Annual Report

Funding Programme:	**Helmholtz Joint Research Groups**
Project ID No.:	HRSF-0002
Project Title:	**New avenues in information and data science: advanced imaging applications at the XFEL and cryo-EM frontier**
Principal Investigator:	Prof. Dr. I.A. Vartaniants
Report Period (=Calendar Year):	01/2019-12/2019

1) Group Structure
   Please report briefly on the structure and personnel development of your group.

Group members on German side:

Prof. Dr. Ivan A. Vartaniants, PhD, senior scientist, group leader, DESY.
Prof. Dr. Wilfried Wurth, PhD, leading scientist, DESY, Hamburg University
Dr. Adrian Mancuso, group leader, Eu. XFEL
Dr. Sergey Lazarev, staff scientist, DESY
Dr. Luca Gelisio, PhD, staff scientist, DESY
Dr. Young Yong Kim, staff scientist, DESY
Mr. Ruslan Khubbutdinov, PhD student, DESY
Mr. Dmitry Lapkin, PhD student, DESY
Mrs. Dameli Assalauova, PhD student DESY
Dr. Ruslan Kurta, staff scientist, Eu. XFEL
Dr. Giuseppe Mercurio, staff scientist, Eu. XFEL
Dr. Jerome Carnis, staff scientist, DESY
Dr. Alexandr Ignatenko, staff scientist, DESY

Group members on Russian side:

Prof. Dr. Vyacheslav Ilyin, PhD, leading scientist, NRC "Kurchatov Institute"
Dr. Alexander Vasiliev, PhD, leading scientist, NRC "Kurchatov Institute"
Anton Teslyuk, leading scientist, NRC "Kurchatov Institute"
Dr. Sergey Bobkov, PhD, staff scientist, NRC "Kurchatov Institute"
Ksenia A. Ikonnikova, PhD student, NRC "Kurchatov Institute"
Timur N. Baymukhametov, PhD student, NRC "Kurchatov Institute"
Evgeniy B. Pichkur, PhD student, NRC "Kurchatov Institute"
Yury M. Chesnokov, PhD student, NRC "Kurchatov Institute"
Sergey I. Zolotarev, PhD student, NRC "Kurchatov Institute"

On German side two scientists (PostDocs) were hired in 2019. These are: Alexandr Ignatenko and Jerome Carnis. Alexandr Ignatenko works on machine learning approaches with applications to single particle imaging data and Jerome Carnis is developing phase retrieval algorithms with applications to coherent X-ray scattering data.
In the year 2019 Max Rose has finished his appointment at DESY, but we keep contacts with him to finalize the work where he is involved.

S. Lazarev has finished his appointment at DESY in September 2019.
W. Wurth passed buy occasionally in 2019 year.

2) Network/ Meetings
Please describe how the group works together. Have there been any international meetings organized by or attended by the group? What is the contribution of the group to the networking of international partners and the Helmholtz Centre?

The group was actively working together. We have two Workshops organized on a German (DESY) and Russian (Moscow) sides (see the schedule of these Workshops in Appendixes).

The first Meeting was organized at DESY on April 1-4, 2019.
The second Meeting was organized at Helmholtz Center in Moscow on November 19-20, 2019.

Besides that we have few short term visits from German side to Russia and from Russia to Moscow for discussions and updates of the project as well as for participation of European XFEL and DESY Photon Science Users Meetings and experiments performed at European XFEL.

We had a longer term (two months) visit of S. Bobkov and S. Zolotarev (NRC "Kurchatov Institute") to DESY, when they were working on the data analysis obtained in several single particle imaging (SPI) experiments at European XFEL.

Results of the research performed in the frame of this Project were reported on a number of National and International Conferences and Workshops (see for the list of Conferences Appendixes).

3) Scientific Progress / Milestones
How has your work plan progressed? What important milestones could be achieved during the report period? Is the progress of your work in accordance with original planning or has the work plan been changed?

Description of work performed in the reporting year and scientific results obtained

A joint project supported by the Helmholtz Association (Germany, HRSF-002 grant) and the Russian Science Foundation (RSF, grant № 18-41-06001) has been carried out by the research teams of DESY (Hamburg) and European XFEL (Schenefeld) on German side and NRC "Kurchatov Institute" (Moscow) on the Russian side from the beginning of 2018 on the topic "New avenues in information and data science: advanced imaging applications at the XFEL and cryo-EM frontier".

Two workshops were organized in the reporting 2019 year. One was organized at DESY, Hamburg (Germany) on April 1-4 (2019) and one in Moscow on November 19-20 (2019). These Workshops were attended by the majority of the project participants from the Russian and German sides. The list of talks presented at these Workshops may be found in the attached files.

Members of the German team (I.A. Vartaniants, Y.Y. Kim, D. Assalauova, A. Ignatenko) together with the members of the Russian team (A. Teslyuk, S. Bobkov, K. Ikonnikova, S. Zolotarev) participated in a three SPI experiments performed at Eu. XFEL during 2019 year (Proposal 2145, May 2019, SPB beamline Eu. XFEL; Proposal 2146, July 2019, SQS beamline Eu. XFEL; Proposal 2316, October 2019, SPB beamline Eu. XFEL).

S, Bobkov and S. Zolotarev stayed at DESY for about two months each (June – August, 2019) to perform research and evaluation of data from these experiments in collaboration with the DESY team.

The main goal of the project is to provide data processing and analysis of streaming data obtained in experiments at the European X-ray Free-Electron Laser (European XFEL) and modern cryogenic electron microscopes (cryo-EM) to study the three-dimensional (3D) structure of single nanoscale particles (viruses, large biological molecules and other biological objects) in the quasi-real-time regime as these data are acquired at the listed experimental facilities.

In 2019, the following results were obtained.

An intermediate software layer for the containerized software platform was developed that is universal for two basic applications - processing of SPI XFEL data and cryo-EM experiments. Development is based on the Docker containerization technology and Kubernetes technology for orchestration of the operation of applied modules in a containerized environment. In this containerized environment in 2020, the application modules will be implemented for forming user versions of the developed software platform with installations on the resources of NRC "Kurchatov Institute" and DESY/Eu-XFEL. On these results the article is prepared, which will be published in early 2020 [11].

An important aspect of the work in 2019 was the coupling of a software platform with the working versions of the platform on the analysis of SPI XFEL and cryo-EM data. On this basis, processing and analysis of SPI XFEL and cryo-EM data was carried out. Analysis of the first SPI data of the end of 2017 experiment at Eu-XFEL, in which participants from the teams of NRC "Kurchatov Institute" and DESY/Eu-XFEL made a key contribution. It was demonstrated that diffraction patterns of individual particles in SPI experiments on Eu-XFEL can be collected using X-ray pulses with the megahertz pulse repetition rate. The results obtained open the way to the use of high-speed XFELs at design frequency to generate diffraction patterns of individual of particles. Based on these results, the SPI Collaboration (8 participants of which are the members of the joint Helmholtz-RSF project) prepared the first reporting article on the experimental study of single nanoscale particles at Eu-XFEL, that will

be published in 2020 [13].

A new module has been developed to estimate the resolution of 3D biomolecule structures in SPI XFEL experiments based on the algorithm of ResMap, used in cryo-EM data analysis. A reporting article has been published on these results [9].

The results of 3D structure recovery and the results of testing of the developed software have been obtained. These results are based on the data obtained at the AMO beamline (LCLS) as part of the SPI Collaboration. The pipeline of SPI reconstruction has been redesigned, additional methods for correction of background scattering have been developed, the existing methods have been modified. It is shown that these results provide an opportunity to eliminate some of the following drawbacks of experimental data: inaccessibility of information from half of the detector, low fraction of diffraction patterns from single particles, lack of information about the central fringe due to the detector protection beamstop. It was demonstrated that the upgraded conveyor system allowed for the 3D reconstruction of the PR772 bacteriophage virus without symmetry constrains. The resolution obtained was better than 8 nm, which was limited by the scattering intensity during the experiment and the number of diffraction patterns of single-particle images. Based on these results the teams of DESY and NRC "Kurchatov Institute" are preparing an article, which will be published in 2020.

A number of results have been obtained on research of three-dimensional structures of biomolecules and viruses in cryo-EM experiments. These results were obtained using the individual steps of the containerized software platform. As such, the platform that is currently under development was tested in the real case studies of reconstruction of 3D biomolecule structure from cryo-EM data. Among the obtained results are the results of research on Chaperonin structures - biomolecules involved in the coagulation of other proteins as well as cryo-EM analysis results on cryo-EM tomography data and small-angle X-ray scattering data on Dps-DNA structures. These results formed the basis for two reporting publications that will be published in 2020 [14, 15].

In addition to this work DESY and XFEL participants of the Project were strongly contributing to research performed at different FEL facilities [1, 2, 12]. A femtosecond resolution X-ray free-electron laser pump-probe experiment with solvated PtPOP metal complex molecules was analyzed by our teams [1]. The molecules were pumped with linear polarized laser pulses creating an excited state population with a preferred orientational (alignment) direction. Two time scales of 1.961.5 ps and 46610 ps were revealed by angular X-ray Cross-Correlation Analysis (AXCCA) associated with structural changes and rotational dephasing of the solvent molecules, respectively. We demonstrate the structural sensitivity and accuracy of the x-ray standing wave technique at a high repetition rate free-electron laser, FLASH at DESY in Hamburg was demonstrated, by measuring the photoelectron yield from

the surface SiO2 of Mo/Si multilayers [2]. These experiments open up the possibility to obtain an unprecedented structural information of adsorbate and surface atoms with picometer spatial and femtosecond temporal resolution. And, finally, we reported on a pump-probe diffraction experiment performed at the LCLS on a colloidal crystal [12]. The IR laser intensity was sufficient to form a periodic plasma state on top of the colloidal crystal. The periodicity of the colloidal crystal and thus created plasma allowed us to study the plasma dynamics with a picosecond time resolution via Bragg peak analysis.

In the frame of FEL studies the group at DESY is developing new imaging schemes based on quantum imaging protocol, the corresponding paper was accepted for publication in the end of 2019 [10]. In this work the results of a classical ghost imaging experiment accomplished at an XUV FEL source FLASH are presented. We demonstrate the possibility of image formation, a double bar in our case, in the beam that has never interacted with the sample. With this experiment we extend the quantum optics methodology to the FEL community.

Group at DESY worked as well on the development of various methods of data analysis and, especially, on the method of AXCCA. An overview of this relatively new technique describing the potentials and applications of this technique to study soft- and hard-condensed matter samples was published this year [5]. This approach in combination with X-ray nanodiffraction was applied to study the formation and correlation of domain boundaries in mesocrystalline superlattices of PbS nanocrystals with face-centered cubic structure [7].

Important developments were obtained in the study of catalysis problem by the DESY group [3,8]. Using coherent X-ray diffraction imaging (CXDI) as an in situ tool, we determined the shape and strain state of a platinum nanoparticle [3]. The experiment was performed at a temperature of 400 K under continuous gas flow conditions of pure Ar and Ar/CO mixtures. Our analysis suggests that under mixed Ar/CO flow at 400 K reshaping of the nanoparticle occurred. New high index facets developed, leading to a stronger lattice expansion, also propagating into the nanoparticle bulk. Our high-resolution experiments pave the way for future CXDI experiments under operando catalytic reaction conditions.

Another important topic of research of the DESY group was understanding of coherence properties of 4-th generation storage rings with ultra-low emittance values [6]. It is presently expected that a storage ring with emittance values of 10 pm rad will reach diffraction limit at hard X-rays. Our analysis have shown that, for the parameters of the storage ring considered in this work, the diffraction limit will be reached for soft X-ray energies. About ten modes will contribute to the radiation field at 12 keV photon energy and even more modes give a contribution at higher photon energies. This analysis shows that, to reach the diffraction limit for high photon energies, electron beam emittance should go down to 1 pm rad and below.

Conferences participation

The results of our joint work were presented on a number of national and International Conferences and Workshops (see list of Conferences attached below). To list just one event, our joined German – Russian group was invited to present our research in the frame of the Helmholtz Associations Initiative and Networking Fund and Russian Science Foundation grant at the IV Russian young scientists forum «Science of future – science of young people» in the frame of III International science conference «Science of future», Sochi, May 14-17, 2019. This was a special day event dedicated to Helmholtz-Russia collaboration and called "Russian-German day". Presentation was made jointly by N. Mukharamova (DESY), I.A. Vartaniants (DESY), and V. Ilyin (NRC "Kurchatov Institute") with the topic: "New avenues in information and data science: advanced imaging applications at the XFEL and cryo-EM frontier".

4) Financial Plan / Time Schedule
Can you comply with the financial plan and time schedule or do you see a need for adjustment?

Financial plan and time schedule looks fine and we do not see any needs for adjustment.

It was some left over of consumables cost money, which was transferred to this year and will be spend this year.

5) Publications of the Group

List of publications in the year 2019 with acknowledgements to grant funding

1. P. Vester, I.A. Zaluzhnyy, **R. P. Kurta**, K. B. Møller, E. Biasin, K. Haldrup, M. M. Nielsen, and **I.A. Vartanyants**, "Ultrafast structural dynamics of photo-reactions observed by time-resolved x-ray cross-correlation analysis", Struct. Dyn., **6**, Issue 2, 024301 (2019). DOI: 10.1063/1.5086374, Impact factor: 1.617.
2. **G. Mercurio**, I. A. Makhotkin, I. Milov, **Y. Y. Kim**, I. A. Zaluzhnyy, S. Dziarzhytski, L. Wenthaus, **I. A. Vartanyants**, and **W. Wurth**, "Towards Time-Resolved Atomic Structure Determination by X-Ray Standing Waves at a Free-Electron Laser", New J. Phys. **21** 033031 (2019). DOI: 10.1088/1367-2630/aafa47, Impact factor: 3.773.
3. M. Abuin, **Y. Y. Kim**, H. Runge, S. Kulkarni, S. Maier, D. Dzhigaev, **S. Lazarev**, **L. Gelisio**, Ch. Seitz, M.-I. Richard, T. Zhou, V. Vonk, Th. F. Keller, **I. A. Vartanyants,** and A. Stierle, "Coherent X-ray Imaging of CO-Adsorption-Induced Structural Changes in Pt Nanoparticles: Implications for Catalysis", ACS Appl. Nano Mater. **2** 4818-4824 (2019). DOI: 10.1021/acsanm.9b00764.
4. **S. Lazarev**, D.J. O. Göransson, M. Borgström, M. E. Messing, H. Q. Xu, D. Dzhigaev, O. M. Yefanov, S. Bauer, T. Baumbach, R. Feidenhans'l, L. Samuelson, and **I. A. Vartanyants**, "Revealing misfit dislocations in InAs0.26P0.74-InP core-shell nanowires by x-ray diffraction", Nanotechnology **30** 505703 (2019). DOI: 10.1088/1361-6528/ab40f1. Impact factor: 3.399.
5. I.A. Zaluzhnyy, **R. P. Kurta**, M. Scheele, F. Schreiber, B. I. Ostrovskii, and **I. A.**

Vartanyants, "Angular X-Ray Cross-Correlation Analysis (AXCCA): Basic Concepts and Recent Applications to Soft Matter and Nanomaterials", Materials, **12**(21), 3464 (2019). DOI: 10.3390/ma12213464. Impact Factor: 2.972.

6. **R. Khubbutdinov**, A. P. Menushenkov, **I. A. Vartanyants**, "Coherence properties of the high-energy fourth-generation X-ray synchrotron sources", J. Synchrotron Rad. **26**(6), 1851-1862 (2019). DOI: 10.1107/S1600577519013079. Impact factor = 3.232.

7. **N. Mukharamova**, **D. Lapkin**, I. A. Zaluzhnyy, A. André, **S. Lazarev**, Y. Y. Kim, M. Sprung, **R. P. Kurta**, F. Schreiber, **I. A. Vartanyants**, M. Scheele, "Revealing Grain Boundaries and Defect Formation in Nanocrystal Superlattices by Nano- diffraction", Small, 1904954 (2019). DOI: 10.1002/smll.201904954. Impact factor = 10.856.

8. T. Kawaguchi, Th. F. Keller, H. Runge, **L. Gelisio**, Ch. Seitz, **Y. Y. Kim**, E. R. Maxey, W. Cha, A. Ulvestad, S. O. Hruszkewycz, R. Harder, **I. A. Vartanyants**, A. Stierle, and H. You, "Gas-induced segregation in Pt-Rh alloy nanoparticles observed by in-situ Bragg coherent diffraction imaging", Phys. Rev. Lett. **123**, 246001 (2019). DOI: 10.1103/PhysRevLett.123.246001. Impact factor = 9.227.

9. **K.A. Ikonnikova, A.B. Teslyuk, S.A. Bobkov, S.I. Zolotarev, V.A. Ilyin** Reconstruction of 3D structure for nanoscale biological objects from experiments data on super-bright X-ray free electron lasers (XFELs): dependence of the 3D resolution on the experiment parameters Procedia Computer Science (2019 г.)

10. **Y. Y. Kim**, **L. Gelisio**, **G. Mercurio**, S. Dziarzhytski, M. Beye, L. Bocklage, A. Classen, Ch. David, O. Yu. Gorobtsov, **R. Khubbutdinov**, **S. Lazarev**, **N. Mukharamova**, Yu. N. Obukhov, B. Roesner, K. Schlage, I. A. Zaluzhnyy, G. Brenner, R. Roehlsberger, J. von Zanthier, **W. Wurth**, and **I. A. Vartanyants**, "Ghost Imaging at an XUV Free-Electron Laser", Phys. Rev. A (2020) (accepted).

11. **A. Tesliuk**, **S. Bobkov, V. Ilyin**, A. Novikov, A. Poyda, V. Velikhov, "Kubernetes container orchestration as a framework for flexible and effective scientific data analysis." Proceedings of the ISPRAS Open conference (ISPRAS OPEN 2019), IEEE Xplore digital library. (2020) (accepted)

12. **N. Mukharamova**, **S. Lazarev**, J.-M. Meijer, O. Yu. Gorobtsov, A. Singer, M. Chollet, M. Bussmann, D. Dzhigaev, Y. Feng, M. Garten, A. Huebl, Th. Kluge, **R. P. Kurta**, V. Lipp, R. Santra, M. Sikorski, S. Song, G. Williams, D. Zhu, B. Ziaja-Motyka, Th. Cowan, A. V. Petukhov, and **I. A. Vartanyants**, "Femtosecond laser produced periodic plasma in a colloidal crystal probed by XFEL radiation", Nature Communications (2019) (submitted).

13. E. Sobolev, **S. Zolotarev**, K. Giewekemeyer, J. Bielecki, …, **S. Bobkov**, H. N. Chapman, …, **L. Gelisio**, …, **V. Ilyin**, …, **M. Rose**, …, **A. Teslyuk**, …, **I. Vartanyants**, V. S. Lamzin, A. Mancuso, F. R. N. C. Maia, "Megahertz single-particle imaging at the European XFEL", Communication Physics (2019) (submitted).

14. **R. Kamyshinsky**, **Yu. Chesnokov**, L. Dadinova, A. Mozhaev, I. Orlov, M. Petoukhov, A. Orekhov, E. Shtykova, **A. Vasiliev**, "Polymorphic protective Dps-DNA co-crystals by Cryo Electron Tomography and Small Angle X-ray Scattering", Biomolecules (accepted) (2020).

15. T. B. Stanishneva-Konovalova, P. I. Semenyuk, L. P. Kurochkina, **E. B. Pichkur**, **A. L. Vasilyev**, M. V. Kovalchuk, M. P. Kirpichnikov, O. S. Sokolova, "Cryo-EM reveals an asymmetry in a novel single-ring viral chaperonin", J. of Structural Biology (accepted) (2020).

6) External Funding

7) Patent Applications   *No. of pending/granted patents*
We did not submitted any Patent Applications
8) Awards received by Group Members
M. Rose received 2019 PhD Award of the Association of the Friends and Sponsors of DESY for his Thesis.

Appendixes: I

Conferences where results in the frame of the grant funding were presented

1. European XFEL Users' Meeting and DESY Photon Science Users' Meeting "Research with Synchrotron Radiation and FELs". DESY Hamburg (Germany), 23 - 25 January 2019, https://indico.desy.de/indico/event/21832/overview

   Satellite Meeting: Coherent X-ray scattering and imaging at P10 / PETRA III (January 24, 2019)

   Oral presentations:
   I.A. Vartaniants (DESY)
   "Basics of Coherent X-ray Scattering Technique"
   N. Mukharamova (DESY), **D. Lapkin** (DESY), I.A. Zaluzhnyy (DESY), A. André, **S. Lazarev** (DESY), **Y.Y. Kim** (DESY), M. Sprung, **R.P. Kurta** (DESY), F. Schreiber, **I.A. Vartanyants** (DESY), and M. Scheele,.
   "Revealing Grain Boundaries and Defect Formation in Nanocrystal Superlattices by Nanodiffraction"

   Posters:
   S.A. Bobkov (NRC KI),
   "First elements of data flow processing pipeline for SPI experiments at European XFEL",

   S. Zolotarev (NRC KI),
   "Classification of diffraction images from the first SPI experiment at European XFEL".

   D. Lapkin (DESY), **N. Mukharamova** (DESY), I. Zaluzhnyy, **R.P. Kurta** (DESY), **R. Khubbutdinov** (DESY), **Y.Y. Kim** (DESY), E. Morozova, A. Andre, D. Dzhigaev, M. Osterhoff, M. Sprung, F. Schreiber, **I.A. Vartanyants** (DESY), and M. Scheele,
   "X-ray Cross-Correlation Analysis of PbS-Cu4APc Mesocrystals"

   D. Assalauova (DESY),
   "Data analysis of single particle imaging experiments of viruses at XFELs"

   R. Khubbutdinov (DESY), R. Chernikov, K. Klementiev, A. P. Menushenkov, and **I. A. Vartanyants** (DESY),
   "Coherence properties of 4th generation synchrotron sources.".

   Y. Y. Kim (DESY),
   "Ghost Imaging at Free-Electron Laser".

2. EMBL Industry Workshop – Cryo-EM in Industry and Academia, EMBL Heidelberg (Germany), 6-8 February 2019, https://www.embl.de/training/events/2019/CPP19-01/Pre-conference-Workshops/Leica/.

   Posters:
   K. V. Boyko, **T.N. Baymukhametov** (NRC KI), **Yuri M. Chesnokov** (NRC KI),…
   Alexander Vasiliev (NRC KI) et al.,

"3D structure of natural tetrametric form of human butyrylcholonesterase obtained by Cryo-electron microscopy".

3. IV Russian young scientists forum «Science of future – science of young people» in the frame of III International science conference «Science of future», Sochi, May 14-17, 2019, https://www.sfy-conf.ru.

   Invited talk at the «Russian-German day» May 16, 2019.
   N. Mukharamova (DESY), **I.A. Vartaniants** (DESY), and V. Ilyin (NRC KI),
   "New avenues in information and data science: advanced imaging applications at the XFEL and cryo-EM frontier".

4. Russian International Conference on Cryoelectron Microscopy 2019 (RICCEM2019), Lomonosov MSU (Moscow, Russia), June 2-5, 2019, http://riccem.org)

   Posters:
   T.N. Baymukhametov (NRC KI), **Yu.M. Chesnokov** (NRC KI), Zh.A. Afonina, **A.L. Vasiliev** (NRC KI),
   «Cryo-ET pipeline on the example of structural analysis of polyribosomes».

   Zh.A. Afonina, **T.N. Baymukhametov** (NRC KI), D.N. Lyabin, **Yu.M. Chesnokov** (NRC KI), **A. L. Vasiliev** (NRC KI),
   «Cryo-ET structural analysis of polyribosomes from HeLa cells».

5. 8th International Young Scientists Conference on Computational Science (YSC2019), Heraklion (Greece), June 2019, http://ysc.escience.ifmo.ru

   Oral presentations:
   K. Ikonnikova (NRC KI),
   "Reconstruction of 3D structure for nanoparticle biological objects from experiments data on super-bright X-ray free electron lasers (XFELs): dependence of the 3D resolution on the experiment parameters", http://ysc.escience.ifmo.ru/files/YSC_program.pdf

   D. Assalauova (DESY),
   «Data analysis of single particle imaging experiments of viruses at the XFEL sources», http://ysc.escience.ifmo.ru/files/YSC_program.pdf

6. SILS 2019 - Annual Meeting of the Italian Synchrotron Radiation Society
   Camerino (Italy) 9-11 September 2019
   https://www.unicam.it/
   L. Gelisio, Y. Y. Kim, S. W. Lim, D. Nam, I. Eom, M. Kim, X. Li, H. Lee, R. Khubbutdinov, M. Daka, K. R. Beyerlein, M. Altarelli, P. Fornasiero, S. Kim, M. Ree, C. U. Kim, and I. A. Vartanyants «Structural evolution of Platinum nanostructured thin films driven by ultrashort IR radiation»

7. The 27th International Symposium Nuclear Electronics and Computing (NEC'2019), Budva (Montenegro), 30 September – 4 October 2019, http://indico-ew.jinr.ru/event/738/.

Oral presentation:
A.B. Teslyuk (NRC KI)
«Containerized services for FEL data processing»,
https://indico.jinr.ru/event/738/material/paper/13.pdf,
https://indico.jinr.ru/event/738/session/18/contribution/192/material/slides/0.pdf;

V.A. Ilyin (NRC KI), invited talk on International student school in the frame of symposium NEC'2019,
«Use of advanced computer science technologies for quasi-online data processing and primary analysis in the pipe-line approach – on example of experiments on EU-XFEL and CryoEM in structural biology», https://indico.jinr.ru/event/907/page/8.

8. Artificial Intelligence Applied to Photon and Neutron Science, ESRF Grenoble (France), 12-14 November 2019, https://workshops.ill.fr/event/209/overview.

   Posters:
   S.A. Bobkov (NRC KI), **A.B. Teslyuk** (NRC KI), **S.I. Zolotarev** (NRC KI), **V.A. Ilyin** (NRC KI), **A. Ignatenko** (DESY), **D. Assalauova** (DESY), **L. Gelicio** (DESY), SPI consortium, F. Maia, **I.A. Vartanyants** (DESY)
   "Machine learning for Single Particle Imaging at European XFEL".

   A. Ignatenko (DESY), **D. Assalauova** (DESY), **S. Bobkov** (NRC KI), **L. Gelisio** (DESY), SPI consortium@LCLS, A. Aquila, **I. A. Vartaniants** (DESY)
   "Image classification for Single Particle Imaging experiments with a fast object detection system based on a Convolutional Neural Network"

9. 2nd Round Table on Machine Learning and Deep Learning at DESY, Hamburg Germany), November 29, 2019, https://indico.desy.de/indico/event/24634/

   Oral presentation:
   A. Ignatenko (DESY)
   "Image classification for Single Particle Imaging experiments with a fast object detection system based on a Convolutional Neural Network"

10. Open Conference in the Institute for System Programming V.P. Ivannikova RAS, Moscow, 5-6 December 2019. https://www.isprasopen.ru

    Oral presentation:
    A.B. Teslyuk (NRC KI), **S.A. Bobkov** (NRC KI), A. Novikov (NRC KI), A. Poida (NRC KI), **V.A. Ilyin** (NRC KI), V. Velikhov (NRC KI)
    «The use of Kubernetes as a framework for building flexible and effective scenarios for scientific data processing»
    https://www.isprasopen.ru/docs/Agenda_ISP_RAS_Open_RU.pdf.

Appendixes: II

RSF-Helmholtz Meeting April 1-4, 2019
DESY Bld. 25f, Seminar Rm. 456
Schedule draft
April 1, 2019

Arrival to DESY

15:00 – Visit to European XFEL

April 2, 2019

8:45 – 9:00 E. Weckert(DESY) – Welcome to DESY

9:00 – 9:15 I. Vartaniants (DESY) – Status of the Project DESY view

9:15 – 9:30 V. Ilyin (NRC "Kurchatov Institute") – Status of the Project Kurchatov Institute view

9:30 – 10:00 A. Vasiliev (NRC "Kurchatov Institute") – Cryo-EM, Status of the Project

10:00 – 10:30 W. Wurth (DESY, HH University) – FLASH2020 and Big Data evaluation challenges

10:30 – 11:00 Coffee break

11:00 – 11:30 P. Vagovic (European XFEL) – SPB/SFX Instrument at European XFEL, first results of operation

11:30 – 12:00 A. Teslyuk (NRC "Kurchatov Institute") – On progress in setting up data processing workflow in containerized computing infrastructure at Kurchatov Institute

12:00 – 12:30 G. Mercurio (European XFEL) – Status of the SCS instrument at European XFEL

12:30 – 14:00 Lunch

14:00 – 14:30 S. Bobkov (NRC "Kurchatov Institute") – Automatic preprocessing, filtering and classification of SPI data on the basis of LCLS amo34117 experiment.

14:30 – 15:00 R. Kurta (European XFEL) – Fluctuation x-ray scattering from a heterogeneous mixture of particles

15:00 – 15:30 Ev. Pichkur (NRC "Kurchatov Institute") – Recent advances in the first stages of Cryo-EM processing

15:30 – 16:00 Coffee break

16:00 – 16:15 R. Kamyshinskii (NRC "Kurchatov Institute") – Cryo electron tomography study of processes of byocrystallization for DNA protection

16:15 – 16:30 T. Baymukhametov (NRC "Kurchatov Institute") – Cryo-EM of polysoms issues in 3D reconstruction

16:30 – 16:45 Yu. Chesnokov (NRC "Kurchatov Institute") – Data processing for cryo-electron tomography study of Dps-DNA nanocrystals

16:45 – 17:00 S. Zolotarev (NRC "Kurchatov Institute") – Viability analysis of alterations of EMC algorithm based on modifications to underlying EM method

17:00 – 17:15 K. Ikonnikova (NRC "Kurchatov Institute") – Analysis of 3D structure resolution limits in X-ray single particle diffraction imaging with different experimental parameters

17:15 – 17:30 D. Assalauova (DESY) – Progress of analysis of data from the last SPI experiment at LCLS

17:30 – 17:45 Y.Y. Kim (DESY) – Towards high resolution reconstruction from the SPI XFEL data

17:45 – 18:00 D. Lapkin (DESY) – XCCA analysis of mezocrystal samples

18:00 – 18:15 L. Gelisio (DESY) – Time resolved melting experiment on thin Pt films at PAL XFEL

18:15 – 18:30 I. Vartaniants (DESY)
Summary of the first day and tasks for the second day

19:00 – Dinner (DESY Bistro)

April 3, 2019

9:00 – 10:30 Discussion of the milestones of the Project

10:30 – 11:00 Coffee break

11:00 – 12:30 Discussion of the milestones of the Project

12:30 – 14:00 Lunch

14:00 – 15:00 Discussion of the milestones of the Project

15:00 I. Vartaniants (DESY) & V. Ilyin (Kurchatov Institute)
Concluding remarks and close of the Meeting

Meeting of the Joint RSF-Helmholtz project
RSF № 18-41-06001, Helmholtz grant № HRSF-002
"New avenues in information and data science: advanced imaging applications at the XFEL and cryo-EM frontier"
19-20 November 2019, Moscow

Place – Malaya Pirogovskaya, dom 7.

November, 19, 10.00 -17.00

1. V. Ilyin (NRC "Kurchatov Institute"). Open remarks. "Status of the German-Russian Project (Russian side)" 15 min
2. I. Vartaniants (DESY). "Status of the German-Russian Project (German side)", 15 min
3. A. Vasiliev (NRC "Kurchatov Institute"). "Status of the cryoEM research in the project", 15 min
4. Anton Teslyuk (NRC "Kurchatov Institute"), "On the progress of development containerized data analysis pipeline for FEL data", 45 min

   Coffee break 11:30-12:00

5. A. Ignatenko (DESY), "Image classification from the Single Particle Imaging (SPI) experiments with a fast object detection system based on a Convolutional Neural Network (CNN)", 30 min
6. Sergey Bobkov (NRC "Kurchatov Institute"), "Automatic data processing organization for SPI
   analysis pipeline", 30 min
7. D. Assalauova (DESY), "Reconstruction of PR772 viruses from the Single Particle Imaging (SPI) experiments at LCLS, 30 min

   Lunch 13:30-14:30

8. Yury Chesnokov (NRC "Kurchatov Institute"), «Problem of preferred orientation in single-particle cryo-EM», 30 min
9. Sergey Zolotarev (NRC "Kurchatov Institute"), "Combining heterogeous data for orientation
   recovery via Dragonfly", 30 min
10. D. Lapkin (DESY), "CuZrTi metallic glasses. "Study of the local structure by the electron diffraction", 30 min

    Coffee break 16:00-17:30

11. Valeria Samigina (NRC "Kurchatov Institute") " TVEV characterization for XFEL experiment ", 30 min
12. Timur Baymukhametov (NRC "Kurchatov Institute"), «Project start: "New approaches in studying mechanisms of translation using cryo-electron microscopy"», 30 min
13. Ksenia Ikonnikova (NRC "Kurchatov Institute"), "Local resolution estimation for FEL data", 30 min

Welcome party 18:00.

November, 20, 10.00-15.00

14. Alexander Kryukov (SINP MSU). Invited talk "Machine learning in analysis of astrophysical data"   10:00-10:30
15. R. Khubbutdinov (DESY), "Hanbury Brown and Twiss experiment at SCS Instrument at European XFEL", 10:30-11:00
16. Eugene Pichkur (NRC "Kurchatov Institute"), «Recent advances in cryoEM software" (by Skype), 11:00-11:30   30 min

    Coffee break 11:30-12:00

17. Alexander Vasiliev (NRC "Kurchatov Institute"), "Recent advances in cryoEM experiments", 12:00-12:30   30 min
18. Round table "The project 2019-2020 planning and general discussion", 12:30-14:30
19. Closing remarks