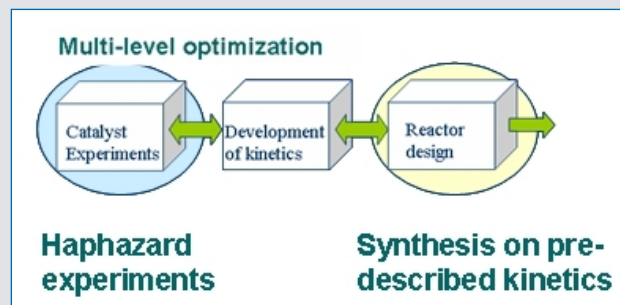
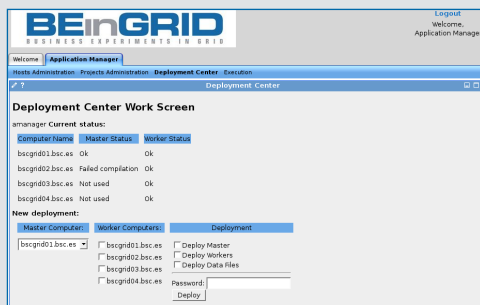


New Product & Process Development



Situation

Process industries are capital intensive and depend on innovative designs of products and processes, which are increasingly dependent upon computer aided experiments. These involve a large industrial sector comprising chemistry, materials design (specialty chemicals, design and structure of the materials) and pharmaceuticals. The path to new products and the economical use of in-vitro experiments require computing tools that enable experiments with ideas and alternative products.

A typical product development road map has a sequential number of basic stages required for each design experiment and implies extensive repetition of the procedure, because each experiment recalculates the design with different process conditions, intermediate products, catalysts, and process equipment. A Grid solution is highly recommended in this scenario because a new development methodology would become possible that significantly reduces the R&D effort and also helps to find innovative solutions.

The partners involved in the presented solution are:

- BSC, with a group expert in programming models for the Grid.
- UCM, whose main aim is to offer a loosely coupled meta-scheduler.
- UniS, with a research group of excellence dedicated to the integration of IT technologies in production manufacturing.
- LIKAT, a research institute which performs R&D on catalysis, reaction and process engineering.

Challenges

In the process industries, catalyst and inorganic materials sectors are growing; however, the chemical/petrochemical industry is undergoing changes owing to the shift away from oil as a raw material. This situation is forcing companies to innovate quickly instead of introducing improvements gradually. A prominent example is the current trend in the transesterification of vegetable oils or animal fats to make biodiesel, which augments and/or replaces petroleum-based diesel.

Process and product development comprise several stages, some of them computing intensive (combination of simulation models with process screening), and with heterogeneous data (databases, computer models, property and cost data). Current development processes involve tackling this problem in a sequential and manual way.

Grids offer a natural environment to exploit all the available computing power but they do not yet have the coordinated environment required by such experiments. Currently available solutions require too much development effort from the end user, which is an adoption barrier for this technology.

Solutions

Our products focus on the gridification of the process of product development. Sequential independent development efforts are integrated into a common one which saves time and generates synergies that are absent from independent development. The computing power and the integration features of a Grid enable this integration.

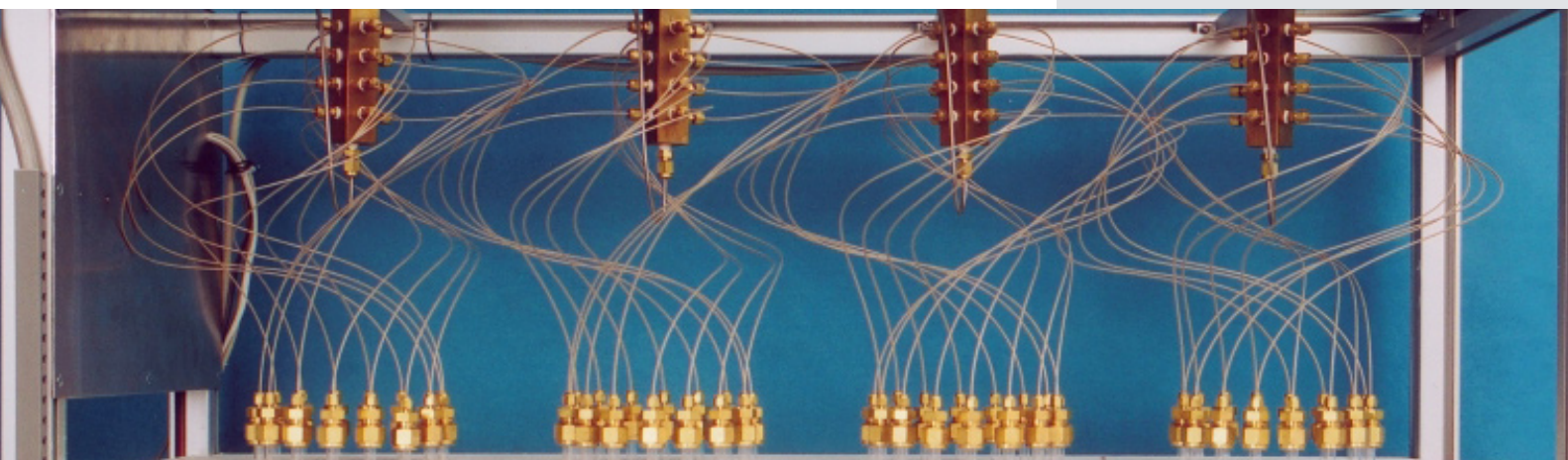
PIGridS (Process Industries integrated Grid Solution) offers a novel and innovative approach to systematise product and process development and the creation of patents and new products, while maintaining the competitiveness of the process industry. It is based on GridAD.

GridAD (Grid Applications Development solution) is a complete solution for the development of applications in the Grid, with a high-level programming model (where the Grid remains almost invisible), automatic parallelisation and gridification, and powered by a metascheduler, with advanced scheduling capabilities. GridAD is the result of the integration through the DRMAA OGF standard of two powerful Grid tools: GRIDSs and GridWay.

With the use of PIGridS, large reductions in the time taken by processes and hence product time-to-market are foreseen, from some years to only a few months. This will have a large impact on the business models concerned.

The main benefits for firms interested in using our solution are the following

- Easy grid adoption by means of grid-unaware development tools
- Use of grid portals to support new and innovative products
- Enabling of large-scale optimisation and simulation experiments
- Enabling of high-throughput and rapid design analysis
- Integration of computing resources across company borders



Business Impact

- PIGridS implies a change from the traditional business model where the product was a software license. In the new business case, PIGridS is offered as a service. Our business case study shows that a start-up company providing consulting and training services for PIGridS can be profitable with a small investment and with an expected ROI of 50% from the second year of operation.
- Companies can out-source the computational part of the process development (e.g. large companies) or get access to services they do not have available (e.g. SMEs).
- Time to market will decrease thanks to a reduction of the computing time, due to parallelisation and integration of methods.
- GridAD is offered as open source software with a business model based on training, support and consultancy for the development of new Grid-enabled applications. The software is generic and can be applied to a large number of industrial sectors.

Perspectives

PIGridS is the first product currently available that completely integrates the features available into a user-friendly solution. PIGridS is the first Grid-enabled solution available worldwide to integrate the process and product development in the process industries. It can solve more complex problems than its competitors. This will allow the development of integrated applications with immense opportunities for innovation.

The GridAD solution is a complete solution, with high level programming, automatic parallelisation and gridification, and includes a metascheduler. Currently there is no equivalent solution on the market. The new portal interface will enable GridAD to overcome barriers to Grid adoption. There is huge potential for this solution since it is generic and can be applied to several sectors of industrial applications.

Partners

Barcelona Supercomputing Centre – Centro Nacional de Supercomputación leads the consortium and provides one of the core technologies (GRIDSs) in GridAD. **Universidad Complutense de Madrid** provides one of the core technologies (GridWay) for GridAD. **University of Surrey** contributes group expertise in the integration of IT technologies in production manufacturing. **LIKAT** provides expertise in catalysis, reaction and process engineering.



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“Thanks to the grid technology we are now able to introduce a new generation of powerful algorithms with applications across the spectrum of engineering.”
David Linke, LIKAT