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ICCS 2014. 14th International Conference on Computational Science

Procedia Computer Science

Volume 29, 2014, Pages 2284–2294



The WorkWays problem solving environment

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Abstract

Science gateways allow computational scientists to interact with a complex mix of mathematical models, software tools and techniques, and high performance computers. Accordingly, various groups have built high-level problem-solving environments that allow these to be mixed freely. In this paper, we introduce an interactive workflow-based science gateway, called WorkWays. WorkWays integrates different domain specific tools, and at the same time is flexible enough to support user input, so that users can monitor and steer simulations as they execute. A benchmark design experiment is used to demonstrate WorkWays.

Keywords: Scientific Workflow, Science Gateways, Interactive workflow-based Science Gateways, Computational Steering.

1 Introduction

Computational science is becoming increasingly complex. Computational experiments often combine computational models, analytical tools and data stores. Furthermore, components are often executed in parallel and/or in distributed environments. This makes the creation and execution of computational experiments challenging. Scientific workflow technology aims to simplify this task by providing a high level environment in which users connect a set of previously defined components, implementing a computational pipeline which meets their needs.

There have been a large number of scientific workflow engines produced in recent years, providing similar capabilities and functionality. For a detailed taxonomy of scientific workflow systems, we refer the readers to [1].

Science gateways are increasingly used to interface application scientists with their computations. A science gateway is a Web portal integrating community-specific tools, applications and data collections, that allows seamless user-interaction via a Web interface [2]. Science gateways are

popular for several reasons. First, they provide simplified, often graphical, interfaces to complex applications, and leverage [users'](#) familiarity with Web technology. Second, the Web separates the user interface from the computation, which simplifies the deployment of new applications. Third, user machines can be relatively low powered since heavy computations are performed remotely.

Using science gateways, users can launch large-scale experiments without concern for the underlying middleware or hardware details. Computations are launched behind the gateway, and these can be individual applications or complete workflows. Workflow-based gateways are extensible because workflows can be used to connect multiple, otherwise independent packages to form a single application. This approach has been taken by many workflow-based gateways such as CAMERA [3] – a Kepler workflow portal supporting microbial ecology researches, the LEAD portal [4] – a BPEL workflow portal for atmospheric research, or Galaxy [5] – a portal running the Galaxy workflow engine, and many more.

One area that has not received a lot of attention is the interaction between users and an executing scientific workflow, which is often executed in batch mode. Science gateways are typically only used to set up parameters, execute a workflow and collect computational outputs. In our opinion, gateways could support complex interactions between the running workflow and users, facilitating monitoring and steering of the execution as it progresses. This is important because human decision-making is an important component of real-world computational science.

We are building a generic workflow-based science gateway, called WorkWays, capable of supporting *man-in-the-loop* computation. This high-level problem-solving environment allows users to integrate different domain specific tools, as well as automates steps in an experiment, and at the same time, being flexible enough to support user interactions. In detail, WorkWays supports:

- * Integration of various domain specific tools that acquire, analyze and visualize scientific data in a visual programming environment;

- * Computational experiments on different high performance computing platforms; and

- * Monitoring and steering the simulations.

The paper begins with a review of existing scientific workflow engines, and corresponding science gateways. It then discusses the system design and implementation of WorkWays. We then demonstrate WorkWays in a use case study in aerodynamics optimization design.

2 Background and Related Works

2.1 Background

A workflow is an abstract description of tasks required for executing a particular real world process, and interactions between them. Each task is defined by a set of activities to be conducted, either by people or system functions [6]. Workflow technologies can be categorized into two broad families: business workflow (BWF) and scientific workflow (SWF). While BWF is control-flow oriented, focusing on control of the system, SWF tends to have a [dataflow-oriented](#) execution model.

A number of SWFMSs have been developed, as listed in Table 1. Several business workflow systems [have also been](#) adapted and used in workflow-based [science](#) gateways [4][16]. A detailed description of those works can be found in [9].

The concept of a science gateway was originally proposed in the context of the TeraGrid to bridge the gap between scientists and TeraGrid's computational resources [2]. Most science gateways provide users with either Web clients, desktop clients or both, to interact with the applications and simulations. These clients hide the underlying computational complexities from scientists and allow them to run scientific applications without concern of where the computation takes place.

There [has been much effort](#) to create and improve various science gateways in [a variety of](#) domains. [Here](#) we only review workflow-based science gateways in the context of this paper.

<i>Science Gateways System</i>	<i>Workflow Engine</i>	<i>Target</i>
CAMERA [3]	Kepler	Meta-genomics
BioWep [10]	Taverna, BioWMS	Bioinformatics
CrowdLab [11]	VisTrail	Visualization
Pegasus portal [12]	Pegasus	General purpose
OOPS [13]	Swift	Bioinformatics
GTLab [14]	DAGMan, Taverna	General purpose
LEAD [4]	BPEL	Weather forecast
SciencePipes [15]	Kepler	Zoology
GPFlow [8]	Windows Workflow Foundation	Bioinformatics
Ergatis [16]	Ergatis	Bioinformatics
Galaxy [17]	Galaxy	Bioinformatics

Table 1: Science Gateways

Table 1 presents a list of workflow-based science gateways and their corresponding workflow systems. A common approach is to deploy the workflow engine at the business layer. A Web interface is provided to select the workflow to be executed, to set up the initial parameters, and to monitor the execution. Once the workflow is passed to the [execution](#) engine, this Web interface can be detached from the [portal](#). To support long running experiments, emails are used to notify status of the execution, so that users can collect the experiment results [3][12][10].

The listed gateways can be divided into two groups in terms of user interaction. The **first group** includes the top 7 gateway systems in Table 1. This group mainly focuses on providing an easy to use interface; user interactivity is limited in these gateways. These systems usually differentiate between workflow developers [and](#) workflow users. [Developers](#) build commonly used workflows locally in their own [development](#) environment, which are then uploaded, and made available to users. [Users](#) only need to set up parameters, start the execution and collect the results afterwards. This approach is very helpful [for](#) novice users since it does not require [them](#) to have [detailed](#) knowledge of [the underlying](#) technology. The **second group**, composed of more recently developed gateways, provides more advanced user interaction capabilities. GPFlow [8], Ergatis [16], Galaxy [18] and SciencePipes [15] [allow](#) users to create [and](#) edit workflows [via](#) the Web. This is important since it enables users to interact with workflows [through](#) a uniform Web interface, i.e. the gateway. Amongst those, Galaxy offers [a](#) unique and intuitive mechanism [for](#) creating workflows. It allows users to experiment with analytical tools, which can be already in the system, or integrated by the users. [A](#) history of these experiments is kept and workflows are created by linking experiments together. In all of the listed gateway systems, GPFlow is the only system that allows [the execution of a](#) workflow both batch and interactively[8].

2.2 Related Work

To our knowledge, GPFlow is the only gateway that supports man-in-the-loop scientific workflows. GPFlow workflows are state-based [8]. At each component, the workflow can be [in a](#) “*running*” or “*suspended*” state, and user inputs are processed at “*suspended*” state. GPFlow supports interactions between running workflows and users by associating a Web interface with each component. Any [change made to a running workflow causes](#) the workflow to be restarted from that point. [The](#) main limitation is that it only supports acyclic [graphs](#), making GPFlow [unsuitable for](#) [implementing](#) feedback loops. [In this paper we include a cyclic graph based workflow.](#)

WorkWays can be classified as a computational steering environment using [a](#) dataflow model, similar to SCIRun [19] and IRIS Explorer [20]. [These systems](#) allow users to control the computational model while viewing the results of the calculation, [giving an](#) ability to focus on the productive region of parameter space. However, since SCIRun and IRIS Explorer are desktop

applications, they need to be installed and configured on each workstation. WorkWays, on the other hand, is more accessible by delivering these computational steering functionalities via the Web.

3 System Architecture

Kepler was chosen as [the](#) workflow engine [for](#) several reasons. The main reason is its unique actor-oriented modeling approach, which separates the execution model (Kepler's director) from the workflow components (Kepler's actors). This feature allows the same workflow to be executed [with](#) different execution modes. Additionally, Kepler offers a rich set of components performing various tasks in scientific processes in different domains [21], on multiple computing platforms.

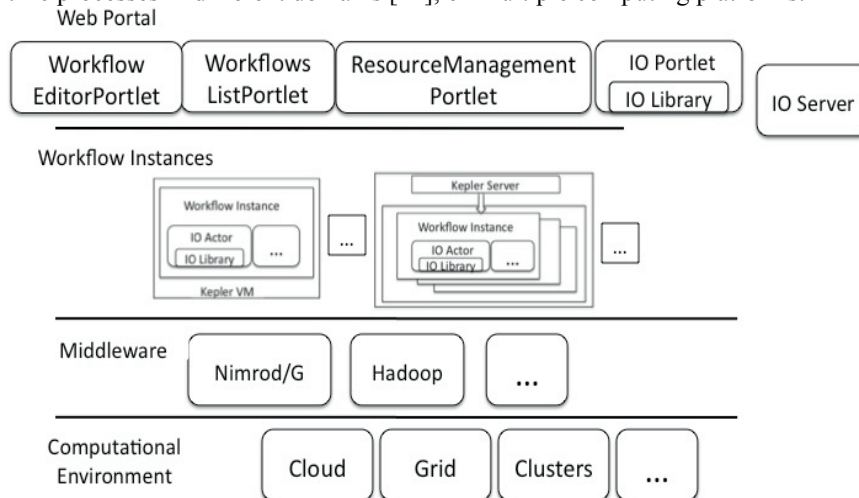


Figure 1: WorkWays architecture

Similar to other science gateways, WorkWays' Web components [are](#) portlets, conforming to JSR 286 standard. This makes WorkWays' Web UI components deployable as plug-ins to any existing gateways supports the same standard.

Figure 1 shows the overall architecture of WorkWays, which will be described in this section.

3.1 IO Framework

The IO framework creates [connections](#) between IO actors and the Web interface, allowing data to be inserted into, or exported out of running workflows. IO actors act as data sources, which initiate the connections. The Web clients (data sinks) then display the data from the IO actors, [obtaining](#) user inputs and transferring these inputs back to appropriate IO actor.

[A client-server](#) architecture is used for connections between IO actors and Web clients. This allows the Web clients and IO actors (and thus workflows) to be [placed](#) in different machines. Additionally, [this also makes it](#) easier to manage connections between data sources and sinks, e.g. how many Web clients can connect to an IO actor at the same time, or whether a Web client can connect to an IO actor, etc.

Figure 2 shows the components of the IO framework, which consists of four components:

IOServer

The *IOServer* is responsible for handling the connections between multiple clients (data sources and sinks), and routing the messages between them. The server is implemented in *nodejs* [22], with its *socket.io* library for communication protocol. Web socket is the main protocol being used, but

socket.io can fallback to other protocols such as JSONP polling, AJAX polling, etc. Messages transferred between *IO Server* clients are in Javascript Object Notation (JSON).

IO Server uses a publish-subscribe mechanism to route messages between clients. Each data source (IO actor) is associated with a unique channel, which is created when the data source connects to the server. Any data sink [that](#) wishes to communicate with the source needs to subscribe to this channel. Although multiple data sink can subscribe to [the same](#) channel, only the first subscriber can publish messages back to the data source, this is to avoid synchronization between multiple sinks.

Messages going through the *IO Server* are stored in a MongoDB database [23]. We use MongoDB because this nonSQL database is more suitable than SQL databases to store the weak-type JSON messages transferred between clients.

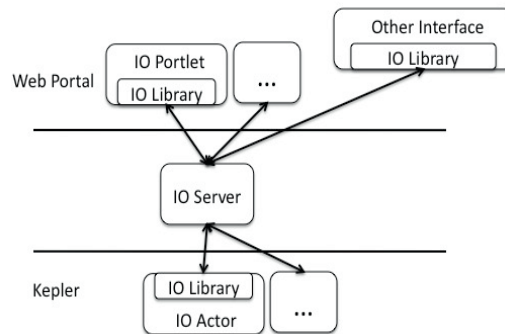


Figure 2: IO Framework components

IOLibrary

This library defines an abstract interface for creating connections to the server. This allows the system to support different connection protocol without affecting the upstream classes i.e. IO clients (*IOPortlet* and *IOActor*).

IOActor

IOActor is a *generic* and *configurable IO actor*, developed to simplify the tasks of creating actors for new IO operations. Instead of implementing new actors, workflow developers can generate new actor from this *IOActor* with IO operations specified declaratively. Figure 3 illustrates how a new actor can be [created](#). The description typically contains the following information:

- * *name*: name of the actor
- * *description*: optional description about the actor
- * *configuration*: information about the *IO Server*, and authentication.
- * One or more *IO operations*, each operation corresponds to a port in the generated actor.

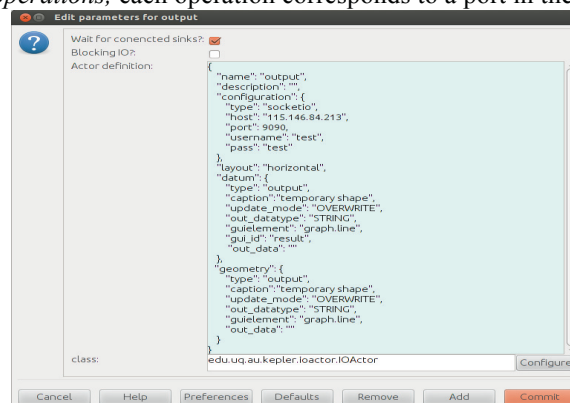


Figure 3: Generic *IOActor*, actor declaration and the generated actor.

IOPortlet:

Vaadin [24] [is used](#) to implement [the](#) IOPortlet. Vaadin is a framework for building rich Web applications as if they are Java desktop applications. Its main advantage is the ability to export applications to different targets, e.g. JSR-286 portlets, Web applications, and smart phone applications.

When a user executes a workflow (using the *WorkflowListPortlets*), a new page [which](#) contains all the *IOPortlets* instances requested by the workflows' IO actors [is created](#). Each *IOPortlet* [is](#) initialized with the name of the IO actor and the id of the workflow containing that actor. This *IOPortlet* creates a connection to the *IOServer* to [allow it to](#) subscribe to the actor's channel. Once [a](#) connection to the actor is created, the portlet generates UI elements as declared by the actor, [and as illustrated](#) in the *guielement* in Figure 3.

On each *IOPortlet*, users can switch between live data and recorded data. In the recorded data mode, the portlet queries the *IOServer* for all the data sent by the IO actor corresponding to this portlet. A slider is provided on the *IOPortlet* to navigate through the history of the data.

3.2 Workflow Authorization, Deployment and Execution

Workflow Authorization

There have been several attempts to create a [Kepler](#) Web-based editors, including SciencePipes, Hydrant and KFlex [25]. The common approach is to translate Kepler's XML declarative file to Web components and vice versa. Due to the complexity of Kepler's XML file, this is not straightforward. [Further](#), the Web interface needs to keep up-to-date with Kepler's XML changes.

We [chose a different approach, and used](#) Kepler's [own](#) editor. This [removes the](#) need to translate [between the web form and the XML](#), or to keep up with changes [in Kepler's XML description](#). [When a](#) user [edits](#) a workflow, WorkWays launches a virtual machine bundled with Kepler and a VNC server. The desktop environment with Kepler running [is](#) streamed to the *WorkflowEditorPortlet* (Figure 1), which is a VNC client. Changes to the workflow will be saved back to WorkWays' database once the user finishes the editing. Currently, WorkWays [has been implemented as](#) virtual machines on the NeCTAR cloud platform [26].

Workflow Deployment

An in-house headless Kepler server was developed to handle workflow deployment. This server receives workflow XML declaration files provided from the *WorkflowListPortlet*, the server then launches the workflow in a separate execution thread. From *WorkflowListPortlet*, users can then collect the data once the execution is done.

This centralised Kepler server might suffer from loading problems when multiple workflows are being executed at the same time. This load needs to be distributed to multiple locations. This can be achieved by:

- ***Partially distributing*** the workflows between multiple Kepler servers, and deploy a *balancer* to balance [the](#) load between them.
- Or ***completely distributing*** the workflows to the ratio of one workflow to one available workflow host.

WorkWays uses the second approach, in combination with [the](#) workflow authorization mechanism. Once [the user](#) finishes editing [a](#) workflow, execution [occurs](#) on the same VM being used for editing. This implementation does not require Kepler server on the VM, and each VM acts like a separate desktop with Kepler running. WorkWays will launch a new VM in case the user wants to edit or execute another workflows.

[Despite the load problem, WorkWays still utilises the centralised approach. This is to overcome security restrictions of some clusters, in which computational jobs cannot be submitted externally.](#)

Kepler servers are deployed at those clusters' head nodes, and executing workflows from the Web portal.

Workflow Execution

In WorkWays, Nimrod/K [30] is used to [implement](#) parallel workflows. Nimrod/K is a [Kepler](#) extension of the Nimrod family toolkit. It augments Kepler with a director, called [the Nimrod/K director](#), [which implements a](#) Tagged Dataflow architecture to expose and manage parallelism in the workflows [30]. Nimrod/K provides actors capable of sending jobs [in parallel](#) to Nimrod/G, which [subsequently distributes](#) and [executes them](#) on a combination of HPC platforms, including clusters, the Grid and the Cloud [38]. [In WorkWays](#), Nimrod/K is pre-installed in the Kepler virtual machines.

WorkWays users can manage resource using the *ResourceManagementPortlet*. This portlet allows users to add/remove/modify Nimrod/G resources, i.e. PBS, SGE, Condor, Globus, OpenStack, EC2 and Azure. From the *WorkflowsListPortlet*, resources [can be assigned](#) to workflows.

4 Case Study

This section demonstrates WorkWays [on](#) an aerodynamic design optimization case study, in which human input [is](#) used to guide [the](#) optimization of a 2D airfoil section [27]. This section first explains the optimization process, and then [demonstrates](#) how this process is [written into a](#) workflow using WorkWays.

4.1 Optimization Process

The optimization process [used here](#) is closely based on the experiment described by Kipouros *et al.* [27]. The new candidate airfoil geometries are generated by local and global modifications using the Free-Form Deformation (FFD) technique [28] (Figure 4). The leading and trailing edges of the airfoil section are kept unchanged to ensure fixed chord length and angle of attack. The parameter space of the optimization problem is defined by the movement of four control points in the Cartesian space, as highlighted in Fig. 3. The open source flow analysis tool Xfoil [29] is used to evaluate each new design vector for the prediction of the lift, drag and moment coefficients. In this example, the combined objective function targets to express maximum lift and minimum drag, subject to a set of hard geometrical constraints of the thickness at 25% and 50% of the chord that maintain the practicality and complexity of this benchmark engineering design case study [27].

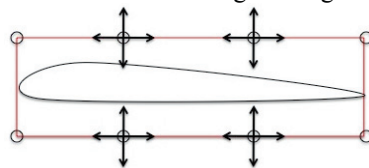


Figure 4: FFD with four control points (Modified from [27]).

Once an optimization process is successfully completed, scientists and engineers are interested [in](#) [identifying](#) the physical and behavioral relationships between design parameters and performance metrics. This is not a trivial task since it involves multi-dimensional data analysis of the parameter space and objective function(s) space simultaneously. In Kipouros *et al.* [30] a method based on Parallel Coordinates visualization [31] has been introduced for the post-analyses of turbo-machinery compressor blades, and in Kipouros *et al.* [32] this method has been expanded further for higher order of data dimensionality and human interaction. This technique has been then tested in Hettenhausen *et al.* [33] and found to be superior over the direct design optimization approaches, in the context of computational engineering design. The knowledge that can be acquired from such analyses can be used to reduce the number of design variables, or reduce the ranges of variability of some of the

design parameters, and ultimately succeed in the reduction of the size of the design space and hence accelerate the design convergence. Furthermore, the domain expert who interacts with such design systems can identify the region of interest of the design parameters that will reveal more interesting and realistic optimum design configurations in shorter time. Hence, a dynamic and interactive relationship should be supported between the human design expert and the computational design system. In the current work, we improve this method by enabling such human-in-the-loop computational design approaches within workflow management frameworks.

4.2 Optimization workflow with WorkWays

Figure 5 shows a workflow performing the 2D airfoil optimization. This workflow uses three IO actors: *Output* and *Optimum* actors for visualising temporary and optimum shape of the foil, and *ParallelCoordinates* actor for analyzing relationships between design and object space. All these three IO actors are generated from the generic *IOActor*. The *WorkflowEditorPortlet* allows users to modify and experiment the workflow before the full-scale execution.

The *DefineSearchSpace* actor initiates the optimization by defining the domain of the search; in this case, this domain is the combination of possible coordinates of the four control points. The starting points will be selected from this domain by the *SelectPointsActor*, and will be sent to the optimization actor. This workflow uses the simplex optimization method, other optimization algorithms, for instance Hook-Jeeves, Genetics Algorithm, etc., can be used just by replacing the optimization actor. The optimization actor generates set of points that are sent for evaluation. In this workflow, FFD and Xfoil are combined into one composite actor: *Compute xfoil*. This composite actor evaluates starting points from the optimization actor, and results of the evaluation are used to decide the next generation of points. This cycle stops when convergence criteria specified in the optimization actor are met. Note that there can exist multiple optimum solutions.

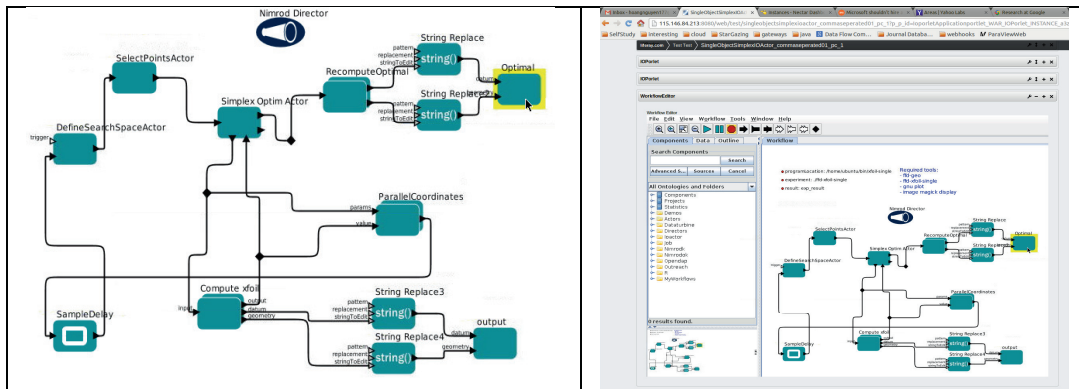


Figure 5: The airfoil workflow (left) being edited in the *WorkflowEditorPortlet* (right).

Figure 6 displays the *Web* page created by WorkWays. The *WorkflowEditorPortlet* is collapsed to reduce the size of the *figure*. There are three *IOPortlets* corresponding to three *IOActors* in the workflow. These portlets are automatically invoked by WorkWays when the workflow is executing. The visualization on each portlet depends on the IO operation defined by the corresponding *IOActor*. The two *IOPortlets* on the right display the temporary and optimum airfoil shapes while the parallel coordinate *IOPortlet* is shown on the left. This parallel coordinate plot has 9 dimensions, consisting of 4 Cartesian coordinates of the control points, and the evaluation result. In order to guide the optimization to a particular parameter space, the users choose a sub-region of each dimension. Once the user clicks the submit button, this information is sent back to the *ParallelCoordinates* actor. This triggers the *DefineSearchSpaceActor* to generate new set of starting points.

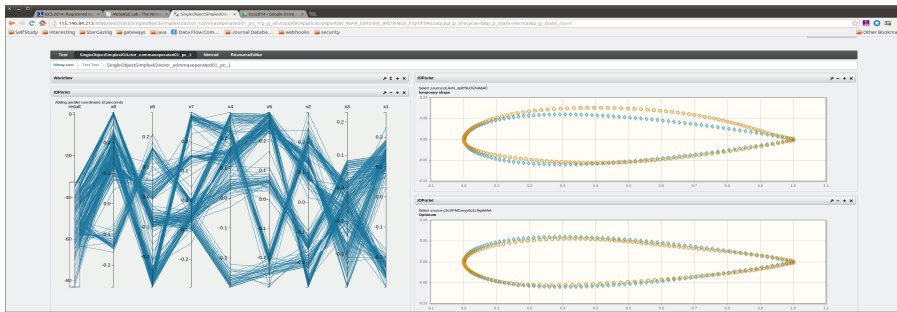


Figure 6: Workflow execution with *IOPortlets* showing parallel coordinates and 2D airfoil shape.

This example illustrates how WorkWays supports an interactive optimization as a problem-solving environment. An editor based on Kepler GUI is provided to allow users to [create, edit](#) and experiment with the [workflows](#). [Our solution is flexible and makes it possible to](#) integrate different domain specific tools into the [experiments](#). [Here we have shown](#) FFD and xfoil [as](#) an example. During the construction of the workflow, the *IOActor* is used to create actors performing different IO operations. This simplifies the tasks of creating new IO actors since no programming is involved. Once deployed and executed, *IOPortlet* and the generated IO actors allow users to monitor and steer the running experiment.

5 Conclusions and Future Work

In this paper we have presented WorkWays, a workflow-based science gateway capable of supporting man-in-the-loop workflows and potentially computational engineering design processes. We have discussed the WorkWays' general architecture. We use Kepler as the workflow engine, and JSR 286 standards for Web components. We also discussed the IO framework, which allows users to insert data into, or export data out of a running workflow. The IO framework has a configurable *IOActor* that can be used to generate new IO actors from simple definition files. This simplifies the creation of new IO actors since no programming [is required](#). WorkWays also provides an intuitive editor that is based on Kepler GUI editor. This is important since it allows users to interact with the workflows [through](#) a uniform Web environment. We also discussed the usage of Nimrod toolkit family in the architecture of WorkWays to manage and execute parallel workflows. An optimization study of 2D airfoil section is used to demonstrate the system.

There are several improvements we would like to make to our system. First, we [would like to](#) enrich the type of objects supported by IO actors and IO portlets. This will allow WorkWays to support more studies in different disciplines. Second, we [will](#) improve the way IO operations are defined. The text-based declaration of IO operations is error-prone; a GUI-based approach would be [more](#) user-friendly. Third, we [will](#) support different types of clients, beside Web client. One of such client is the OptiPortal tiled display wall [34]. This will enable visualization of high-resolution data, which often requires [very](#) large [screens](#).

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