



*CASP*i*E*

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Working Toward Unattended Student Access to Remote Instrumentation

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The CASPiE Model for Instrumentation

- Research-quality data requires research-quality instrumentation.
- Because of cost only one copy of each device will be purchased.
- Each instrument will be equipped with an autosampler and be capable of remote control.
- Beginning students will submit samples, with the raw data and data-processing software stored on an Internet-accessible server.
- Advanced students will run their own samples remotely.

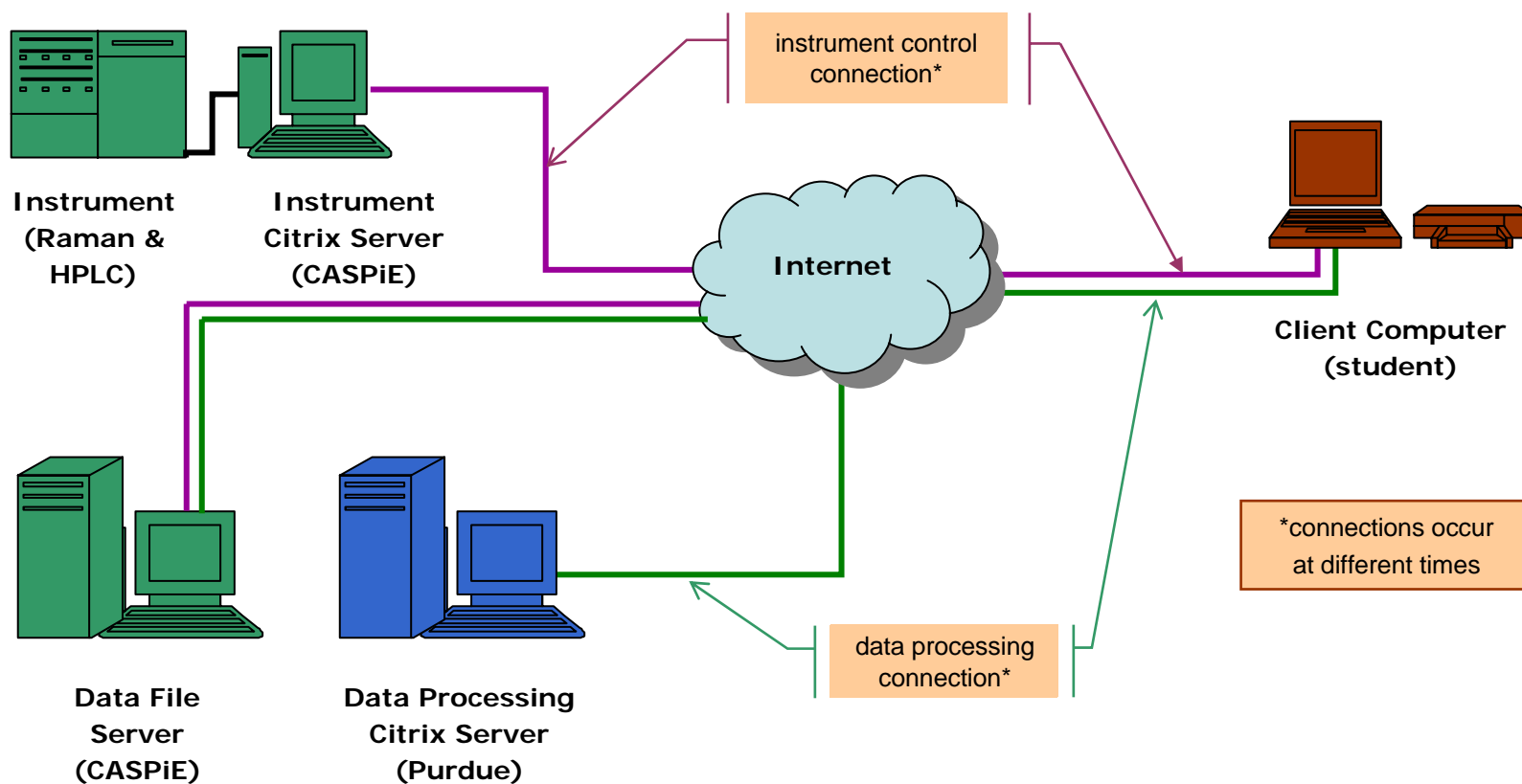


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Network Diagram and Connections





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Number of Participating Students

Spring/Summer/Fall 05: ~20/term working out "bugs"

Spring Term 06: 30 remote Raman, 20 batch HPLC

Spring Term 07: 30 remote Raman, 360 batch HPLC

High Student Numbers Demand High Throughput.

Devise strategies to facilitate high student and sample throughput:

- *Improve turnaround efficiency*
- *Increase instrument in-service time*



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Improving Efficiency

- 1) Automated Access – Instrument time must be efficiently allocated and students held to reservation time.
 - Access to an instrument's controlling application is determined by membership in a specific Active Directory group.
 - Student accounts are moved in and out of the instrument access Active Directory group automatically using an Active Perl script which is driven by reservation information in a SQL database.
 - The instrument application is 'wrapped' in a timing program which either chides the user to exit or forces a logoff at the end of a reservation.



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Improving Efficiency

- 2) Minimize Sample Load Time – When possible, samples are shipped in autosampler trays. Sample sequence files will be generated by users to minimize transcription error.





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Improving Efficiency

- 3) Minimize Sample Run Time – Consider ‘fast’ method technology e.g. “Fast” GC/LC. “Fast” methods can reduce chromatographic run times by a factor of 10 or more.

- 4) Web-Based Reservation System – Allow students and instructors to reserve time based on instrument host institution determined boundaries.



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Increasing Instrument Time

Offline Data Processing

Data review, re-processing, and printing should not consume valuable instrument time.

- We use the Purdue's Citrix Server farm for offline access to the same software package used for instrument control.
- The number of concurrent users can be controlled via Citrix to satisfy license agreements.



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Increasing Instrument Time

Unattended Student Remote Access

With high student numbers we anticipate not being able to accommodate all users during their scheduled lab hours. Consequently, students will be unsupervised during remote sessions.

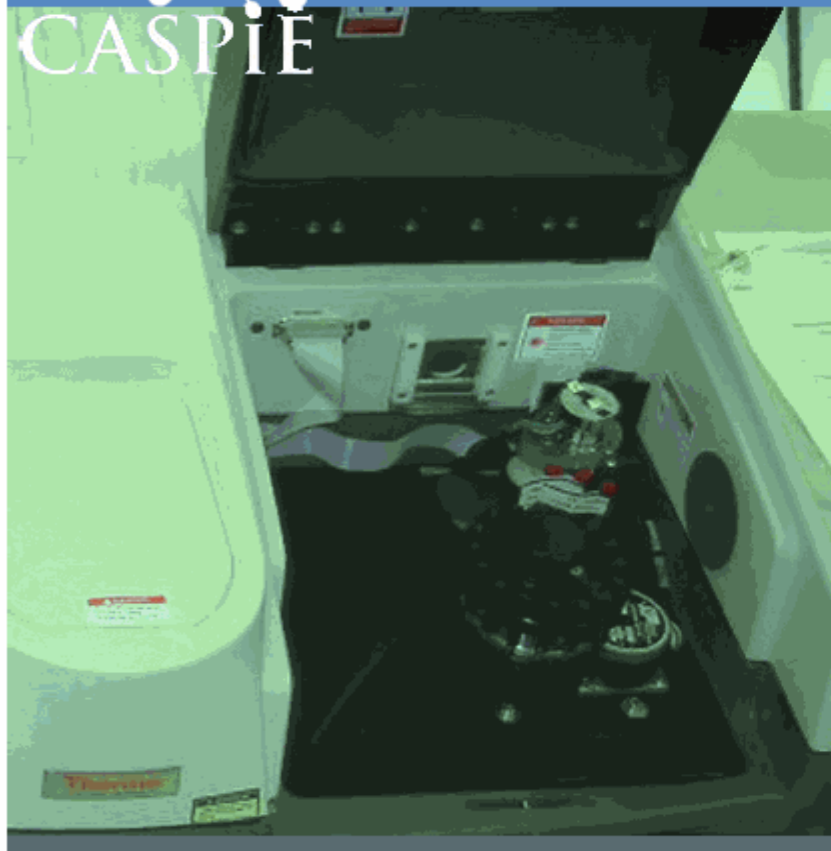
Challenges

- 1) Training and tutorials – Provide in-lab training sessions as well as online tutorials.
- 2) Security - Access and authorization must be secure to protect *computer, instrument, and data files*.



The Center for Authentic Science Practice in Education

July 10, 2006 - 4:21 pm

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CASPIE Tutorials

Introduction to the Raman Instrument

The CASPIE Raman instrument is not a standalone instrument but rather an accessory attachment on a Fourier Transform Infrared Spectrometer (FTIR). Only the FT-Raman accessory has an autosampler and can be run remotely. The Raman autosampler holds 16 sample tubes in a circular wheel. The wheel turns to move a selected sample tube into the path of the Raman laser. The tubes are special 3-in NMR tubes which can accommodate both liquid and solid samples. An infrared laser strikes the sample in the autosampler stimulating the Raman signal. The Raman scatter is directed to an interferometer inside the FTIR which encodes all of the signal frequencies into an interferogram. The light is then passed to the detector which records the encoded signal. The interferogram is decoded by a computer using a mathematical function called a Fourier Transform which gives the frequency spectrum of the Raman signal. The Raman frequency spectrum contains information about the functional groups present in the sample.

[Preparation of Solid Samples for Raman Analysis >>>](#)

[Introduction to the CASPIE Raman Instrument \(Movie File\) >>>](#)

[Instructions for Collecting Raman Spectra \(Printable PDF Document\) >>>](#)

[Raman Instrument FAQ >>>](#)

[Raman Data Processing \(PDF Documentation\) >>>](#)

Online Tutorials



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Unattended Student Remote Access - Security

- 1) Restrict Access to Instrument Application – Experience with laboratory computers shows that computer function must be protected.
 - We prevent students from accessing the instrument computer "desktop" by employing Citrix Metaframe Presentation Server.
 - Applications execute on a server and only screen updates, mouse movements and keystrokes are transmitted to and from the client computer.
 - Client-side software installs as a downloaded plug-in and can handle virtually any client operating system.



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Unattended Student Remote Access - Security

- 2) Individual Student Accounts – Group accounts are considered a security risk.

- 3) Limit Instrument Control Features – Restrict student access to method files and calibration features.
 - Instrument software must have customizable user permissions. Many software packages have this feature to be compliant with FDA's Title 21 Code of Federal Regulations (21 CFR Part 11).



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Full Control

Limited, Customized Control

OMNIC For Raman - [Window1]

File Edit Collect View Process Analyze Raman Report Window Help

Experiment Experiment Setup... Ctrl+E
Match Spectrum Settings

Collect Raman... Ctrl+S
Collect Reference... Ctrl+B
Display Reference
Raman Autosampler - Display Spreadsheet
Raman Autosampler - Reset Wheel
Raman Autosampler - Move To Position ...
Raman Autosampler - Move To Next Allowed Position
Raman Autosampler - Spin Sample
Raman Autosampler - Exit

80
75
70
65

OMNIC For Raman - [Window1]

File Edit Collect View Process Analyze Raman Report Window He

Collect Raman... Ctrl+S
Raman Autosampler - Reset Wheel
Raman Autosampler - Move To Next Allowed Position
Laser On
Laser Off
Stop Collection

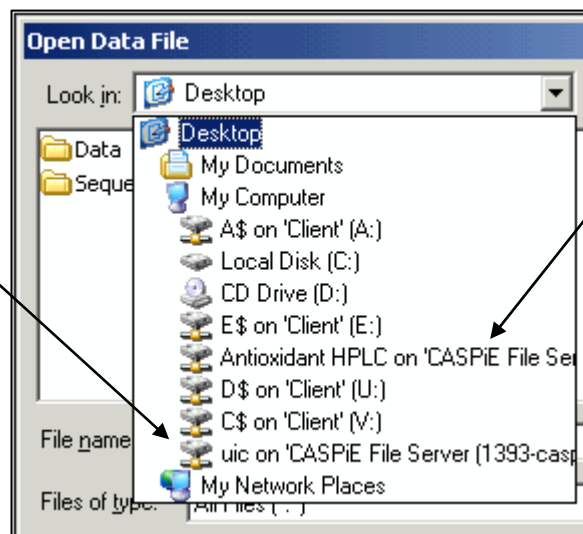
90
80
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60
50



Unattended Student Remote Access - Security

- 4) Restrict Data File Access – Students should only be able to open and manipulate their own data.
- Map drive to specific file server share folder at login.
 - Set share permissions to allow data modification but not deletion.

Data folder –
read/write
access



method and
template folder –
read only access



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Increasing Instrument Time

Remote Access Outside Normal Working Hours

Can instruments be effectively and safely operated remotely without staff on hand? (nights and weekends)

Challenges

- 1) Staff unavailable for troubleshooting.
 - Online FAQs for common problems.
- 2) Instruments and servers must be protected from the consequences of client disconnects.



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Managing Client Disconnects

The consequences of a client disconnect on instrument status/condition must be considered and ameliorated.

- For our Raman instrument a client disconnect leaves the IR laser on.
- Code was included in the 'wrapper' program which detects disconnects, terminates the instrument application, and signals the laser to shut down.
- *This solution required obtaining code from the instrument vendor.*



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