

CASE FOR SUPPORT

PART 1: Previous track record of investigators

General experience of investigators in this area

Prof. W.S. Kendall (WSK) has worked in probability for 35 years (the last 20 at Warwick Statistics), authoring about 100 papers and 6 co-authored or co-edited books. He has served in various editorial rôles, including inaugural Coordinating Editor for the section *Stochastic Geometry and Statistical Applications* of *Advances of Applied Probability*, and Chief Editor for *Electronic Communications in Probability*. He was Scientific Secretary for the Bernoulli Society 1996-2000, Scientific Programme Chair for its Sixth World Congress in 2004, and currently is President-Elect. He was PI for the 2008 EPSRC Warwick workshop “New scaling limits in probability”, initiating a biennial series of UK probability meetings. Since 2006 WSK has served as co-director and PI of the EPSRC-funded Academy for PhD Training in Statistics, annually training 80 Statistics first-year UK PhD students.

Prof. M. Williams (MW) is Deputy Head of the Digital Manufacturing Theme group at WMG. MW is a Chartered Engineer and Fellow of the Institution of Mechanical Engineers and worked as a Dimensional Control consultant in a wide range of industries before joining WMG in 2003. MW established the WMG Product Evaluation Technologies (PET) research group and has managed a diverse portfolio of applied research projects totalling over £30M funded by EPSRC, TSB and EU. This has led to MW publishing over 50 academic papers in peer reviewed journals and international conferences. Independently audited socio-economic impact of this research includes 1500 jobs safeguarded, £20M process savings, and £7.5M of incremental R&D investment. Current research interests include Advanced Metrology Systems, Digital Prototyping, and the Human Machine Interface (HMI).

Dr. J.A. Brettschneider (JAB) earned a probability PhD with applications to statistical mechanics 10 years ago. Since then JAB has worked in methodological applied statistics and interdisciplinary projects, with co-authors from mathematical sciences, genomics and medical research. She has supervised many interdisciplinary Masters projects in applied statistics and probability, and is currently co-supervising two PhD students. JAB has worked on statistical consulting projects eg with the Risk Initiative and Statistical Consultancy Unit based in the Department of Statistics. She sits on Bernoulli Society Council, and was a main local organiser of the statistical computing conference `user!2012`.

Dr. T. Nichols (TN) has worked on modelling and inference of medical imaging data for 20 years and authored 100 peer-reviewed publications. He won the Organization for Human Brain Mapping’s Young Investigator Award in 2009 and is an editor for *NeuroImage*. He combines industrial and academic experience, having worked as a Director of Modelling and Genetics at GlaxoSmithKline, 2006-2009. Currently a Principal Research Fellow joint between Warwick Statistics and WMG, he is ideally placed to coordinate Statistics and WMG project activity.

Dr. G. Gibbons (GG) joined WMG in 1997 as head of the Additive Layer manufacturing (ALM) department. His research interests include ALM processing of novel materials, quality and reliability management of ALM systems, and ALM in clinical practice and education. He works across many sectors (motorsport, aerospace, defence, healthcare, fashion etc) to provide ALM manufacturing solutions. GG has received over £650k of EPSRC funding and recently he led the ALM research activities within the EPSRC / ERDF funded Premium Vehicle Customer Interface Technologies programme, and is currently PI for the EU funded FP7 AirPROM project (2011 - Euros 693k).

Specific experience of the investigators relevant to this proposal

WSK has co-authored the major monograph in the area of stochastic geometry [11] (third edition now in preparation) as well as recently co-editing and contributing to a collection of expository articles describing recent research in the area [7]. Many of his papers concern work on the interfaces between probability, statistics and geometry, including influential work on perfect simulation, networks, point processes, and recent work on detection of curvilinear and quantal structure.

MW has co-authored [8, 9], GG has co-authored [4, 6] and MW and GG are co-presenting a paper [3] at “1st Annual EPSRC Manufacturing the Future Conference”.

JAB has been working on high-dimensional data from gene expression microarray data with an emphasis on quality assessment, including computational aspects and the special case of time course experiments [2, and references therein]. She has worked on asymptotic bounds for large deviation events for random fields and on related ergodic theorems [1, and references therein].

TN has extensive experience in modelling large, complex data, including multiple testing inference for brain imaging [5] detecting changes in the brain while controlling false positives; highly relevant to developing spatial testing procedures that localize faults in ALM objects scanned with CT. TN has also worked on Positron Emission image reconstruction Tomography [10], closely related to CT reconstruction, and facilitating work either in CT ‘projection’ domain or the volume image domain.

Research environment

The Warwick Statistics Department is located in the modern Zeeman Building, providing an attractive working environment with all facilities required for world-leading research. The Statistics Department runs a thriving series of workshops on its own account through the major EPSRC-funded CRiSM initiative (Centre for Research in Statistical Methodology), and owns and runs a small departmental computing cluster (40 fast processors, 80GB of memory) supporting computationally intensive research. The Warwick probability group is shared between Statistics and Mathematics (in the same building) and works closely together in running research seminars, and hosting visitors and conferences (the probability research workshop series mentioned above returned to Warwick this year as part of the EPSRC-funded Year of Probability 2011-2012). We will use local expertise in both Statistics (Dr Elke Thönnies) and Mathematics (Profs Mackay and Farber) for specific technical input.

WMG is an internationally recognised group based in five dedicated co-located buildings adjacent to the Zeeman Building, with a range of research grants and industrial funding working in advanced materials and manufacturing processes, totalling £70M per year.

The Product Evaluation Technologies (PET) research group owns a 225/320kV Micro X-Ray scanner capable of producing Computed Tomography reconstructions at a resolution of up to 5 microns. The group has also access to the latest digital laser scanning technology for capturing high accuracy three dimensional surface models and photorealistic visualisation and digital prototyping software for data interpretation. This will be crucial in capturing and categorising the internal and external characteristics of ALM samples used to test and validate statistical methods developed by the project.

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CASE FOR SUPPORT

PART 2: Proposed research. Inside-out: Statistical methods for CT validation of complex structures in Additive Layer Manufacturing

1 Background

Additive layer Manufacturing (ALM) develops products directly from their digital design data by the layer-wise addition of material. ALM is a tool-less process, so responds cost-effectively to changing customer demand, and has potential to be a paradigm-shift in manufacturing. It enables creation of innovative products through realisation of complex, even “impossible”, geometries [25], and integration of new materials for enhanced performance [17]. ALM is now being explored in many sectors, eg aerospace [12], healthcare [20], motorsport [6]. Potentially it enables new business models, products and supply chains, shifting manufacture away from large scale mass production to collaborative (customers engaged in the design process) or even democratised (customers design and manufacture their own products) manufacture. In combination with E-business advances, ALM is opening up a whole new product service industry model of Mass Customisation, offering the customer the ability to personalise a product [10]. Despite these enormous opportunities, ALM market penetration by 2020 is only forecast to be 8% [27]. The recent TSB report on national competency in ALM [24] identifies two key issues restricting market growth: inconsistency part quality, and lack of in-process measurement. Inconsistent part quality can arise from internal flaws: porosity due to lack of consolidation pressure, inconsistent surface energies of melt and solid layers and non-uniform layers (Marangoni flow), or stress-induced cracks arising from solidification and phase changes [11]. Moreover the application of reliability management tools for ALM is in its infancy [16], due mostly to inability to obtain useful quality data from the ALM system. Thus the TSB has proposed [24] that new rapid in-process and end-of line product measurement techniques should be a key future ALM research focus for the UK. The proposed research will deliver a means to rapidly assess the internal quality of ALM manufactured components, unachievable with current technology, enabling the cost and time-effective delivery of fit for purpose ALM products with assured quality levels.

2 National Importance

The UK has a healthy High Value Manufacturing sector, and a particularly strong aerospace manufacturing presence. UK aero engine manufacturing is ranked world 2nd. Key players, including BAE Systems, Bombardier, EADS, and Rolls-Royce, are worth £23.5bn in 2011-12, and predicted to reach £26.2bn in 2016-17. The UKs biomedical sector, and especially the orthopaedic and implantables market, is worth over £400m (UK) and over £10bn globally, and is expanding at a CAGR of over 7%, with key players such as S&N, Zimmer, Stryker, Biomet. Both sectors will benefit from the ability to deliver cost-effective new products with enhanced customer benefit (advanced fuel injectors and combustion systems with improved fuel performance, customised biomedical implants for improved fit and longevity). Increased uptake in these and other sectors will benefit ALM and CT Original Equipment Manufacturers (OEMs) through increased revenues. It has been estimated that overcoming the current limitations of ALM and gaining market acceptance would enhance penetration from 8% to 92% by 2020, in a market worth £66bn globally. This research will deliver new CT-based methods for quality assessment of complex products through Additive Layer Manufacturing. This aligns directly with EPSRCs Manufacturing the Future Theme, addressing ‘Performance and Inspection of Mechanical Structures and Systems’ within the Innovative Production Processes sub-theme. It also directly addresses ‘development of non-destructive evaluation techniques’, underpinning a range of sectors such as aerospace, defense, healthcare and manufacturing. There is a significant strategic fit with the recently launched High Value Manufacturing Catapult, principally providing a method for the validation of light-weight ALM derived structures and developed under the structural optimisation theme within WMG. This research will help to develop the existing relationship between WMG and

the Statistics department, linking novel mathematical research techniques (new statistical methods) with novel manufacturing research (rapid, reliable and robust quality assurance methodologies for Additive Layer Manufacturing), addressing an important manufacturing research challenge. The focus is on using a technology (CT) in a manufacturing process (ALM) for product data capture and analysis, which is one of the areas identified in the Industrial Mathematics KTN and the HMV Catapult Centre workshop. The Future Manufacturing with Mathematical Sciences initiative offers the opportunity to bring together cutting edge research capability and expertise in manufacturing (WMG) and statistical mathematics (Department of Statistics), fostering collaboration, increasing manufacturing intelligence, and enabling new technologies for the UK to meet the future manufacturing global challenges.

3 Work Programme and Methodology

This project therefore aims to build statistical and probabilistic methods to reliably detect defects in ALM-produced objects with cone-beam computed tomography (CT), with an emphasis on minimizing the time needed to make such inferences. The work programme divides into three objectives:

1. to undertake *detailed investigation of random variation* for the CT data collected;
2. to determine methods to supply *statistical process control of printed objects*;
3. to develop statistical methods for *assessing geometry and topology* of printed objects.

3.1 Detailed investigation of random variation

Objectives 2 & 3 depend on an accurate model for the deterministic and stochastic features of the CT data collected, in both projection (raw data) and 3D volume image domains. The first objective therefore is the development of a mean value model in both these domains, using tools based on computed aided design (CAD) models of the manufactured item, together with determination of an appropriate model for measurement noise.

CT uses X-rays to measure object density *via* a sequence of 2D radiographs, which in turn can be reconstructed into a 3D volume image. The cone-beam CT device at WMG PET is a commercially available device (Nikon metrology XTH320LC), comprised of a fixed X-ray source 873mm away from a flat panel detector. Samples are placed between source and detector and rotated by a precision manipulator to produce the sequence of radiograph images; note that this is different from medical fan-beam CT, where source and detector rotate about the patient. The flat panel detector consists of a scintillator sandwiched against a semiconductor consisting of $2000 \times 2000 \cdot 0.2^2$ mm² light-sensitive photodiodes. The scintillator absorbs X-rays and emits visible light to be detected by the photodiodes.

A simple model of the relationship between X-ray intensity and object density at detector i is

$$I_i = I_{0,i} \exp\left(-\int_{\mathcal{X}_i} \mu(x)dx\right)$$

where I_i is the intensity measured with the object present, $I_{0,i}$ is the intensity measured with no object present (calibration scan), $\mu(x)$ is the linear attenuation coefficient at location x in the object, and \mathcal{X}_i is the path through the object between source and detector i . The data available from the scanner takes the form of $Y_i = -\log(I_i/I_{0,i})$, $i = 1, \dots, I$, where i indexes over all 2D projection pixels over all rotation angles. While I_i would ideally consist of Poisson-distributed X-ray photon counts, instead the photodiodes report a continuous response proportional to X-ray intensity. The observed data reflect a variety of other sources of variation, including X-ray tube current instability, varying photodiode efficiency and photodiode electronic noise.

We will construct an accurate (though necessarily approximate) noise model in the projection domain. Our starting point will be the ‘‘Poisson + Gaussian’’ model [22], actually a Gaussian model where each projection element is assumed independently distributed with variance derived from scaled Poisson counting noise and Gaussian electronic noise. This model depends on the object mean (described next), a Poisson scaling factor θ and electronic noise variance σ^2 that possibly varies from pixel-to-pixel; θ and σ^2 must be estimated from data.

Line integrals through the Computer Aided Design (CAD) model that generated the ALM object will provide the basis for the (defect-free) mean model, $m_i = \int_{\mathcal{X}_i} \mu_{CAD}(x) dx$, where μ_{CAD} is the relative density of the object ($\max_x \mu_{CAD}(x) = 1$, $\mu_{CAD}(\text{“air”}) = 0$). The data mean $E(Y_i) = f(m_i)$ requires a mapping function $f(\cdot)$, a low-order polynomial based on calibration scans of simple solid objects (e.g. a cylinder). Ideally the mapping would just be $f(m) = \mu_{material} \times m$ to reflect the unknown linear attenuation coefficient of the ALM material, but instead may require curvature to reflect “beam hardening” [2], a nonlinearity due to a multispectral beam source. If needed, we will additionally consider the effects of scintillator afterglow (which induces a blurring between detectors), and scatter (which induces a haze and artifacts).

We will use Nikon Metrology’s filtered back projection (FBP) algorithm to reconstruct 3D volume data from projection data. At highest resolution the reconstructed volume has $\approx 8 \times 10^9$ voxels with 3^3 micron³ voxels. While FBP has no noise model and suffers under low count rates, we generally will have a good count rate due to initial focus on small, light objects. We can consider large, dense objects, but then low count rates will require the use of “statistical reconstruction” methods [8]. In the volume domain, the CAD model gives the (defect-free) mean up to a scalar multiple (possibly accounting for rigid-body registration). A surface model can be constructed from observed data, in preparation for topological comparisons. Variance estimation in the volume domain, unfortunately, is a challenging and on-going research area in the reconstruction literature (see, e.g., [28]). If projection-domain efforts (where variance is available) do not sufficiently locate defects, we will explore the use of repeated, short scans to derive empirical variance estimates.

To test the null hypothesis of no defects, we will use our mean and noise model in the projection domain to construct test statistics at each projection element. Large test statistic values indicate disparity between the actual and defect-free CAD model (e.g. pores, cracks, shape errors). In the volume domain we will examine the extracted surface and its geometry relative to the CAD model.

The test statistics in the projection domain and the estimated surface model in the volume domain feed into parts 2 and 3 of this project, respectively. Where feasible, the projection domain approach offers considerable time advantages, as volume reconstruction is computationally very costly. Still greater time savings can be gained if a small number of angles are sufficient to detect defects.

This part of the work programme depends on tight collaboration between TN, JT and Stats-PDRA (S-PDRA). S-PDRA will develop the noise model, working closely with JT for calibration data. JT will build the mean model from the CAD model with close interaction with Nikon Metrology, and interact with S-PDRA to use this to build test statistics; JT will also build surface models from volume data, matched to CAD models. TN will coordinate, drawing on his image reconstruction experience.

3.2 Statistical process control of printed objects

Development of ALM technology beyond rapid prototyping to higher throughput production is hindered by the bottleneck of immature quality control. Particular statistical shortcomings include inconsistency between batches, lack of monitoring methods, absence of standards and limited accessible performance data [24, Table 3]. Highly complex (and often internal) part geometry resists direct inspection. We plan to develop a suitable statistical process control (SPC) methodology based on geometrical outcomes (e.g. curvature). Exploiting the flexibility of the ALM approach for mass customisation (e.g. medical implants), we may permit specifications to vary over the production run.

CAD model M , manufactured object X , and estimates \hat{X} can all be represented as random fields in d -space. The volume domain ($d = 3$) is natural, but the projection domain corresponds to higher (over-specified) dimensionality. Quality assessment based on the deviation $V = M - \hat{X}$, leads to statistics such as $|\max_i V_i|$, for i running over all possible voxels. Beyond that, we will explore the scanning statistics to test for general types of signals shapes (corresponding to defects) T in noisy environment. Bounds for tail probabilities under the Null can be derived by studying finite horizon versions of large deviation probabilities using likelihood ratio methods [14, and references therein]. For example, let $\{Z_n(t), t \in T\}$ be the random field of standardized score statistics for n observations and $x = o(n^{1/4})$. Under certain distributional assumptions for the noise and its impact on the signal, $P(\sup_{t \in T} Z_n(t) \geq x) \approx x^{d-1} (2\pi)^{-d/2} \phi(x)$, up to an $o(1/x)$ term.

As geometrical features depend on (infinitesimal) local or even global characteristics (cf Section

3.3), a functional data approach has recently been introduced in the monitoring of profiles [26, and references therein] and geometric properties (e.g. roundness, flatness) based on the symbolic language of geometric dimensioning and tolerancing (GD&T) [5, and references therein]. They replace *a priori* strategies for the sampling of measurement points by adaptive strategies derived by regression models (e.g. SARX) and the use of PCA in multivariate statistical process control (MVSPC) [1]. We will use this to develop adaptive sampling strategies for CT scans. Further aims include development of control charts for selected geometrical outcomes and study of their run-length performance.

Searching for arbitrary defects over the entire object leads to a huge multiple testing task. Recent progress in this field [7, for a review] provide a range of multiple testing error measures and control strategies. We will determine suitable approaches using estimates of the correlation structure.

We will evaluate and compare our methods on the basis of statistical properties (e.g. sensitivity), simulations and tests on faulty items designed for this purpose. The ALM community will be given access to the data as well as to a catalogue of typical defects, their shapes in the projection space and appropriate test statistics. This is motivated by experiences from the microarray community, where calibration data affycomp.biostat.jhsph.edu and a defect catalogue plmimagegallery.bmbolstad.com have triggered further methodological improvements and quality benchmarks.

Beyond its use for outlier detection, the proposed work embeds into a broader quality engineering context. It leads to continuous process improvement by assigning *special causes or poor quality*, as Shewhart put it. ALM applications are as different as aero engines and limited edition jewellery. Following Taguchi's emphasis on the functionality, we allow spatially inhomogeneous targets and different priorities (e.g. maximal thickness, minimal variation, smoothness).

Our primary aim is to develop a solid methodology for *a posteriori* assessment of the object. Given the urgent need for in-line process control as the new technology is taken up, we prioritize potential adaptability for in-line monitoring schemes. This includes minimisation of the number of time consuming CT scans, quality assessment in the projection domain and adjustable detection error rates allowing to operate QC simultaneously on two time scales (quick in-line screening calibrated to detect a maximal amount of faulty items with a minimum amount of scans but at high false detection rate, and a slower follow-up test with low false detection rate applied to items screened out as faulty).

In this section of the project, novel statistical methodology will be produced by developing test statistics corresponding to a range of defect types, exploring distributions and correlation structures in the ALM application, deriving bounds for corresponding tail probabilities, suggesting techniques for multiple testing error control and implementing all these techniques in concrete SPC tools. Most of these results would be of interest beyond ALM applications.

TN and JAB will collaborate closely to develop/evaluate statistical tests, supported by the S-PDRA, using joint work by WSK and JAB on geometry. JAB, WSK and TN will have input into JT's design of sample datasets. Aspects of MVSPC will be explored by the S-PDRA under supervision of JAB and WSK, consulting with MW and GG. Overall evaluation will involve the entire team.

3.3 Assessing geometry and topology

Workers in stochastic geometry etc have developed various estimation methods for geometry and topology of random structures, and these are directly applicable to two-phase 3D structures as in simple ALM. We will apply these methods to statistical analysis of small-scale structural variations and texture for use in quality control. Initially we will work in the volume domain; later we will investigate robustness of the measures to the kind of degradation arising from measurement by reduced numbers of radiographs, and explore relationships to significant deviations in the projection domain.

We give three examples. Firstly, the classical Minkowski functionals and measures from integral geometry. As in [21], these can be defined in terms of the volume of a dilation of the object K . For a bounded convex body the Minkowski functionals are defined by the *Steiner formula* (3D case)

$$\text{Volume}(K \oplus b(o, r)) = W_0(K) + 3W_1(K)r + 3W_2(K)r^2 + W_3(K)r^3,$$

where $A \oplus B = \{a+b : a \in A, b \in B\}$ and $b(o, r)$ is the ball of radius r . This definition may be extended by use of C -additivity relations (namely, $W_i(K_1 \cup K_2) = W_i(K_1) + W_i(K_2) - W_i(K_1 \cap K_2)$), producing

geometric valuations on wider families of non-convex bodies, serving as good models for the objects studied in ALM. There is an extensive and informative theory [18]. The first two functionals correspond to conventional volume and surface area, but W_2 and W_3 measure mean and Gaussian curvature. They can be approximated from thresholded data [13] and can be localized to produce curvature measures. Recently this has been applied to generate graphical aids to diagnosis for emphysema using lung CT data [23], and this application serves as a useful model for our investigation.

Secondly, there is a very recent generalization of the Minkowski functional theory to the tensor-valued case, using symmetric tensor products of position vectors with surface normals to generate tensor valuations. [19] introduces the extensive theory, and makes software freely available. As noted in [19], these additional valuations permit quantification of anisotropy effects.

These investigations deliver graphical presentations of curvature and anisotropic features, distributed over the external and internal surfaces of the object of interest. At appropriate levels of accuracy, this allows quantification of small-scale anomalous geometric deviations. This will then be assessed to determine the amount of radiograph information required to deliver reliable information, based on our model for random variation. In ALM applications the geometry of the nominal object is already known; therefore the assessment will be based on a statistical perturbation analysis informed by our detailed analysis of random variation. The objective is to limit the amount of effort (in terms of radiographs) required to obtain useful information about small-scale geometric deviations.

As well as geometry, one can measure quantitative topological features using persistent homology [4]. This is computed by considering a judicious distribution of points over the surface of the body to be considered (representative “witness” points), dilating each point using a ball of radius ε , and computing the homology of the resulting union of balls, viewed as a function of ε . This gives information about the topology of the structure at varying length scales, typically presented using a so-called bar-code diagram. The calculation carries a high computational burden: however recent statistical work considers alternative approaches using particular choices of ε based on curvature constraints [3, 15]. Additionally there is an interpretative problem: a possibly substantial fraction of the reported topology will arise from random fluctuation. We believe we can address this, based on stochastic geometry ideas concerning the statistical behaviour of large vacancies and other artefacts in critical high-intensity Boolean models as indicated in [9, Section 3.6]. Such a result will deliver a statistical perspective on whether bar-code diagrams are producing evidence of real structure; this deliverable should have impact beyond the ALM application.

WSK will work with the S-PDRA to construct estimators of spatial distribution of curvature and anisotropy, consulting with JW and GG on engineering significance, and using sample objects generated at Renishaw and WMG, and analyzed using Nikon Metrology facilities (with JT as liaison). WSK and JAB will work on relating persistent homology to Boolean model asymptotics.

4 Academic Impact

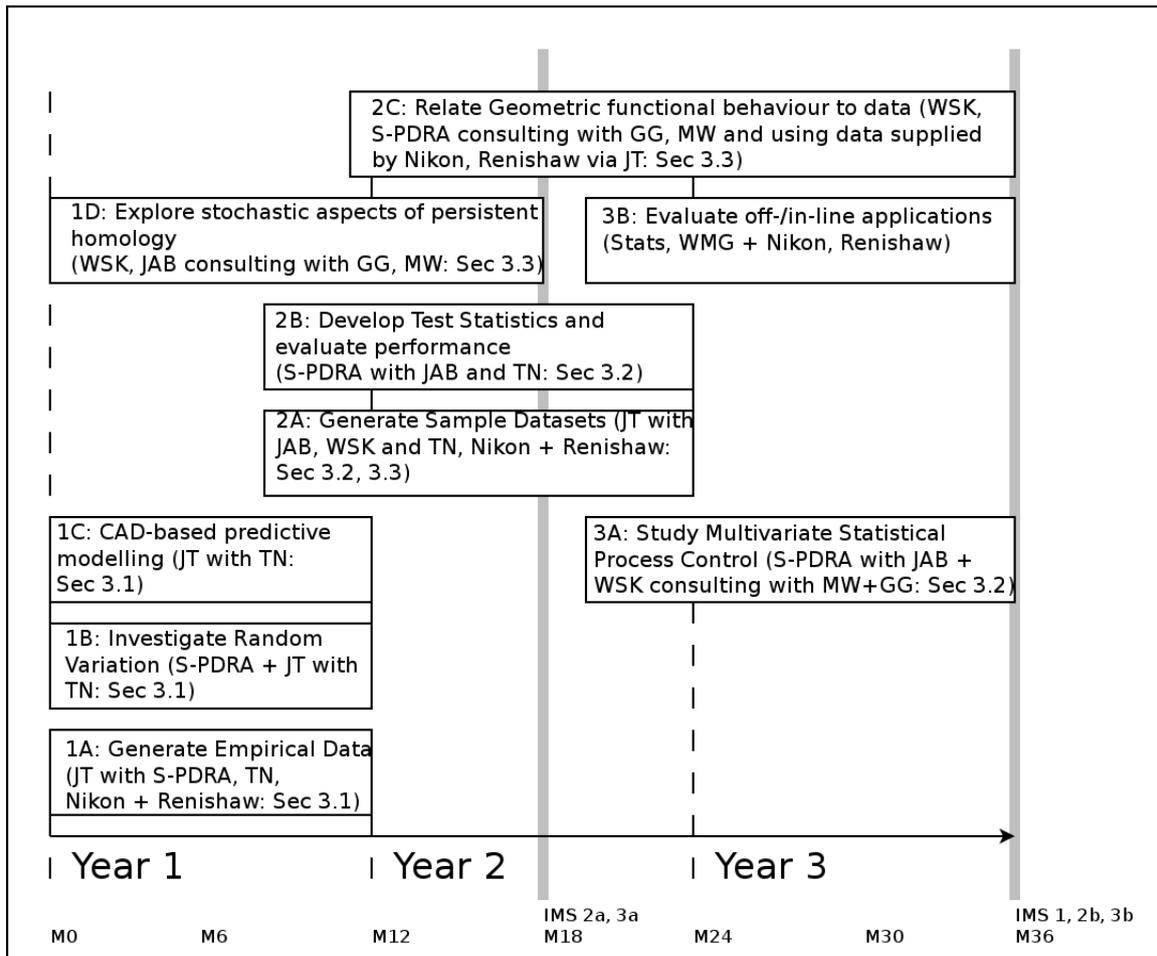
The careful exploration of the impact of random variation in a new application area is invariably of considerable interest and stimulus to applied statisticians; invariably such new applications have a strong innovative effect. Further innovation will be supplied by application to statistical process control of methods from random field theory, stochastic geometry, and ideas from microarray analysis. We aim to generate at least two major papers describing these developments to the statistics and engineering research communities, and additionally present the work at major national and international academic conferences. Early dissemination will use the arXiv preprint server and Warwick research repositories.

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WORK PLAN



Project Management & Responsibilities

The PI (WSK) and the senior WMG CI (MW) oversee the general direction of the research and share the responsibility of chairing

- monthly project progress meetings**, at which the group will discuss detailed progress towards fulfilment of tasks and milestones, and review potentially exploitable developments, and
- six-monthly steering group meetings**, at which the group together with industrial advisors will discuss potentially exploitable developments more fully.

Detailed research rôles are as annotated on the work diagram.

WSK will oversee the work of the Statistics PDRA (S-PDRA).

The second WMG CI (GG) will oversee the work of JT (the WMG PDRA) and will take responsibility for developing industrial links as the work programme progresses.

Close liaison between the two PDRAs will be facilitated because WMG and Statistics are geographically close, allowing for regular collaboration meetings. Good liaison between the WMG and Statistics parts of the collaboration will be facilitated by the joint position held by TN.

Milestones (from Pathways to Impact):

IMS 1 Researchers trained in generic skills

IMS 2a, 2b (1+1)×Journal publication

IMS 3a, 3b (2+2)×Conference presentations & proceeding publications