High-Throughput Experimentation and Tessella

High-Throughput Experimentation (HTE) is finding increasing use across a range of industries as a means of accelerating the R&D process, developing innovative technologies, and bringing products to market faster.

HTE has a broad range of applications in the development of formulations, coatings, chemical synthesis, polymers and catalysts, as well as applications in the study of biological systems. HTE has been successfully applied at sample sizes ranging from micro-well plates and micro-arrays through to vessels and reactors of hundreds of millilitres.

However, HTE isn't just about doing more experiments faster. To get the most from HTE requires a new approach and a new toolset. Through our work across many industries, including coatings, pharmaceuticals, consumer products and other speciality chemicals, Tessella has experience and capability across the software and informatics tools needed for this emerging discipline.

Workflow design

HTE requires workflows at a number of levels: from capturing the high-level business process, including planning and data analysis, down to workflows that represent the experimental protocol, process automation and robotic control.

Tessella has extensive experience of workflow systems at all of these levels, including editors for end-users to design automated laboratory processes, automated data processing chains, and high-level experimental protocols for long running studies covering weeks or months of elapsed time.

Experimental design

Although not all HTE applications make a clear distinction between workflow, protocol and experimental design, it is useful to think of DoE (Design of Experiment) as an activity in its own right that is concerned with what varies between samples (such as sample composition and process parameters) rather than the mechanics of creating and testing samples. Tessella can develop tools to design experiments within a specified design space, or, rather than reinvent, integrate existing best-of-breed statistical DoE tools into your HTE solution.

Modelling

Even with the higher sample processing capacity possible using HTE, a design space with more than a few composition or process variables may still be too large to cover adequately with a reasonable number of samples in screening and optimization experiments.

For some applications it is possible to model the variable space to predict outcomes and identify the most fruitful areas of the space to explore. These models can then be refined with actual experimental data to improve prediction capabilities.

Tessella has applied modelling to HTE and has extensive modelling capabilities including adaptive techniques that allow model refinement based on results of real-world experiments.

Instrument control and integration

Tessella has a wealth of experience in controlling and interfacing to laboratory instruments and robotics, whether through vendor-supplied interfaces or low level interfaces to custom hardware. Our experience covers liquid handling robotics, plate handlers, robot arms, HPLC/MS and a host of other laboratory automations devices. We have particular experience working with HTE platforms from Bosch Lab Systems and Symyx.

Data management, analysis and reporting

An HTE system requires an integrated data management system to deal with the large volume of data that are generated. To make the most of the valuable data resource needs query, mining and reporting capabilities suited to the multi-dimensional nature of HTE data.

Tessella has over 25 years experience of scientific data management, including work in regulated environments. Our capabilities include data management, long-term data preservation, reporting, analysis and visualization.

A Selection of Tessella's HTE Experience

Tessella and Bosch Lab Systems

Bosch Lab Systems produces HTE automation technology for the synthesis and characterization of new materials and formulations:

http://pa.bosch.com/boschlabsystems

Tessella is working in cooperation with Bosch to develop HTE software to provide the chemist's user interface and experiment management system to Bosch's HTE hardware platform (for a number of different clients).

Tessella is developing software to allow chemists to create experimental protocols and experimental designs, to translate those experiments into instructions to be passed to Bosch's HTE systems, and to collect and manage the output data returned by the hardware. These software solutions are being customized for each client's particular requirements and interfaced to their corporate systems when required.

Automated coatings recipe evaluation

A global coatings company needed an automated system to evaluate a large number of theoretical recipes. An instrumentation company developed a robotic system and Tessella defined the interfaces between the respective components, allowing the development of the hardware and software systems to be undertaken in parallel.

Tessella's software was responsible for experiment design, sample recipe selection and batching, sample queue management and submission to the robotic system. The software is also responsible for the retrieval and analysis of the experimental results. The experiment design and analysis were complemented by a model to predict the physical properties of the product that could then be evaluated by comparison with the measured properties of the experimental samples.

Consumer product HTE research

Tessella undertook a root and branch review of data management and HTE for a large consumer products client. This resulted in the design and implementation of a bespoke system to help their scientists through the execution of their HTE experiments. The web-based system allows the users to define plate layouts, protocols, execute experiment designs and gather the results within a data management framework.

The system interfaces to many pieces of HTE equipment including Spectramax and Tecan Sunrise plate readers in both stand-alone mode and when integrated with robotic systems from manufacturers such as Tecan, Hamilton, Zinnser, PAA, and Caliper Life Sciences.

In addition, web services were developed in order to facilitate data input and output to bespoke hardware and workflow systems such as Pipeline Pilot.

HTE strategy study

Tessella worked with a leading HTE research centre to help define their IT strategy. This involved organizing a number of workshops with the various stakeholder groups, drafting a User Requirements document, and then assessing the various commercial products (LIMS, Electronic Lab Notebooks etc) against the requirements, as well as obtaining detailed costings for the implementation of each.

The final outputs of this project were the User Requirements document, a report defining how well the various solutions fulfilled those requirements, and a proposed strategy for the research centre.

Symyx Renaissance support

Tessella supported the HTE group of a large chemical company. This involved interfacing Symyx Renaissance to a variety of bespoke high throughput instruments for measurements such as rheometry and light transmission through suspensions. This was achieved by extending Renaissance with custom components to add the desired functionality. In addition, Tessella maintained the databases and application servers and ensured the smooth running of the system.

Parallel reaction optimization

Tessella helped GSK develop a system called PROSPER, which controls a robot, enabling chemists to run up to 52 litre-sized reactions in parallel. This is used for investigating and optimizing chemical reaction processes.

Salts and Polymorphs

Tessella developed an Automated Salts And Polymorphs software system for GSK. The system is designed to evaluate different salts of a drug and identify and characterize the salts' different crystal forms (polymorphs). The software manages the whole experimental process from design experimental protocols and screening experiments through to process automation and data management.

To find out how Tessella might help with your High Throughput Experimentation requirements please email *info@tessella.com*

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