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Academic appointments

Lawrence Berkeley National Laboratory, Molecular Biophysics and Integrated Bioimaging Division, Principal Investigator Paul Adams.

2020-present	Computer Research Scientist
2017-2020	Bioinformaticist Project Scientist
2014-2017	Computational biologist postdoctoral fellow
2007-2013	Institute of Mathematical Problems of Biology of Russian Academy of Sciences, Laboratory of Macromolecular Crystallography, junior research scientist, supervisor Vladimir Lunin.
2008-2009	Lomonosov Moscow State University (Pushchino branch), lecturer of courses "Programming languages and translation methods", "Computer practical course"
2005-2007	Izhevsk State Technical University, lecturer

Education

2013	Ph.D. in Biophysics. Institute of Theoretical and Experimental Biophysics of Russian Academy of Sciences, Pushchino, Russia Thesis: "Detection of alternative conformations in protein crystals by analyzing the mobility of atoms in unrestrained refinement".
2009	M.S. in Applied mathematics and informatics (with honors). Pushchino State University, Pushchino, Russia Thesis: "Unrestrained refinement of biological macromolecules as a tool for detection of alternative conformations".
2007	M.S. in Computer Science (with honors). Izhevsk State Technical University, Izhevsk, Russia Thesis: "Online resource for theoretical study of hydration of biopolymers".

Research activities

2014-present I participate in development of *cctbx* and *Phenix* [7] – software library and suite for the automated determination of molecular structures using X-ray crystallography and other methods (www.phenix-online.org) under supervision of Prof. Paul Adams. I introduced a number of performance improvements of existing code resulted in significant speed up of programs in *Phenix* suite by refactoring and implementing new algorithm in Python as well as in C++. I take part in overall quality assurance including developing new tests and adjusting existing tests, user support and bug fixing including legacy code.

My responsibilities include maintaining *Phenix* tools in compliance with the latest developments in mmCIF format, participating in format development as a member of mmCIF/PDBx working group [9]. I remain in close contact with developers on

wwPDB team to clarify any inconsistencies and ensure rapid implementation in *Phenix*.

Selected projects:

- Rama-Z score for protein backbone validation in close collaboration with PDB-REDO team to ensure consistent results with their implementation [5].
- Collaborations with other software packages including cryo_fit [8] and Schrödinger.
- Core tools including model information handling widely used across the suite. Developing new generation of secondary structure restraints, NCS handling, new validation techniques [11-15].
- Algorithms for protein secondary structure idealization along with appropriate restraints to facilitate low-resolution refinement.
- New type of geometry restraint – parallelity conducted in collaboration with Alexandre Urzhumtsev [16]. This type of restraint will facilitate low-resolution refinement of nucleic acids.
- Implementation of flood-fill algorithm for the search of connected regions in various maps [19], results were used in [6, 10, 17].
- Improving restraints for disulfide bonds in protein structures [18].

2007-2013 Analysis of atomic shifts in unrestrained refinement conducted with Prof. Vladimir Lunin. Refinement of more than 200 high-resolution structures from PDB with phenix.refine and Refmac. Resulted in 5 papers [20-23, 25] and two programs: *Shift_plot* and *AC_prediction* (previously named *DETAC*). The programs were written on Python with matplotlib. Bash scripts were used for automatic structures refinement.

2008-2009 Application of cluster analysis to *ab initio* low-resolution phasing conducted with Prof. Vladimir Lunin and Prof. Alexandre Urzhumtsev (international collaboration between RAS and CNRS). Resulted in a paper [24] and program *ClanGR* used in Buehler *et al*. Acta Cryst D**65**, 644-650. *ClanGR* has graphical user interface based on wxWidgets library and implements interface between Python and Fortran code.

2007 The development of web server for calculation of hydration parameters of biopolymers conducted with Dr. Dmitry Tikhonov. Resulted in a paper [26] and web-site. Involved object-oriented C++ programming, PostgreSQL, HTML, CSS, XML.

Professional activities

Peer review:

- Scientific Reports
- Plos One

Advisory panels:

- Member, mmCIF/PDBx working group (2017-present)

Meetings and symposia

Invited speaker:

2022 4th International Symposium on Cryo-3D Image Analysis, Lake Tahoe, CA, 2022.

2017 RosettaCon 2017. Leavenworth, WA, August, 8-11, 2017.

Oral presentations at international meetings

2014-present 11 talks at Phenix developers semi-annual meetings in Berkeley, Los Alamos, Cambridge and Duke

2020 Bay Area Cryo-EM meeting

2015 XXII West Coast Protein Crystallography Workshop, Monterey, CA, USA
2014 Gordon research seminar: Diffraction methods in structural biology, Lewistone, MA, USA
2013 28th European Crystallographic Meeting, Warwick, England
2012 27th European Crystallographic Meeting, Bergen, Norway
2011 XXII Congress and General assembly of the International union of crystallography, Madrid, Spain

Poster presentations

2019 XXIV West Coast Protein Crystallography Wrokshop, Asilomar, CA, USA
2018 Gordon research conference: Diffraction methods in structural biology, (Lewistone, MA, USA)
2017 XXIII West Coast Protein Crystallography Wrokshop, Asilomar, CA, USA
2014 Gordon research conference: Diffraction methods in structural biology, (Lewistone, MA, USA)
2010 International School of Crystallography, 42th Course (Erice, Italy)
2008 International School of Crystallography, 40th Course (Erice, Italy)

Participation in international schools and workshops

2010 International School of Crystallography, 42th Course (Erice, Italy)
2009 PHENIX Workshop (Strasbourg, France)
2008 International School of Crystallography, 40th Course (Erice, Italy)
2007 Mathematics for Biomedical Engineering Summer School (Warwick, England)

Research Grants

Principal investigator

2012-2013 "Development of objective methods for the identification of alternative conformations of amino acid residues in the protein crystals in X-ray diffraction studies", Russian Foundation for Basic Research, 12-04-31096.

Honors and awards

2017 Best poster presentation at XXIII West Coast Protein Crystallography Workshop, Asilomar, CA, USA
2013 3rd degree diploma of Pushchino competition of young scientists for the best project
2012 Diploma for the best section presentation at 16-th International Pushchino school-conference for young scientists "Biology – science of XXI century"
2009 M.S. Diploma with honors of Pushchino State University.
2008 Diploma for the best section presentation at 12-th International Pushchino school-conference for young scientists "Biology – science of XXI century"
2008 Diploma for the best section presentation on II regional scientific conference for young scientist and students of South of Moscow Region
2008 The "Moscow Region" scholarship from the government of Moscow Region.
2007 M.S. Diploma with honors of Izhevsk State Technical University

Research papers

1. Gydo C.P. van Zundert, Nigel W.Moriarty, **Oleg V.Sobolev**, Paul D.Adams, Kenneth W.Borrelli. (2021) "Macromolecular refinement of X-ray and cryoelectron microscopy structures with Phenix/OPLS3e for improved structure and ligand quality". *Structure*. 913-921.
2. T. C. Terwilliger, **O. V. Sobolev**, P. V. Afonine, P. D. Adams, C.-M. Ho, X. Li and Z. H. Zhou. (2021). "Protein identification from electron cryomicroscopy maps by automated model building and side-chain matching", *Acta Cryst*. **D**77. 457-462.
3. Wang, L., Kruse, H., **Sobolev, O. V.**, Moriarty, N. W., Waller, M. P., Afonine, P. V., Biczysko, M. (2020). Real-space quantum-based refinement for cryo-EM: Q|R#3. *Acta Cryst* **D**76. 1184-1191.
4. Terwilliger, T. C., **Sobolev, O. V.**, Afonine, P. V., Adams, P. D., Read, R. J. (2020). Density modification of cryo-EM maps. *Acta Cryst* **D**76. 912-925.
5. **Sobolev, O. V.**, Afonine, P. V., Moriarty, N. W., Hekkelman, M. L., Joosten, R. P., Perrakis, A., Adams, P. D. (2020). A global Ramachandran score identifies protein structures with unlikely stereochemistry. *Structure*. 28. 1249-1258
6. Terwilliger, T. C., Adams, P. D., Afonine, P. V., **Sobolev, O. V.** (2020). Cryo-EM map interpretation and protein model-building using iterative map segmentation. *Protein Sci*. **29**. 87-99.
7. Liebschner, D., Afonine, P. V., Baker, M. L., Bunkóczi, G., Chen, V. B., Croll, T. I., Hintze, B., Hung, L. W., Jain, S., McCoy, A. J., Moriarty, N. W., Oeffner, R. D., Poon, B. K., Prisant, M. G., Read, R. J., Richardson, J. S., Richardson, D. C., Sammito, M. D., **Sobolev, O. V.**, Stockwell, D. H., Terwilliger, T. C., Urzhumtsev, A. G., Videau, L. L., Williams, C. J., Adams, P. D. (2019). Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix. *Acta Cryst.* **D**75. 861-877.
8. Kim, D. N., Moriarty, N. W., Kirmizialtin, S., Afonine, P. V., Poon, B. K., **Sobolev, O. V.**, Adams, P. D., Sanbonmatsu, K. cryo_fit: Democratization of Flexible Fitting for Cryo-EM. 2019. *Journal of Structural Biology*. **208**. 1-6.
9. Adams, P. D., Afonine, P. V., Baskaran, K., Berman, H. M., Berrisford, J., Bricogne, G., Brown, D. G., Burley, S. K., Chen, M., Feng, Z., Flensburg, C., Gutmanas, A., Hoch, J. C., Ikegawa, Y., Kengaku, Y., Krissinel, E., Kurisu, G., Liang, Y., Liebschner, D., Mak, L., Markley, J. L., Moriarty, N. W., Murshudov, G. N., Noble, M., Peisach, E., Persikova, I., Poon, B. K., **Sobolev, O. V.**, Ulrich, E. L., Velankar, S., Vonrhein, C., Westbrook, J., Wojdyr, M., Yokochi, M. & Young, J. Y. (2019). Announcing mandatory submission of PDBx/mmCIF format files for crystallographic depositions to the Protein Data Bank (PDB). *Acta Cryst*. **D**75, 451-454.
10. Terwilliger, T. C., Adams, P. D., Afonine, P. V., **Sobolev O. V**. (2018). Map segmentation, automated model-building and their application to the Cryo-EM Model Challenge. *J Struct Biol*. **204**. 338-343.
11. Terwilliger, T. C., Adams, P. D., Afonine, P. V. & **Sobolev, O. V.** (2018). A fully automatic method yielding initial models from high-resolution cryo-electron microscopy maps. *Nature Methods*. **15**, 905-908.
12. Afonine, P. V., Klaholz, B. P., Moriarty, N. W., Poon, B. K., **Sobolev, O. V.,** Terwilliger, T. C., Adams, P. D. & Urzhumtsev, A. (2018). New tools for the analysis and validation of cryo-EM maps and atomic models. *Acta Cryst.* **D**74, 814-840.
13. Afonine, P. V., Poon, B. K., Read, R. J., **Sobolev, O. V.,** Terwilliger, T. C., Urzhumtsev, A. and Adams, P. D. (2018). Real-space refinement in PHENIX for cryo-EM and crystallography. *Acta Cryst*. D**74**, 531-544.

14. Terwilliger, T. C., **Sobolev, O. V.,** Afonine, P. V. and Adams, P. D. (2018). Automated map sharpening by maximization of detail and connectivity. *Acta Cryst.* D**74**, 545–559.
15. Liebschner, D., Afonine, P. V., Moriarty, N. W., Poon, B. K., **Sobolev, O. V.**, Terwilliger, T. C. & Adams, P. D. (2017). Polder maps: improving OMIT maps by excluding bulk solvent Acta Cryst. D**73**, 148-157.
16. Sobolev, O.V., Afonine, P.V., Adams, P.D. & Urzhumtsev, A. (2015). Programming new geometry restraints: parallelity of atomic groups. *J. Applied Crystallography*. **48**. 1130-1141.
17. Afonine, P.V., Moriarty, N.W., Mustyakimov, M., **Sobolev, O.V.**, Terwilliger, T.C., Turk, D., Urzhumtsev, A. & Adams, P.D. (2015). FEM: feature-enhanced map. *Acta Cryst* D**71**. 646-666.
18. Sobolev, O.V., Moriarty, N.W., Afonine, P.V., Hintze, B.J., Richardson, D.C., Richardson, J.S. & Adams, P.D. (2015). Disulfide bond restraints. *Computational Crystallography Newsletter*. **6**. 13.
19. Sobolev, O.V., Afonine, P.V. & Adams, P.D. (2014). Connectivity analysis tools in CCTBX. *Computational Crystallography Newsletter*. **5**. 35-37.
20. Sobolev, O.V. Detection of alternative conformations: *Shift_plot* and *AC_prediction* programs. (2013). *J. Appl. Cryst.* **46**. 554-559.
21. Sobolev, O.V. and Lunin, V.Y. Detection of alternative conformations by unrestrained refinement. (2012). *Acta Cryst*. D**68**. 1118-1127.
22. Sobolev, O.V. DETAC: tools to detect alternative conformations by unrestrained refinement. (2012). *Computational Crystallography Newsletter*. **3**. 32-34.
23. Sobolev, O. V., Lunin, V. Y. The use of Refmac crystallographic refinement program for the detection of alternative conformations in biological macromolecules. (2012). *Mathematical Biology and Bioinformatics*. **7**. t16-t24.
24. Sobolev, O.V., Lunina, N.L., Lunin, V.Y. The use of cluster analysis methods for the study of a set of feasible solutions of the phase problem in biological crystallography. (2010). *Computer Research and Modeling*. **2**. 91-101 (in Russian)
25. Sobolev, O. V., Lunin, V. Y. Unrestrained reciprocal space refinement of macromolecular structures as a tool to indicate alternative conformations. (2008). *Mathematical Biology and Bioinformatics*. **3**. 50-59 (in Russian).
26. Sobolev, E.V., **Sobolev, O.V.**, Tikhonov, D.A. Online resource for theoretical study of hydration of biopolymers. (2008). *SAR and QSAR in Environmental Research*. **19**. 303 – 315.