

White paper FUJITSU Software HPC Cluster Suite – HPC Gateway

Engineers, analysts and researchers using HPC systems face their own challenges in optimising designs, interpreting data and discovery. Dealing with everyday complications of working with HPC systems, infrastructure and tools should not be one of them. Enabling HPC Simplicity means capturing knowledge and expertise within a solution that broadens HPC access and eases work, even for experienced users. This whitepaper describes just some of the ways the HPC Gateway offers this simplicity.



Introduction

High Performance Computing is a market often characterised by floating-point performance, interconnect bandwidth and memory throughput. These factors yield easily digestible numbers that allow us to track progress of systems and absolute capability. Yet what they don't reveal is whether end-users and project managers are fully able to exploit this potential, and particularly how new users and market sectors can integrate HPC into their business.

Routes into HPC

There are many routes to HPC adoption. Organisations who have worked with HPC systems and applications for years have built up significant internal competence to use and operate such environments. Others are more recently launching projects to take advantage of the scale and speed that HPC systems can offer their applications, for instance through a migration from workstations onto clusters. All have similar needs to ensure that users can effectively utilise the HPC servers.

- An intuitive and productive working environment.
- Mechanisms to capture and preserve best practice methods and processes.
- Ways to combine these methods with information to assemble and grow a learning system to sustain and disseminate HPC competence across the organisation.

Simplifying HPC

All HPC activity rests on the same foundation: prepare and run applications, monitor and control jobs, access and manipulate data. These steps can be just a tool supporting the actual business of the organisation. Equally, if organised and managed appropriately in themselves they can become part of the distinctive competence of the business. Either way, it is the ability to simplify the use of HPC, and embed methods and actions into a common expert environment that are key to improving the relative value from HPC investments.

HPC user desktop

There are clear benefits from "ready-to-go" HPC systems: optimal application performance, system readiness, faster deployment. Now, with the PRIMERGY HPC Gateway included in its HPC Cluster Suite (HCS), Fujitsu extends its offer beyond machine deployment and system management to the daily on-going business use of HPC.

This integrated web environment simplifies HPC for both current and potential users of HPC. New or occasional users will find it easy to prepare, launch and monitor work with no tuition. The Gateway aims to convert the sometimes obscure language of the HPC environment into terms more natural for the business user. Rather than multiple screens and command line operations, the user will interact through a central interface, piloting their workload with mouse-clicks, drop-down lists, concise application profiles and pre-defined workflows.

HPC Simplicity

PRIMERGY HPC Gateway

The PRIMERGY HPC Gateway is a complete web-based environment to simplify all aspects of HPC work management. Within this same environment you have the ability to manage all HPC work, handle files on any HPC server, monitor application execution as well as batch and system status, exchange documents, read user guides, collaborate with the team at any location through the forums and knowledge base. The gateway tool bar and desktop layout is configurable according to your preferred scheme.

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		Process Manager is the central point for all your HPC work and data access.
		Built-in features include:
		1. Run a wide range of pre-defined HPC applications. 2. On-board your own application scripts.
		Access and handle data across multiple filesystems from a single global explorer.
		Submit automated and robust best-practice workflows built around your end-to-end technical business processes.

Application catalogue

Clearly the central function of an HPC gateway web environment must be to run applications. A catalogue of common application interfaces is available to add to your HPC Gateway installation. One-step operations add these methods to your Gateway. Final association to the local application package installation are quickly made through an environment setup in the web desktop.

Additional interfaces can be added rapidly, either developed to a user-requested design or through the application on-boarding mechanism. This second capability offers a fast-path to make any application with existing run scripts available from the Gateway – runnable by end-users in just a few minutes.

Workflow automation

What really sets the PRIMERGY HPC Gateway apart is its workflow capability, dedicated to the automation of HPC application process orchestration and data movement. This workflow system provides a robust value-adding approach to encode HPC business processes, capturing how HPC is used to solve problems, as compared to running an HPC workload as a set of individual job transactions.

Standardise and reuse

Programmed workflows are used in the PRIMERGY HPC Gateway to automate any type of HPC business application process. By encapsulating multiple steps for a given experiment overall throughput is increased: the user is freed to focus on decision and analysis, while the system manages file movement, simulation task scheduling and synchronisation. For the same project users might select from several workflows, choosing the one most appropriate to that experiment. Standardisation of the organisations' best-practice processes makes individuals more effective in their domain of expertise since they are using HPC in terms of the business purpose. Re-use of tuned workflows brings more reliability in each experiment, reduces waste from misplaced data and enhances traceability for the whole project.

A key advantage of this approach is the way it allows newer users of HPC to simply and intuitively drive even quite complex simulations and analyses. Organisations currently using HPC can broaden adoption across their engineering and research teams, while new entrants are helped through the integral expertise and guidance.

Process evolution

Organisations can continue to adapt their workflows as new processes are identified and tuned. Either by linking tasks in new ways, or importing pre-developed workflows, the overall portfolio of methods can be expanded and enhanced.

Pre-developed workflows can be imported and run in any edition of the FUJITSU HPC Cluster Suite Gateway. To develop your own workflows requires the HCS Advanced edition.

Automating business workflows

Process Manager

The Process Manager is the primary portlet contained within the same gateway environment. It can be opened within the same browser page or a separate tab, and provides capabilities including:

- Run a wide range of pre-defined HPC applications.
- Run your own on-boarded scripts.
- Access and handle data across multiple filesystems (possibly across multiple servers) from a single global explorer.
- Submit automated and robust best-practice workflows built around your end-to-end technical business processes.
- Monitor applications during execution.
- Maintain a portfolio of job profiles to track progress of the experiment.

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Projects and teams

HPC is a solution normally used by groups or teams within the context of common projects. Therefore the scope of HPC solutions needs to incorporate facilities beyond job submission. Data generated through running HPC applications is ultimately turned into information and knowledge for the actual business purposes of the company.

Share and exchange information

There are many ways to engage end-users with the PRIMERGY HPC Gateway. Wikis are a way for individuals to create descriptions of methods and procedures they have found most effective. For example, usage guides for the Gateway catalogue applications can be added as wiki pages. Other types of documents – reports, research papers, presentations – can be stored and disseminated through the Documents library.

Accumulate knowledge

Forums are a place where users discuss issues and work out resolutions, and where individuals add to the collective knowledge of the organisation, in a structured and searchable manner. Eventually articles can be generated within the KnowledgeBase so that they can be referenced and applied on future projects.

Active process reporting

The capabilities of the Gateway unlock the potential to create a complete and dynamic reporting system. By creating specific reporting services and incorporating them into an application workflow it is easily possible to obtain continuous and immediate summary report generation. Statements can be output on the precise setup of every job and the movement of files between tasks and resources used for each computational stage. Summary information on the application-level results of a simulation may also be included into the reporting mechanism. And to increase overall visibility and clarity on the project such reports may be instantly added to the shared document library, so that the individuals and the team can actively monitor progress experiments.

Conclusion

Advances in HPC technology bring opportunities to tackle newer, more difficult problems or enable existing processes to become more efficient or effective. However there is a hidden cost in this advancement: complexity. Ease of use is sometimes overlooked when looking at clock speeds, bandwidths and capacity of advanced technology. We believe the best way to embrace new technology is to ensure it is delivered to end-users without complicating their daily processes.

Fujitsu's PRIMERGY HPC systems provide leading capabilities in terms of performance, quietness, low-power consumption, and packaging; from data centres to in-office clusters. The PRIMERGY HPC Gateway in the FUJITSU HPC Cluster Suite has been designed to capture end-user processes and methods behind the daily HPC operations, to allow tuning of their business processes and the creation of integrated solutions. This combination provides a clear value-adding offer: a simplified HPC experience with expertise designed-in – ready for use.

Contact

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