An Innovative Collaborative High-Performance Platform for Simulation

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This paper presents an innovative collaborative visualization platform for the simulation-based design applications. Following the scope and the main objectives, the general architecture based on the internet standard technologies is explained. Based on a multi-domain approach, several demonstrators are involved crossing interests of industrial and academic communities. Related to the field of process engineering, we adapt and deploy a web-based architecture research application on the targeted platform.

1. Introduction

The Collaviz project[1] develops an innovative multi-domain remote collaborative platform for the simulation-based design applications. The major value brought to the scientific and industrial community is to make remote analysis and collaboration easily available and scalable. Web-based technologies, on the top of shared high-performance computing and visualization centers, will permit researchers and engineers handling very large data sets, including 3D data models, by using a single workstation, wherever in the world. Just a “standard” internet connexion should be needed.
This paper introduces this ambitious project and exposes potential benefits and opportunities that this project could bring to CAPE community. Taking advantage of the open-source high-performance platform delivered by the project at the end of 2010, we have to experiment such approach for CAPE domain applications.
The first section presents the overall project (budget, stakeholders, scientific objectives, main deliverables, timeline …). The second part details the platform and its web based technologies and architecture. One goal is to generalize the concept of distributed and remote services and apply it to collaborative scientific visualization and data processing.

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1 French ANR Program 2008 - Conception et Simulation – COSINUS, Ref: ANR-08-COSI-003 2009-2011 (36 months), Budget: 4 M€, Effort: 554 m.m

In this approach, every visualization process is done through a set of open source tools available locally or remotely for any scientific computing applications. The third part shows the opportunities offered by the Collaviz platform for scientific simulation application through a demonstrator for each application addressed by the project. Especially we present our application scenario for Computer-Aided Process Engineering in the fourth part. Finally we conclude the paper with the current state of our CAPE demonstrator and the next planned developments.

2. Presentation of the Collaviz Open Platform

The classical approach for remote collaborative platform for simulation-based design applications is not adapted anymore. An overview of different solutions can be found in (Grimstead et al., 2005). This approach cannot support efficiently those applications which generate Terabytes and even Petabytes of data. The worldwide networks are still not strong enough, especially with 10Mb/s or less for the common daily network of users to transfer back these data from centralized supercomputer centers where the data are computed to the local client for processing. Furthermore, researchers' and engineers' local computing resources are not suited to treat this kind of volume of data anymore.

Collaviz has been created in order to break some technological bottlenecks for scientists to collaborate and process their data remotely at any place and any time in the world with just a standard internet connection. With the participation of more than 17 academic, industrial and associated partners, it deals with several main challenges. The main and strong idea is to provide to academics and engineers from any simulation domain an "easy-to-integrate" platform! Its characteristics should be open process, web-based technologies, remote reliable architecture, HPC capability, 3D visualization, collaborative facility, common bandwidth thin client-access (browser) and rich client-access (any modeling environments).

Collaviz will deal with 4 major challenges. First, it will provide applications designed for habits of very different communities (geophysics, fluid dynamics, structure, biochemical, drug design…). It has to consider mainstream technologies for the service access (low bandwidth internet access, standard hardware for visualization…). Its assets will be in interactive and participative collaboration, not only remote "shared display" visualization. Moreover, these technologies have to be accessible easily, and Collaviz will provide the proper tools to manage all the services from a user and administrator point of view, to have a full transparent access to these scalable resources: visualization clusters, grid computing, etc.

3. Architecture and middleware

With high expectations from different partners, the architecture had to answer to different problems. Collaviz aims not only at providing users with a complete solution from a simple internet connection, but also at allowing developers to easily provide new functionalities and customizations. In order to achieve this, the platform needed to be highly modular. Based on the outputs of previous projects dealing with remote collaboration such as Part@ge (French ANR Program, 06TLOG031, 14 partners) or with remote scientific visualization such as SCOS/V3D (French ANR Program, 06TLOG028, 22 partners), and also “state of the art” analysis, the Collaviz architecture has been designed following SOA (Services Oriented Architecture) concepts, with clients connecting to a system providing services distributed on different servers (Figure 1).

The resulted platform implementation ended at the end of 2010, with various demonstrators being worked since the beginning of 2011. Those demonstrators are detailed in section 4.

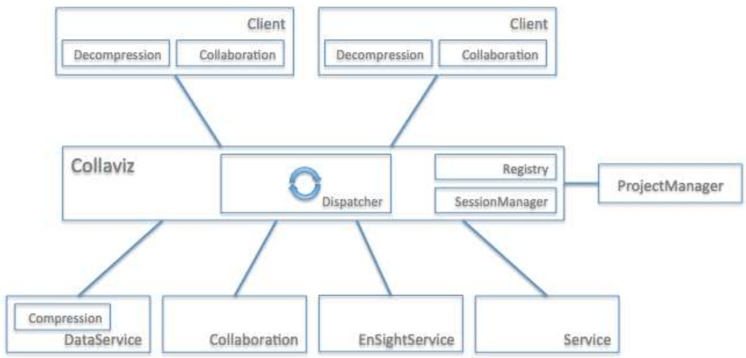

Figure 1. General architecture of the Collaviz platform

The Collaviz middleware is the core component of this architecture, ensuring the consistency of the information across the whole system. It is composed of four main modules:

- Dispatcher, the communication sub-system, acting as an event loop and allowing clients, services and core components to exchange commands and notifications,
- Registry, the service description database, keeping track of all functionalities provided by plugged-in services,
- Session, the session management component that handles client connections and the processing pipeline,
- Data proxy, the data exchange sub-system, which compresses and adapts data (including 3D data) to the client and network capabilities.

The Dispatcher component also provides the communication modules for clients and services to connect to the platform. To ease customization, all the API of the different components have been described before implementation to be able to replace one implementation with another if the default one, provided by the project, does not suit the user’s needs. For example, the project provides communication layers for TCP, HTTP and HTTPS protocols between the clients and the middleware but another can be added if necessary.

Services are the processing modules of the system. A service connecting to the middleware must describe the different functionalities it offers to users. Several “core” services are implemented by the project such as a Data Service exposing files from a shared file system, a Collaboration Service allowing people to interact on the same processing pipeline on different clients but also real processing services. For example, two different 3D data post-processing engines have been implemented, exposing the features of Kitware' Paraview and CEI' Ensight, two of the most used tools for scientific visualization (Figure 2). As services are accessed remotely, they can be distributed on different servers and, if needed, be deployed on high performance computing cluster. With this approach, even if your client application runs on a simple laptop, you can benefit of all the computing power of the infrastructure on which the Collaviz platform you connect to has been installed.

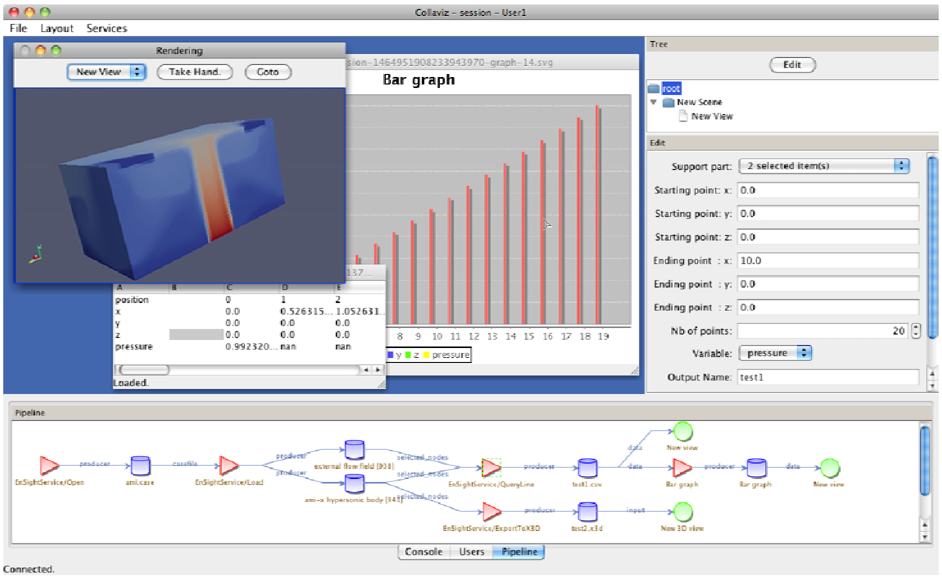

Figure 2. Collaviz client screenshot

A generic client is also implemented by the project with 2D and 3D visualization capabilities. As the middleware sends to each client at connection time a complete description of all the processes exposed by the registered services and its rights to use them, this generic client provides a graphical user interface to the processing pipeline offering all the possibilities of the platform. Other clients can be developed and existing visualization software can also be adapted to the Collaviz platform to take advantage of it.

4. A multi-domain approach

Several demonstrators are involved in Collaviz project since the beginning of 2011. The demonstrators will show the advantages provided by the platform on a truly multi-domain approach, crossing interests of industrial and academic communities.

Each code will be deployed on the basis of the integrated software and hardware test infrastructure provided by the project. The needed software adaptation and new and domain-specific functionalities will be developed by each partner and will be integrated on the targeted test platform.
All users will provide a full range of test cases integrated on the test guide (scenario) attached to one of the diverse demonstrators. Test of usability (functionalities & GUI), access easiness, performance and proposal of feature improvements will be the major result of the experiments. Each demonstrator (provided by partners such as EDF, INPT, EGID, NECS, MEDIT, Techviz and BRGM) will follow the same process: multiple remote web access to achieve collaborative analysis of scientific computed simulations datasets. The used infrastructures will be HPC ones (Virtual Nodes, HPSlab, CEA/DIF-TER@TEC), user workstations and SCILAB specific client.
If most of the uses of Collaviz platform are generic, major differences remain in the specificities of: (i) the field of research: geophysics, structure, drug design, process engineering…; (ii) specific formats of data used by the communities involved (HDF5, MED, Ensight…); (iii) ergonomics related to specific needs and habits of each research community.
The use of several and domain-specific demonstrators with different needs will assure that the results of the Collaviz project are not limited to one specific use. The goal behind this is to share as much as possible knowledge and to provide several generic and/or specific functionalities while staying focused on the real expectations of the users. While the core of the system will be conceived in a generic way, several demonstrators are planned to illustrate the versatility of the concept, with at stake, the ability for real user to appropriate the platform.

5. CAPE Application

As a demonstrator related to the fields of chemistry, our researches will be in charge of adapting, integrating and deploying a web-based architecture research application called Ternary Diagram Web Simulation (TDWS) on the targeted test platform taking advantage of partners support and project HPC infrastructure.
TDWS aims to design and visualize ternary diagram. The software does necessary numerical calculations from CAPE-OPEN unit operation models (Belaud et al., 2003) and draws ternary diagrams for different types of CAPE application such as L-L or L-L-V equilibrium calculation, distillation residual curves simulation, ... As example, our researchers are using this tool for understanding and developing distillation column model with chemical reactions inside (Thery et al., 2004). Also this tool allows us to validate and test our modern methods combining algebra and numerical calculation (Alloula et al., 2009) for solving NLAE and DAE CAPE models.
The challenge is to succeed in adapting, integrating and deploying the TDWS application on the targeted Collaviz platform taking advantage of partners support and project HPC infrastructure. Once the current state of TDWS application is adapted successfully to the platform architecture and technologies, we would like to improve our software by adding advanced functionalities such as:

- Collaborative work: At present several collaborators (research engineer and researchers) cannot work on a same session simultaneously from different geographic location. TDWS opens a dedicated and separate session to each client access.
- Display different residual curves in the same diagram and ternary diagram 3D picture: Our scientific model enclosing in the eXMSL part allows doing simultaneous calculations but this function is not yet available through TDWS architecture. Having several residual curves on a same diagram would obviously improve the study. In the same way, it is very interesting to work on a 3D visualization according to different CAPE specific dimensions (such as basically for a ternary system with respect to a state variable i.e. pressure). That is an actual great demand coming from our research department. Of course that requests to update our scientific models.
- The software could get benefit from HPC: If the current status of TDWS requests a common quadri-processors Windows server, to add 3D interactive model and data, collaboration process and multiple curves calculation dependant on parameter study will benefit from an HPC infrastructure.
- The software could simulate other phenomena: New functions request a non-trivial effort as TDWS were just developed for specific calculations and viewing. This point is out of the Collaviz scope. However subsequent to the project we plan to extend our approach to other CAPE functionalities.

6. Conclusion

The first version of our collaborative high-performance platform for simulation is released at the end of 2010. The integration project of our CAPE application into Collaviz platform has started in early of 2011.

The Collaviz project should open new prospects and our demonstration prototype should validate the general idea: to exploit an “easy-to-integrate” advanced services platform for CAPE oriented simulation applications.

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