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Citation for published version (APA):

Matser, V., Apostolov, R., Carter, A., De Groot, B. L., Harrow, I., Hospital, A., Ippoliti, E., Melquiond, A., Soiland-Reyes, S., & Trellet, M. (Accepted/In press). *Building biomolecular modelling communities through BioExcel Interest Groups*. Poster session presented at ISMB/ECCB 2017, Prague, Czech Republic.

Citing this paper

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Building biomolecular modelling communities through BioExcel Interest Groups

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BioExcel is an EU-funded Centre of Excellence for computational biomolecular research. Despite the importance and increasing adoption of biomolecular simulation techniques, the user communities in Europe are fragmented, possibly excepting communities built around specific codes (e.g. HADDOCK, GROMACS). Support and maintenance of codes is done by small to mid-sized groups, and there is a noticeable lack of overall interactions to ensure coordinated approaches, knowledge transfer and structured initiatives.

The BioExcel vision is to become a focal point for advances in software development, knowledge exchange and support, as well as a networking facilitator for the wider community of computational biomolecular researchers. BioExcel addressed this by creating user-led Interest Groups (IGs), the current IGs are: Entry Level Users, Integrative Modelling, Free energy, Hybrid Methods, Workflows, Industry IG, Training IG. The aim of the IGs are (1) to share BioExcel expertise with members of the groups through workshops, forums and training, (2) to learn from IG members, this could be informal feedback on training needs, software improvement but also more formalised, where IG members join the BioExcel Scientific Advisory Board, (3) enhance the interactions between IG members, including between industry and academia or training professionals. In this poster we present the different Interest Groups, the approaches that each IG has taken to facilitate community building (e.g. newsletter, webinar, online discussions) and what metrics will be used to measure success (e.g. number of active members, workshop attendance). To increase interconnections all IGs are involved in a BioExcel community forum event.