

Oleg V. SOBOLEV

Lawrence Berkeley National Laboratory
1 Cyclotron Road Mailstop 33R0345, Berkeley, CA, USA, 94720
Email: oleg.izhevsk@gmail.com ; Phone: +1 (510) 990-2107 (cell),

Academic appointments

- 2017-present Lawrence Berkeley National Laboratory, Molecular Biophysics and Integrated Bioimaging Division, Bioinformaticist Project Scientist, Principal Investigator Paul Adams.
- 2014-2017 Lawrence Berkeley National Laboratory, Molecular Biophysics and Integrated Bioimaging Division, Computational biologist postdoctoral fellow, Principal Investigator Paul Adams.
- 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 honours). 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 honours). Izhevsk State Technical University, Izhevsk, Russia
Thesis: “Online resource for theoretical study of hydration of biopolymers”.

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.

Meetings and symposia

Invited speaker:

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

Oral presentations at international meetings

- 2015 XXII West Coast Protein Crystallography Wrokshop, 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

- 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 activities

- 2014-present Participation in development of *Phenix* – software 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.
 Development and implementation of algorithm for protein secondary structure idealization along with appropriate restraints to facilitate low-resolution refinement. Conference abstract [2]. Paper is in preparation.
 Development and implementation of new type of geometry restraint – parallelity conducted in collaboration with Alexandre Urzhumtsev resulted in paper [5]. This type of restraint will facilitate low-resolution refinement of nucleic acids.
 Number of performance improvements of existing code resulted in significant speed up of programs in *Phenix* suite.
 Implementation of flood-fill algorithm for the search of connected regions in various maps. Resulted in paper [8], the results were used in paper [6].
 Improving restraints for disulfide bonds in protein structures, resulted in paper [7].
- 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 [9-12, 14] 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 1 paper [13] and program *ClanGR* used in Buehler *et al.* Acta Cryst D65, 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 1 paper [15] and web-site. Involved object-oriented C++ programming, PostgreSQL, HTML, CSS, XML.

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 honours 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 honours of Izhevsk State Technical University

Publications

Research papers

1. 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.* **D74**, 814-840.
2. 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.* **D74**, 531-544.
3. 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.* **D74**, 545–559.
4. 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.* **D73**, 148-157.
5. **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.
6. 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* **D71**. 646-666.
7. **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.
8. **Sobolev, O.V.**, Afonine, P.V. & Adams, P.D. (2014). Connectivity analysis tools in CCTBX. *Computational Crystallography Newsletter.* **5**. 35-37.
9. **Sobolev, O.V.** Detection of alternative conformations: *Shift_plot* and *AC_prediction* programs. (2013). *J. Appl. Cryst.* **46**. 554-559.
10. **Sobolev, O.V.** and Lunin, V.Y. Detection of alternative conformations by unrestrained refinement. (2012). *Acta Cryst.* **D68**. 1118-1127.

11. **Sobolev, O.V.** DETAC: tools to detect alternative conformations by unrestrained refinement. (2012). *Computational Crystallography Newsletter*. **3**. 32-34.
12. **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.
13. **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)
14. **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).
15. 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.

Conference abstracts

1. **Sobolev, O.V.**, Afonine, P.V., Urzhumtsev, A., Moriarty, N.W. & Adams, P.D. (2015). Improving low-resolution refinement of nucleic acids in Phenix. XXII West Coast Protein Crystallography Workshop. March, 15-18, 2015.
2. **Sobolev, O.V.**, Afonine, P.V., Adams, P.D. (2014). Extending Phenix tools for low-resolution refinement against crystallographic and EM data. Gordon research conference and seminar, report and poster. July, 27- August, 1, 2014.
3. Sobolev, O.V. Programs for detection alternative conformations by unrestrained crystallographic refinement. (2013). 17-th International Pushchino school-conference for young scientists “Biology – science of XXI century”, April, 21-26. Proceedings. 85-86.
4. Sobolev, E.V., Pyatkov, M.I., **Sobolev, O.V.** Framework for scientific web-servers. (2013). 17-th International Pushchino school-conference for young scientists “Biology – science of XXI century”, April, 21-26. Proceedings. 79. (in Russian).
5. **Sobolev, O.V.** The detection of alternative conformations during determining molecular structure by X-ray diffraction. (2012). International conference for young scientists “Theoretical and experimental biophysics’12” 22-24 October 2012, Pushchino, Russia. Book of Abstracts. 73.
6. **Sobolev, O.V.**, Lunin, V.Y. Analysis of atomic shifts in crystallographic unrestrained refinement can indicate alternative conformations of amino acid residues. (2012). 4th International Conference Mathematical Biology and Bioinformatics, 14 – 19 October 2012, Pushchino, Moscow region. 143-144.
7. **Sobolev, O.V.**, Lunin, V.Y. The values of atomic shifts in unrestrained refinement can hint alternative conformations. (2012). IV Russian Biophysics Congress, 20-26 August 2012, Nizhny Novgorod. Symposium 1. Book of Abstracts. 273. (in Russian).
8. **Sobolev, O.V.**, Lunin, V.Y. Atomic shifts in unrestrained refinement can indicate alternative conformations. (2012). *Acta Cryst.* **A68**. s81.
Sobolev, O.V., Lunin, V.Y. Atomic shifts in unrestrained refinement can indicate alternative conformations. (2012). 27th European Crystallographic Meeting August 6-11, 2012, Bergen, Norway. Book of abstracts. 88.
9. **Sobolev, O.V.** Statistical evaluation of the decision-making procedures of presence of alternative conformations with macromolecular unrestrained refinement. (2012). 16-th International Pushchino school-conference for young scientists “Biology – science of XXI century”, April, 16-21. Proceedings. 83-84 (in Russian)
10. **Sobolev, O.V.**, Lunin, V.Y.. Unrestrained reciprocal space refinement can indicate alternative conformations. (2011). *Acta Cryst.* **A67**. C104-C105.

- Sobolev, O.V.**, Lunin, V.Y. Unrestrained reciprocal space refinement can indicate alternative conformations. XXII Congress and General assembly of the International union of crystallography, 22-30 August 2011 Madrid, Spain. Book of abstracts. C104-C105.
11. **Sobolev, O.V.** The analysis of atom's mobility during unrestrained refinement. (2011). 15-th International Pushchino school-conference for young scientists "Biology – science of XXI century", April, 18-22. Proceedings. 218 (in Russian)
 12. **Sobolev, O.V.**, Lunin, V.Y., Lunina, N.L., Baumstark, M.W. The use of cylindrical models and cluster analysis for phasing Low Density Lipoprotein particles. (2011). 3rd International Conference Mathematical Biology and Bioinformatics, 10 – 15 October 2010, Pushchino, Moscow region. 173-174.
 13. **Sobolev, O.V.**, Lunin, V.Y., Lunina, N.L., Baumstark, M.W. The use of cylindrical models and cluster analysis in X-ray study of Low Density Lipoprotein particles. (2010). International School of Crystallography, 42th Course Structure and Function from Macromolecular Crystallography: Organisation in Space and Time, Erice, Italy, 3-13 June 2010, Programme, Lecture Notes & Poster Abstracts. 229.
 14. **Sobolev, O.V.** The use of cylindrical models and cluster analysis for phasing of Low-density Lipoproteins. (2010). 14-th International Pushchino school-conference for young scientists "Biology – science of XXI century", April, 19-23. Proceedings, vol.2. 292 (in Russian).
 15. **Sobolev, O.V.** Program ClanGR for cluster analysis of electron density Fourier syntheses. (2009). 13-th International Pushchino school-conference for young scientists "Biology – science of XXI century", September, 28 – October, 2. Proceedings. 262-263 (in Russian).
 16. **Sobolev, O.V.** Unrestrained reciprocal space refinement as a tool to indicate alternative conformations. (2008). 12-th International Pushchino school-conference for young scientists "Biology – science of XXI century", November, 10-14, Proceedings. 341-342 (in Russian).
 17. **Sobolev, O.V.**, Lunin, V.Y. Unrestrained reciprocal space refinement as a tool to indicate alternative conformations. (2008). Proceedings of the II International conference on mathematical biology and bioinformatics. 156-157.
 18. **Sobolev, O.V.** Atomic resolution unrestrained reciprocal space refinement may indicate alternative conformations. (2008). International School of Crystallography, 40th Course From Molecules to Medicine: Integrating Crystallography in Drug Discovery, Erice, Italy, 29 May - 8 June 2008, Programme, Lecture Notes & Poster Abstracts. 384.
 19. Sobolev, E.V., **Sobolev, O.V.**, Tikhonov, D.A., Online resource for theoretical study of hydration of biopolymers. (2007). Fourth International Symposium Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2007), Mocsow, Russia, September 1-5, 2007. 153.
 20. **Sobolev, O.V.**, Sobolev, E.V., Tikhonov, D.A. Hydration microscope. (2007). Proceedings of 11-th International Pushchino school-conference for young scientists "Biology – science of XXI century" October, 29 – November, 2. 61 (in Russian).