

SIG No: 9
Reported Period: 2012-2013
Report Date: 17/07/2014
Reported by: Harry Powell

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1. Introduction. (50 words max.)

SIG9 offered help to the IUCr Commission on Crystallographic Computing for their Computing School to be held before IUCr 23. We are also in the early stages of organising a Workshop for younger developers immediately before ECM29 in Rovinj.

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-paymenthtm>)

SIG 9 ecacomsg 178

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: Getting more from your electron density \(joint with SIG7\)](#)

[MS 30: Beyond harmonic treatment](#)

[MS 31: Photocrystallography](#)

+ keynote speakers:

KN5: Zbigniew Dauter, *National Cancer Institute, Argonne National Laboratory, Argonne, IL 60439, USA. "The Brain as a Validation Tool"*

KN9: Lukas Palatinus, *Institute of Physics of the AS CR, Na Slovance 2, 18221 Prague, Czechia* "Charge flipping & Co.: dual space algorithms in crystallography".

+ Software Fayre

7. Prizes sponsored/coordinated

Poster prize sponsored by OlexSys - first awarded at ECM28

A software competition was held for one free registration to ECM28 (open to young members). It was won by Dmytro Guzenko of the University of Leuven, Belgium.

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 ECM29.

Number of Participants: unknown.

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 different software packages.

Title: Younger Developers' Workshop (prior to ECM29)

Number of Participants: 30 +

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.)

An opportunity for younger crystallographic developers (across powder, small molecule and protein crystallography) to meet and discuss their individual software developments and techniques.

10. Other matters. (50 words max.)

We helped the IUCr Commission on Crystallographic Computing to organise their workshop prior to IUCr XXIII in Montreal, Canada which was cancelled due to low registration.

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

Very little.

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 Roces, 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)