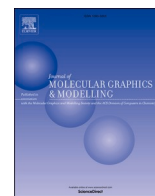




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From the archives: the origins of a society and a journal for the field of molecular graphics and modelling

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The Molecular Graphics and Modelling Society (MGMS) was instrumental in founding the Journal of Molecular Graphics (JMG) that later became the Journal of Molecular Graphics and Modelling (JMGM) of today. Based on the archives of the MGMS, this short article will provide a brief overview of the inception of the UK Molecular Graphics Group, which later evolved into the Molecular Graphics Society (MGS) and then MGMS; we cover the period from Nov 17, 1981 to the Group's first annual general meeting on April 14, 1983. It was during this period that the need for a new journal focussed on the emerging area of molecular graphics was recognised, as outlined in the article by Prof. Graham Richards in this issue.

The MGMS today is a successful society that promotes education and research into molecular graphics and modelling through a range of meetings, prizes, lecture tours, bursaries and other activities. Molecular graphics and modelling are now key and integrated tools across biology and chemistry, including in drug design. However, the Society dates back forty years, to a time when the application of computers in scientific research and visualization of molecules was still nascent.

As indicated above, the forerunner to the MGMS was the UK Molecular Graphics Group. The initial letter of invite to its inaugural conference, dated November 17, 1981, stated that the Group's aim was the "formation of an energetic group that will benefit all its members." This meeting was organised by Andy Morffew of IBM, as acting secretary of the Group, and the Group's name was abbreviated to UKMGG; this meeting followed on from the initial informal gathering he called at Balls Park in September 1981 to scope out the idea, as described in Prof. Richards' article in this issue. As will become evident from the highly active programme of activities in its first year and a half, the Group was very successful in realising this goal, to the point where the Group was presented as the Molecular Graphics Society at its first Annual General Meeting in 1983. From this AGM, the minutes of the Chairman's report reads that "The MGS has been in existence for nineteen months since the first seeds were sown in September 1981. Originally, it was launched as the United Kingdom Molecular Graphics Group but its reception in

Europe and the USA as the only society trying to deal exclusively with the problems of molecular graphics has greatly broadened its outlook." As has been pointed out elsewhere [1], the term "molecular graphics" in the 1980s had a somewhat different meaning from later years, embracing not only visualization and graphics techniques but the application of molecular calculations to solve problems in chemistry and biology, i.e. at this point in time, the definition encompassed implicitly modelling as well as graphics. In the 1990s, both the Society and the Journal added the term "modelling" into their titles to explicitly recognise this activity [1].

The inaugural conference of the UKMGG took place at Leeds University on the January 8, 1982, chaired by Andy Morffew and J. G. (Andy) Vinter. Located at the Astbury Department of Biophysics, the conference featured talks by several speakers, including Prof. Tony North on "Applications of display systems in studying molecular structures and interactions", Prof. Tom Blundell on "The use of the Birkbeck Interactive Computer Graphic System in molecular biology", and Dr. W. A. Thomas on the "Application of computer graphics to drug design" (Fig. 1).

In addition, proposals for rules of the UKMGG to "promote communication of all aspects of molecular graphics" were discussed, as were ideas (pencilled in the margin of an archived document) to become "part of a larger organisation? BBS, Chem Soc, BCA". The UKMGG did not choose this route, and the Society might have looked different in shape to the MGMS today if it had. A proposal at the Leeds meeting for a quarterly newsletter where members may publish review articles was approved. Among the 84 attendees were such future stalwarts of the MGMS and the discipline as a whole as Frank Blaney, then of Beecham Pharmaceuticals and Graham Richards of Oxford University; representatives from a range of other bodies were present including from the Cancer Research Campaign Group (S. Neidle and S. Islam), SERC Daresbury (S. Hull and P. Machin), the ICI Plant Protection Division (A. Marchington and K. Heritage), Fisons (F. Ince and D. Payling), Boots (G. Haran), Glaxo (A. Casson, P. C. Cherry and J. Elks), and Shell (A.

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UK MOLECULAR GRAPHICS GROUP
 INAUGURAL MEETING
 at
 ASTBURY DEPARTMENT OF BIOPHYSICS
 LEEDS UNIVERSITY
 on
 Friday 8 January 1982

A G E N D A

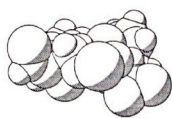
CHAIRMAN : Dr A J MORFFEWE

- 10.45 Discussion
 12.15 PROFESSOR A C T NORTH
 "Applications of Display Systems in studying Molecular Structures and Interactions"
 13.00 LUNCH

CHAIRMAN : Dr J G VINTER

- 14.00 Dr W A THOMAS
 "Application of Computer Graphics to Drug Design (provisional)"
 14.45 PROFESSOR T L BLUNDELL
 "The use of the Birkbeck Interactive Computer Graphic System in Molecular Biology"
 15.30 TEA
 15.45 Dr D N J WHITE
 "A Strategy for Energy Minimisation with Molecular Graphics"
 16.40 Dr A J MORFFEWE
 "Computing Science and the development of Molecular Graphics Systems"
 17.15 Finish

Fig. 1. Agenda of the inaugural conference of the UKMGG (Jan 8, 1982).



UK MOLECULAR GRAPHICS GROUP

Fig. 2. Front page banner of the first newsletter of the UKMGG (April 1982).

Dearing). Interestingly, Butterworths Publishers of Sevenoaks was also represented at this inaugural conference, by M. Slade.

The first workshop of the UKMGG was proposed at the inaugural Leeds conference, and subsequently took place on March 22-24, 1982 at Oxford. This was hosted by local organiser Graham Richards at Lady Margaret Hall. The workshop was planned with the goal of promoting

"opportunities for discussion" under the headings of "docking routines, drug design, surface presentation, linking graphics and batch programs, the man/machine interface, novel graphics routines, plotting programs and recent advances in graphics hardware". Conference fees at the Oxford workshop were £80 for residents and £20 for non-residents.

The workshop featured a broad range of speakers; this included Alwyn Jones from the University of Uppsala, Sweden, who, as described in a subsequent report of the event, discussed "the philosophy behind the [FRODO] system"; and Bob Langridge of UCSF who "showed how perception of the molecule is improved using the surface representation and colour." At the workshop, Rod Hubbard of York University (a future MGMS chair and JMGM editor) was reported to have described the "system that he has produced on a micro. This system has been built in a very short time and created a great deal of interest, especially among those who do not have large capital expenditure budgets. He also used a video to great effect." This early work and exposure through the MGS

Announcing a new quarterly journal from Butterworth Scientific

Journal of

Molecular Graphics

first issue: March 1983

Published in association with the Molecular Graphics Society

EDITOR: Dr A. J. Morfiew (IBM, Winchester, UK)

The use of computers for the investigation of molecular structure, function and interaction has developed in parallel to the technological advances of the last thirty years. One such advance, computer graphics, has been developed into a tool of great importance to chemists, molecular biologists, pharmaceutical researchers and others who need to visualise and interact with molecular models.

Until recently, the literature covering original research and application in this field has been scattered and disunited. The formation of the Molecular Graphics Society (formerly UK Molecular Graphics Group) in Europe together with the launch of the *Journal of Molecular Graphics* will provide more effective communication between workers from different backgrounds.

The *Journal of Molecular Graphics* will be international in both scope and readership and essential to research workers in the fields of:

- Biochemistry
- Biophysics
- Chemistry
- Crystallography
- Molecular biology
- Pharmaceutical research
- Polymer science
- Quantum chemistry
- Software development

SCOPE
The scope of the journal will focus on the following areas

- Hardware and software of molecular graphics systems
- New algorithms and procedures
- New representations of molecular structures
- Useful parametric plots
- Molecular modelling using computer graphics
- Results of projects using molecular graphics

The *Journal of Molecular Graphics* will feature original research papers and short communications together with occasional invited review articles. All contributions will be rigorously refereed to ensure a high scientific content. It is planned to include 4 pages of colour plates in alternate issues of the journal.

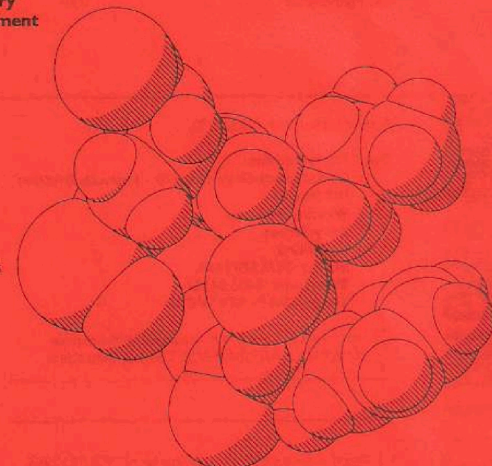


Fig. 3. Flyer from 1983 announcing the scope and content of the forthcoming quarterly journal from Butterworths Scientific, namely the Journal of Molecular Graphics.

gave him the experience that led to his subsequent development of the HYDRA and QUANTA software packages for molecular graphics, modelling and design. Quantum mechanics was also being linked with drug design at the workshop, as demonstrated by a talk on the “Application of interactive graphics and semi-empirical energy calculations using drug binding to DHFR as an example” by Liz Potterton, a research student of Keith Prout at Oxford University. Once again, the attendees of this UKMGG event represented a number of countries and spanned

academia and industry.

Meeting minutes of the UKMGG committee held at the workshop deemed the first workshop to be going well, although noting that travel on Sundays could be problematic. Suggested future topics for workshops and meetings included PERQ workstations and UNIX, micro systems, graphics peripherals, networking and database searching. This was also the first time that plans for a dedicated journal were mooted, in response to two publishers independently approaching the UKMGG on the matter,

one of which was Butterworths. At the committee meeting, a variety of possible publishers were discussed, including Butterworths.

Prior to this meeting, in January 1982, under the auspices of the UKMGG, Andy Morffew generated a Bibliography for Molecular Graphics. Some articles on molecular graphics that were highlighted and annotated in this compilation included:

- C. Levinthal. *Scientific American*, 1966, 214, 42. "A classic and the stimulus for many other workers in this field. Also appeared in the IBM proceedings in 1965."
- C. D. Barry & A. C. T. North. *Cold Spring Harbor Quant Biol.* 1971, 36, 577. "A classic, still one of the best descriptions of molecular graphics."
- D. Tsernoglou, G. Petsko, J. McQueen, J. Hermans. *Science* 1971, 197, 1378. "The first publication of a protein fitted on a computer graphics system."

The first UKMGG Newsletter was published in April 1982 (Fig. 2), starting with a list of committee members of the Group on page 1: M. S. G. Clarke (Beechams), D. J. Gilman (ICI Pharmaceuticals), A. J. Morffew (IBM UK Scientific Centre), A. C. T. North (Leeds University), W. G. Richards (Oxford University), J. G. Vinter (Wellcome Research) and D. N. J. White (Glasgow University). This committee can rightly be viewed as comprising the founding members of the subsequent Society, all being part of the core group that organised the inaugural conference on January 8, 1982.

The news section of the circular noted that "Michael Connolly is joining Arthur Olson's group at Scripps Clinic, La Jolla" and "joining Michael and Arthur will be Libby Getzoff and John Taner [sic] from the Richardsons' group at Duke University." The newsletter also announced two one-day meetings, to be organised by Andy Vinter from Wellcome and by David Gilman from ICI; and reported the UKMGG currently had 92 members, including from Australia, Switzerland, Germany, France and Belgium. It featured a book review of "Fundamentals of Interactive Computer Graphics" by J. D. Foley and A. van Dam (Addison-Wesley, 1982). At 664 pages in length, the review remarked that "Undoubtedly, this is the most comprehensive book available on computer graphics." Also, alongside a report of the first workshop, the desire to produce a new journal, which would allow colour pictures, was reiterated in the newsletter.

A second newsletter was published in October 1982; in this was listed some groups who had recently purchased mainframe machines: a Megateck 7000 was procured by Ciba-Geigy in Basle; and a Ramtek 9460 was obtained by the IBM UK Scientific Centre; an Evans & Sutherland system was being considered by Wellcome Research; and interestingly, a PS300 was obtained by University of North Carolina from Evans & Sutherland, apparently as part of their "give away scheme". The newsletter also featured a discussion of graphics standards, where the ANSI voted to accept GKS (the Graphics Kernel System) as a standard, provisional on some amendments. There was also a review article on red-green stereoscopy, and a mention of the forthcoming Royal Institution meeting on molecular graphics (to be held on December 7, 1982). Finally, the newsletter reported that Butterworths had agreed, on August 12, 1982, to publish the proposed Journal, setting out that this would consist of 32 A4 pages, with a four-page section of colour plates. Subsequent journal guidance indicated that the author would need to obtain prior agreement of the Journal to print colour figures, for which "transparencies should be supplied".

The first edition of the Journal of Molecular Graphics was published

in March 1983, in association with the newly named Molecular Graphics Society (Fig. 3). The first editor was Andy Morffew. The announcement of the Journal (Fig. 3) stated that:

"The use of computers for the investigation of molecular structure, function and interaction has developed in parallel to the technological advances of the last thirty years. One such advance, computer graphics, has been developed into a tool of great importance to chemists, molecular biologists, pharmaceutical researchers and others who need to visualise and interact with molecular models. Until recently, the literature covering original research and application in this field has been scattered and disunified. The formation of the Molecular Graphics Society (formerly UK Molecular Graphics Group) in Europe together with the launch of the Journal of Molecular Graphics will provide more effective communication between workers from different backgrounds."

Contemporaneous with the journal launch, a letter was sent to members (on March 29, 1983) indicating the intention to seek approval to become a Charity in Law, with a vote to take place at the AGM the following month. The vote was carried at the first AGM, on April 14, 1983 at the University of Sussex. At this meeting, the UKMGG now MGS reported a busy year, including five meetings, four newsletters, and the journal launch. It set a membership fee of £15, with 153 members comprising 67 academics and 86 from industry; 26 were students and 28 from outside the UK including members from West Germany, USA, Belgium and Switzerland.

It was noted by the Chairman Andy Morffew that the Society's "very existence has increased awareness in the field of molecular graphics and enhanced communication and education among its members both in the lecture hall and the bar. Of particular importance is the roughly equal proportion of academic and industrial members which has benefited the liaison and understanding of the two environments (perhaps the government can take a lesson). Finally the Society has endeavoured to foster an atmosphere which can aid research into the possibilities and applications of molecular graphics. Bringing together molecular graphics people and encouraging papers from them no matter what their interest, background or place of work may be, represents the Society's *raison d'être*." Plans were then put forward at the AGM to "increase the momentum", highlighting that the Society "is its members and without their input, enthusiasm and encouragement the Society and its offices cannot exist."

In conclusion, the success of the MGMS and JMGM owes a great deal to the early pioneers of the field represented by the UKMGG and MGS.

Declaration of competing interest

The authors declare that they have no known competing financial interests in regard to the content of this article.

Acknowledgements

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Reference

- [1] R.E. Hubbard, D.B. Boyd, *Reinvention of the Journal of Molecular Graphics and Modelling: defining a discipline*, *J. Mol. Graph.* 16 (1998) 113–114.