# **MSc AI Dissertation Project Proposal Form**

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| **Student number** |  | **Date** | 13/02/2025 |
| **Student name** | **Joshua Hellewell** | | |
| **Supervisor name** | **Chandrasekhar Kambhampati** | | |
| **Project title:** | **Exploring geometry representation methods in AI for efficient design space exploration and optimisation.** | | |
| **Project description – background, aims, objectives, research question(s), brief reflection on novelty/originality** | | | |
| Engineering is propelled by effective design space exploration and optimisation. As is common, numerical tools are used to substitute expensive physical testing; for example, computational fluid dynamics can, by solving physical numerical equations, provide engineers with flow field information such as surface pressure fields and velocity profiles. Such simulations are computationally expensive and not optimised for fast, iterative design exploration, which can be partly attributed to the input geometry complexities (unstructured mesh files, point clouds, etc.) inhibiting simple parameterisation that would enable an interpretable representation of complex features and geometries. In the absence of such a concise description of how shapes are related, design space exploration and optimisation is constrained to a high-dimensional landscape, inheriting computational challenges and falling victim to the curse of dimensionality, which suppresses efficient design exploration. Complex shapes, such as those found in typical aerodynamic applications, can be composed of millions of elements described by vertices, edges, and faces, and therefore exploring all combinations is computationally infeasible. Having a low-dimensional representation of complex shapes that concisely represents the defining features and nuances enables optimisation methods such as grid search, Monte-Carlo methods, or gradient-based optimisation to be performed more efficiently. This research aims to identify, investigate, and compare different approaches to addressing this high-dimensional challenge.  Despite industry application mainly residing in the 3D space, the computational burden and data availability introduce unnecessary challenges that detract from the underlying concepts proposed in this research, and that for that reason, we will focus on 2D geometries and optimisation problems.  The objectives of this project will be to research and compare different AI models for encoding geometries into low-dimensional spaces and to assess how such representations facilitate design space exploration for optimising geometric quantities of interest, analogous to real optimisation problems in complex engineering design. The project will also analyse the structure and smoothness of the learned geometry representations and their suitability for use in different optimisation approaches such as gradient-based, genetic algorithms, and Bayesian optimisation. Finally, we aim to identify which approaches to geometry representation provide the most interpretable and controllable representation that can be harnessed to conduct targeted design modification and optimisation.  Generative models, such as auto-encoders, encoder-decoders, and generative adversarial networks, are finding use cases across engineering. Despite auto-encoders emerging in the 1980s, their applications across engineering are increasing to enable conventionally high-complexity and compute-resource-hungry processes to be approached in an intermediary low-dimensional search space. Additionally, design space exploration and optimisation are a critical enabler to design innovation, and doing so in a cost-efficient manner is sought in industry whereby conventional numerical simulations are intractably resource-hungry for such highly complex components and systems. In addition to investigating methods for compressing the high-dimensional complexity of geometries, we will deploy the learned representations to a simple 2D optimisation problem, area to perimeter ratio – which may be perceived as the 2D equivalent of surface area to volume ratio, which is often used as a parameter to control heat loss; however, this approach could be extended to other industry problems, such as optimising the lift to drag coefficient for an airfoil. | | | |
| **Methodology – rationale, data selection and collection, recruitment of participants, analytical process** | | | |
| The project will be conducted by firstly identifying a comprehensive dataset of 2D shapes that will be used to represent the geometry space, albeit simplified into the 2D domain to avoid computational limitations associated with data formats such as voxel grids, point clouds and mesh grids. Optionally, the UIUC 2D airofil dataset may be used, however, this dataset is smaller and spans a more similar library of geometries (i.e., all airfoils). In the 3D domain, publicly available datasets such as Shapenet may be used, however, this research will focus on 2D geometric shapes (squares, circles, triangles etc). For 2D shapes, the inputs will be treated as images, analogous to the MNIST image digits datasets commonly used for classification benchmarking.  All data will be stored locally and processed using Python. Specifically, for working with ML models the data will be stored as .h5 files for efficient storage and access. Any neural network models will be built using Metas’ PyTorch architecture, and training using the CUDA implementation for efficient, parallelised model training.  A literature review will be conducted that will identify techniques for representation high dimensionality data into a low dimensional space, alongside design exploration and optimisation methods that can be used for engineering design. This review will aim to identify state-of-the-art techniques to latent space representation and identify opportunities to build on or leverage technologies for design space exploration. | | | |
| **Theoretical framework and intended tools/technologies** | | | |
| Generative models may include Auto-encoders, Variational Auto-encoders, Denoising Auto-encoders, Sparse Auto-encoders, Contractive Auto-encoders. Generative Adversarial Networks. Implicit Neural Representations. | | | |
| **Key literature identified for literature review (include references)** | | | |
| Park, J. J., Florence, P., Straub, J., Newcombe, R., & Lovegrove, S. (2019). Deepsdf: Learning continuous signed distance functions for shape representation. *Proceedings of the IEEE Computer Society Conference on Computer Vision and Pattern Recognition*, *2019-June*. <https://doi.org/10.1109/CVPR.2019.00025>  Zhu, Z., Wang, X., Bai, S., Yao, C., & Bai, X. (2016). Deep Learning Representation using Autoencoder for 3D Shape Retrieval. *Neurocomputing*, *204*. https://doi.org/10.1016/j.neucom.2015.08.127  Li, P., Pei, Y., & Li, J. (2023). A comprehensive survey on design and application of autoencoder in deep learning. In *Applied Soft Computing* (Vol. 138). https://doi.org/10.1016/j.asoc.2023.110176  Sun, JM., Wu, T. & Gao, L. Recent advances in implicit representation-based 3D shape generation. Vis. Intell. 2, 9 (2024). <https://doi.org/10.1007/s44267-024-00042->  Sharp, N., Attaiki, S., Crane, K., & Ovsjanikov, M. (2022). DiffusionNet: Discretization Agnostic Learning on Surfaces. *ACM Transactions on Graphics*, *41*(3). https://doi.org/10.1145/3507905  Wu, Z., Song, S., Khosla, A., Yu, F., Zhang, L., Tang, X., & Xiao, J. (2015). 3D ShapeNets: A deep representation for volumetric shapes. *Proceedings of the IEEE Computer Society Conference on Computer Vision and Pattern Recognition*, *07-12-June-2015*, 1912–1920. https://doi.org/10.1109/CVPR.2015.7298801  Qi, C. R., Su, H., Mo, K., & Guibas, L. J. (2017). PointNet: Deep learning on point sets for 3D classification and segmentation. *Proceedings - 30th IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2017*, *2017-January*, 77–85. https://doi.org/10.1109/CVPR.2017.16 | | | |
| **Industrial partner (if appropriate)** | | | |
| **Rolls-Royce,**  **Mark Hobbs –** [**Mark.Hobbs@Rolls-Royce.com**](mailto:Mark.Hobbs@Rolls-Royce.com) **| Technical Specialist Future Methods** | | | |
| **Project management** | | | |
| Table: Project timeline and key outputs (expand table as needed)   |  |  | | --- | --- | | **Week** | **Activity** | |  |  | |  |  | |  |  | |  |  | |  |  | |  |  | | | | |
| **Resources and Research Data Management Plan (Describe the resources required and the data you expect to acquire or generate during this research project, how you will manage, describe, analyse, and store the data and what mechanisms you will use to share and preserve your data.**) | | | |
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| **Planned outputs/publications/research datasets/impact/dissemination** | | | |
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| If successful, I undertake to carry out the research according to the University’s Ethics code of Practice. I realise that I will not proceed into data collection without an ethical approval in place  (Applicant’s signature required) |  |
| Date and signature of Supervisor approval |  |