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Prospects for mathematical crystallography[1]

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The potential of mathematical crystallography as an emerging field is examined from a sociological point of view. Mathematical crystallography is unusual as an emerging field as it is also an old field, albeit scattered, with evidence of continued substantial activity. But its situation is similar to that of an emerging field, so we analyse it as such. Comparisons with past emergent efforts suggest that a new field can grow if given an economic demand for its product and a receptive environment. Developing a field entails developing a sense of identity, developing infrastructure and recruiting practitioners.

1. What is mathematical crystallography?

It is a commentary on the state of mathematical crystallography that we should start by attempting to determine what 'mathematical crystallography' is. Unlike mathematics (whose subject has been a major topic of philosophical debate for over two millennia) and crystallography (whose subject seems well defined despite cataloguing questions about topics like quasicrystals and periodic structures of fewer than three dimensions), the subject of mathematical crystallography itself seems uncertain.

This is ultimately a sociological issue, but the most readily available data lie in information science. We look at two catalogues, the Library of Congress (which helpfully has a section labelled 'geometrical and mathematical crystallography') and zbMATH (which does not). We find that the two catalogues give two quite different pictures of the field, suggesting that an inclusive notion of 'mathematical crystallography' will incorporate more than one community, and possibly several.

En route, we will encounter evidence that while a somewhat central community of practitioners has a relatively coherent view of the subject, much activity in what we might call *mathematics for crystallography* is not captured by that coherent view.

1.1. Mathematical crystallography as a self-identified field

In the Library of Congress system,[2] chemistry occupies QD 1–999, crystallography occupies QD 901–999 and mathematical crystallography occupies QD 911–919. The complete list of Library of Congress codes for mathematical crystallography, and the number of works actually in the Library of Congress, are listed in Table 1; almost all mathematical crystallography books are listed under QD 911, General Works.

It may be more useful to look at what individual authors call 'mathematical crystallography'. In his seminal – or perhaps more accurately, Promethean – work, Harold Hilton (1903) wrote that 'the object of this book is to collect for the use of English readers those results of the mathematical theory of crystallography which are not yet proved in the modern textbooks on that subject in the English language'. Notice that he was not attempting to define a field; he was merely providing access to it for researchers unfamiliar with German. The book is divided into point groups and space groups, although there is a brief mention of a model of crystal growth.

One could undertake a survey of works published, or a survey of views of practitioners, to get a comprehensive description of the field. But for now, a superficial gist may be obtained by reviewing a biased sample of books available at the University of South Florida (Tampa) library (and one other book, Schwarzenberger, 1980). Here, the QD 911 section appears to contain three kinds of truly general works. There are books primarily in geometric crystallography, which we could define as crystallographic groups and combinatorial structures – the latter being discrete sets of points, graphs and complexes, patterns and tilings – used to model crystals. These are books like Altmann (1977), Boisen & Gibbs (1985), Brown *et al.* (1978), Buerger (1971), Engel (1986), Hilton (1903), Jaswon (1965), O'Keeffe & Hyde (1996), Schwarzenberger (1980), Sunada (2013), Wells (1977) and Whittaker (1985). Then there are books on crystal structure determination, which we could regard as the extension of geometric crystallography to include diffraction analysis. These are books like Giacovazzo (2002), Hauptman (1972), Julian (2008), Kitaigorodskii (1961), Prince (1994), Rollett (1965) and Shmueli (2007). And there are books on physical properties arising from (deducible from) these structures, like Nowick (1996) and Wooster (1973). In addition, there are specialized works, and books on ancillary subjects such as quasicrystals and

[1] This article forms part of a special issue dedicated to mathematical crystallography, which will be published as a virtual special issue of the journal in 2014.

[2] The primary competitor for the Library of Congress system is the Dewey Decimal System, whose schedule includes 500 Natural Sciences & Mathematics > 540 Chemistry > 548 Crystallography > 548.0151 Mathematical Principles and 548.7 Mathematical Crystallography. We will use the Library of Congress in this article in order to count titles more readily.

Table 1
The Library of Congress classification codes for 'Geometrical and mathematical crystallography' as of 2009 (Library of Congress, 2009), and the number of items in the Library of Congress under those codes as of 30 July 2013, according to their online catalogue.

Code	Description	No. of items	Comments
QD 911	General works	234	Items on geometric crystallography (including aperiodicity), supporting theory, tables, methods and software
QD 912	Fundamental systems; including tetragonal, orthorhombic, monoclinic systems	1	One book published in 1971
QD 913	Diagrams	16	Books of tables and diagrams published between 1866 and 1973, inclusive
QD 915	Goniometric measurements	4	All published between 1825 and 1934, inclusive
QD 919	Statistical methods	1	One book published in 1995

colour groups. These are books like Jawson & Rose (1982), Patera (1998) and Senechal (1995). So what do these books have to say about their subject?

Many of these books began with statements by the authors on the nature of the field or the intent of the book. Starting with geometric crystallography, Altmann (1977) wrote that 'This is an applied group theory book', while Boisen & Gibbs (1985) are more specific about their two goals: 'The first is to derive the 32 crystallographic point groups, the 14 Bravais lattice groups and the 230 space groups. The second is to develop the mathematical tools necessary for these derivations . . . '. Engel (1986) stated that mathematical crystallography has 'found increasing interest' during the previous decade, with '[s]ignificant results . . . obtained by algebraic, geometric and group theoretic methods'. O'Keeffe & Hyde (1996) focused on how the atoms of a crystal are arranged in space, which requires 'learning the methods appropriate for describing infinite periodic objects', in particular, point and space symmetry groups and 'simple geometric patterns that underlie crystal structures', *i.e.* 'polyhedra, . . . , plane patterns, . . . , sphere packings, cylinder packings, nets, . . . '.

Sampling from our examples among the books focusing on crystal structure determination, Julian (2008) took a position similar to that of O'Keeffe & Hyde: 'Crystallography is the science of finding the locations of atoms in crystals', and the goal of the text is '. . . understanding not only how atoms are arranged in crystals but also how crystal systems are related to each other'. Prince (1994) had different criteria for inclusion: 'Either they are things that I have had to learn, or look up frequently because I didn't use them enough to retain the details in ready memory, or they are things that I have frequently explained to other colleagues'; one could describe the topics in Prince's text as matrices, symmetries of finite and infinitely repeating objects, vectors and tensors, data fitting, uncertainty estimates and statistical significance, data fitting in crystal structure determination, and the fast Fourier transform.

Finally, sampling from our remaining examples, Jawson & Rose (1982) wrote, 'The central problem of mathematical crystallography is to determine the independent microscopic symmetries consistent with every macroscopic crystal symmetry.' Nowick (1996) was concerned with '. . . the effect of crystal symmetry in determining the tensor properties of crystals', which is a position similar to Wooster's (Wooster, 1973), who proposed to apply group theory to 'vibrations of atoms and molecules'. Senechal (1995) stated that her primary concern was crystal classification, and '. . . the problem of relating the geometry of discrete point sets to the diffraction spectra of functions associated to them . . . '.

In her historical account of geometric crystallography, Senechal (1990) wrote, 'Geometrical crystallography includes the study of crystal form, the mathematical representation of crystal structure and the relations between them.' That view of the past is certainly what one gets from the antiquarian work by Dana (2011), which focused on macroscopic crystal form. The biased sample of books above suggests that while mathematical crystallography has remained primarily concerned with geometry, the subject has shifted from the study of macroscopic crystal form to microscopic (in fact, nanoscopic) crystal form.

With the interesting exception of Prince (1994), our sources suggest that mathematical crystallography has retained its identity while expanding its reach. But since the subject is over a century old, and since it is central to crystallography (at least from the traditional point of view), one would expect that

Table 2
Searches for the string 'mathematical crystallography' in leading databases, searched on 24 August 2013.

Both Google Scholar and WorldCat spread very wide nets and we would expect inflated numbers.

Database	No. of items listed under 'mathematical crystallography'
Amazon (books)	53
American Chemical Society publications	27
Google Scholar	597
American Mathematical Society Mathematics Reviews (MathSciNet)	23
SciFinder Scholar (contains the former Chemical Abstracts)	10
Web of Knowledge (contains the former Science Citation Index)	14
WorldCat ('WorldCat connects you to the collections and services of more than 10 000 libraries worldwide')	195
World Wide Web of Science ('maintained by the US Department of Energy's Office of Scientific and Technical Information')	74
Zentralblatt für Mathematik (zbMATH)	17

Table 3
The string 'crystal' appears in eight sub-subfields of the MSC 2010 table posted at http://www.ams.org/msc/pdfs/classifications2010.pdf.

For the moment, we will take the core of 'mathematics in crystallography' to be 74E15, 74N05 and 82D25

Field	Subfield	Sub-subfield
14 Algebraic geometry	14F (Co)homology theory	14F30 *p*-adic cohomology, crystalline cohomology
20 Group theory and generalizations	20H Other groups of matrices	20H15 Other geometric groups, including crystallographic groups
52 Convex and discrete geometry	52C Discrete geometry	52C23 Quasicrystals, aperiodic tilings
74 Mechanics of deformable solids	74E Material properties given special treatment, especially anisotropy and crystalline structure	74E15 Crystalline structure
74 Mechanics of deformable solids	74N Phase transformations in solids	74N05 Crystals
76 Fluid mechanics	76A Foundations, constitutive equations, rheology	76A15 Liquid crystals
82 Statistical mechanics, structure of matter	82D Applications to specific types of physical systems	82D25 Crystals
82 Statistical mechanics, structure of matter	82D Applications to specific types of physical systems	82D30 Random media, disordered materials (including liquid crystals and spin glasses)

the phrase 'mathematical crystallography' would appear frequently in titles, abstracts and keywords. But as we can see from Table 2, it does not. This suggests that as a self-identified field, or at least as a field identified by the Library of Congress, mathematical crystallography is in a more quiescent mode, but not dormant, since the dates of publication of the books on the shelf of QD 911 suggest that the recent slowdown is moderate, and may be reversing: see Fig. 1.

1.2. The mathematics in crystallography

Another approach is to suggest that mathematical crystallography consists of the mathematics developed for, or (directly) inspired by, crystallography. This would be hard to measure, but we can take a brief and superficial look at the mathematics done in association with crystallography.

There are two major databases for mathematical literature: the old Zentralblatt für Mathematik und ihre Grenzgebiete (now zbMATH, maintained by the Heidelberg Academy, Springer and the FIZ Karlsruhe–Leibniz Institute for Information Infrastructure), and the new Mathematical Reviews (now MathSciNet, maintained by the American Mathematical Society). zbMATH and MathSciNet receive articles and books and send many of them to volunteer reviewers to compose paragraph-long micro-reviews, which are then published (now posted online).

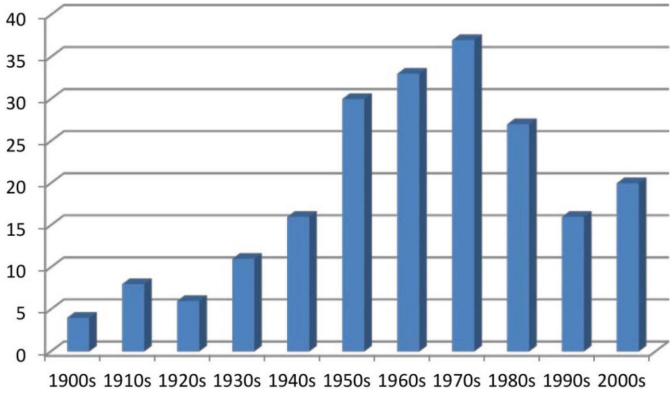

Figure 1
During the 20th century, publications of items shelved in the Library of Congress under QD 911 peaked during the 1960s and 1970s. Query conducted 24 August 2013.

In addition, zbMATH and MathSciNet collaborate in maintaining a Mathematical Subject Classification (MSC, see American Mathematical Society, 2009), which is organized as follows. First, mathematics is subdivided into fields, each of which is assigned a two-digit code. Then each of these fields is subdivided into subfields, each of which is assigned an additional letter from the alphabet. Finally, each of these subfields is subdivided into sub-subfields, and each of these sub-subfields is assigned an additional two-digit code. Thus 05 is Combinatorics, 05B is 'Designs and configurations', and mathematical crystallographers may be particularly interested in 05B35 ('Matroids, geometric lattices'), 05B40 ('Packing and covering') and 05B45 ('Tessellation and tiling problems'). There are about 6000 sub-subfields altogether.

When an editor of zbMATH or MathSciNet sends an article or a book out to be reviewed, the editor assigns tentative 'primary' and 'secondary' subject codes (and keywords). The reviewer will take these into account when proposing the subject codes (and keywords) to be used. Many items will thus have multiple codes, and most will have at least one.

This practice facilitates data mining. For example, the string 'crystal' appears in eight sub-subfields in the MSC 2010 table, although some of these are apparently subjects that arose from mathematical crystallography long ago and have since gone their own way (but may be of interest to crystallographers again, some day). All eight are listed in Table 3.

We can now use zbMATH to estimate research activity (zbMATH states on its website that it covers 'over 3000' journals). Since most sub-subfields in mathematics are essentially pure, we take the parsimonious view and query only about three of these sub-subfields: 74E15 Mechanics of deformable solids > Material properties given special treatment, especially anisotropy and crystalline structure > Crystalline structure; 74N05 Mechanics of deformable solids > Phase transformations in solids > Crystals; and 82D25 Statistical mechanics, structure of matter > Applications to specific types of physical systems > Crystals. We get 4486 items containing at least one of these three codes.[3]

[3] This query was conducted on August 23, 2013.

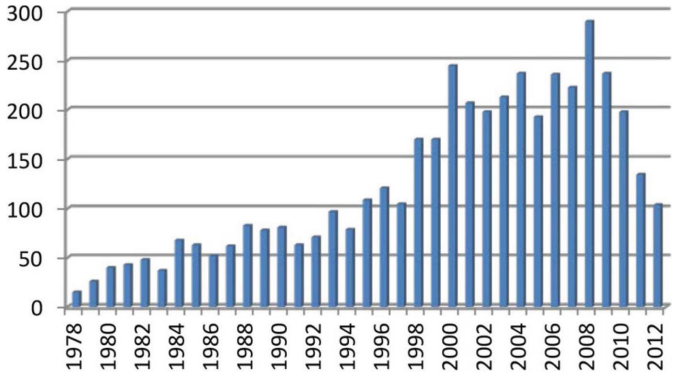

Figure 2
From 1978 to 2012, the number of items listed per year in zbMATH under sub-subfields 74E15 . . . > Crystalline structure; 74 N05 . . . > Crystals; and 82D25 . . . > Crystals has increased substantially. Slow turnaround may affect reports for 2011 and 2012. Query conducted 22 August 2013.

We can see the growth of the field – or perhaps (being realistic), the growth of its coverage. zbMATH allows subsearches by year, and while the oldest record in this search is dated 1872, the first year with at least ten entries was 1978 and the first with at least 100 was 1995. The number of entries in zbMATH per year for items with codes 74E25, 74N05 or 82D25 are shown in Fig. 2.

But what are the producers of these items researching? We can get a rough picture by using the fact that items frequently have multiple codes, and we look for the other codes occurring with the codes 74E15, 74N05 and 82D25 among these 4486 items. Just looking at the fields, we see that besides the 2990 items with field 82 (Statistical mechanics, structure of matter) and the 2210 items with field 74 (Mechanics of deformable solids), there are eight other fields with over 100 items each; these are enumerated in Table 4.

We can obtain a more precise picture by applying the following algorithm to this population of 4486 items. In most (but not all) of these fields, there may be one very dominant subfield which, in turn, may have one very dominant sub-subfield. For each of these areas, we determine the most heavily populated subfield, and for that subfield, we determine the most heavily populated sub-subfield. The results of this algorithm applied to these eight fields is presented in Table 5. Incidentally, if we narrow our focus to those items with codes from 'pure' mathematics (all codes below 69, and thus including statistics and computer science as pure mathematics), we obtain 1741 items.

zbMATH's picture of the mathematics associated with crystallography is now a bit different from the Library of Congress picture of mathematical crystallography. While many items involve the symmetries and discrete structures associated with mathematical crystallography, there are also items in differential equations, statistics and numerical analysis (as well as physics). These other subjects remind us of Prince's (Prince, 1994) pragmatic approach to selecting topics: the mathematics in crystallography is the mathematics that crystallographers find useful – or that mathematicians think crystallographers will find useful.

Table 4
Eight fields were listed with over 100 items each among the 4486 items coded 74E15, 74N05 and 82D25.

Field	No. of items	Percentage
20 Group theory and generalizations	493	11%
35 Partial differential equations	367	8.2%
52 Convex and discrete geometry	342	7.6%
81 Quantum theory	336	7.5%
65 Numerical analysis	210	4.9%
78 Optics, electromagnetic theory	179	4%
80 Classical thermodynamics, heat transfer	168	3.7%
51 Geometry	137	3.1%

This is, of course, a very naive and superficial picture; a more careful comprehensive review would be desirable.

1.3. Uncertainties and caveats

These two pictures, from the Library of Congress and zbMATH, suggest that 'mathematical crystallography' is something slightly different from the mathematics done for crystallography. In fact, comparing Figs. 1 and 2, we can see that publications in QD 911 declined at the same time that publications in 74E15, 74N05 and 82D25 were rising.

One caveat is immediate. In §1.1, we listed 24 books (besides Dana, 2011). What does zbMATH say about them? Twelve are not listed at all – apparently mathematical content was not what zbMATH had in mind – and two old books are listed, but with no MSC codes. That leaves ten, and among these, the code 74E15 did not occur, 74N05 occurred once and 82D25 occurred five times. This strongly suggests that the mathematics recognized by zbMATH in these three (relatively applied) sub-subfields is somewhat different from traditional 'mathematical crystallography'. Incidentally, while 24 codes turned up among these nine items, only four showed up more than once: 20H15 ('Other geometric groups, including crystallographic groups') eight times, 51F15 ('Reflection groups, reflection geometries') five times, 82D25 ('Crystals') four times, and 01A60 ('History and biography > History of mathematics and mathematicians > 20th century') twice.

Perhaps mathematical crystallography is an old field with a relatively large penumbra. This view might be supported by considering the last two meetings of the Society for Industrial and Applied Mathematics' activity group on Mathematical Aspects of Materials Science, each of which had over 200 attendees attending about 100 two-hour minisymposia, many of them focusing on crystallographic topics, but only one to three of which were on 'mathematical crystallography'.

Perhaps mathematical crystallography, considered inclusively, is a panoply of fields with uncertain internal connections and communication, and thus uncertain self-identification. Consider a genuinely new field. Nanoscience and nanotechnology have been studied by academics in information science using keyword and other string searches (*e.g.*, Porter *et al.*, 2008; Islam & Miyazaki, 2010) employing data-mining techniques of the sort described in Porter & Cunningham (2004). Grienesen & Zhang (2011) argue that in

Table 5
Eight fields were listed with over 100 items each among the 4486 items coded 74E15, 74N05 and 82D25.

The rightmost column is the percentage of the items of a field that are listed in the given subfield(s) or sub-subfield(s); thus 91.5% of the items with codes 74E15, 74N05 or 82D25 that also have code 20 (Group theory) are assigned code 20H15.

Subfield (and sub-subfield, if there is a concentration)	No. of items	Percentage of the field
20H15 Other groups of matrices > other geometric groups, including crystallographic groups	451	91.5%
35Q Equations of mathematical physics and other areas of application	194	52.8%
52C23 Discrete geometry > quasicrystals, aperiodic tilings	119	34.8%
81Q General mathematical topics and methods in quantum theory and 81V Applications to specific physical systems	273	81.3%
65C Probabilistic methods, simulation and stochastic differential equations and 65M Partial differential equations, initial value and time-dependent initial-boundary value problems and 65N Partial differential equations, boundary value problems and 65Z Applications to physics	142	67.6%
78A General	174	97.2%
80A Thermodynamics and heat transfer > 80A22 Stefan problems, phase changes *etc.* and 80A23 Inverse problems	137	81.5%
51F15 Metric geometry > reflection groups, reflection geometries and 51M20 Real and complex geometry > polyhedra and polytopes; regular figures, division of spaces	113	82.5%

the 1990s, there was less consensus in 'nanoscale studies' over what keywords practitioners should use in their publications; this would make it more difficult for other researchers interested in the same or related topics to find those publications, and it would make it more difficult for information scientists to survey the field.

Researchers studying mathematical crystallography may face similar obstacles, which (as we shall see) may have an effect on how the field develops. Mathematical crystallography is not new, but if it is re-emerging from a panoply of scattered subfields, it may resemble a new field in significant ways.

2. Newly emerging science and technology

Emergence has become an academic subject in its own right – or, more accurately, emergence has become several academic subjects in philosophy, history, sociology, business and (for tracking it) information science. While the literature on innovation appears essentially descriptive, patterns discerned among the successes and failures have led several scholars to offer advice, if not prescriptions, for participants in emerging fields. In this section, we review some basics about emerging fields and innovations of science and technology, and we apply them to mathematical crystallography.

2.1. About emergence

Friedel (2007) proposed that technology advances incrementally from the work of innovators who have their own agendas – agendas that may not have much to do with what posterity makes of those innovations. For example, group theory arose during the 18th and 19th centuries partly because of efforts to solve polynomial equations – or prove that they were insoluble (in terms of finitary expressions), and then work out what could be said about the solutions (Wussing, 1984). Seven decades after Leonhard Euler's implicit use of what we call 'groups', Evariste Galois launched the word 'group' in 1831, and even then it wasn't until 1846 that Augustin-Louis Cauchy proposed 'groups of permutations' (within hailing distance of the 'groups of actions' in contemporary algebra and crystallography) as a subject of study in itself.

Of course, group theory is a branch of science, not technology, but the theory of emergence spreads an even wider net than that. For example, consider the question of whether an innovation needs a publicly identifiable champion. A century ago, Cubism arose as an artistic movement that initially had no public leadership until critics hailed Pablo Picasso and George Braque over a decade after the movement took over Paris (Sgourev, 2013). Meanwhile, the rise of Surrealism was almost immediately trumpeted by André Breton's *Manifeste de surréalisme* (Nadeau, 1982). These two near-simultaneous developments in art in France suggest that a visionary public leadership may or may not be a characteristic of a new movement.

There seem to be two pre-eminent models of emergence.

Donald Campbell (1960, 1987) proposed that knowledge and creation arose from innovators combining and adjusting extant notions and then selecting the useful results. Science and the arts evolve rather as life does, with a diversity of ideas and a system of selection. This model was adjusted by Dosi (1982), who proposed that as industrial systems arose, they tended to carve various 'paths' that they then tended to follow. For example, David (1985) describes how the QWERTY keyboards that (almost) all of us use came into dominance almost by accident, but once QWERTY was in place, the inconvenience of changing keyboards and the natural conservatism of human beings conspired to keep QWERTY long after it ceased being the optimal choice.

Thomas Kuhn (1965) claimed that 'normal science' consists of 'puzzle solving' under the auspices and conscious and unconscious constraints of an overarching 'paradigm'. The paradigm incorporates not only the accepted theory, but also the accepted views of what is important, what the major problems and goals of the field are, and so on. When a paradigm comes under sufficient pressure, and if there is an apparently superior competitor (superior in the view of enough participants), there may be a 'paradigm shift' to the competitor. Like Campbell, Kuhn proposes that selection depends on the participants choosing from their own agendas and points of view: again, innovation is a social process.

Economics is the dismal science, and the economic view of emergence lies in the shadow of Joseph Schumpeter's (1942) notion of *creative destruction*, in which people used to well worn paths are forced elsewhere. Resistance to emergence is also a subject of much study; but the problems caused by emergence raise the question of why anyone would bother. Darden (1978) proposes that if we regard an academic field as having as its subject a major problem or challenge, then an

emerging field would attract interest if it addressed the problem in an effective or compelling way. Recall Wussing's (1984) outline of the emergence of group theory, which attracted interest because of its utility in addressing the challenge of computing, or even describing, roots of polynomials. In a very different field, the construction of the unprecedented wide, tall domes of the Basilica of St Mary of the Flower in Florence, St Peter's Basilica in Rome and St Paul's Cathedral in London exhibited the utility of statics and novel design principles in architecture (Cowan, 1977).

The community may be slow to accept the most useful innovations, even if the innovations were something the community (or at least, powerful players in the community) want. For example, Crowe (1967) describes Hermann Grassmann's development of a 'barycentric calculus' which he communicated to the world *via* large books that leading mathematicians attempted to read and failed to understand. Mathematicians tried reading the books because they suspected that Grassmann's calculus might be the algebra of three-dimensional space that they increasingly desired. But because Grassmann was unable to communicate, the barycentric calculus largely disappeared. Half a century later, Willard Gibbs – who communicated *via* preprints to targeted European colleagues – successfully sold his new 'vector algebra', which was similar to the barycentric calculus, but apparently more accessible.

Turning to biology, Charles Darwin did not propose any mechanism for inheritance to underlie his theory of natural selection, with the result that mechanisms of inheritance became a major part of the subsequent controversy. Gregor Mendel's theory of genetic inheritance was what Darwin desired, but either because Mendel did not bring his results to the attention of the right people in the right way (Eiseley, 1958), or because Mendel's theory was radically different from what contemporary botanists were prepared to accept (Barber, 1961), Mendel's theory would not be popularized until long after Mendel and Darwin were dead.

Sometimes the innovation is ahead of its time in the sense that it appears before the machinery that it will ultimately articulate with. Daylight (2012) outlines the development of the modern computer from the 1930s to the 1960s, and he presents various engineers developing the first electronic computers during the 1940s. Only in the 1950s, well after the logician Alan Turing became active in computing, did the first software engineers stumble across Turing (1936) and decide that Turing's abstract machine was a model for what they were doing. Although Turing's paper chronologically preceded the inventions (plural) of the electronic computer, its impact came later.

The array of obstacles to innovation is itself a topic for research and commentary. Barber (1961) enumerated several forms of resistance within the scientific community itself, including entrenched interests, limited imagination and preconceptions about mathematics. Crane (1972) wrote about the effects of isolation among geographically scattered practitioners, and the need for infrastructure (journals, conferences, organizations) to connect practitioners of a new field. (Some movements get started and established at one place – *e.g.*, Paris for cultural movements like Cubism – before spreading out.) Fagerberg & Verspagen (2009) warned that new fields face credibility problems when interacting with practitioners of other fields, especially when competing for resources.

One way to address the problems of access to resources and infrastructure is to build one's own. For example, a century ago biology had an anti-mathematical bias, and when the Council of the Royal Society told Francis Galton that mathematical papers should be kept separate from papers on applications of mathematics to biology, Galton's reaction was to ask Karl Pearson if he should resign from the Society. Pearson advised Galton to found his own journal, and *Biometrika* was the result (Barber, 1961).

For infrastructure and allocation of resources to be issues, the identity of a field must itself be an issue. But self-identity can be problematic. For example, a decade ago, Schummer (2004) described nanoscience and nanotechnology as a panoply of different fields, and recall that Grienesen & Zhang (2011) warned that using 'nano*' as a search term for data mining 'nanoscale studies' in the 1990s will miss many publications. Perhaps during the 1990s, the self-identity of 'nanoscale studies' had not jelled to the point it has today. A lack of identity complicates communication: if a field's identity is so weak that a participant cannot recognize a fellow participant – or if a potential recruit cannot recognize a participant – then building a network of contacts in that field will be difficult.

Recruitment of new participants, either graduate students or researchers from other fields, may be critical. Bettencourt *et al.* (2008) developed a simple formula comparing the number of publications per year to the number of new authors appearing each year, and applied it to the emergence of cosmological inflation, cosmic strings, prions, H5N1 influenza, carbon nanotubes and quantum computing. They concluded that the development of an emerging field depends substantially on recruitment, which suggests that it depends on the population of potential recruits and the networks of contacts between participants and that population.

These desiderata are almost surely interdependent. Assuming Friedel's (2007) point that a major innovation is developed incrementally by many players, a network among participants is necessary for the innovation to be developed into something more than an appealing notion. And a visible application or accomplishment of a field would make it more attractive to potential recruits, who would go on to make more accomplishments.

2.2. The (re-)emergence of mathematical crystallography

To do justice in describing mathematical crystallography as a 'newly emerging [field of] science and technology' (AKA a NEST; see, *e.g.*, Guo *et al.*, 2012) we would have to conduct the sort of investigation described in Robinson *et al.* (2013); but here, all we can do is expand on the point of Guo *et al.* (2012) that the future of an emerging field is uncertain. However, we can outline how some of the extant generic advice might be

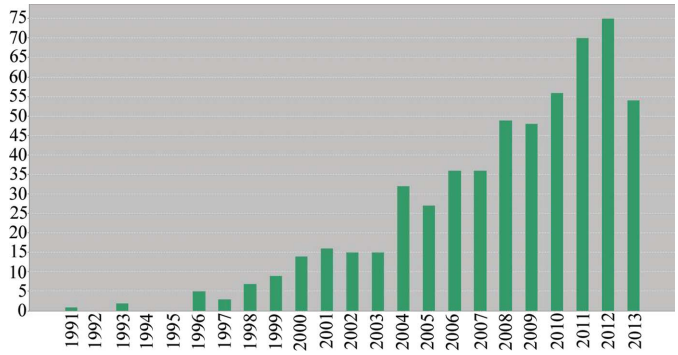

Figure 3
Results from the Web of Knowledge search for items under TOPIC = 'crystal structure prediction' (including quotes) conducted 3 September 2013. This graph is purportedly of 'all items' under that topic, and as the first item appeared in 1991, Maddox (1988) is not listed in the Web of Knowledge under that topic. However, Maddox (1988) is listed (under different topics), with 237 citations within that database. Query conducted 3 September 2013.

adapted to mathematical crystallography. We will focus on three issues: Darden's (1978) suggestion that a field advances by solving problems, the suggestion of Bettencourt *et al.* (2008) that recruitment of new participants is critical and Crane's (1972) emphasis on infrastructure.

If mathematical crystallography facilitated a major advance in crystallography, that would demonstrate its utility to the community. Let us consider an example. One of the major challenges of modern crystallography is the design of crystals in advance of synthesis, along with predictions of the hypothetical crystal's properties, so that the design is useful in the synthesis of the crystal and the resulting product possesses the predicted properties. The apparent inability to accomplish this by the 1980s was described by Maddox (1988) as a 'continuing scandal'. In his introduction to the 2011 anthology *Modern Methods of Crystal Structure Prediction*, Oganov (2011) writes that 'the situation began to change in 2003–2006, and this avalanche-like development of this important field can be called a scientific revolution that continues to this day'. This statement is largely supported by the very naive search in the Web of Knowledge shown in Fig. 3.

The articles in Oganov's anthology articulated to a wide range of mathematical fields. Blatov & Proserpio (2011) presented the underlying combinatorial (or perhaps 'topological') view of the structures being predicted. Wales (2011), Tipton & Hennig (2011), Schöne & Jansen (2011), Goedecker (2011) and Lyakhov *et al.* (2011) described applications of several popular optimization techniques, while Martonák (2011) and Leoni & Boulfelfel (2011) described simulations of phase transitions, *i.e.* of dynamic situations. If, for example, an application of mathematical techniques provided a reliable method for rapidly generating both predictions of crystal structures and reliable procedures for synthesis, that would attract favourable attention to the field.

Crystal structure prediction provides only one of several classes of challenges where mathematical crystallography could make a considerable contribution and raise its profile in the process. That would encourage recruitment, so let us now look at that issue. Since mathematical crystallography is an interdisciplinary field in the intersection of chemistry, physics and mathematics, we could start with challenges facing interdisciplinary scientific fields. In their 1995 review of *Mathematical Challenges from Theoretical/Computational Chemistry*, the National Research Council (1995) concluded with several 'cultural issues and barriers to interdisciplinary work'. Some of these should be familiar. For example, faculty in one department may have difficulty receiving appropriate credit for work in another field. And students seeking credentials in an interdisciplinary field may have difficulty completing the prerequisites for the courses that they desire. The National Research Council even brought up the fact that at many universities, chemists and mathematicians are in separate buildings and have limited daily interaction. And there is a considerable language barrier between chemists and mathematicians. The language barrier may be central to a problem that the National Research Council did not directly address: the alleged difficulty of mathematics.

Popular culture agrees that 'Math is hard'.[4] Tobias (1978) claims that the problem is the attitude towards mathematics, but others claim that mathematics is intrinsically hard. Smith (2002) argues that the difficulty is linguistic: in mathematics, language is used in a more artificial way. One might go beyond Smith to argue that one difference between chemistry and mathematics is that in the latter, both discovery and verification are linguistic exercises. Meanwhile, in chemistry, both discovery and verification rely on instruments and experiment. The result is that, in mathematics, there is a greater burden on the language, which then becomes more difficult for novices to master.

Whatever the reason, math appears hard. It may even be hard for mathematicians. One place to see the difference between chemistry and mathematics at work is to compare journal backlogs. The IUCr Executive Committee (International Union of Crystallography, 2013) reported the mean publication times during 2011 for their eight journals, and the range was from 0.7 months to 5.4 months, with a mean of 3.8 months. Meanwhile, the American Mathematical Society (2012) surveyed 114 journals and reported the median times in 2011 from submission to *acceptance*; these ranged from 2 months to 18.2 months, with a mean of 7.8 months. There may be several reasons for the longer review time, but the explanation that 'math is hard' is a likely one, although (as we shall see), there may be a subcultural reason.

Recruitment into a recognizably hard subject poses challenges, no matter how rewarding it might be. It is even more necessary than usual to make the field accessible to newcomers, and that brings us to infrastructure.

Traditionally, newcomers would learn a field by listening – taking classes and tutorials or talking to participants – or by reading. The traditional infrastructure thus consists of meetings, books and journals. Meetings and journals are institu-

[4] What Mattel's popular Barbie doll said was, 'Math class is tough' (New York Times, 1992).

Table 6
The five journals that had published the most articles in sub-subfields 74E15, 74N05 and 82D25, with the number of articles published in each (under column 'All').

Then for each of the eight subfields with the largest intersection with 74E15, 74N05 and 82D25, the three journals that had published the most articles, with the number of articles published in each (under columns '20', '35' *etc.*). Search conducted 21 October 2013.

Journal	All	20	35	51	52	65	78	80	81
Acta Cryst. A	165	88		10	34				
Arch. Mech.								6	
Dokl. Akad. Nauk, Ross. Akad. Nauk									10
Int. J. Mod. Phys. A									10
Int. J. Solids Struct.	167								
Int. J. Heat Mass Transfer								6	
Int. J. Plasticity	218								
J. Math. Phys.									10
J. Comput. Phys.			19			27		8	
J. Mech. Phys. Solids	286								
J. Phys. A Math. Theor. (formerly *J. Phys. A Math. Gen.*)	224	40	17	7	59		9		51
Math. Models Methods Appl. Sci.						7			
Mod. Phys. Lett. B							8		
Physica D			16					6	41
Phys. Lett. A						10	27		
Z. Kristallogr.		23		7	19				

tional, while books are usually results of individual effort. This brings us to institutional infrastructure.

There are several organizations relevant to mathematical crystallography. Probably foremost is the International Union of Crystallography (IUCr), whose Commission on Mathematical and Theoretical Crystallography organizes workshops and tutorials on the foundations of crystallography at locations around the world. In addition, the IUCr has member organizations, 'adhering bodies', usually national crystallographic organizations, which form 'national committees for crystallography' to liaise with the Union. These organizations may organize meetings and workshops.[5] And the IUCr maintains several journals (including this one) and publishes texts and monographs in association with Oxford University Press.

Mathematical crystallography is interdisciplinary, so several scientific societies provide usable resources. Many of these societies are national, often with articulation agreements to analogous organizations in other nations. The larger organizations include:

(i) For chemistry, the American Chemical Society and the Materials Research Society.

(ii) For mathematics, the American Mathematical Society, the European Mathematical Society and the Society for Industrial and Applied Mathematics (SIAM).

(iii) For physics, the American Physical Society, the Deutsche Physikalische Gesellschaft (DPG) and the European Physical Society (which has the DPG as a member).

Some of these organizations have activity groups focusing on crystallography; for example, the DPG has a Fachverband Kristallographie, while SIAM has a Mathematical Aspects of Materials Science activity group, which includes crystallography. One major service these organizations provide is sponsoring meetings. Many meetings are open for unsolicited contributed talks, but more to the point, some meetings facilitate recruitment and network building by accepting proposals for symposia, minisymposia and special sessions at the meetings. A few accept proposals for tutorials.

Meetings are expensive (in both money and time) to organize and to attend, which leaves books, journals and the internet as more convenient, if more detached, alternatives. Let us take a brief look at the journals, which nowadays are largely internet resources.

Returning to zbMATH, one can identify the journals that published the most articles in a given field. In Table 6, we list the journals that had published the most articles in the sub-subfields 74E15, 74N05 and 82D25, and those that had published the most articles in those sub-subfields that were also in the eight fields of mathematics listed in Table 3. The journals ranged from the *International Journal of Plasticity*, which published 218 articles in the three sub-subfields but was not among the top three journals in any of the eight fields of mathematics, to the *Journal of Physics A*, which published 224 articles in the three sub-subfields and was also among the top three journals in six of the eight fields of mathematics of Table 3. The journals that were among the top three in at least three of the eight fields were the *Journal of Physics A*, *Acta Crystallographica A*, *Zeitschrift für Kristallographie*, the *Journal of Computational Physics* and *Physica D*. All journals listed cover either general science, crystallography, physics or materials science; there is one applied mathematics journal and no chemistry journals.

From this point of view, despite the Library of Congress and Dewey Decimal classifications of crystallography as a subfield of chemistry, physics may have a greater footprint in mathematics for crystallography than chemistry. Perhaps this is because there is more crystallographic activity in physics than in chemistry. Perhaps this is because physics is more mathematical than chemistry and so mathematical and theoretical crystallographers might be more inclined to publish in physics journals. Perhaps there is a different reason.

Recall one of the major conclusions of §1: (classical) mathematical crystallography is not the same thing as mathematics for crystallography (as measured by zbMATH). In addition, although there is enormous activity in crystallography with geometric and mathematical issues (in crystal prediction alone, there are metal–organic frameworks, zeolites and other polymer structures), there are no chemistry journals listed in Table 6. The crystallography in chemistry journals are not listed by zbMATH.

It seems that there are at least two communities of practitioners working in this multidisciplinary field and possibly

[5] In 2014, the IUCr itself, and other groups, are organizing events around the United Nations International Year of Crystallography.

several more. In this survey, we have not encountered evidence of strong lines of communication between these communities, and such a lack of self-identification or of recognition of common interests can limit access to or use of infrastructure. Lack of communication may make subcultural obstacles more difficult to surmount.

For example, consider the longer review times for mathematics journals (as opposed to crystallography journals). This may reflect different expectations of journal editors, which may in turn reflect cultural differences that could complicate collaborations. For example, crystallography journals do not expect reviewers to verify the reported results; that would require replicating the experiments. But mathematics journals do expect reviewers to state whether the results appear 'sound'. This may be a reason why mathematics referee reports take longer.

If a journal receives a paper, it has certain expectations about how that paper should be dealt with. If a journal finds itself dealing with a multidisciplinary paper with referees (and authors) having varying expectations, that can make the process and the ultimate decision on whether to publish more difficult. This is merely another example of a subcultural barrier to multidisciplinary research.

Considering the situation, how should mathematical crystallographers move forward?

3. Prospects and prescriptions

The prospects for mathematical crystallography would appear to be good. We start with the relatively non-controversial claim that many of the leading technological challenges of the 21st century will be critically dependent on advances in materials science. Crystals, including nanocrystals and quasicrystals, are already a major part of materials science: as of 1 November 2013, the Web of Science has 1.8 million items of topic 'crystal' and 3.0 million of topic 'materials'. We would expect the economic demand for crystallography to continue (if not grow) through the century.

That probably means an economic demand for mathematical crystallography. Recalling the characterizations of crystallography as the determination of the positions of atoms in crystals – either for designing novel crystals or for classifying or determining properties of crystals – the problem is and remains heavily mathematical. Let us return to crystal prediction to see how this might work.

A number of material design efforts are under way, and some of them rely on 'big data' methods, *i.e.* having a computer program generate reams of prospective material designs and then having another computer program winnow through them, seeking designs promising enough to bring to human attention. For example, White (2013) described the work of Gerbrand Cedar of MIT, Stefano Curtarolo of Duke and Alán Aspuru-Guzik of Harvard on the 'rational and systemic design of future high-performance materials': they use computer programs to predict materials, and then after (attempting to) synthesize the predicted materials, they use more programs to analyse and catalogue the results. 'The initiative's ultimate goal is to use this iterative process to significantly reduce the time and cost to bring new materials from the laboratory to the marketplace.'

Automating combinatorial chemistry – and thus having computers conduct combinatorial analysis – has its limitations. The number of combinations to generate and then check explodes exponentially with the number of components (atoms or molecular building blocks) per unit, and it is quite simple to devise a search that would exhaust the world's computer memory and take geologic time to compute. 'Not only do we not understand the basic physical principles we need to model, there are at the moment no computers powerful enough to predict how certain material structures yield particular properties', wrote Johnson (2007). 'When it comes to solid matter, systems are so complex that current computer modelling tools quickly run out of steam.' Johnson contended that '... material by design isn't even on the horizon, certainly not for the production of bulk commercial materials'.

Mass generation of designs is already being done in crystal prediction. For example, the *Atlas of Hypothetical Zeolite Structures* (Foster & Treacy, 2010) lists over 5 million 'crystal nets' (just for zeolites) which can be regarded as (rather Spartan) blueprints. The problems are generating and identifying chemically feasible crystal nets.

Mathematicians have been developing workable algorithms for thousands of years. The motivation was often that, for the given problem, there was no extant algorithm, or that all extant algorithms were unsatisfactory. If what is desired is a mathematical toolkit for crystal prediction, we know whom to ask. With that in mind, the probable economic demand for materials by design should assure a future for mathematical crystallography in this century. But as Robert Farley (2008) observed in a different context, just because something must happen does not mean it will. The unfortunate histories of Grassmann's barycentric calculus and Gregor Mendel's discrete genetics – both developments greatly needed by the scientific community, and yet neglected for decades – suggest that the prospects for mathematical crystallography may require more than a solution to an extant problem.

If mathematical crystallography is to generate major applications, then an evolutionary epistemologist might recommend recruiting a diverse community of participants. That would greatly increase the odds of finding associations of ideas that will produce useful innovations. If one believes in the potential of mathematical crystallography, then recruiting participants – either colleagues in other fields, or graduate students – is the most promising strategy.

One possibility is to advertise. This article is in a virtual issue of *Acta Crystallographica A*, which was inspired by a sequence of minisymposia on mathematical crystallography in the Society of Industrial and Applied Mathematics' 2013 meeting on Mathematical Aspects of Materials Science. Meetings like this one may be useful for recruiting, and so may semi-popular works like Weyl (1952), Senechal & Fleck (1988) and Conway *et al.* (2008). In addition, manifestos like Yaghi *et al.* (2003) and Nespolo (2008) may serve as advertising.

Recalling Grassmann, Mendel and Turing, advertising in itself may not be enough: there has to be extant activity to advertise. For example, Toumey (2009) notes that while several researchers have told him that they recalled Feynman's 1959 *There's Plenty of Room on the Bottom* speech (published as Feynman, 1960) being the subject of much conversation during the following two decades, there were only seven citations during those two decades; citations became more common only after the nanotechnology developments of the 1980s.

One must have something to advertise, and the advertisement should be presented in terms that potential recruits are prepared to hear.

In McColm (2007), mathematical truth was represented as an invisible edifice: our knowledge was represented as a vine that grows up the edifice. Mathematicians are thus gardeners. When a mathematician finds a new balcony, turret or gargoyle, she leads colleagues to that architectural element by growing a vine there: the accessibility of this new discovery depends critically on the passage of the vine.

Recalling Grassmann and Gibbs, inaccessibility may have delayed the dissemination of a three-dimensional (and in fact, n-dimensional) algebra by half a century. Accessibility is critical for recruiting colleagues. And as for recruiting graduate students, recall the metaphor of a vine growing up an invisible edifice. The vine is more readily climbed by novices if it has some very climbable trunks, with lots of strong low branches placed in a navigable pattern. Exposition and education may be as critical as discovery itself in making an innovation succeed.

At the SIAM meeting, Michael Zaworotko listed as one of the primary challenges building a common vocabulary accessible to chemists, crystallographers, mathematicians, physicists and other participants. In a similar vein, writing about nano* research, Porter & Youtie (2009) recommend that 'Minimizing jargon and acronyms (and we know that we use them here!), and checking understandability by researchers from other disciplines, should reduce the barriers to nano research knowledge transfer.' A related step would be that multidisciplinary articles be relatively self-contained, in that [strictly necessary (!)] jargon and acronyms be defined within the article itself: when attracting novices, conciseness may be a lesser virtue than clarity or accessibility.

4. Discussion

We anticipate a substantial need for mathematical crystallography, a need that is probably already extant. Converting that need into an economic demand – making contemporary scientists and engineers aware of that need and persuading them that the field is worth the effort and resources to develop – is another matter.

In addition, there is substantial research activity not only in what we might call classical mathematical crystallography, but also in mathematical topics related to crystallography outside of the classical topic. The self-identification among all these researchers and practitioners as 'mathematical crystallographers is probably limited, and these participants probably make up several communities – or even several fractions of various ancillary communities – rather than an identifiable community of mathematical crystallographers. This lack of self-identification and social connections may hamper the development of the field, and the growth of mathematical crystallography may depend on building a sense of community as well as connections to related fields in chemistry, physics and mathematics.

Building a sense of community may entail recruitment and infrastructure. But beyond the effects of such consolidation and encouragement, the prospects of mathematical crystallography will depend on what it can provide for the scientific and engineering worlds as they address the challenges of the 21st century.

This article arose from a project to map mathematical crystallography as a field, with progress posted on the Crystal Mathematician weblog at http://blogs.iucr.net/crystalmath/; the mapping project will continue. I would like to acknowledge the assistance and advice of those who responded to postings and correspondence, especially Mike Grienesen, Mike O'Keeffe, Alan Porter, Lorenzo Sadun, Marjorie Senechal and Peter Strickland. I would also like to acknowledge the advice of the two referees, whose comments led to major improvements in this paper.

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