Open Marketplace for Simulation Software on the Basis of a Web Platform

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Simulations and distributed computing (1/3)

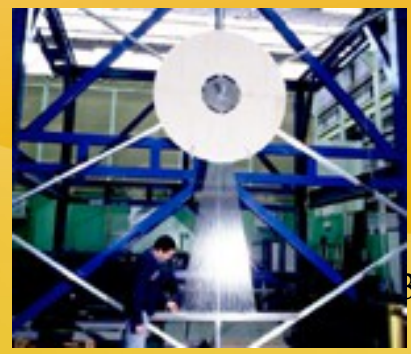
- Simulation of complex systems is a time expensive and resource consuming task
- Statistical validation of simulation models or the need to compare the system behavior in several different conditions require many simulation runs
  - ⇒ often local resources are insufficient
- a viable solution to speed up the process is to run the simulations on a distributed system
  - a good example: WLCG project

Simulations and distributed computing (2/3)

- The Worldwide LHC Computing Grid (WLCG)
  - It was designed by CERN to handle the prodigious volume of data produced by Large Hadron Collider (LHC) experiments in high-energy (elementary particle) physics
    - approximately 25 petabytes per year
  - an international collaborative project
  - **grid**-based computer network infrastructure incorporating over 170 computing centers in 36 countries

CMS ***LHCb*** ***ATLAS*** ***ALICE***



Simulations and distributed computing (3/3)

- Inspired by the WLCG success, grid computing became popular beyond the high-energy physics
  - bioinformatics, nanotechnology, geophysics, etc.
    - to share and combine the power of computers
    - and sophisticated, often unique, scientific instruments
- The most ambitious attempt to extend the grid technology to other scientific areas was undertaken in the framework of a series of European projects

DataGrid → EGEE → EGI (2001 - 2015)

Grid → Web platforms

- With the growth of performance of individual resources (supercomputers, data storages, cloud systems, etc.) the grid conception began to lose a significant part of its appeal
  - a large-scale distributed computing grid infrastructure ⇒ high overheads
    - ⇒ requires powerful unifying organizational structure, maintaining a cumbersome grid infrastructure (WLCG — CERN)
  - the focus in the development of a new generation of middleware shifts to building convenient and efficient means for accessing individual computing resources
    - **web platforms** for remote access to individual computing resources

Remote access to HPC resources

- in many cases researchers need to run a large number of similar computing tasks
  - the Software as a Service model, **SaaS**
  - Web platform (WP) for remote access to computing resources: a set of specialized web services + web application interfaces
- Having in their disposal a set of pre-configured "tools", users only needs to formulate the essence of a specific request in a natural language
  - "a **tool**" = pre-arranged task (*a launch of an application package, an access to a data storage, etc*)
  - A series of tasks depending on each other in a hierarchical way are called **workflows**

Types of Web Platforms (WP)

1. WPs for job submission: remote submission, monitoring, and obtaining the job results;
2. WPs for job submission and software installation: item 1 + remote installation and configuring of application packages (tools);
3. Web hubs: items 1, 2 + providing the features of professional social networks (sharing experiences, rating of tools, etc);
4. WPs of application software market: items 1, 2, 3 + services for interaction between the providers and consumers of «tools» on market principles (analogue App Store, Google Play etc.).

Basic Functional Requirements to WPs (1/2)

- management of user credentials granting the right to use the available resources
  - Authentication, authorization delegation
- remote administration of the web platform via a web browser
  - Accounts, granting the rights to use of sets of tools; accounts of tool providers

Basic Functional Requirements to WPs (2/2)

- job execution management
  - composition of jobs from the available tools; converting commands into the resource format; launching jobs; monitoring; receiving results; remote vizualization
- data files transfer management
  - transfer of input/output data to/from local computer/ storage system
- tools (web services) management
  - registration of new tools, creation of toll templates

Examples of WPs Implementations (1/4)

- web platform of educational-methodical software package «Multiscale modeling in nanotechnology» (Photochemistry Center of the Russian Academy of Sciences (RAS); http://www.nanomodel.ru);
- «Personal virtual computer» system (South Ural State University; http://supercomputer.susu.ac.ru/pvc);
- UniHUB, the technological platform of the National «University Cluster» program (Institute for System Programming of RAS; https://unihub.ru);

Examples of WPs Implementations (2/4)

- computing cloud platform of the Ural Branch of the RAS (Instit. of Math. and Mechanics, UrB RAS);
- web portal of the supercomputer management system (Glushkov Institute of Cybernetics of NAS of Ukraine; http://melkon.com.ua/ru/cms);
- Everest web platform (Institute for Information Transmission Problems of the RAS; http://everest.distcomp.org)
- multifunctional instrumental and technological platform for cloud computing support CLAVIRE (SPbg State University of Information Technologies, Mechanics and Optics; http://clavire.ru);

Examples of WPs Implementations (3/4)

- nanoHUB, web hub in nanotechnology (consortium of the US universities; http://www.nanohub.org);
- eQUEUE, web platform for the remote job submission (Advanced Clustering Technologies, Inc.; http://www.advancedclustering.com/products/software/equeue);
- Nucleonica, scientific web portal (Institute for Transuranium Elements; http://www.nucleonica.net);

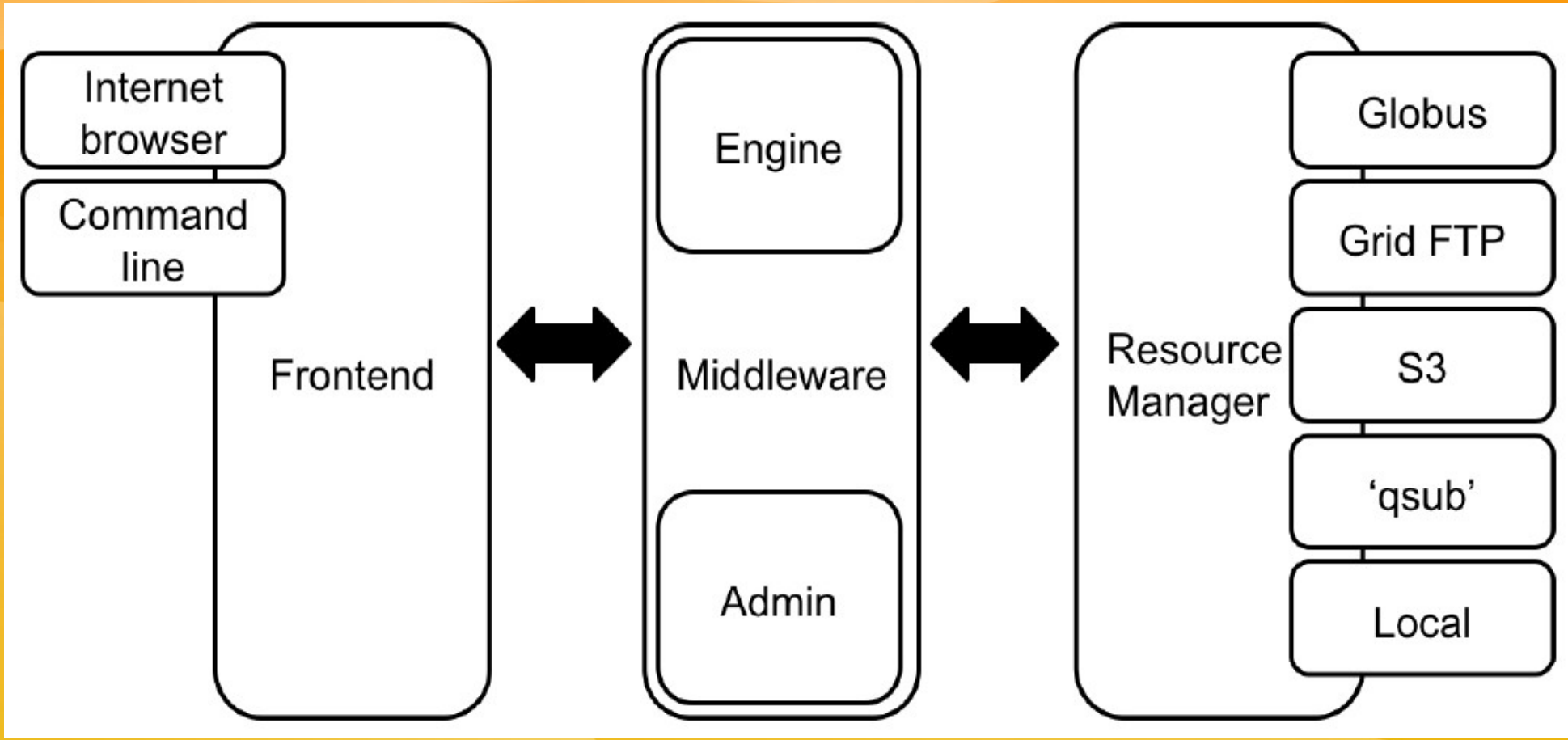
Examples of WPs Implementations (4/4)

- WebMO web platform (Hope College, Holland, USA; http://www.webmo.net);
- WP e-Science Central (Newcastle University, UK; http://www.esciencecentral.co.uk).
- Yabi web platform (Centre for Comparative Genomics, Murdoch, Australia; https://ccg.murdoch.edu.au/yabi)

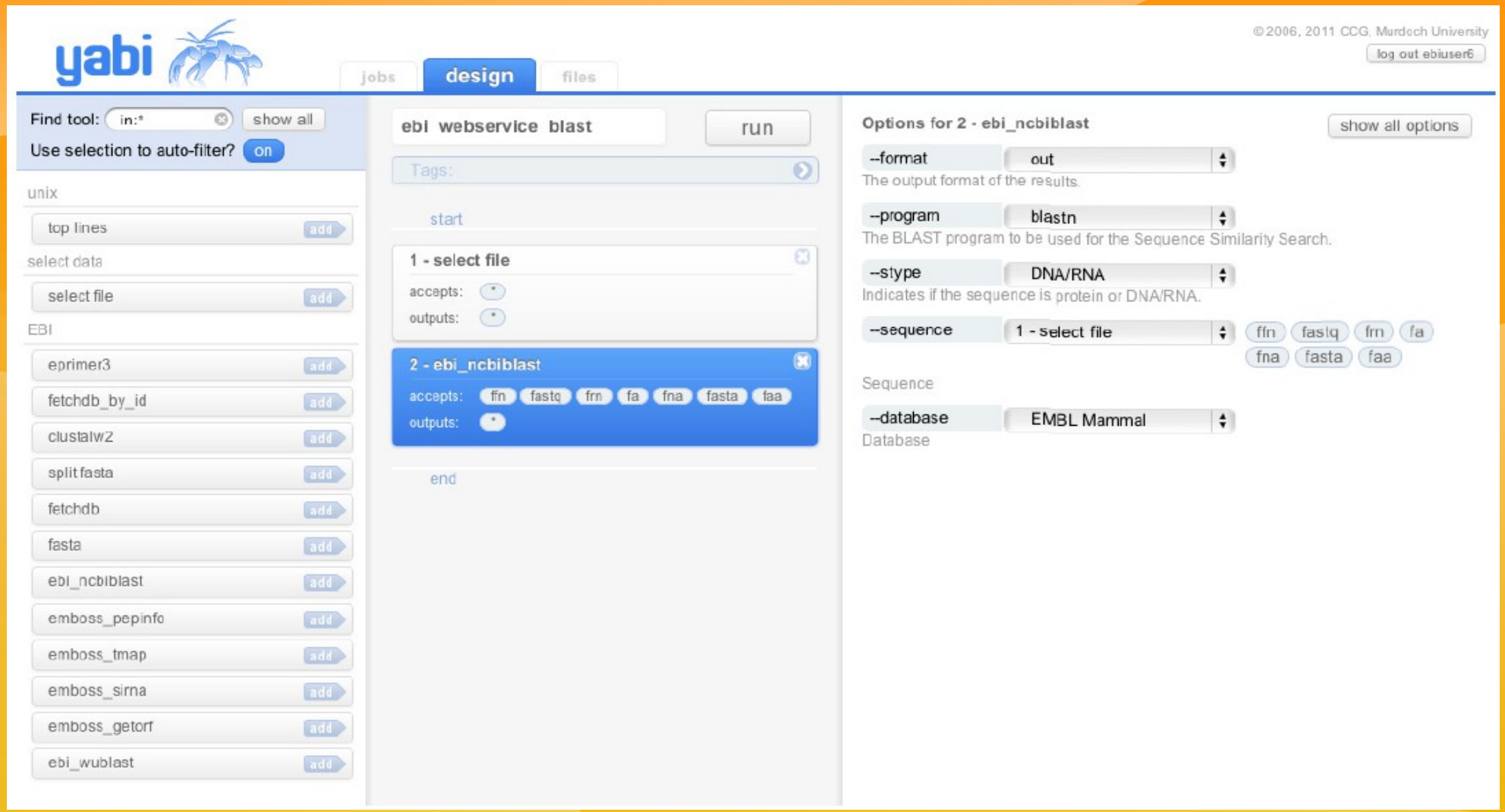
Typical example: Yabi Project

- provides the execution of workflows consisting of successive tasks
  - accesses to databases,
  - use of the results as input for computing tasks etc.
- has well developed and convenient administrative interface for
  - configuring the "tools"
  - controlling the user access to these tools
- GNU GPL v3 (noncommercial use)

Yabi Project: architecture



Yabi Project: Web GUI



Yabi Project: administration

Creation of tools

WPs Implementations:

- all of these developments ensure the provision of end-users in advance preset simulation tools
- they are still insufficient to ensure the creation of a web platform capable of performing the whole range of tasks characteristic for a free open market

Open Marketplace Paradigm

Functions of marketplace – appropriate WP modules.

- Information: Marketplace gives participants the information about quantity and quality of producs.
  - WP provides calalog of available applications, blog for discussion and means for assigning rating marks.
- Matchmaking of users and SW providers:
  - API and Web interfaces both for SW providers and users.

Open Marketplace Paradigm

Functions of marketplace – appropriate WP modules.

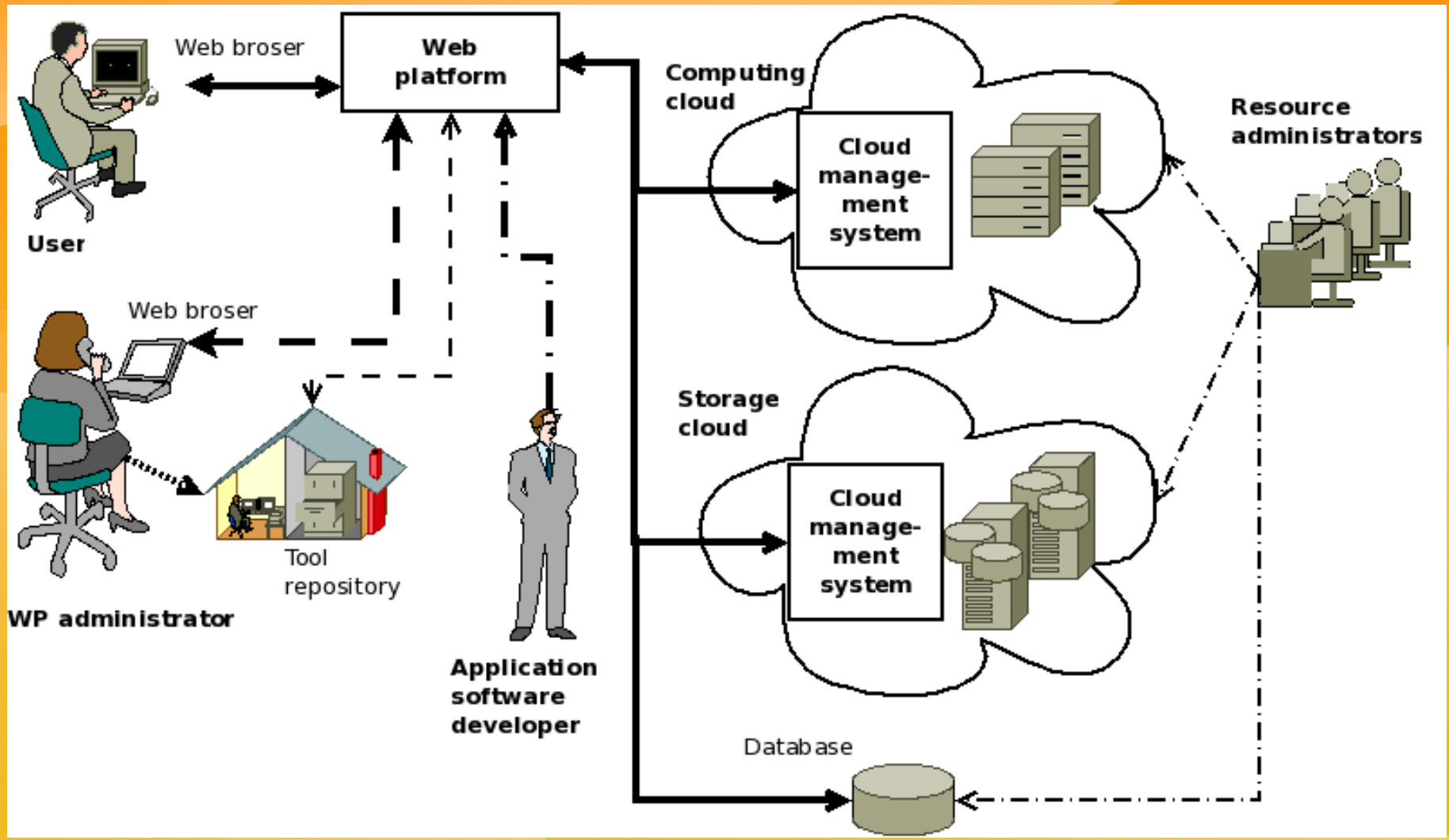
- Service price forming: price formed on the market on the basis of supply and demand, taking into account the competition
  - Pricelist and importance of offered software.
- Regulation: Market balances the supply and demand
  - WP as a whole

Open Marketplace Paradigm

Functions of marketplace – appropriate WP modules.

- Stimulating innovation products: Market stimulates the development of innovation products, the reduction of costs and increase the quality.
  - WP as a whole
- Coordination: market encourages producers to create the necessary economic benefits to the community at the lowest cost and a reasonable return.
  - Blog and rating facilities
- Identification of inefficient producs.
  - Billing

General WP architecture (1/2)



General WP architecture (2/2)

- Software developers interact with the cloud management system via the WP
  - PaaS model
  - software deployment + convertation into the web tool
- WP contains modules needed for market-like interrelations between providers and users of tools
  - monitoring
  - logging and billing
  - Blog
  - Rank module

Current status of the project

- A prototype of such a platform is currently being developed at SINP MSU (1st year of the project)
  - General architecture, set of modules
  - API both for users and providers has been developed
- From a technological point of view, the WP prototype be implemented as a set of web services
  - with extensive use of architectural style REST
  - data exchange between the services - in the JSON format

Conclusion (1/3)

- Further line of development of the web toolkit may be related not only with the quantitative increase in the number of web-based platforms for remote access and the expansion of scientific, engineering, and manufacturing areas in which they are used,
- but also with the improvement of the technology of remote deployment of new application software on resources interacting with the web platforms
- This approach will help to overcome an important problem associated with the use of the SaaS model in scientific areas, namely, limited set of application packages offered by SaaS providers

Conclusion (2/3)

- Currently, the provision of services for providers of application software in the context of scientific-oriented web platforms is not developed enough.
  - Although some implementations (for example, e-Science Central) have services for remote application software deployment, they are still insufficient to ensure the creation of a web platform capable of performing the whole range of tasks characteristic for a free open market.

Conclusion (3/3)

- The technology of creating such web platforms market of application software can be based both on the original solutions and on the synthesis and adaptation of the solutions used in research hubs (e.g., nanoHUB; nanohub.org), cloud and grid systems, as well as in on-line app stores.
- However, it seems that unlike the on-line app stores, the platform should not only provide information services for searching the tools needed by users, but also provide the feasibility of direct using of the necessary tools.
- Thus, the future web platforms will provide a single entry point both for web service providers and for their customers.