

SIG No:9 Crystallographic Computing

Reported Period: 2012-2013

Report Date:

17/06/2013

Reported by:

Harry Powell

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1. Introduction. (50 words max.)

SIG9 now has a website and has been organising a computing school to take place before ECM28. We have secured funding for a poster prize to be awarded at this and future ECMs. We are running a software competition.

2. SIG web site:

SIG 9 url: <http://sig9.ecanews.org/>

3. Number of ECA individual members registered with the SIG according to

(<http://www.xray.cz/eca/im-payment.htm>)

SIG 9	ecacomsg	169
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4. Existence of a SIG mailing list Yes / No

No (an informal list is kept by HRP; a list is held on IUCr web server but does not seem to elicit any replies)

Address of the mailing list:

Number of members in the SIG mailing list : 92

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate)

~200 (based on the mailing list and knowledge that most researchers in this field are not on the list).

6. List of MS organized by the SIG at the last ECM

MS 29 Likely to be useful: Statistical software packages

MS 30 Buy one, get one free: Software for twin handling

MS 41 Dynamics in crystals: experimental techniques and software

MS 45 Advances at lower resolutions: new experimental and modeling approaches

+ keynote speaker: Simon Parsons, University of Edinburgh, Edinburgh, Scotland: Absolute Structure Determination

+ Software Fayre

7. Prizes sponsored/coordinated

Poster prize sponsored by OlexSys - to be awarded first at ECM28

A competition will be held for one free registration to ECM28 (open to young members).

8. Past Activities other than Microsymposia at ECM

none this year

For Each Activity

Title:

Number of Participants:

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers
 endorsed (SIG logo on the web page/leaflets)
Sponsored by ECA?
 Yes/ No

Other Sponsors/Organizers:
Short Description: (50 words max.)

9. Future/Programmed Activities.

For Each Activity

Title: Software Fayre at ECM28 - now a MS rather than run separately over two days.

Number of Participants: unknown, since this is a new format.

Level of involvement of SIG in the activity:

- ECA Individual members registered with the SIG involved in the organizing committee 1
 ECA Individual members registered with the SIG involved as lecturers unknown
 endorsed (SIG logo on the web page/leaflets) no

Sponsored by ECA?

Yes/ No no

Other Sponsors/Organizers: no

Short Description: (25 words max.)

Interactive lectures based on use of ~4 different software packages.

Title: Introduction to Software Development for Crystallographers (prior to ECM28)

Number of Participants: 40 +

Level of involvement of SIG in the activity:

- ECA Individual members registered with the SIG involved in the organizing committee 2
 ECA Individual members registered with the SIG involved as lecturers ~5
 endorsed (SIG logo on the web page/leaflets) yes

Sponsored by ECA?

Yes/ No No

Other Sponsors/Organizers: CCP4, CCDC, Rigaku, Dectris, Agilent, Bruker, OlexSys

Short Description: (25 words max.)

lectures and in-depth tutorials outlining how to start implementing crystallography in software - planning, developing pipelines with existing software, use of existing libraries, visualising results, GUI essentials, manipulating matrices, symmetry and space groups, using Fourier methods.

10. Other matters. (50 words max.)

We will be helping the IUCr Commission on Crystallographic Computing to organise and run their workshop prior to IUCr XXIII in Montreal, Canada.

11. Brief annual activity report (100 words max.)

Appointed a SIG Secretary who has been extremely helpful in organising the Computing School.

12. List SIG officers, name and e-mail, and specify their main function in the SIG:

Chairman - Harry Powell, harry@mrc-lmb.cam.ac.uk or hrp1000@cam.ac.uk

Deputy Chairman - Martin Lutz, m.lutz@uu.nl

Secretary - Andrea Thorn, andrea.thorn@WEB.DE

Committee: Laura Rocas, laura.uniovi@gmail.com

Garib Murshudov, garib@mrc-lmb.cam.ac.uk

Rocco Caliandro rocco.caliandro@ic.cnr.it

Supplementary Materials.

(List of all supplementary materials, if any, related to the SIG report)

- Addendum 1 to n (to be sent in separate files)