

BEAR Conf '25

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Acknowledgements

We would like to thank all the people who contributed to this publication.

Front Cover

Whispers of Vortices from a Covert-Inspired Leading-Edge Flap
Chandan Bose (University of Birmingham) & Hibah Saddal (University of Birmingham).

Cite

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Foreword

Dr Dietmar Heinke

Chair of the BEAR user group



The proceedings summarize the content of the BEAR PGR Conference in 2025. At this conference BEAR users came together to hear about the fascinating research that Postgraduate Researchers (PGRs) and academic staff undertake on the University's supercomputer, BlueBEAR. The BEAR PGR Conference is an annual event where we give PGRs an opportunity to get experience in running a conference, gaining skills that will enrich their CV.

This year the conference was a one-day event including poster presentations and talks. The presenters came from a wide range of disciplines such as mechanical engineering, financial economics, investment management, aero dynamics, climate research, chemical engineering; physics & astronomy; applied health research; social policy and computer science. We also had two excellent keynote speakers: Dr. Loïc Lannelongue (University of Cambridge) and Dr Xilin Xia (University of Birmingham). Loïc introduced the Green Algorithms project which aims to reduce the environmental impact of supercomputers. Xilin provided very interesting insights into the latest advances in research into climate change.

I hope you find these abstracts very stimulating and will inspire you to go and find out more about the presenters' research and how BlueBEAR may help you with your own research.

The conference concluded by announcing the best poster and talk winners. It was a difficult choice with such an excellent range of presentations, but the winner of the best poster was Oskar Soulas, with his engaging and clear presentation and the winner of the best talk Zhuangchen Wu, with his highly visual and impactful talk. We would like to thank Lenovo for providing the prizes (Motorola smart phones) for the winners.

These proceedings and the conference would not have been possible without the tremendous amount of work that goes on behind the scenes by many dedicated individuals. So a big thank you to the organizing committee for their excellent work: Poppy Aves, Aaron Wiggins, Brandon Ingram, Margarita Saranti, Hibah Saddal, Simone Ausilio, Ni Yang, Nina Adler and the advisory Committee: Aslam Ghumra, Dr. Stephanie Thompson and Debbie Carter.

Dietmar Heinke

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Winner best presentation
Zhuangchen Wu

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Winner best poster
Oskar Soulas

Conference Agenda

Start Time	Duration	Event	Title/Topic
10:00	00:30	Registration & Refreshments	
10:30	00:10	Welcome	Introduction by Dietmar Heinke - Chair of the BEAR User Group
10:40	00:45	Xilin Xia	Keynote: Development and application of computational models for natural hazards and climate risk assessment
11:25	00:20	Ben Jenkins (ONLINE)	Outcomes and Learnings from 4 Years of Research on DEM Calibration
11:45	00:20	Chandan Bose	Unleashing GPU-Accelerated Computing: Aerodynamics of Butterfly Swarms
12:05	00:15	Break	
12:20	00:20	Son Nguyen	Don't Cry Over Spilled Oil: Stock Market Punishment for Environmental Missteps
12:40	00:20	Hibah Saddal	Modelling Bio-Inspired Fluid-Structure Interaction Problems Using Open-Source Codes
13:00	01:00	Lunch + Posters	
14:00	00:45	Loïc Lannelongue	Keynote: Green Algorithms, Green DiSC and GREENER principles: making computational science more environmentally sustainable
14:45	00:20	Yibo Zhang	When She Holds the Purse Strings: Intrahousehold Female Status and Household Resilience under Natural Disaster Exposure
15:05	00:15	Break	
15:20	00:05	Liu Tong	Structural monetary policy and firms' green innovation

A G E N D A

Start Time	Duration	Event	Title/Topic
15:25	00:05	Nina Adler	Effect of laser pulsing and interlaying machining on residual stresses in laser direct energy deposition
15:30	00:05	Lamya Majeed	Induced Resistance: Programming Tomatoes for Resilience
15:35	00:05	Zhenyi Zhai	The impact of airport expansion on local housing prices: evidence from the UK
15:40	00:05	Zhuangchen Wu	Ratings, popularity, and price setting
15:45	00:05	Haonan Tian	Speed Limits, Noise Abatement, and House Prices: Evidence from a Quasi-Natural Experiment in Wales
15:50	00:05	Mohammad B M A J Aldoub	Information shock and belief heterogeneity in the peer-to-peer secondary market
15:55	00:10	Break	
16:05		Prizes and Wrap-up	

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KEYNOTE : DEVELOPMENT AND APPLICATION OF COMPUTATIONAL MODELS FOR NATURAL HAZARDS AND CLIMATE RISK ASSESSMENT

Xilin Xia

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Due to Climate Change, there will be more extreme weather events such as intense rainfall storms in the future. These events often cause hydrological hazards such as flooding, landslides and debris flows. Modelling the risk from these rainfall-related hazards is essential for increasing resilience. It underpins important applications that reduces risk or enables faster recovery. In this presentation, I will present my recent research on developing cutting-edge modelling methods for climate and weather-related hazards, including both hydrodynamic and machine learning based approaches, and their applications in risk assessment and real-time forecasting.

OUTCOMES AND LEARNINGS FROM 4 YEARS OF RESEARCH ON DEM CALIBRATION

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Simulating granular materials through the Discrete Element Method (DEM) faces several challenges, with one of the main issues being the calibration of coefficients that define the forces between particles. Accurate calibration is essential to ensure that DEM simulations reflect real-world behaviour at all scales, from individual particle interactions to the collective dynamics of large systems. However, a lack of universally accepted calibration standards has led to inconsistent and often inaccurate results in DEM simulations, hindering its wider adoption in both research and industry [1]

This work focuses on indirect calibration methods using powder characterisation instruments, which infer the interaction properties needed for DEM simulations by mapping bulk behaviours to particle interactions. Our studies have identified the optimal instruments, combinations, and regression models for effective calibration as summarised in Figure 1. Over the past four years, significant progress has been made in developing a more standardised calibration model, offering valuable insights and best practices for DEM simulations. These findings could serve as a foundation for future advancements in numerical powder simulation, benefiting both researchers and industry practitioners.



References

[1] C. R. K. Windows-Yule and A. Neveu. "Calibration of DEM simulations for dynamic particulate systems". In: Papers in Physics 14 (July 2022). doi: 10.4279/pip.140010. url: <https://www.papersinphysics.org/papersinphysics/article/view/795>.

UNLEASHING GPU-ACCELERATED COMPUTING: AERODYNAMICS OF BUTTERFLY SWARMS

Chandan Bose

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The study of robotic butterfly swarms presents futuristic opportunities for understanding complex aerodynamic interactions in bio-inspired flight formations. However, simulating large-scale robotic swarms is computationally intensive due to intricate flow interactions, moving boundaries, and nonlinear phenomena. In this research, we harness the power of GPU-accelerated computing to accelerate aerodynamic simulations significantly using an Immersed Boundary Method and overset meshing strategy. Our GPU-accelerated flow solver efficiently handles the complex flow interactions inherent to the flapping wings of robotic butterflies, enabling detailed characterization of aerodynamic performance metrics such as lift, thrust, and propulsion efficiency. Through high-resolution computational fluid dynamics simulations, we explore critical aerodynamic features emerging within robotic butterfly swarms, including wake interactions, vortex formation, and aerodynamic synchronization between multiple units. These insights not only deepen our fundamental understanding of swarm aerodynamics but also directly inform the design principles of next-generation robotic aerial systems. Ultimately, this study demonstrates the transformative potential of GPU-computing in computational aerodynamics, offering robust and scalable tools capable of unlocking new paradigms in bio-inspired engineering and robotics research.

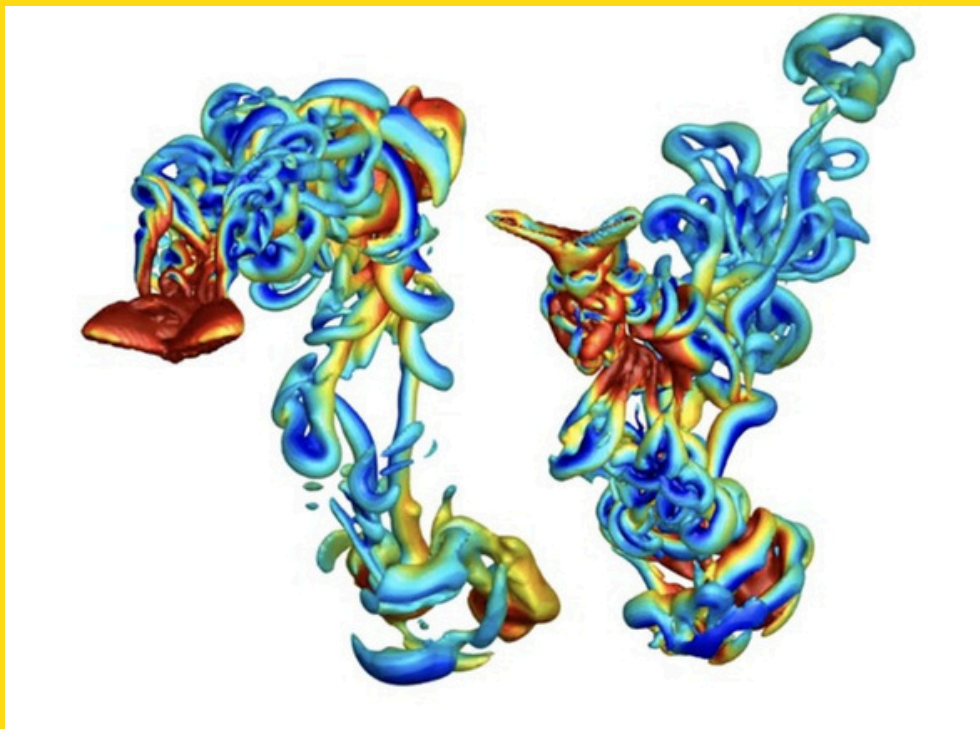


Figure 1: Unsteady flow-field around two butterflies.

DON'T CRY OVER SPILLED OIL: STOCK MARKET PUNISHMENT FOR ENVIRONMENTAL MISSTEPS

Son Nguyen

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We investigate the stock market consequences of corporate environmental offences, with a focus on the role of environmental scandals - the heightened public and media scrutiny following regulatory violations. Using an international panel of 8,298,782 firm-month observations across 34 countries from 2010 to 2025, we construct a comprehensive event study to examine how environmental misconduct affects stock returns. Among 1,753 public firms tracked, we identify 678 firms involved in environmental offences, and explore how market reactions vary across firms. Our findings show that environmental violations lead to significant monthly stock return declines, and this effect is exacerbated when the firm has a history of high-profile environmental scandals. We argue that scandals amplify investor reaction by intensifying reputational risk beyond the financial penalty alone. Further, we uncover heterogeneity in the market response: firms with higher carbon emissions (reflecting the pollution premium) and younger firms in early life-cycle stages face stronger stock price punishments, while mature firms exhibit relative resilience. This study is among the first to analyze the financial consequences of environmental scandals at a global scale, integrating regulatory, reputational, and firm-specific risk dimensions in understanding market discipline.

MODELLING BIO-INSPIRED FLUID-STRUCTURE INTERACTION PROBLEMS USING OPEN-SOURCE CODES

Hibah Saddal

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Hibah Saddal(1) and Chandan Bose(1)

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This study investigates the modelling of bio-inspired flexible flaps and morphing foils [1] in the low Reynolds number regime using open-source codes. The incompressible fluid flow is governed by the Navier-Stokes equations and solved using the finite volume method in OpenFOAM. The structural parts are simulated using the finite element based solver CalculiX. Two-way coupling between the fluid and structural solvers is facilitated via preCICE, which enables efficient parallel execution and data exchange between both solvers. The radial basis function interpolation technique is employed for data mapping at the fluid-structure interface, while the Interface Quasi-Newton Inverse Least Squares (IQN-ILS) acceleration scheme enables partitioned strong coupling between the fluid and solid solvers. The numerical simulations investigate the effects of governing parameters such as dimensionless bending rigidity

$$(K_B = \frac{EI}{\rho_f U_\infty^2 L^3}) \text{ and mass ratio } (\mu = \frac{\rho_s h}{\rho_f L}) / \text{density ratio } (\rho^* = \frac{\rho_s}{\rho_f})$$

on the wake dynamics, where EI is the bending rigidity, ρ_f is the fluid density, ρ_s is the solid density, U_∞ is the free-stream velocity, h and L are the thickness and the length of the flap, respectively. By varying the flexibility of bio-inspired flaps and optimising their locations along the wing surface, we have found that the stall can be significantly delayed, leading to increased lift. In another study, we show that passive morphing mitigates spatial-temporal gust effects, improving aerodynamic efficiency. Refer to the representative computational results presented in Figure 1. We aim to present a detailed computational efficiency comparison of different coupling algorithms and data-mapping schemes for these problems. This research provides a robust open-source numerical framework for studying fluid-structure interaction problems, with potential applications in optimising micro aerial vehicles and unmanned aerial vehicles under gusty environments.

MODELLING BIO-INSPIRED FLUID-STRUCTURE INTERACTION PROBLEMS USING OPEN-SOURCE CODES

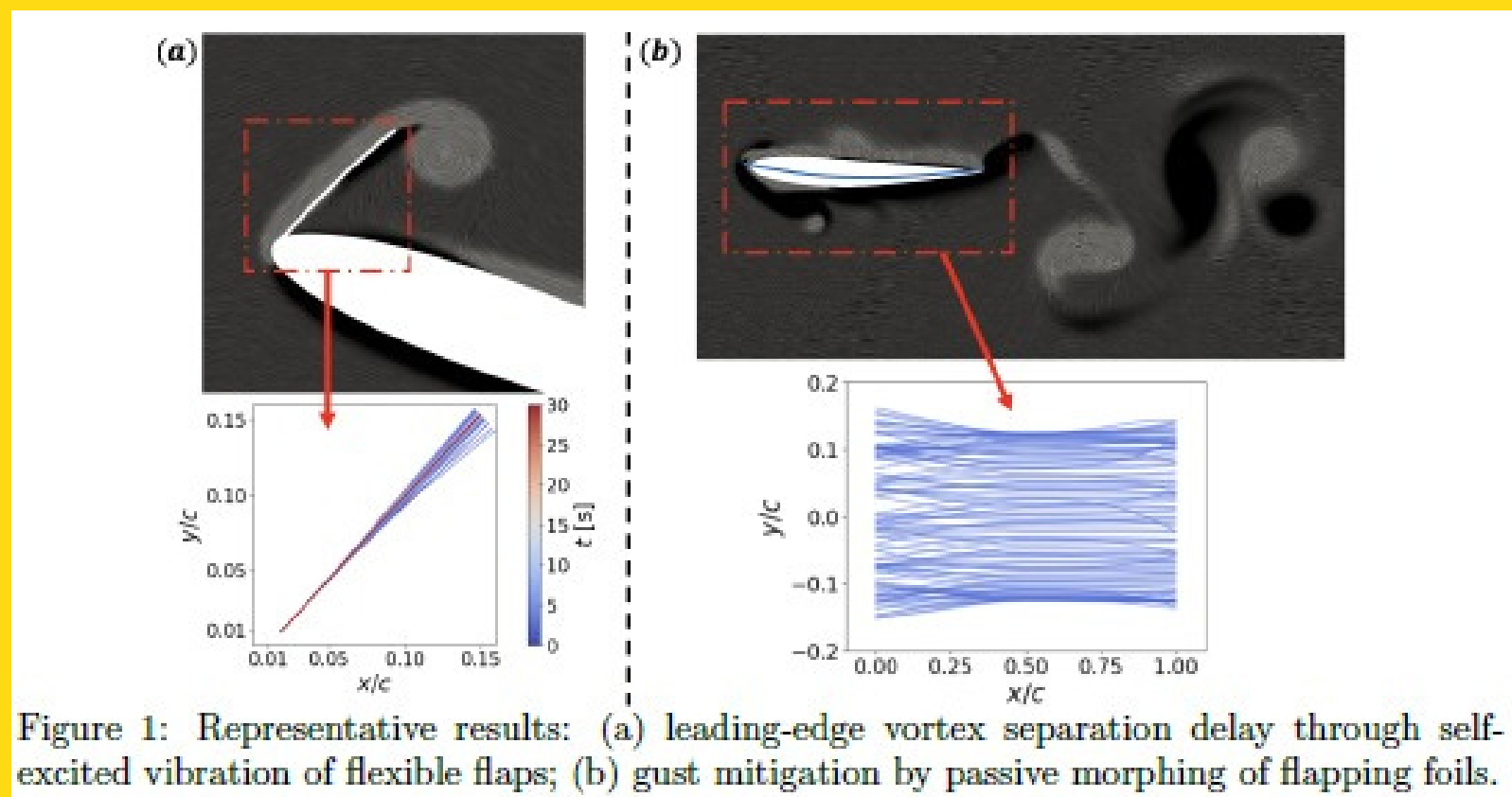
Continued from previous page

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1. LI, D., ZHAO, S., DA RONCH, A., XIANG, J., DROFELNIK, J., LI, Y., & DE BREUKER, R. (2018). A REVIEW OF MODELLING AND ANALYSIS OF MORPHING WINGS. PROGRESS IN AEROSPACE SCIENCES, 100, 46-62.

KEYNOTE : GREEN ALGORITHMS, GREEN DISC AND GREENER PRINCIPLES: MAKING COMPUTATIONAL SCIENCE MORE ENVIRONMENTALLY SUSTAINABLE

Loïc Lannelongue

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From genetic studies and astrophysics simulations to AI, scientific computing has enabled amazing discoveries and there is no doubt it will continue to do so. However, the corresponding environmental impact is a growing concern in light of the urgency of the climate crisis, so what can we all do about it? Tackling this issue and making it easier for scientists to engage with sustainable computing is what motivated the Green Algorithms project. Through the prism of the GREENER principles for environmentally sustainable science, we will discuss what we learned along the way, how to estimate the impact of our work and what hurdles still exist. It will also be a chance to highlight how the new Green DiSC certification framework can support scientists and institutions in making their research more sustainable.

WHEN SHE HOLDS THE PURSE STRINGS: INTRAHOUSEHOLD FEMALE STATUS AND HOUSEHOLD RESILIENCE UNDER NATURAL DISASTER EXPOSURE

Yibo Zhang

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Yibo Zhang, Alessandra Guariglia

This study investigates the role of intrahousehold female status in shaping household development resilience under the impact of natural disasters. Utilising panel data from the China Financial Panel Studies and the Emergency Events Database spanning 2014–2022, our analysis reveals that households where women are financial managers exhibit significantly greater resilience following adverse events. This relationship is particularly pronounced among households with less affluent families, low education, and fewer children, suggesting that female leadership may foster an environment conducive to sustained intra-household economic growth. In summary, our findings underscore the pivotal role of female status in enhancing household resilience after disasters, while explaining the growing prevalence of women as household financial managers.

STRUCTURAL MONETARY POLICY AND FIRMS' GREEN INNOVATION

Tong Liu

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Tong Liu, Alessandra Guariglia, David Dickinson

Using a panel of Chinese listed firms over the period 2015–2022, we examine the impact of the 2018 expansion of the Midterm Lending Facility (MLF) collateral to include green credit on corporate green innovation. We measure firms' exposure to MLF based on their loan relationships with banks holding different levels of green credit.

Using a difference-in-differences (DID) approach, we find that the 2018 MLF expansion increased the number of green patents granted by approximately 8.8%. This increase is mainly attributable to a 9.1% rise in green utility model patents, while green invention patents remain unaffected.

Firms headquartered in developed eastern regions, operating in heavily polluting industries, and those without sufficient credit ratings to issue bonds drive our results. Because they respectively exhibit higher innovation efficiency, face stronger regulatory pressure to green their operations, and rely more heavily on bank credit.

Mechanism analysis shows that, the 2018 policy raised firms' total bank loan by 0.74%, mainly through a 0.79% rise in long-term loans. Short-term borrowing was not affected, consistent with the medium-term nature of the MLF and its role in encouraging longer-term financing. This provides evidence for the bank credit channel of MLF.

Overall, the policy significantly expanded bank credit and stimulated corporate green innovation.

EFFECT OF LASER PULSING AND INTERLAYING MACHINING ON RESIDUAL STRESSES IN LASER DIRECT ENERGY DEPOSITION

Nina Adler

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Additive manufacturing will play a crucial role on the path to more sustainable manufacturing. The ability to produce near-net shape builds reduces waste, saves material, and minimizes the need for post-processing, hence less energy and time. However, before additive manufacturing is widely adopted, significant challenges need to be overcome so it can substitute traditional manufacturing processes. One of these is to control residual stress caused by the rapid heat cycle the material has to overcome during the laser melting. Current methods are mainly based on post-process treatment. However, this leads to an increase in process time. To cope with this ongoing problem, my PhD investigates two in-process methods, pulsed laser and interlayer machining.

To validate the experimental work of both methods, I am currently developing simulations using the simulation software Abaqus on Blue-Bear. I calculate residual stress development and heat distribution in these simulations on my manufactured samples.

At the BEAR PGR Conference (2025), I would like to present how interlayer machining and pulsed lasers can decrease residual stress in direct energy deposition. My focus will be on the reduced heat induction caused by pulsed lasers, the relieving effect interlayer machining can have on the stress distribution of the printed layers, and how BlueBEAR helps understand these processes. Only a few works were done on interlayer machining. Therefore, we still do not fully understand how machined layers influence residual stress. This could further enhance our understanding of residual stress and improve additive manufacturing processes to get one step closer to sustainably manufactured products. Finally, I would like to show my simulations on this topic.

INDUCED RESISTANCE: PROGRAMMING TOMATOES FOR RESILIENCE

Lamya Majeed

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Botrytis cinerea, the causal agent of grey-mould disease, poses a significant threat to global tomato production, with post-harvest yield losses reaching up to 50%. Our research investigates whether priming elicitors, such as β -aminobutyric acid (BABA), can enhance intrinsic plant defenses and provide sustainable disease control alternatives. We have demonstrated that BABA-induced resistance (BABA-IR) is long-lasting and mediated by epigenetic mechanisms, including DNA methylation. Using whole genome bisulfite sequencing, we observed reduced DNA methylation in CHH contexts in young tomato plants compared to older plants, indicating greater epigenetic imprinting capacity at early developmental stages.

Transcriptomic analysis through RNA-sequencing revealed that gene expression changes associated with BABA-IR are strongly influenced by the developmental stage of the tomato plant. Notably, we see that BABA-IR is consistently effective in plants treated at two to three weeks of age but declines after four weeks, coinciding with flowering—a pivotal developmental transition. Furthermore, we identified key genes and molecular markers linked to these early developmental stages that are likely involved in establishing long-lasting resistance in the tomato fruit. These genes are also differentially expressed with BABA treatment, as well as during infection with *Botrytis cinerea*, which further highlights the effectiveness of BABA-IR when treatment is at these early developmental stages.

Our findings provide new insights into the relationship between plant development, epigenetics, and induced resistance, offering a mechanistic understanding of how BABA establishes durable immunity in tomato. This work highlights its potential application in improving crop protection strategies in other plant systems.

THE IMPACT OF AIRPORT EXPANSION ON LOCAL HOUSING PRICES: EVIDENCE FROM THE UK

Zhenyi Zhai

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This study investigates the relationship between airport expansion and house prices in the UK. As airports develop to accommodate growing demand for air travel, their expansion projects can bring benefits (such as improved accessibility and regional economic growth) and costs (including increased noise, air pollution and congestion). These opposing effects make the net impact on the value of nearby residential property an important but unresolved empirical question. This study focuses on major airport expansion projects in England between 2011 and 2019 and uses a difference in-differences framework for analysis. The analysis aims to isolate the causal effect of airport development on the housing market while controlling for local economic trends and geographical characteristics. The study contributes to the wider literature on urban economics and infrastructure policy by examining how large transport projects affect real estate dynamics. The results of this study can guide the behaviour of future policymakers and real estate investors.

RATINGS, POPULARITY, AND PRICE SETTING

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Using data from online menus of restaurants in the United Kingdom, we explore how ratings affect price-setting behavior. In this paper, ratings from online consumers are used as a measurement of levels of “consumer anger”. We find that the frequency of price changes in British restaurants negatively correlates with ratings, which is consistent with the consumer anger theory. However, the effects of consumer anger are diminished as the restaurants gain higher popularity (a larger number of reviews). Also, the “consumer anger” story is more pronounced for independent restaurants, price increases, and main dishes. These results suggest that the consumer anger theory might only work for independent sellers with limited bargaining power rather than chains with large market shares.

TEMPORAL CLUSTERING OF SEVERE EUROPEAN WINTER WINDSTORMS ON INTRASEASONAL TIMESCALES

Sophie Feltz

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Severe European winter windstorms cause high economic loss and environmental damage. When these extreme storms cluster in time, these impacts are amplified. Yet, the behaviour and drivers on shorter, intra-seasonal timescales have not been fully investigated. The impact-relevant footprint of the storm system is identified using the wind based impact-oriented tracking algorithm WiTRACK (Leckebusch et al., 2008), for the core winter seasons (DJF) 1980/01-2022/23 from ERA5 reanalysis. Derived from a Poisson Process, we quantify the magnitude of clustering through the widely established dispersion statistic (Mailier et al., 2006). On fixed 45- and 30-day timescales, the spatial distribution of the dispersion statistic has been analysed. The time-development of the dispersion statistic on shorter time horizons is investigated through 21-, 15- and 11-day moving windows.

Preliminary results reveal an increase in clustering in the latter half of the winter season on the fixed 45- and 30-day timescales. Shorter time horizons reveal clear peaks at the middle and the end of the season. To analyse mechanisms that drive the defined intraseasonal behaviour on the shorter time horizons (<30 -days), we examined the roles of several large-scale variability modes, namely the North Atlantic Oscillation (NAO), the East Atlantic pattern (EA), and the Scandinavian pattern (SCA). Results reveal a correlation between intra-seasonal variability of clustering and the occurrence of such large-scale modes, suggesting the EA as a key driver for increasing clustering. In addition, the individual contributions of large-scale modes to clustering at different times of the season can be diagnosed.

SPEED LIMITS, NOISE ABATEMENT, AND HOUSE PRICES: EVIDENCE FROM A QUASI-NATURAL EXPERIMENT IN WALES

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This study investigates the causal effect of traffic noise reduction on residential property prices by leveraging a quasi-natural experiment: the 2018 speed limit reduction (from 70 to 50 mph) on five motorways in Wales. Combining granular housing transaction data from the UK Land Registry (2013–2023) with geospatial road boundaries manually digitized from Google Earth, we employ a Difference-in-Differences (DiD) design to estimate localized housing market responses.

Results reveal that lowering speed limits significantly reduced traffic noise, leading to a 6.6% increase in house prices for properties within 150 meters of treated motorway segments compared to control areas. The price premium diminishes spatially, declining to 2%–3% at 400 meters and disappearing beyond this threshold, a pattern consistent with the physical decay of noise propagation. Mechanism validation aligns these effects with engineering estimates of noise reduction (3–5 dB under similar policies), confirming that the policy’s impact operates primarily through environmental improvements rather than confounding factors.

Methodologically, our integration of high-resolution spatial data with housing characteristics (e.g., energy efficiency ratings from the Domestic EPC dataset) strengthens causal identification and addresses spatial spillovers. The findings highlight the economic value of noise mitigation, demonstrating that speed limit policies can serve as dual-purpose tools to enhance environmental quality and property values. Furthermore, the spatial heterogeneity of effects underscores

opportunities for targeted urban planning, such as prioritizing speed reductions near noise-sensitive zones like schools or residential clusters. As the first causal evidence in the UK linking traffic noise abatement to housing market outcomes, this study provides policymakers with actionable insights for balancing mobility, sustainability, and equitable development.

INFORMATION SHOCK AND BELIEF HETEROGENEITY IN THE PEER-TO-PEER SECONDARY MARKET

Mohammad B M A J Aldoub

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Novel to the literature, this paper identifies the differences in investors' opinions in the secondary market of peer-to-peer (P2P)[1] lending and how they are influenced by negative information shock. Using Bondora's[2] database, with around 17 million observations, we create the dependent variable as the dispersion in investors' opinions, calculated as the standard deviation of the price of notes (share of the loans) traded within the same week. We have found that when there is a negative or peculiar shock (information) regarding a loan, i.e., loan default, investors' opinions diverge. This indicates that investors will begin to value loans differently if a negative shock occurs suddenly.

We use DS-Heckman method, which is an extension of the Heckman model that uses the lasso method for both the selection and outcome equations, which is a more robust way of Heckman model.

The results also show that as risk increases, dispersion of beliefs increases, but that at a certain point, as risk becomes extreme, dispersion will decrease and herding behaviour will become more prevalent.

We also evaluate the impact of loan defaults during holidays and crises, finding that the dispersion of defaults will be less during holidays than during regular days. In a crisis, we test the COVID-19 pandemic (three phases), finding that investors are more uncertain at the beginning but follow each other's behaviour during the second and third waves. Furthermore, different negative shocks and spread measures are used for robustness, and the results remain consistent.

[1] P2P lending platforms are technological platforms that bypass traditional intermediaries by connecting borrowers directly with lenders without the need to pass through a financial institution as a middleman.

[2] Bondora is a peer-to-peer (P2P) lending platform operating in Europe.



Asim Abbas, Mark Lee,
Niloofar Shanavas, Venelin Kovatchev,
Mubashir Ali

TEAM MEMBERS MOTIVATION

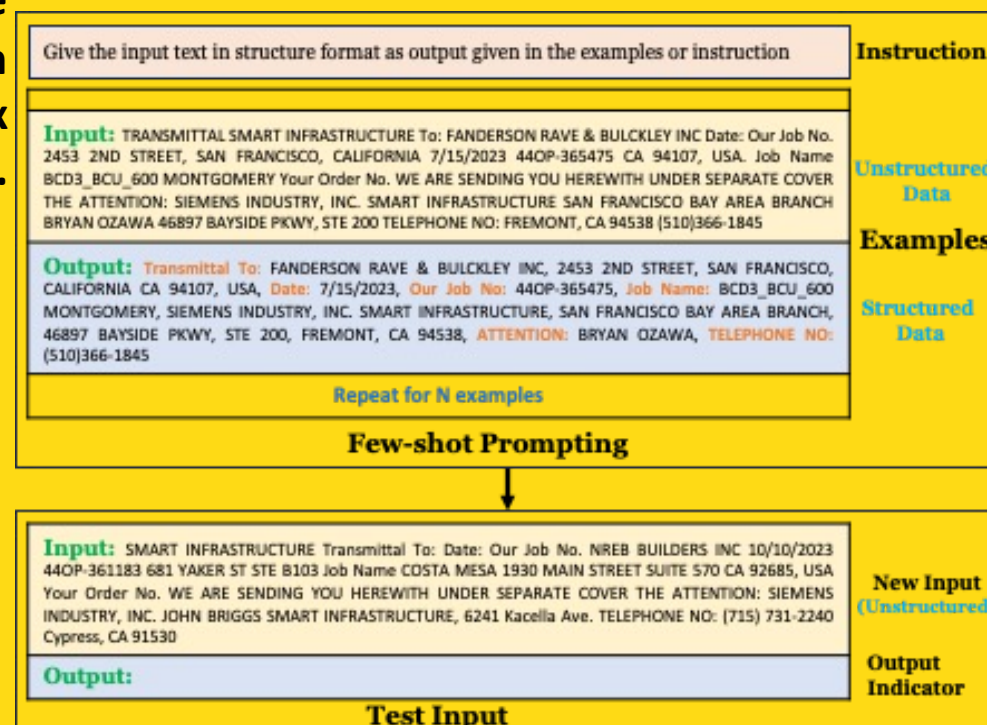
Q To automate the multiple and composite tender entities extraction process from complex tables using NLP techniques.

Q Extracting composite tender entities structurally from complex tables is an ongoing research problem. While extracting text from complex table structures, the context is often lost, making it difficult to understand for both humans and machines.

FEW-SHOT LEARNING APPROACH

q The table structure is highly complex due to frequent merging and splitting of rows and columns, leading to inconsistencies during data extraction.

qEntities are scattered across multiple columns and rows, requiring careful extraction.



Average Relative Distance (ARD): Pre-Fewshot Learning and Post-Fewshot Learning Approach

Model	$\alpha = 0\%$	$\alpha = 50\%$	$\alpha = 100\%$
FVPDF2	0.71	2.21	3.04
PDPDFnumber	0.43	2.76	3.64
Unstructured.io	0.79	3.32	3.84
PDM-Miner	0.49	2.96	4.27
PSMUPDF	2.88	3.22	3.41

Average BLEU Score: Pre-Fewshot Learning and Post-Fewshot Learning

Model	$\alpha = 0\%$	$\alpha = 50\%$	$\alpha = 100\%$
FVPDF2	0.95	0.77	0.82
PDPDFnumber	0.91	0.8	0.8
Unstructured.io	0.94	0.84	0.85
PDM-Miner	0.92	0.8	0.84
PSMUPDF	0.85	0.77	0.78

$$\text{ARD} = \frac{1}{N} \sum_{i=1}^N |p_i - q_i| \quad (1)$$

$$\text{BLEU}_{\text{avg}} = \frac{BP \cdot \exp \left(\sum_{n=1}^N w_n \cdot \log(p_n) \right)}{T} \quad (2)$$

Entities	PDFMiner		PYMUPDF		Unstructured.io		PDFPlumber		PYPDF2	
	Pre	Post	Pre	Post	Pre	Post	Pre	Post	Pre	Post
To Company	89	100	97.63	100	82.67	100	85.33	100	81.67	100
By Ayles	90	100	95	100	92	100	70.33	100	63	95.33
Date	100	100	100	100	95	100	100	100	95	100
Tender No	100	100	100	100	100	100	100	100	95	100
Tender Name	95	100	97.3	92	80	100	91.67	100	94.33	100
From Company	100	100	90	92	90	100	89.33	100	83.67	100
From Address	98.67	100	97	90	90	100	87.33	100	82	100
Attention	94.33	100	91.33	92	80.33	100	37.67	100	38	100
Telephone No	100	100	90	100	92.67	100	63.33	100	49.67	100

$$S_{actual} = \sum_{i=1}^n S_i = \sum_{i=1}^n (2F_i + P_i - N_i - 2W_i), \quad (3)$$

$$Accuracy(\%) = \left(\frac{S_{actual} - S_{min}}{S_{max} - S_{min}} \right) \times 100 \quad (4)$$

Full Match(Fi): 2 points, Partially Match(Pi): 2 points, Not Match(Ni): -1 point and Wrong Match(Wi): -2 points.

CONCLUSION

The study combined LLMs, text extraction tools, rules, and regular expressions in a few-shot learning setup to enhance structured text extraction and tender entity classification from complex PDF tables. Few-shot learning with LLMs significantly improved performance and accuracy in structured text extraction, addressing the limitations of individual tools.

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USING DEM TO INVESTIGATE THE IMPACT OF PARTICLE-PARTICLE PROPERTIES ON MIXING EFFICIENCY IN A RAM

Emily Allman
Supervisors: Aaron Wiggan, Jack Grogan, Kit Windows-Yule
University of Birmingham, School of Chemical Engineering
Conducted as part of MEng Chemical Engineering Final Year Research Project

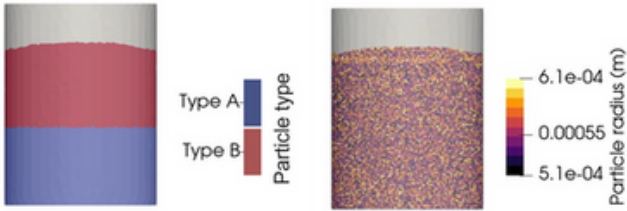
INTRODUCTION

Resonant Acoustic Mixers (RAM) are a versatile non-contact mixing technology, capable of delivering efficient mixing using oscillations. They have been shown to demonstrate superior mixing efficiency compared to traditional mixing technologies, causing widespread application across industries such as pharmaceuticals, energetics and construction. As RAM applications continue to expand, research is being conducted to understand the factors effecting its mixing performance. This study aims to assist in the optimisation of industrial mixing processes.

METHODOLOGY

1

DEM simulations run on LIGGGHTS, for varying fill heights and particle-particle properties. Discrete Element Method (DEM) modelling simulates the movement of particles through equations, such as Newton's 2nd law.



2

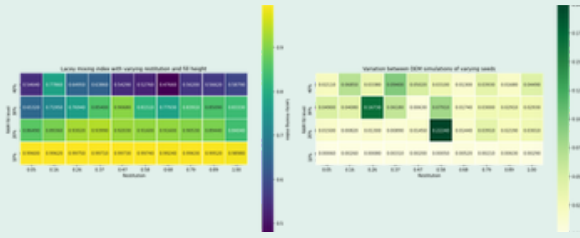
The analysis assessed mixing efficiency using:

- Lacey mixing index to quantify mixedness, ranging from 0 (complete segregation) to 1 (perfect random mixing).
- Mixing rate to evaluate particle dispersion speed - higher rates indicate improved efficiency.
- Mixing time to measure how quickly uniformity is achieved - shorter times suggest optimal energy transfer.
- ParaView to visualise simulations and analyse parameter effects interactively.

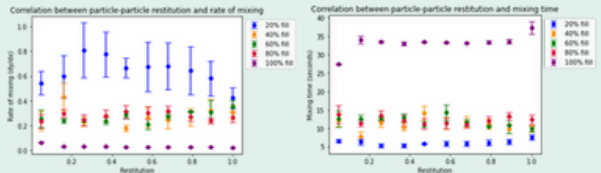
RESULTS AND DISCUSSION

RESTITUTION

- Little correlation seen for Lacey mixing index after 3 seconds of mixing or after the full run time of 12.5 seconds
- Shown to influence mixing performance at the start of mixing, at low fill heights

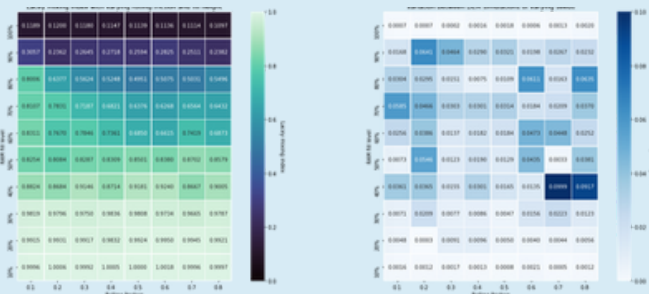


- Further studies recommended to reduce variance, to analyse relation between mixing efficiency, mixing rate and mixing time
- Fill height has more significant impact on mixing efficiency - negatively impacting the performance, by reducing mixing rate and increasing mixing time

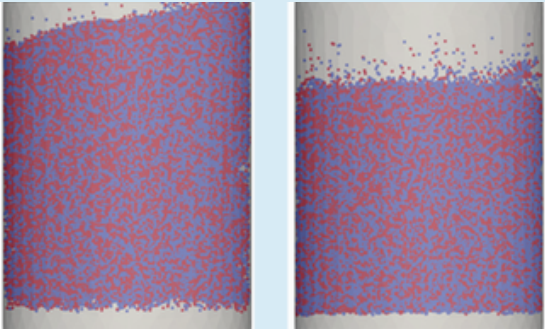


ROLLING FRICTION

- Defined gradient between Lacey mixing index and rolling friction at varying fill heights, reflecting findings of Zheng et al.



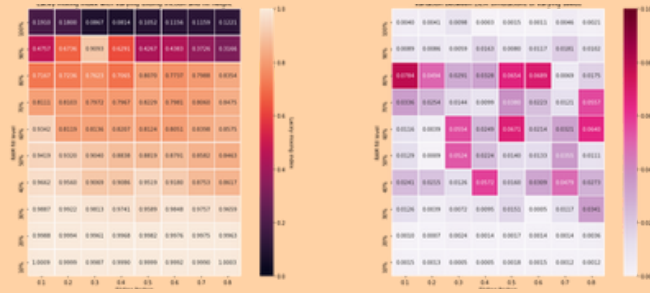
- Reduced mixing efficiency at high rolling friction values, due to the formation of MCC particle clusters



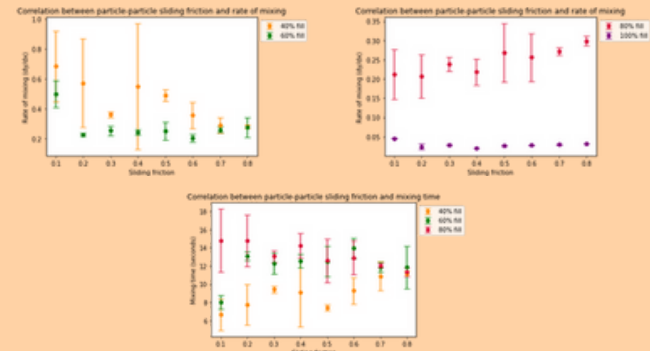
- Increased rolling friction attributes to reduced mixing rate and increased mixing time - reducing mixing efficiency

SLIDING FRICTION

- 2-way gradient observed, whereby mixing efficiency is best at low fill height with low sliding friction, and high fill height with high sliding friction



- Balance required to achieve effective mixing - free movement of particles associated with low fill height and low sliding friction, and resistive effects from high fill height and high sliding friction, supporting findings of Rong et al.



CONCLUSION

- Fill height is a predominant influence on mixing efficiency in RAM, supporting findings of Vandenberg and Wille, and contradicting claims of Osorio and Muzzio
- Restitution has a minimal impact on mixing efficiency, mostly seen at the start of mixing at low fill heights
- Increasing rolling friction attributes to reduced mixing efficiency
- Impact of sliding friction in RAM is a balance between the free movement of particles and resistive effects

FURTHER RESEARCH

- Investigation into the impact of varying particle-particle and particle-wall properties in situ on the mixing efficiency
- Experimental validation of this study

Scan for to view
Research Project Report
and full reference list



KEY REFERENCES
A. Vandenberg and K. Wille, "Evaluation of resonance acoustic mixing technology using ultra high performance concrete". In: Construction and Building Materials 164 (2018), pp. 716–730. ISSN: 0950-0618. DOI: <https://doi.org/10.1016/j.conbuildmat.2017.12.217>.
J.G. Osorio and F.J. Muzzio, "Evaluation of resonant acoustic mixing performance". In: Powder Technology 278 (2015), pp. 46–56. DOI: <https://doi.org/10.1016/j.powtec.2015.02.033>.
Q.J. Zheng et al. "Interparticle forces and their effects in particulate systems". In: Powder Technology 436 (2024). DOI: <https://doi.org/10.1016/j.powtec.2024.119445>.
W. Rong et al. "Sensitivity analysis of particle contact parameters for DEM simulation in a rotating drum using response surface methodology". In: Powder Technology 362 (2020), pp. 604–614. DOI: <https://doi.org/10.1016/j.powtec.2019.12.004>.

Understanding the roles of novel transcription factors involved in pancreatic beta cell development

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UNIVERSITY OF BIRMINGHAM



BetaCell Birmingham

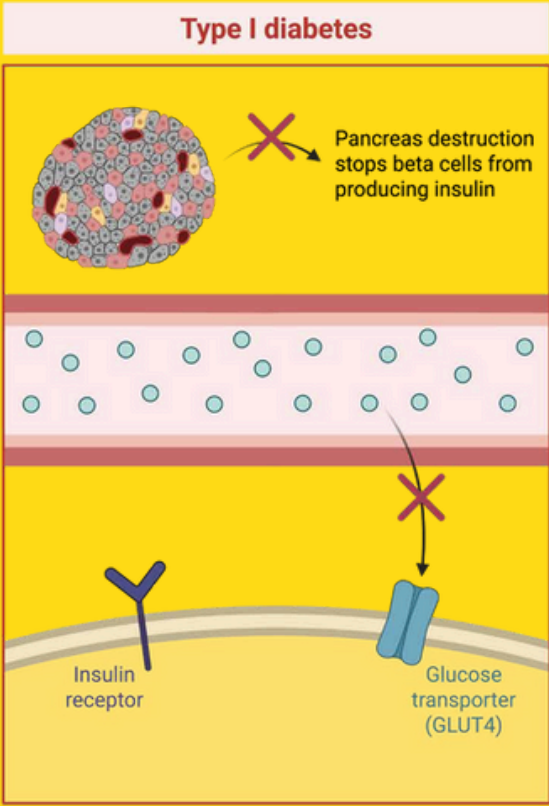
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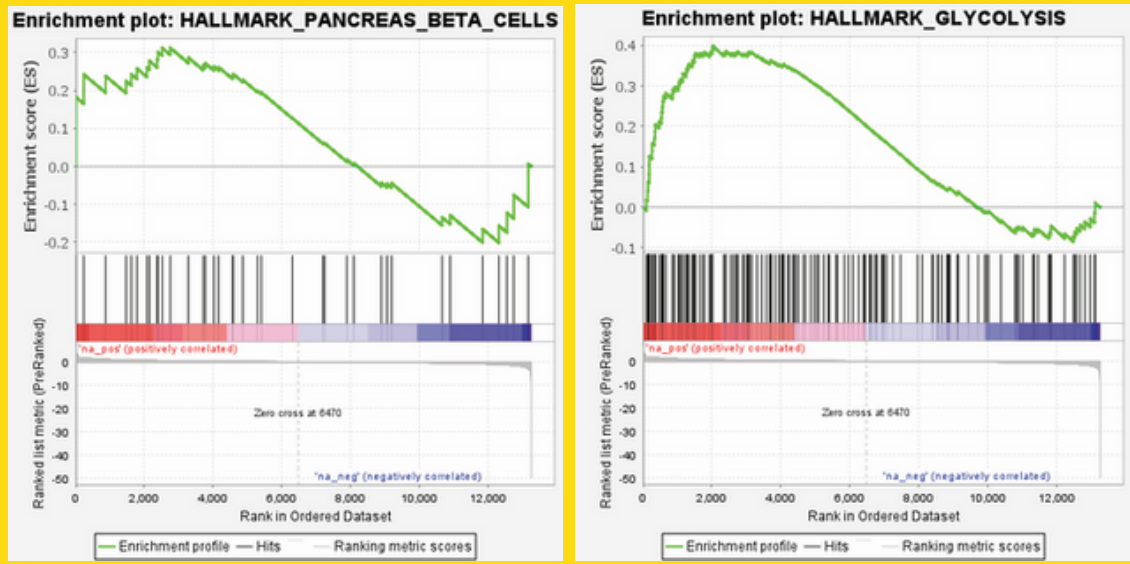
National Centre for the Replacement Refinement & Reduction of Animals in Research

1. Introduction

- Type I diabetes (T1D) is an autoimmune disease where the immune system destroys the pancreatic beta cells with the islets of Langerhans, resulting in insufficient insulin secretion [1]. • Cell replacement therapy has become a promising therapeutic option of T1D. With lab-grown insulin-producing stem cell-derived beta cells (sBCs), we can replace destroyed beta cells and restore insulin production and secretion. • However, sBCs generated in vitro are functionally and transcriptional immature compared to primary beta cells in human body [2-4].
- **We are interested in understanding the transcriptional profiles by identifying novel factors that may play essential roles in beta cell-specific functions. We hope that will help us to generate better beta cells for more clinical applications.**

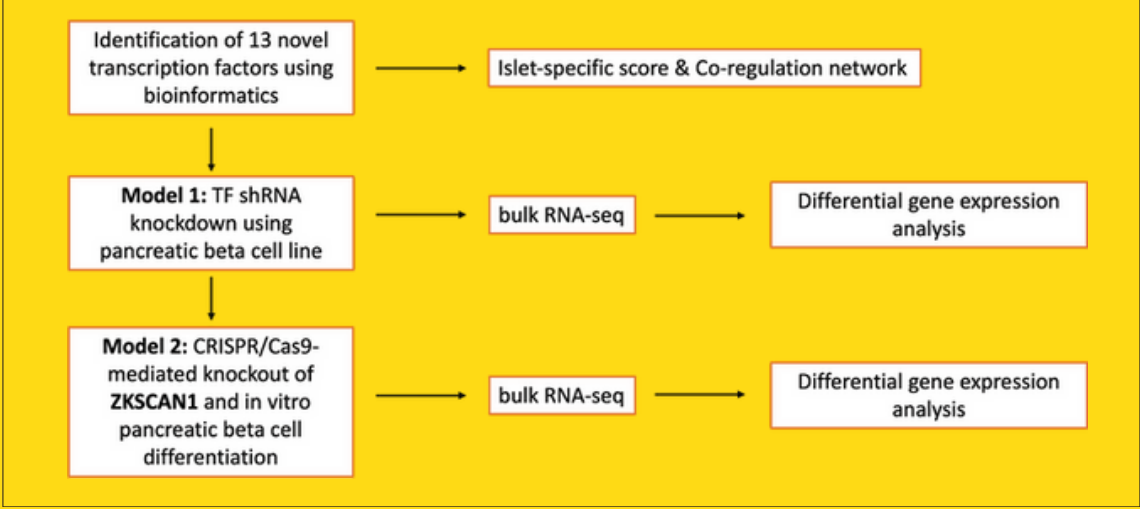


4. Gene Set Enrichment Analysis

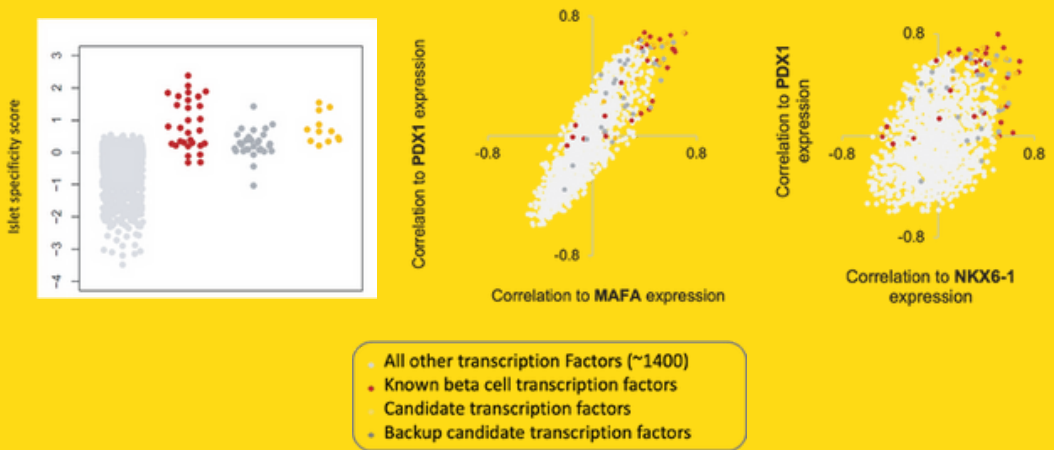


- We knockdown ZKSCAN1 using shRNA in a beta cell line (EndoC-βH3) and sent for bulk RNA-seq.
- Gene set enrichment analysis (GSEA) showed that differential expressed genes (DEGs) upon knockdown of ZKSCAN1 are enriched in pancreas beta cells and glycolysis.
- This suggests ZKSCAN1 have a role in regulate beta cell-specific genes and beta cell metabolism.

2. Workflow

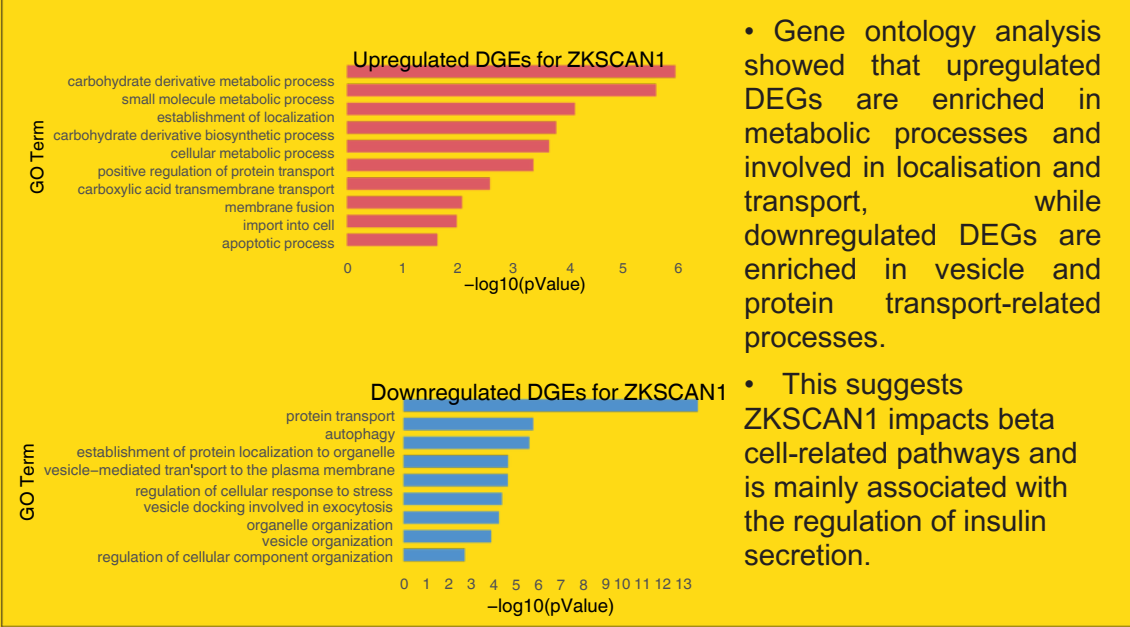


3. Identification of novel transcriptions



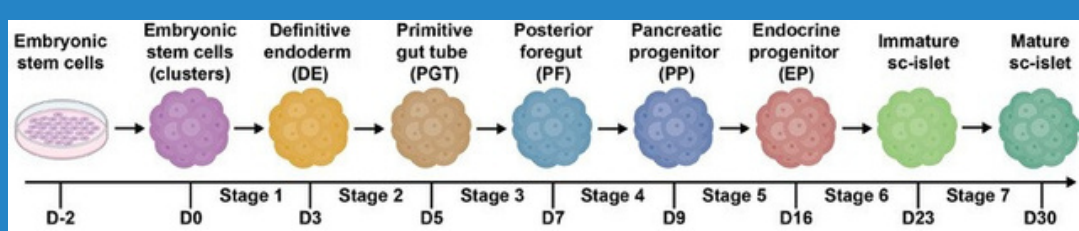
- Approach 1 examined islet-specific gene expression patterns in 208 human islet samples and 384 non-islet tissue samples. This described the expression patterns of all transcription factors (TFs) in human islet and to identify candidate TFs with islet- and beta cell-specific expression patterns.
- Approach 2 examined the transcriptional network of candidate TFs with well-known beta cell regulators. Candidate TFs showed positive correlations with the key mature beta cells regulators – PDX1, NKX6.1 and MAFA.
- **With bioinformatic analysis, we identified 13 novel TFs that are related to beta cell development or function. This project focuses on a particular TF called ZKSCAN1 (zinc finger with KRAB and SCAN1 domain 1).**

5. Gene Ontology Analysis



- Gene ontology analysis showed that upregulated DEGs are enriched in metabolic processes and involved in localisation and transport, while downregulated DEGs are enriched in vesicle and protein transport-related processes.
- This suggests ZKSCAN1 impacts beta cell-related pathways and is mainly associated with the regulation of insulin secretion.

6. Current Work



- We are using in vitro differentiation of human embryonic stem cells (hESCs) towards insulin-producing beta cells to understand the developmental roles of ZKSCAN1.
- **We plan to identify transcriptional and genomic targets of ZKSCAN1 at different developmental stages during differentiation. We will carry out bulk RNA-seq and ChIP-seq using ZKSCAN1 WT and KO stem cell lines generated by CRISPR/Cas9, followed by bioinformatics analysis.**

References:

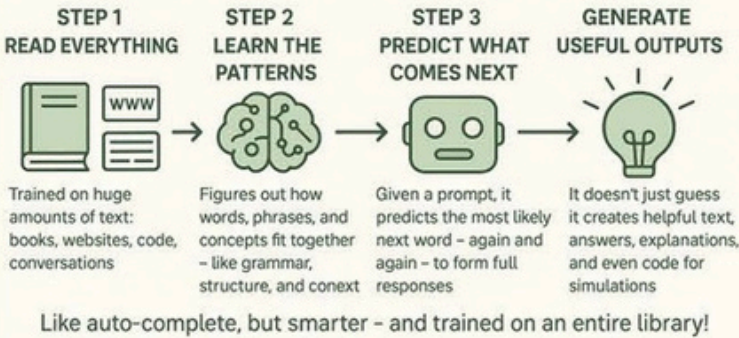
- [1] Forbes JM, Cooper ME. Mechanisms of diabetic complications. *Physiol Rev*. 2013 Jan;93(1):137-88. doi: 10.1152/physrev.00045.2011.
- [2] Karimova MV, Gvazava IG, Vorotelyak EA. Overcoming the Limitations of Stem Cell-Derived Beta Cells. *Biomolecules*. 2022 Jun 9;12(6):810. doi: 10.3390/biom12060810.
- [3] Augsornworawat, P., Hogrebe, N.J., Ishahak, M. et al. Single-nucleus multi-omics of human stem cell-derived islets identifies deficiencies in lineage specification. *Nature Cell Biology* 25, 904–916 (2023). <https://doi.org/10.1038/s41556-023-01150-8>
- [4] Veres, A., Faust, A.L., Bushnell, H.L. et al. Charting cellular identity during human in vitro β-cell differentiation. *Nature* 569, 368–373 (2019).

From Text to Tech: Simplifying Physics-Based Simulations with Large Language Models

Author: Ossama Shafiq | Supervisors: Dr Bahman Ghiassi & Dr Alessio Alexiadis | School of Engineering | School of Chemical Engineering

How Does an LLM Work?

Think of it like a supercharged language brain trained to predict words and patterns.



Introduction

Setting up physics-based simulations in **civil and chemical engineering**—like stress analysis in beams or fluid flow in reactors—is often slow and complex. Engineers must manually define geometry, mesh domains, and configure solvers, creating a barrier for rapid design. We explored how **large language models (LLMs)** like GPT-4, LLAMA, and Phi-3 can automate this process. Our **Text to Tech** pipeline translates natural language into geometry and simulation input files. Through benchmarking, we assessed each model’s strengths and weaknesses—finding that small, fine-tuned models can match larger ones for many geometry tasks. To go beyond text, we developed a **Vision to Tech** extension: engineers sketch a shape, and a vision-language model turns it into a valid .geo file. Using **Low-Rank Adaptation (LoRA)** fine-tuning on vision LLMs, we trained systems that reliably convert hand-drawn sketches into simulation-ready geometries. Together, these contributions demonstrate that LLMs—both in text-only and multimodal forms—can significantly reduce the barrier to entry for simulation-driven engineering.

Methods

1 Input File Generation

Used 9 LLMs (e.g., GPT-4o) to generate: **Geometry files (.geo)** for GMSH and **Simulation files (.sif)** for ELMER.

2 Simulation Setup

Tested two geometries: **Square Bar** (Simple) and **Wheel & Axle** (Complex) Simulations were run under static load using linear elastic properties.

3 Evaluation Metrics

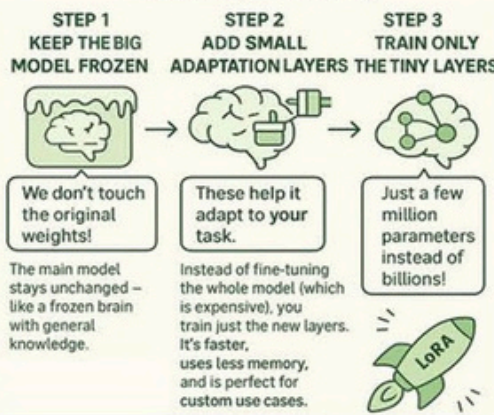
Scored outputs on: **Geometry Fidelity, Correctness of Parameters, Completeness of Files and Simulation Success.**

4 Prompting Pipeline

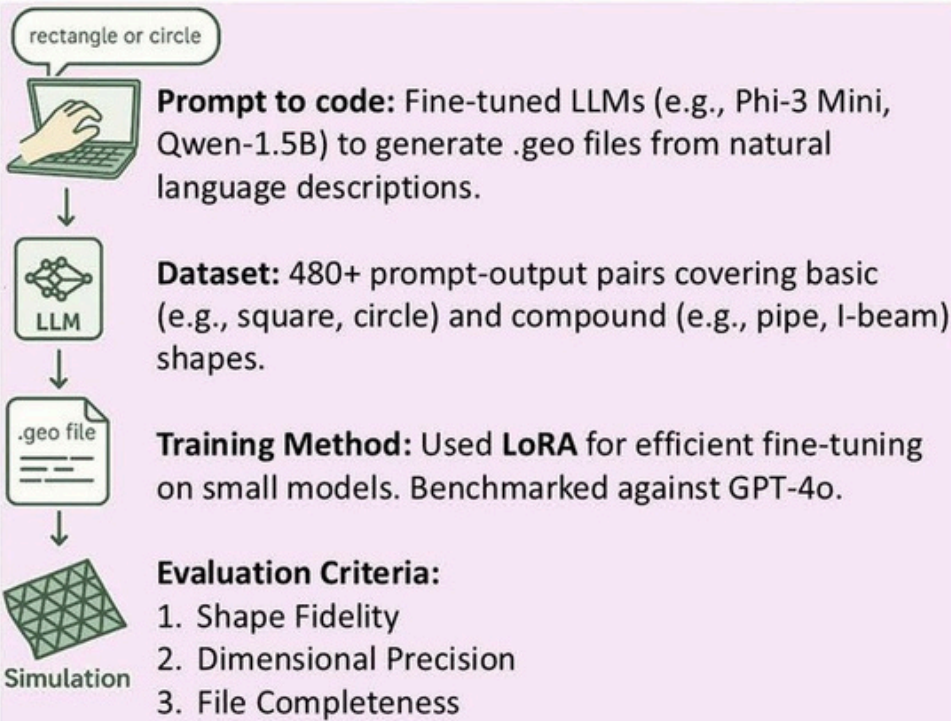
Used Python/ LangChain: 1. Templates for prompts 2. Outputs cleaned + tested in GMSH/ELMER 3. Visuals checked against simulation results

What Is LoRA?

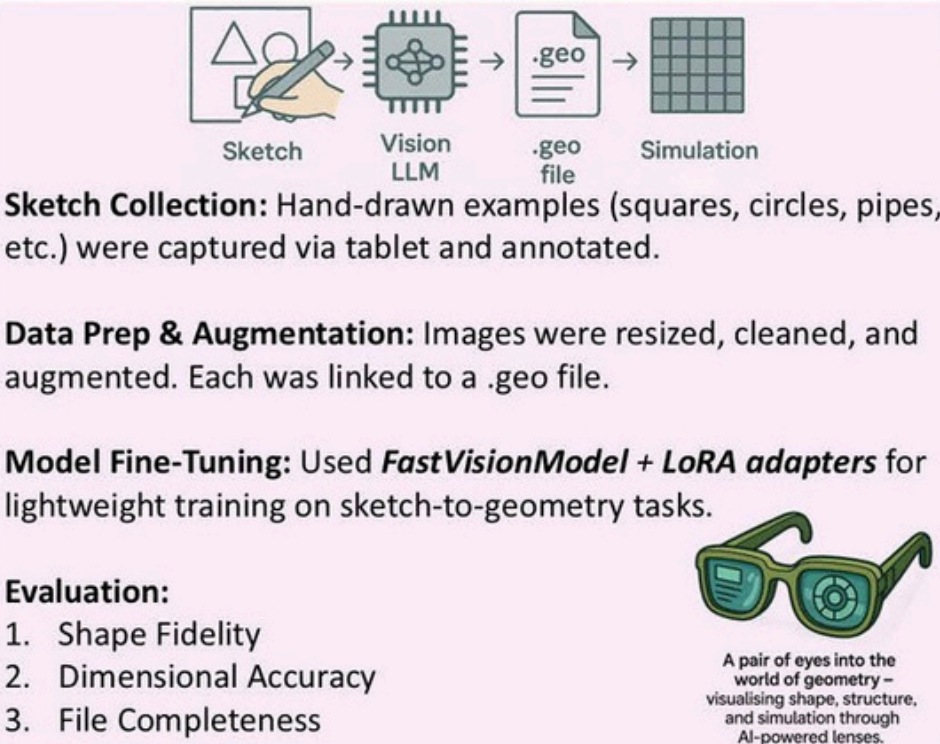
Think of it like “plugging in” new knowledge to a model without retraining the whole thing.



Text to Tech: Automating Geometry with Language Models



Vision to Tech: Interpreting Sketches with Multimodal AI



Conclusion

This project demonstrates how large language models (LLMs) can transform simulation workflows in civil and chemical engineering by automating the generation of geometry and simulation files.

We began by evaluating the capabilities of general-purpose and fine-tuned LLMs in converting text prompts into simulation-ready .geo and .sif files. Our **Text to Tech** pipeline showed that even lightweight models, when fine-tuned, can achieve near-perfect results in geometry fidelity, dimensional accuracy, and simulation completeness—rivaling larger models like GPT-4o.

To extend automation to conceptual design stages, we developed a **Vision to Tech** pipeline that accepts hand-drawn sketches as inputs. Using the Unsloth FastVisionModel and LoRA adapters, we fine-tuned vision-language models on annotated image-geometry pairs. In our comparative study, **Gemma 3 4B** significantly outperformed other vision models (e.g., Qwen 2.5 VL 3B & 7B), accurately translating sketches into valid .geo files across a range of geometries.

Together, these pipelines demonstrate that LLMs—both in text-only and multimodal forms—can reduce technical barriers, speed up simulation setup, and improve accessibility for engineers working on real-world physical systems.

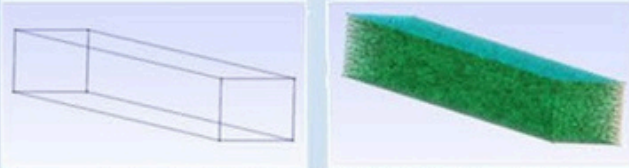
Email | oxs391@student.bham.ac.uk
LinkedIn | ossama-shafiq-776809167



Results

1 Simple Geometries

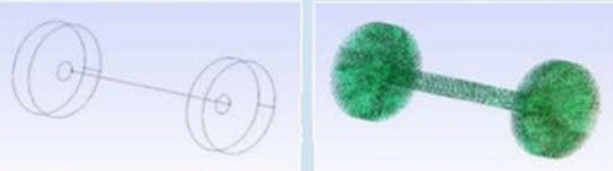
Top Models: GPT-4o, GPT-4, LLAMA-3-70B, MIXTRAL 8X22B
→ Near-perfect .geo files (96-100/100)
→ GPT-4o used Boolean operations-most advanced.



Struggled: LLAMA-2-70B, LLAMA-3-8B, PHI-3 Mini
→ Low accuracy and missing structure

2 Complex Geometries

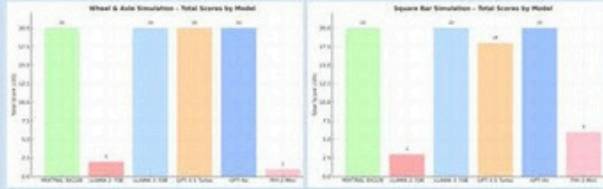
Top Models: GPT-4o (96), LLAMA-3-70B & GPT-4 (91)
→ Correct alignment and full file outputs



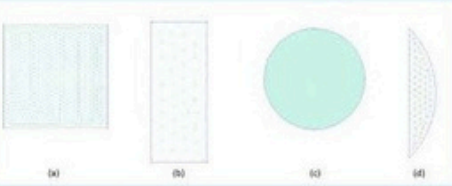
Challenges: LLAMA-2-70B, PHI-3 Mini
→ Failed due to structural issues

3 Simulation Input Files

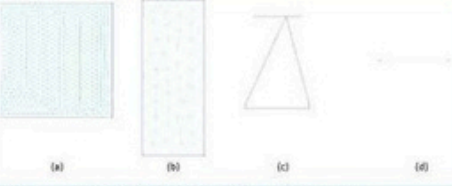
Square Bar + Wheel & Axle Tasks:
→ GPT-4o, GPT-4, LLAMA-3-70B, MIXTRAL = 20/20
→ PHI-3 Mini & LLAMA-2-70B = 1-6/20 (unusable files)



Before Fine Tuning



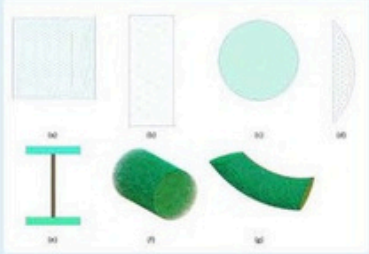
GPT-4o: Top performer across basic shapes. Struggled with bent pipe.



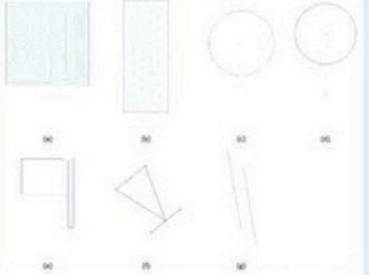
Qwen-2.5 14B: Moderate accuracy; struggled with complex forms.

Phi-3 Mini & Qwen-1.5B: Weak baseline; errors in dimensions and syntax.

After Fine Tuning

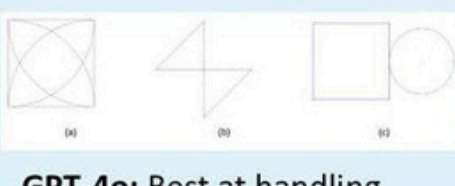


Phi-3 Mini: Perfect scores (60/60) across all shapes. **Qwen-1.5B:** Strong improvements but slightly less consistent.



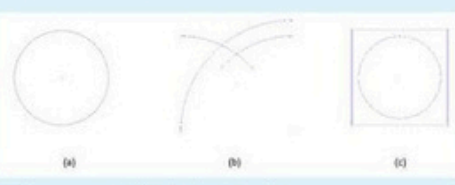
Qwen-2.5 14B: Better on basics, challenged by complex shapes.

Multi-Geometry Prompts



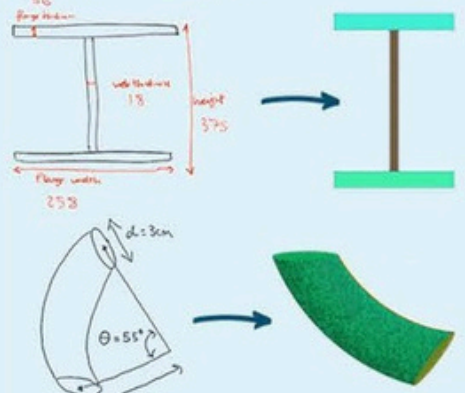
GPT-4o: Best at handling multiple shapes in prompt ‘circle next to a square’.

Small fine-tuned models: Unable to render the correct geometries.



Prompt: ‘circle inside a square’

Gemma 3 4B: Successfully fine-tuned to convert sketches into accurate .geo scripts. Handled complex shapes (I-beams, bent pipes) with high precision.



Qwen 2.5 VL 3B & 7B: Struggled to generate correct outputs despite strong visual models. Outputs were incomplete or incorrect for most geometries.

When She Holds the Purse Strings...

Yibo Zhang, Alessandra Guariglia

University of Birmingham

Abstract

This study investigates the role of intrahousehold female status in shaping household development resilience under the impact of natural disasters. Utilising panel data from the China Financial Panel Studies and the Emergency Events Database spanning 2014–2022, our analysis reveals that households where women are financial managers exhibit significantly greater resilience following adverse events. This relationship is particularly pronounced among households with less affluent families, low education, and fewer children, suggesting that female leadership may foster an environment conducive to sustained intra-household economic growth. In summary, our findings underscore the pivotal role of female status in enhancing household resilience after disasters, while explaining the growing prevalence of women as household financial managers.

Introduction

Natural disasters, as sources of unpredictable adverse shocks, not only undermine macroeconomic stability (Andi Duqi et al., 2021; Battiston et al., 2021) but also erode household welfare (Gallagher and Hartley, 2017). It also contributes to persistent poverty and long-term social exclusion (Rui et al., 2022).

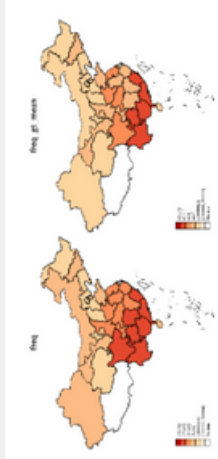


Figure 1: Natural Disasters by Province

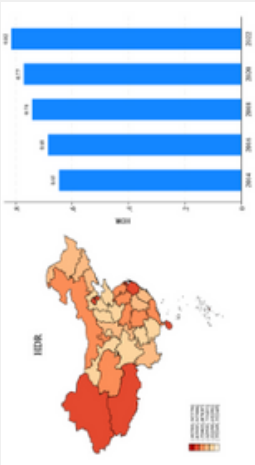


Figure 2: HDR by Year and Province

Therefore, resilience has become a central focus in anti-poverty strategies (Fernandez-Gimenez et al., 2010, 2012; Hallegatte et al., 2016). It is defined as "the capacity over time of a person, household or other aggregate unit to avoid poverty in the face of various stressors and the wake of myriad shocks. If and only if that capacity is and remains high over time, then the unit is resilient" (Barrett and Constanas, 2014).

With the improvement of women's status within the family, the question of how this affects family resilience, especially in the aftermath of natural disasters, has become an urgent issue that needs to be addressed.

Important Result

Intrahousehold Female Status and Resilience

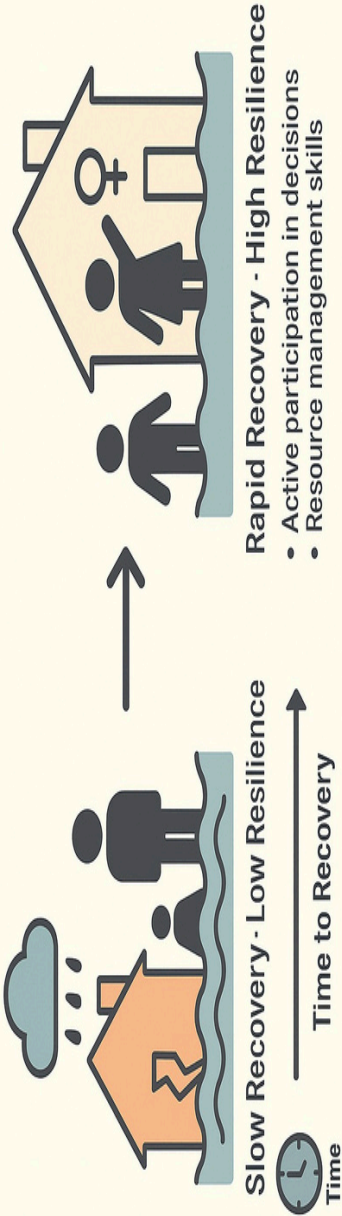


Figure 4: Main result

Data

1. Household Survey Data: China Family Panel Studies (CFPS).

Through this database, we divide households by household type: couple and non-couple households. The first type is defined as households with two married or cohabiting spouses. Non-couple households include single-person and other households (e.g., single mothers with children)

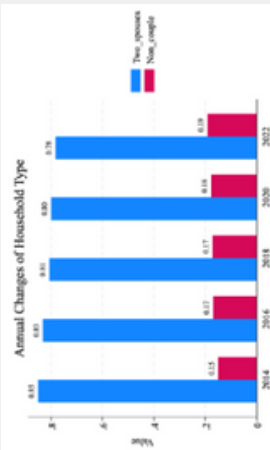


Figure 3: Household Type and Survey Year

2. Natural Disasters Data: Emergency Events Database (EM-DAT).

EM-DAT data include all disasters from 1900 until the present. Therefore, all the households have experienced more than one disaster in our sample.

Method

We use the following methodology to examine the impact of intrahousehold female status on the HDR after natural disasters:

$$\begin{aligned} HDR_{it} &= \beta_0 + \beta_1 FW_{it} \times NaturalDisasters_{it} \\ &+ \beta_2 FW_{it} + \beta_3 NaturalDisasters_{it} \\ &+ \beta_4 X_{it} + \delta_p + \theta_t + \epsilon_{it} \end{aligned}$$

Conclusions

- Female control of finances in the household can increase the resilience of the household to thrive after a disaster.
- This relationship is particularly pronounced among households with less affluent families, low education, and fewer children.
- This relationship is particularly pronounced among earthquakes and extreme temperatures.

Acknowledgements

I would like to express my sincere gratitude to Professor Alex and her research team for their expert guidance on empirical design.

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Searching for the Ground State Structure of Lithium Imide

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UNIVERSITY OF
BIRMINGHAM

Introduction

Traditional lithium-ion batteries currently use an electrolyte consisting of a lithium-based salt dissolved in an organic solvent. However, traditional electrolytes are not ideal as they are flammable and can contain toxic compounds as a result there is a desire to switch to a safer form of electrolyte. Solid electrolytes are far safer when compared to traditional electrolytes making them the preferred choice for next generation batteries. We have been computationally studying lithium imide as a potential solid electrolyte. Lithium imide is an ideal solid electrolyte as it has a high ionic conductivity comparable to liquid electrolytes.¹ This means that there would be no performance lost if the switch was to be made. As well unlike other solid electrolyte lithium imide only consists of very light elements making the batteries lighter. This makes lithium imide an ideal electrolyte for devices where the weight of battery is important such as electric vehicles and portable electronics.

Defects will occur in any solid material that is not at absolute zero as they are entropically stabilizing. Defects within a solid electrolyte are of great interest as they can drastically alter the properties of a solid electrolyte hence why we are interested in studying the defect chemistry of lithium imide. Before we can study the defect chemistry of lithium imide, we must first make sure that we are basing our calculations on the lowest energy or ground state structure at absolute zero. This is because otherwise our predictions about the defect present in lithium imide will be incorrect and as these defects are very important in understanding how lithium imide functions as a solid electrolyte, we want to ensure that they are correct. The problem is that this was a topic of debate in the early 2000's with many different structures being proposed however no conclusive answer was ever reached. This means that before we can study the defect chemistry of lithium imide, we must first ensure that we have the ground state structure.

Lowest Energy From the Literature

The first step was to determine which of the structures proposed in the literature was the lowest in energy. This was done using Density Functional Theory (DFT) which is a computational method that can be used to predict structural properties.

Seven proposed structures were taken and relaxed using DFT.²⁻⁸ It was found that the structure proposed by Mueller & Ceder was the lowest in energy, see figure 1.2 In this structure the nitrogen's form a Face Centred Cubic (FCC) sub-lattice, with a hydrogen bound to each while lithium occupies the octahedral sites between the nitrogens.

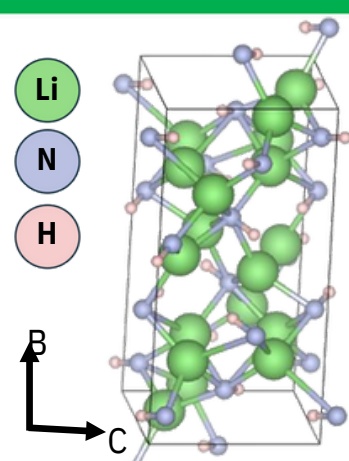


Figure 1: Structure proposed by Mueller & Ceder.²

Structure Search Analysis

Even though the MLP didn't work the structure search continued, over 4000 more structures have been generated and relaxed using DFT. Through these structures some trends can be seen among the lowest energy structures.

We took 1000 of these AIRSS structures and extracted information about the local coordination environment of each lithium ion using Pairwise Controlled Manifold Approximations (PaCMAP). This was combined with the energy of each local environment to produce figure 3. By looking at figure 3 we can see that there is only around 0.5 eV difference in energy between lithium environments implying that energetically they are quite similar. This is further supported by the fact the PaCMAP values determine for each lithium have them cluster together with no clear clusters emerging within the graph this implies that all lithium ions are in very similar local environments with no clear distinction between them. By looking at some structures we can see that this is indeed the case as most lithium tend to lie in a tetrahedral coordination environment of some distorted version of such an environment, see figure 4 for examples. This tetrahedral coordination lithium environment is also present in Mueller & Ceder's structure, see figure 1, This is strong support that the lithium ions in the Mueller and Ceder structure are indeed in their lowest energy conformation and that a lower energy configuration does not exist.

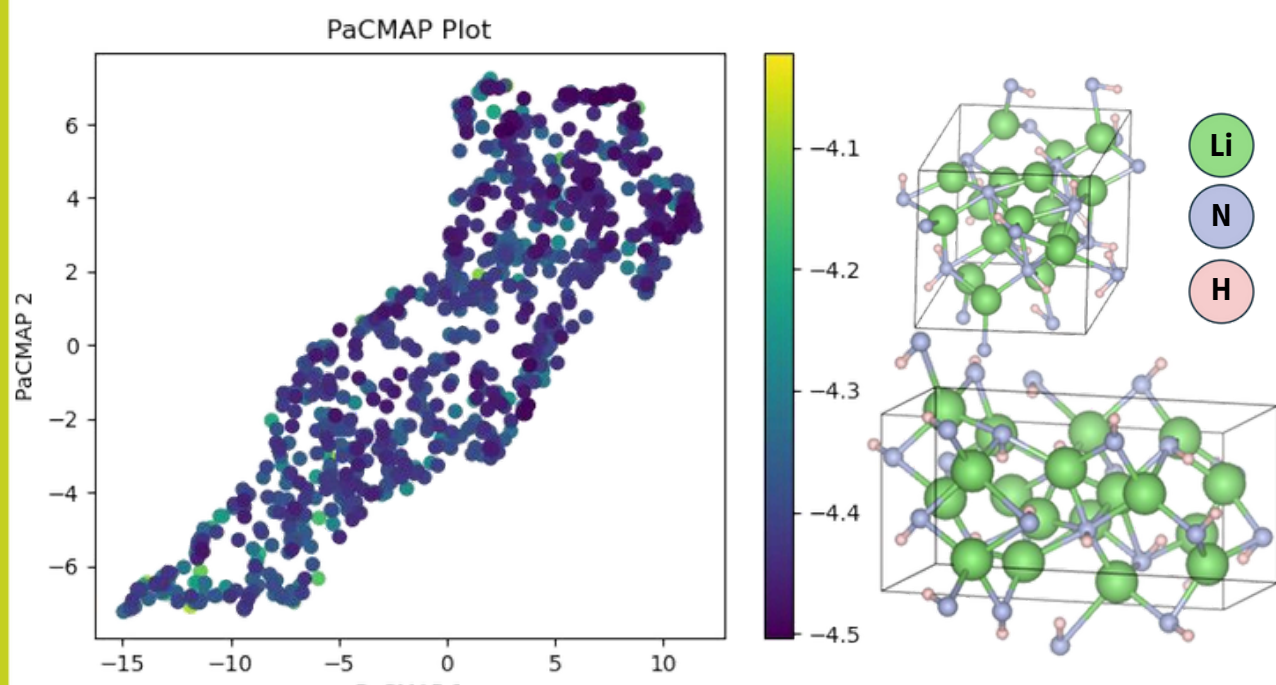


Figure 3: PaCMAP plot of lithium's various coordination environments

Figure 4: example structures generated by AIRSS

MLP-Assisted Structure Search

To ensure that we did indeed have the ground state structure of lithium imide we performed Ab-Initio Random Structure Searching (AIRSS) to see if we could find a structure lower in energy. We also decided to generate a Machine Learnt Potential (MLP) to see if it would help speed up the structure search. The first step to creating an MLP is generating a set of training data. This was done by creating 2000 AIRSS structures before relaxing them with DFT. Using the DeePMD software package we were able to train an MLP using this data. To test its effectiveness 200 more structures were generated using AIRSS. These test structures were relaxed with both DFT and our MLP with the energies given from each being plotted to see how accurate the MLP is in comparison to DFT, see figure 2. From figure 2 we can see that there is no correlation between the energies given by the MLP and DFT, meaning that this MLP will not be of use in continuing the structure search and it would most likely be easier to continue with the aid of an MLP.

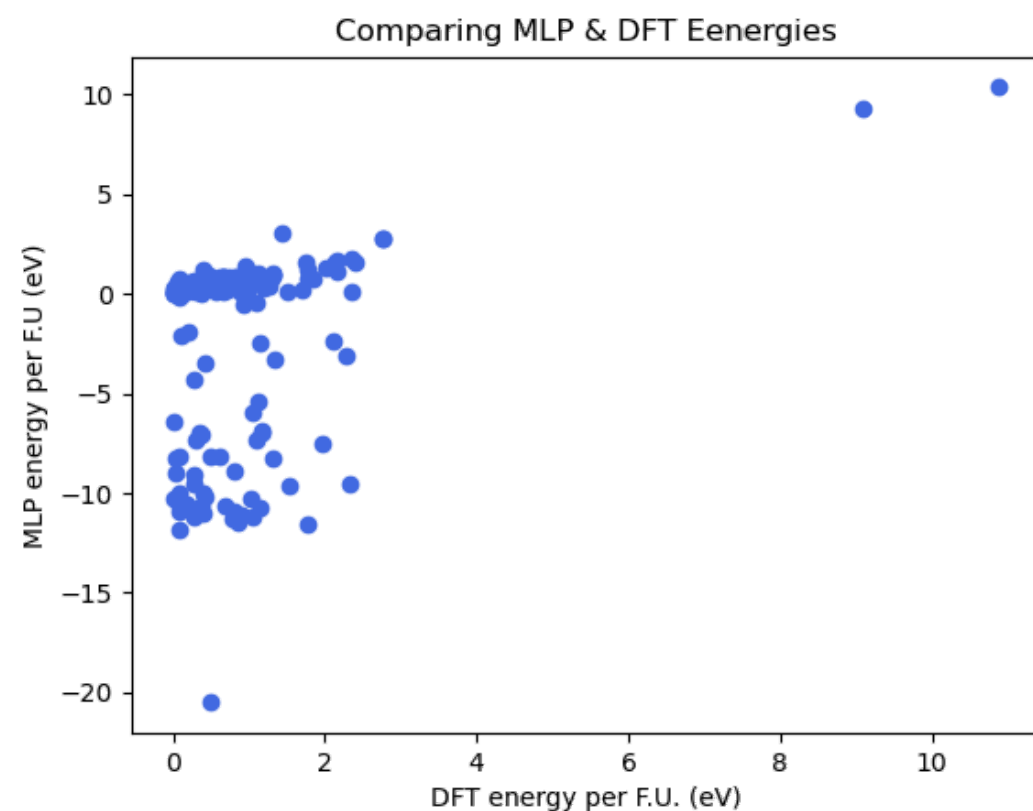


Figure 2: A comparison between the energy of each system per formula unit calculated by DFT vs MLP

Conclusion & Further Work

In this poster we have discussed which among the various lithium imide structures proposed by other research groups is the lowest in energy. We have also described our own structure search and the attempt at using an MLP to quicken the search although unsuccessful. We have also discussed the similarities among the AIRSS structures and how it seems lithium prefers to sit tetrahedrally between nitrogen atoms much like the Mueller & Ceder structure which supports its claim as the lowest energy lithium imide structure. However, further work must be done so that we can be confident in our answer. This would include continuing our structure search as well as analysing nitrogens and hydrogens preferred local coordination environments

All of the computations described in this poster were performed using the University of Birmingham's BlueBEAR HPC service, which provides a High Performance Computing service to the University's research community. See <http://www.birmingham.ac.uk/bear> for more details.

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VASP



Effect of laser pulsing and interlayer machining on residual stresses in laser directed energy deposition

by Nina Eva Adler



INTRODUCTION

Additive manufacturing (commonly known as 3D printing) will play a crucial role on the path to more sustainable manufacturing. The ability to produce near-net shape builds reduces waste, saves material, and minimizes the need for post-processing, hence less energy and time. However, before additive manufacturing is widely adopted, significant challenges need to be overcome so it can substitute traditional manufacturing processes. One of these is to control residual stress caused by the rapid heat cycle the material must overcome during the laser melting. Current methods are mainly based on post-process treatment. However, this leads to an increase in process time. To cope with this ongoing problem, my PhD investigates two in-process methods, pulsed laser and interlayer machining [4].

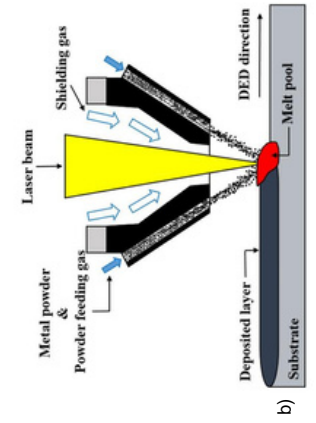
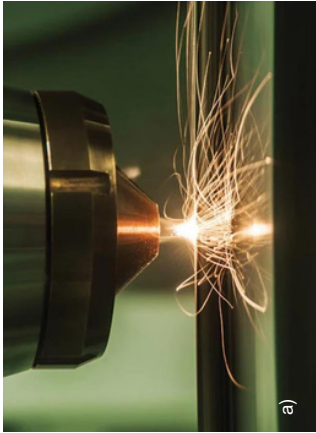


Figure 1: Concept of Directed Energy Deposition, explanation of the deposition process
a) Photo during the deposition process of Directed Energy Deposition [1]
b) Schematic illustration of powder deposition, powder melting and printing of a single layer [2]

Motivation

METHODOLOGY

Hybrid Manufacturing

Pulsed Laser: The aim of using a pulsed laser in additive manufacturing is to reduce the energy and heat input into the printed sample. With a noncontinuous laser, the printed lines experience a cooling cycle before another melting cycle induces heat. Thus, the temperature gradient can be better controlled, and residual stress and distortion can be reduced.

Interlayer Machining: The goal is to machine off the first part of the printed top layer. The theory is that most

stresses evolve around the surface area, and machining the top part can introduce some relief effects.[3]

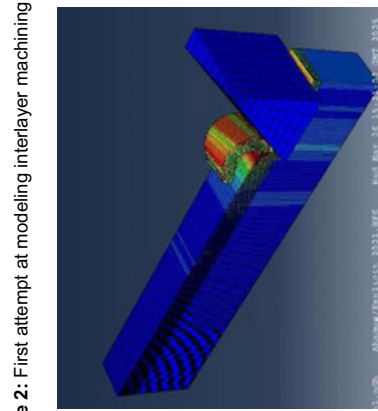


Figure 2: First attempt at modeling interlayer machining

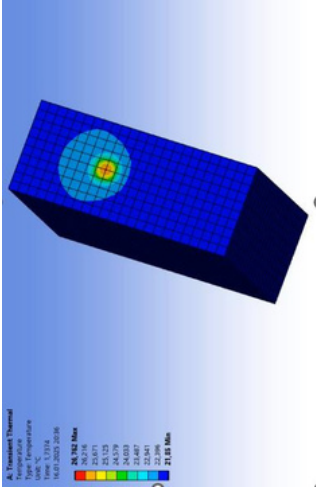


Figure 3: First attempt at modeling pulsed laser



Figure 4: Printed single wall: 450 W laser power and 8 mm/s printing speed

Set Up

Experiments

The design of the experimental setup is based on five stages:

- 1) **Printing single lines** and investigating optimized parameters
- 2) **Printing thin walls** and again determining the optimized parameters in terms of microstructure and geometrical properties
- 3) **Printing thick walls** with proper scan strategy and finding the correct parameter set
- 4) **Add hybrid manufacturing** to the optimized parameter set of stage 3: interlayer machining and pulsed laser
- 5) To validate the experimental work of both methods, I am currently **developing simulations** using the simulation software Abaqus and Ansys on Blue-Bear high-performance computer).

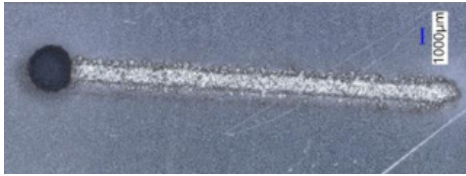


Figure 5: Printed single line

RESULTS

During the first stages, the main criteria for validating the quality of a single track is the ratio between the height and the depth of the substrate (dilution).

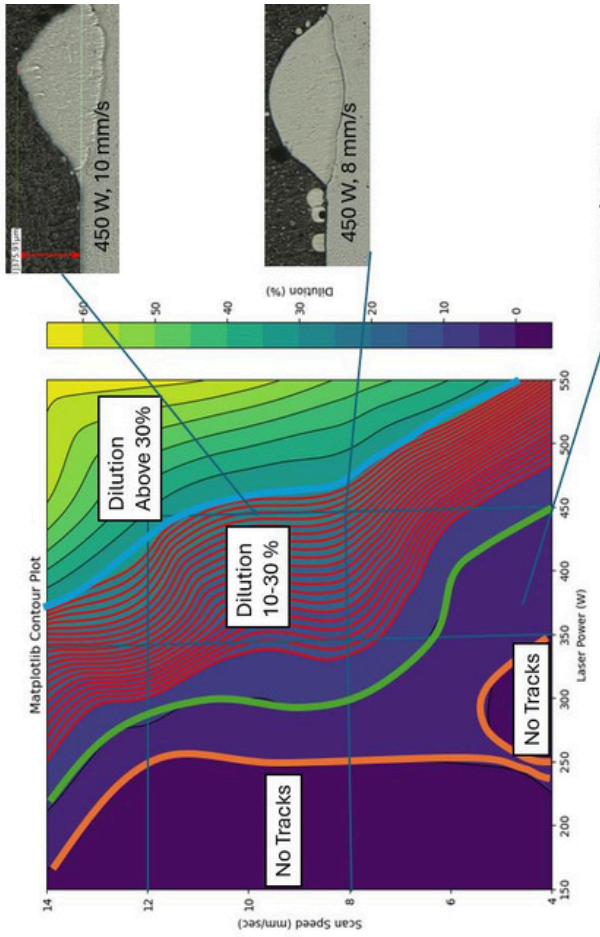


Figure 7: The visualization of the used parameter set to print single lines. The optimized parameters based on the optimal dilution (height and depth ratio) are marked on the blue square.

Current Status

Sources

- [1] <https://www.lboro.ac.uk/research/amrg/about/the7categoriesofadditivemanufacturing/directedenergydeposition/>
- [2] J.-S. Lim, W.-J. Oh, C.-M. Lee, and D.-H. Kim, "Selection of effective manufacturing conditions for directed energy deposition process using machine learning methods," Sci Rep, vol. 11, no. 1, p. 24169, Dec. 2021, doi: 10.1038/s41598-021-03622-z
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Origins of High Ionic Conductivity in Lithium Imide Solid Electrolytes

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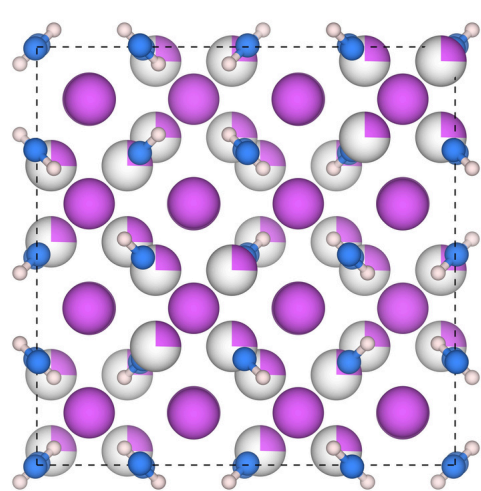


Figure 1: Li₂NH supercell. Li: Purple, N: Blue, H: Grey

Lithium imide (Li₂NH) (**Fig. 1**) was previously studied for H storage, but was first identified as a Li conducting solid electrolyte in 2016.¹

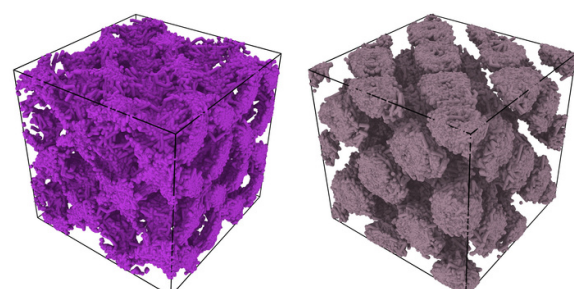


Figure 2: Atom trajectories from AIMD. Li: Purple, H: Grey

Li₂NH has 2 dynamic species. We investigate the factors affecting Li mobility for its optimisation.

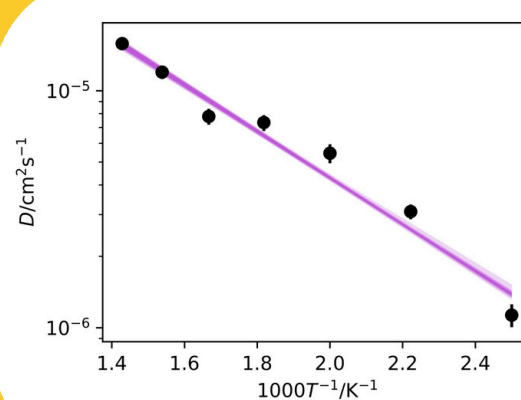


Figure 3: Arrhenius plot of Li diffusion

Part 1: Lithium Dynamics

AIMD simulations run at a selection of temperatures for a minimum of 150 ps until diffusion coefficients converged.

Conductivity peaks at the pure imide composition. The difference between artificial and naturally balanced compositions shows Li content isn't the sole factor affecting mobility.

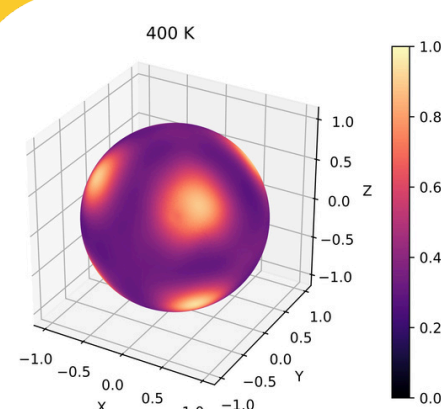


Figure 6: H densities at 400 K

Part 3: Hydrogen Dynamics

Analysis of the AIMD trajectories of H gives some insights as to its preferential arrangement in tetrahedral Li vacancies (**Fig. 6**). This is consistent with clustering (**Fig. 7**), and also allows us to compare Li diffusion with H occupation (**Fig. 8**).

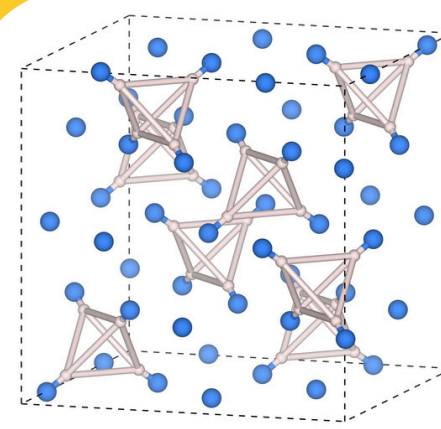


Figure 7: Anion FCC Sub-Lattice with clustered H. N = Blue, H = Grey

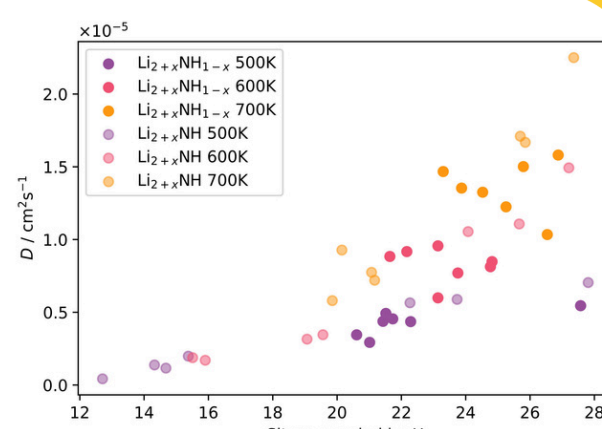


Figure 8: Diffusion coefficients vs sites occupied by H

Li conductivity is good, but can it be improved with disorder/off-stoichiometry?

There is a correlation between sites being occupied by H and Li diffusion. Therefore, an increase in H clustering reduces conductivity.

Part 2: Solid Solutions

Various compositions were investigated as a solid solutions of imide, amide and nitride groups (**Fig. 4**).

Li rich and deficient systems balanced with an artificial charge rather than with H were used to observe the effect of adding or removing Li whilst maintaining the FCC anion sub-lattice (**Fig. 5**).

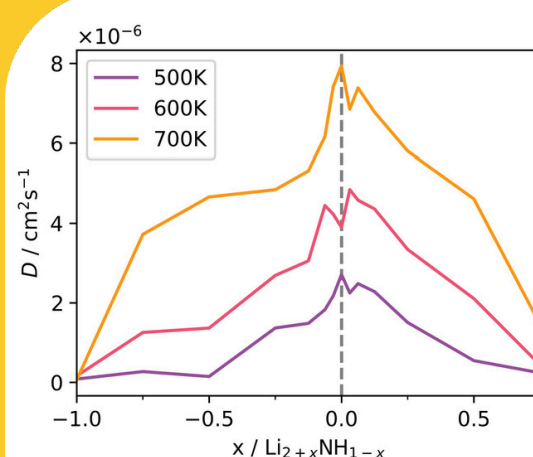


Figure 4: Solid solution diffusion coefficients

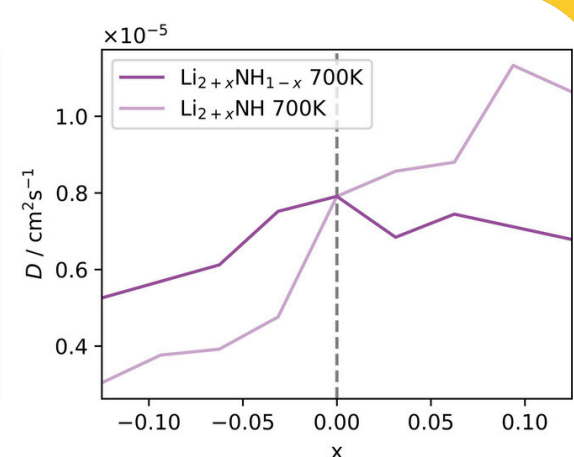


Figure 5: Diffusion coefficients for artificially and non-artificially charge balanced compositions

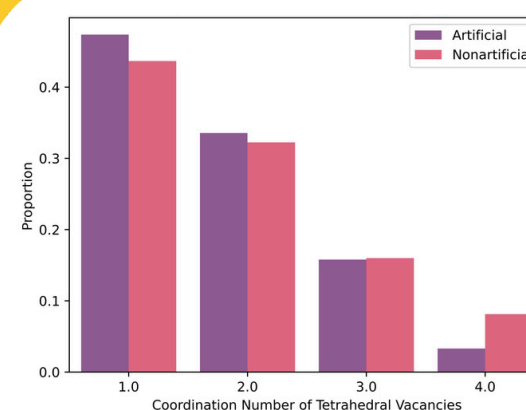


Figure 9: Coordination number distribution of vacant Li tetrahedra

Part 4: Lithium Clustering

Previous studies found that Li₂NH's lowest energy structures have Li clusters around vacant tetrahedra, that trap carriers and resist breaking apart.² This is clear when comparing the +2 artificially balanced system to its nitride-balanced counterpart (**Fig. 9**).

The removal of H when balancing with a nitride results in the increased clustering of Li, explaining the reduction in conductivity.

Now that the factors affecting Li mobility have been identified, we can look to maximise conductivity for use in Li-ion batteries.

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Some of the computations described in this poster were performed using the University of Birmingham's BlueBEAR HPC service, which provides a High Performance Computing service to the University's research community. See <http://www.birmingham.ac.uk/bear> for more details.

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2.G. Miceli et al., *J. Phys. Chem. C* 2011, 115, 7076–7080.