**Integrative/Hybrid (I/H) methods meeting summary, Thursday June 8th, 2017**

We organized a "large" I/H methods virtual meeting with representatives from the I/H methods task force members and the wwPDB partners. Thirteen participants from various groups attended the meeting. Meeting invites were sent to representatives from the following groups.

*I/H methods task force representation and validation sub-group members*

Andrej Sali (UCSF, USA) sali[at]salilab.org

Torsten Schwede (SIB, Switzerland) torsten.schwede[at]unibas.ch

Gerhard Hummer (MPI, Germany) gerhard.hummer[at]biophys.mpg.de

Jens Meiler (Vanderbilt, USA) jens.meiler[at]vanderbilt.edu

Frank DiMaio (U. Washington, USA) dimaio[at]u.washington.edu

Emad Tajkhorshid (UIUC, USA) emad[at]life.illinois.edu

*ChimeraX developers*

RBVI (UCSF, USA) <http://rbvi.ucsf.edu>

*wwPDB partners*

RCSB PDB (Rutgers, USA) <http://www.rcsb.org/>

PDBe (EBI, UK) <https://www.ebi.ac.uk/pdbe/>

PDBj (Osaka U, Japan) <https://pdbj.org/>

BMRB (U. Wisconsin) <http://www.bmrb.wisc.edu/>

*Research groups working on I/H modeling*

Marc Marti-Renom (CNAG, Spain) martirenom[at]cnag.crg.eu

**Meeting Attendees (representatives from the above groups)**

Ben Webb (UCSF, USA) ben[at]salilab.org

Tom Goddard (RBVI, UCSF, USA) goddard[at]cgl.ucsf.edu

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Maggie Gabanyi (RCSB, USA) – Scribe maggie.gabanyi[at]rcsb.org

**Meeting Agenda**

1. Update on I/H methods project - Ben Webb, Brinda Vallat

2. Live demo: Visualization of the Nup84 integrative model using ChimeraX - Tom Goddard

3. Open discussion - Everyone

**Meeting Summary**

1. Brinda Vallat provided an update on the I/H methods project.

* Dictionary is evolving and so are the models. Refer to the IHM extension dictionary at <https://github.com/ihmwg/IHM-dictionary> and the PDB-Dev repository at <https://pdb-dev.rcsb.rutgers.edu/>
* Follow up with other members of this group to obtain dictionary compliant integrative models
* Ensemble coordinates in binary format: Currently testing DCD format for coordinates with topology inferred from the mmCIF file
* Next steps: Generate a multi-state integrative model, enable ChimeraX to write integrative models as mmCIF files, publish the current work

1. Tom Goddard gave a live demonstration of visualizing the Nup84 integrative model with ChimeraX.

* ChimeraX daily build can be downloaded from: <https://www.rbvi.ucsf.edu/chimerax/download.html>
* The Nup84 integrative model can be obtained from: <https://pdb-dev.rcsb.rutgers.edu/>
* Nup84 publication: Yi Shi, Javier Fernandez-Martinez, Elina Tjioe, Riccardo Pellarin, Seung Joong Kim, Rosemary Williams, Dina Schneidman-Duhovny, Andrej Sali, Michael P. Rout, and Brian T. Chait, [Structural characterization by cross-linking reveals the detailed architecture of a coatomer-related heptameric module from the nuclear pore complex](http://mcponline.org/content/early/2014/08/26/mcp.M114.041673), Molecular & Cellular Proteomics, 2014, mcp.M114.041673.
* The live demonstration highlighted the following aspects:
* The coarse-grained structure of the best scoring model comprising of the seven subunits in the Nup84 sub-complex of the yeast nuclear pore complex
* The starting structural models (homology models and X-ray crystal structures) of the seven Nup84 subunits
* Templates and sequence alignments that were used to obtain the homology models
* Spatial restraints derived from experiments: chemical crosslinks (satisfied and violated) and 2DEM class average image. Note: There may be other restraints used in the modeling (such as restraining dimer interface contacts from crystal structures) that are not explicitly defined in the dictionary. These are part of ongoing discussions about whether to include modeling implementation details that are case-specific.
* Visualization of ensembles (accessed as binary DCD files, using the DOI provided in the mmCIF file) and associated localization densities
* Statistics pertaining to chemical crosslinks (histograms of crosslink distances across ensembles)

1. Questions and open discussion followed the presentation. There were questions regarding visualization of validation metrics for crosslinks and visualization of large scale structures of genomes. In the interest of time, some of these in-depth discussions will be carried forward to the regular weekly meetings.