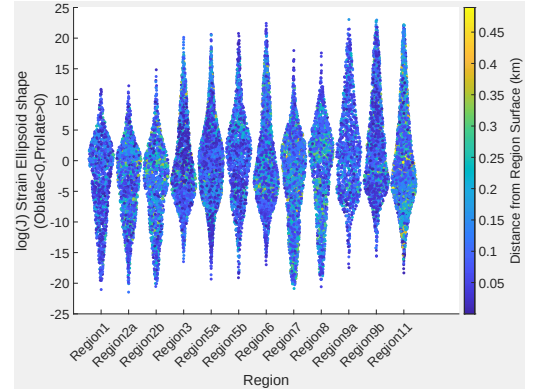
(a) Nadai-Hsu finite strain for strain ellipsoid shape ($\log J$) regions.



(b) Orientation of the major principal strain axis for strain ellipsoid shape ($\log J$) regions.



(c) Topology by contact surface area for strain ellipsoid shape ($\log J$) regions.



(d) Swarm chart for strain ellipsoid shape ($\log J$) of the passive markers in each region .

Figure 4.26: Transpressional with both pure and simple shear boundary condition strain region analysis for strain ellipsoid shape ($\log J$) using a tensor convolution of size (5, 5, 5) (4.25).

4.4 Discussion

A computational approach that can automatically determine strain partitioning from computational geodynamic models was presented and implemented. This was applied to a 3D thermo-mechanical model of viscous folding. This is also applied to the domain-ing/segmentation of the multi-scale curvature of the upper and lower contact surfaces based on the material markers from the numerical model. The criteria used for partitioning were the kinematic vorticity W_k and strain ellipsoid shape $\log J$, which align with the flow partitioning definition Lister and Williams [13]. Both of these methods are objective and repeatable and can be used to treat strain partitioning in a consistent manner across different scales. The automated curvature and strain partitioning was applied two different scales using the manifold harmonic transform and Riemannian manifold tensor averaging respectively. Both of these multi-scale computational methods have never been applied to structural geology or geodynamics.

The relationship between material scale and rheology is an active area of research [24], but as far as studies that consider the macroscopic scale of deformation and the scale-dependencies of observations there are few [23]. Strain partitioning, which is closely related to the nature of deformation scale, in early studies was applied to micro-structure deformation mechanisms such as distinguishing between cataclasis and crystal plasticity [21]. There are few field studies that validate macroscopic strain partitioning with the microscopic, a notable exception being the study of Mitra [15] which validates the classic study of Cloos [4], but regional studies can be found in the literature, albeit without numerical validation [8; 9].

Using the superpixel method applied to the kinematic vorticity (W_k) and strain ellipsoid shape ($\log J$), the degree of strain partitioning within a regional deformation can be quantitatively and objectively demonstrated. The results confirm that transpressional deformation does have a greater degree of strain partitioning than pure compressional deformation, but also show that the simplification of zones of pure shear and localised planes of simple shear are not necessarily valid [10]. Moreover, it is also noted, that while the regional deformation in the pure compression case is coaxial in terms of the velocity boundary condition, locally structures can appear as transpressional. Thus, the need to quantitatively and statistically consider scale and strain partitioning should be applied more widely for regional studies.

A limitation of the numerical models is that only one competency contrast and thickness ratio is considered. An area for further study would be to consider how more competent layers would affect the degree of strain partitioning. Since this will include a greater degree of flexural slip strain partitioning would presumably increase too [5]. Moreover, using non-linear (power law) viscosities would also account for dislocation deformation mechanisms and would allow for an interesting approach to study on the degree of strain partitioning.

While velocity boundary conditions do you have the ability to apply a consistent regional deformation, how realistic this is for crustal plate motion should be studied

and developed further within geodynamic computational models. The validation of this numerical approaches though can only be achieved by testing how they scale to expected localised strain field observations though. The methods used in this chapter can be used to assist in this.

While velocity boundary conditions can apply a consistent regional deformation that can reliably be solved numerically, this isn't necessarily realistic for crustal plate kinematics and dynamics of crustal plate motion. These limitations of geodynamic numerical codes are often expressed in terms of strain compatibility and smoothly varying strain heterogeneity [11]. Numerical modelling that use a finite element though can often incorporate fairly complex geometric and boundary condition setups so that strain compatibility is ensured [19]. But in terms of scale, these finite element models often rely on weak seeds to induce brittle behaviour. While this allows for the development of strain partitioning, together with strain hardening mechanisms [14], this doesn't allow for the multi-scale viscous growth of instabilities that is so characteristic of ductile structures [2]. The development of multi-scale geometric and mechanics methods can be used for validating some of these finite element numerical approaches by testing how they scale to expected localised finite strain field observations. For example, observed structures such as anastomosing shear zone networks and their multi-scale S-C fabric development curvature.

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Chapter 5

Case Study: Padtherung Syncline

5.1 Introduction

The methods for multi-scale curvature are developed for a regional ductile structure in the Hamersley province, Western Australia. The regional geology and data used are first introduced. An implicit modelling approach using universal co-kriging is applied to generate the 3D model of the syncline. The multi-scale curvature is then applied and subsequent interpretation is presented.

5.2 Geology

The Padtherung Syncline[49] is found in the central Hamersley province, Western Australia (see Figure 5.1) and lies on the northern limb of the Wonmunna Anticline (see Figure 5.2). It consists of an E-W trending near horizontal doubly-plunging syncline. It is slightly north verging with a planar south dipping northern limb and a folded north dipping southern limb (see Figure 5.3).

The syncline has outcropping of the economically important Mt Newman member bedrock of the Marra Mamba Iron Formation which is overlain by the West Angelas Member of the overlying Wittenoom Dolomite [30]. Moreover, cementation of the base of the detritals has formed an haematite-rich conglomerate commonly referred to as canga [23]. These detritals are a relatively small but important iron ore resource in the Hamersley province, Western Australia, derived from the breakdown of bedded ores, as well as BIF and shale units.

The rock units of the Hamersley province have gone through a number of compressional and extensional deformation events with only low grade metamorphic overprint, which I summarize in Table 5.1. The major deformation of the Hamersley group in the region is the Ophthalmian Orogeny which is dated to 2195-2145 Ma[41; 44]. This orogeny formed the Ophthalmian Fold Belt and is interpreted to record the collision of the Glenburgh Terrane to the southern margin of the Pilbara Craton[7; 49]. The intensity of deformation across the fold belt varies across the province, with the western-half being comprised of E-W trending dome and basin folds that have the Archean granitoid-greenstone basement

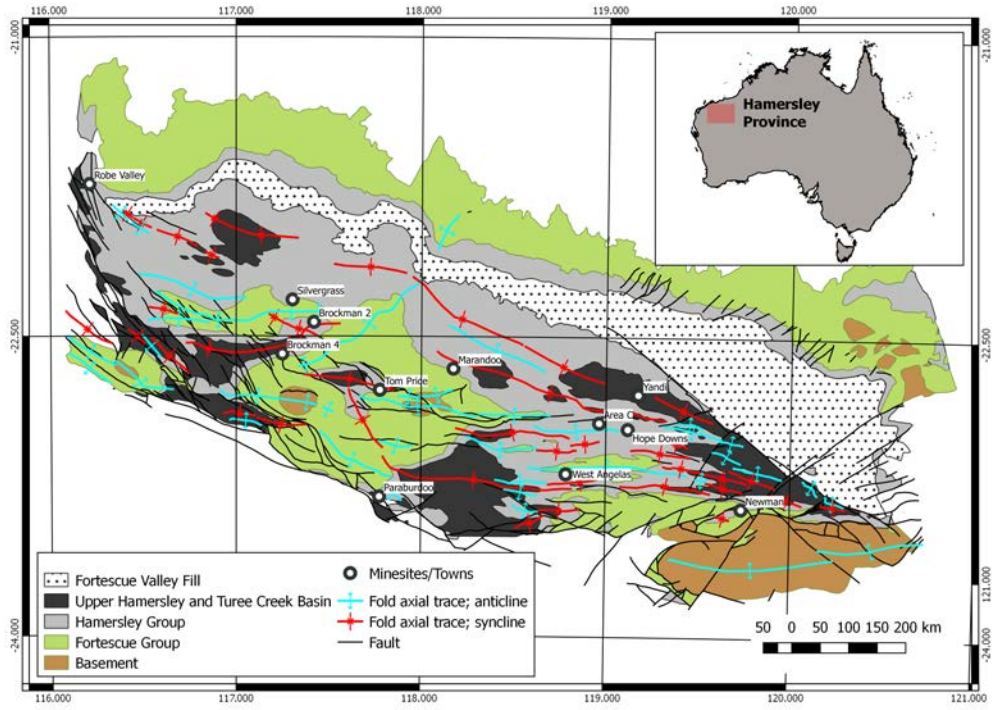


Figure 5.1: Geological map of the Hamersley province with major structures [16]

exposed in the core of the domes, and a E-W trending thin-skinned fold and thrust belt in the eastern-half, for example the Wonmunna Anticline [11]. The other major folding event for the region is the northwesterly trending 2.0 Ga Panhandle Orogeny (D3) [38; 39; 45]. The last deformational event of the region occurred during the Capricorn Orogeny (D4) around 1.78 Ga and is recorded in the southern margin of the Hamersley Province by minor N-W trending folds and a tilt towards the SW [24; 49]. While the E-W large-scale upright D2 are easily distinguishable, the coaxial D3 Panhandle and D4 Capricorn are often difficult to differentiate [10; 11; 45]. The D3 Panhandle folding, while particularly well developed in the western Turner and Brockman syncline [11], is less pronounced in the central and eastern region so that northwesterly trending folding has also been interpreted as the result of progressively deformed D2 structures that have been re-oriented [6].

Mapping Data The input data used for the three-dimensional implicit geological modelling (Universal Co-Kriging) is outlined here. The input data used is the field measurements of bedding orientations together with bedding contacts are traces (strings) the points are extracted from map polygons.

Orientation data used for interpolation included 1677 bedding orientation measurements (S_0). Bedding surface points for the base of units were sampled at 50m intervals along the mapped contacts for the base of the West Angelas, Mount Newman, MacLeod and Nammuldi members. The spacing of 50m was determined by the mean spatial density of orientation measurements and the original mapping scale. The basal contact between the Marra Mamba Iron Formation and the volcanic Fortescue Group is poorly exposed

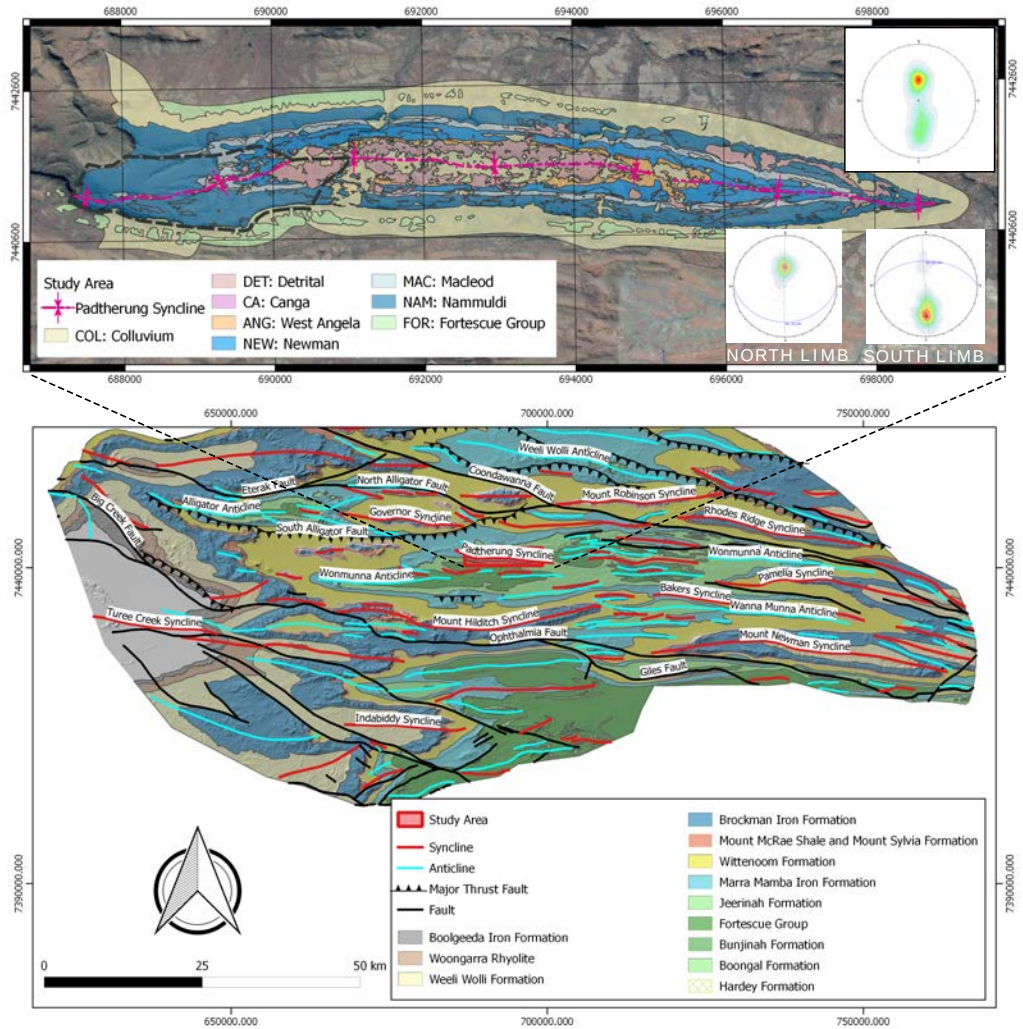


Figure 5.2: Surface Geology(top) of the Padtherung Syncline major structural elements and the study area structural domain [14]. ANG corresponds to the West Angelas member, NEW the Mt. Newman, MAC the Macleod member, NAM the Nammuldi member and FOR the Fortescue Group basement. (bottom) Linear structures and bedrock geology of the central and eastern Hamersley province [17]

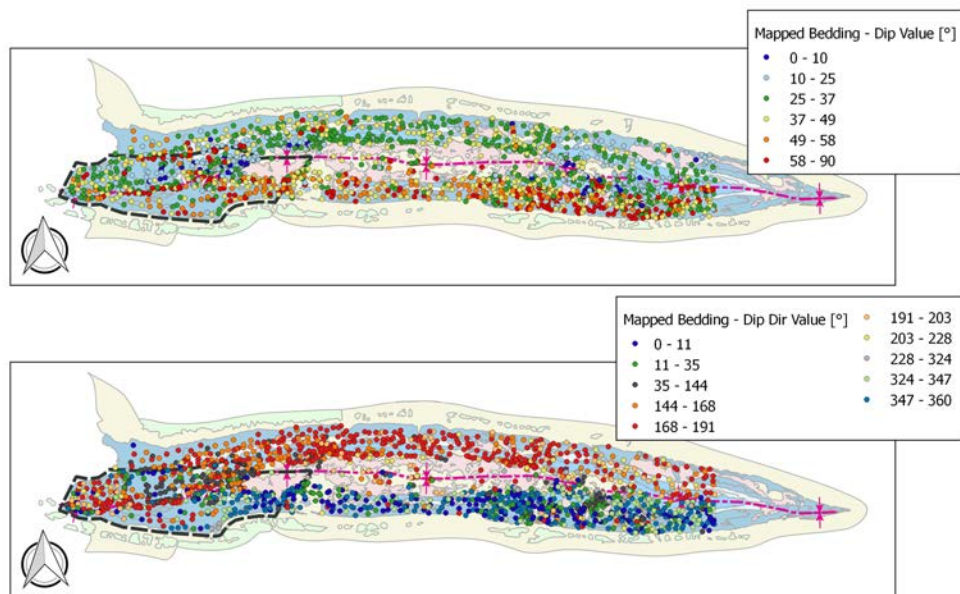


Figure 5.3: Padtherung Syncline dip and dip-direction domains based on mapped bedding

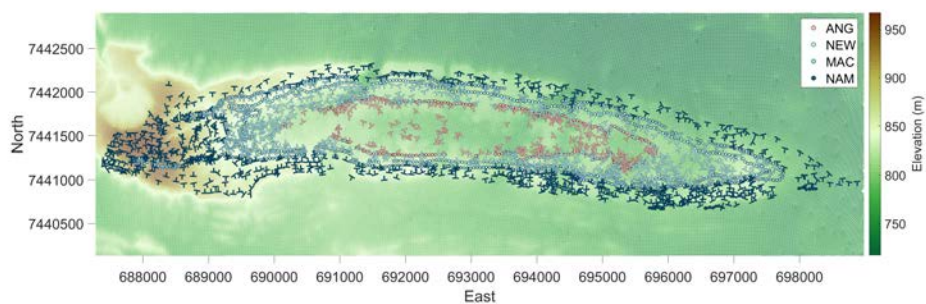


Figure 5.4: Input traces and bedding orientations for implicit model.

	D4: CAPRICORN OROGENY (or <i>Ashburton orogeny</i>)	1780 – 1830 Ma. [24; 48; 49] Minor upright folding. Dextral strike-slip faults as a result of reactivation of NW normal faults (E2). SW tilt of Southern Margin
	E3: Panhandle Extension	~ approx. 2008 Ma. WNW trending normal faulting and dolerite dyke intrusion (mostly showing NW-SE strike), after reactivation of E2 normal faults. NW-striking dolerite dikes intruded along E3 normal faults during the later stages of the E3 event at 2008 Ma. [38].
	D3: PANHANDLE OROGENY	2008 – 2031 Ma. [38] WNW to NW trending, north verging, inclined to overturned, open to tight folds and associated south over north thrust faults, as well as NW striking dolerite dikes. Increases in intensity from west to east of the Hamersley Basin. Interference of D2 and D3 folds generated an asymmetrical dome-basin pattern (Type 1, Ramsey, 1967). It is still a subject of debate if D3 is a progressive deformation phase related to the Ophthalmia orogeny tectonic phase (eg Cawood and Hollingsworth [6]) or a separate orogenic phase (eg Taylor et al. [45]).
	E2: Ophthalmia Extension	~ approx. 2209 Ma. [35] – stratigraphic constraint NNW to NW striking, mostly NE dipping normal faults; tilted during later phases of extension, to sub-horizontal to gently dipping faults
	D2: OPHTHALMIA OROGENY	2145 – 2195 Ma. [41; 44] Large scale E-W folding producing the thin-skinned fold belt throughout the Eastern Hamersley Basin, and large E-W dome and basin in the Western Hamersley Province. Strain decreases northwards.
	D1: Basin compaction and extension	2444 – 2629 Ma. [47; 52] Syn-diagenesis, early vertical loading and NW-SE extension. Podding and local slump folding of the BIF units.

Table 5.1: Tectonic event summary table for the Hamersley Province with principal strain axis orientation (left). Modified from Taylor et al. [45] and Brown et al. [4]. After Dalstra [11]; Dalstra and Rosière [12]; Martin and Morris [34]; Powell et al. [39]; Taylor et al. [45]; Tyler and Thorne [49]

and difficult to constrain, particularly in the more folded southwest margin of the deposit. This resulted in a total of 1056 surface points and 1677 orientations used as input for the interpolation (see Figure 5.4).

	West Angelas	Mt Newman	Macleod	Nammuldi
Field Measurements of Bedding	221	493	275	688
Bedding Contact	212	393	429	22
Trace Points				
TOTAL	433	886	704	710

Table 5.2: Number of input values for implicit modelling of surface by stratigraphic units.

The grid resolution for the interpolation was chosen to be 140-by-50-by-100 (X, Y, Z), with the extents set to 687177 – 699615 in the X direction, 7439967 – 7443060 in the Y

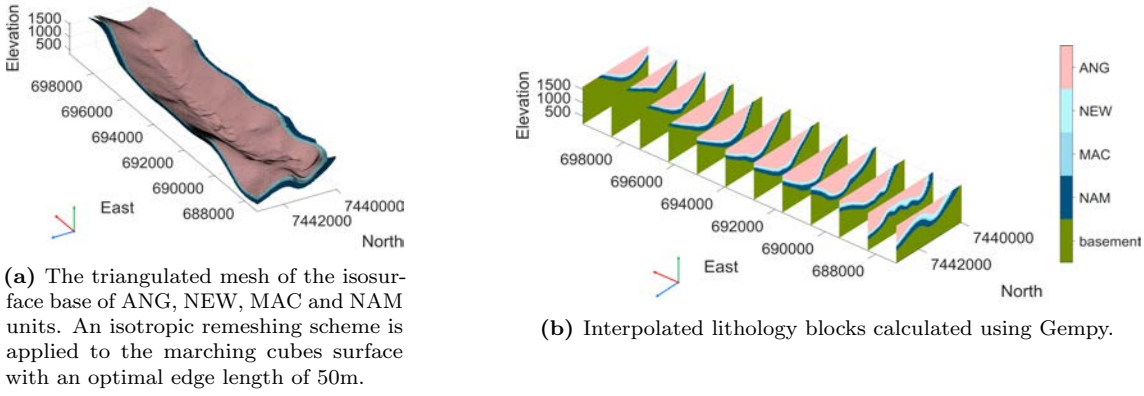


Figure 5.5: Results of Universal Co-Kriging using Gempy [13] for the Padtherung Syncline.

direction, and 200 – 1600 in the Z direction in a Mercator projection grid (EPSG : 28350). The block size for this grid resolution is then given as 89m-62m-14m ($X - Y - Z$). This was chosen so that interpolation could be made using a laptop with 32GB of memory. The kriging parameters used include a covariance range of 3.81×10^6 , drift equations of (3,0) in the (X, Y) direction, nugget gradient of 0.01, and nugget scalar of 1×10^{-6} , which are calculated as the Gempy default parameters [13]. The stratigraphic series interpolated 5 units: the West Angelas Member (ANG), the Mount Newman Member (NEW), the MacLeod Member (MAC), the Nammuldi Member (NAM) and the basement Figure 5.5.

The isosurfaces are extracted from the interpolated scalar field using the standard marching cubes algorithm [28]. The triangular face aspect-ratio can vary significantly when using marching cube isosurfaces since inter-grid slices introduce irregular vertices [3]. This will adversely affect any subsequent curvature analysis. To overcome this we apply an isotropic triangular local smoothing remeshing scheme [21]. The algorithm linearly scales with the number of vertices and can be efficiently computed to optimize for edge length globally across the re-meshed surface. A target edge length of 50m for the resulting triangular mesh which is derived as half the average distance between bedding field observations.

Study Area I outline western-most part of the Padtherung Syncline here as the study area. The hinge of the major structure shows evidence of rotation and hence evidence of fold morphology complexity [5]

The western area of the syncline contains several antiform-synform pairs that are exposed within the Nammuldi member (see Figure 5.6). The increased topographic relief and relative competency of the Nammuldi member also preserves some structures that coincides with possible D2-D3 interference.

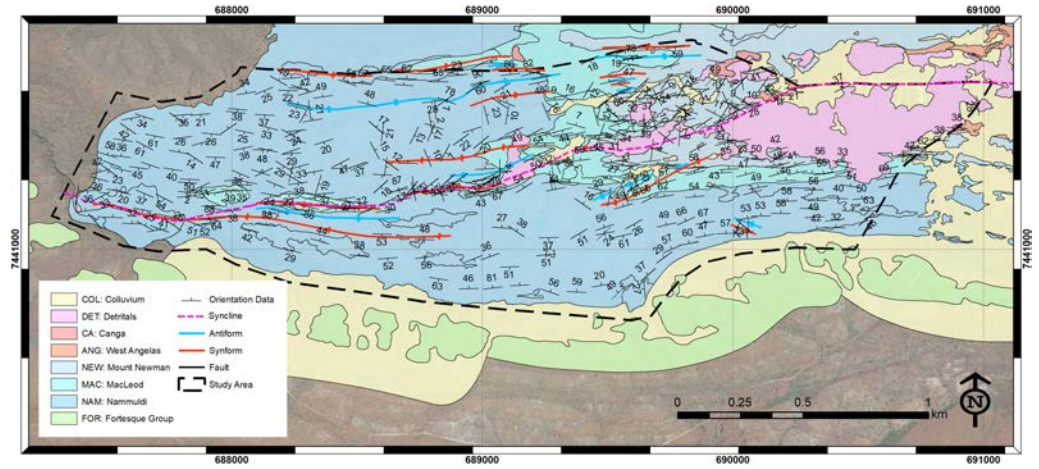


Figure 5.6: The study area structural map with manually interpreted form lines.

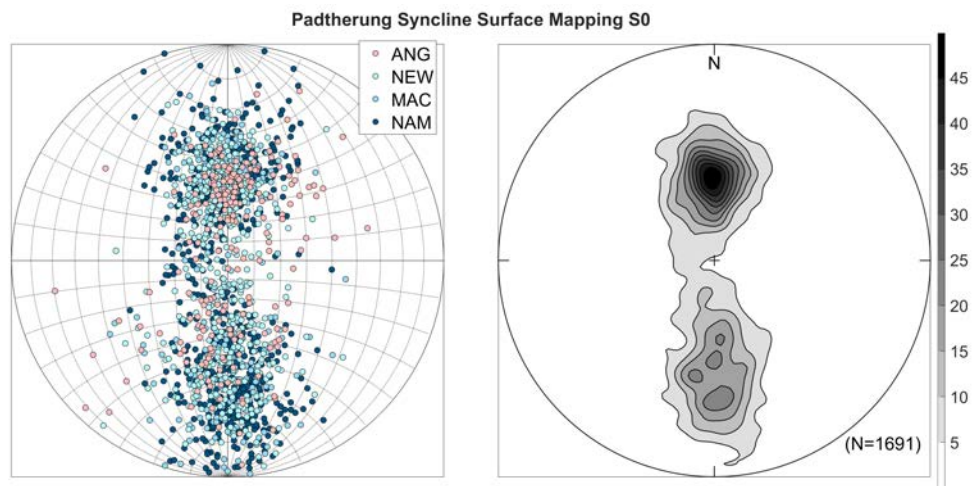


Figure 5.7: Equal-area scatterplot of surface mapping in the study area (left), Kamb contour plot of the surface mapping using $\sigma = 3$, 10 contour intervals (right).

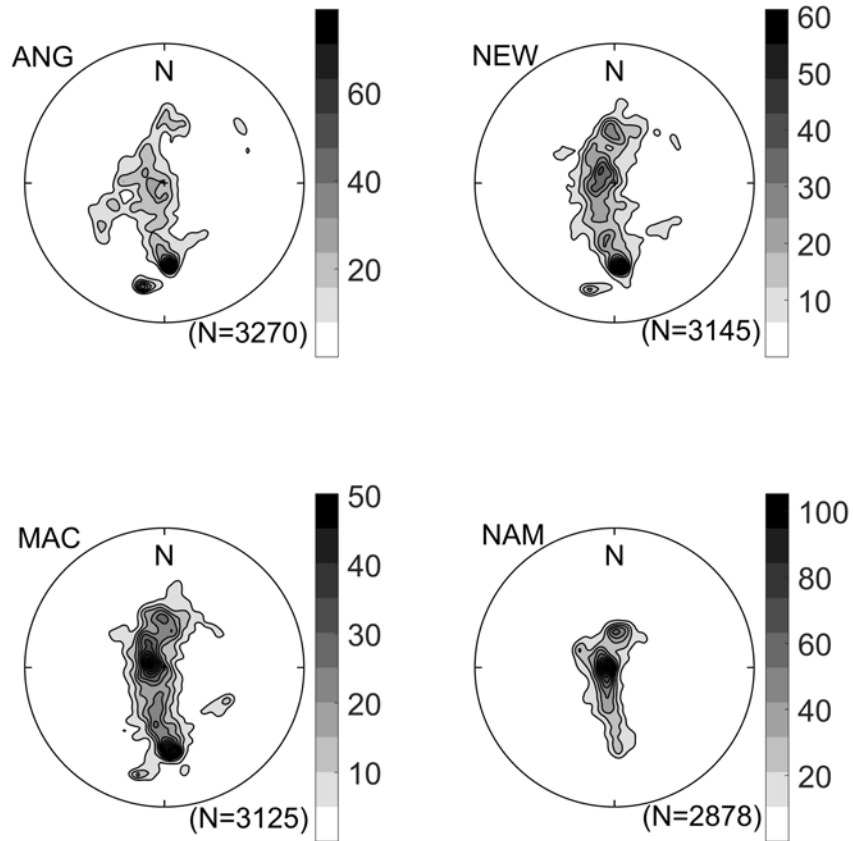


Figure 5.8: Kamb contour plot of the interpolated surfaces for the base of the West Angelas (ANG), Mount Newman (NEW), MacLeod (MAC) and Nammuldi (NAM) units. $\sigma = 3$ and 10 contour intervals are used. Note that NEW and MAC have similar amounts and styles of folding, while NAM is least folded and ANG is the most.

5.3 Methods

The multi-scale curvature based on eigenscales developed in Section 2.3.2 are applied to the triangulated meshes in Figure 5.5a. The method of discretization is outlined here.

The cotangent discretization of the Laplacian (Figure 5.9) for a mesh with n vertices is a matrix L with entries

$$L_{ij} = \begin{cases} \cot\alpha_{ij} + \cot\beta_{ij}, & j \in N(i) \\ 0, & j \notin N(i) \\ -\sum_{k \neq i} L_{ik}, & i = j \end{cases}, \quad (5.1)$$

where $N(i)$ are the neighbouring vertices to vertex i and α_{ij}, β_{ij} are the angles opposite to the edge between vertices ij . These angles behave in such a way that if we treated the triangulated mesh not as a surface but instead made up of volumes or elements, then the differential coordinates on the surface could be fully derived from the cotangent angles [37].

To calculate the eigenscales of the mesh we then multiply the Laplacian matrix by the per-vertex area. This is called the mass-matrix M and is a diagonal $n \times n$ matrix where the diagonals correspond to A_i . When this is multiplied with the cotangent Laplacian it can be considered as a discretization of the Laplace-Beltrami matrix (L_S) for a mesh surface $\mathcal{S}$. The generalized eigenproblem can then be solved as

$$L_S \mathbf{v}_i = \phi_i \mathbf{v}_i. \quad (5.2)$$

Where L_S is the Laplace-Beltrami matrix, $\mathbf{v}_i$ is an eigenvector and ϕ_i is an eigenvalue. Moreover, since the only non-zero entries of L_S correspond connected vertices, efficient algorithms for finding eigenvalues and eigenvectors in sparse matrices can be used [27]. The smallest eigenvalue corresponds to the lowest spatial frequency on the manifold surface which is the inverse of the wavelength of the shape. The eigenvector $\mathbf{v}_i$ for a given harmonic i contains the amplitude at each vertex for i . This amplitude it should be noted is defined on the manifold surface so that it is not directly measured for the absolute vertex coordinate values. We can then transform the eigenvectors into the canonical basis by multiplying them by M^{-1} . This can be considered as analogous to the frequency-space used in Fourier analysis so that we can specify how many eigenvectors to use in the inverse transform to regenerate the mesh at larger harmonic. This transform is commonly referred to as the Manifold Harmonic Transform [50].

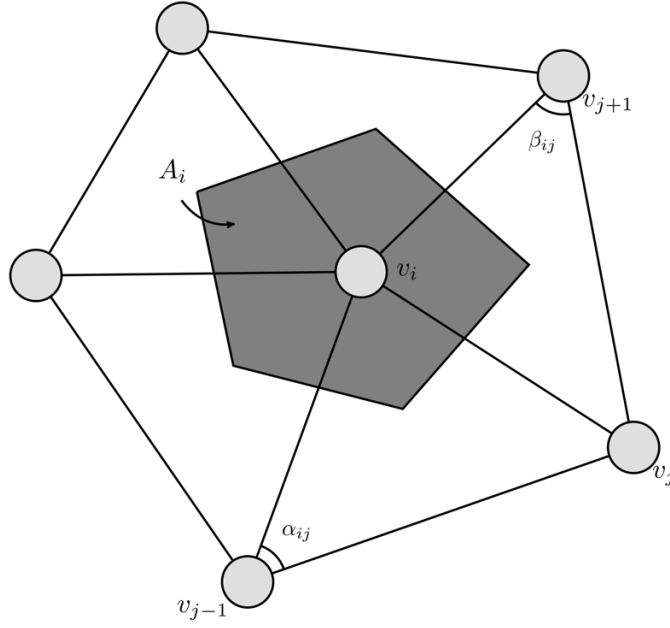


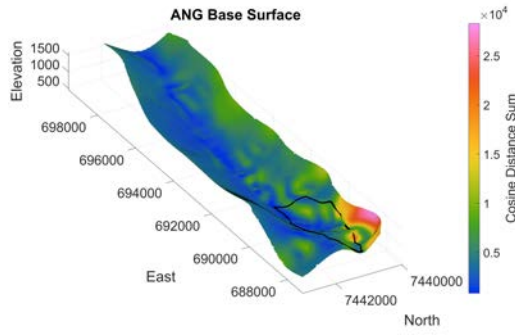
Figure 5.9: The angles α_{ij}, β_{ij} and the (dark grey) barycentric area A_i used to discretize the *Laplace-Beltrami* operator at a vertex v_i . Figure based on Botsch et al. [3].

5.4 Results

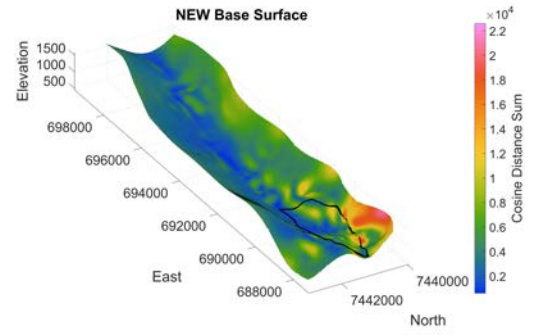
Study Area A set of 500 eigenbasis derived from the surface normal is used to reconstruct the interpolated surface of the West Angelas, Mount Newman, MacLeod and Nammuldi base. The eigenvalue scales range from 3876m to 80m. The surface complexity of each mesh is calculated and mapped (see Figure 5.12), and this is compared against the surface mapped bedding orientation measurements and manually interpreted form lines for analysis.

It can first be observed from Figure 5.12 that each surface has a different range of cosine distance sums with the highest to lowest range being ANG, NEW, MAC and NAM respectively. The ANG and NEW member are both approximately 70m-80m in thickness, while the MAC member is 30m-40m and the NAM member is approximately 130m with a maximum of 203m [29; 31; 32; 33]. The shale-dominated dolomite ANG and BIF-dominated NEW have similar cosine distance sums suggesting a similar amplification-rate. The similar thickness of the members of approximately 80m and considering the lower bound eigenvalue scale of 80m for calculating the cosine distance sum, suggests a zone of contact strain [40], between the more competent NEW and less competent ANG. The thick competent NAM member lack of cosine distance sum compared to the thinner MAC member also suggests that the MAC unit may act as the dominant member within a structural lithic unit [9]. This suggests that the NAM unit is less folded than the MAC, which corresponds with the understanding that the fold nucleation starts in thinner stiff layers of structural lithic units rather than thick competent units [46].

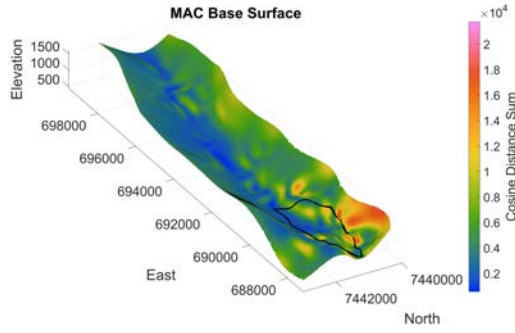
The area A in Figure 5.12 has high cosine distance sums across all surfaces. The bedding measurements suggest that an antiform may exist that complements the manually interpreted synform. The structural contours for NEW and MAC though show that the



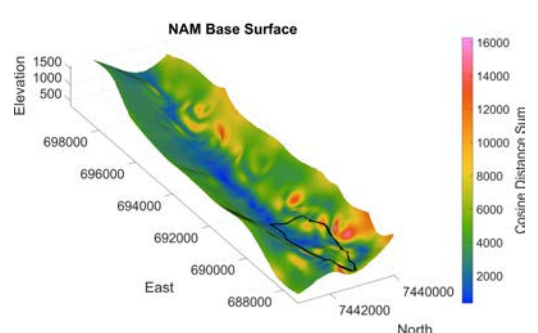
(a) Cosine distance sum for the basal contact surface of the West Angelas member (ANG).



(b) Cosine distance sum for the basal contact surface of the Mount Newman member (NEW).



(c) Cosine distance sum for the basal contact surface of the MacLeod member (MAC).



(d) Cosine distance sum for the basal contact surface of the Nammuldi member (NAM).

Figure 5.10: The surface complexity using the cosine distance sum for the four basal surfaces facing South-East along the Padtherung Syncline. The study area domain in Figure 5.12 is outlined in black. Note that the southern limb has higher values than the north. All units implicitly interpolated using universal co-kriging.

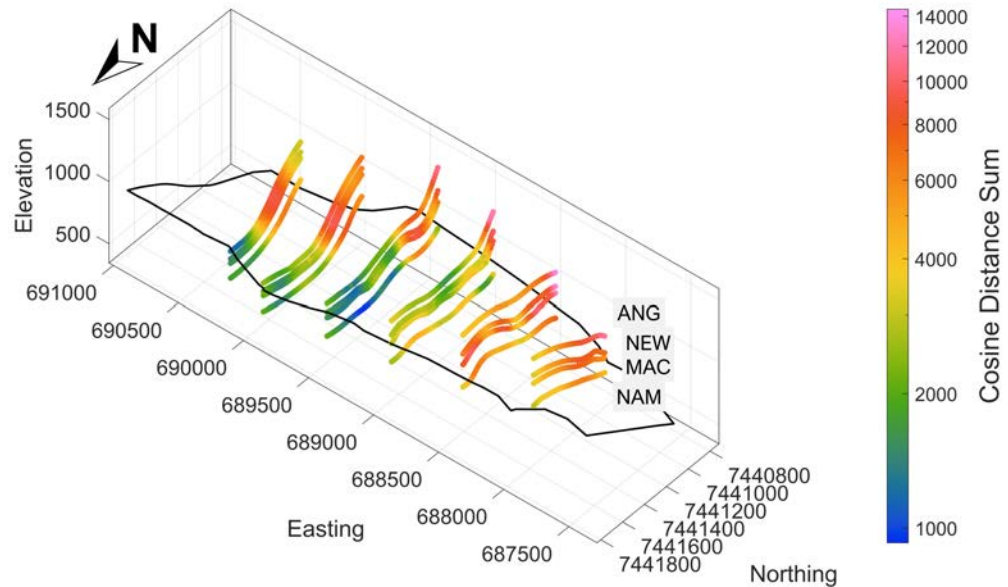


Figure 5.11: Cross-section slices in the easterly direction of the cosine distance sum surfaces. Values are higher towards the west and south, with the NAM surface having lower values as well.

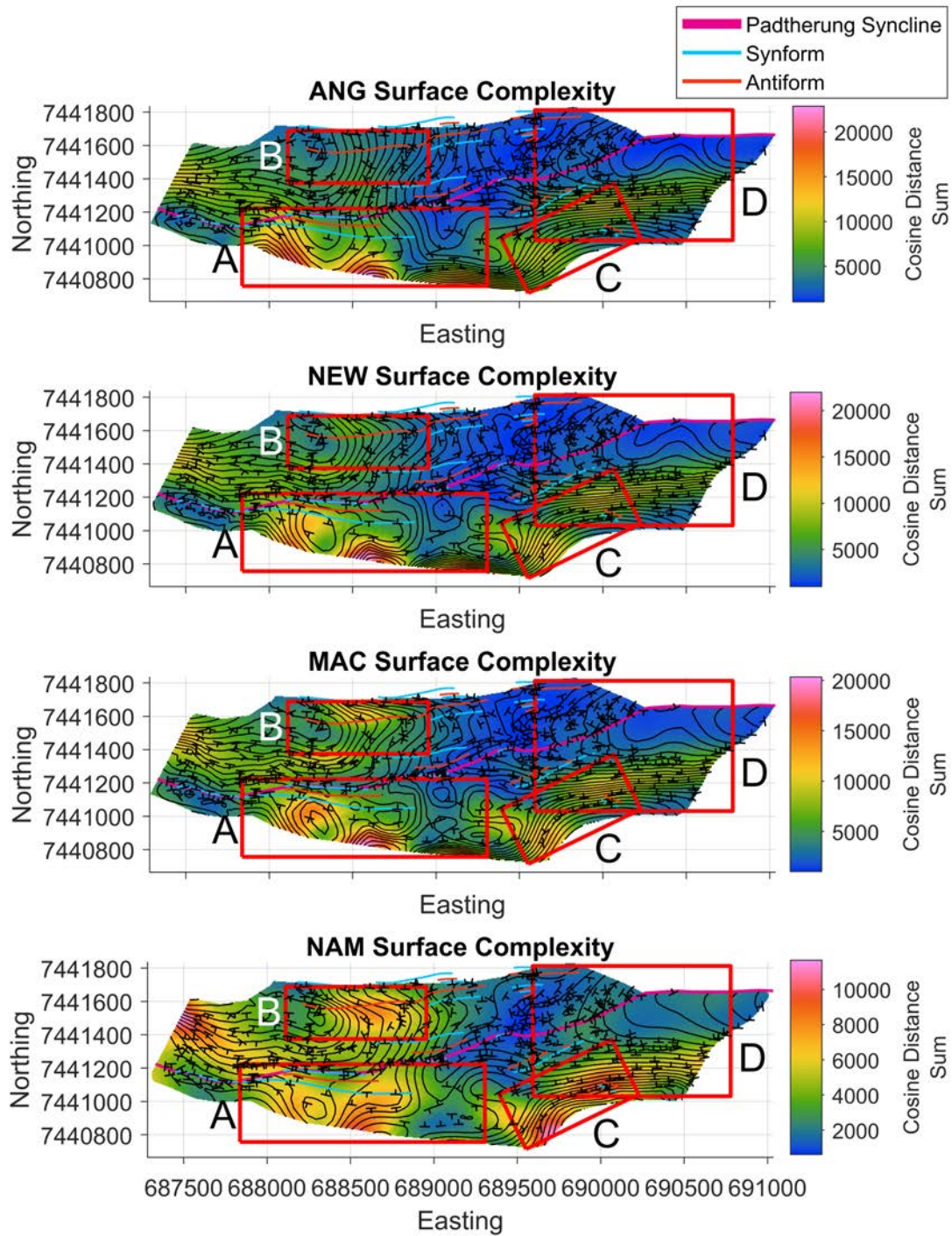


Figure 5.12: Surface structural complexity maps with input bedding S0 measurements, manually interpreted form lines , and domain outlines. Structural contour intervals are 20m.

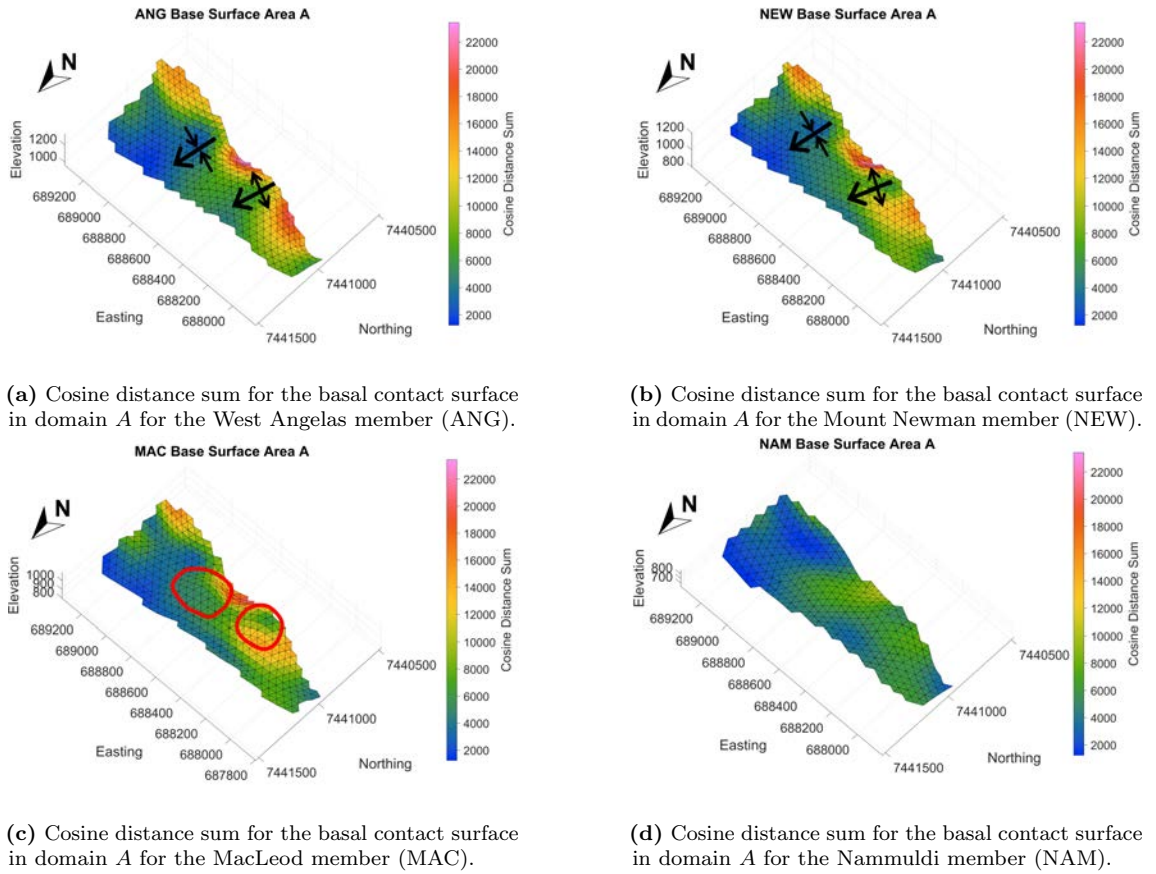


Figure 5.13: The cosine distance sum for the area A in Figure 5.12. Potential hinge locations annotated on ANG and NEW surface, while domes which may form a continuous pericline are circled in red on the MAC surface.

lack of bedding measurements on the southern margin of A as well as the lack of NAM base contact points has resulted in two dome structures that most likely actually form one cylindrical or periclinal structure Figure 5.13c.

The area D in Figure 5.12 shows how the cosine distance sum structural complexity is higher along the limbs of the syncline and lower near the hinge being consistent with the synthetic model Figure 4.5. The southern limb of the Padtherung Syncline in this area is also higher than the northern limb which is consistent with the interpretation that it is more folded Figure 5.3.

The areas enclosed by A and C across all four surfaces have successive culminations and depressions along the cosine distance sum on the southern limb that are non-cylindrical and have trends facing North-South. This contrasts with area B where the cosine distance sum trends appear more East-West trending as minor folds. This together with the change in orientation of the axial surface of the Padtherung Syncline suggests a possible progressive polyclinal fold development with hinge-lockup in the southern limb [5; 6].

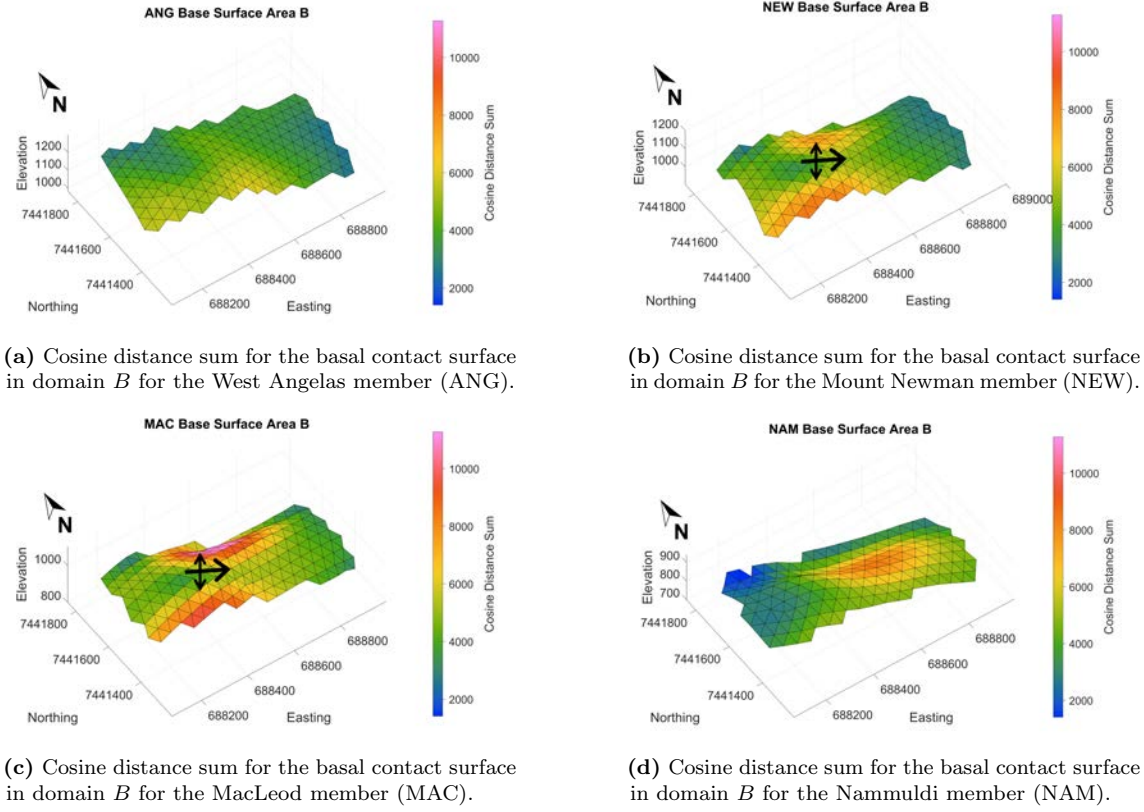
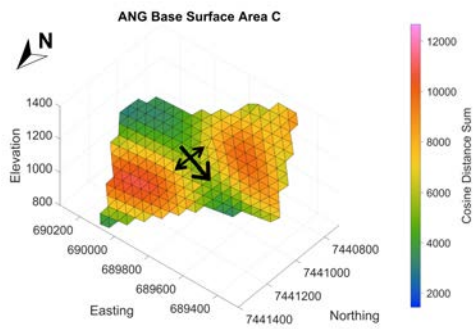


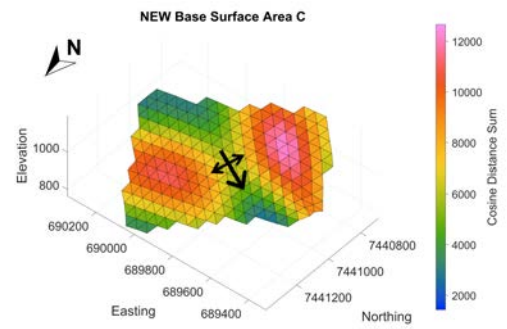
Figure 5.14: The cosine distance sum for the area B in Figure 5.12. Note the E-W trending axial traces interpreted from hinge zones.

5.4.1 N2U Gaussian Curvature Segmentation

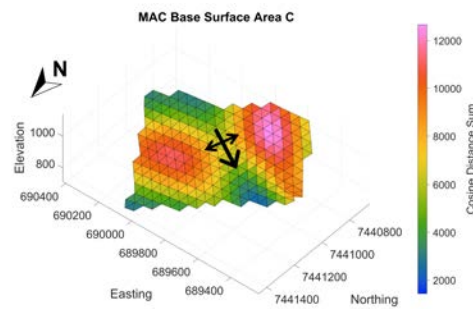
The multi-scale curvature segmentation developed previously is applied to three-dimensional resource surface model. This model was constrained by drillhole data, including gamma logs and several acoustic and optical televiewer measurements, and interpolated using an implicit modelling approach. The unit is upper portion of the Mount Newman member, described as N2U within the Hamersley and is noted to be closed surface. The value of using κ_{gauss} can be seen in Figure 5.17b and Figure 5.17c, since because it is an intrinsic measure, even though the surface normals would have opposite directions, the segmentation regions show a spatial consistency in the map view. Clusters 1 and 4 appear as symmetric in scale between saddle regions and domes/basins as seen in Figure 5.17 and Figure 5.18. Moreover, Cluster 5,3,2 appear on dome/basin edges and can be seen to have three distinct scales high negative curvature. This could imply three distinct fracture characteristics.



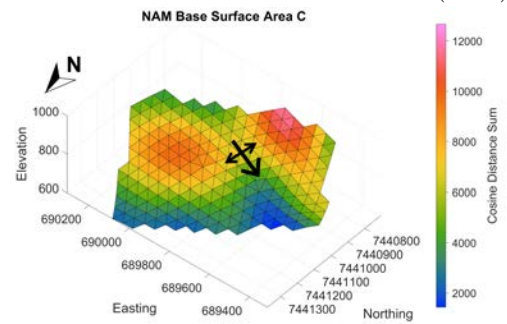
(a) Cosine distance sum for the basal contact surface in domain C for the West Angelas member (ANG).



(b) Cosine distance sum for the basal contact surface in domain C for the Mount Newman member (NEW).

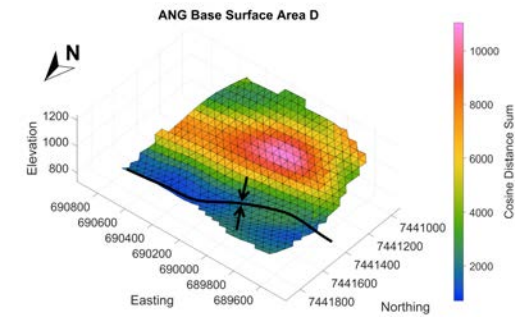


(c) Cosine distance sum for the basal contact surface in domain C for the MacLeod member (MAC).

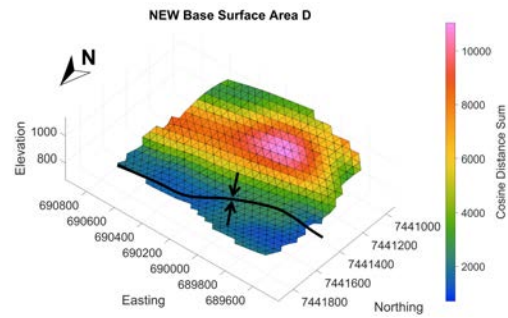


(d) Cosine distance sum for the basal contact surface in domain C for the Nammuldi member (NAM).

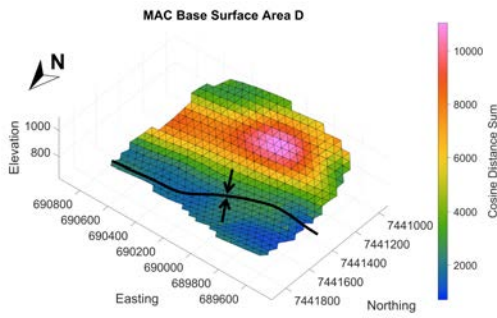
Figure 5.15: The cosine distance sum for the area C in Figure 5.12. Steeply plunging hinge lines are interpreted between areas of high cosine distance sums.



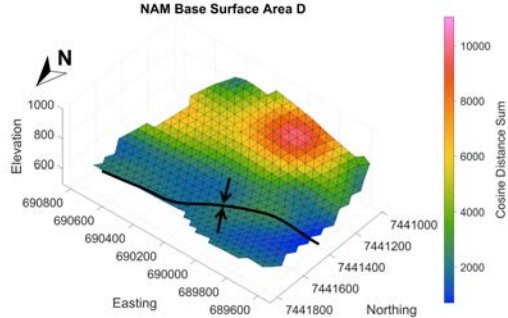
(a) Cosine distance sum for the basal contact surface in domain D for the West Angelas member (ANG).



(b) Cosine distance sum for the basal contact surface in domain D for the Mount Newman member (NEW).

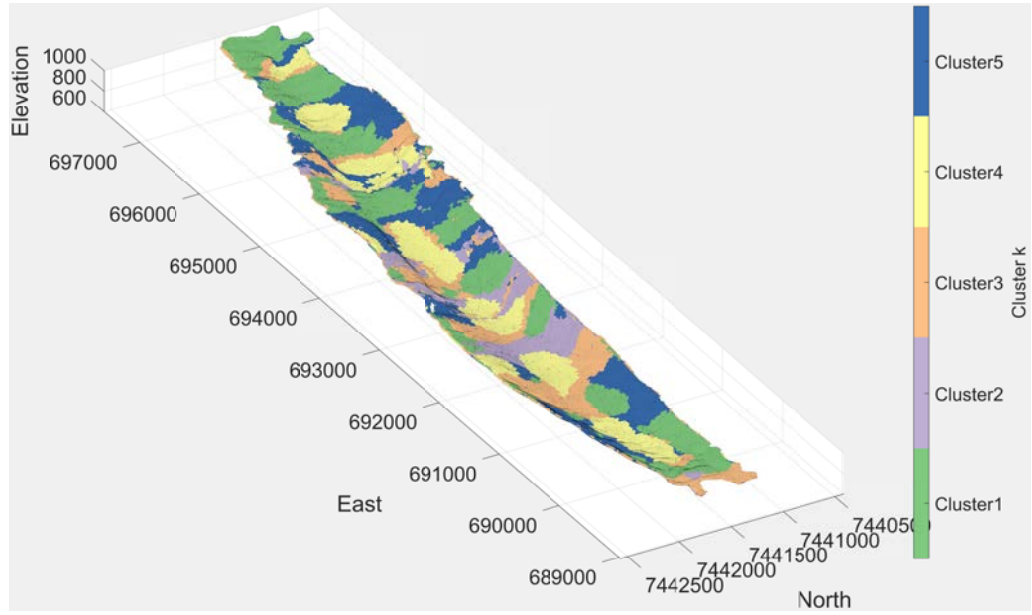


(c) Cosine distance sum for the basal contact surface in domain D for the MacLeod member (MAC).

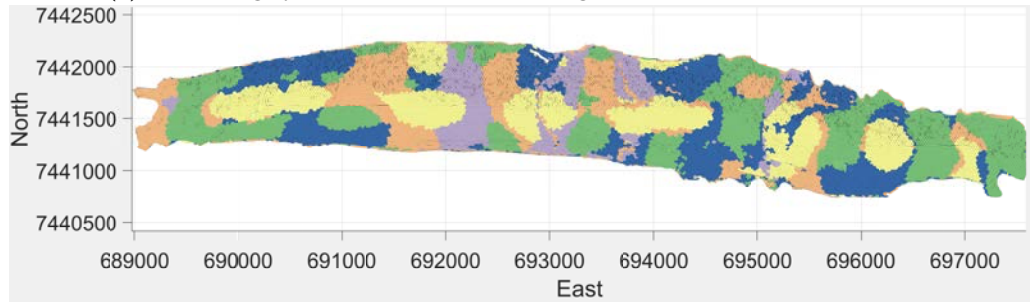


(d) Cosine distance sum for the basal contact surface in domain D for the Nammuldi member (NAM).

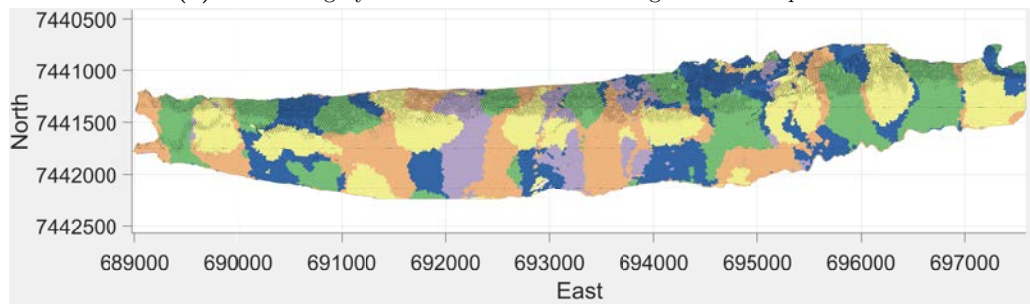
Figure 5.16: The cosine distance sum for the area D in Figure 5.12, with the approximate location of the Padtherung Syncline. Note that the southern limb has higher cosine distance sum values than the northern limb.



(a) Padtherung Syncline Gaussian curvature segmentation three-dimensional view.



(b) Padtherung Syncline Gaussian curvature segmentation top view.



(c) Padtherung Syncline Gaussian curvature segmentation bottom view.

Figure 5.17: The Gaussian Curvature (κ_{gauss}) segmentation using $K = 5$.

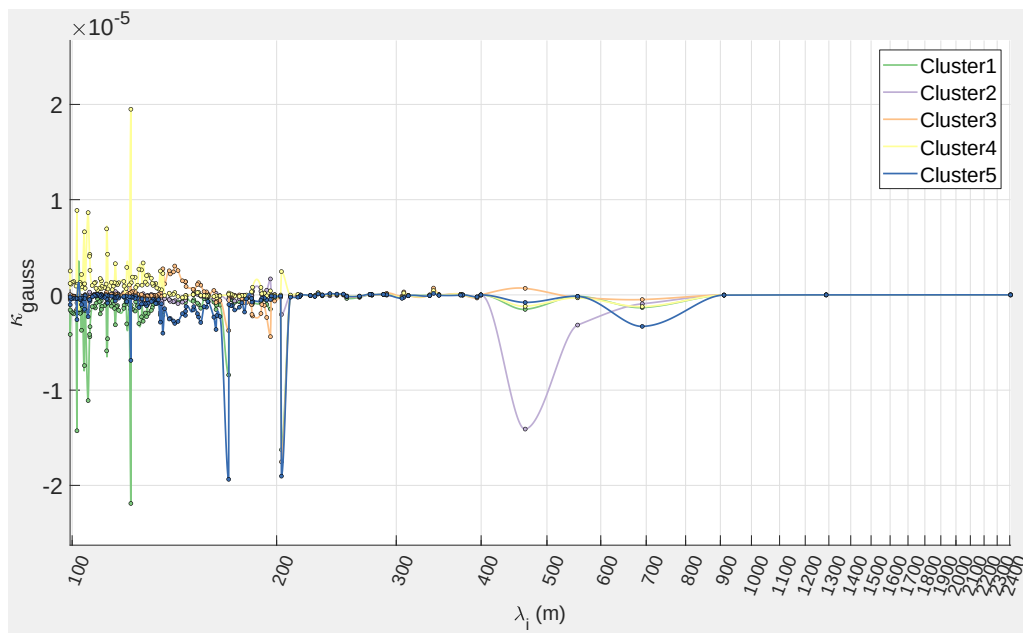


Figure 5.18: Padtherung Cluster Centres.

5.5 Discussion

The application of the discrete cotangent Laplacian to mesh representations of geological surfaces, provides a robust approach to characterizing the scale of surfaces. The eigenvalues of the Laplacian matrix starting from the smallest value can be computed so that we are able to extract the largest wavelength harmonics of the mesh surface. By comparing the orientation of individual mesh faces for a set of eigenvalues, we can determine the local variability of the orientation as a function of scale. To quantify this variability, I take the pairwise cosine distance between the orientations of a mesh face for the computed set of scales.

A three-dimensional structural model of the Padtherung Syncline, located in the central Hamersley province, Western Australia, was developed to evaluate the surface complexity measure. An implicit model using the dual form of universal Co-Kriging [8] was applied to bedding measurements and contacts for four conformable layers using the python library Gempy [13]. While other implicit interpolation methods can incorporate specific structural elements such as axial surface fields [18; 26], enforcing a global model of polyphase deformation for structures that develop progressively or that are deformed coaxially will not produce reliable geometries, particularly for folds with curved and/or rotated hinges [5]. The application of local anisotropy measures using linear functional constraints with radial basis functions [20] though has the potential for capturing the non-cylindrical local strain partition geometries.

Another limitation with the universal Co-Kriging approach lies in characterizing global thickness variation [26] which is important for enforcing hinge-thickness variation in fold styles as well as sedimentation rates. This is particularly important when conditioning geological models by drill hole data [1; 19; 22; 51]. An alternate approach could also be to use an energy penalization approach to implicit structural modelling [42].

I interpret the culminations in the cosine distance sum to be identified with fold limbs while the depressions to be coincident with fold hinge regions specifically with reference to the passive simple shear fold model. Interpreting other kinematic modes is important piece of contextual information that can also be used for model refinement, i.e. regions of flexural slip vs simple shear for balanced restoration [15]. This can be frame as an energy minimization problem too similar to bending energy in fault-related folding [25]. Incorporating buckling energy and enforcing constraints across multiple layers though may require the simulation of viscous flow [43].

Another area for future work for multi-scale curvature measures would be to incorporate more localized harmonics. In an approach similar to wavelets, localized harmonics can be efficiently calculated [36]. A further enhancement can be made by learning localized shape descriptors that also incorporate directional anisotropy given domain classes [2].

The surface curvature cosine distance sum also allows the interpretation of the Padtherung Syncline as a progressive deformed $D2$ structure rather than a $D2 - D3$ fold interference structure. The observation that fold interference patterns in the central Hamersley can be explained by progressive $D2$ deformation has previously been described [6]. The

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development of asymmetric folds in competent layers (parasitic to the Wonmunna anticline) causes thickened hinges and short limbs to behave more rigidly, which subsequently causes local strain partitioning [5]. As the antithetic rotation causes the shorter limb hinge to lock-up (Price, 1990), which in the case of the Padtherung Syncline may explain its non-planar axial surface or polyclinal geometry, together with the increased buckling along the southern limb, i.e. the shorter limb.

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Chapter 6

Conclusion

6.1 Summary

Multi-scale curvature analysis using the co-tangent Laplacian provides a novel and robust method for identifying areas of structural complexity. The developed cosine distance sum in this thesis of mesh face orientations is an objective repeatable measure that can be used to compare different surfaces and areas. Since surface curvature is related to strain distribution, these measures can have important applications in minerals targeting and engineering, as well as in reservoir characterization as indicators of fracture distribution.

A set of computational methods that consider scale from a geometric as well from a deformation mechanics view were developed. This was applied to a 3D thermo-mechanical geodynamic model of viscous folding to investigate how strain partitioning and curvature segmentation behave across scales. The ability to scale parameters that are dependent on deformation such as fracture density or geotechnical parameters such as rock quality designation is important as aspect of the the work of coupling geometric and deformation scale.

The multi-scale curvature methods are then applied to a case-study of the Padtherung Syncline in the East Hamersly, Western Australia. An implicit 3D model based on field measurements of bedding and contact points is developed and used as the basis of the curvature analysis. The identification of curvature patterns of buckling on the shorter southern limb suggests the kinematics of a progressively deformed hinge rotation with the shorter limb locking up.

6.2 Conclusion and Outlook

The application of geodynamic numerical models of folding also presents the potential for the development of new and novel methods of structural interpolation for modelling. The ability of using thermo-mechanical simulations to generate training data for geometries in the context of temporal difference learning, in terms of spatial agents [8] and flow networks [1]. In particular, the work of Hjelle [5] should be noted in developing a numerical framework for scalar field interpolation using the Hamilton-Jacobi equation and Ramsay's

dip-isogon fold classification [11]. The Hamilton-Jacobi equations as applied to anisotropic wavefront propagation [6] are also known as the continuous form of the Bellman equations which play an essential role in reinforcement learning [16].

Future work using the methods of multi-scale curvature analysis developed in this thesis I also suggest could consist of blending scalar fields in a manner similar to Hjelle [5], but using the front propagation of Gaussian curvature rather than dip-isogons. A geometric deep learning approach using appropriate convolution neural network (CNN) operations [3; 13; 15] to create generative models that spatially and geometrically encode realistic and rheologically-constrained curvature. When applied using temporal (which in the context of geological modelling would be a conformable sequence of layers) difference learning to the front propagations, the *flow network* of the multi-scale curvature distribution would theoretically produce multi-scale non-cylindrical 3D fold geometries that are parameterised by factors such as competency contrast and relative thickness. Another interesting application of this would be to track 3D hinges (segments of connected maximal curvature) through the interpolated scalar field for constructing fold axial surfaces. Properties such as tortuosity of hinges and identification of localised non-cylindrical regions in axial surfaces would indicate highly-prospective dilatational jogs for hinge-parallel fluid flow [2; 12].

Another potential application rather than generative front propagation could be to interpolate curvature *interpolation* across an individual surface using generative directional field synthesis [14], in a manner similar to Hillier et al. [4]. It should be noted that a significant component necessary for the work of Hjelle [5] is in the mathematical formulation of tangent spaces that can be applied numerically for the scalar field interpolation. This is an active area of research within the field of geometry processing where it falls under *directional fields* [17] or more generally (or abstractly in the mathematical sense) *frame field operators* [10]. Many of the shortcomings of co-tangent Laplacian tetrahedral discretizations noted by Hillier et al. [4] and Irakarama et al. [7], can be mitigated by using the frame field based boundary condition formulation of [9; 10].

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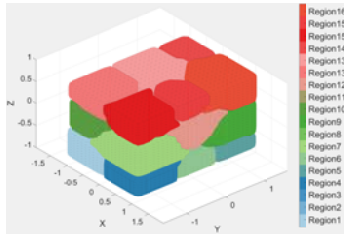
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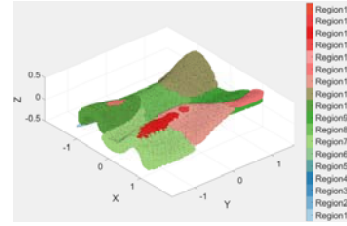
Appendix A

Pure Compression free-slip base

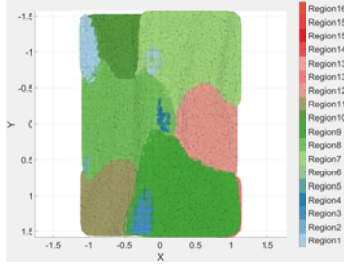
The results in this appendix correspond to the Section [4.3.2](#). The Compressional Pure Shear with free-slip base boundary condition parameters can be found in Table [4.3](#). The results for the large scale averaged W_k strain partition mesh and the $\log J$ strain and mesh figures.



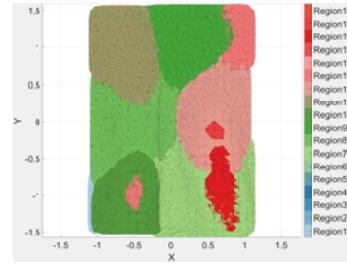
(a) Superpixel regions by kinematic vorticity(W_k).



(b) Superpixel regions by kinematic vorticity(W_k) clipped by surfaces.

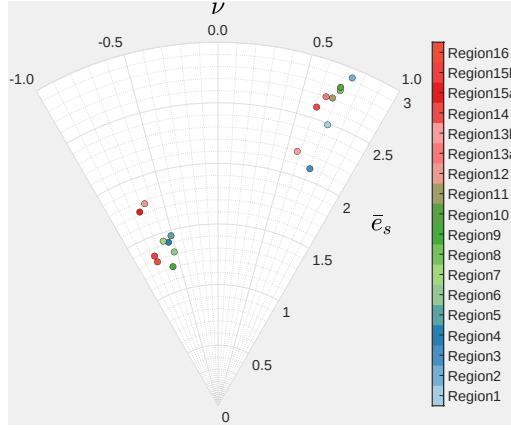


(c) Superpixel regions clipped bottom view.

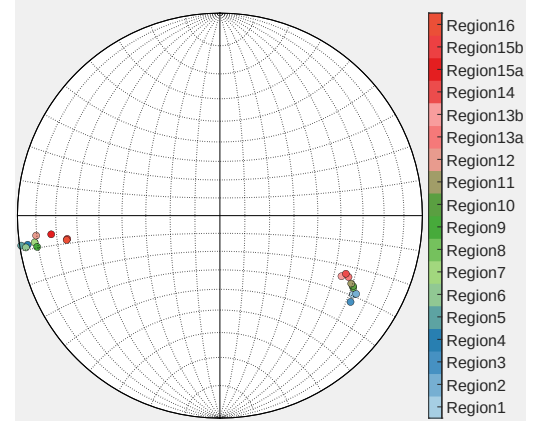


(d) Superpixel regions clipped top view.

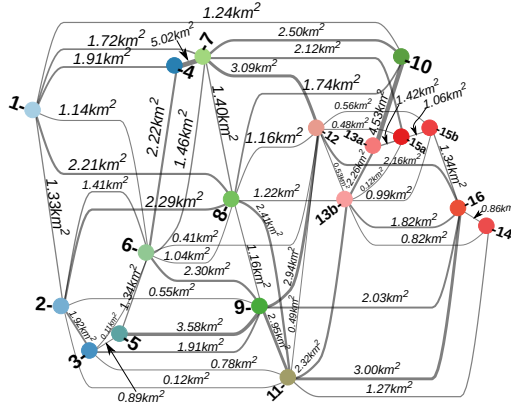
Figure A.1: Compression pure shear with free-slip base boundary condition after 15.1562Myr. Superpixel region results using kinematic vorticity(W_k) using a tensor convolution of size (5,5,5). Two anticlinal ridges develop: one more symmetric (regions 8, 11, 12, 14) and one more asymmetric (regions 10, 13, 16, 17).



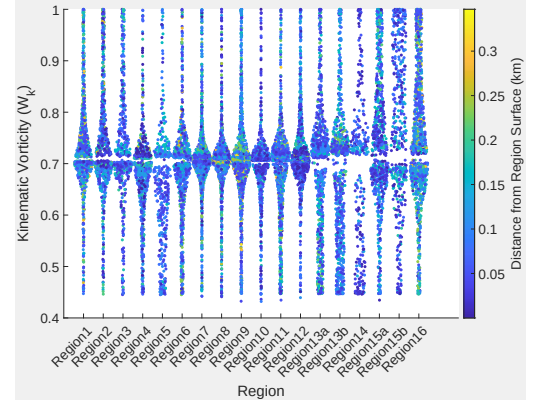
(a) Nadai-Hsu finite strain for kinematic vorticity (W_k) regions.



(b) Orientation of the major principal strain axis for kinematic vorticity (W_k) regions.



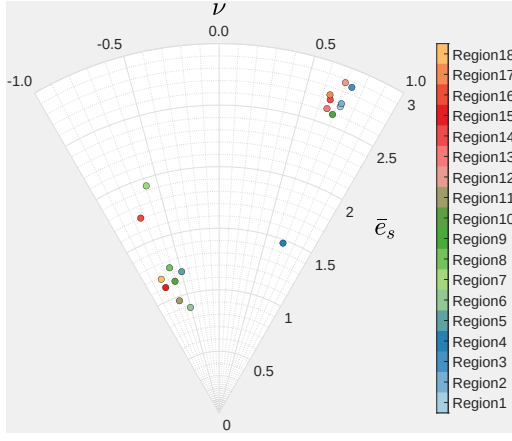
(c) Topology by contact surface area for kinematic vorticity (W_k) regions.



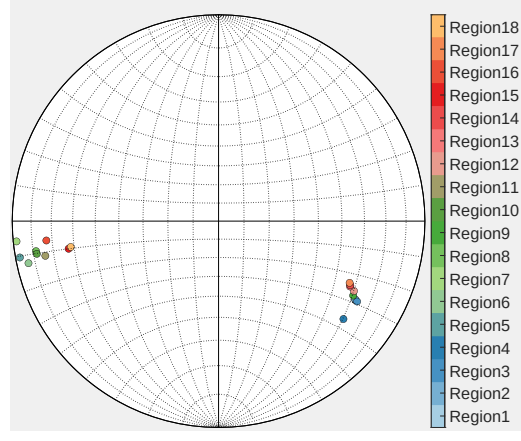
(d) Swarm chart for kinematic vorticity of the passive markers in each region.

Figure A.2: Compression pure shear with free-slip base boundary condition after 15.1562Myr. Strain region analysis for kinematic vorticity(W_k) using a tensor convolution of size (5, 5, 5) (Figure A.1)

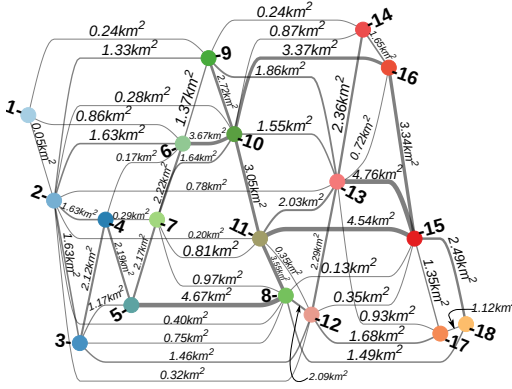
A. PURE COMPRESSION FREE-SLIP BASE



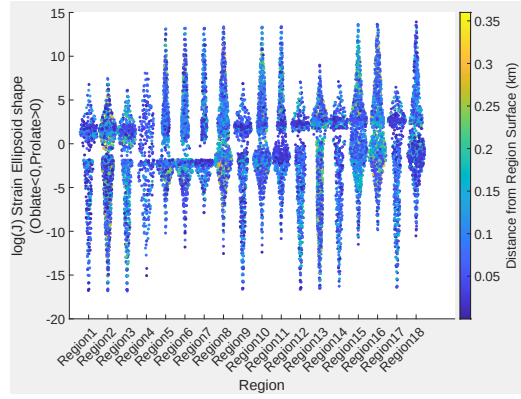
(a) Nadai-Hsu finite strain for strain ellipsoid shape ($\log J$) regions.



(b) Orientation of the major principal strain axis for strain ellipsoid shape ($\log J$) regions.

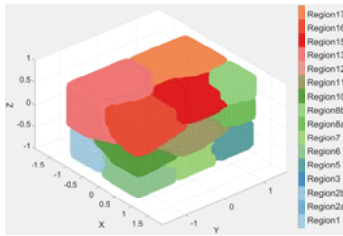


(c) Topology by contact surface area for strain ellipsoid shape ($\log J$) regions.

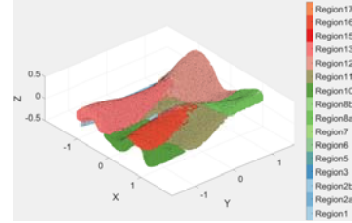


(d) Swarm chart for strain ellipsoid shape ($\log J$) of the passive markers in each region .

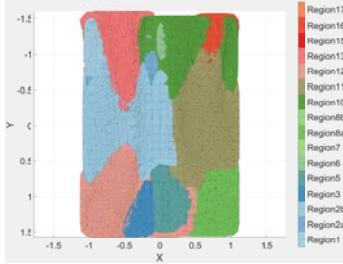
Figure A.3: Compression pure shear with free-slip base boundary condition strain region analysis for strain ellipsoid shape ($\log J$) at full marker resolution (Figure 4.15).



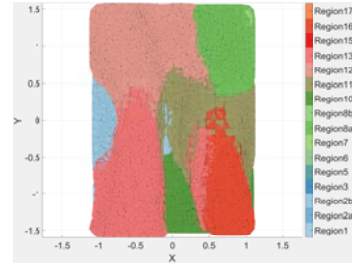
(a) Superpixel regions by strain ellipsoid shape ($\log J$).



(b) Superpixel regions by strain ellipsoid shape ($\log J$) clipped by surfaces.

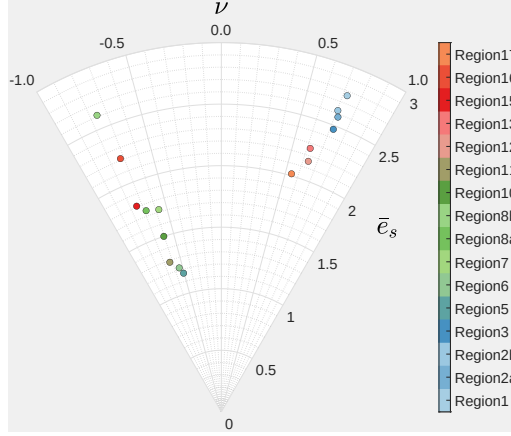


(c) Superpixel regions clipped bottom view.

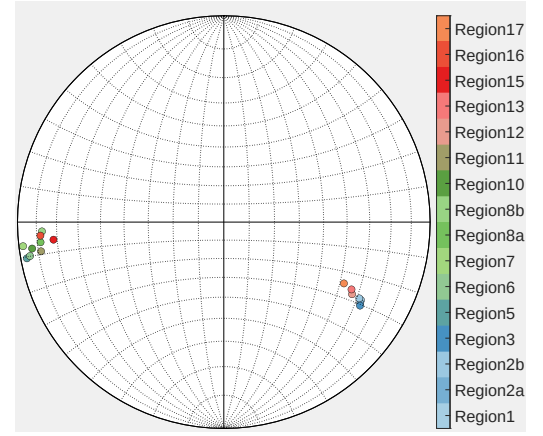


(d) Superpixel regions clipped top view.

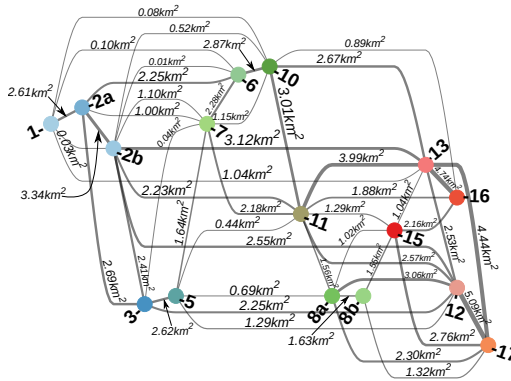
Figure A.4: Compression pure shear with free-slip base boundary condition after 15.1562Myr. Superpixel region results using strain ellipsoid shape ($\log J$) using a tensor convolution of size (5, 5, 5). Two anticlinal ridges develop: one more symmetric (regions 10, 11) and one more asymmetric (regions 11, 12, 13, 15).



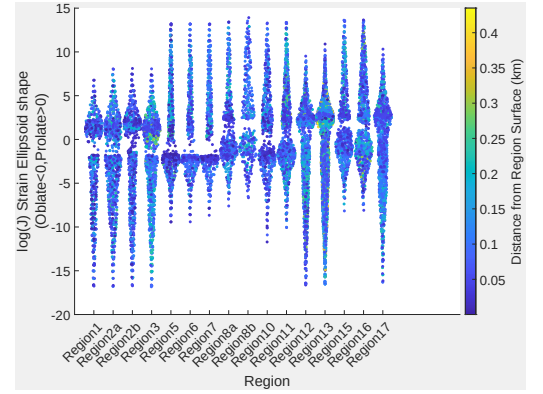
(a) Nadai-Hsu finite strain for strain ellipsoid shape ($\log J$) regions.



(b) Orientation of the major principal strain axis for strain ellipsoid shape ($\log J$) regions.



(c) Topology by contact surface area for strain ellipsoid shape ($\log J$) regions.



(d) Swarm chart for strain ellipsoid shape ($\log J$) of the passive markers in each region .

Figure A.5: Compression pure shear with free-slip base boundary condition strain region analysis for strain ellipsoid shape ($\log J$) using a tensor convolution of size (5, 5, 5) (Figure A.4).

Appendix B

Compressional Pure Shear with noslip base

The results in this appendix correspond to the Section [4.3.2](#). The Compressional Pure Shear with no-slip base boundary condition parameters can be found in Table [4.3](#). A no-slip base implies a greater degree of bulk shortening and can be interpreted as having kinematics like a detachment fold.

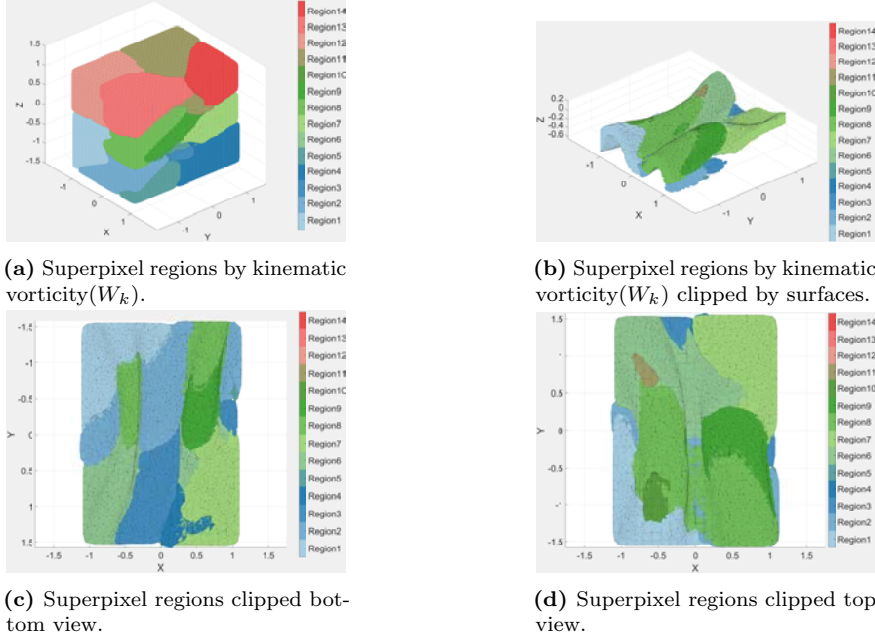


Figure B.1: Compression pure shear with noslip base boundary condition after 15.1562Myr. Superpixel region results using kinematic vorticity(W_k) at full marker resolution.

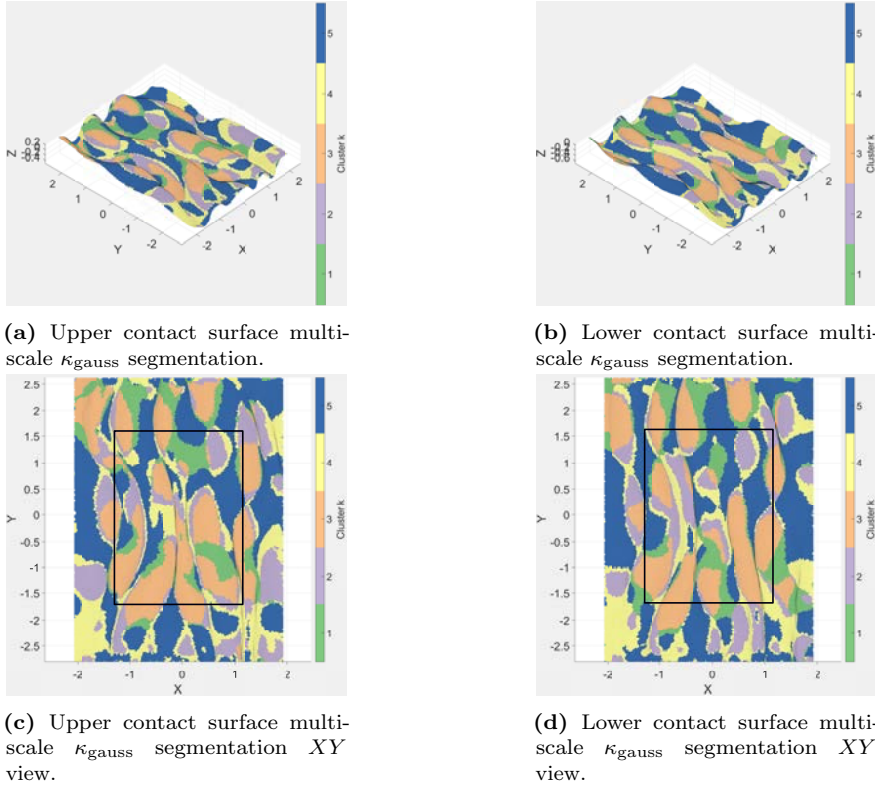
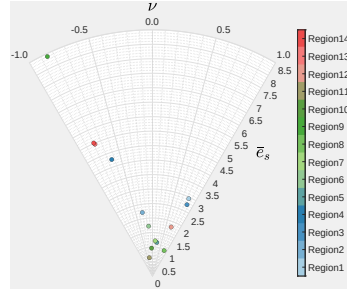
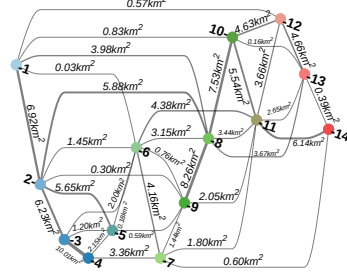


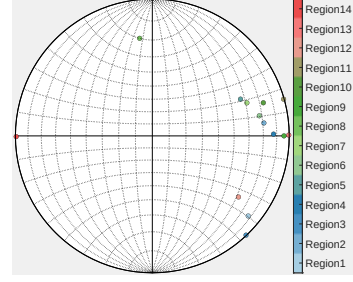
Figure B.2: Compression pure shear with noslip base boundary condition after 15.1562Myr. Multi-scale Gaussian(κ_{gauss}) curvature segmentation. The range of eigenvalues that form the basis is **min** $\lambda_2 = 1.77$ km to **max** $\lambda_{150} = 0.13$ km, with $K = 5$ clusters.



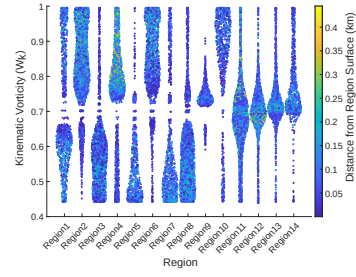
(a) Nadai-Hsu finite strain for kinematic vorticity (W_k) regions.



(c) Topology by contact surface area for kinematic vorticity (W_k) regions.



(b) Orientation of the major principal strain axis for kinematic vorticity (W_k) regions.



(d) Swarm chart for kinematic vorticity of the passive markers in each region .

Figure B.3: Compression pure shear with noslip base boundary condition after 15.1562Myr. Strain region analysis for kinematic vorticity(W_k) at full marker resolution (B.1).

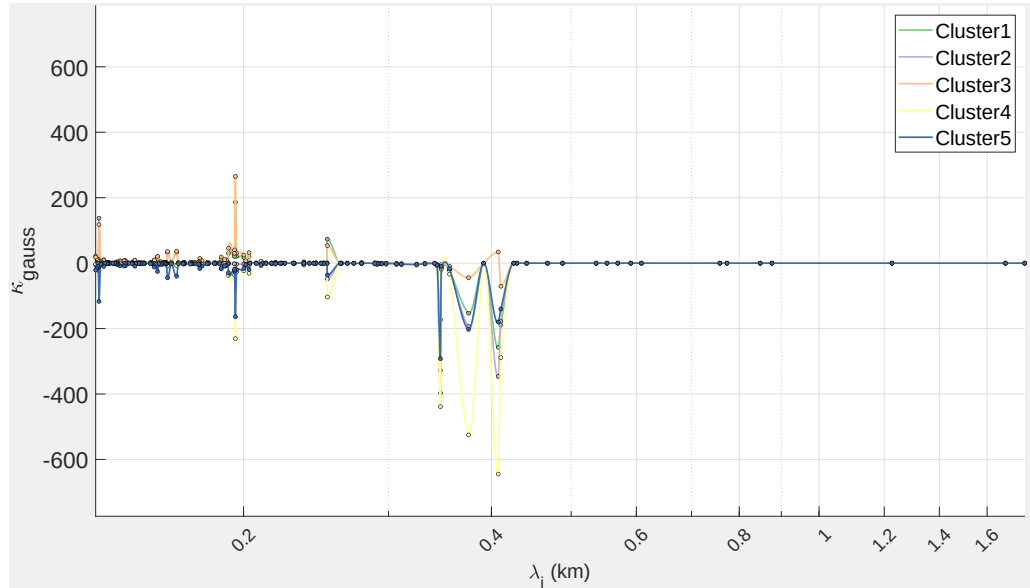


Figure B.4: The cluster centres of the Gaussian(κ_{gauss}) curvature segmentation for the compression pure shear with noslip base boundary condition model(B.2). Each cluster is a 148 = (150 – 2) dimensional vector where each dimension corresponds to a κ_{gauss} value. Note that $\kappa_{\text{gauss}} < 0$ values imply that locally the shape is saddle-shaped and $\kappa_{\text{gauss}} > 0$ values imply the shape is locally dome/basin (2.6).

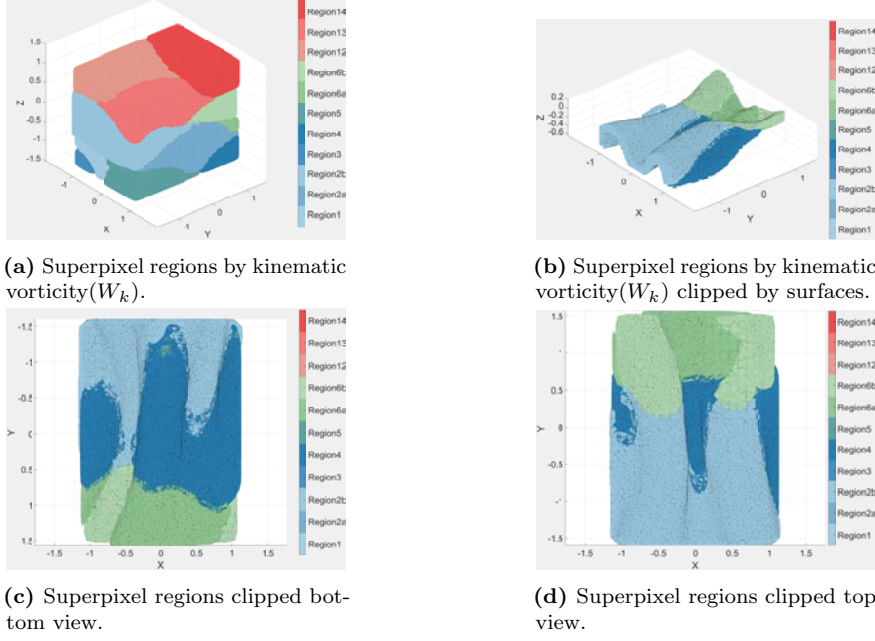


Figure B.5: Compression pure shear with noslip base boundary condition after 15.1562Myr. Superpixel region results using kinematic vorticity(W_k) using a tensor convolution of size $(5, 5, 5)$.

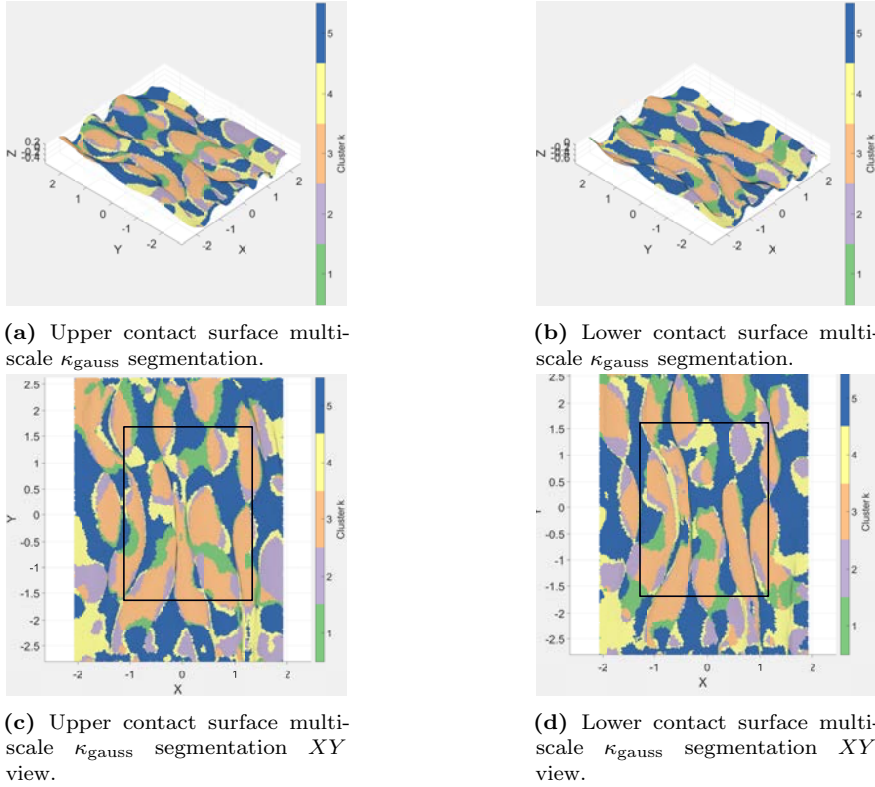
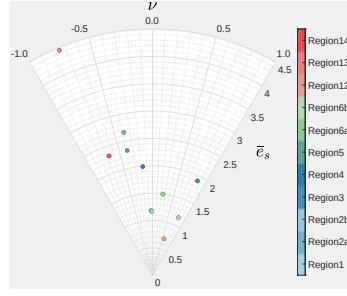
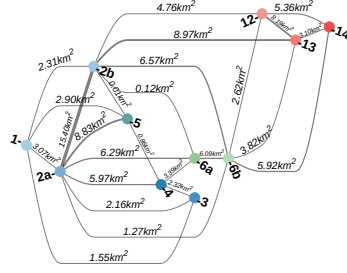


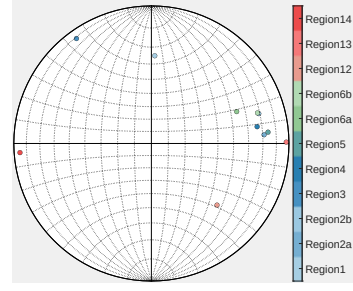
Figure B.6: Compression pure shear with noslip base boundary condition after 15.1562Myr. Multi-scale Gaussian(κ_{gauss}) curvature segmentation. The range of eigenvalues that form the basis is $\min \lambda_{61} = 0.21$ km to $\max \lambda_{150} = 0.13$ km, with $K = 5$ clusters.



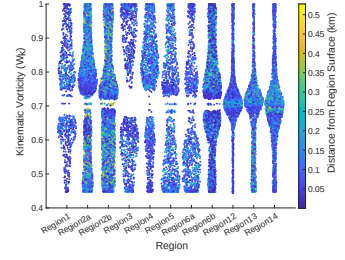
(a) Nadai-Hsu finite strain for kinematic vorticity (W_k) regions.



(c) Topology by contact surface area for kinematic vorticity (W_k) regions.



(b) Orientation of the major principal strain axis for kinematic vorticity (W_k) regions.



(d) Swarm chart for kinematic vorticity of the passive markers in each region .

Figure B.7: Compression pure shear with noslip base boundary condition after 15.1562Myr. Strain region analysis for kinematic vorticity(W_k) using a tensor convolution of size (5, 5, 5) (B.5)

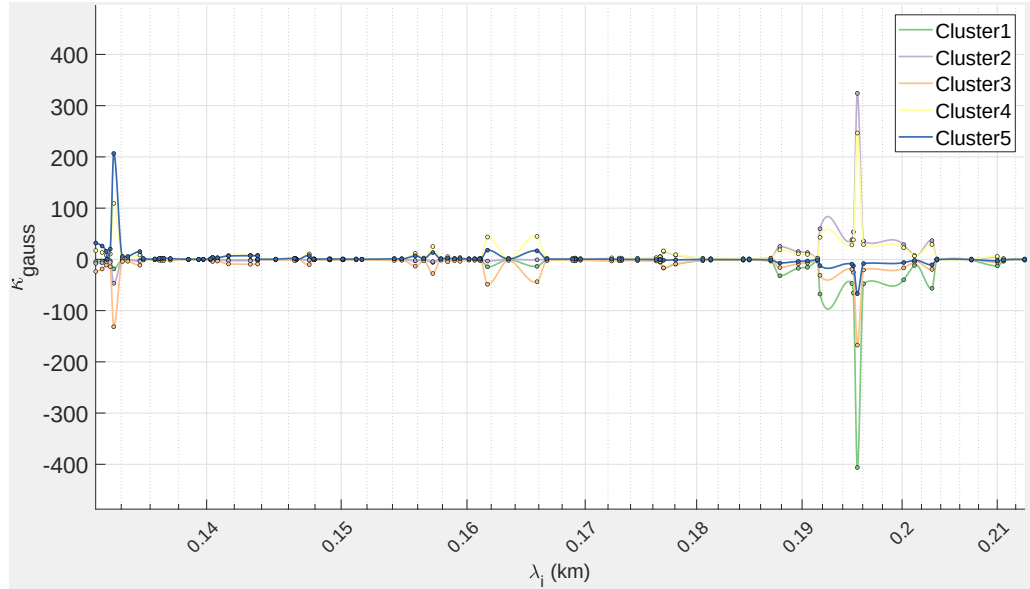


Figure B.8: The cluster centres of the Gaussian(κ_{gauss}) curvature segmentation for the compression pure shear with noslip base boundary condition model (B.6). Each cluster is a $89 = (150 - 61)$ dimensional vector where each dimension corresponds to a κ_{gauss} value. Note that $\kappa_{\text{gauss}} < 0$ values imply that locally the shape is saddle-shaped and $\kappa_{\text{gauss}} > 0$ values imply the shape is locally dome/basin (2.6).

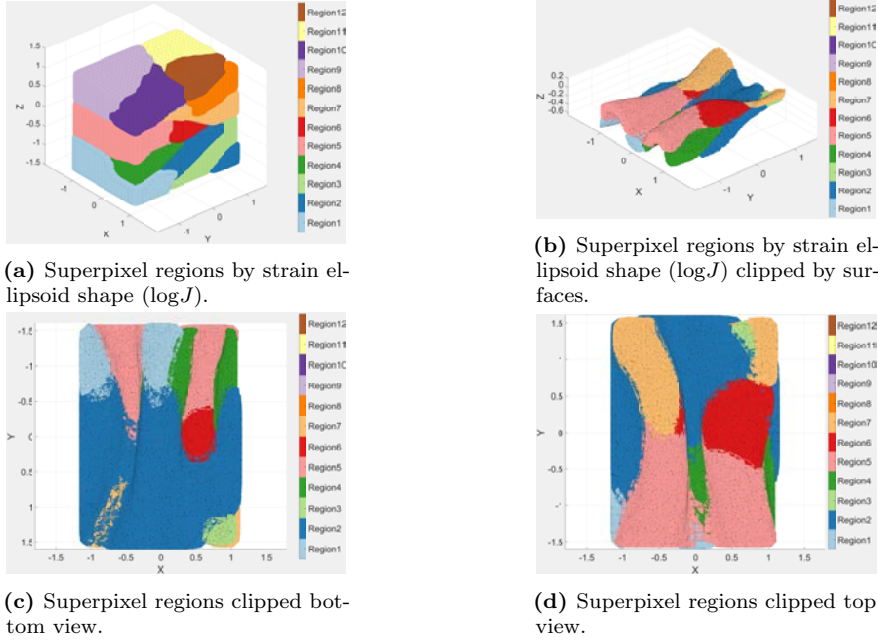


Figure B.9: Compression pure shear with noslip base boundary condition after 15.1562Myr. Superpixel region results using strain ellipsoid shape ($\log J$) at full marker resolution.

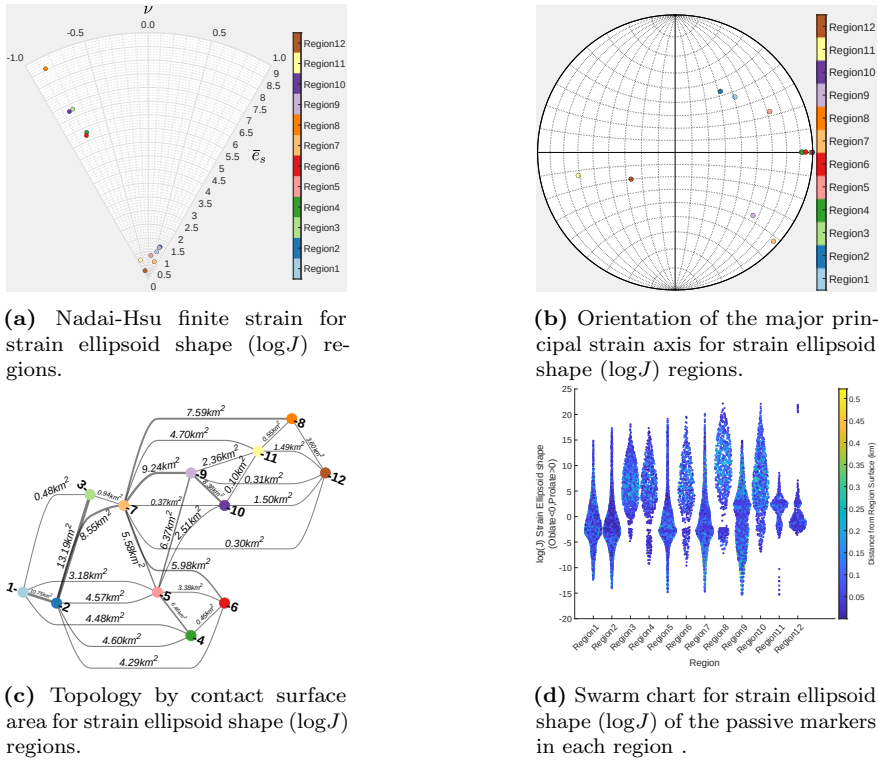
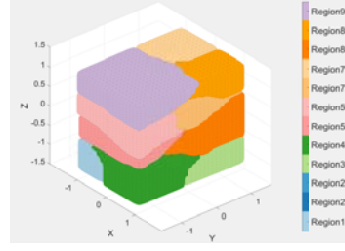
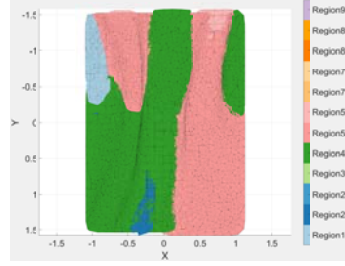


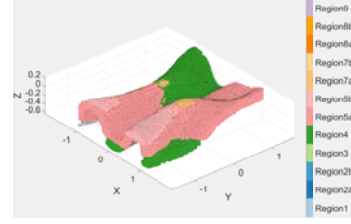
Figure B.10: Compression pure shear with noslip base boundary condition strain region analysis for strain ellipsoid shape ($\log J$) at full marker resolution (B.9).



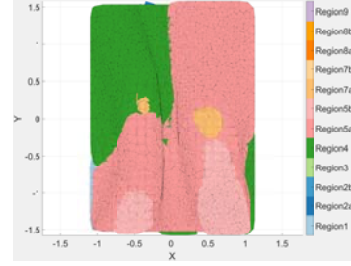
(a) Superpixel regions by strain ellipsoid shape ($\log J$).



(c) Superpixel regions clipped bottom view.

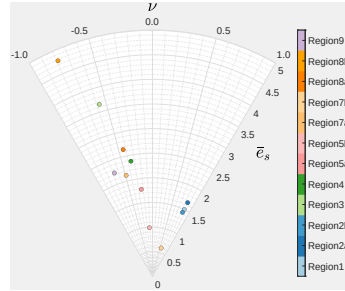


(b) Superpixel regions by strain ellipsoid shape ($\log J$) clipped by surfaces.

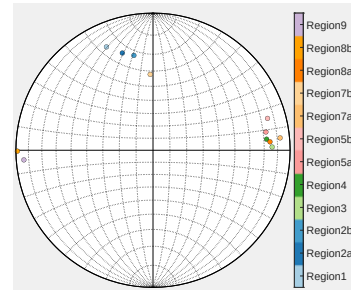


(d) Superpixel regions clipped top view.

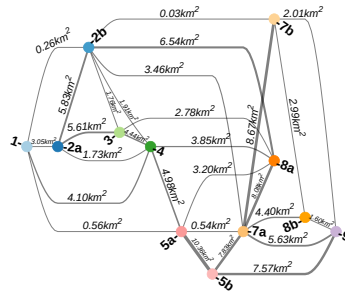
Figure B.11: Compression pure shear with noslip base boundary condition after 15.1562Myr. Superpixel region results using strain ellipsoid shape ($\log J$) using a tensor convolution of size $(5, 5, 5)$.



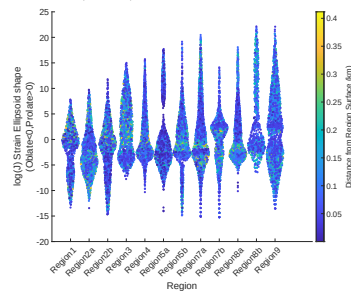
(a) Nadai-Hsu finite strain for strain ellipsoid shape ($\log J$) regions.



(b) Orientation of the major principal strain axis for strain ellipsoid shape ($\log J$) regions.



(c) Topology by contact surface area for strain ellipsoid shape ($\log J$) regions.



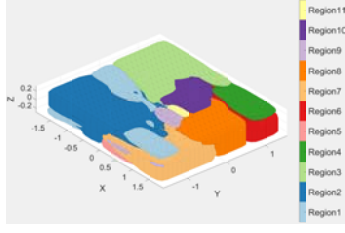
(d) Swarm chart for strain ellipsoid shape ($\log J$) of the passive markers in each region .

Figure B.12: Compression pure shear with noslip base boundary condition strain region analysis for strain ellipsoid shape ($\log J$) using a tensor convolution of size $(5, 5, 5)$ (B.11).

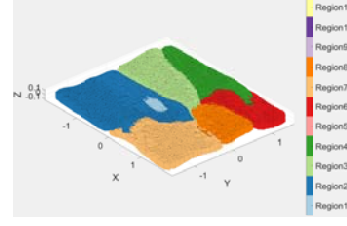
Appendix C

Strike-Slip Simple Shear

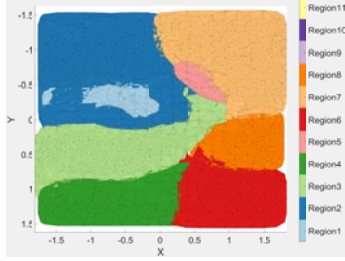
The results in this appendix correspond to the Section [4.3.2](#). The Strike-Slip Simple Shear boundary condition parameters can be found in Table [4.3](#), and a visualization of how the velocity conditions appear is found in Figure [4.3](#). The fold growth is smaller than the other models, and thus hasn't developed the Type 1 interference and hinge rotation that is common to high strain shear zones.



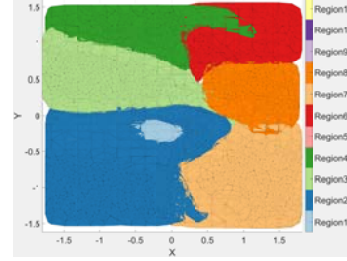
(a) Superpixel regions by kinematic vorticity(W_k).



(b) Superpixel regions by kinematic vorticity(W_k) clipped by surfaces.

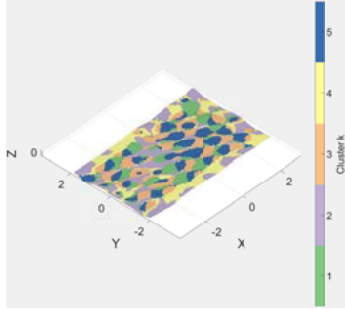


(c) Superpixel regions clipped bottom view.

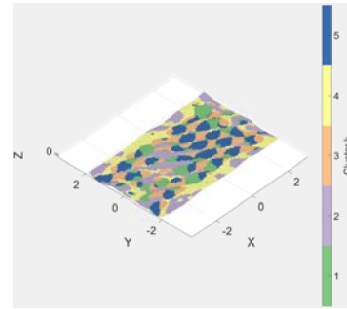


(d) Superpixel regions clipped top view.

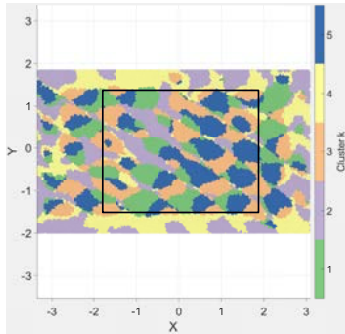
Figure C.1: Strike-Slip simple shear boundary condition after 15.1562Myr. Superpixel region results using kinematic vorticity(W_k) at full marker resolution.



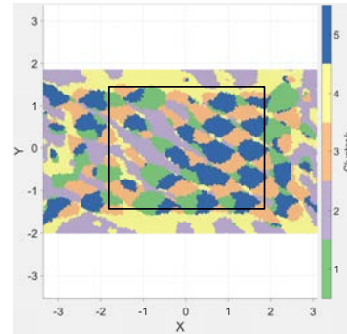
(a) Upper contact surface multi-scale κ_{gauss} segmentation.



(b) Lower contact surface multi-scale κ_{gauss} segmentation.

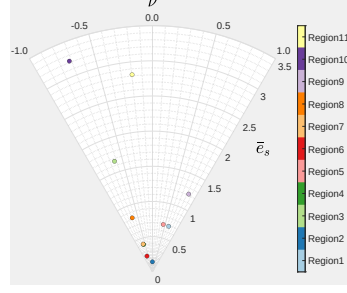


(c) Upper contact surface multi-scale κ_{gauss} segmentation XY view.

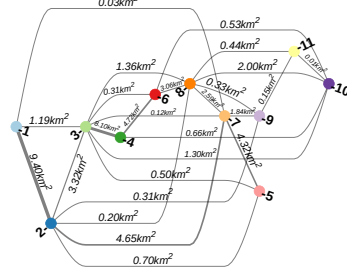


(d) Lower contact surface multi-scale κ_{gauss} segmentation XY view.

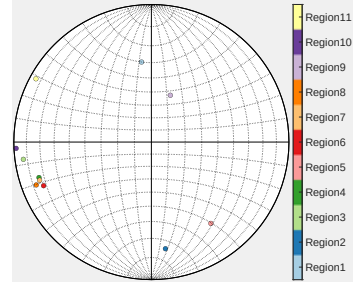
Figure C.2: Strike-Slip simple shear boundary condition after 15.1562Myr. Multi-scale Gaussian(κ_{gauss}) curvature segmentation. The range of eigenvalues that form the basis is **min** $\lambda_2 = 1.77$ km to **max** $\lambda_{150} = 0.13$ km, with $K = 5$ clusters.



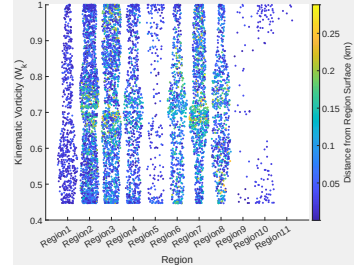
(a) Nadai-Hsu finite strain for kinematic vorticity (W_k) regions.



(c) Topology by contact surface area for kinematic vorticity (W_k) regions.



(b) Orientation of the major principal strain axis for kinematic vorticity (W_k) regions.



(d) Swarm chart for kinematic vorticity of the passive markers in each region .

Figure C.3: Strike-Slip simple shear boundary condition after 15.1562Myr. Strain region analysis for kinematic vorticity(W_k) at full marker resolution (C.1).

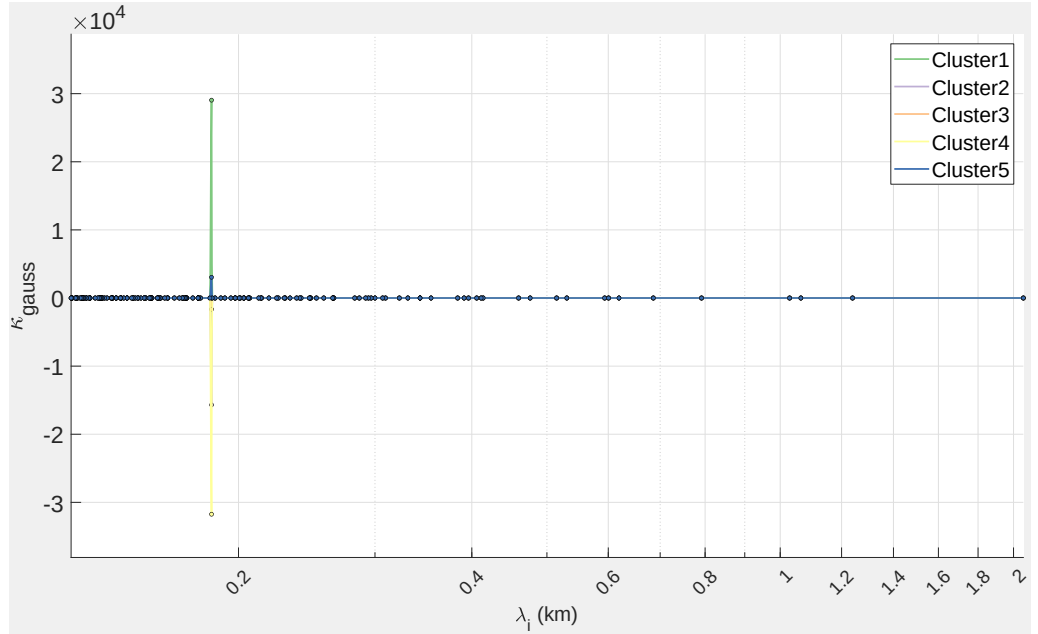
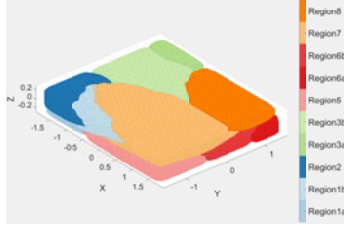


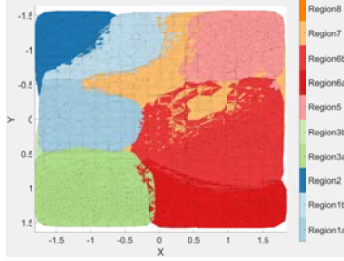
Figure C.4: The cluster centres of the Gaussian(κ_{gauss}) curvature segmentation for the Strike-Slip simple shear boundary condition model(C.2). Each cluster is a $148 = (150 - 2)$ dimensional vector where each dimension corresponds to a κ_{gauss} value. Note that $\kappa_{\text{gauss}} < 0$ values imply that locally the shape is saddle-shaped and $\kappa_{\text{gauss}} > 0$ values imply the shape is locally dome/basin (2.6).



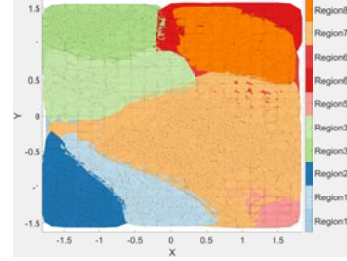
(a) Superpixel regions by kinematic vorticity(W_k).



(b) Superpixel regions by kinematic vorticity(W_k) clipped by surfaces.

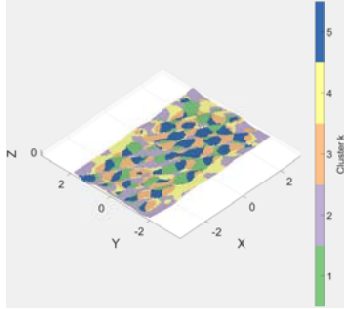


(c) Superpixel regions clipped bottom view.

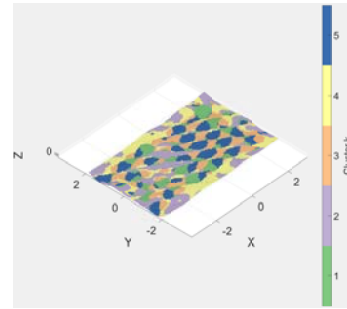


(d) Superpixel regions clipped top view.

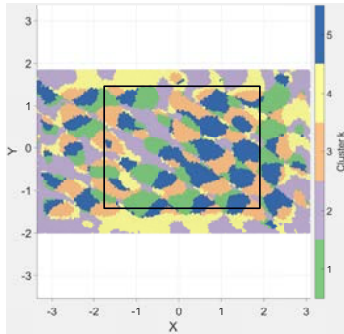
Figure C.5: Strike-Slip simple shear boundary condition after 15.1562Myr. Superpixel region results using kinematic vorticity(W_k) using a tensor convolution of size $(5, 5, 5)$.



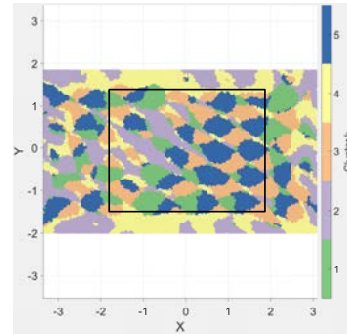
(a) Upper contact surface multi-scale κ_{gauss} segmentation.



(b) Lower contact surface multi-scale κ_{gauss} segmentation.

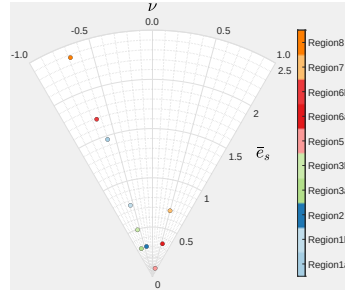


(c) Upper contact surface multi-scale κ_{gauss} segmentation XY view.

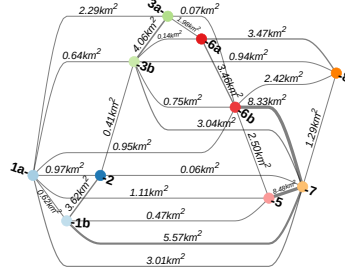


(d) Lower contact surface multi-scale κ_{gauss} segmentation XY view.

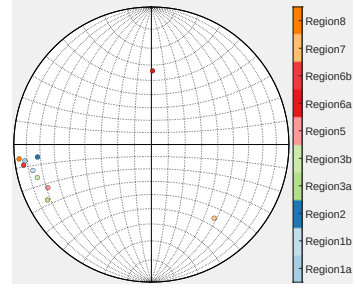
Figure C.6: Strike-Slip simple shear boundary condition after 15.1562Myr. Multi-scale Gaussian(κ_{gauss}) curvature segmentation. The range of eigenvalues that form the basis is $\min \lambda_{61} = 0.21$ km to $\max \lambda_{150} = 0.13$ km, with $K = 5$ clusters.



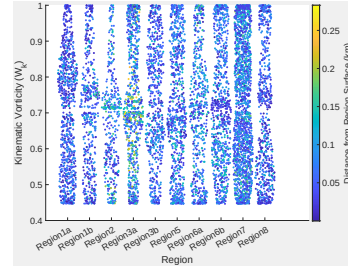
(a) Nadai-Hsu finite strain for kinematic vorticity (W_k) regions.



(c) Topology by contact surface area for kinematic vorticity (W_k) regions.



(b) Orientation of the major principal strain axis for kinematic vorticity (W_k) regions.



(d) Swarm chart for kinematic vorticity of the passive markers in each region .

Figure C.7: Strike-Slip simple shear boundary condition after 15.1562Myr. Strain region analysis for kinematic vorticity(W_k) using a tensor convolution of size (5, 5, 5) (C.5)

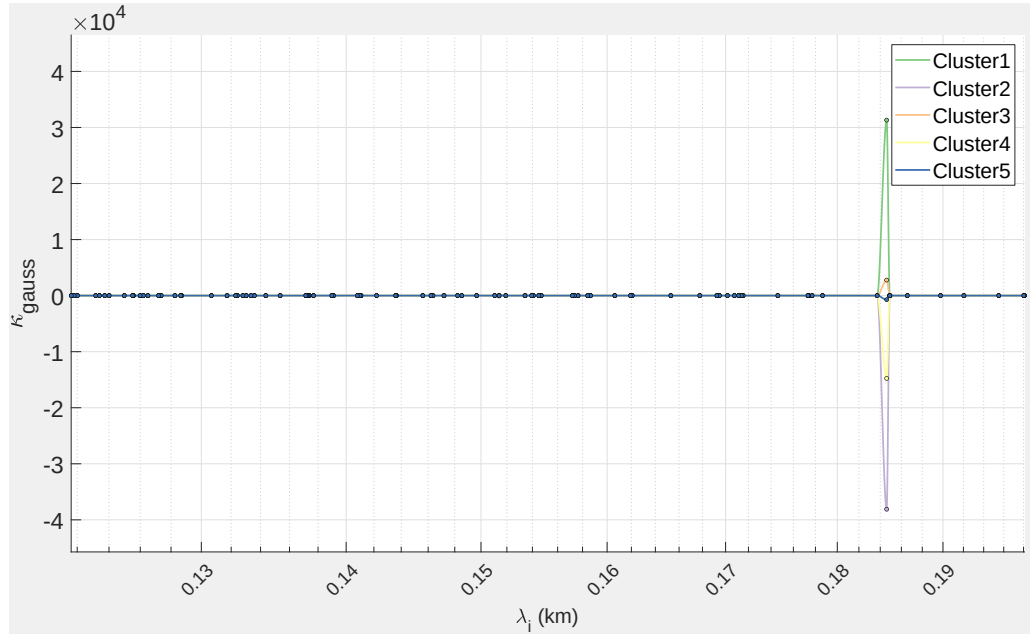
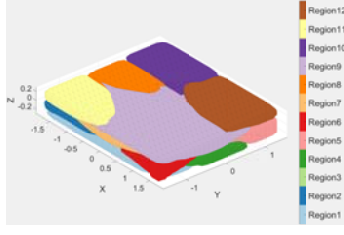
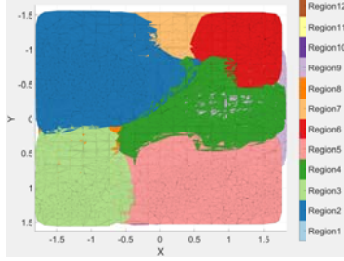


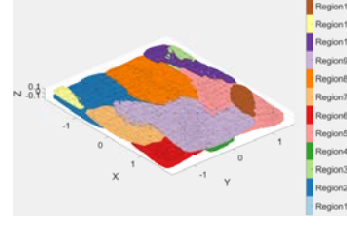
Figure C.8: The cluster centres of the Gaussian(κ_{gauss}) curvature segmentation for the Strike-Slip simple shear boundary condition model (C.6). Each cluster is a $89 = (150 - 61)$ dimensional vector where each dimension corresponds to a κ_{gauss} value. Note that $\kappa_{\text{gauss}} < 0$ values imply that locally the shape is saddle-shaped and $\kappa_{\text{gauss}} > 0$ values imply the shape is locally dome/basin (2.6).



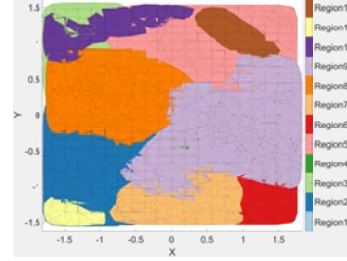
(a) Superpixel regions by strain ellipsoid shape ($\log J$).



(c) Superpixel regions clipped bottom view.

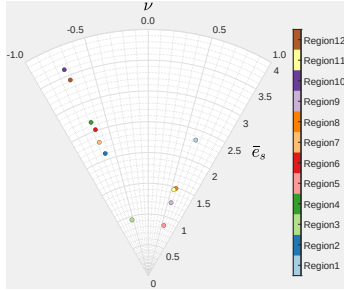


(b) Superpixel regions by strain ellipsoid shape ($\log J$) clipped by surfaces.

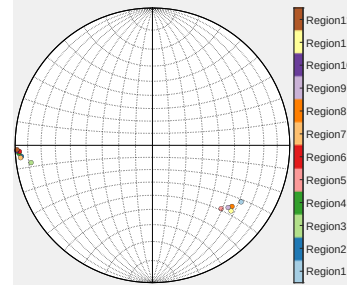


(d) Superpixel regions clipped top view.

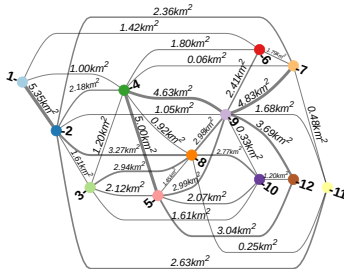
Figure C.9: Strike-Slip simple shear boundary condition after 15.1562Myr. Superpixel region results using strain ellipsoid shape ($\log J$) at full marker resolution.



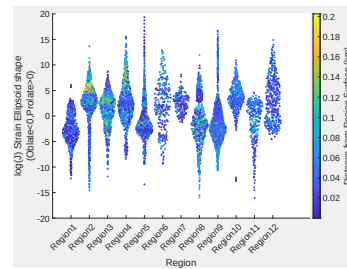
(a) Nadai-Hsu finite strain for strain ellipsoid shape ($\log J$) regions.



(b) Orientation of the major principal strain axis for strain ellipsoid shape ($\log J$) regions.

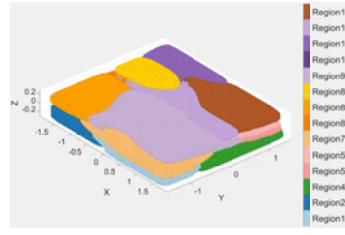


(c) Topology by contact surface area for strain ellipsoid shape ($\log J$) regions.

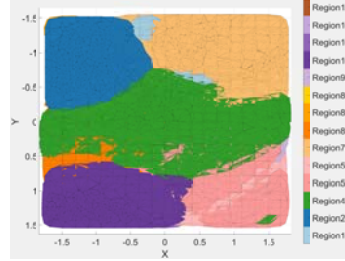


(d) Swarm chart for strain ellipsoid shape ($\log J$) of the passive markers in each region .

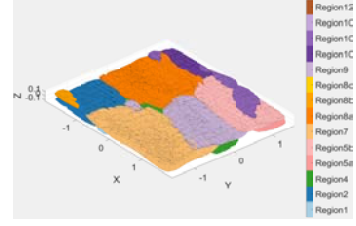
Figure C.10: Strike-Slip simple shear boundary condition strain region analysis for strain ellipsoid shape ($\log J$) at full marker resolution (C.9).



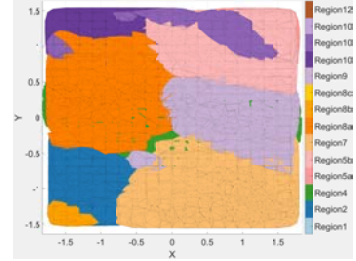
(a) Superpixel regions by strain ellipsoid shape ($\log J$).



(c) Superpixel regions clipped bottom view.

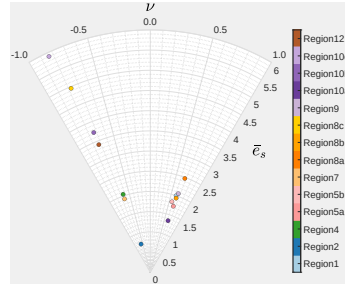


(b) Superpixel regions by strain ellipsoid shape ($\log J$) clipped by surfaces.

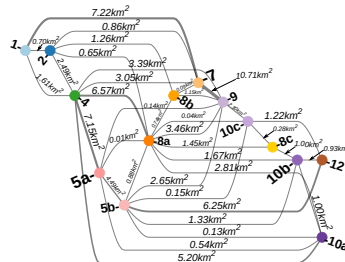


(d) Superpixel regions clipped top view.

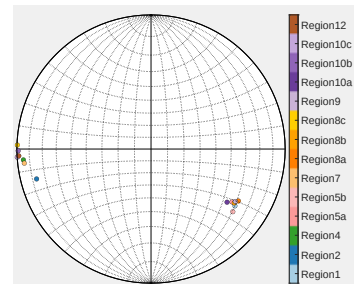
Figure C.11: Strike-Slip simple shear boundary condition after 15.1562Myr. Superpixel region results using strain ellipsoid shape ($\log J$) using a tensor convolution of size $(5, 5, 5)$.



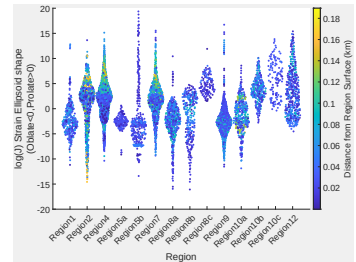
(a) Nadai-Hsu finite strain for strain ellipsoid shape ($\log J$) regions.



(c) Topology by contact surface area for strain ellipsoid shape ($\log J$) regions.



(b) Orientation of the major principal strain axis for strain ellipsoid shape ($\log J$) regions.



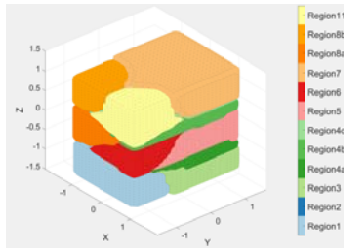
(d) Swarm chart for strain ellipsoid shape ($\log J$) of the passive markers in each region .

Figure C.12: Strike-Slip simple shear boundary condition strain region analysis for strain ellipsoid shape ($\log J$) using a tensor convolution of size $(5, 5, 5)$ (C.11).

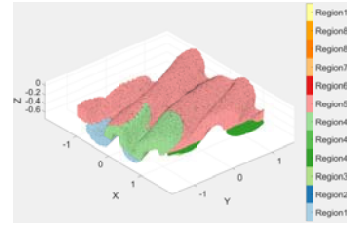
Appendix D

Transpression Pure and Simple Shear

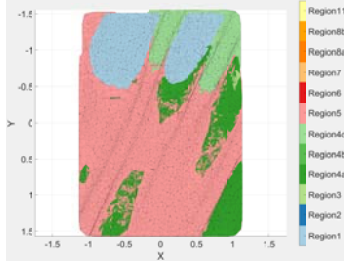
The results in this appendix correspond to the Section [4.3.2](#). The Transpressional Pure and Simple Shear boundary condition parameters can be found in Table [4.3](#). The results that make up this section include the mesh and strain region analysis for the larger average scale kinematic vorticity results.



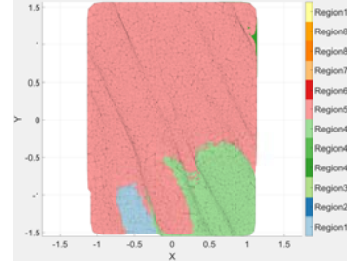
(a) Superpixel regions by kinematic vorticity(W_k).



(b) Superpixel regions by kinematic vorticity(W_k) clipped by surfaces.

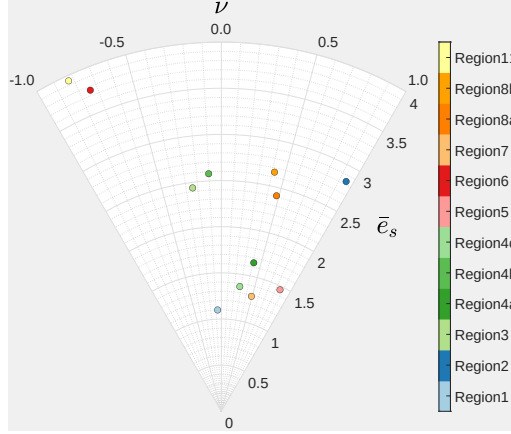


(c) Superpixel regions clipped bottom view.

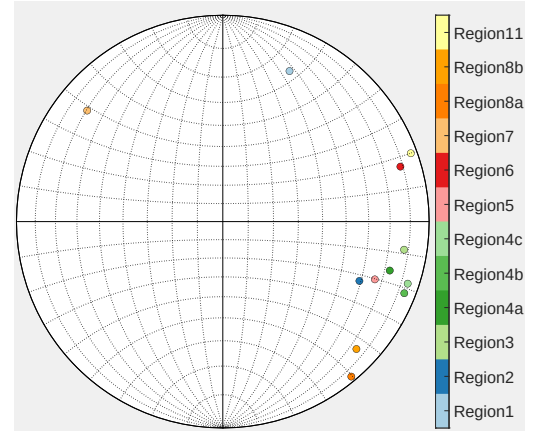


(d) Superpixel regions clipped top view.

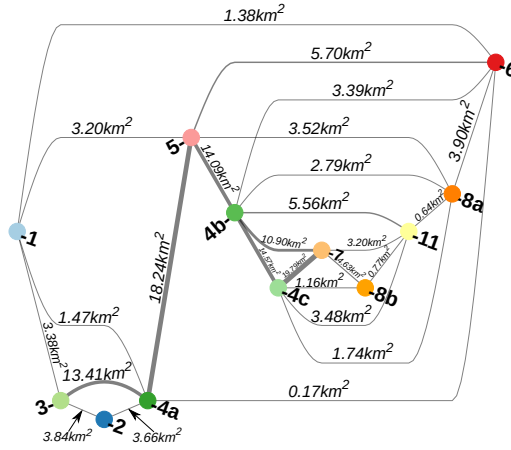
Figure D.1: Transpressional with both pure and simple shear boundary condition after 15.1562Myr. Superpixel region results using kinematic vorticity(W_k) using a tensor convolution of size (5, 5, 5).



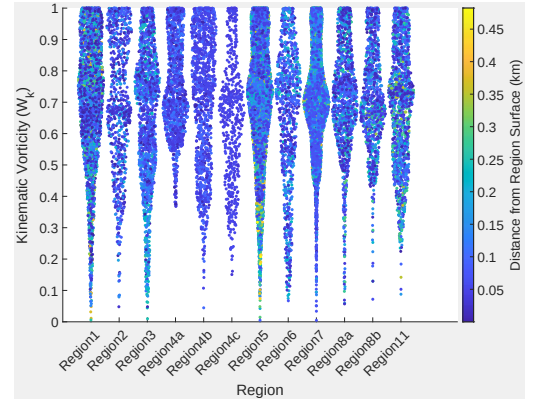
(a) Nadai-Hsu finite strain for kinematic vorticity (W_k) regions.



(b) Orientation of the major principal strain axis for kinematic vorticity (W_k) regions.

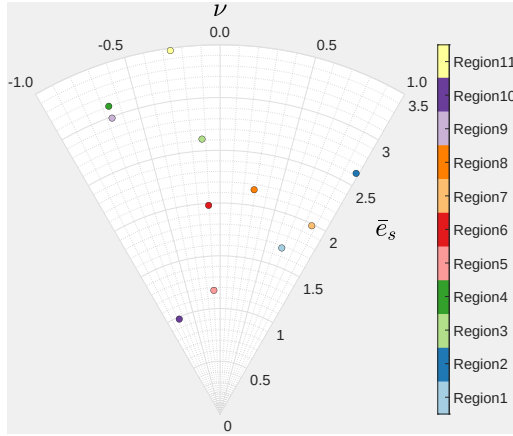


(c) Topology by contact surface area for kinematic vorticity (W_k) regions.

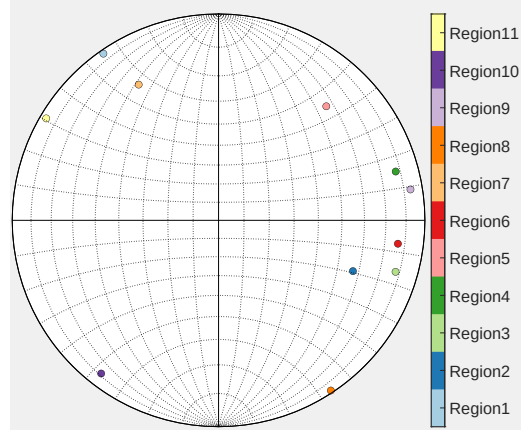


(d) Swarm chart for kinematic vorticity of the passive markers in each region .

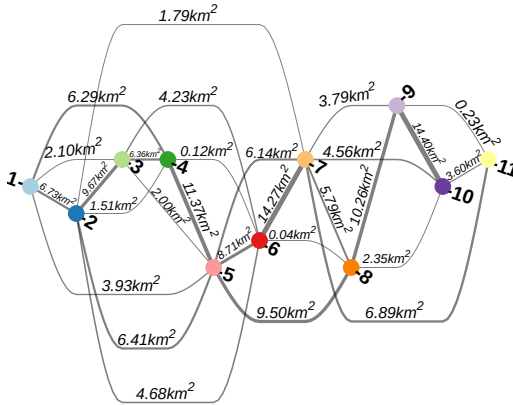
Figure D.2: Transpressional with both pure and simple shear boundary condition after 15.1562Myr. Strain region analysis for kinematic vorticity(W_k) using a tensor convolution of size (5, 5, 5) (D.1)



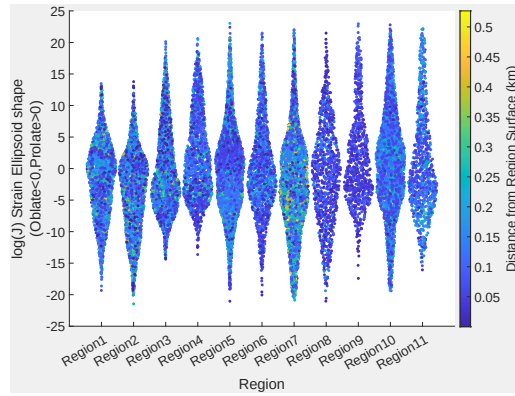
(a) Nadai-Hsu finite strain for strain ellipsoid shape ($\log J$) regions.



(b) Orientation of the major principal strain axis for strain ellipsoid shape ($\log J$) regions.



(c) Topology by contact surface area for strain ellipsoid shape ($\log J$) regions.



(d) Swarm chart for strain ellipsoid shape ($\log J$) of the passive markers in each region .

Figure D.3: Transpressional with both pure and simple shear boundary condition strain region analysis for strain ellipsoid shape ($\log J$) at full marker resolution (4.24).