The importance of applying computational creativity to scientific and mathematical domains Paper type: Position Paper

Abstract

Science and mathematics are currently vastly underrepresented in the computational creativity (CC) community. This is at best a wasted opportunity, and at worst a significant problem for computational creativity. We discuss why the CC community should apply their work to scientific and mathematical domains, and argue that this would be mutually beneficial for the domains in question, demonstrating our position throughout the paper by reference to mathematics and geology. We propose a research programme for building closer relationships between CC and the scientific community, focusing on understandability of science and the role that AI is currently playing in scientific research.

Introduction

Despite the best efforts of successive ICCC organising committees and the computational creativity (CC) community, CC has always attracted substantially more interest from researchers in artistic than scientific and mathematical domains. In their 2017 study of application domains in CC, (Loughran and O'Neill 2017) found that, of 16 categories, papers on Maths, Science and Logic accounted for only 3% of the 353 papers on CC across 12 years. Of course, some work is domain independent, or at least not easily assigned to an academic discipline, such as the body of work on CC and curiosity (for instance (Grace et al. 2017)). Even taking this into account, it is clear that science and mathematics are vastly under-represented in our community.

There are potentially many reasons why this may be the case. Firstly, AI researchers in scientific domains may well be doing creativity-related work in other contexts but not engaging with the CC community. Automated reasoning and automated scientific discovery are both thriving subfields of AI, with internationally recognised journals as outlets for publication and engagement; certainly these will contain work relevant to our field but couched in different terminology with different methodologies. Secondly, it may be that other, practical, priorities in scientific domains have led to a focus on techniques such as search, data-mining and automated deduction. Since these generate results of interest to domain experts, the more difficult, fluid and tenuous concept of creativity may be seen as unnecessary, risky or simply not a priority. This may particularly be the case given the

various "AI winters" in the twentieth century (the second of which ended in 1993, just six years before the first workshop on CC), and the need for AI to "prove itself". Thirdly, CC researchers may consider that even if generation is possible within scientific domains, evaluation is too difficult. How we should evaluate our work and our systems has always been a contentious – albeit important – issue in CC, with few proposed evaluation metrics and the majority of researchers still arguing for value along the lines of "we/people liked the system's output" or "we/people couldn't distinguish the system's output from human produced work". It might be the case that in science, the main evaluation metric – "is it true?", or "does it work?" – is considered simply too expensive or difficult to demonstrate.

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We argue here that neglecting scientific and mathematics domains in CC is at best a wasted opportunity, and at 66 worst a significant problem for CC. While computationallyproduced work in the arts is currently novel, this may have a limited lifespan. We call this the *Saturation Problem*. In ten or twenty years, people may ask themselves whether we still want more computer-generated paintings or poems. There may or may not be a good answer to this. The question as to whether we still want more computer-generated science or mathematics, however, seems less likely to be asked: we always want more science and mathematics. We believe that it is essential to the health of our field that we reach out as a community at this stage, both to domain experts in science and maths and to those in related AI areas. The benefits of doing so will go both ways. As AI is used more and more in science, there is greater dependence on blackbox machine learning systems. While providing greater predictive power, this often comes at the cost of understanding. Que We call this the *Understandability Problem* and argue that it will become a big issue in science, which we will have to address. Twenty years of thinking about computational creativity has provided us with valuable tools for thinking about these problems. This paper is a call to arms to CC researchers to apply their work to science, thus solving both the saturation problem and the understandability problem.

Loughran and O'Neill argue that "tackling scientific, logical or realistic issues could help bring the reputation of CC away from a purely aesthetic domain towards developing solutions for real world problems." (Loughran and O'Neill 2017, p.7) and that "It is imperative that the field remains

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Congos cethod Filds this Congos other hove done this Materiation? balanced as it grows and that we remember to reflect on all areas of growth." [Ibid.]. In this paper we support and present further arguments for this position, alongside practical recommendations for doing so.

What is science?

The concept of science is not a straightforward one. The division of the origins of learning and systematic production of new knowledge into disciplines as we know them tends to takes into account at least some of the following: methodologies, objects of study (which can be shared with other disciplines), a body of accumulated knowledge (which is generally not shared with other disciplines), theories and concepts, terminology and an institutional manifesto (so that it can reproduce itself) (Krishnan 2009, p9). Sciences include Natural sciences, which are subdivided into physical sciences (chemistry, physics, astronomy), life sciences, or biology (zoology, botany, ecology, genetics) and earth science (geology, oceanography, meteorology, palaeontology); Social sciences (psychology, sociology, economics, law, political science); Formal sciences (mathematics, logic, theoretical computer science, statistics); and Applied sciences, which are subdivided into engineering (computer science, civil engineering, electrical engineering, mechanical engineering); health sciences (medicine, dentistry, pharmacy) and agriculture. The number and variety of sciences makes generalisations difficult, and core values vary accordingly. However, values commonly associated in particular with the (rather unhelpfully named) "hard sciences" include repeatability, reproducibility, predictability, generality and understandability. This last value is particularly cherished: for instance, Roger G. Newton sums it up as "The primary aim of most physical scientists is to understand and explain the workings of Nature." (Newton 2000, p. 4).

The arts are just as difficult to define. These are sometimes divided into the "seven arts": Architecture, Sculpture, Painting, Literature, Music, Performing, and Film. Julie Van Camp, writing in the context of United States Congressional policy on arts education, provides the following extensional definition:

The term 'the arts' includes, but is not limited to, music (instrumental and vocal), dance, drama, folk art, creative writing, architecture and allied fields, painting, sculpture, photography, graphic and craft arts, industrial design, costume and fashion design, motion pictures, television, radio, film, video, tape and sound recording, the arts related to the presentation, performance, execution, and exhibition of such major art forms, all those traditional arts practiced by the diverse peoples of this country. (sic) and the study and application of the arts to the human environment.²

	Science	Arts
Aesthetic:	truth	beauty
Approach:	problem-driven	artefact-driven
Task:	analytic	generative
Terminology:	discover	create
Status:	objective	subjective
Goal:	knowledge	self-expression

Table 1: Possible differences between the sciences and the arts

As a starting point – generalising (and controversially) – we could suggest some of the differences between the sciences and the arts as shown in Table 1. Of course, the real-world everyday lived experience of doing science or doing art is far more complex than Table 1 would suggest. Studies of interpretations of seismic data in geology, for instance, show the large number of different expert interpretations of the same seismic section, highlighting the subjectivity involved (Bond et al. 2007). These interpretations are used to analyse subsurface geology, and form the basis for many exploration and extraction decisions. Even in cases where interpreters report that an interpretation is relatively straightforward, there are significant differences in interpretation, leading to significantly different predictions, for instance about gross pore volume in a pool or gross you rock volume (Rankey 2003). While clearly objectivity is to see the second secon the goal here, such studies may suggest that this aspect of geological practice is closer to visual art interpretation than it is to some other scientific domains. Similarly, studies of the back stage production of mathematics show that beauty is often a guiding value (Inglis and Aberdein 2015); there is a high level of disagreement amongst experts about the validity of certain proofs (Inglis et al. 2013); and proofs and theories are often considered to be constructed rather than discovered (Lakatos 1976). Less structured knowledge such as our ability to reason logically has been shown to be highly context dependent (for instance, participants in the Wason Selection Task were unable to solve a problem at an abstract level but could solve it correctly when it was framed in a familiar context (Wason and Shapiro 1971)); constructing grounding metaphors to the physical world and abstract linking metaphors found to be fundamental to our understanding and construction of mathematical knowledge (Lakoff and Núñez 2000); and even the language in which reasoning occurs affecting our preconceptions, perceptions and assumptions (Dehaene et al. 2008; Barton 2009).

Dibbets expresses the relationship between arts and sciences well:

But in the end, we all do very much of the same. All scientists, artists, composers and writers are intensively occupied imagining something that does not yet exist. They find themselves at the borders of areas where up to then hardly anyone found himself, trying to solve problems that are incomprehensible to others, trying to answer questions no one has ever asked. Here, they

 $^{^{1}}A$ visualisation of the fields of knowl-Wikipedia's of disbased on list academic edge ciplines sub-disciplines be found and can here: http://www.thingsmadethinkable.com/item/fields_of_knowledge.php ²http://web.csulb.edu/jvancamp/361_r8.html

share a vision on things that are not yet real. (Dibbets 2002, p. 1)

Some of these interdisciplinary features are recognised in curriculum design and teaching featuring transferable skills, in which one skill may be learned within a scientific context and developed or employed in an arts context, or vice versa (see for instance (Gaff and Ratcliff 1996)). Indeed, the STEM to STEAM movement (expanding the acronym Science, Technology, Engineering, and Mathematical disciplines to include Art) explores the role of arts integration, collaboration, and experience centered learning in knowledge creation (Ghanbari 2015). Of course, the need for so many interdisciplinary initiatives (and related concepts such as transdisciplinarity, pluridisciplinarity, and multidisciplinarity) may suggest that some traditional discipline boundaries are no longer drawn in a helpful way. The evolving role and functionality of AI systems further complicates things. The focus of AI researchers, particularly in machine learning, is often on the skills they hope to simulate rather than a particular domain in which they are usually employed. This may be more a more productive approach than the typical CC focus on domain over skill.

The Saturation Problem in Computational Creativity

The saturation problem in CC is potentially an identity problem for us. Recent developments in other areas of AI – principally machine learning (ML) – have led to astonishingly rapid progress in generative processes. Research in Constructive Machine Learning has led to impressive generative results in both the arts and sciences, including painting, music, poetry, gaming, drug design, and gene design – usually in collaboration with domain experts. Our concern is that the sheer size and combined resources of the ML community may render generative work in CC untenable.

CC has long been seen as more than "mere generation"³, with many other aspects of the creative act modelled, in particular aesthetic judgements, but also (more controversially) the importance of framing information and meta-level processes. As generative results in other areas of AI become more sophisticated, we may need to focus on these other aspects of the creative act. However, even with this in mind, we are concerned that the arts domains *may* reach a saturation point for CC: as the novelty and backstory of computergenerated art grows old, society may question whether and why we want more computer-produced artistic artefacts. In order to keep the field alive, we propose that as well as focusing on other aspects of creativity, we find other application domains.

The Understandability Problem in Science

Roger Newton's quote above about the primary aim of physical scientists being to understand and explain nature is uncontroversial, but difficult to unpack. Ever since the entirety

of our collective scientific knowledge became too big for a single polymath to comprehend, we have had to outsource our understanding to others. The institutionalised ways in which trust of others' understanding and progress is handled started with the early universities, and developed with the invention of the printing press, academic journals, the peer review process and so on. Knowledge and understanding is a social process, as argued in (Martin and Pease 2013), but even in the human-only case this gets complicated. The longest proof in history, of the Classification of finite simple groups, is over 10,000 pages, spread across 500 or so journal articles, by over 100 different authors from around the world, and took 110 years to complete. What does understanding mean here? Perhaps a handful of people understand the proof in its entirety, and when they die it is not obvious that any single person will ever again understand the entire proof (in part because it may be replaced with a simpler proof).

Shinichi Mochizuki's 500-page proof in 2012 of the abc conjecture provides another perspective on the importance of understanding in mathematics. The abc conjecture, proposed in 1985, on relationships between prime numbers, is considered to be one of the most important conjectures in number theory (more significant than Fermats Last Theorem - in fact Fermats Last Theorem would be a corollary of the proof). A proof would be "one of the most astounding achievements of mathematics of the twenty-first century. [Goldfeld, in (Ball 2012)]. Mochizuki has a good track record as a mathematician, having proved "extremely deep" theorems in the past [Conrad in (Ball 2012)]. The problem is that the techniques and mathematical objects which Mochizuki has developed to use in his proof are so strange and new that it would take a reviewer or mathematical colleague most of their career to understand them, before they were able to understand and verify the proof. Despite some efforts from Mochizuki and a handful of his followers to make his work accessible, currently his proof is neither published nor accepted by mainstream mathematicians, for the simple reason that they don't understand it.

Crowd-sourced mathematics, in which open conjectures are solved collaboratively via online fora (amongst other things), has been used for around ten years now by a subset of the mathematical community as a new way of producing mathematics through collaboration and sharing (Gowers and Nielsen 2009). Neilsen argues that this has resulted in "amplifying collective intelligence" in his book *Reinventing Discovery* (Nielsen 2011). It has certainly resulted in some original and significant new proofs. Here it is perfectly possible (in fact it would be surprising if it were not the case) for a person to be a co-author but not fully understand the proof in their paper.

Adding computers to the social process, to form a combination of people, computers, and mathematical archives to create and apply mathematics – a "mathematics social machine" (Martin and Pease 2013) – further complicates matters. *Automated theorem proving* is the task of deciding whether a given formal statement follows from a given set of premises (Sutcliffe and Suttner 2001). The least informative approaches, algorithms based on the *resolution* rule (Robin-

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³The slogan at the 2012 ICCC conference was "scoffing at mere generation for more than a decade." - although this has been challenged, for instance by (Ventura 2016))

son and others 1965), produce merely a "yes", "no" or "unknown" response. Not only is this devoid of *explanation*, but it also hides the effects of any bugs; requiring the user to either trust the results, or verify the implementation.

Both of these issues can be mitigated by having the system instead generate a *proof object*: a formal argument for *why* a given statement follows or does not follow. Once generated, a proof object's validity can be checked without requiring any knowledge of how it was created, thus avoiding the need to trust or verify the (potentially complicated) search and generation procedures. The *de Bruijn criterion* (Barendregt and Wiedijk 2005) describes theorem provers which produce proof objects that are trivial to check by independent *proof checker* programs (which are themselves easily verified, due to their simplicity); examples are Coq (Barras et al. 1997) and Isabelle (Nipkow, Paulson, and Wenzel 2002).

Proof objects are not a complete solution to understandability, since they can still be quite inscrutable to human users. This often depends on how closely the chosen formal system is able to encode the user's ideas: for example, the formal proof of the Kepler Conjecture was performed using a system of Higher Order Logic (HOL) (Hales et al. 2015) whose proof objects (natural-deduction style derivations), whilst tedious, are in principle understandable to a user experienced with both the software and problem domain. The same cannot be said of the Boolean Pythagorean Triples problem, a statement of Ramsey theory involving the structure of the natural numbers. Rather than taking a high-level approach like HOL, the authors of (Heule, Kullmann, and Marek 2016) analysed sets $\{0..n\}$ for larger and larger n, encoding these restricted versions of the problem into the language of boolean satisfiability (SAT), and found that the problem is unsatisfiable for n = 7825, and hence for the natural numbers as a whole. In this case, the proof object demonstrates this unsatisfiability using 200 terabytes of propositional logic clauses (compressable to 68 gigabytes). Not only is this far too much for any human to comprehend, but the concepts used in the proof (boolean formulae) are several layers removed from the actual problem statement (natural numbers, subsets and pythagorean triples).

Whilst "low level" formalisms like SAT are less understandable or explanatory for users, they are far more amenable to automation than more expressive logics. Despite the proof for the Boolean Pythagorean Triples problem being many orders of magnitude larger than that of the Kepler Conjecture, the latter is well beyond the ability of today's automated theorem provers due to its encoding in HOL. Instead, it took 22 collaborators 9 years just to formalise the proof (Hales had previously produced a less formal proof, hundreds of pages long and accompanied by unverified software; yet another reminder that humangenerated artefacts are not necessarily understandable either).

The situation is even worse in automated scientific discovery. The widespread use of *machine learning* (ML) to find patterns in scientific data has been criticised by Genevera Allen in her recent talk at the 2019 Annual Meeting of the American Association for the Advancement of Science

(AAAS)⁴. She highlighted accuracy and reproducibility issues with scientific discoveries made by machine-learning techniques. Understandability is another huge problem with such discoveries; often with a tradeoff between the generality of an approach and how easily its resulting behaviour can be understood. The understandability problem concerns this last issue.

Proposed solutions

Here we propose three different approaches that the CC community can take to address the understandability problem. Each approach, at the same time, would solve the saturation problem, by focusing on science. We end each subsection with a concrete recommendation towards a new Research Programme in CC.

The "human-like computing" approach

Human-like computing research is a research programme developed for a UK funding initiative by the Engineering and Physical Sciences Research Council. This programme "aims to endow machines with human-like perceptual, reasoning and learning abilities, which support collaboration and communication with human beings.", with one of the stated motivations to "inspire new forms of computation based on human cognition, especially on tasks where humans currently exhibit superior abilities."

We believe that a focus on more human-like computing would result in systems whose output more closely resembled human produced work. If this were the case, then we hypothesise that there would be greater understandability. In the context of science and mathematics, there is much theoretical work on how people work in these domains and how knowledge is constructed. For instance, the philosophy of informal mathematics and the study of mathematical practice and cultures are thriving communities with annual research events and a good number of published books and papers. We can build on this work by building human-like computing systems which model theoretical findings.

The CC community is particularly well equipped to work in this research programme. The FACE evaluation model (Colton, Pease, and Charnley 2011) is based on the multiple aspects involved in the human creative act, including aesthetic judgements, concept development, framing information and meta-level processes which can generate, for instance, the means by which an artefact is generated. This might be reflected in automated theory formation approaches to Automated Reasoning, which consider a far wider view of mathematical knowledge production than the traditional narrow focus of Automated Theorem Proving, including the automatic generation and evaluation of new conjectures, concepts, examples explanations, and so on (see (Pease, Colton, and Charnley 2013) for an example). In some ways, given the closeness of some (aspects of some) sciences to artistic domains, this may be low hanging fruit

⁴https://eurekalert.org/pub_releases/2019-02/rucwt021119.php

⁵https://epsrc.ukri.org/newsevents/pubs/human-like-computing-strategy-roadmap/

for system developers to apply their systems to scientific and mathematical domains.

Recommendation 1: Apply your system to scientific domains.

The "Framing" approach

Enhancing software with explanatory functionality would also help to mitigate the understandability problem. The "F" from the FACE model stands for *Framing*, and we advocate a dual-approach of software generating framing information alongside an artefact, problem solution or new data pattern. We foresee this being an increasingly important area of research in CC, with an increasing level of sophistication, from explanation to justification to argument and dialogue with a user about the value, method of production, motivation etc behind the output.

Many ML approaches can be characterised as constructing a computer program (or "model") consisting of two parts: an overall structure or architecture, which remains fixed; and a set of adjustable parameters, which are inferred or "learned" from data (e.g. training data of desired input/output examples). One particularly simple architecture is the decision tree: nested boolean queries of the input, often used for classification (Safavian and Landgrebe 1991). These queries are parameters, and are chosen based on how efficiently they separate the classes given in the training data. Decision trees are nominally understandable, since their behaviour on a given input traces a single path through these queries; yet they perform poorly compared to other ML algorithms. The random forest approach yields better results by combining many decision trees and having them vote on the overall outcome (Breiman 2001), although such ensemble behaviour is more difficult to reason about than that of a single tree.

Recent research has focused on highly expressive classes of models such as differentiable programming (Wang et al. 2018), whose architectures output not only a (numerical) answer, but also partial derivatives with respect to the parameters; and probabilistic programming, which samples from a distribution conditioned on the training data. Both frameworks allow arbitrary architectures, specified via Turing-complete languages, and provide efficient, composable methods for optimising the parameters (e.g. Stochastic Gradient Descent and Markov Chain Monte Carlo, respectively) to minimise arbitrary loss functions (e.g. the squared output error on a training data set).

With such expressive formalisms, the conflict between the generality of a model and its understandability becomes clear. Task-specific architectures require fewer parameters than general-purpose approaches and perform well with little training data, for example hand-written characters can be classified based on a single example if we allow our model to assume the given images are generated by pen strokes (Lake, Salakhutdinov, and Tenenbaum 2015). Likewise we can infer parameters of a 3D scene (such as object position and lighting) from images if we embed a ray-tracer into our model (Li et al. 2018); embedding a physics engine can provide predictions about these scenes, which are useful e.g.

for robot controllers (Degrave et al. 2016).

The parameters of such programs are easily understood: they describe the pen strokes, geometric and physical properties of the simulated system, inferred from the given images. However, such specificity makes these implementations unsuitable for anything else. The choice of such highlevel, task-specific components is performed by the user, and encodes some of their domain knowledge into the structure of the solution, such that it doesn't have to be learned. This is similar to how logics like HOL can directly represent high-level concepts (e.g. natural numbers and sets) but whose proof methods have limited reusability due to the difficulty of automating such high-level reasoning.

At the other end of the spectrum we have differentiable programs with general purpose architectures, like *neural networks* (capable of universal function approximation (Funahashi 1989)). These are compositions of a large number of identical sub-expressions ("neurons"), whose parameters ("weights") scale the input values, and hence the contribution of each sub-expression to the whole. Such architectures encode essentially no domain knowledge, requiring much larger training sets than task-specific algorithms in order to "learn" these details. The behaviour of general purpose models depends so heavily on their (many) parameters, that understanding their behaviour becomes difficult and they are often treated as inscrutable "black boxes"; akin to the large (un)SAT proof described above.

Full generality is seldom required: even if we don't want to constrain a model's internal operation, the input and output data formats will always be known. Such knowledge can be encoded in the architecture through the use of *convolutional layers*, for example forcing a 2D grid structure when dealing with images (Krizhevsky, Sutskever, and Hinton 2012). Introducing task-specific components like this can aid in understanding the resulting models, since they are constrained to operate on 2D patches of image content (like shapes or textures), rather than potentially arbitrary numerical relationships between pixels.

Understanding exactly how these programs make their decisions is an active area of research, known as explainable artificial intelligence (XAI) (Došilović, Brčić, and Hlupić 2018; Doshi-Velez and Kim 2017; Molnar 2018), with popular approaches such as saliency maps (Simonyan, Vedaldi, and Zisserman 2013) tending to reverse-engineer the factors which lead to a model's decisions (judging the saliency of each pixel based on how strongly it would effect the output prediction if adjusted). These methods appear intuitive, e.g. producing visualisations highlighting a particular object in a scene as the reason for its classification; akin to the proof objects emitted by theorem provers. Yet this can obscure the difficulty of interpreting such high-dimensional decision boundaries. In particular, these explanations or justifications can be fundamentally altered by imperceptible adjustments to the input (Ghorbani, Abid, and Zou 2017). Similar adjustments can also change a model's output, leading to the field of adversarial machine learning (Goodfellow, Shlens, and Szegedy 2014); adjustments to even a single pixel can not only cause a system to mislabel an input, but to give high confidence to its erroneous result (Su, Vargas, and Sakurai

interesting, Com i set this ? 2019). Such fragility and opaqueness has important implications as these techniques begin to have decision making applications in life-critical domains such as automotive control (Bojarski et al. 2016) and medical diagnosis (Esteva et al. 2017).

Recommendation 2: Enhance your system with framing capabilities.

The "forgoing understandability" approach

It may be the case that, given the increase in power, generality and predictiveness that ML approaches give, we decide to forgo understandability in science. As a community we would be in a unique position to develop thinking on this, and to answer questions such as whether we should try to replace understandability with something else. Previous work such as (Colton et al. 2015) identifies stakeholder groups in CC research and practice: this can be extended to scientists and mathematicians to ensure that we develop in directions which will be fruitful and useful to society.

Recommendation 3: Produce philosophical work on what computational creativity should mean, and what science done with computers should entail.

Concluding Remarks

Deep learning and ML are making inroads everywhere: generative arts, processors, windfarms, Go, machine vision, and so on, and we need to consider as a community where this leaves us. Our suggestion in this paper is to focus on science and mathematics, where we have much to contribute.

Of course, both science and CC are fluid disciplines and will evolve as technology and culture change. One possible solution to the problems described here would be to adapt our view of what is valuable, and what is an artefact. For instance, could a neural network itself be considered to be a scientific discovery? It may be that AI systems become objects of study in the same way as the human brain is currently an object of study, with methods and approaches from neural science, psychology, cognitive science and so on employed to understand an AI system and its behaviour and interactions.

People are not naturally good at science. The history of science and scientific methodology, the length of time it takes to train a scientist and the high number of published research findings in science which are considered to be false or sub-standard⁶ all hint at the difficulty of the scientific enterprise. This is partially due to political and institutional factors such as pressure to publish, conflicts of interest and a culture which is often more competitive than collaborative; but also partially due to the constant battle to avoid the large number of cognitive biases that adversely affect our reasoning and judgements (Haselton, Nettle, and Andrews 2005; Sutherland 2013). On the other hand, the arts – while also

difficult to do well – do not usually go against our natural way of thinking, and can be seen as a celebration of our humanity. In many ways science should be an obvious application domain for computational creativity. This paper is a call to arms for the whole CC community, to apply their systems to scientific and mathematical domains, to enhance their systems with framing functionality, and to produce philosophical work on new directions in our field.

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