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The DisVis and PowerFit web servers: Explorative and Integrative Modeling of Biomolecular Complexes harvesting EGI GPGPU resources

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Structure determination of complex molecular machines requires combination of an increasing number of experimental methods with highly specialized software geared towards each data source to properly handle the gathered data. Recently we introduced the two software packages PowerFit [1,2] and DisVis [3]. These combine high-resolution structures of atomic subunits with density maps from cryo-electron microscopy or distance restraints, typically acquired by chemical cross-linking coupled with mass spectrometry, respectively. To facilitate their use by a broad community, they have been implemented as web portals harvesting both local CPU resources and GPGPU-accelerated EGI HTC resources [4], making use of GPGPU-enabled Docker containers developed under the MoBrain competence center of EGI-Engage[5] and the INDIGO-Datacloud EU project [6]. The web portals offer user-friendly interfaces, while minimizing computational requirements, and provide a first interactive view of the results. The portals can be accessed freely after registration via http://milou.science.uu.nl/services/DISVIS and http://milou.science.uu.nl/services/POWERFIT.

1. G.C.P. van Zundert and A.M.J.J. Bonvin. Fast and sensitive rigid-body fitting into cryo-EM density maps with PowerFit. *AIMS Biophysics.* **2**, 73-87 (2015).
2. G.C.P van Zundert and A.M.J.J. Bonvin. Defining the limits and reliability of rigid-body fitting in cryo-EM maps using multi-scale image pyramids. *J. Struct. Biol.*, **195**, 252-258 (2016).
3. G.C.P. van Zundert and A.M.J.J. Bonvin. DisVis: Quantifying and visualizing accessible interaction space of distance-restrained biomolecular complexes. *Bioinformatics.* **31**, 3222-3224 (2015).
4. http://www.egi.eu
5. https://mobrain.egi.eu
6. http://www.indigo-datacloud.eu

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