Final report from the e-IRG Task Force, providing recommendations on

Sustained Maintenance of Scientific Software

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Background

• European e-Infrastructure ecosystem for (research) computation is established, primarily via EGI and PRACE
• Maintenance and improvement of the application software is now an urgent issue
• Paradigm shifts: Faster cores -> more cores, accelerators, tera-petascale -> peta-exascale, ...
• Significant efforts needed on new or significantly renewed application codes, including new algorithms and methods
• Application software is an essential part of e-Infrastructure
• Several efforts have been initiated, but there is a clear need to develop a consistent strategy, taking a holistic view of the application software ecosystem.
Delineate possible structures supporting the maintenance, scaling, and performance improvements of scientific application software of European interest using a holistic approach covering the full spectrum of problems ranging from small over medium to extreme scale (exascale).

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2. The Scientific Software Crisis

3. Centres of Excellence for Scientific Software

4. Summary of main recommendations

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Main Recommendation

To address the software crisis, the EC and the member states should provide support and funding for the establishment of Centres of Excellence for Scientific Software (CESS), currently focusing on scientific software on the application layer using a holistic approach and building up and retaining the necessary competence of future European software developers.
Scientific Applications normally exist in an environment of a complex software stack comprising:

1. Operating System
2. Compiler
3. Libraries
4. Programming language/paradigm
5. Scientific simulation/analysis software
6. Frameworks (workflow systems, resource access/management frameworks/middleware)
7. Portals, GUIs
Characteristics and Attributes of a CESS

A CEES should...

...support the **entire software lifecycle on all levels** within the European e-Infrastructure ecosystem

A variety of competences are needed in an **interdisciplinary setting**:
- Parallel computing in general
- Programming models
- Tools and environments for debugging and performance optimization
- Numerics-oriented libraries and toolkits
Characteristics and Attributes of a CESS

A CEES should...

…create a collaborative environment facilitating the “co-design” (applications and programming environment) of academic community and industrial scientific software

• Open standards and interfaces
• Use of non-restrictive licenses
• Provide paths for ISVs to provide value-added software and services
Characteristics and Attributes of a CESS

A CEES should...

...provide a transparent process for requirements gathering and prioritization

Forms of requirements gathering:
- Surveys, observations, document review, ... (existing req.)
- Feature requests, focus groups, interviews, ... (known new req.)
- Brainstorming, prototypes, usage analysis (unknown req.)

Issues in requirements prioritization:
- Importance
- Added value
- Tractability
- Opportunity
- Stage
Characteristics and Attributes of a CESS

A CEES should...

...implement **interfaces** to the **e-Infrastructure providers** and vice versa, while establishing clear responsibilities for operations on the one side and development on the other side.

- e-Infrastructure providers rely on the software developed by the software centres of excellence to
  - Operate, maintain and manage their resources
  - Deploy and operate basic services for scientific users
  - Provide specific functionalities on higher levels of abstractions for scientists to perform their scientific tasks
- The quality of the software is therefore part of user satisfaction concerning the services provided by the e-Infrastructure providers
- The CESS require interaction with the e-Infrastructure providers specifically for:
  - Evaluation (feasibility) or large research collaborations’ needs
  - Deployment and testing of software and updates
Characteristics and Attributes of a CESS

A CEES should...

…work with other organizations to develop and promote appropriate curricula across Europe that provides researchers with a foundation in computational science and distributed computing.
Characteristics and Attributes of a CESS

A CEES should...

...have a governance model, ensuring that user communities drive the scientific strategy.

Experts on governance need to be involved in the setup of a CESS.
The different potential organizational and funding schemes need to be discussed further to derive sustainable solutions for CESSs. It would be best to perform a design study project in order to investigate possible impacts and the advantages and disadvantages of different models.