Analytical Instrument Control using XML-based Web Service

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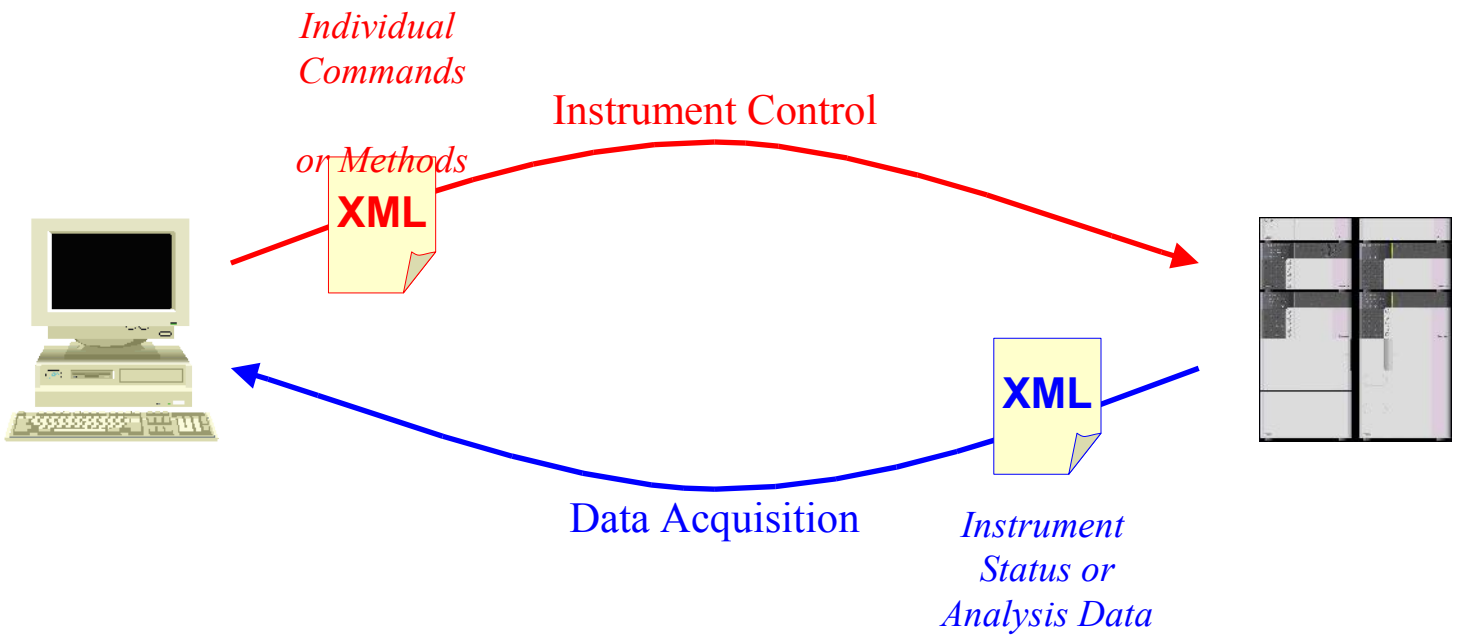
Introduction

- Labs have heterogeneous mix of instruments, vendors and software
- Instruments are controlled in a proprietary way for each vendor
- The number of requests for a multi-vendor support of analytical instrument control and data processing software is increasing every year
- However, for multi-vendor support, there are still many problems remaining such as development costs, software maintenance caused by upgrading of analytical instruments, upgrading an operating system, etc.
- XML Web service can be implemented on various platforms including an embedded system like an analytical instrument, and its proxy program can be easily generated by using many development tools.
- Development work at Shimadzu for a multi-vendor instrument control object model using XML Web service was introduced in the new HPLC system (Prominence, LC20A)

Introduction

- Growing need to integrate Instrument Control and Data Acquisition Systems with LIMS, E-Lab notebook, Process Automation software, etc.
- The integration requires the ability to interchange analysis data as well as execute instrument control from different software layers
- New complex multi-instrument systems (“super” systems) require special custom developed software for automation
- Increasing regulatory requirements result in more validation work
- Validation is an overhead and it needs to be reduced

Instrument Control Model using XML



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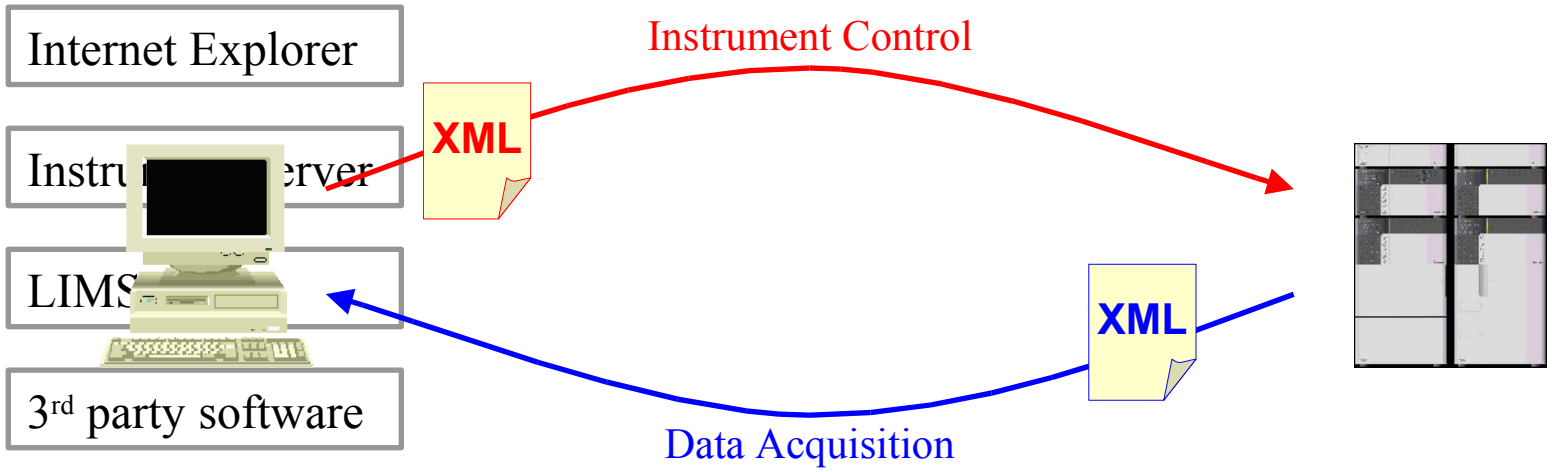
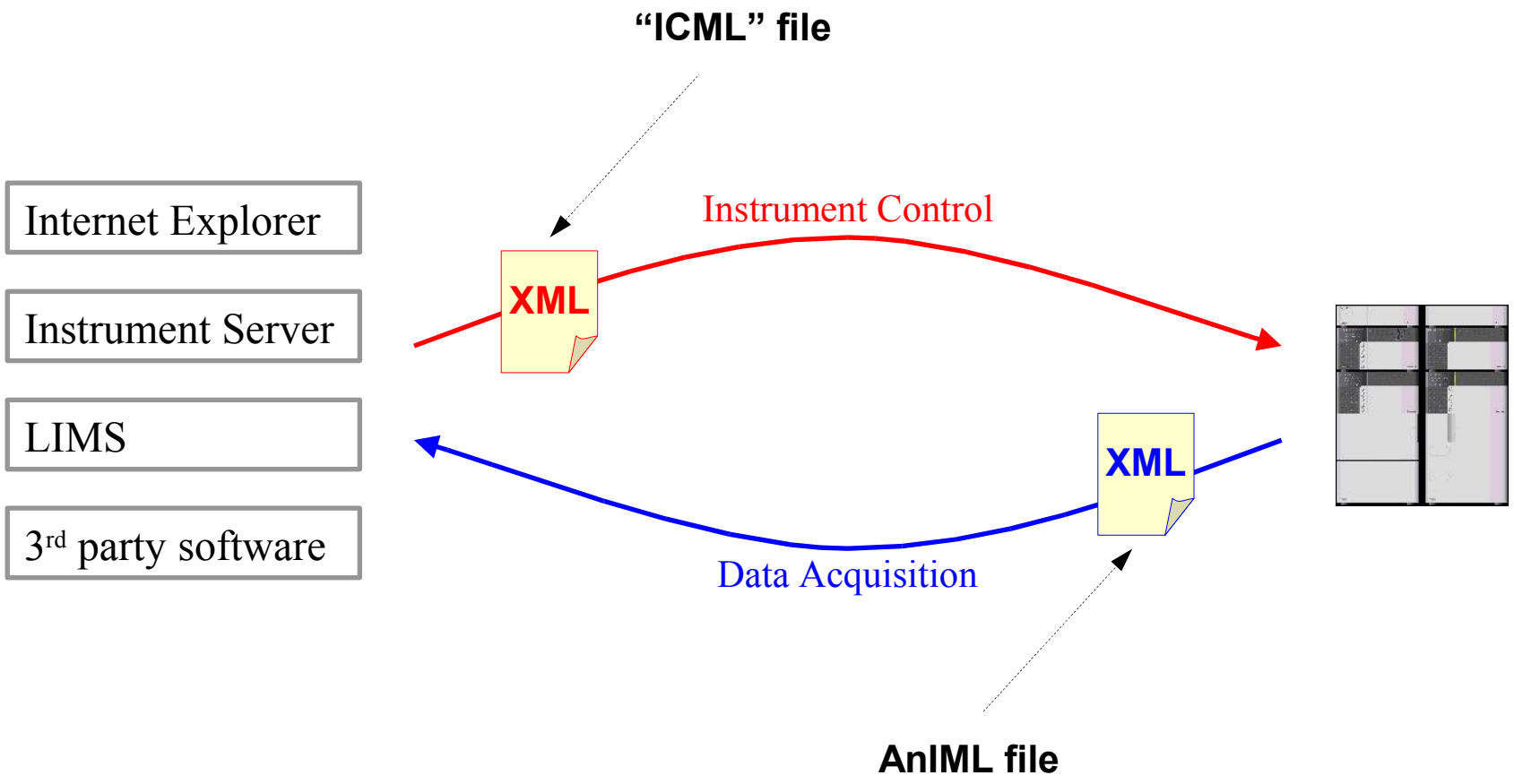


Standard Formats in XML-based Communication



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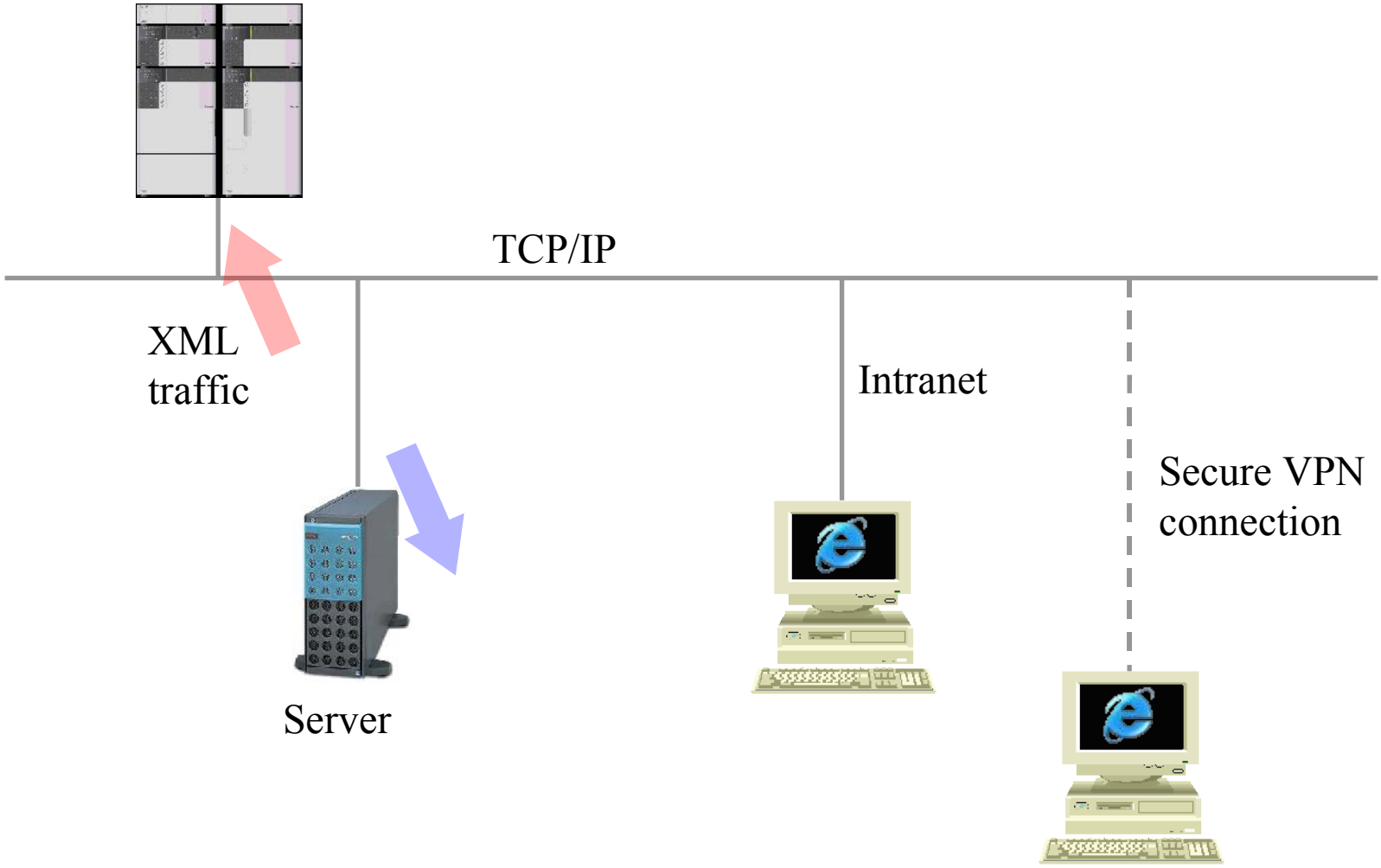
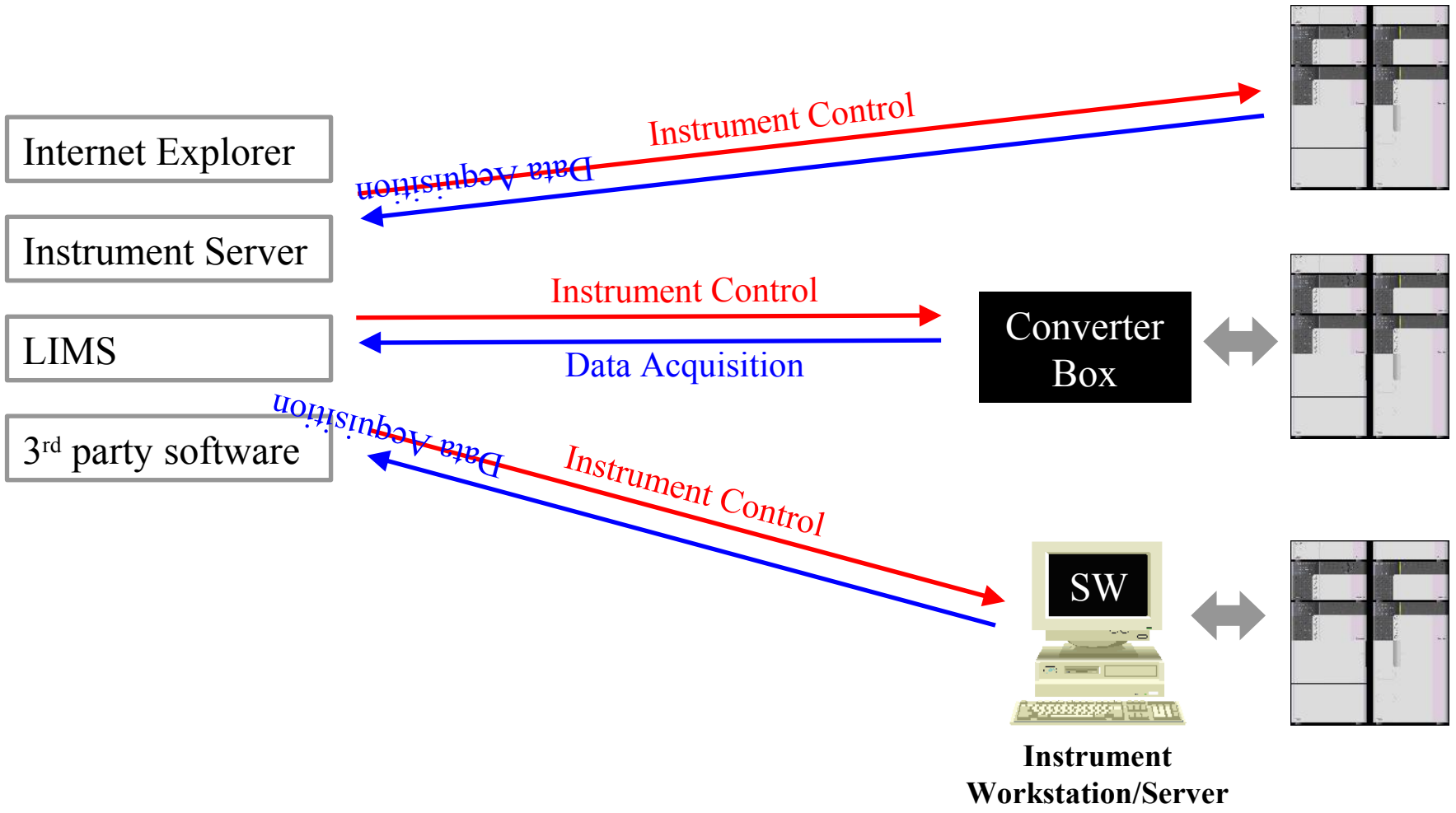


Possible Migration Scenarios

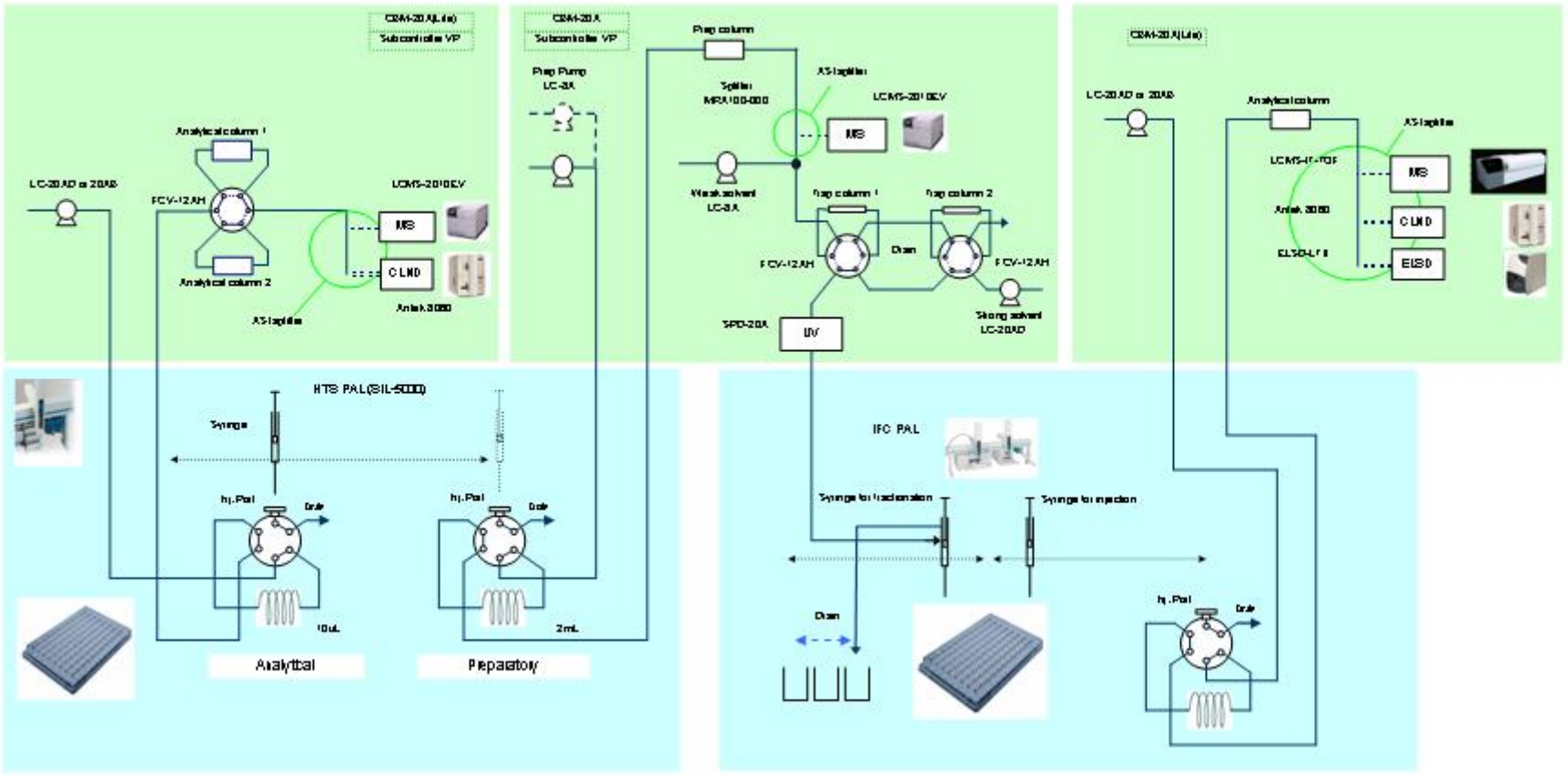


Example of a “Super” LC System

Preliminary Analysis

Purification

Final Analysis



Software Aspects of Controlling a "Super" System

- Most COTS instrument software can only operate a conventional system – "super" systems are handled as independent systems
- Must be treated by the software as one super-instrument
- There maybe myriads of possible configurations
- Each configuration is unique and requires a custom approach to operate the system
- The software is not likely to be commercially available – a custom application need to be developed
- All the negatives of custom applications: expensive development, documentation, maintenance, validation, etc.
- The application has a limited niche use

Handling Conventional and "Super" Systems via XML

- Individual system components (pump, detector, etc.), conventional analytical instruments (HPLC system) and "super" systems can be handled in a unified way.

Conventional LC System:

System Controller
- Pump
- Autosampler
- Oven
- Detector

"Super" LC System:

System Controller 1
- Pump1
- Autosampler1
- Oven1
- Detector1
- Valve 1

System Controller 2
- Pump2
- Autosampler2
- Oven2
- Detector2

- Component and System level objects

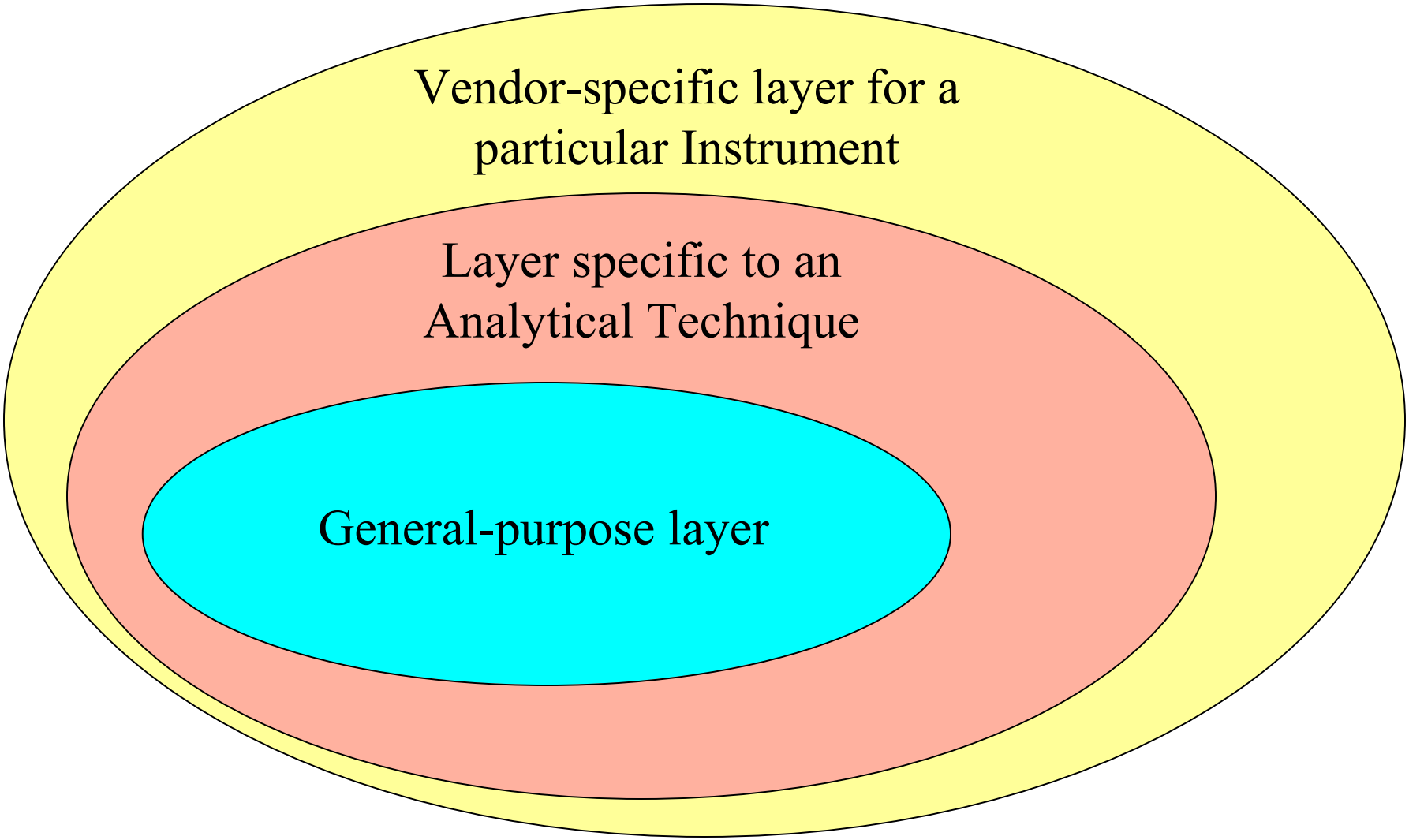
Handling Conventional and “Super” Systems via XML

- A system of any complexity can be described in an XML file in a consistent way
- No need for a custom application to handle a specific configuration of a “super” system
- Generic software can be developed for handling individual system components (pump, detector, etc.), conventional analytical instruments (HPLC system) and “super” systems in a consistent way

HPLC Web Control

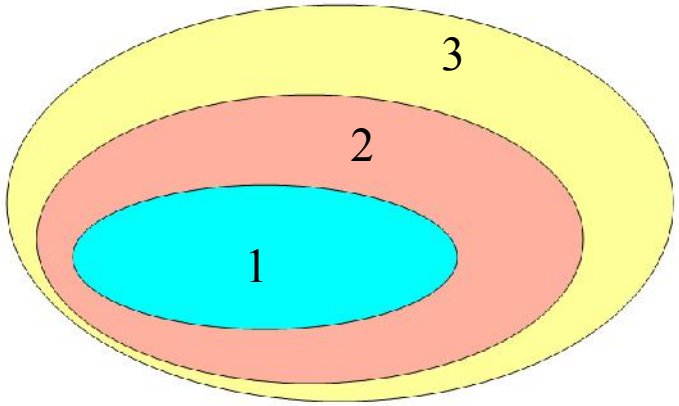
Prominence

Multi-vendor Instrument Control Object Model



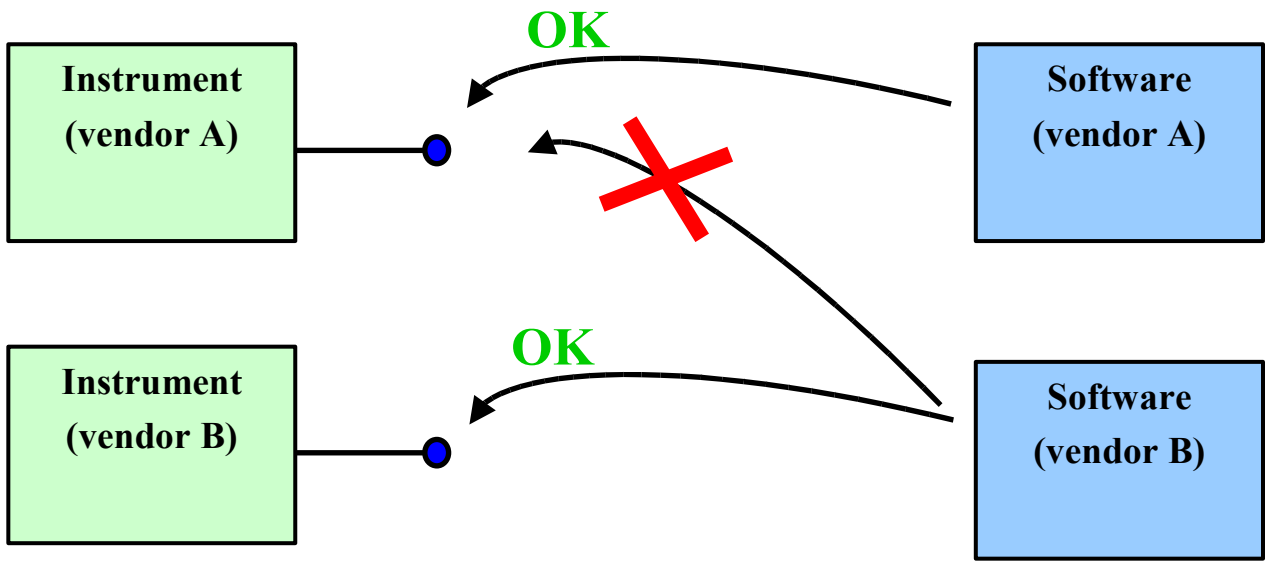
Multi-vendor Instrument Control Object Model

1. General-purpose layer handles general properties of a method. Used for reporting method parameters.
2. Layer specific to an Analytical Technique handles general properties of an HPLC technique. Used for basic instrument control.
3. Vendor-specific layer for a particular Instrument handles all aspects of the instrument method. Used to fully control the instrument including vendor-specific functions.



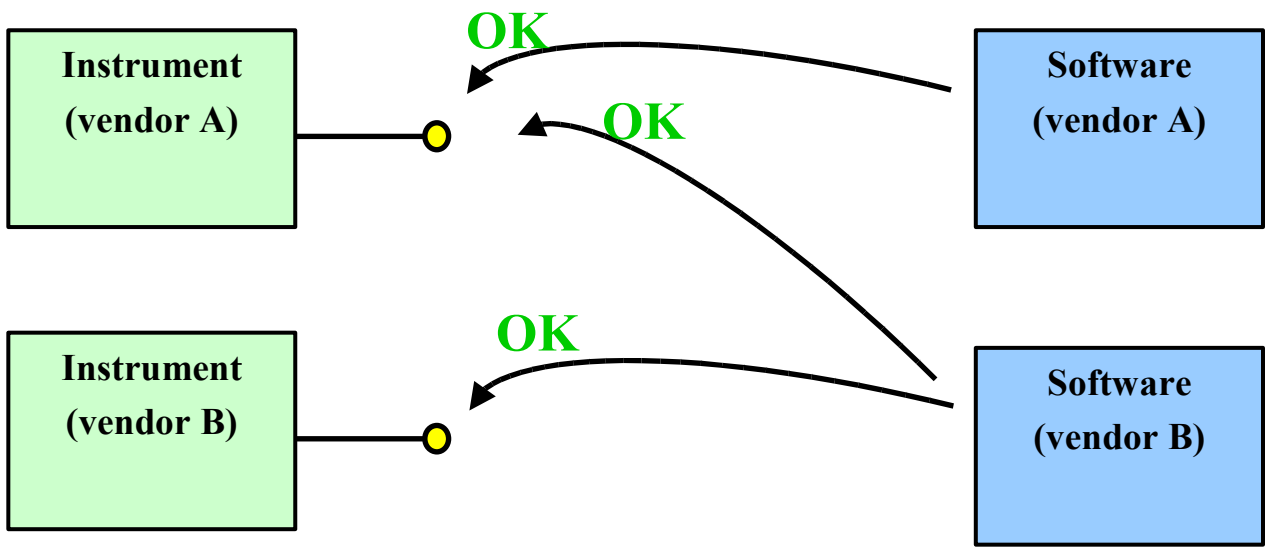
Vendor-specific Interface

- Each instrument has a vendor-specific interface
- It's possible to fully control an instrument by a vendor-specific interface
- But it is NOT possible to control another vendor's instrument



Technique-specific Interface

- If an instrument has an interface common to an analytical technique…
- It is possible to have basic control of the instrument via such interface
- But it is still not possible to fully control the instrument (vendor specific functions)

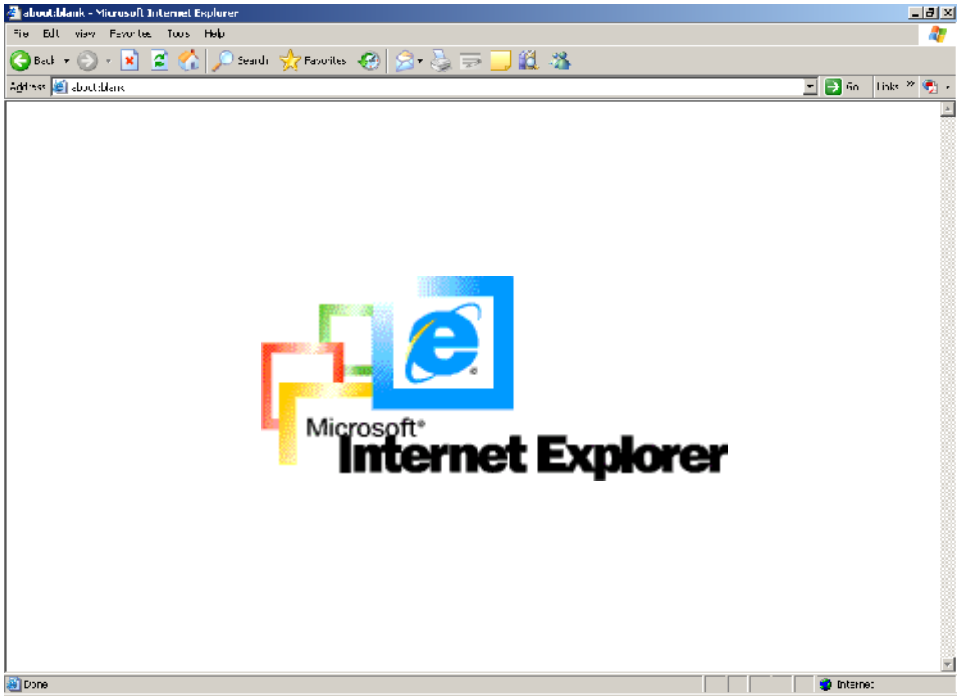


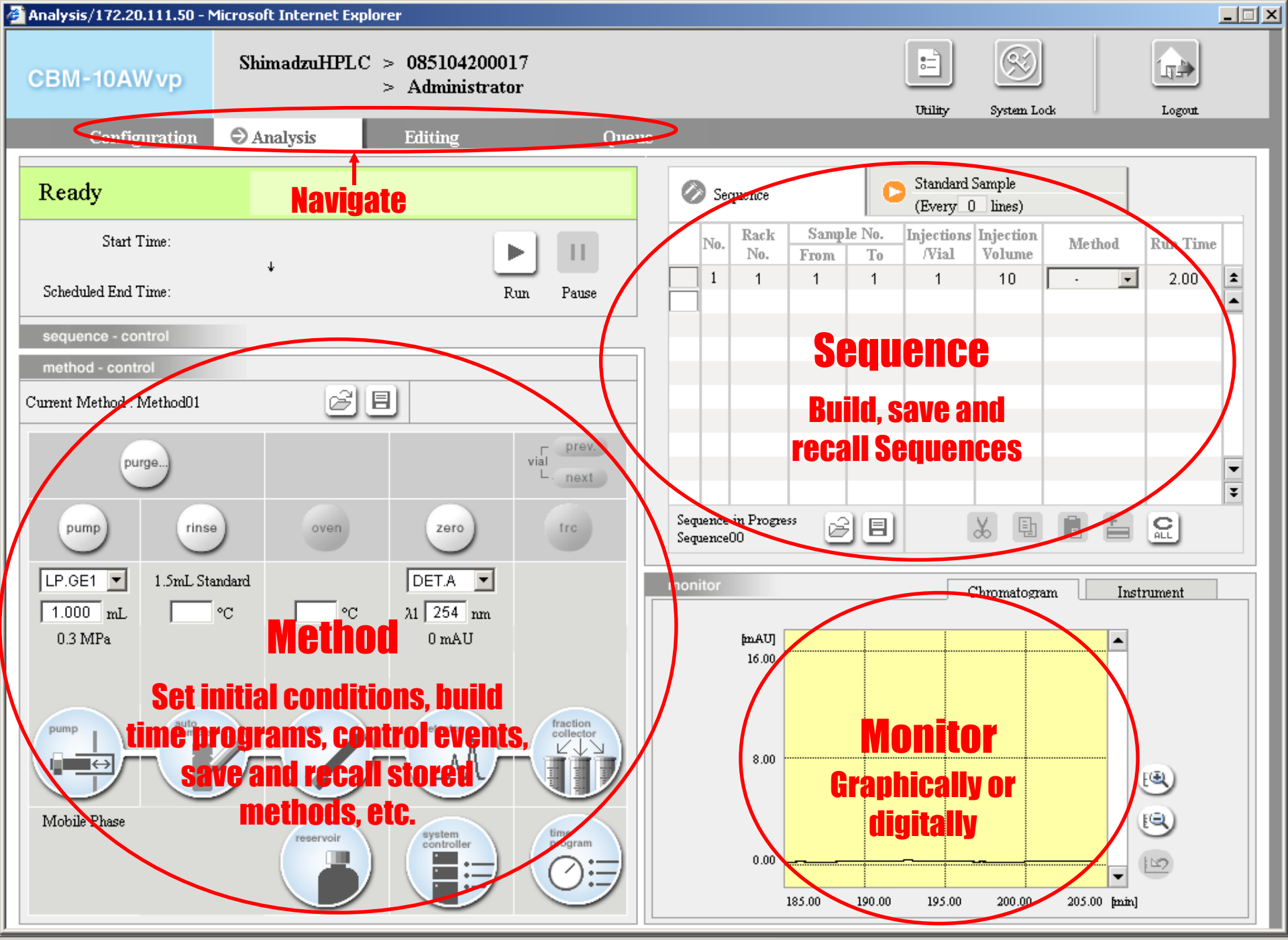
Capabilities of the New Instrument Control Module

- Web control
  - Control
  - Monitor
  - Perform Instrument Maintenance
  - Access from any PC on the network, intra- or internet via Internet Explorer browser
- Data buffering capability
  - If the network goes down, the analytical results are secured
- Capability to directly connect HPLC to the network
  - Capability to directly connect the HPLC to the network via the TCP/IP connection

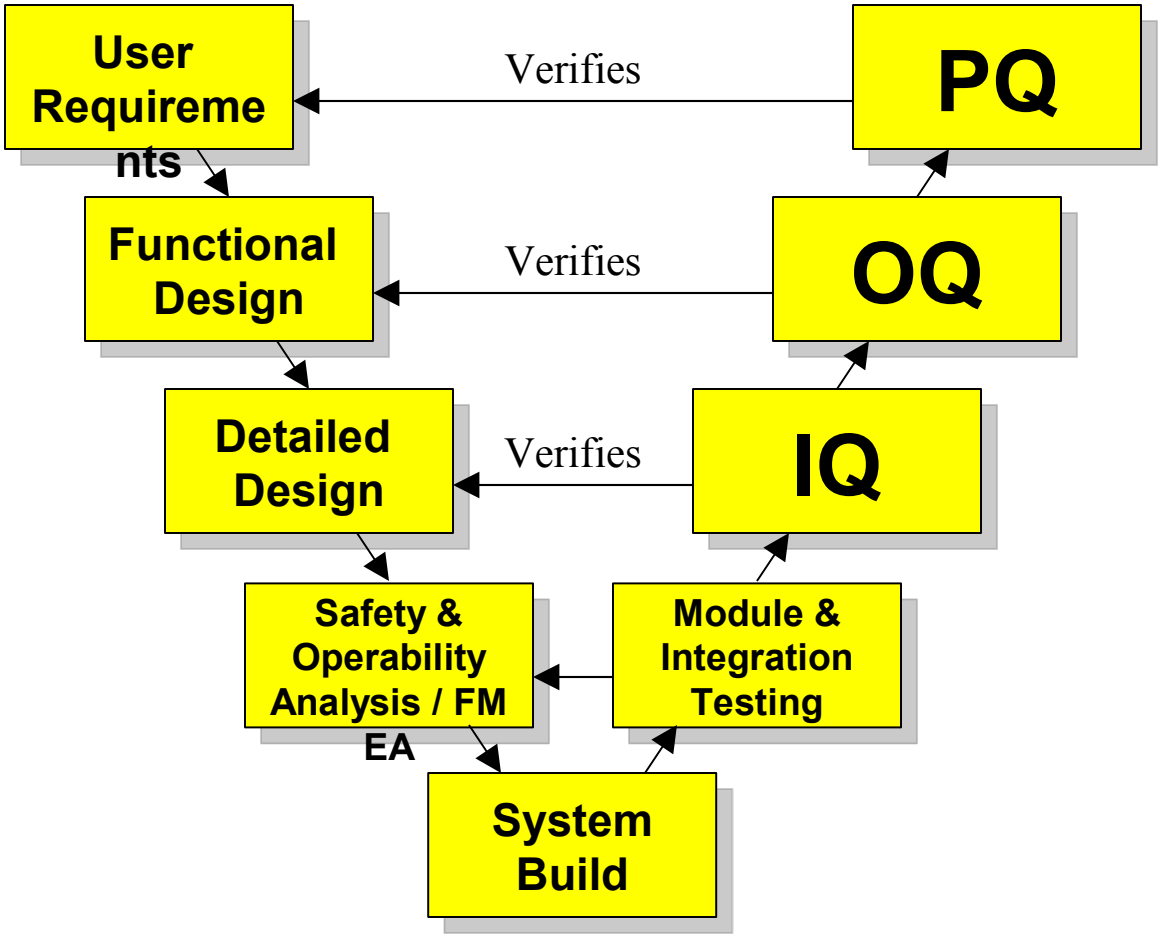
How do we use it ?

- From any computer on the network Launch Internet Explorer and type the IP address of the instrument (HPLC)
- A DNS can also be set up to use unique names instead of IP addresses such as “HPLC1”
- Enter the User ID and Password




Analysis/172.20.111.50 - Microsoft Internet Explorer
CBM-10AWvp
ShimadzuHPLC > 085104200017
> Administrator
Utility
System Lock
Logout
Configuration
Analysis
Editing
Queue
Navigate
Ready
Start Time:
Scheduled End Time:
Run
Pause
sequence - control
method - control
Current Method : Method01
purge...
prev.
vial
next
pump
rinse
oven
zero
frc
LP.GE1
1.000 mL
0.3 MPa
1.5mL Standard
°C
°C
DET.A
λ1 254 nm
0 mAU
Method
Set initial conditions, build time programs, control events, save and recall stored methods, etc.
pump
auto sampler
fraction collector
Mobile Phase
reservoir
system controller
time program
Sequence
Standard Sample
(Every 0 lines)
No.
Rack No.
Sample No.
From
To
Injections /Vial
Injection Volume
Method
Run Time
1
1
1
1
1
10
2.00
Sequence
Build, save and recall Sequences
Sequence in Progress
Sequence00
ALL
monitor
Chromatogram
Instrument
[mAU]
16.00
8.00
0.00
185.00
190.00
195.00
200.00
205.00
[min]
Monitor
Graphically or digitally
Slide 15 of 19
Maneki Neko
English (U.S.)

Benefits in Software Validation



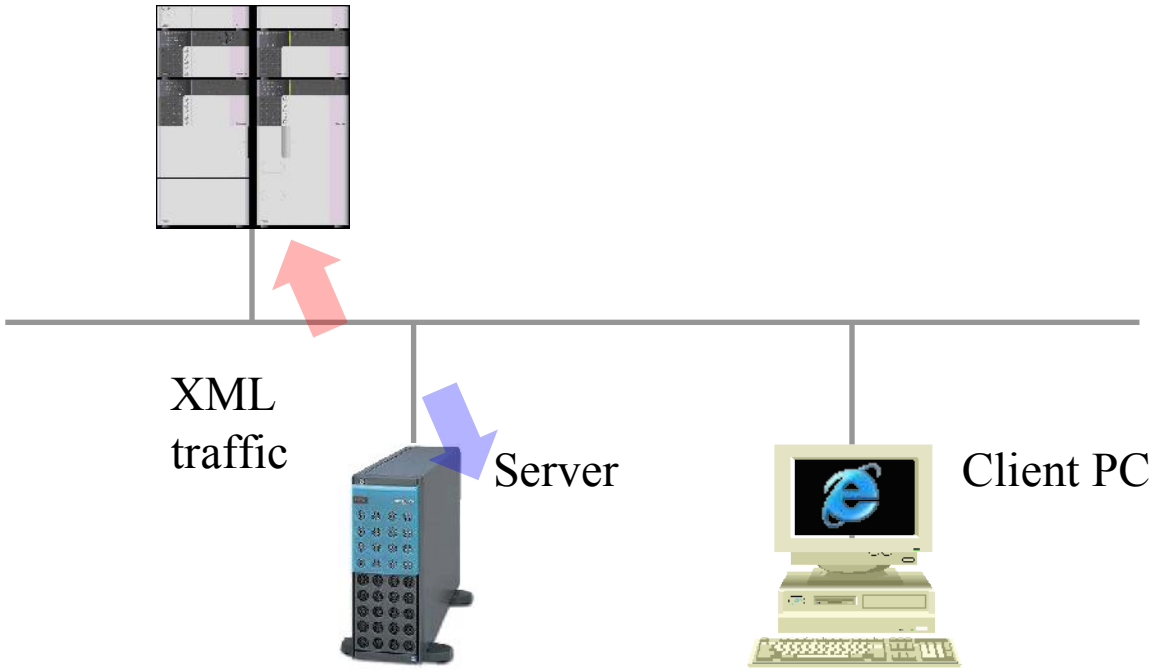
Benefits in Software Validation

Cat.	Software Type	Validation Approach
1	Operating System	Record version. The OS will be challenged indirectly by the functional testing of the application.
2	Firmware	For commercial firmware record version and configuration. Calibrate as necessary and verify operation against user requirements. Manage custom firmware as GAMP Cat. 5.
3	Standard Software Packages	Record version and verify operation against user requirements. Consider auditing the supplier for critical and complex applications.
4	Configurable Software Packages	Record version and configuration, and verify operation against user requirements. Consider auditing the supplier for critical and complex applications. Manage any custom programming as GAMP Cat. 5.
5	Custom Software	Audit supplier and validate complete system.

RISK

Benefits in Software Validation

- Instrument Control and Data Acquisition software on a client PC (Cat.4) is replaced with Internet Explorer (Cat.3)
- Significant reduction in the amount of validation work
- From stand-alone application to a client/server scenario, thin client (Citrix) and virtually “empty client”.



Thank You !

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