NGI H2020 Profile

**NGI AEGIS**

15-05-2014

# Target user communities

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|  | Research Community/Project description (list in order of descending priority) |
| Community 1 | **Physical sciences community** * Operations and maintenance of the current system, and its extension;
* Seminars and trainings on new middleware features;
* Adaptation of the existing middleware technologies to support novel hardware architectures;
* Extension of the middleware schedulers with testing queue capability.
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| Community 2 | **Chemistry community*** Operations and maintenance of the current system, and its extension;
* Seminars and trainings on workflow concepts, and application porting;
* Extension of the currently available workflow technologies;
* Introduction of an application performance monitor.
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| Community 3 | **Agriculture community*** Porting of new agriculture applications and standardization of Grid porting process;
* Development of concept of data-driven approach and data-driven job management system;
* Customization of the existing document-oriented database technologies, and their integration to middleware.
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# Resource provisioning for target communities

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|  | **Compute and storage capacity currently available (or available in the future) to deal with the data growth** | **Access policy** | **Available funding or funding models (present and future)** | **What existing resources the e-infrastructures can offer, their current usage, the limitations and plans to deal with the data deluge** |
| **Community 1** | * **PARADOX cluster**1696 Intel Xeon E5-2670 @ 2.6 GHz Sandy Bridge processors with 2 GB of RAM per core; 106 NVIDIA Tesla M2090 with 6 GB of RAM; 100 TB of disk storage space; Infiniband QDR non-blocking interconnection
* **AEGIS01-IPB-SCL Grid site**704 Intel Xeon E5345 @ 2.33 GHz processors with 1 GB of RAM per core; 50 TB of disk storage space; Gigabit Ethernet interconnection
* **5 NGI AEGIS production Grid sites**300 Intel Xeon processors; 10 TB of disk storage space; Gigabit Ethernet interconnection
 | AEGIS VO acceptable use policy available at the NGI AEGIS web ste. | NGI AEGIS is actively working on securing funding. Partial funds are available from national research projects of active user groups. | Resources coordinated by NGI AEGIS, and listed here. |
| **Community 2** |
| **Community 3** |

# User support skills

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|  | User support skills and related technical and disciplinary areas |
| Training and education | NGI AEGIS User Support has experience in organization and realization of introduction and advanced training events on Grid technology, Grid porting process, and high-performance computing. |
| Technical skills | * Deployment, maintenance, testing, profiling and tuning of available Grid technologies (core services).
* Grid porting, debugging, profiling, and tuning of serial and parallel (MPI, OpenMP, OpenMP/MPI, GPU, XeonPhi) applications in the area of physics, chemistry, engineering, material science, as well as utilisation of advanced Grid scheduler features.
* Deployment, maintenance, and customisation of gUSE workflow technologies, which also includes complex workflow creation, portlet creation, and development of custom interface that envelopes a generic workflow.
* Experience with high-performance software libraries (LAPACK, BLAS, FFTW3, SPRNG, Intel MKL, ScaLAPAC, etc.) and application tools (MPICH, MPICH2, OpenMPI, gcc, gfortran, Intel Compilers, PortlandGroup Compilers, NAMD, CPMD, Firefly, AutoDock Vina, OpenEye, etc.)
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| Discipline/user-specific skills | * Extensive knowledge and wide user community in Computational Physics, especially in Condensed Matter Physics. The numerical studies range from strongly correlated systems, such as Bose-Einstein condensates, fractional quantum Hall effect, Bose-Hubbard and Fermi-Hubbard models, to studies of electronic structure properties, organic semiconductors, solar cells, and include classical (soft condensed matter) granular materials and molecular dynamics approaches.
* Experience in solving of partial and ordinary differential equations, including discretization strategies.
* Solving of large diagonalization problems.
* Minimization problems and variational approaches.
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# Software development skills and experience

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| Skill | Description |
| Profiling and optimization | In-depth knowledge of profiling and optimization techniques for serial and parallel codes (OpenMP, MPI, CUDA, OpenCL), as well as benchmarking and scalability testing. |
| Development of operational tools | Development of DCI-oriented operational and monitoring tools. |
| Development of high-level interfaces | Development of custom interfaces that envelopes a generic Grid ported workflow, as well as RESTful interfaces on the top of Grid ported application. |