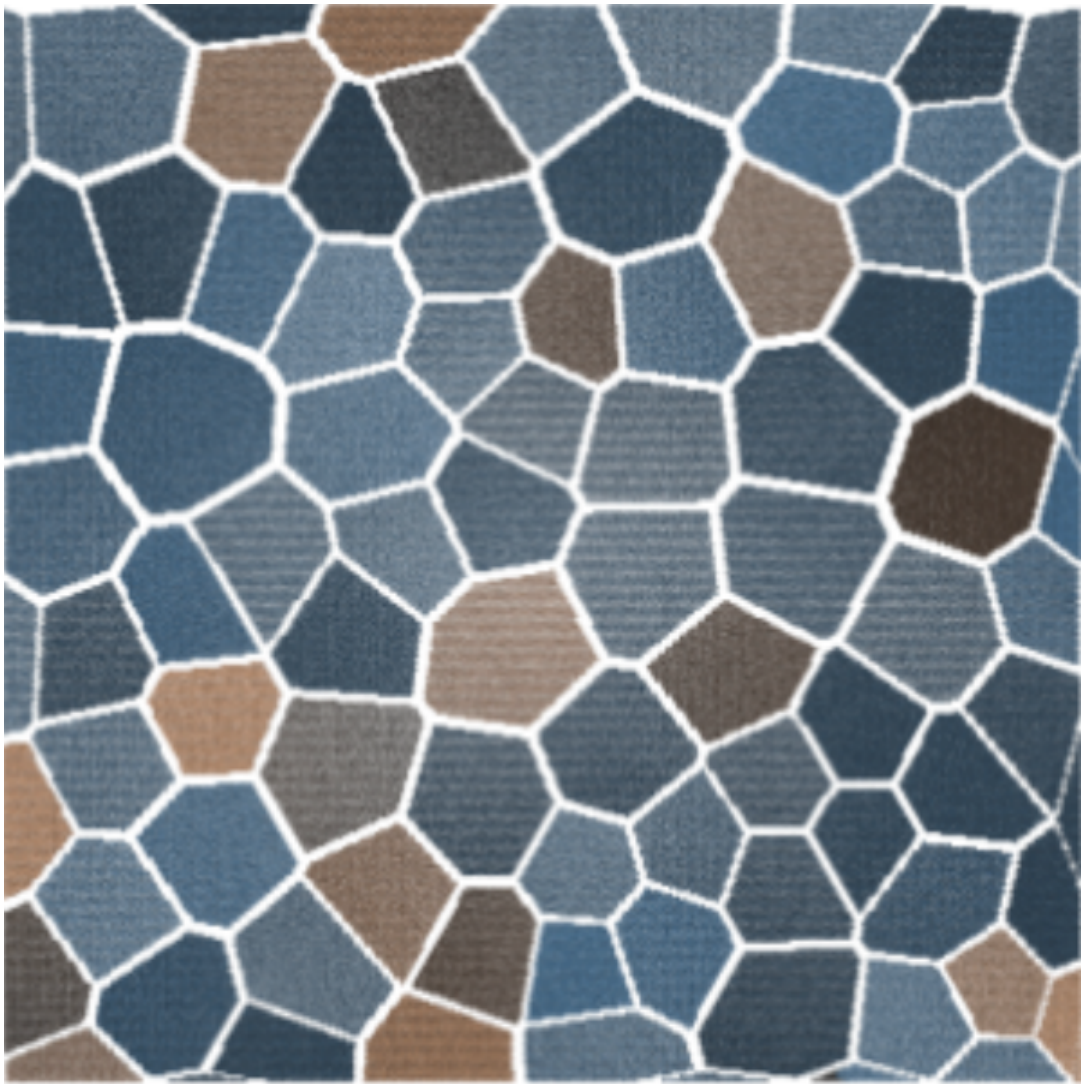
2022

IOP | Institute of Physics
Computational Physics Group

Newsletter



Spin Dynamics Simulations of Iridium Manganese Alloys.
(image courtesy of Dr Sarah Jenkins)

Newsletter Contents

This Newsletter

Dear Readers,

The feature article for this edition of the newsletter is an invited contribution by Dr Sarah Jenkins from the University of York, the winner of the 2021 IoP Computational Physics Group PhD Prize, on **'Spin Dynamics Simulations of Iridium Manganese Alloys'**.

We also summarise conferences and workshops that took place over the last year and a half. The reports provided by our members offer a great summary of the activities that our Group is involved in.
Despite the pandemic continuing in 2021, the Group was involved in a number of exciting events, collaborating with other IoP special interest groups. We have also had an opportunity to organise first hybrid/in-person meetings since the start of the pandemic. Those members who are involved in teaching, will find the report from the conference, `Lessons Learned in Lockdown` particularly useful.
We are also planning new events, regular and one–off, that we hope will bring our already strong Community closer together and enable new and exciting collaborations. Make sure to regularly check our Group blog `www.compphysics.org` to stay up to date on the upcoming events.

Most URLs in the newsletter have web hyperlinks and clicking on them should take you to the corresponding page. The current and previous editions of the newsletter can be found online at:
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If you have any suggestions on how to improve this newsletter, or have any articles/news that you would like to seen publish, please let us know!

Enjoy this edition!

On behalf of the The Computational Physics Group Committee:
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Spin Dynamics Simulations of Iridium Manganese Alloys

Dr Sarah Jenkins
The University of York

Introduction

Every year there is a demand for computers to become smaller, faster and have a higher data density. To keep up with this, computational power must increase exponentially as described by Moore's law. To increase the computing power a new wave of research in "beyond Moore's law" technology [26] is being developed. One of these technologies is a subfield of spintronics, known as anti-ferromagnetic (AFM) spintronics which uses the AFM as the active element to store, read and write information, contrary to conventional spintronic devices which use ferromagnets (FM) as the active element.
These devices have the potential to greatly outperfom their ferromagnetic counterparts as AFM materials are ultrafast, and very robust to external fields [17]. One of the challenges in designing anti-ferromagnetic spintronic devices is the control and detection of the magnetisation of the anti-ferromagnet due to its lack of stray fields. A promising way of achieving this is via the exchange bias effect, which occurs when a FM is coupled to an AFM and causes a shift of the magnetic hysteresis loop. Despite the widespread use of exchange bias in magnetic recording devices there is still little knowledge of the microscopic origins of the effect because our knowledge of AFMs still lacks a basic understanding [17]. Recently, many novel experimental developments have been created in an attempt to probe the spin structures such as using optical approaches [25] and investigating spin transport effects [3, 11]. However, none of these can probe into the interfaces or observe the atomistic level properties at a high enough frequency as is required to properly understand the ultra fast dynamics of AFM materials. To investigate these materials, advanced computational models are required. The computational modelling of FM materials relies heavily on continuum models however, these break down for antiferromagnetic or ferrimagnetic materials. Recent developments in computational power have meant that it is now possible to model systems at an atomistic level where each atom is given a local magnetic moment. Only using these advanced atomistic computational models can the magnetic properties of AFM's be properly understood.
The AFM most widely used in spintronic devices is Iridium Manganese (IrMn). Its main advantage is its high magnetic ordering (Néel) temperature and high magnetic anisotropy. In these devices IrMn is used in thin film form, and in many compositions has a non-collinear magnetic structure. Here I present a full theoretical study of the anti-ferromagnetic material Iridium Manganese using an atomistic spin model, determining the properties of IrMn in extraordinary detail, paving the way for a full understanding of this complex and interesting material and the interfaces which are responsible for exchange bias.

Modelling anti-ferromagnets

Iridium Manganese has a very complex magnetic structure, as depending on the order and composition of the Ir and Mn concentrations the number of sublattices and magnetic ground state changes. This means that previously there has been a lot of confusion around the magnetic spin structures of IrMn and incorrect assumptions have often been made in the literature[23, 9, 19].
One of the largest problems in modelling this system is the anisotropy. In disordered IrMn alloys determination of the anisotropy term in the spin Hamiltonian presents a significant challenge as each atom has a different local crystalline environment, leading to a unique anisotropy value at each site. Ideally, the system would be modelled using a completely *ab-initio* approach, but this is only feasible for up to a few 100 atoms. Instead, the Néel pair anisotropy model is used, a model first proposed by Néel in 1954 [21] to model the surface of a crystal. The model assumes that the lack of bonds at surfaces causes an anisotropy.

I have extended the Néel pair anisotropy model to model the non magnetic Ir atoms as non-magnetic impurities.
The atomistic model used in the simulations is the vampire software package [8]. The energetics for IrMn is described by the spin Hamiltonian:

$$\mathscr{H} \quad = \quad -\sum_{i<j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - \frac{k_N}{2}\sum_{i\neq j}^{n_z}(\mathbf{S}_i \cdot \mathbf{e}_{ij})^2 - \sum_i k_{\mathrm{u}}(\mathbf{S}\cdot\mathbf{e}_z)^2 - \sum_i \mu_{\mathrm{s}}\mathbf{S}_i \cdot \mathbf{B},$$

where the first term is the exchange energy, the second term is the anisotropy energy and the third term is the applied field Hamiltonian. $\mathbf{S}_i$ describes the spin direction on site i. J_{ij} is the effective exchange interaction which was limited to nearest ($J_{ij}^{\mathrm{nn}} = -6.4 \times 10^{-21}$ J/link) and next nearest ($J_{ij}^{\mathrm{nnn}} = 5.1 \times 10^{-21}$ J/link) neighbours [15, 14]. $k_N = -4.22 \times 10^{-22}$ is the Néel pair anisotropy constant and $\mathbf{e}_{ij}$ is a unit vector from site i to site j, n_z is the number of nearest neighbours. Spin Dynamics simulations were done solving the stochastic Landau-Lifshitz-Gilbert equation with a Heun numerical scheme [7].

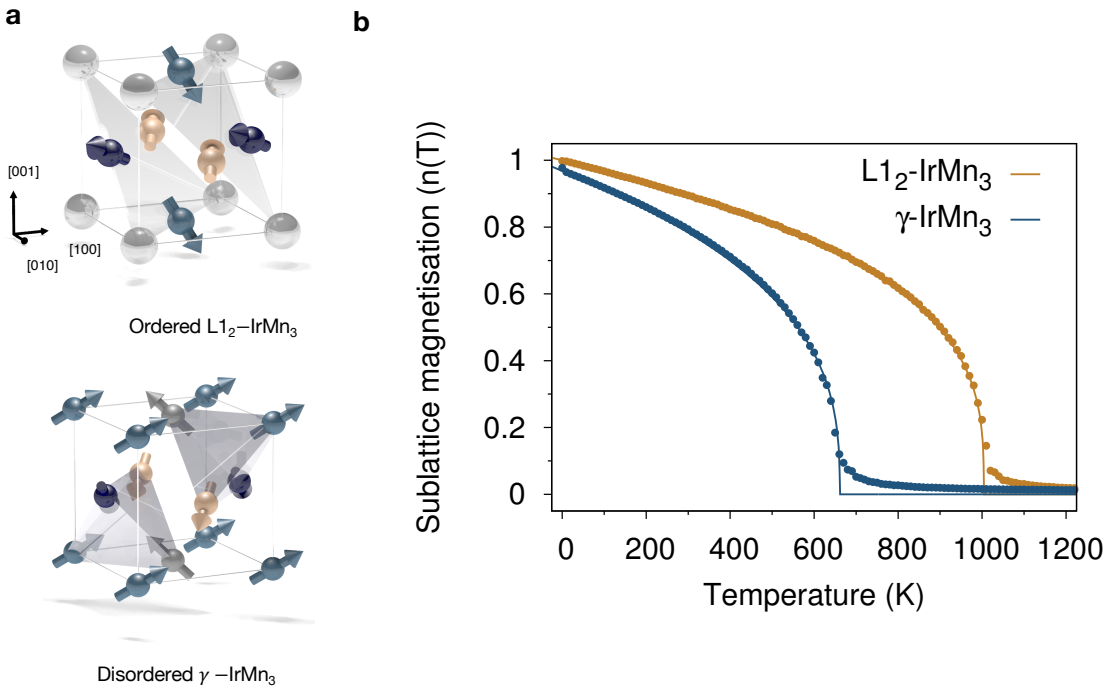

Figure 1: **Visualisation of the simulated ground state spin structures of IrMn$_3$ and simulated magnetisation vs temperature curves** (a) Simulated spin structures of ordered L1$_2$-IrMn$_3$ and disordered γ - IrMn$_3$. The spins show an average spin direction of each magnetic sublattice direction over the whole sample. In the case of L1$_2$-IrMn$_3$ the corner atoms are all Ir and so have no net magnetic moment and are therefore represented by the spheres. (b) Magnetisation vs temperature curves for ordered and disordered IrMn$_3$

To validate our model, magnetic ground states and Néel temperatures will be compared to previously known experimental and theoretical results for IrMn to check the model in many states. The ground state spin structures are shown in Fig.1 (a) and the Néel temperatures are shown in Fig.1 (b). I find that ordered L1$_2$-IrMn$_3$ has a triangular ($T1$) spin structure where the magnetic moments lie in plane along the (111) planes with an angle of 120° degrees between them pointing along the [211] directions and that disordered γ-IrMn$_3$ has a tetrahedral ($Q3$) spin structure [19]. These are both in agreement with previous

experimental [19] and *ab-initio* results [27]. Our simulations reproduce the Néel temperatures for the $L1_2$ ($T_N \sim 1000$ K) and γ ($T_N \sim 700$ K) phases of $IrMn_3$.

The complex magnetic Anisotropy in IrMn

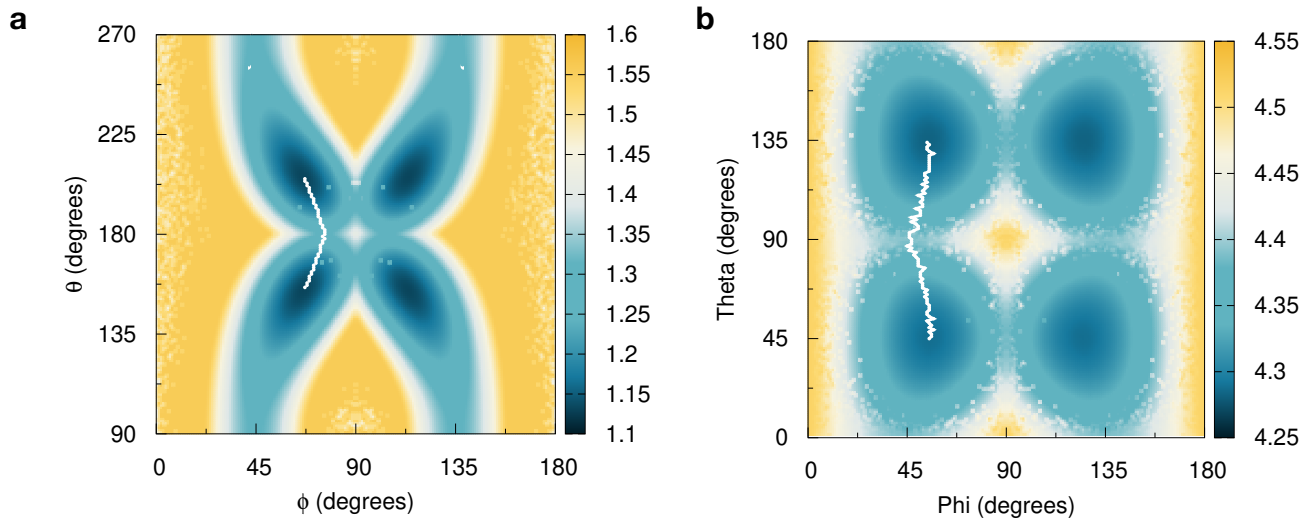

Figure 2: **Anisotropy of IrMn** The energy surface for (a) ordered $L1_2$ $IrMn_3$ and (b) disordered $IrMn_3$ the white lines show the minimum energy paths between ground states.

The magnetic anisotropy of antiferromagnets plays a crucial role in stabilising the magnetisation of many spintronic devices. In non-collinear antiferromagnets such as IrMn the symmetry and temperature dependence of the effective anisotropy are poorly understood. Theoretical calculations [27] and experimental measurements [28, 5] of the effective anisotropy constant for IrMn differ by two orders of magnitude, while the symmetry has been inferred as uniaxial in contradiction to the assumed relationship between crystallographic symmetry (cubic) and temperature dependence of the anisotropy. The energy barrier separating two ground states is the minimum energy path for the spins to rotate from one ground state to another. At a finite temperature the anisotropy constant is a free energy difference arising from spin fluctuations. To calculate the energy barrier, we use a constrained Monte Carlo [2] (CMC) algorithm to determine the entire energy surface and then calculated the minimum energy between two ground states.
In $IrMn_3$ both ordered and disordered structures have very different anisotropy surfaces as shown in Fig. 2. For ordered $L1_2$ - $IrMn_3$ it was found that the energy surface is unusually complex although shows the usual four fold symmetry expected from cubic anisotropy. In disordered γ - $IrMn_3$ the energy surface shows a usual cubic symmetry. This is expected from the cubic nature of the IrMn crystal. In ordered $L1_2$ $IrMn_3$ the calculated 0K energy barrier is 1.78×10^6 J/m^3, and for disordered $IrMn_3$ the energy difference is slightly lower at only 9.96×10^5 J/m^3. These values are an order of magnitude lower than that calculated by Szunyogh *et al* [27] for a rigid spin rotation around the (111) plane. This reduction in the energy barrier is due to meta stable spin structures, which lower the overall energy barrier [14]. Our results have resolved the discrepancy between previous experimental and theoretical results and have contributed massively to the understanding of anisotropy in AFM materials. Our results demonstrate the importance of non-collinear spin states on the thermal stability of antiferromagnets with consequences for the practical application of antiferromagnets in devices operating at elevated temperatures.

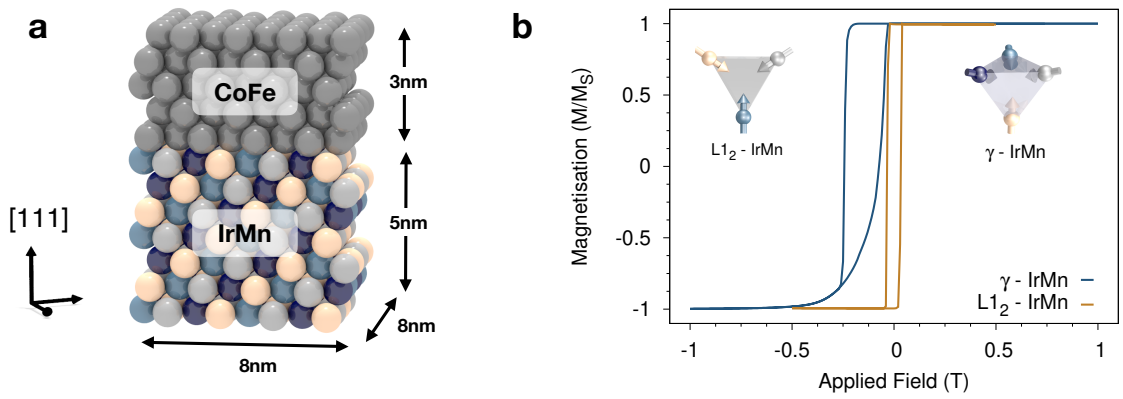

Figure 3: **Schematic representation of the bilayer and simulated hysteresis loops.** (a) Schematic representation of the IrMn/CoFe bilayers. (b) T= 0K hysteresis loops for the ordered and disordered phases of IrMn. The magnetic structures of both γ - $IrMn_3$ and $L1_2$ - $IrMn_3$ are shown within (c).

Exchange Bias

Many theoretical models have been proposed to explain the exchange bias effect [22, 6, 20]. However, previous models have all assumed that exchange bias occurs either due to domains [22] or grain boundaries in the AFM. Here I present a natural atomistic model of exchange bias applied to γ-$IrMn_3$/ CoFe bilayers, and prove that domains or grain boundaries are not necessary exchange bias to occur [16]. In fact, exchange bias can occur in a single grain with no grain boundaries, domains or interface mixing. I discover that the exchange bias comes from the underlying anti-ferromagnetic structure. Initially, only a single grain is investigated, once the underlying cause of exchange bias is found the model is extended to a more realistic multiple grain system then interface mixing and disorder is investigated.

To study the exchange bias effect, the disordered $IrMn_3$ is coupled to a FM to form a bilayer as shown in Fig. 3 (a). The direction of the exchange bias is set by a simulated field cooling process in a 0.1 T field applied along the x-direction. After cooling, the field is removed and the system relaxes to an equilibrium state. For the disordered γ-$IrMn_3$, the CoFe magnetisation tilts around 19 degrees out of the plane due to imprinting from the underlying antiferromagnetic spin structure. After the exchange bias is set, a hysteresis loop is simulated which shows an exchange bias field of $B_{\mathrm{EB}} = 0.14$ T [16]. Assuming a reduction in the exchange bias due to temperature effects, this value is close to typical experimental measurements [23]. In contrast, if the AFM is swapped with the perfectly ordered $L1_2$-$IrMn_3$/CoFe system there is no canting during the equilibration stage and the simulated hysteresis loop shows no exchange bias and very low coercivity as shown in Fig. 3 (b). These results suggest that the exchange bias therefore must come from the intrinsic ordering within the system.

To determine the cause of exchange bias, the direction and magnitude of the interface magnetisation is observed throughout the hysteresis loop in the disordered IrMn system. The interface moment of the AFM exhibits hysteretic behaviour with the same exchange bias and coercivity as the FM, the large coercivity suggest the interface has a large reversible interface moment as has been predicted experimentally [24]. It can also be observed that the AFM exhibits a small vertical shift, this vertical shift arrises due to the interface exchange field causing irreversible spins which do not rotate during the hysteresis cycle. From this, we can conclude that our interface moment is comprised of a reversible moment and an irreversible moment. The magnitude of the irreversible moment is directly proportional to the vertical shift in the hysteresis loop and it is these spins which pins the AFM magnetisation and are responsible for the shifted hysteresis loop observed in the exchange bias effect. The existence of irreversible spins is a direct output of our simulation and quantitatively correlates with the computed exchange bias field with a physically realistic magnitude. Importantly this is observed without the need for AFM grains or interface mixing. But

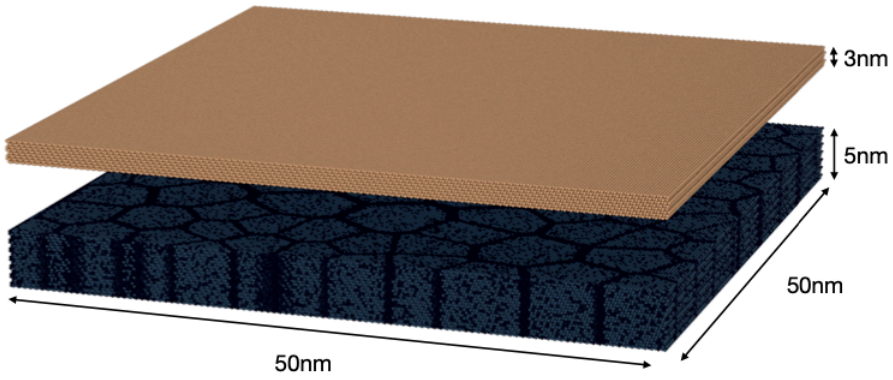

Figure 4: **Schematic diagram of the AFM/FM multigranular bilayer**

what is the nature of these uncompensated spins?
To this end we consider the nature of the atomic structure of disordered γ-$IrMn_3$ where 25% of the atoms in each sublattice are Ir. The 25% which are Ir (non magnetic) are chosen randomly using a probability function. The random nature of the removal means that although on average 25% are removed from each sublattice in reality a slightly different number will be removed from each sublattice. For an infinite grain the difference would balance out but as our grain is of a finite size the system can end up with large differences between the numbers in each sublattice. The difference leaves a net magnetic moment along the direction of the sublattice with the largest number of Mn atoms remaining. This explains the observation of exchange bias in the disordered $IrMn_3$ phase and the lack of exchange bias in the ordered phase where there is no disorder present in the system. This unexpected finding resolves one of the long standing puzzles of exchange bias and provides a route to developing optimised nanoscale antiferromagnetic spintronic devices. This is the first model of simulate exchange bias without replying on AFM domains or grain boundaries neither of which have been experimentally proven to exist.
Now we have uncovered the origin of exchange bias, the model is extended to a more realistic multigranular system comparable to realistic device sizes as shown in Fig 4 [13]. Previously, due to the large system sizes, only micromagnetic simulations have been possible, with an assumed distribution of antiferromagnetic anisotropy directions. Using the atomistic model the anisotropy directions occurs naturally and no assumptions are required. I performed large scale simulations of exchange bias containing over 1.5 million atoms. The granular structure was created using a Poisson distribution, this created a lognormal distribution of grain volumes comparable with experimental observations [1] as shown in Fig. 5 (a).
The exchange bias is simulated using the same procedure as for the single grain system, the system had a lognormal distribution of grains with a median size of 6 nm and a standard deviation of 0.37 nm. The simulation gave a realistic values of exchange bias as shown in Fig. 5 (b) as compared to experiments [23]. By varying the average grain size in the system the grain size dependence of exchange bias can be calculated. The grain size dependence shows the expected peak observed experimentally as shown in Fig. 5 (c). This peak occurs due to the competition between the superparamagnetic nature of small grains at temperature and a reduction in the statistical imbalance in the number of interfacial spins for larger grain sizes as shown in Fig. 5 (c). So far, all of the simulations have been done at 0K, realistic devices will need to use temperatures of room temperature and above, the next step was to investigate the temperature dependence of exchange bias and check that the exchange bias from the intrinsic structure holds with higher temperatures and domain walls/grain boundaries are still not necessary. The simulations show a strong temperature dependence of the exchange bias in agreement with experimental observations. At the block-

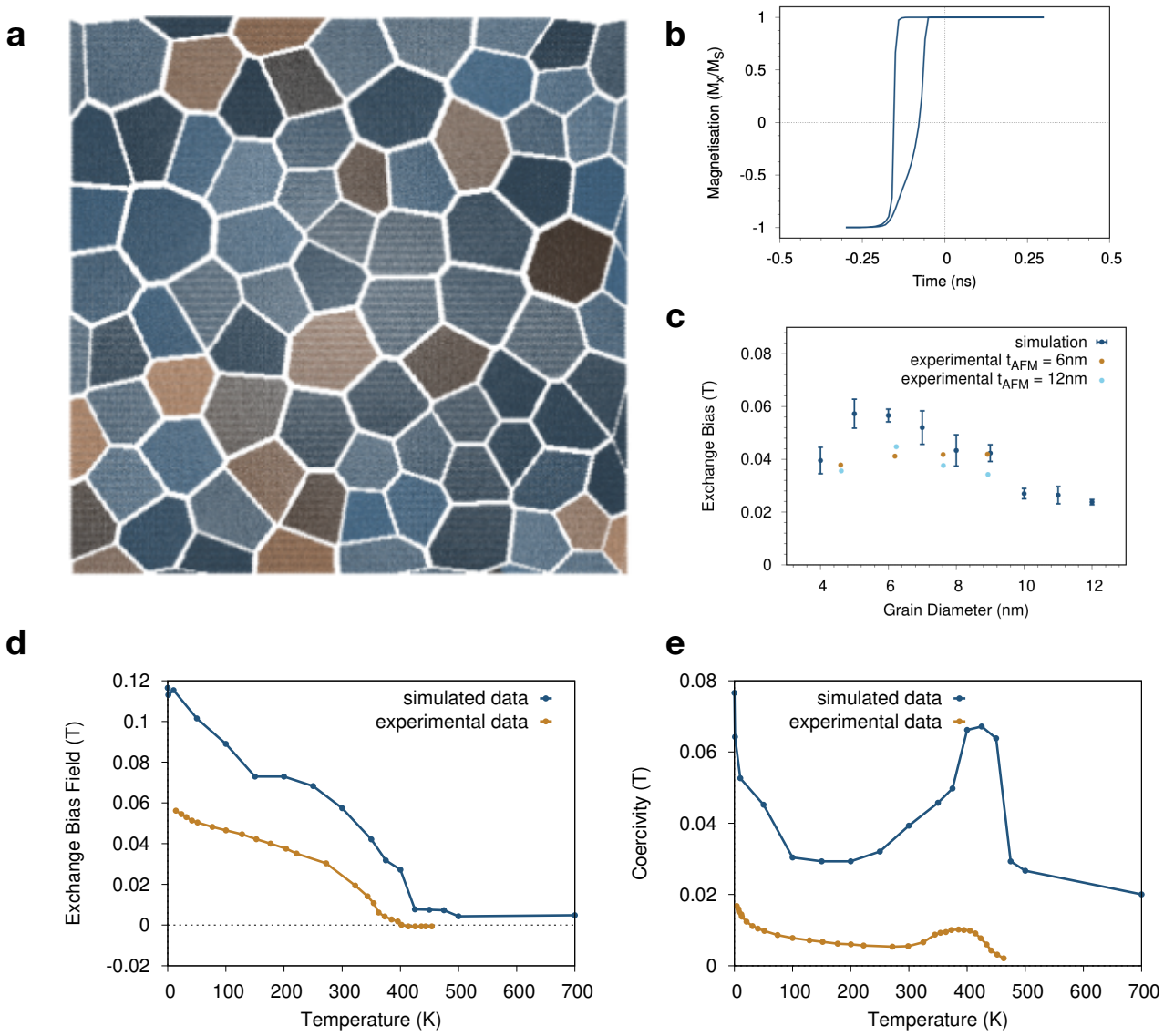

Figure 5: **Exchange Bias in multigranular systems**(a) Example simulated granular structure on the AFM. (b) Example exchange bias in a mutigranular hysteresis loop. (c) Grain size dependence of exchange bias matching the experimental observations of [23] (d) Temperature dependence of exchange bias (e) Temperature dependence of the coercivity.

ing temperature the exchange bias is observed to be zero as shown in Fig. 5 (d) as at this temperature the AFM grains can switch superparamagnetically between ground states. The coercivity, however, massively increases as shown in Fig. 5 (e). It was discovered that the increase in coercivtiy occurs due to the flipping of the antiferromagnet. The flipping of the AFM means that instead of the AFM adding a unidirectional anisotropy now it adds a uniaxial anisotropy meaning it gives exchange bias in both directions. This means that after flipping the exchange bias is now in the opposite direction and has been thermally reset during the hysteresis loop. This thermal resetting therefore causes the increase in coercivity and the system has exchange bias in both the positive and negative direction giving no net shift in the hysteresis loop.
One of the largest problems in the detection and control of the magnetisation of AFM materials is the training effect. The athermal training effect causes a large drop in the measured exchange bias after the first hysteresis loop. The origin of athermal training is still a widely disputed problem due to the difficulty

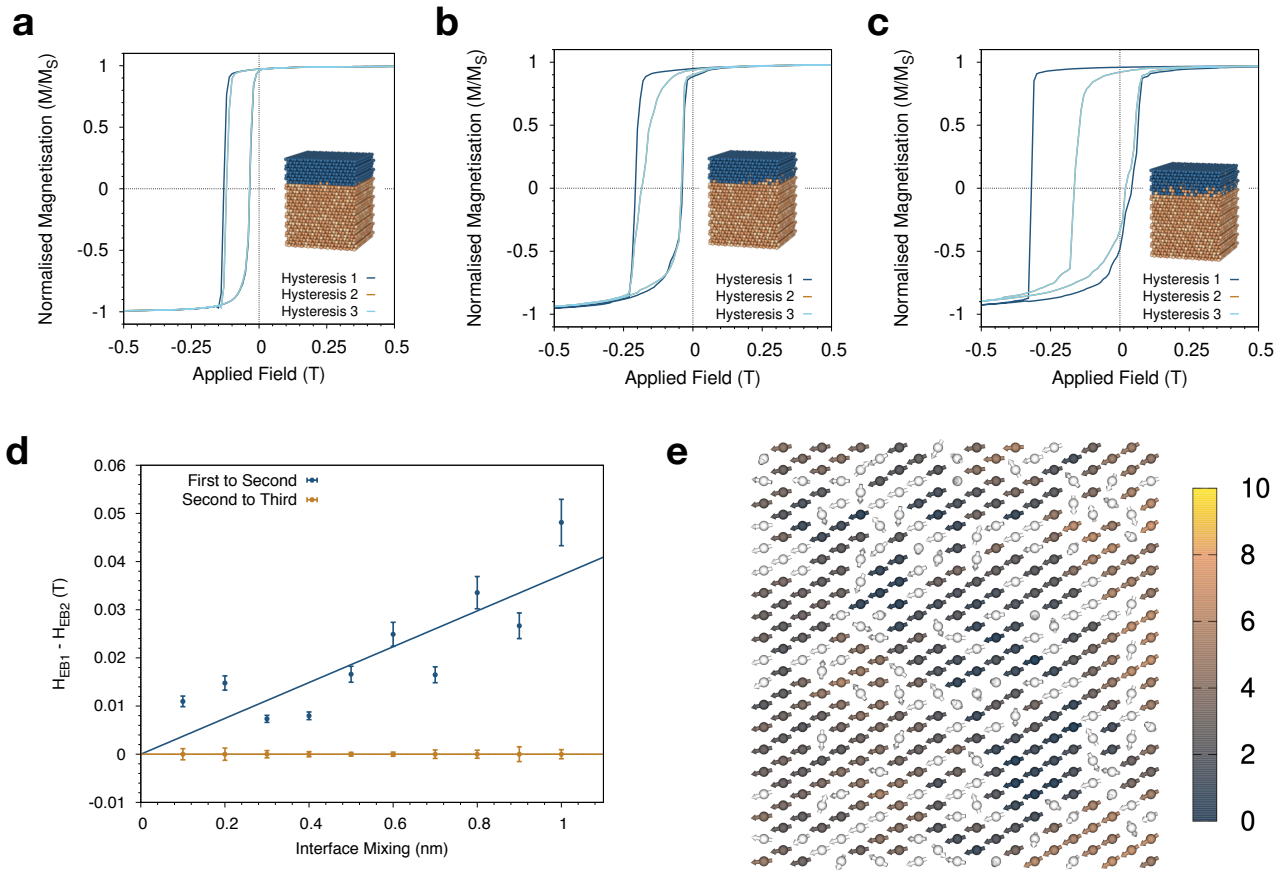

Figure 6: **The first three simulated hysteresis loops for different intermixing widths,the change in exchange bias and the average rotation of each layer of the Mn between the start and end of the first hysteresis loop.** The interface mixing widths were (a) 0.1nm, (b) 0.5nm and (c) 1nm. The insets show a subsection of the bilayer to demonstrate the level of interface mixing. (d) The change in the exchange bias between consecutive hysteresis loops, with lines of best fit to guide the eye. (e) The change in interface spin structure between the start and end of the first hysteresis for an interface mixing width of 1 nm. The change in colour shows the change in angle in degrees as shown by the scale bar on the side. The white atoms are CoFe and are always aligned with the applied field.

in experimentally probing the rearrangement of AFM spins at the interface. It has been proposed to be due to the degree of order of the AFM at the interface [4] or changes in the configuration of the antiferromagnet during the hysteresis cycle [10]. To prove this hypothesis a second hysteresis loop was simulated for the system shown in Fig. 5 (a), this has no interface disorder. In this system the first and second hysteresis loops exactly matched and therefore the athermal training effect did not occur [12]. This matches the prediction of Bitternas *et al* that the athermal training effect occurs due to disorder at the interface.

The next step was to systematically investigate the effect of the intermixing and how this affects the exchange bias and then whether the simulations show the athermal training effect. Simulations were run with interface mixing widths between 0.1 nm and 1 nm. The simulations showed that the exchange bias, coercivity and switching field all increase with increased intermixing as shown in Fig. 6 (a) (b) and (c). We can see from Fig. 6 (d) that the simulations have showed the athermal training effect and there is a large change in the exchange bias between the first and second hysteresis loops which increases with the level of interface mixing. However, no change in exchange bias is found between the second and third hysteresis loops agreeing with previous experimental measurements of low temperature systems, where

a large decrease in the exchange bias is found between the first and second measured hysteresis loops only [18]. To understand what is causing the training effect, the magnetisation in the interface layer was observed. It was found that there is a change in magnitude of the Mn interface magnetisation between the start and the end of the first hysteresis loop, this is because the interfacial spin state after the setting is highly frustrated and is in a metastable spin state. This metastable spin state leads to a large effective exchange coupling and thus large initial switching field. After the first hysteresis cycle these metastable spins drop into a reversible ground state that is repeatable for all subsequent hysteresis cycles. The change in spin configuration means that the first and second hysteresis loops will start from different interface spin structures. To quantify this change, a subsection of the interface spin structure was visualised and the change in angle from start to end of the hysteresis loop was calculated. The angles between the initial and final positions of the spins are shown in Fig. 6 (e). Our simulations provide new insights into the role of interface mixing and the importance of metastable spin structures in exchange biased systems which could help with the design an optimisation of antiferromagnetic spintronic devices.

Conclusion

AFM materials could hold the key to the creation of novel AFM spintronic devices which will give smaller, faster, devices with lower power consumption to keep up with Moore's law. This thesis focused on increasing the understanding of the technologically relevant AFM, IrMn, using an atomistic spin model. This is the first comprehensive atomistic investigation into IrMn alloys, simulated with details which are not possible using micromagnetic or current *ab-initio* approaches. The model gives results which match experimental measurements and from this more complex structures such as finite size systems and different material alloys can be studied. It is the first model of an exchange biased bilayer which does not rely on grain boundaries, impurities or AFM domains to create the exchange bias field. The highly parallel, scalable nature of VAMPIRE means that exchange bias can be simulated in systems of comparable size to those in real devices such as hard drive read heads. Details such as interface mixing and the effect of composition can be simulated and the model can be used to determine the atomistic cause of macroscopically observable effects such as exchange bias and the athermal training effect.

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Conference and Workshop reports

• The International Society of Quantum Biology and Pharmacology (ISQBP) 2021 President's Meeting

29th June – 1st July 2021 (online) - https://www.isqbp.org/events/2021-isqbp-presidents-meeting

The International Society of Quantum Biology and Pharmacology (ISQBP) 2021 President's Meeting was held from June 29 - July 1, 2021 via a virtual platform organized from Strasbourg, France.

We counted over 180 participants from all over the world, thanks to the professional services of PREMC, the meeting went off with no technical problems. The talks started at 4 pm Paris time and went until about 10 pm for the three days. Besides the talks, there was an active poster session each day that allowed young researchers to expose their work and generally interact through a virtual networking platform.

Professor Alex MacKerell from the University of Maryland (Baltimore, USA) was presented with the 2020 award in Computational Biology and gave a talk entitled 'CHARMM Additive and Drude Polarizable Force Fields: The Long and Winding Road....to....Hey Jude'. The MacKerell lab is well known for being responsible of developing and maintaining the empirical force fields used in a number of simulation packages including the program CHARMM (Chemistry at HARvard Macromolecular Mechanics). The group is also well known for developing CADD methodologies including SILCS (Site-Identification by Ligand Competitive Saturation) and CSP (Conformationally Sampled Pharmacophore).

Other speakers included Charles L. Brooks (University of Michigan, USA), Marco Cecchini (University of Strasbourg, France), Thomas E. Cheatham (University of Utah, USA), Franca Fraternali (Kings College, London, UK), William Jorgensen (Yale University, USA), Klaus Liedl (Leopold-Franzens-University Innsbruck, Austria), Adrian Mulholland (University of Bristol, UK), Lennart Nilsson (Karolinska Institutet, Sweden), Modesto Orozco (University of Barcelona, Spain), Montgomery Pettitt (University of Texas, USA), Carol Post (Purdue University, USA) and Maria Ramos (University of Porto, Portugal). They highlighted in their talks recent advances in modelling and simulation in biophysics and biochemistry.

Report kindly provided by Prof Carmen Domene

• Lessons learned in Lockdown – Joint meeting of the Higher Education Group and Computational Physics Group

14th April 2021 (online)

The Higher Education Group and the Computational Physics group ran a joint meeting on the teaching of computational physics in lockdown. The lively meeting had a maximum 40 simultaneous attendees with nearly 30 engaging in the discussions when time ran out. This one-day fully-online meetings consisted of 3 sessions, which focused on the most important issues facing teachers and educators during the pandemic:

Opportunities for dynamic delivery

In this varied session the speakers presented a wide range of technological solutions that had been used successfully to deliver teaching in a range of computing languages and with wide range of platforms. There are clearly many solutions available with different pros and cons. There were common issues with the technology available to students producing disparities in student experience. It was noted that some universities could be galvanised into action by lockdown to provide e.g. servers.

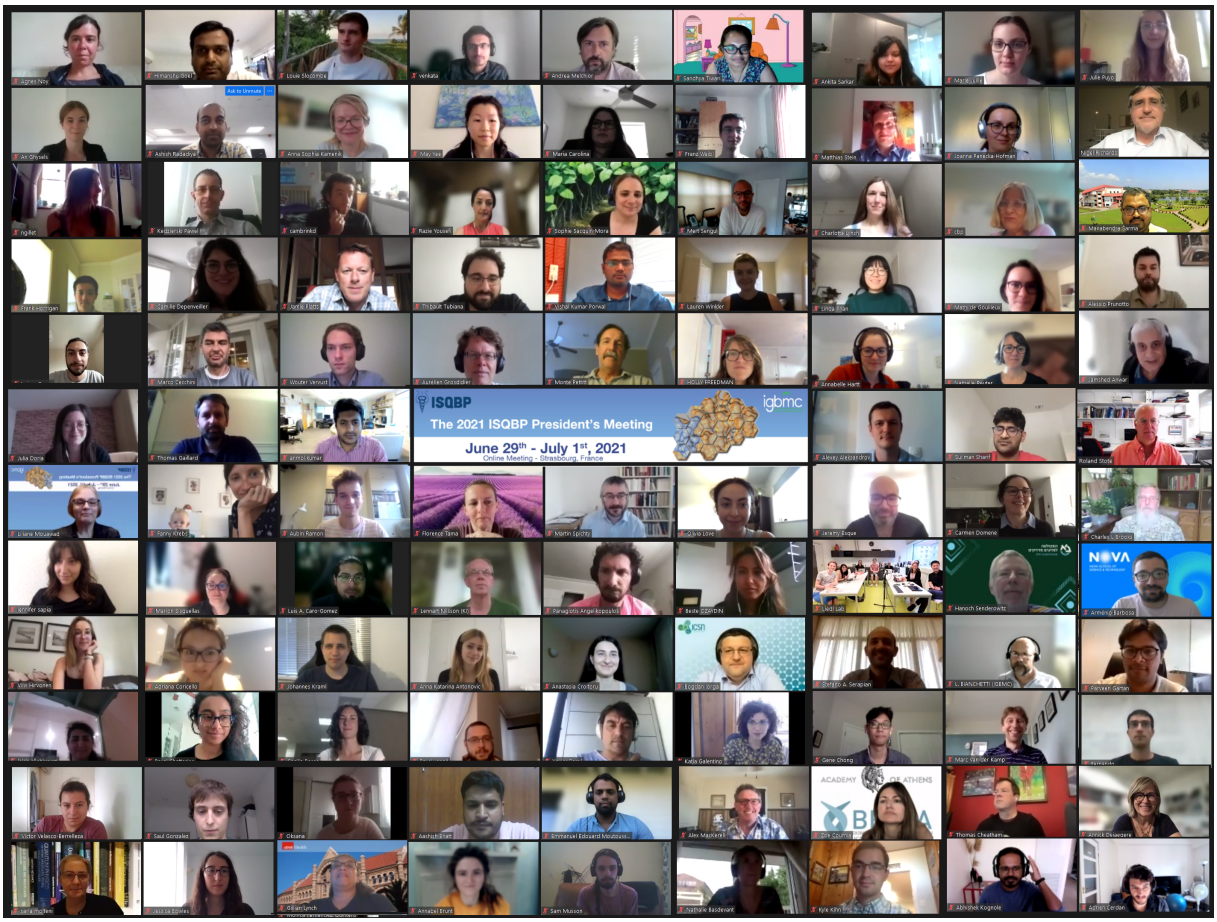

Figure 7: Attendees of the ISQBP 2021 President's Meeting.
Image courtesy of Dr. Roland Stote (IGBMC - CNRS UMR 7104 - Inserm

The first session identified common themes that reappeared during the day for example students had been presented with material in advance but had not always engaged with it, turning online sessions into delivery of teaching.

A major theme identified was the difficulty of engaging students with demonstrating online. Trying to replicate the "over the shoulder" type help is very difficult. Ideas included using gather.town which seemed to have worked well both for demonstrating and promoting interaction amongst students. Teams allowed quick switches from chatting to video calls. Polls had been introduced in one course where every hour students were polled on their progress so that demonstrators could help those in most need. In discussion it was reported that discord had been used with success.

Autograding had eased the burden of marking for large classes. This allows quick feedback, but it is difficult to make precise and unambiguous questions that are not trivial. Students tend to get perfect grades or do poorly, but it can be very useful for formative feedback.

Encouraging Engagement

Following on from the issues identified in the morning session the first half of the afternoon focused on methods to improve engagement with a study of whether providing solutions to problem on demand rather than at a fixed time made a difference to attainment. We heard about the potential for using augmented reality in teaching. We also heard how a computational project prize based on solving a challenging problem had motivated students with a lot of programming experience -even after the prize had been awarded elsewhere! Padlets for asynchronous chats had been successfully used.

We were encouraged to be honest about how coding works. To show that we do google solutions to programming problems.

A final talk in this session was on teaching physics to visual artists to get them to produce accurate representations of physical effects without maths, was illustrated by some Kurzgesagt explanations of physical phenomena – do check out the webinar recording. A 3rd year Physics class is being asked to do the same thing. It would be interesting to see the results.

Prospects for Project work

We hear an illuminating talk on the software carpentry approach to teaching computing with an important feature being I code. . . You code. This live coding in front of students, with the inevitable mistakes made by the teacher was felt have many good points including giving students permission to make mistakes themselves and was compared to the success of online gamers who attract large audiences. The course described had presented Python to postgraduate students but assumed no knowledge. Students who were experience were encouraged to act as helpers. This approach was also reported as having been successful elsewhere and solution to the variety of experience that students have in computing course.

We heard about the use of dedicated breakout rooms for students to get individual support in a 1st year computing lab project and the variety of approaches being used to take experimental work online. And as a final thought that remote teaching is likely to be in place next year at least for some students.

Discussions raised many questions and issues:

- Is there now "more computational material" because of COVID issue or is this a trend exacerbated by COVID?
- Do we understand how students interact? Discord as reported as being popular with students and has a mix of video chatting and text. Asynchronous chatting is well used and this may impact the choice or platform as in some cases chat disappears.
- We need to remember how important computation skills are using real world examples.

- Despite difficulties with engagement and technology in most courses many students have performed very well.

Report kindly provided by Dr Tyler Shendruk

• Motility in Microbes, Molecules, and Matter

6^{th} - 7^{th} December 2021, London / online

The Computational Physics Group was delighted to co-organise an interdisciplinary meeting "Motility in Microbes, Molecules, and Matter" which was held on 6-7 December 2021 in London. This event was co-organised with the Biological Physics Group and Marco Mazza (Loughborough).

Our aim was to cast together a group of physicists and biologists working on systems as different as cell motility in tissue growth and cancer, synchrony in flagellar dynamics, structural rearrangements within biofilm communities, nuclear motor proteins, and artificial microswimmers. We also decided to mix advances in experimental investigations and novel computational methods to tackle these challenging, far-from-equilibrium problems. The result was a joyful (and controlled) chaos of scientific discussion.

We had a superb selection of speakers (senior and junior) who discussed the role of motility at different length scales in both biological and artificial systems. The event hosted 90 participants (62 in person and 28 remotely) and was one of the first meetings held also in-person after the restrictions of the COVID lockdowns. Thus, it had a particularly high values for PhD students and junior postdocs who could present their results. In fact, a highlight of the 2-day meeting was the poster session, which saw lively discussions and nascent collaborations amongst Early Career Researchers. The success of the event, and the strong interest of the community in this meeting at the interface between physics and biology, theory and experiments, convinced us of the need to organise a second edition in the Autumn of 2022.

Report kindly provided by Dr Tyler Shendruk

Computational Physics Group News

- ## The Computational Physics Annual PhD Thesis Prize

  Each year, the IoP Computational Physics Group awards a Thesis Prize to the author of the PhD thesis that, in the opinion of the Committee, contributes most strongly to the advancement of computational physics.

  The winner of the 2021 Thesis Prize is Dr Sarah Jenkins for her thesis entitled *'Spin Dynamics Simulations of Iridium Manganese Alloys'*, which was undertaken at the University of York. A feature article describing her work appears in this edition of the CPG Newsletter.

  Applications are now being accepted for the 2022 Thesis Prize. Eligibility and deadline are as follows:

  – Applications are encouraged across the entire spectrum of computational physics.
  – Applicants conducted their research at an institution in the UK or Ireland.
  – The PhD examination has taken place since 1st January 2021 and up to the submission deadline.
  – **The submission deadline is 30th April 2022** (though early submissions are encouraged).

  Submission format:

  – A four page (A4) abstract, describing the background and main achievements of the work.
  – A one page (A4) citation from the PhD supervisor, including confirmation of the date of PhD examination, that the student passed and whether the thesis has also submitted to another IoP group for a PhD thesis prize.
  – A one page (A4) confidential report from the external thesis examiner.

  Entries (PDF documents preferred) and any questions relating to the Prize should be sent by email, with "IoP CPG Thesis Prize" as the subject header, to Dr Shendruk (✉ t.shendruk@ed.ac.uk).

  Further details about the thesis prize can be found on the `Group page`.

- **IoP Computational Physics Group - Research Student Conference Fund**

The Institute of Physics Computational Physics Group is pleased to invite requests for partial financial support towards the cost of attending scientific meetings relevant to the Group's scope of activity. During the pandemic, the Fund can be used to cover the costs of attending online conferences. The aim of the scheme is to help stimulate the career development of young scientists working in computational physics to become future leaders in the field.

- **Computational Physics talks series**

After the first event, which took place last year, we will be relaunching the series of talks for the members of the Computational Physics Group, in a new format. These informal, online lunchtime meetings will take place every two months and will last an hour, with 45 minutes dedicated to the talk. The remaining time will be used for questions, discussion and other social activities, as required. The meetings are designed to bring Members of our Group together, encourage discussion on the subjects of our research and foster existing and start new collaborations.
We invite the Members to submit an short abstract for a short talk about their work and research that they would like to share with other Members of our Community. We especially welcome contributions from PhD students and Early Career Researchers. Depending on the popularity and the number of abstracts we receive, the frequency of the meetings and the length of the talks may be adjusted throughout the year.

For abstract submission, any questions or suggestions, please contact Mateusz Malenta at
✉ mateusz.malenta@gmail.com

Related Newsletters and Useful Websites

The Computational Physics Group works together with other UK and overseas computational physics groups. We list their newsletter locations and other useful websites here:

- Newsletter of the Computational Physics Division of the American Physical Society:
  `www.aps.org/units/dcomp/newsletters/index.cfm`
- Europhysicsnews newsletter of the European Physical Society (EPS):
  `www.europhysicsnews.org/`
- Computational Physics Group blog (CPG):
  `www.compphysics.org`