Domain-Specific Services in Polish e-Infrastructure

Jacek Kitowski[1,2], Kazimierz Wiatr[1], Łukasz Dutka[1], Tomasz Szepieniec[1], Mariusz Sterzel[1], and Robert Pająk[1]

[1] AGH University of Science and Technology, ACC Cyfronet AGH, ul. Nawojki 11, 30-950 Kraków, Poland

[2] AGH University of Science and Technology, Faculty of Computer Science, Electronics and Telecommunications, Department of Computer Science, al. Mickiewicza 30, 30-059 Kraków, Poland

Abstract. Modern e-infrastructures provide huge computational power and storage capacities to their users. While increasing capacity and progressing with technological advancement is gradually ceasing to be a problem, making these infrastructures easy-to-use for their users is still a challenge. The barrier the users have to overcome to use an e-infrastructure in their scientific experiments is still high – it is almost impossible to do this without prior training on the infrastructure usage and without knowledge of UNIX-like systems. At the same time, the user is offered more and more easy to use tools in many other fields. The increasing gap between the users' skills and competence required to effectively use the e-infrastructure services needs to be bridged with a new layer of services which are specific to a given domain of science and more easy to use by researchers. The paper introduces the foundations of the PL-Grid Infrastructure, the objectives of the PLGrid Plus project and shortly describes several sample domain-specific services and tools, developed and deployed in the Polish computational e-infrastructure to overcome the aforementioned problems.

Keywords: domain-specific solutions, computing services, IT infrastructure.

1 Polish Grid Infrastructure

The Polish Grid Infrastructure [1] has been created within the PL-Grid project (2009-2012) [2,3]. It was then that the basic infrastructure has been developed. Soon, in March 2010, the PL-Grid Infrastructure turned out to be the first operational National Grid Initiative (NGI) in Europe. Since then, the users not only have been able to conduct interdisciplinary research on a national scale, but also have been given transparent access to international grid resources. Next, the PLGrid Plus project (2011-2014) [4] was started, aiming at the infrastructure extension with specific environments, solutions and services, developed according to the identified needs of different groups of scientists. Both projects were

M. Bubak et al. (Eds.): PLGrid Plus, LNCS 8500, pp. 1–15, 2014.

maintained by the Polish Grid Consortium [5] and co-funded by the European Regional Development Fund as a part of the Innovative Economy program.

This development was possible thanks to the experience the members of the Polish Grid Consortium had gained in previous years – by coordinating big infrastructure projects (e.g. [6]) or participating in their accomplishment [7], as well as in development of tools (e.g. [8]) or applications porting (e.g. [9]).

2 Domain-Specific Services – PLGrid Plus Solution

Contemporary science shows a great demand for networking, data storage, computing provided by e-infrastructures. However, from the point of view of a domain scientist, using the modern computing systems, services and tools of these infrastructures often becomes relatively difficult. Therefore, the scientists need assistance and close collaboration with service providers.

The main aim of the PLGrid Plus project [4] is to lower the barriers required for the researchers to use the infrastructure provided in PL-Grid, and, thus, attract new communities of the users, who need the computational power and large disk space of supercomputers but have no or little skills in using it. To achieve this, a number of domain-specific environments, i.e., solutions, services and extended infrastructure (including software) has been developed to serve researchers from specific domains of science. To enable and facilitate development of these domain-specific environments, the project relies on a broad cooperation with representatives of various disciplines (domain experts), often grouped in domain consortia. Direct cooperation with them, mostly through involvement in the project activities, ensures matching of computing, software, databases and storage services to the actual needs.

The domain-specific services are built on top of PL-Grid core services that are used to communicate with the computing and storage infrastructure (see Fig. 1). These core services include e.g. middleware – at present, PL-Grid Infrastructure users can choose from three major middleware suites to run their computations: gLite [10], UNICORE [11] and QosCosGrid [12].

The domain-specific services hide the complexity of the underlying infrastructure and, at the same time, expose the actual functions that are important to the researchers of the given domain (see Section 3). In this way, the users are provided with exactly the functionality they need. What is more, it is exposed to them in their domain-specific manner to achieve maximum intuitiveness and usefulness.

The activities realized in the PLGrid Plus project, aiming at the development of the domain-specific services, can be grouped into several categories:

- Integration Services: dedicated portals and environments, unification of distributed databases, virtual laboratories, remote visualization, service value (utility and warranty) facilities, SLA management – all at national and international levels,
- Computing-Intensive Solutions: specific computing environments, adoption of suitable algorithms and solutions, workflows, cloud computing, porting scientific packages,

– Data Intensive Computing: access to distributed scientific databases, homogeneous access to distributed data, Big Data (data discovery, processing, visualization, validation, etc.), 4th paradigm of scientific research (data intensive scientific discovery),
– Instruments in Grid: remote transparent access to instruments, sensor networks,
– Organizational: organizational backbone, professional support for specific disciplines and topics, rich international collaboration (EGI.eu [13], EGI-InSPIRE [14], EMI [15], PRACE [16], etc.).

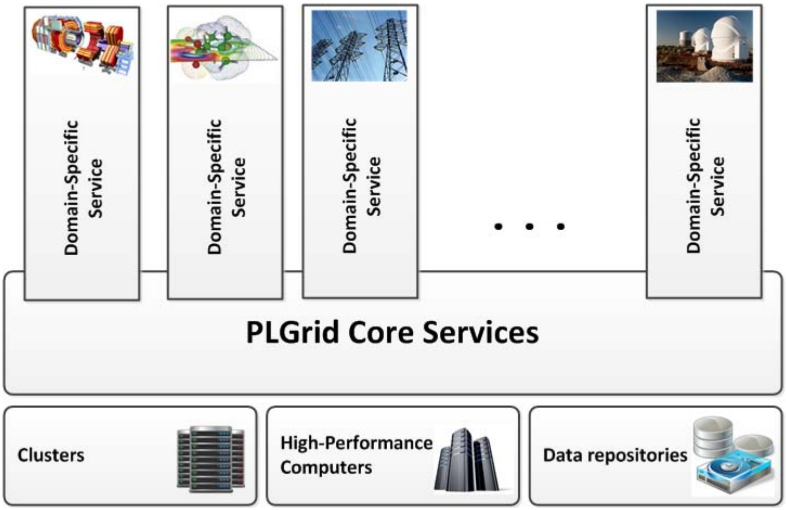

Fig. 1. Layered view of the PL-Grid Infrastructure

To provide support for building the domain-specific services, interdisciplinary teams have been established, gathering both e-infrastructure and domain experts. The teams work in short cycles providing the required functionality. The design of a particular service is based on the needs articulated by the researchers from a respective domain of science. Then, the service is developed in cooperation of computer scientists and domain experts, until it can be deployed and connected to the infrastructure. Finally, it is published and, after acceptance tests, made accessible to all the users who request it.

Currently, the PLGrid Plus project supports 13 different domains of science with their domain-specific services: Acoustics, AstroGrid-PL, Bioinformatics, Quantum Chemistry and Molecular Physics, Ecology, Energy Sector, Health Sciences, HEPGrid, Life Science, Materials, Metallurgy, Nanotechnologies, and SynchroGrid. Each of them requires different approach and different tools.

Introduction of domain-oriented solutions for these 13 communities [17,18] broadened the scope of use of the project's results to various research groups. Moreover, the experience in building domain services along with the existing offer of general services should make the integration of new groups smooth and much less expensive.

Access to the PL-Grid Infrastructure's computing resources is free to Polish researchers and everyone involved in scientific activities who is associated with a university or research institute in Poland. To obtain an account in the PL-Grid Infrastructure that enables access to its computing resources and domain-specific services, one needs to register using the PL-Grid portal [19]. Researchers who do not have Polish citizenship, should first contact an appropriate person from the university or research institute in Poland they cooperate with, and, with its help, proceed with the registration process.

3 Analysis of the Services Functionality

The scientists conducting their research with the use of computers have a need for different aspects of interactions with the computer or the infrastructure. The domain-specific services developed around the PL-Grid Infrastructure cover the following functions:

- visualization (see Sections 4.1 and 4.6),
- graphical interfaces supporting: repeatable experiments, data management, domain application-specific interface (with input preparation support, output visualization), running complex scenarios with parallel tasks, remote access through an Internet browser (see Sections 4.2 and 4.12),
- stand-alone services that are used in computing, e.g. databases (see Sections 4.8 and 4.11),
- efficient domain-specific data access, analysis and management (see Sections 4.3 and 4.7),
- deploying new, efficient algorithms solving domain-specific problems (see Sections 4.2 and 4.10),
- interfaces to complex physical instruments (see Sections 4.3 and 4.4),
- tools which enable management of computations from the users' personal devices, running both: Linux and MS Windows as well as mobile operating systems (see Sections 4.2, 4.11 and 4.12).

All the above-mentioned functions help to tailor the domain-specific services to the needs of different groups of scientists, thereby fitting the PL-Grid computational infrastructure to the topics of research.

4 Examples of Domain-Specific Solutions and Services Deployed in the PL-Grid Computational Infrastructure

It is not possible to provide in this paper a detailed view of all the domain-specific services including those already developed and deployed in the infrastructure, and the ones being planned for implementation. Therefore, only several sample services – already deployed or scheduled for deployment in the nearest future – representing all 13 scientific domains, have been chosen to be briefly presented within this section.

4.1 Acoustics

Hearing. The main part of the service is the Psychoacoustical Noise Dosimeter, which is based on utilizing the modified psychoacoustic model of hearing. The primary function of the Dosimeter is to estimate, in real time, auditory effects, which are caused by exposure to noise [20]. The user can define detailed conditions of exposure to noise such as: noise level, exposure time, and energy distribution in the frequency domain. The outcomes are presented in a form of cumulated noise dose and characteristic of temporary shift of the hearing threshold (see Fig. 2).

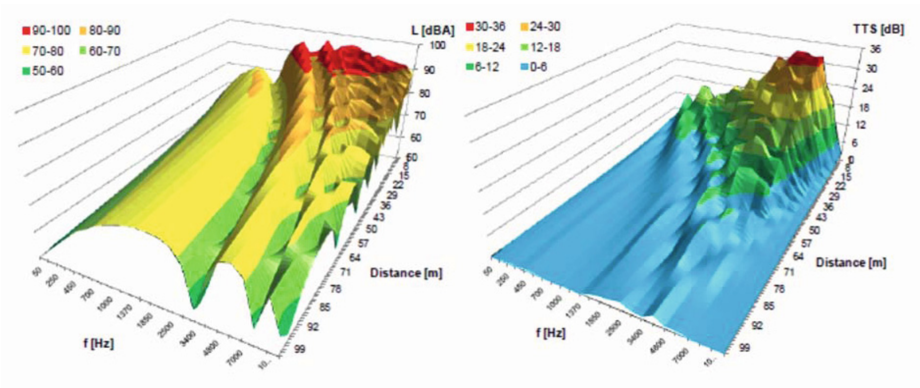

Fig. 2. Spectrum distribution of acoustic energy of noise source (left) and TTS (temporary threshold shift) effect evoked by the exposure to this noise expressed in critical bands as a function of distance from the noise source (right)

Noise Maps. The application generates noise maps in urban environments based on the data provided by the user. Integration of the software service with the network of distributed sensors allows for making automatic updates to noise maps for a specified time period. Operations are performed employing a dedicated noise prediction model, optimized for a computer cluster. In addition, predicted maps may be adjusted, using real noise level measurements [21,22].

4.2 AstroGrid-PL (Astrophysics)

InSilicoLab for Astrophysics. The service aims to support launching complex astrophysical computational experiments in the PL-Grid Infrastructure [23,24].

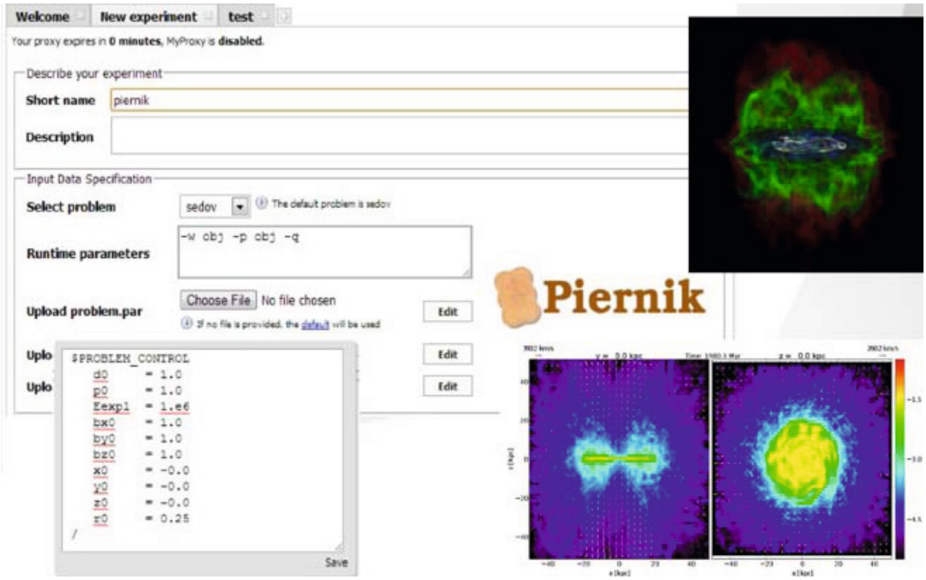

Fig. 3. InSilicoLab for Astrophysics with the first provided code – PIERNIK

These experiments facilitate performing numerical simulations without the need for unassisted and, often, very complex, astrophysical code compilation. InSilicoLab for Astrophysics serves as an interface grid-enabling numerical codes. The first code implemented in this form is a multi-purpose, magnetohydrodynamical, open-source code PIERNIK [25] (see Fig. 3).

4.3 Bioinformatics

Genetic Data Processing. The service allows to run a sequence of programs for analysis of bioinformatics data obtained from a genomic sequencer. Programs that can be activated in a cascade of data processing tasks, are: GS Run Processor, GS Reference Mapper, GS Reporter, GS Assembler and BLAST. Preparation of calculations is done in a graphical client of the UNICORE environment – UNICORE Rich Client [26,27].

Genetic Data Storage. The service implemented for all users who want to store – safely, in the long-term – large amounts of data on storage resources of the distributed computational infrastructure. The transmitted data is encrypted – ensuring confidentiality of the users data, and stored – providing an adequate level of security and access control [28].

4.4 Ecology

Automatic Phenology Observations Service (APheS). Gives an opportunity to observe the flora, together with important processes running in it [18]. The service is based on the KIWI Remote Instrumentation Platform – a framework for building remote instrumentation systems [29]. The platform provides a set of components to control and manage scientific equipment or sensors like cameras, weather, air pollution and water flow sensors, and others (see Fig. 4).

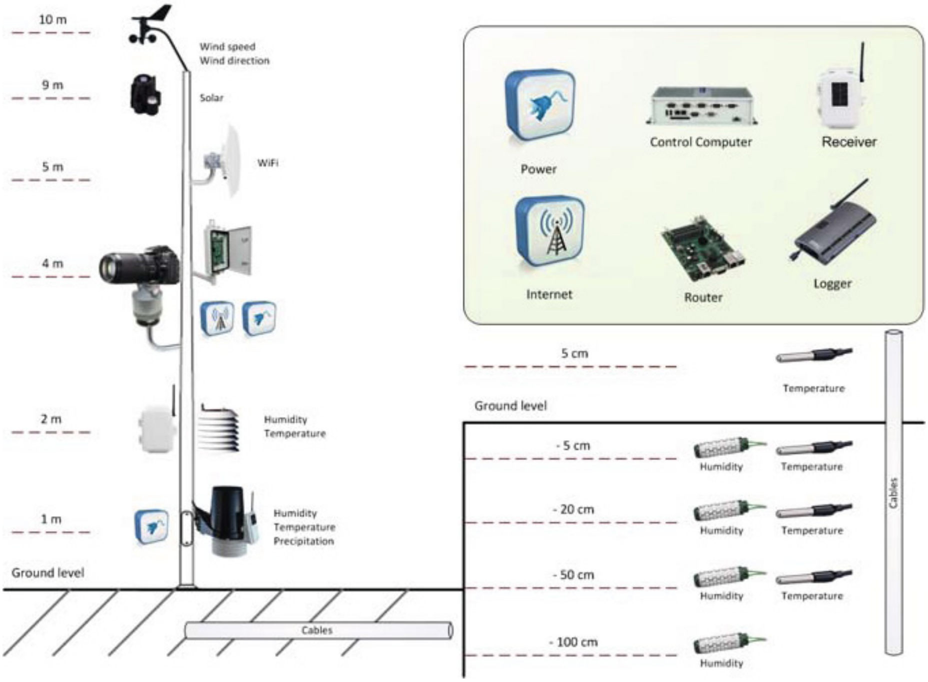

Fig. 4. Automatic phenology observations – infrastructure

Among several scenarios, designed to fully utilize the instrumentation system's potential and provide scientists with data, are:

– defining the phenological year seasons, climate local to the data-gathering site or phenophases for plants cultivated on the nearby arable area,
– examining the effects of cultivation conditions on the duration of vegetation,
– determining the relation between air humidity and wild plants growth.

For each scenario, in order to deliver results, analysis of raw and processed meteorological data and/or photos is performed. As a result of these studies, pictures accessible through the KIWI system may be tagged with information determined by the scientist.

The APheS service constitutes a unique and innovative tool that allows phenological observations to become automated, remote measurements. This solution, developed and deployed within the PLGrid Plus project, is of great value, as it was developed in close collaboration with scientists from the natural sciences domain.

4.5 Energy Sector

πESA (Platform for Integrated Energy System Analysis). The service enables to perform an integrated analysis of the development of the Polish energy system [30]. The main tools included in the πESA platform are:

- TIMES – a tool allowing for building models of energy systems,
- Polyphemus – an air quality modeling system, and
- MAEH – a model to assess the impact of pollution on the environment and human health.

πESA allows users to build energy scenarios by identifying their main assumptions and performing studies of the environmental, economic and social impacts of energy use. For the energy scenarios developed by the users, πESA provides various kinds of practical information on, among others, 1) energy carriers balances, 2) cost, 3) energy conversion techniques used, 4) emissions of pollutants and their atmospheric dispersion, the size of their concentrations and deposition on the territory of Poland at a selected geographical resolution and their impact on human health and the environment.

OptiMINE. The service enables analysis of variants of mining and selection of the best of these variants with respect to plans of coal mining in the given mine. The input data, i.e.: the parameters of the planned excavation (determined data) and the progress of work (as random variables) are entered by the researcher. As a result of the application, the researcher receives adequate values of progress in the various workings and for a distribution of work over time which will ensure fulfillment of the planned extraction.

4.6 Health Sciences

Data Processing for Visualization. The service enables processing of medical data (segmentation, detection of distortion, comparison and search for relevant fragments) for advanced visualization, for scientific and diagnostic needs. Such an analysis is a key element to both research and medical diagnostics. This data processing requires high computing power, which is provided by the PL-Grid Infrastructure. Due to importance of the data, an adequate level of security and data access control is ensured.

4.7 HEPGrid (High Energy Physics)

CVMFS. The service provides catalogs of software and data needed to reconstruct and analyze data in HEP experiments (see Fig. 5). It operates on a dedicated server installation on a read-only virtual file system CERNVM-FS, installed by the FUSE module in the local user space. With this service, all the versions of the software and any modifications made to the central servers are immediately available ensuring reasonable usage of the local storage resources.

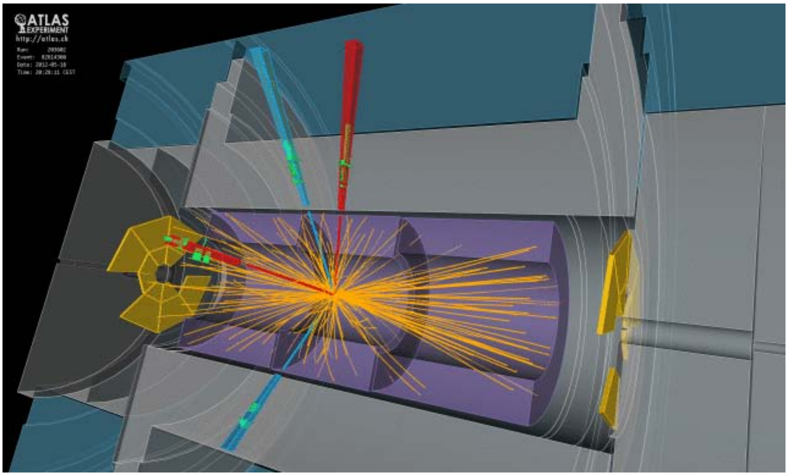

Fig. 5. Visualization of production and decay of the Higgs boson to two electrons and two positrons in the ATLAS detector (figure courtesy of CERN)

Proof on Demand (PoD). The service is designed to perform the final physical HEP analyses. It enables parallel data processing in the ROOT environment [31] using partitioning of input data and its processing by independent processes, and provides merging of the output results. In this way, the processing time of large quantities of data can be reduced by a factor of $1/n$ where n is the number of running PoD processes.

4.8 Life Science

Advanced Microarray Analysis Tool – Integromics. The service was developed for people conducting biological research using DNA microarrays, providing information on the level of gene expression in test samples [17]. Integromics is a tool that helps analyze this information and correlate expression levels with other clinical data on the studied organisms. The service is a unique web application, which supports a range of complex analyses, including, among others:

- quality control and normalization for the most popular microarray types (Affymetrix and Agilent), ensuring that differences in intensities are indeed

due to differential expression, and not merely printing, hybridization, or scanning artifacts,
- Artificial Neural Network (ANN) analysis, capable of creating and training a neural model (a perceptron), and subsequently using it to distinguish between healthy and abnormal tissue based on gene expression profile data (see Fig. 6),
- integromics analysis, which combines gene expression data with lipidomic or proteomic information in order to find interesting correlations, patterns and associations.

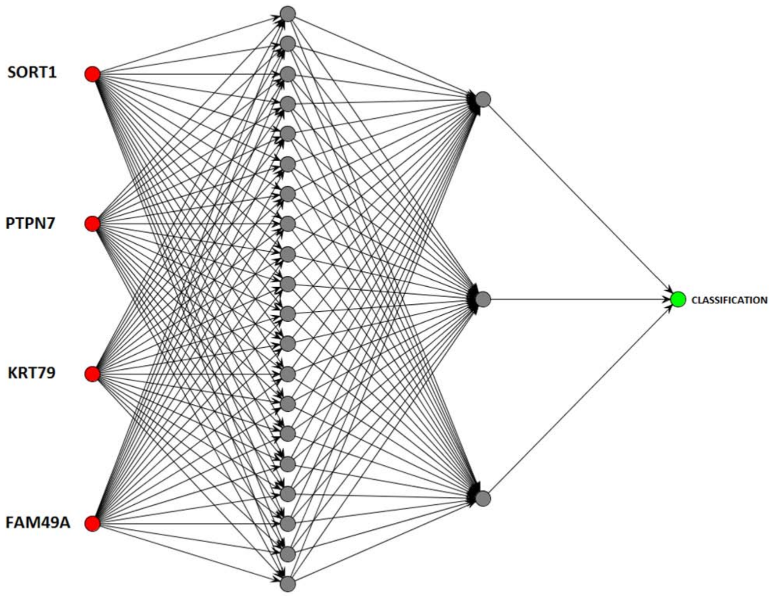

Fig. 6. Schematic representation of a sample artificial neural network, developed for classification based on gene expression profiles

4.9 Materials

Advanced Maintenance of the Material Modeling Software on the UNICORE Platform. The service provides grid access to some popular software packages used in the modeling of materials – VASP, Siesta, QE, Abinit and OpenMX through the UNICORE platform (middleware). It also provides support in executing typical task sequences.

Visualization of 3D Data in the VisNow Software Package. The results of programs such as VASP, Siesta, QE, Abinit, OpenMX are often large sets of data describing spatial distribution of a given quantity, e.g., electron density. Within the described service, a visualization software – VisNow – has been extended by a module enabling efficient preview of the aforementioned results, and, based on it, drawing required charts and maps.

4.10 Metallurgy

SSRVE. The service is used to generate a Statistically Representative Volume Element (called SSRVE) for microstructures of materials. The service is designed for people involved in large-scale modeling using a representation of microstructure of two-phase metallic materials [32] (see Fig. 7).

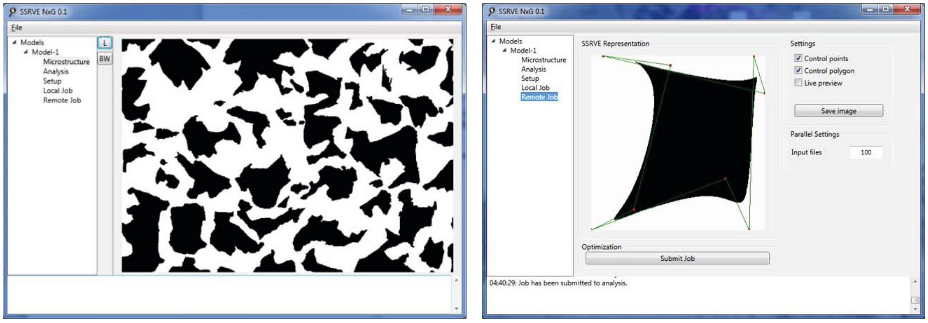

Fig. 7. Full representation of microstructure (left) and generated SSRVE (right)

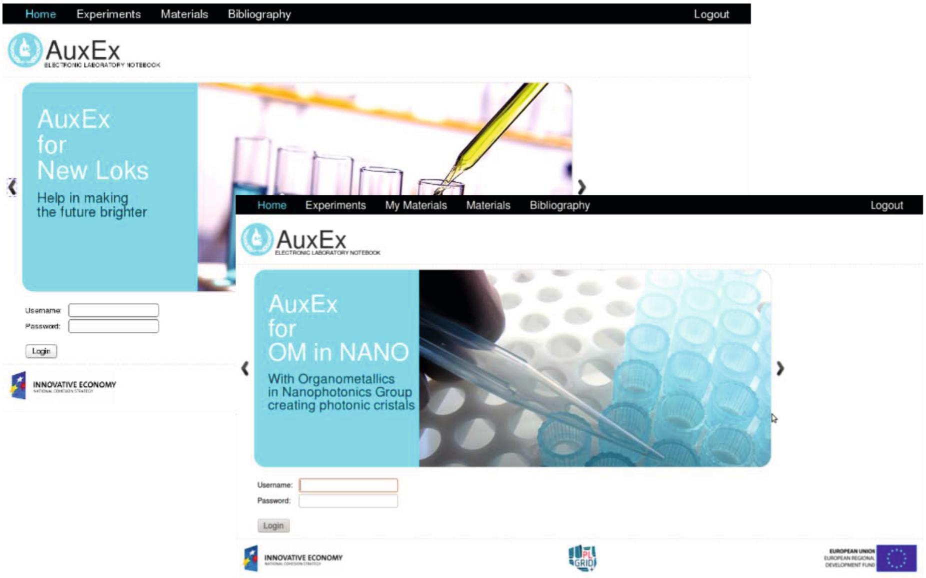

Fig. 8. AuxEx service portals

Extrusion3d. The service relates to the modeling and optimization of extrusion profiles. It can assist a user in the process of designing tools and technologies. Owing to the implemented criterion of loss of cohesion, it also enables analyzing the extrusion process for cracks in the extruded material [33].

4.11 Nanotechnologies

AuxEx. The service is designed for teams of researchers, who, in their daily work, face the problem of managing and sharing large amounts of heterogeneous data. AuxEx is a dedicated software tailored to the needs of a particular team. It allows for a maximum effective cooperation in a specific research project. The service can be used within the PL-Grid Infrastructure or as an application deployed locally on the user's servers [34] (see Fig. 8).

Nanomechanics Portal. The service is designed for people who use methods from Molecular Dynamics as a basic research tool. It provides a number of tools, including: 1) tools to prepare and perform a molecular-dynamic simulation, 2) tools for analysis of the simulation results, in particular for structure characterization of materials simulated numerically.

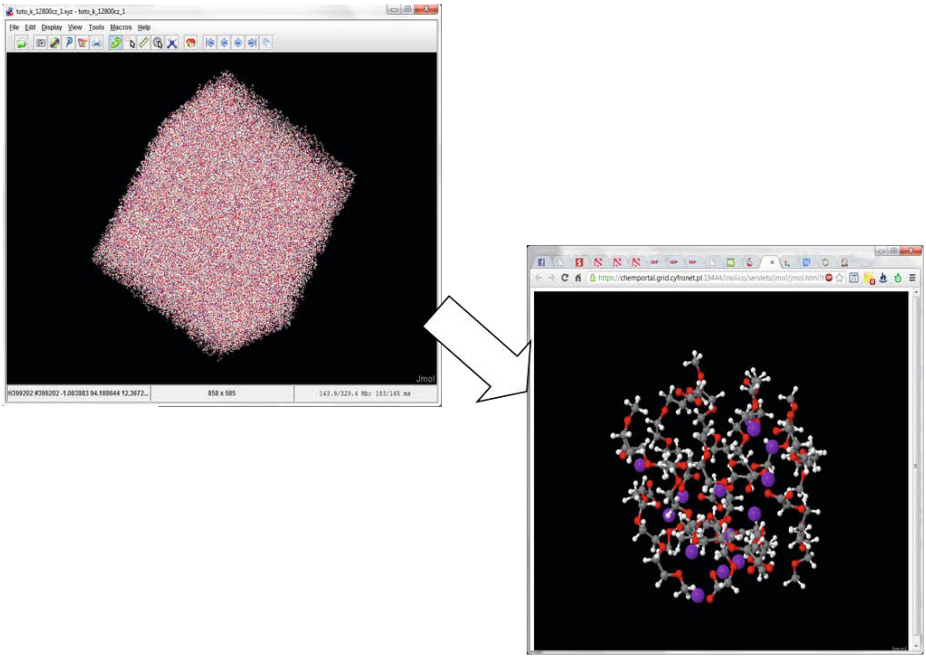

Fig. 9. An example of Trajectory Sculptor usage: an MD frame of 400 000 atoms reduced to a few selected molecules

4.12 Quantum Chemistry and Molecular Physics

InSilicoLab for Chemistry. The service supports launching of complex computational quantum chemistry experiments on the PL-Grid Infrastructure [23], [35,36]. These experiments facilitate planning of sequential computation schemes that require preparation of series of data files, based on a common schema. The first two experiments offered to the chemistry domain within InSilicoLab are: 1) general quantum-chemistry experiment and 2) Trajectory Sculptor [37]. The latter is a tool applicable to a wide range of systems, including binary or ternary solvent mixtures, electrolyte solutions or ionic liquids (see Fig. 9).

4.13 SynchroGrid

Elegant. The service developed for those involved in design and operation of a Synchrotron. The service consists in: 1) provisioning of the Elegant (ELEctron Generation ANd Tracking) application in parallel version on a cluster, 2) configuring the Matlab software to read output files produced by this application in Self-Describing Data Sets (SDDS) format and to generate the final results in form of drawings [38].

5 Conclusions and Future Work

The presented approach to construction of big e-infrastructures and opening their features to scientists, developed in the framework of the PL-Grid and PLGrid Plus projects, presents a way of providing advanced IT infrastructure to modern scientific research. The resulting solution provides Polish researchers with capability for collaboration with international research organizations.

The described approach also proves that the most important goal of the PLGrid Plus project – expansion of the existing computational infrastructure towards domain-specific solutions for research teams – allows for conducting more effective and valuable research. The results of most of these scientific computations can be applied in various branches of science and technology.

With the development of the domain-specific solutions, it became possible to reach beyond the traditional community of IT infrastructure users and create interdisciplinary teams, enabling them to achieve better scientific results, construct, implement and maintain domain services, as well as to introduce improvements to the functioning of the PL-Grid Infrastructure. Many of these users were directly involved in the PLGrid Plus project and supported its activities, thus, significantly contributing to the accomplishment of the final project's results.

In the future, we plan to focus on other domains of science and to offer a wider range of cloud and big data services. Modernization of software environments (i.e., toward EMI components) and hardware solutions (with more GPGPUs and Intel phi) are also foreseen.

References

1. The Polish Grid Infrastructure web site, http://www.plgrid.pl
2. The PL-Grid project web site, http://projekt.plgrid.pl
3. Bubak, M., Szepieniec, T., Wiatr, K. (eds.): PL-Grid 2011. LNCS, vol. 7136. Springer, Heidelberg (2012)
4. The PLGrid Plus project web site, http://www.plgrid.pl/plus
5. The Polish Grid (PL-Grid) Consortium web site, http://www.plgrid.pl/en/contacts
6. Bubak, M., Malawski, M., Zając, K.: Towards the CrossGrid architecture. In: Kranzlmüller, D., Kacsuk, P., Dongarra, J., Volkert, J. (eds.) PVM/MPI 2002. LNCS, vol. 2474, pp. 16–24. Springer, Heidelberg (2002)
7. Marco, J., Campos, I., Coterillo, I., et al.: The interactive European grid: Project objectives and achievements. Computing and Informatics 27(2), 161–171 (2008)
8. Dutka, Ł., Kitowski, J.: Application of component-expert technology for selection of data-handlers in CrossGrid. In: Kranzlmüller, D., Kacsuk, P., Dongarra, J., Volkert, J. (eds.) PVM/MPI 2002. LNCS, vol. 2474, pp. 25–32. Springer, Heidelberg (2002)
9. Funika, W., Korcyl, K., Pieczykolan, J.: Adapting a HEP application for running on the Grid. Computing and Informatics 28(3), 353–367 (2009)
10. gLite – Lightweight Middleware for Grid Computing, http://glite.cern.ch/
11. UNICORE – Uniform Interface to Computing Resources, http://www.unicore.eu
12. QosCosGrid Middleware, http://www.qoscosgrid.org/
13. EGI.eu web site, http://www.egi.eu/
14. EGI-InSPIRE project web site, http://www.egi.eu/about/egi-inspire/
15. EMI web site, http://www.eu-emi.eu/
16. PRACE web site, www.prace-ri.eu/
17. Kitowski, J., Dutka, Ł., Mosurska, Z., Pająk, R., Sterzel, M., Szepieniec, T.: Development of Polish Infrastructure for Advanced Scientific Research – Status and Current Achievements. In: Proceedings of 12th International Symposium on Parallel and Distributed Computing, ISPDC 2013, IEEE Conference (2013)
18. Kitowski, J., et al.: Development of Domain-Specific Solutions within the Polish Infrastructure for Advanced Scientific Research. In: Wyrzykowski, R., Dongarra, J., Karczewski, K., Waśniewski, J. (eds.) PPAM 2013, Part I. LNCS, pp. 237–250. Springer, Heidelberg (2014)
19. The PL-Grid portal web site, https://portal.plgrid.pl
20. Kostek, B., Kotus, J., Czyżewski, A.: Noise Monitoring System Employing Psychoacoustic Noise Dosimetry. In: Proceedings of the 47th AES Conference, Music Induced Hearing Disorders, New Technologies for Measurement and Prevention, Columbia College, Chicago, Illinois, USA, June 20-22 (2012)
21. Szczodrak, M., Kotus, J., Czyżewski, A., Kostek, B.: Application of Noise Mapping Tool Deployed in Grid Infrastructure for Creating Noise Maps of Urban Areas. The Computer Science Journal 14(2), 231–242 (2013)
22. Szczodrak, M., Kotus, J., Kostek, B., Czyżewski, A.: Creating Dynamic Maps of Noise Threat Using PL-Grid Infrastructure. Archives of Acoustics 38(2), 235–242 (2013)
23. Kocot, J., Szepieniec, T., Sterzel, M., Golik, M., Wojcik, P., Twarog, T., Grabarczyk, T.: A Framework for Domain-Specific Science Gateways. In: Bubak, M., Turała, M., Wiatr, K. (eds.) CGW 2013 Proceedings, pp. 93–94. ACK CYFRONET AGH, Kraków (2013)

24. The InSilicoLab for Astrophysics service web site, http://insilicolab.astro.plgrid.pl/
25. Ciecieląg, P., Hanasz, M., Kowalik, K., Kundera, T., Stachowski, G., Borkowski, J.: Grid-enabled platform for astronomers. In: Bubak, M., Turała, M., Wiatr, K. (eds.) CGW 2013 Proceedings, pp. 57–58. ACK CYFRONET AGH, Kraków (2013)
26. Borcz, M., Kluszczynski, R., Skonieczna, K., Grzybowski, T., Bala, P.: Using PL-Grid Infrastructure to Store and Process DNA Sequence Data from GS FLX Instrument. In: Bubak, M., Turała, M., Wiatr, K. (eds.) CGW 2012 Proceedings, pp. 67–68. ACK CYFRONET AGH, Kraków (2012)
27. Borcz, M., Kluszczyński, R., Skonieczna, K., Grzybowski, T., Bała, P.: Processing the biomedical data on the grid using the UNICORE workflow system. In: Caragiannis, I., Alexander, M., Badia, R.M., Cannataro, M., Costan, A., Danelutto, M., Desprez, F., Krammer, B., Sahuquillo, J., Scott, S.L., Weidendorfer, J. (eds.) Euro-Par Workshops 2012. LNCS, vol. 7640, pp. 263–272. Springer, Heidelberg (2013)
28. Borcz, M., Kluszczynski, R., Marczak, G., Chrupala, R., Benedyczak, K., Skonieczna, K., Grzybowski, T., Bala, P.: PL-Grid services for bioinformatics community. In: Bubak, M., Turała, M., Wiatr, K. (eds.) CGW 2013 Proceedings, pp. 67–68. ACK CYFRONET AGH, Kraków (2013)
29. KIWI Remote Instrumentation Platform web site, http://kiwi.psnc.pl/
30. Wyrwa, A., Pluta, M., Zysk, J., Skoneczny, S., Mirowski, T.: Modelling the mid-term development of the energy system with the use of technology explicit partial equilibrium model. In: Bubak, M., Turała, M., Wiatr, K. (eds.) CGW 2013 Proceedings, pp. 55–56. ACK CYFRONET AGH, Kraków (2013)
31. ROOT environment web site, http://root.cern.ch/drupal/
32. Rauch, L., Pernach, M., Bzowski, K., Pietrzyk, M.: On application of shape coefficients to creation of the statistically similar representative element of DP steels. Computer Methods in Materials Science 11(4), 531–541 (2011)
33. Milenin, A., Kustra, P.: Optimization of extrusion and wire drawing of magnesium alloys using the finite element method and distributed computing. In: Proceedings of the InterWire 2013 International Conference (2013) (in press)
34. Banach, G., Mikolajczyk, M.M., Uchronski, M., Tykierko, M.: Auxiliar Experimentorum – a different approach for creating and developing scientific applications. In: Bubak, M., Turała, M., Wiatr, K. (eds.) CGW 2013 Proceedings, pp. 65–66. ACK CYFRONET AGH, Kraków (2013)
35. Kocot, J., Szepieniec, T., Harężlak, D., Noga, K., Sterzel, M.: InSilicoLab – Managing Complexity of Chemistry Computations. In: Bubak, M., Szepieniec, T., Wiatr, K. (eds.) PL-Grid 2011. LNCS, vol. 7136, pp. 265–275. Springer, Heidelberg (2012)
36. Kocot, J., Eilmes, A., Szepieniec, T., Sterzel, M., Golik, M.: Molecular Modeling of Complex Systems with InSilicoLab. In: Wiatr, K., Kitowski, J., Bubak, M. (eds.) Proceedings of the Sixth ACC Cyfronet AGH Users Conference, pp. 45–46. ACC CYFRONET AGH, Kraków (2013)
37. Eilmes, A., Sterzel, M., Szepieniec, T., Kocot, J., Noga, K., Golik, M.: Comprehensive Support for Chemistry Computations in PL-Grid Infrastructure. In: Book of Abstracts of the Current Trends in Theoretical Chemistry VI Conference, pp. G9–G13. Jagiellonian University, Faculty of Chemistry, Kraków (2013)
38. Stankiewicz, M., Wawrzyniak, A., Goryl, P., Zajac, M., Nowak, M., Zytniak, L., Melka, F., Szymocha, T.: Services for Synchrotron deployment and operations. In: Bubak, M., Turała, M., Wiatr, K. (eds.) CGW 2013 Proceedings, pp. 63–64. ACK CYFRONET AGH, Kraków (2013)