Current State of Chemical Laboratory Equipment Using Virtual Machines

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Abstract

This paper is a study of virtualizing chemical laboratory equipment PCs to extend the life time of the overall laboratory equipment platform. Replacing laboratory equipment based upon depreciation is mentioned as this may serve as a starting point for replacement among businesses and research centers. An overview of virtualization is provided as well as the advantages of virtualization in the laboratory from a business, Information Technology (IT), as well as a laboratory point of view. Two solutions based upon serial connection based equipment are proposed which would extend the life of the instrumentation while maintaining aging operating systems. Initial test results of the proposed solutions are presented indicating that the use of production equipment could be successful. A discussion tying in the triad of business, IT, and the laboratory goals with the testing results is provided and then a suggested course for future work is made to address using virtual platforms to assist in maintaining chemical laboratory equipment and the connected PCs past their depreciated lifetimes.

Keywords: Serial connections, laboratory equipment, virtual machines

1 Introduction

Approaching challenges in a chemical laboratory from a triad of the business viewpoint, Information Technology (IT) viewpoint, as well as the scientific viewpoint may result in solutions which are beneficial from multiple perspectives. From the business point of view, reducing the purchasing intervals of expensive chemical analytical equipment may be viewed favorably as this can enhance the availability of funding for other areas. In contrast to the business aspect, reducing the purchase intervals for laboratory equipment could result in having expensive but unsupported equipment which may impact availability, reliability, and recoverability. Finally from the IT point of view, security and supportability of the equipment may be a significant concern with older equipment. Addressing the concerns and the impact of business, IT, and laboratory decisions from multiple perspectives needs to be accounted for as chemical laboratory equipment can be a critical part of a business or research center.

Businesses and research centers want to ensure that their equipment is available when and where it is needed, provides data and information the equipment was designed for, and assists with meeting their goals. Often business, IT, and laboratory requirements may overlap. For example, all parties desire the analytical equipment to be available and to maximize the useful life. This will ensure that equipment replacement churn is minimized thus allowing the purchase of other items rather than replacement equipment. Another part to also consider is reproducibility and documenting testing environments and archiving these test environments which laboratories may need for regulatory or research purposes. The maintenance and/or replacement of chemical laboratory equipment is thus of interest from the business, IT, and laboratory viewpoints.

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This paper approaches the replacement of analytical laboratory equipment from a depreciation perspective and steps that may be applied to extend the life of the equipment to survive long enough for full depreciation of the asset. Although depreciation may not be the singular reason for replacing equipment, it serves as a starting point when viewed from a business and financial angle. A short overview introducing virtualization is given as well as two solutions based upon converting serial connections to either USB or Ethernet based connections. Ensuring that data is unmodified as the data passes through multiple devices is also a critical step as corrupted or missing data can influence test results, the control and safety of equipment, and the reproducibility of testing. Testing for whether data has been altered between the source and destination will be accomplished by a hashing function measured before and after a simple file transfer between test systems.

2 Depresciation of Equipment

Replacing analytical laboratory equipment in a Chemical Laboratory based upon depreciation indicates that replacement may be at least eight years and in some cases fifteen years or more [4, 9, 19] although laboratories may continue using the equipment well past the depreciation time frame. Analytical laboratory equipment often have PCs as part of the installation and are designed to process the output from the instruments via vendor software and may place the resulting data in text files, databases, or other formats for storage on the PC. Thus, PCs attached to laboratory equipment are considered a part of the overall unit when the laboratory equipment is initially purchased and all are depreciated at the same time as a single unit.

In contrast, business environment PCs are often replaced every three to five years as part of a company life cycle management program or due to the scheduled depreciation of computer assets (e.g. [4, 9, 19]). Despite the regularly scheduled replacement of office PCs, as stated PCs within analytical laboratory environments may not be replaced for eight or more years if connected to laboratory analytical equipment and thus may have negative effects regarding support. In conjunction with the physical PC hardware is the operating system which may not have support by the original vendor after a set number of years. For example, Microsoft operating systems are typically supported for approximately ten to twelve years after first release [15]. After this point the operating system is no longer supported and does not receive updates, fixes, or patches nor is it typically sold by standard vendors. The ramifications can be that while laboratory equipment was purchased approximately mid-way through a PC operating system lifetime (e.g. five years), the laboratory equipment may be in use for a total of ten years with the result that the supporting PC will continue to operate with an unsupported operating system for an additional five years or more. A lack of vendor support for an operating system and the respective security updates increases the potential of the system being undermined unless the system is isolated so as to reduce the opportunity for compromise. To mitigate or overcome areas where the instruments may need to continue operations well past the official operating system and PC support dates, virtual machines may address some of these inherent issues. An observation that Kind et.al. [11] noted in 2009 was that virtualization concepts and techniques were not observed in available literature when applied to chemistry laboratories. Within the past six years however there has been more of a shift to considering virtualization and cloud based solutions as denoted by Calabrese and Cannataro [6], Zhao et.at. [22], Kanwal et.al. [10], Thackston and Fortenberry, [20], and Nocq et.al. [16]. Advantages with the shift to virtualization and cloud computing includes allowing the use of larger data sets and in some cases computing power (CPUs, memory, disk space, etc.). This has the potential of moving the analytical instrument PCs from being locked in to a predefined hardware platform to one that is more flexible, reliable, and recoverable. For a move towards virtualization, there are a number of areas to consider to include security, connection types, and the porting of applications.

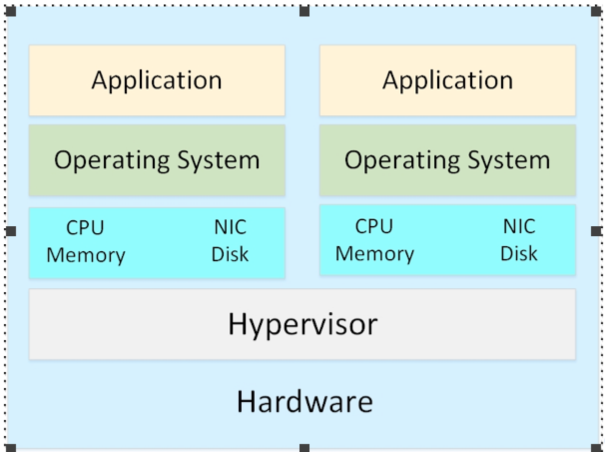

Figure 1: Hardware and Hypervisor [3]

3 Virtualization Overview

A virtual machine (VM) is used to describe a bundle of resources that have been virtualized and reside on a physical host providing equivalent functionality to that of a physical machine [12]. Virtualization is used whereby a VM looks and acts as an independent system with its own CPU, memory, hard disk(s), and other resources with an operating system and applications installed [17].

Virtualization as pointed out by Ribiere [17] is used in IT for many reasons to include:

- Logical partitioning so that several VMs can run on the same hardware.
- Fast provisioning which enables the creation and copying of VMs in a matter of minutes.
- Different operating systems can run independently at the same time on the same hardware.
- Legacy applications can run on emulated hardware with the result that the VM always stays the same regardless of what underlying hypervisor or hardware it is supported by.

A Virtual Machine Monitor (VMM) or hypervisor plays an important role in managing and coordinating access to the resource pool via a software layer. The hypervisor effectively hides the physical resource details and provides the virtualized resources and services for higher level application [1]. Although virtualization is often used as a cost-saving tool by IT, a strategic use can be realized when we look at application deployment and management [21]. Figure 1 depicts how the physical hardware is overlaid with a hypervisor (VMware in this case) and individual VMs with operating systems that “see” the virtual hardware. Advantages of using a hypervisor include security between VMs, device sharing, and performance isolation [18]. These capabilities would be directly applicable to areas that are of concern when dealing with laboratory systems. If the security between virtual machines can be enhanced and the performance can be tuned for the virtual machines assigned to laboratory equipment, this could alleviate security risks and performance degradation of the virtual machines.

In the line of enhancing security, in some cases older software programs require local administrator permissions to run. This is considered an issue in most environments as the elevated permissions could allow malware to run with those same elevated permissions [11]. When the laboratory PC is not attached to a network and is operating in a stand-alone mode, a local administrator login may not be considered a major issue. However, when the same PC is attached to the network then the logged in account may have

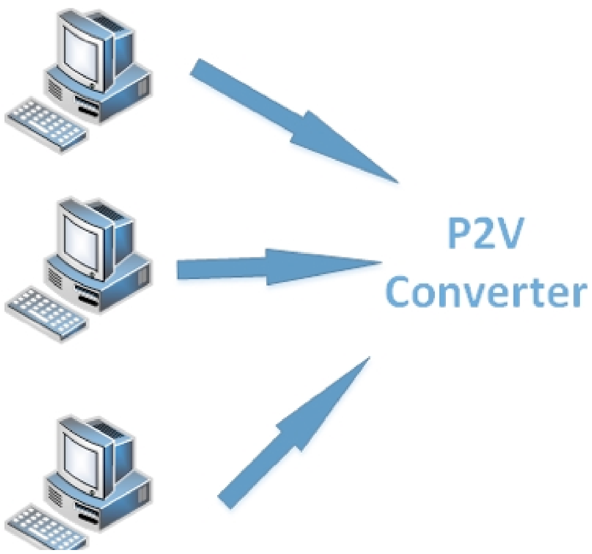

Figure 2: P2V Conversions

additional permissions on the local network which would violate security protocols for many companies. If a virtual machine can be used as a replacement, then isolating the virtual machine on a virtual network may obviate some of the inherent security risks that Kind et.al. [11] have made mention of.

If a virtualization solution is to be considered, there must be a viable pathway to convert a physical PC to a virtual machine. With this in mind, the ability to replace old computers and the related infrastructure while retaining the current software installations may be accomplished via a Physical to Virtual (P2V) conversion [11]. A P2V conversion results in a virtual machine with the same characteristics as the physical machine to include installed software and settings. The conversion also removes the dependencies on specific network card drivers and physical hard disk size limitations which can be advantageous for laboratory PCs. Hypervisors allow the virtual machines to be migrated between hypervisor versions and vendors thus ensuring that there is an extended lifetime of the virtual machine often available which would be much longer than that of a standard physical PC. While on a hypervisor, the physical space allotted to the virtual machine can be adjusted where needed if the amount of data, updates, or other factors dictates an increase in space. Figure 2 depicts running a P2V conversion process on multiple physical PCs resulting in a set of VMs that would reside on a hypervisor platform. With virtualization, the lifetime of the applications and operating system may be extended. However, the limits of virtualization include software restrictions that only support standard hardware including USB, serial, parallel, and SCSI connections, etc. [17]. Although this may be a restriction for some specialized laboratory instruments, standard connections such as serial, USB, and RJ-45 are most often found on standard laboratory equipment. For those that have specialized connections, there may be additional adaptors which could be considered.

4 Virtualizing PCs in the Analytical Laboratory

With the use of virtual machines an operating system can be utilized for a longer period of time as the physical PC hardware is no longer a factor as a dependency. This can also minimize the amount of disruption to operations if hardware changes were required by avoiding the need to reinstall an O/S and applications on new PC hardware [8]. Although plant operations are specifically mentioned by Hodge [8], the same principle applies to chemical laboratories as well. As with some manufacturing processes, chemical laboratories may have specific applications that would need to be ported from older operating systems and hardware to newer operating systems and hardware. Porting applications is often very costly due to the qualification and validation requirements needed to ensure functionality [17].

As an extreme example of validation requirements by Ribiere [17], the life expectancy of a nuclear power plant is 40 years. Many applications may be developed and a qualification and validation process is followed with the result that these applications do not need to change in their functionality or function during the life time of the plant. Meanwhile, PC hardware may have a life span of only three to five years with the result that it is difficult to maintain the original software applications for an extended time.

Within the pharmaceutical industry, the replacement of a PC may also require revalidation which results in very high costs. If systems need to be revalidated every five years or so due to the limiting factors of hardware and software obsolescence, this can add up to a very large cost for business [2]. As an example in the pharmaceutical environment: "Genentech estimated that the costs to upgrade one of its Windows 95 PC-based HMIs to a Windows Server 2003-based system would be approximately $40,000," recounts Anthony Baker, PlantPAx characterization and lab manager at Rockwell Automation (`www.rockwellautomation.com`). "Final figures topped $100,000 because of costs associated with validating the system for use in a regulated industry," adds Baker[2].

Ribiere [17] suggests two solutions that may be used to keep the original applications running to include:

- A stock of old hardware held in reserve which the application software can run on
- Port the applications to new hardware and new operating systems

As Hodge [8], Ribiere [17], and Herbert [2] remark, porting applications can be prohibitively expensive and can cause significant disruption. Stocking old hardware has the disadvantage of determining how much hardware to stock and the associated space restrictions for storage and normal degradation due to aging of the stock items [17]. Depending on the size of the supported organization and mix and age of equipment, stocking old hardware could be expensive and resource intensive. Chemical laboratories may not have the IT knowledge or skill sets readily available for replacing the parts on PCs nor in configuring the device drivers, troubleshooting, or testing. Still, for short term purposes where the equipment may be in a harsher environment, stocking limited hardware may be a very good option.

Although extending the life of legacy systems via virtual systems can result in a significant cost saving by extending the life of a system from five years to ten or more years [2], this can also be coupled with additional advantageous of virtualization such as recovery and reliability. Recovery from a PC failure may not be eliminated by using virtual machines, however reliability is increased by providing a faster mechanism for recovery via virtualization [2]. Along with reliability, another benefit is longer lifecycles for applications which may be critical to chemical laboratories. Rather than a dependence upon the lifecycle of an operating system or PC hardware, virtual machines are dependent upon a hypervisor which typically has a longer lifecycle [2]. In place of upgrading the PC hardware and operating system, the virtual machine can remain with the original tested configuration and when the hypervisor needs to be upgraded or migrated to a different hypervisor, the original virtual machine remains unaffected. This could also be a benefit to laboratories which depend upon a static environment for scientific testing and obtaining consistent results.

In a scientific context, two major issues present themselves when conducting an experiment. The first issue is reliability of results whereby the actual performance of a system can be represented. The second issue is reproducibility whereby the experiments can be run again and still achieve the same results [12]. By creating a virtual machine, the conditions and environment used for experiments can be easily reproduced even if the exact hardware and software are not available [12]. This could be of interest from the documentation perspective as well as reproducibility as a virtual machine that is used for conducting experiments can be saved as a file and then copied off and archived. If there are concerns regarding the setup and configuration of the virtual machine, the virtual machine can be retrieved from

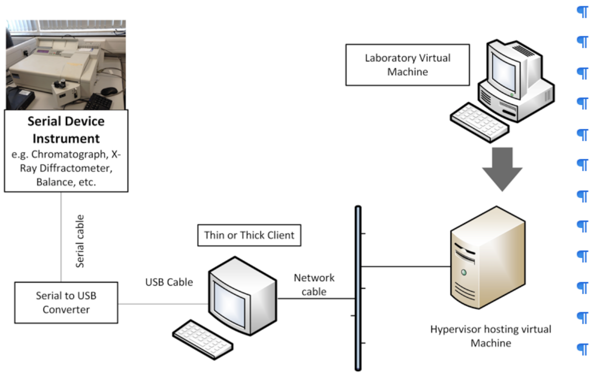

Figure 3: Serial to USB Converter with Virtual Machine

the archive and used in the context of the original experiments. This is something which would be much more difficult to duplicate with physical machines.

Using VMs and leveraging network infrastructures can be a powerful combination that can assist a chemical laboratory. As has been noted, there are a number of benefits that virtual machines can offer, but there are also some issues which may cause concern with the result that virtual machines may not be an ideal solution.

Virtualization products emulate parallel ports, but this is limited to printing only [17]. This can be a concern as some equipment may require the use of a parallel port dongle. Without the detection of the dongle, laboratory equipment software may not work. This situation would be unacceptable and may necessitate the use of a physical PC which has a parallel port.

Other disadvantages if using thin clients include a lack of resources when connecting peripheral devices such as printers. Although port mapping and USB redirection can obviate some of these issues, not all scenarios can be addressed due to the large number of peripheral types possible [7]. The testing of media converters could be explored by laboratories if there is sufficient cause to do so.

5 Suggested Solutions

Establishing a connection between analytical laboratory piece of equipment and a PC for aging (or in many cases current) laboratory equipment may be tested using several solutions. With a focus on analytical equipment with serial connections, serial to USB converters would be a fairly simple solution resulting in a point to point (equipment to PC) connection. As Blansit [5] states however, when a serial to USB converter is used, the number of COM ports also increases each time a device is connected. As devices are tested on a PC, the number of COM ports also increases and therefore a user must be familiar with the Device Manager applet found in the Control Panel. This may be a deterrent if the USB adaptor is not connected to the same port each time.

Using Figure 3 as an example, a serial device instrument is attached to a serial to USB converter with the instruments' serial cable. The serial to USB converter is then attached to a thin/thick client. Once the USB cable is attached to the client, the USB port is redirected to the laboratory virtual machine hosted on a hypervisor (e.g. VMware, Hypver-V, etc.). The laboratory virtual machine with the serial device instrument software can then be accessed via the client. Figure 4 shows an example of a serial to USB converter produced by Moxa whereby up to two serial devices can be connected to the converter which is then connected to a USB port on a PC.

Another possible solution for serial based connections is using a serial device router (serial device

Figure 4: Moxa UPort 1250

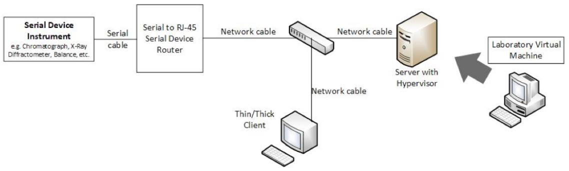

Figure 5: Serial to Serial Device Router

server or serial gateway) as mentioned by Lang [13] which would obviate issues with point to point connections found in serial and USB connections. Serial device routers offer an intelligent serial to IP networking option which leverages the Ethernet infrastructure and takes advantage of performance, security and resiliency of the Ethernet architecture [14]. Serial device routers are also designed for industrial environments and can be hardened to withstand environmental factors such as temperatures, high particulates, high humidity and corrosive environments [14] that may be found in laboratories.

Figure 5 depicts an example setup using a serial device instrument and a serial device router. The serial cable is attached to the laboratory instrument and to the serial device router. The router is assigned an appropriate IP address and the network cable from the serial device router is attached to a network switch. The laboratory virtual machine has the vendor software for the serial device router which allows the simulation of a serial port. The laboratory virtual machine can then be accessed by a network client (e.g. thin or thick). Figure 6 shows an example of a serial device router produced by Moxa which converts a serial DE-9 connection to an Ethernet RJ-45 connection which would allow serial traffic to transverse a network via IP.

Figure 6: Moxa NPort 5110A

6 Initial Testing of Suggested Solutionsl

To determine if the suggested solutions had any validity, a controlled test environment using physical PCs was created to verify if a 1MB file (1024 kilobytes) could be transferred between PCs using a serial to USB converter and a serial device server.

An initial scenario was used to establish the base equipment functionality to include the serial cables, null modem and gender changers, as well as the data tap (see Figures X and Y). The use of virtual machines and any networking communications was initially excluded thus strictly focusing on ensuring that the thick clients and base equipment was functioning as expected. To ensure that data was not modified during transit, a text file was created which was 102,400 bytes in size on the source PC (TestPC01) which simulated a laboratory instrument. A hash was then calculated against this file and used as a reference for all future testing. To test this scenario, the text file was sent from TestPC01 (Figure 7) to TestPC02 which was then captured using a Data Logger. A third PC was used to also capture the text file and acted as a control in future testing scenarios. The data tap, null modem adaptor, gender changers, and serial cable setup is depicted in Figure 8. Once the text file was received by the receiving PCs, a hash value was once again calculated against the received files on TestPC02 and the Monitoring PC and compared to the reference hash value on TestPC01. As depicted in Table 1, the initial scenario revealed that no change in data occurred in the base scenario indicating that the serial cable, data drop, gender changers, and null

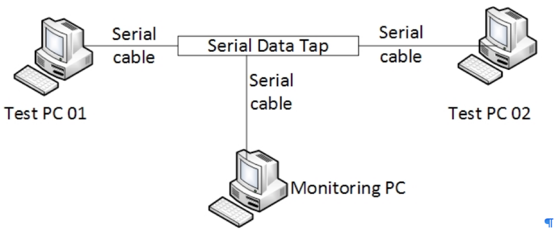

Figure 7: Initial Configuration

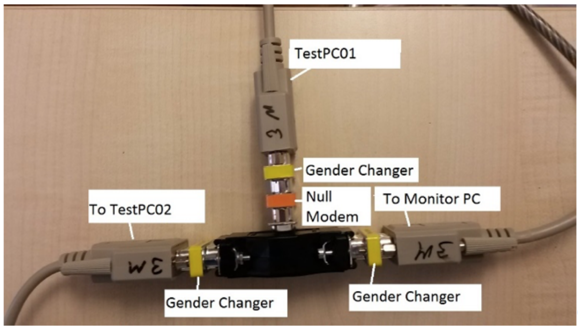

Figure 8: Data Drop Configuration

modem adaptors did not modify the data in anyway as the hash values were consistent across all files.

A second scenario tested sending a text file from TestPC01 via a serial to USB converter to a VM via serial port redirection. In this test TestPC01 sent a text file to the serial port which was captured by the serial to USB converter that was plugged into TestPC02 (Figure 9). TestPC02 then established a RDP session to the Windows 7 VM (Win7SP1VM) using port redirection to pass the file to the Windows 7 VM. Once the file was successfully transferred to the Monitor PC and the VM (Win7SP1VM), the hash value was calculated against the received files. The results of the hash values in Table 2 also indicate that the file was not modified during transmission through the aforementioned equipment nor by the serial to USB converter.

A third scenario used a serial device server to pass the file from TestPC01 to the target systems. This scenario used TestPC02 to access a Windows 7 VM (Win7SP1VM) via RDP (Figure 10). The Windows 7 VM had the serial device server drivers installed and the data was received from the serial device server via IP. The data in the form of a text file was successfully passed from the source PC (TestPC01) which is

Table 1: Initial Configuration Results

PC	Hash Value
TestPC01	DEC61E799CF32E3C45685BA257811B6
TestPC02	FDEC61E799CF32E3C45685BA257811B6
Monitor PC	DEC61E799CF32E3C45685BA257811B6

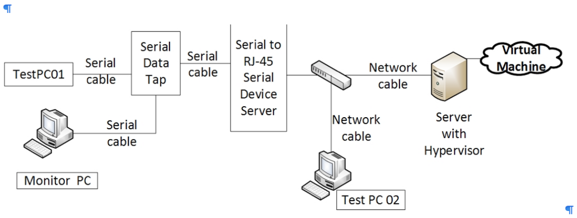

Figure 9: Testing with USB Converter

Table 2: IUSB Converter Test Results

PC	Hash Value
TestPC01	FDEC61E799CF32E3C45685BA257811B6
TestPC02	FDEC61E799CF32E3C45685BA257811B6
Monitor PC	FDEC61E799CF32E3C45685BA257811B6

simulating a laboratory instrument to the Monitor PC and the destination PC (Win7SP1VM) via a serial device server. Based upon the hash values for the three files listed in Table 3, the contents of the files were identical and thus no modifications to the file took place after passing through the serial ports, serial device server, gender changer, null modem adaptor, and the data tap.

7 Discussion

Using virtual machines to extend the life of laboratory equipment may address business goals from the business and financial perspective as the recurrence of replacing equipment may be reduced. This allows the funds that would normally be allocated for equipment replacement to be used for other purposes within the business. From the IT perspective, virtualization is a familiar and supportable technology that offers security, isolation, and the ability to tune the virtual machines for best performance to the benefit of the laboratory. A pathway to converting a physical PC to a virtual machine and supporting the resulting virtual machines is well documented and understood with the result that risks can be mitigated by avoiding untested technologies. From the laboratory perspective the opportunity to extend a validated environment, minimize disruption to operations, increase reliability, as well as offer reproducibility of tests and experiments is very attractive.

Based upon the outcomes of initial testing of the suggested solutions in a controlled environment using PC's to simulate laboratory equipment indicates that data is not modified during transfer through the tested connectors, cables, and converters to the virtual machines. This was established via a standard

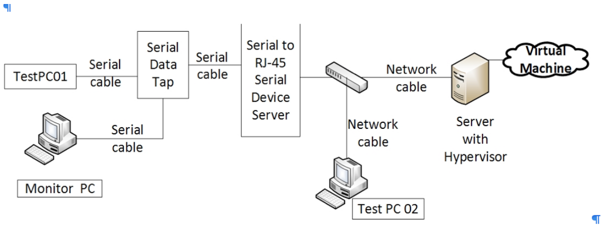

Figure 10: Testing with Serial Device Server

Table 3: Serial Device Server Test Results

PC	Hash Value
TestPC01	FDEC61E799CF32E3C45685BA257811B6
TestPC02	FDEC61E799CF32E3C45685BA257811B6
Monitor PC	FDEC61E799CF32E3C45685BA257811B6

hashing algorithm and the results show that the hashing values are consistent across the tested scenarios. This is important from both the IT as well as the laboratory perspective as data corruption needs to be avoided and ensures confidence regarding the environment. Although the controlled environment indicates that using virtual machines in a laboratory environment may be feasible, further testing using production equipment would validate whether the assumptions and environment are in fact achievable.

Linking these test results back to the triad of business, IT, and laboratory goals, the successful testing and results indicate that using virtual machines to supplant physical PC's could be pursued with a focus on laboratory equipment that utilizes serial connections. Leveraging well-established IT technology and skills assists with the business goals of keeping costs down by using existing infrastructures and knowledge where possible and extending the life of the equipment. Using IT technology could also assist the laboratory environments by enhancing the equipment environment by also providing reliability, recoverability, and security.

8 Conclusion and Future Work

With the advent of virtualization, IT departments have used virtualization capabilities to reduce the number of servers in datacenters, increase the density of machines by using hypervisors, and to enhance reliability and recoverability of the virtualized systems. Using virtualization capabilities is a well-established and well known technology used by IT departments which has provided great benefits to the data centers. However, using virtual machines to replace physical PCs attached to chemical analytical equipment is relatively new with many laboratory personnel unfamiliar with virtualization technology and how it could enhance their laboratories. The triad of business, IT, and laboratory goals could benefit by further discovering the feasibility of virtualization. Exploring virtualization technologies within the laboratories could result in providing enhanced flexibility, recoverability, and the ability to more easily replicate testing environments while also benefiting the business by reducing costs. Based upon the above results, a series of testing focusing on older equipment with standardized interfaces such as DE-9 or USB could be accomplished by using a combination of P2V conversions of the original PC, media converters, serial device router, and a hypervisor server in a production environment. Instrument software can then be checked to verify if the equipment can communicate with the virtual machine and software and whether the instrument software continues to yield expected results while on a virtualized platform. If successful, this would provide an opportunity to extend the life of the instrument while maintaining the older operating system and instrument software and allow easy backups and snapshots to be taken of the virtual machines (VMs). Snapshots of the VMs would allow quick recovery due to misconfiguration, disaster recovery, or if updates to either the instrument software or operating system render the environment less than desirable.

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