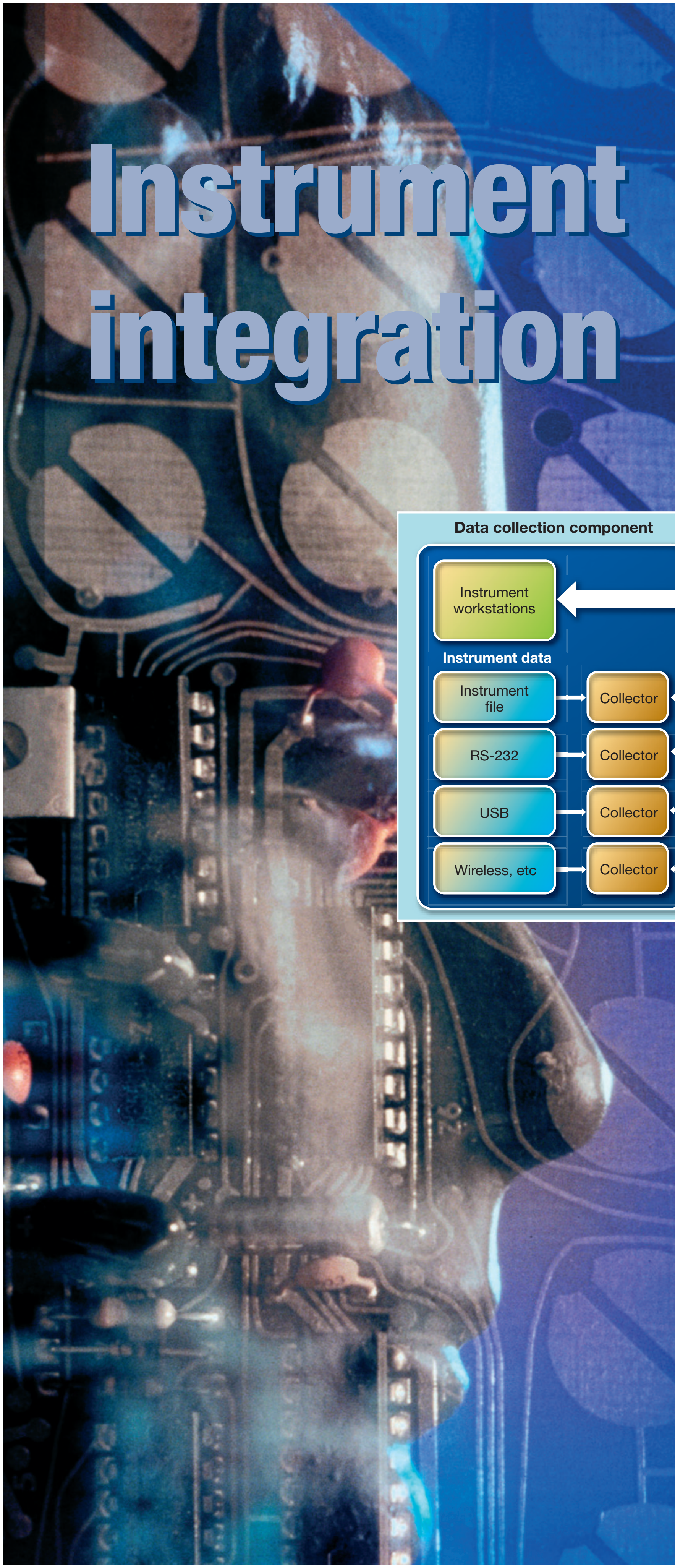
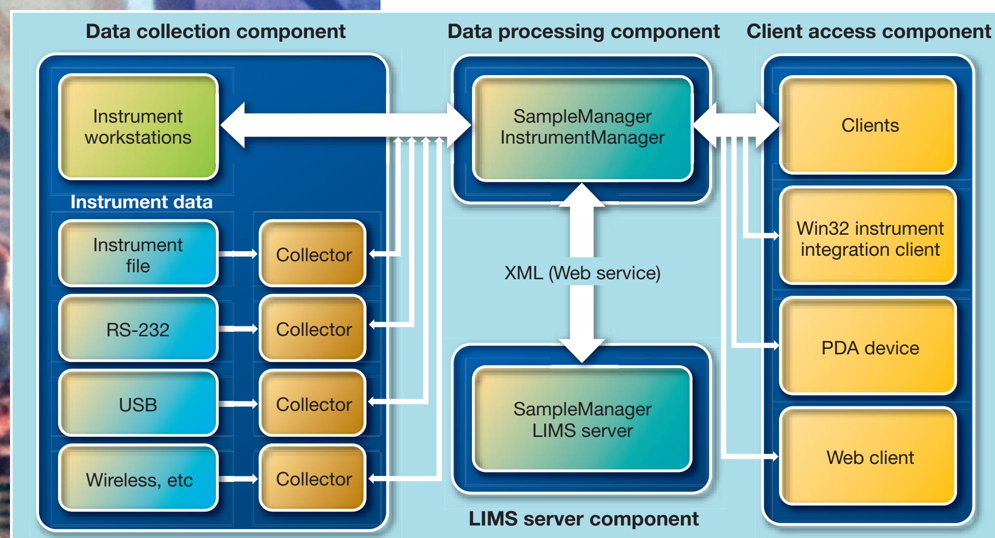
Instrument integration



Technological advances have led to a proliferation of analytical data that must be managed effectively. Colin Thurston, of Thermo Electron Corporation, discusses how Laboratory Information Management Systems (LIMS) integration can help



Advancing technology in laboratory instrumentation along with higher-throughput processes are generating massive volumes of analytical data – even terabytes per project. The challenge is to automate and integrate laboratory operations and procedures wherever possible in order to manage and process these growing data volumes more effectively. A LIMS (Laboratory Information Management System), like any other information system, becomes more responsive and productive when it is integrated with other systems and applications in the laboratory environment. Integrating LIMS with analytical instruments not only automates laboratory functions but also provides data-sharing benefits that add value to the original investment.

LIMS implementation tends to be a high profile undertaking, and effective instrument integration can provide a positive and visible early milestone. Achieving this integration, however, demands not just specific product functionality but a close partnership between the LIMS vendor and the customer.

Traditionally, instrument integration products were designed for single PC operation and struggle with today's networked operations, leaving a clear need for a more flexible, 'scalable' solution. Alternatives are emerging that employ advanced technology and architecture that provide considerably more efficient and effective integration of LIMS with laboratory instrumentation.

Instrument integration systems acquire data automatically, with the primary goal of eliminating errors in transcription and reducing the amount of time needed to manually write or type results. Most systems in the pharmaceutical industry were implemented to ease compliance with regulatory protocols, such as 21 CFR Part 11. Further development has meant that some systems offer instrument connectivity that involves very little coding to be installed and, more importantly, the fault tolerance necessary for 24-hour production environments.

Systems are usually capable of connecting to most instruments that have either an output transmitting ASCII or that can export data as an ASCII file. Also, each PC that runs the instrument integration software is able to connect multiple instruments so that the number of PCs that can be connected to the LIMS is effectively unlimited.

costly specifications

But these types of solutions, often termed 'thick client' solutions by informatics vendors, tend to fall short in a number of areas and can struggle, particularly in laboratories in a high throughput environment. They were not originally designed to handle huge volumes of data from the latest versions of highly sophisticated instruments.

Scalability of hardware can also rapidly become a problem. Each PC dedicated as an instrument workstation needs a full system installation – capable of data acquisition, processing and interchange to the LIMS, while also providing the client interface for the user. This inevitably requires a costly, high specification machine at each workstation. Also, logistical problems may be encountered when integrating instruments 'down the wire', in which case a high specification PC would need to be within the radius of the maximum cable run from each instrument.

In a laboratory with 20-30 instruments spread across a number of locations, providing the administration and security for all workstation PCs can be a major undertaking. Configurations and upgrades of any individual element of the software can require a full installation of the application, including the necessary configuration and subsequent validation.

To cover for events such as hard disk failure, an administrator would require a back-up strategy for each workstation. Maintaining system security and eliminating risk of data loss becomes a significant management challenge – occupying resources that could be more productively allocated elsewhere.

new approaches

A more flexible and scalable instrument integration solution would incorporate an architecture that separates the collection and processing of instrument data into separate software components. In situations where high levels of data processing and modern, reliable networking are required, these software components could be deployed in a distributed configuration. For many global organisations, server-based data processing is the preferable option.

A new approach to integrating LIMS with instrument integration includes a PC that holds a series of instrument file collectors with the workstation and instruments. The function of these collectors is configured at the central server, which instructs each to look for either a data file from a network or hard drive or a stream of data via an interfacing port.

For example, the server can be configured to direct a collector to listen for a stream from a specific port, or to be ready for a particular stream of data and to stop at the termination of the stream. In addition, configuration of the server controls the scheduling of the transfer of the instrument data from the collector. No processing whatsoever need be carried out at the instrument workstation.

As analytical instruments evolve with new technology, collectors may be added to support different types of data output. For instance, access to data via XML (eXtensible Markup Language) based files are becoming more prevalent within pharmaceutical QA/QC laboratories. Connecting these instruments to the LIMS could be as simple as installing a new collector.

An architecture utilising a central server within a dedicated, secure, IT department-controlled strong-room leads to management efficiencies in a number of areas. For example, it provides a single location for updates, for configuration of all parsing scripts (which extract the data from the instrument output) and all mapping scripts (which correlate the data from the instrument to the correct fields in the LIMS).

The single central server also enables the back-up routines and security to be centrally administered and provides the ability to build in hardware fault tolerance, redundancy and back-ups at a single location. In traditional architecture for LIMS/instrument integration architecture, all these critical issues would need to be addressed at each workstation individually.

Taking PC theft as an example, in a workstation-based application a full installation of the application would be required on a replacement PC plus a full configuration determining from where data is to come and in what format (instrument file, COM-based instrument, etc). Reconfiguration of all the parsing and mapping scripts would also be necessary.

This would either result in significant down time, or require laborious manual transcription of results while waiting for the instrument to be reconnected.

Contrast this scenario against a solution using scalable architecture, where a replacement preconfigured PC can be quickly brought online. Only the collector component needs to be installed, along with any local parsing and mapping configurations, for the system to be up and running again.

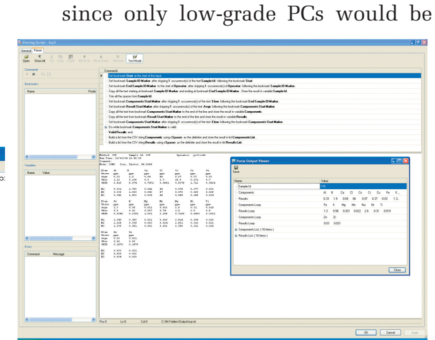
Once the server is directed to the new collector or series of collectors, instrument capture can be restored immediately. Furthermore, savings can be made since only low-grade PCs would be required in this new architecture.

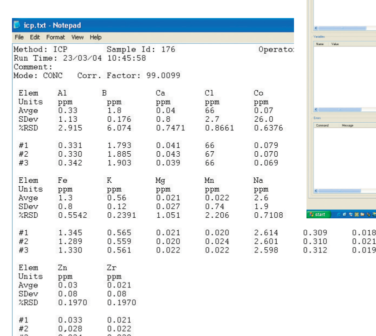
Modern LIMS/instrument integration solutions have been designed to address the data management and security requirements of today's laboratory, such as compliance with 21 CFR Part 11. Organisations can configure different roles and groups for individuals inside and outside the lab, assign appropriate functionality and system menu options to groups or specific end-users, and prevent unauthorised users from accessing specific areas of the system.

Integrated security, password protection, audit trail and electronic signatures allow multi-user access, while ensuring each piece of information is accessible only by authorised personnel.

The trend for larger LIMS vendors ►

Facing page: Diagram showing how the LIMS server component fits in with data collection and client access





Below: Modern instrument integration solutions require advanced data mapping and parsing capabilities to process data from disparate instrument types and multiple vendors, thus eliminating the need for bespoke interfaces for each instrument system.

◀ is toward developing and implementing their own instrument integration solutions as alternatives to separately sourcing third-party products. This approach, taken by Thermo Electron Corporation with its flagship LIMS, SampleManager, provides additional value to existing and future installations.

A standard user interface is utilised for all types and brands of instruments, providing consistency throughout the lab and the organisation, reducing training requirements and accelerating implementation. Automating the transfer of results from analytical instrumentation to SampleManager is eliminating manual typing of results with its associated transcription errors.

Now, even in very high throughput environments, analytical information from sophisticated instrumentation can be delivered accurately and quickly to laboratory management and other authorised decision-makers, increasing productivity in the laboratory and lowering the cost of ownership for LIMS. ■

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Scalable computing architecture explained

Microsoft **.NET technology** is a popular framework for scalable computing architecture and the 'componentising' of software solutions. This technology offers a building block approach to application development utilising XML, enabling interconnectivity as well as integration to larger applications over the Internet. The attributes of XML as a basis for a data file standard have been well documented and it is enjoying widespread acceptance both as a data interchange and storage format, including within the regulated industries. XML is a public domain, platform-neutral data formatting standard. It offers an application-independent way of representing data, however rich, using plain ASCII text.

These technologies provide a 'future-proofing' quality to the LIMS/instrument integration solution. New collectors, for example, can be embedded in the software by an instrument vendor, thereby simplifying integration with the LIMS.

Using architecture based on components rather than single larger applications facilitates customisation of collectors without affecting the whole solution. In a regulated environment, this offers significant savings in the extent of validation required to demonstrate compliance with GXPs.

By using Microsoft .NET within such an architecture, the instrument integration system can be presented to the user in different ways, via a Windows32 client or web pages. The ability for a chemist to configure instruments and review the status of instruments using PDA technology is another possibility.

By using a **Web service** interface to store analytical data in a LIMS as part of this architecture, the processing components can be isolated from variations in multiple LIMS implementations; an important consideration with large pharmaceutical manufacturers operating on a global basis. In brief, a Web service is simply an application that can be delivered as a network service and integrated using standard Internet technologies. Much of the strength of the Web services concept lies in the fact that it combines a simple-to-understand format with proven and well-established communications technology.

Web services are built using a group of XML standards, thereby providing complete platform independence. This allows an organisation to deploy the Web service on the server platform of its choice, and to use the Web service from any application written in any programming language.

A Web service also allows for the reuse of existing business rules within the LIMS. Organisations that have standardised on a LIMS for their laboratories will also have configured the LIMS differently for specific labs – r&d and production environments, for example. Should one of the LIMS be upgraded in this situation, no changes would be required to the instrument integration functionality. This simplifies deployment of new LIMS features, reduces validation efforts, and allows much greater flexibility than conventional LIMS deployments.

LIMS users, in fact users of any software application, will be familiar with how existing applications can mysteriously stop working when they install a new application onto their PC. This is due to conflict between the .dll files in the two applications.

By isolating applications, .NET eliminates this conflict. This means that when installing a new collector, for example, at the instrument workstation there need be no concern when using .NET component-based architecture.

This not only minimises impact on PC performance, but also reduces the amount of validation required in regulated environments.