# CENTRE FOR PARALLEL COMPUTING

HIGH PERFORMANCE CLOUD APPLICATION SUPPORT SERVICE (HP-CLASS)

UNIVERSITY OF TECHNOLOGICAL INNOVATION WESTMINSTER#

# HIGH PERFORMANCE CLOUD APPLICATION SUPPORT SERVICE

### SUPPORT SERVICES FOR HIGH PERFORMANCE CLOUD APPLICATION USERS:

- Analysis of compute- or data-intensive applications
- High performance workflow design for intensive applications
- High performance cloud application prototyping
- P-GRADE web-based toolset training and hand-holding.

### SUPPORT SERVICES FOR HIGH PERFORMANCE CLOUD APPLICATION SERVICE PROVIDERS:

- Support for P-GRADE installation and configuration
- P-GRADE customisation and development
- Access to P-GRADE advanced features
- Cloud- and grid-based infrastructure development
- Research and development.

The Centre for Parallel Computing (CPC) offers a generic support service to users and collaborators based on P-GRADE. The objectives of the service are:

- To enable users with compute- and dataintensive applications to benefit from high performance cloud computing through the P-GRADE toolset
- To analyse, enable and prototype intensive user applications on high performance cloud- and grid-based infrastructure
- To provide technical support to high performance cloud service providers for P-GRADE installation and advanced features, and underlying cloud- and grid-based infrastructure
- To provide training, research and development.

### TOOL ENVIRONMENT BASED ON P-GRADE

P-GRADE (Parallel Grid Runtime and Application Development Environment) is a web-based, service-rich environment for the design, execution and monitoring of computational workflows. It was originally developed for computational grids but is now extended to encompass virtualised cloud environments. P-GRADE significantly accelerates the re-engineering procedure of sequential and parallel applications providing easy-to-use solutions even for nonprofessional programmers. The P-GRADE user interface is based on computational workflow - an everyday familiar concept that allows even non-computing experts to manage their applications. The tool itself hides all low-level computing infrastructure access mechanisms

through high-level graphical web interfaces. Workflows that include parameter-sweep applications (eq. Monte Carlo simulations) and parallel applications (eg. MPI jobs) are readily handled. Each stage of the development life-cycle (design, debugging, testing, monitoring and performance analysis) is addressed in P-GRADE. Its highly portable run-time environment provides dynamic load balancing facilities for long-running parallel applications and fault tolerant execution based on fully automatic checkpointing and migration mechanisms for cluster, grid and cloud applications as well as on-line monitoring facilities and remote performance visualisation.



## EXAMPLES OF APPLICATIONS SUCCESSFULLY PORTED USING P-GRADE

- Rendering Portal a grid-based on-line rendering service – a service operated by the Centre for Parallel Computing at the University of Westminster
- ProSim A Modelling Protein Carbohydrate Recognition In-silico
- VisIVO Visualisation Interface to the Virtual Observatory – for creating customized views of 3D renderings from astrophysical data tables
- Cellular Automata-based Laser Dynamics simulates the dynamics of laser devices
- Extraction of X-ray Diffraction Profiles obtains information about particles hit by X-ray
- SIMAP Simulates and analyses the dynamic behaviour of biochemical models
- WISDOM a meta-middleware for managing and monitoring jobs on the EGEE and OSG Grids

- In silico modelling using Autodock
- Traffic Portal an e-learning portal for transport and logistics studies
- DASP Digital Alias-free Signal Processing, a program defining the class of optimal periodic non-uniform sampling sequences
- Molecular Dynamics Simulation by CHARMm – macromolecular simulation
- Patient readmission analysis with the R statistical package
- CORSIKA Cosmic Ray Simulation for Karlsruhe Shower Core and Array Detector
- BWA Burrows-Wheeler Aligner, alignment of DNA sequences for genomics research
- Image and video rendering with MentalRay
- Classification of hospital patient profiles using the R statistical package GAMESS-UK – ab initio molecular electronic structure program
- MultiBayes for analysing DNA sequences of genes.



Example: Modelling Protein Carbohydrate Recognition in P-GRADE



# CENTRE FOR PARALLEL COMPUTING (CPC)

#### **Company Partners**

CPC have worked with many industrial partners in collaborative research and development projects, including:

- Simsoft Ltd, Turkey
- E-Group Ltd, Hungary
- ETH Zurich, Switzerland
- Scaletools Ltd, Switzerland
- CloudBroker GmbH, Switzerland
- 4D Soft Ltd, Hungary
- INAF Osservatorio Astrofisico di Catania, Italy
- Stichting AlmereGrid, The Netherlands
- Atos Origin S.A. Origin, Spain
- Platform Computing GmbH, Germany
- Microsoft Research.

#### **Academic partners**

- Laboratory of the Parallel and Distributed Systems in the Computer and Automation Research Institute of the Hungarian Academy of Sciences (MTA SZTAKI), Hungary
- Academic Medical Center of the University of Amsterdam, The Netherlands
- ETH Zurich, Switzerland
- Middle East Technical University, Turkey
- Eberhard Karls Universität Tübingen, Germany
- University of Zaragoza, Spain
- INAF Osservatorio Astrofisico di Catania, Italy
- Laurea University, Finland
- Trinity College, Dublin, Ireland

- French National Institute for Research in Computer Science and Control (INRIA), France
- Centre National de la Recherche Scientifique (CNRS), France
- Cardiff University, UK
- Faculdade Ciencias e Tecnologia da Universidade de Coimbra, Portugal
- Universität Paderborn, Germany
- University of Copenhagen, Denmark
- University of Innsbruck, Austria
- Universitätsmedizin Berlin, Germany
- University of Zaragoza, Spain
- Academia Sinica Grid Computing, Taiwan
- Institute for Systems Analysis Russian Academy of Sciences, Russia
- G.V. Kurdyumov Institute for Metal Physics, Ukraine
- JSC Kazakh-British Technical University, Kazakhstan
- Universidade Federal de Campina Grande, Brazil
- School of Computer, Huazhong University of Science and Technology, China
- Centro de Investigaciones Energéticas Medio Ambientales y Tecnológicas (CIEMAT), Spain
- The Foundation for the Development of Science and Technology in Extremadura (Fundecyt), Spain
- University of Southampton, UK
- University of Portsmouth, UK
- University of Manchester, UK.

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