# VIRTUAL COLLABORATIVE PLATFORMS FOR LARGE SCALE MULTIPHYSICS PROBLEMS

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**Abstract.** Multiphysics problems are orders of magnitude more complex than single discipline applications, e.g., climate modeling, flight dynamics simulation, nuclear plant simulation, environmental disaster prevention. Powerful computing technologies are therefore required: security, fault-tolerance, dynamic reconfiguration, real-time monitoring, fail-safe procedures are mandatory. Among these technologies are also broadband networks and distributed computing, using cluster and grid-based environments. It is clear that large supercomputers, PC-clusters and, to a limited extent wide area grids, are currently used for demanding e-science applications, e.g., nuclear and flight dynamics simulation. It is not so clear however what approaches are currently the best for developing multiphysics applications.

We advocate in this paper the use of an appropriate software layer called *upperware*, which, combined with cluster and grid-based techniques, can support their uptake by the users when running multidisciplinary codes. This paves the way for Virtual Collaborative Platforms.

## 1. INTRODUCTION

Virtual environments are tools and facilities dedicated to the design, deployment, execution, monitoring and maintenance of large applications on distributed resources [1]. These resources may be computers, file archives, sensors, visualization tools, etc. The users do not need to own any one of them. He or she may have access to and use any combination of them among a set of available resources whenever he or she is granted the appropriate rights to do so, using a simple laptop or sophisticated apparatus, e.g., an immersive visualization environment

He does not need any technical knowledge of the underlying software and hardware tools, except that one he or she is currently using. The technical infrastructure, may it be a state-of-the-art middleware for grid computing or a large cluster of commodity PC connected to a broadband network, is made almost transparent to him/her.

In order to implement this approach, we need a software layer masking the underlying infrastructure. Because hardware, operating systems and i/o devices are sometimes referred to as *underware*, and because *middleware* is the de facto naming for grid management and interface software, we name this new layer the *upperware*.

The *upperware* is the generic service layer used to virtualize the resources used by the applications. It masks the actual hardware and software resources, making possible the design, management and concurrent use of dynamic, possibly overlapping and cooperating sets of private computing infrastructures. In this respect, the *upperware* enables secure virtual private computing environments to co-exist, in a way similar to virtual private networks (VPN) that are designed to co-exist over communication networks.

The *upperware* is built on top of existing grid middleware. It is therefore made compatible with current and upcoming grid technology standards (OGSA, WSRF, GT4).


## 2. VIRTUAL COLLABORATIVE PLATFORMS

From the user point-of-view, the interface to the applications are high-level graphic interfaces that masks the resource distribution and technical definitions [2]. They are sets of dependent tasks connected by a workflow graph. This approach leaves all the technical aspects to a further step, while focusing on the application logic only. The tasks are connected by a control flow graph formed by sequence, parallel, interleaved and imbedded loops.

Together with the underlying upperware and middleware infrastructures, this forms Virtual Collaborative platforms (VCP).

The tasks correspond to executable codes that are located transparently for the users on remote sites. It is the responsibility of the application designers and providers to define which resources the application needs, where they should be located if required, and which complementary properties they should exhibit (availability, QoS, etc). None of these resources are required to be local and to belong to the users or designers. Brokering protocols and usage grants are therefore supported by the *upperware*. Submission of such grants can be negotiated on a permanent or one shot policy. The *upperware* appears therefore as a general resource broker, negotiating with the remote systems the availability and use of resources, based on the local policies and granted access rights.


## 3. DEPLOYMENT OF VCP

The obvious advantages of the VCP are their ability to hide the technical aspects of heterogeneity and distribution to the application designers and users. The end-users never interact directly with the underlying middleware and networks. The application designers

have to define the abstract tasks involved, the corresponding executable codes (by their name and access paths) and the resulting data files (by their names and access paths also).

## 3.1 Industrial aspects

Among these aspects are the legacy applications and procedures which are among the constraints that hamper the wide dissemination of new technology and business opportunities. Legacy aspects are essential for knowledge and investment preservation.

It is also important that research and projects take into account the existing applications and procedures to enable their seamless integration within future platforms and research. Otherwise, de facto standards based on commercial products will continue to impose existing environments, e.g., CATIA. This could preclude or delay future evolutions, openness and interoperability of application software and collaborative platforms.

Fundamental issues have to be addressed, e.g., scalability, reconfiguration, reliability, fault-tolerance, quality of service and security which are major user concerns.

The industrial aspects also include a better support for the users which are not experts in the technologies they use, e.g., Internet users. This is a clear constraint for example for grid technologies, the uptake of which is hampered by the technology burden they put on the industry and on all the users.

The societal aspects include also the support for dynamic and evolving partnerships on collaborative projects.

This include management of security, confidentiality, authorization, IPR management and other technologies supported basically by all computerized techniques today. But they must be adapted and evolved to support adequately new VCP.

Another question is to what extent are the current Web2.0 concepts compatible with the corresponding very stringent constraints of contracting industries, and how to evolve it to fulfill these requirements?

This raises the issues of software engineering for the platform development and maintenance, e.g., service oriented architectures, service composition, large (petascale) data management, visualization of data,  on the fly management and configuration of the platforms, tools for designing, verifying and evaluating the platforms. No global solution exist today for these issues.

## 3.2 Technological aspects

A number of technologies are emerging today with great potential for industry competitiveness and technological independence in Europe.

Among these are: grids, PC-clusters, Virtual organizations, and Web-based platforms.

This sometimes precludes further breakthrough in industry with the related impact.

For example, grid technology advertises "Virtual organization", "Virtual workspaces" and "virtualization of resources" as novel concepts and functionalities to support user, data and application software integration. The corresponding technologies can improve VCP support.

This has given rise to the *upperware* concept, advertised as a frontier for new services. This is not however clear cut and should be refined.

The way to do this should also clarify the starting points and goals addressed. Is it to adapt existing procedures and tools to include new technology barriers, e.g., cooperation among worldwide distributed teams using grid technologies? Or evolve existing CSCW concepts to include generalized distribution and dynamicity of users, data and applications in project management? Another issue is the milestones that would define the roadmap to future VCP.

Indeed, existing grid technologies potentially include several functionalities that could support next generation VCP: virtualization of resources, virtual organizations, virtual workspaces, etc.

The advertised convergence of grids and Web technologies, via web services and WSRF in Globus for example, may confuse the users with the emergence of Web 2.0 [13], which tends to transform the current Web technologies into generalized application platforms.

Because VCP might benefit from both the grids and the Web 2.0 technologies, which do not overlap, a clear examination of both should be engaged to fertilize on the best available aspects offered by each one.

The conclusion here is that VCP research must include (or be supported by) novel aspects from grids, Web2.0 and communication technologies. Stated otherwise, this means that VCP will be an outcome of the ICT convergence.

It must also include support for the seamless inclusion of legacy applications and procedures.

It should finally answer the fundamental question concerning the opportunity to define and prototype new concepts, e.g., the *upperware*, which must be discussed to extract a proven adequacy, after a clear definition of their functionalities and interfaces with existing (e.g., middleware) and upcoming technologies (e.g., Web 2.0).

Because no prototype can yet play the role of proof of concept, a first step should be to support the development of an experimental *upperware* platform. Next, run multiphysics testcases on it to assess the approach and realize performance benchmarks using various deployment configurations.

There are other important aspects which are usually not well covered. They deal with the openness of the platforms and their interoperability, as well as the connected tools. They are listed below:

- The role of VCP is to include a large variety of software tools, which may be dedicated to modeling, simulation, design and experiments. These tools are used to contribute to large-scale problems and must be used in collaborative ways to ensure consistent achievements of the large-scale projects. It is therefore important that software development, deployment, configuration and execution be designed with open architectures, methodologies and platforms, e.g., Service Oriented Architectures.
- Development prototypes using a single commercial software environment are therefore a threat to openness, and potentially severe technology traps. This can hamper future developments and compliance with upcoming standards The only way is therefore to plug existing tools to open platforms. Compliance of the software tools with communication and software engineering standards will therefore be mandatory.

- Further, raw computing power delivered by thousands of processors linked to clusters or supercomputers will not by themselves solve new problems put forward by the processing of petabytes of data generated by large-scale applications. New categorization and data-mining and access techniques will have to be designed for fast access to pertinent data related to new simulations and visualizations.
- The development, uptake and dissemination of grids, cluster and super-computing will necessarily impact on future industry, not only in engineering projects. This is because there is currently a vast ongoing driving force in grid and cluster communities to incorporate sophisticated resource management features (actual and virtual resources), with the corresponding distributed support (resource discovery and allocation, workflow management, security and confidentiality support, e.g., authentication and authorization). It is the so-called "technology push/application pull" paradigm.
- Also, grid communities work on "virtual workspaces" that go far beyond the original "virtual organizations" concept. The maturing of this technology will impact on VCP and *upperware* development and adoption.
– Simultaneously, virtualization techniques have been marketed for desktop, server and distributed computing, e.g., XEN [11], VMware [12]. Their rapid dissemination is a good indication concerning the roadmap for virtual collaborative platforms.
– Following the DEISA [8], D-Grid and others, initiatives like the Partnership for Advanced Computing in Europe (PACE) are deploying strategic task forces and infrastructures for high-performance computing dedicated to large-scale multiphysics simulation programs [7].
– Last but not least, there is a very large number of workflow management and execution engines used for e-science and e-business applications, e.g., Taverna, GridAnt, Kepler, Bonita [4]. Some of them have been developed specifically to run on grid infrastructures., using web services, and allow composition of complex and potentially multiphysics applications. It is believed that this is the way for future, easy to use, high-performance parallel and distributed computing environments for solving large-scale multiphysics problems.

There is no doubt that all the points mentioned above will influence the development and deployment of future virtual collaborative platforms.


## 4. CONCLUSIONS


Large scale multiphysics problems have focused recently much attention from the industry because complex artifacts, e.g., aircraft, nuclear plants and mobile phones, require extensive simulation and optimization processes. Further, competition and societal requirements imply severe design constraints on innovative products. The solutions to new designs require comprehensive simulations that include several disciplines with different, if not contradictory, requirements: aerodynamics, structural mechanics, flight dynamics, acoustics and electromagnetics for aircraft design, for example. Powerful although versatile and seamless computing environments are required to run these demanding simulation and optimization

processes by non computer science experts. One avenue is to deploy them on supercomputers or clusters of commodity computers. Another interesting perspective is to share computing resources through computing grids, i.e. distributed heterogeneous resources connected by broadband networks.

This paper presents collaborative platforms as a mean to integrate multiple distributed software tools into a unified service envionment that engineers can use seamlessly in order to design complex artifacts involving multiple physics.

## 5. ACKNOWLEDGMENTS

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