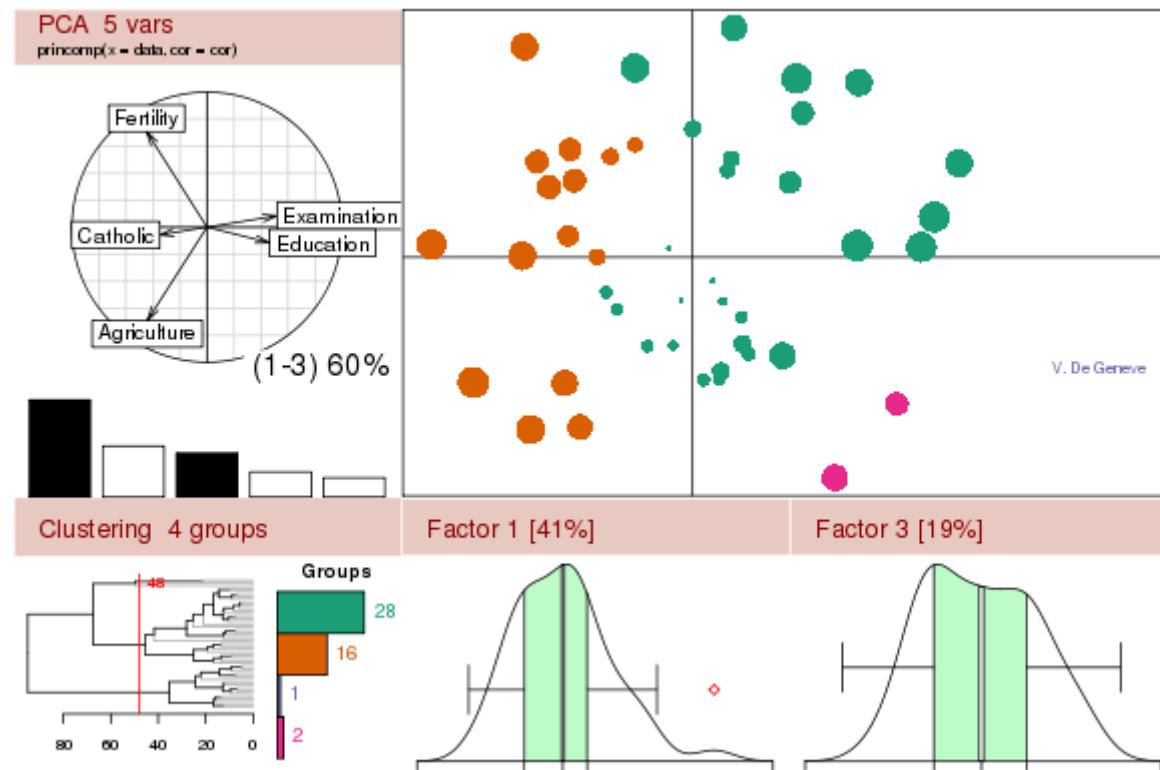


2013 Eric Pitman Summer Workshop in Computational Science



...an introduction to R, statistics, programming, and getting to know datasets

Introducing: Workshop Staff

Jeanette Sperhac, Scientific Programmer, UB CCR

and intrepid assistants:

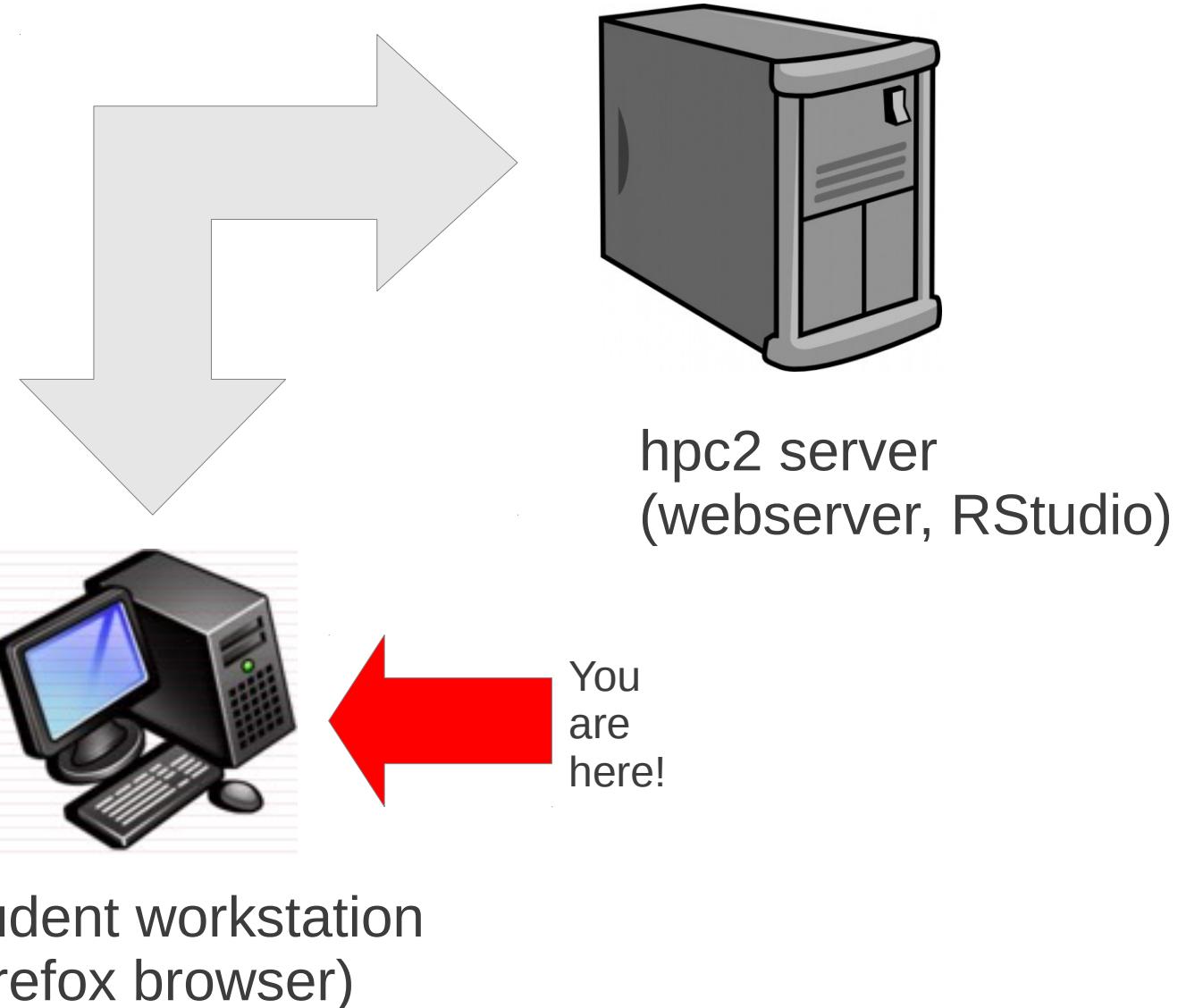
- Ryan Mraz, RIT
- Sam Steffan (alumnus of this workshop!), UNC
- Brian Narby, Pitt



0. Setup on hpc2.org

- Register on hpc2.org
- Intro to RStudio
- Set up RStudio Projects with GitHub
- File transfer: using WebDAV

Workshop computing environment



Register on hpc2.org

You must have an email address...

1. On hpc2.org website, click Register link
2. Fill in required fields; submit
3. Follow link to Create New Account page
4. Choose username and password; specify email address; submit
5. Click link on confirmation email; sign in

Register on hpc2.org

A screenshot of a web browser displaying the hpc2.org website. The URL https://hpc2.org is visible in the address bar. The page features a large red arrow pointing downwards towards the right side of the header. The header includes a navigation bar with links like 'Most Visited', 'Getting Started', 'Disable', 'Cookies', 'CSS', 'Forms', 'Images', 'Information', 'Miscellaneous', 'Outline', 'Resize', 'Tools', 'Source', 'Login', 'Register', and a search bar. Below the header, the hpc logo is displayed with a '2' in a square, followed by the text 'Improved Simulation Through Collaboration'. A subtext below the logo lists member institutions: Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory • NYSERNet. A horizontal menu bar contains links for 'HOME', 'USER INFO', 'ACCOUNTS', 'SOFTWARE', 'ABOUT', 'RESEARCH GROUPS', and 'HELP!'. To the left, a sidebar titled 'The NY State High Performance Computing Consortium' provides information about the partnership and links to 'GETTING STARTED', 'COMPUTING SOFTWARE', 'RESEARCH HIGHLIGHTS', and 'DOCUMENTATION AND TRAINING'. On the right, a large 3D visualization shows a complex fire plume simulation with a color gradient from red to green, overlaid on a wireframe mesh. A caption at the bottom right reads 'Fire Plume Modeling P. E. DesJardins, University at Buffalo'.

Fill in required fields and submit

Screenshot of a web browser showing the hpc2.org/apply page.

The browser toolbar includes: Back, Address Bar (https://hpc2.org/apply), Favorites, Google search, and various icons for file operations.

The menu bar includes: Most Visited, Getting Started, Disable, Cookies, CSS, Forms, Images, Information, Miscellaneous, Outline, Resize, Tools, View Source, and a Help icon.

The header features the hpc logo (with a red '2' in a box), the tagline "Improved Simulation Through Collaboration", and the text: Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory • NYSERNet.

The navigation menu includes: HOME, USER INFO, ACCOUNTS, SOFTWARE, ABOUT, RESEARCH GROUPS, and HELP! (with a question mark icon).

The breadcrumb trail says: You are here: Home

Apply For New Account

Info: Registration is a two part process. The application form, which helps us assign resources for you, and registering an account on the HUB. This application form has 17 required fields, including check boxes, fill-in-the-blank and short answers about yourself and how you will use the supercomputing resources on hpc2. After it is reviewed, you will be invited to use supercomputing sites.

User Information

Applicant Name / PI: required

Name of Institution/Business required

Address line 1: required

Click “Register”



Improved Simulation Through Collaboration

Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory • NYSERNet

[Login](#) | [Register](#) |

Search

[HOME](#) [USER INFO](#) [ACCOUNTS](#) [SOFTWARE](#) [ABOUT](#) [RESEARCH GROUPS](#)

[HELP!](#)

You are here: Home

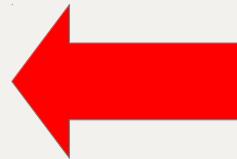
Account Application Validation

Thank You

Thank you for applying for a HPC² account. You should receive an email within 5-10 business days, specifying the supercomputing sites you can run jobs on.

Please continue on to

[Register](#)



If you have any questions or you don't hear back, please use the [site contact](#).

Pick a login name and password

The screenshot shows a web browser window with the URL <https://hpc2.org/register> in the address bar. The browser interface includes standard navigation buttons (back, forward, search, etc.) and a toolbar with various icons like Disable, Cookies, CSS, Forms, Images, Information, Miscellaneous, Outline, Resize, Tools, and View Source.

The main content area features the hpc logo (blue letters with a red square icon) and the text "Improved Simulation Through Collaboration". Below the logo, it says "Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory • NYSERNet". On the right side, there are "Login" and "Register" buttons, and a search bar.

The navigation menu at the top has links for HOME, USER INFO, ACCOUNTS, SOFTWARE, ABOUT, and RESEARCH GROUPS. A "HELP!" link with a question mark icon is also present.

The breadcrumb trail indicates the user is at "You are here: Home » Register".

The main form title is "Create New Account". It contains a "Login Information" section with fields for "User Login" (a required input field), "Password" (a required input field), and "Confirm Password" (a required input field). There is also a "STRENGTH" input field below the password fields. To the right of the form, there is a note about username changes and a password strength indicator.

Login Information

User Login: required

Combination of lowercase letters and numbers. No spaces or punctuation.

STRENGTH

Confirm Password: required

Users cannot be changed. If this poses a serious problem or raises concerns please contact our [support](#).

Password may be changed any time after account creation.

hpc2 new account created

 Improved Simulation Through Collaboration

2

Search

Login | Register | RSS

Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory • NYSERNet

HOME USER INFO ACCOUNTS SOFTWARE ABOUT RESEARCH GROUPS HELP! ?

You are here:  Home » [Register](#) » [Create New Account](#)

Create New Account

✓ Your account has been created successfully.

A confirmation email has been sent to 'jsperhac@gmail.com'. You must click the link in that email to activate your account and resume using hpc2.

hpc2 - Members: My Account: Jeanette Sperhac - Mozilla Firefox

hpc2 - Members: My Account: ...

https://hpc2.org/members/myaccount

Most Visited ▾ Getting Started

Disable Cookies CSS Forms Images Information Miscellaneous Outline Resize Tools View Source

Jeanette Sperhac (jsperhac) Logout My Account 16 New Messages

Search

hpc Improved Simulation Through Collaboration

Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory • NYSERNet

HOME USER INFO ACCOUNTS SOFTWARE ABOUT RESEARCH GROUPS HELP! ?

Dashboard

My Account Jeanette Sperhac

- Getting Started
- Computing Software
- Browse All Software and Materials
- Wish List
- Support
- Machine Status
- Knowledge Base

Personalize Dashboard

Storage (manage) 0% of 0GB

My Groups

- Center for Computational Research approved
- CCR Test Group manager
- jmsperhac group manager

All My Groups All Groups New Group

My Contributions

Tools

- arith2 Status: updated
- arith Status: published
- rstudiotool Status:

All My Messages Settings

Resources

- Simulation Tools

Dashboard

Profile Account Groups Contributions Points Usage Favorites Messages 60

My Tools

- Recent Favorites All Tools
- Jmol: 3D viewer for chemical structures in 3D
- Large-scale Atomic/Molecular Massively Parallel Simulator
- NAMD Scalable Molecular Dynamics
- Quantum ESPRESSO
- R Studio Tool

RStudio

https://hpc2.org/members/myaccount

[Most Visited](#) ▾ [Getting Started](#)[Disable](#) ▾ [Cookies](#) ▾ [CSS](#) ▾ [Forms](#) ▾ [Images](#) ▾ [Information](#) ▾ [Miscellaneous](#) ▾ [Outline](#) ▾ [Resize](#) ▾ [Tools](#) ▾ [View Source](#) ▾ [O](#)

Improved Simulation Through Collaboration

Jeanette Sperhac (jsperhac)

[Logout](#)[My Account](#)[16 New Messages](#)

Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory • NYSERNet

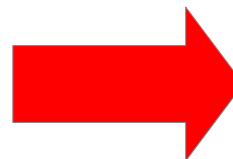
[HOME](#)[USER INFO](#)[ACCOUNTS](#)[SOFTWARE](#)[ABOUT](#)[RESEARCH GROUPS](#)[HELP!](#) You are here: [Home](#) » [Tools](#) » [R Studio Tool](#) » [About](#)

R Studio Tool

By [Jeanette Sperhac](#)¹, [Steve Gallo](#)²

1. SUNY at Buffalo 2. Center for Computational Research, SUNY at Buffalo

RStudio is an IDE for the R language. It provides a multipane window environment for statistical computing and graphics in R.

[Launch Tool](#)

Version 1.0 - published on 12 Feb 2013

 Open source: [license](#) | [download](#)[View All Supporting Documents](#) [Add to your favorites!](#) Share: ...

0 Citation(s)

[About](#) [Citations](#)

SEE ALSO

No results found.

Category

[Tools](#)

Published on

12 Feb 2013

Abstract

The R Studio Tool is a deployment of the RStudio IDE on the hpc2 hub. It provides a multipane window environment for statistical computing and graphics in R.

R Studio provides syntax highlighting, code completion, and smart indentation; ability to execute R code from the source editor; ability to easily manage multiple working directories using projects; and ability to quickly navigate code using type-ahead search.

hpc2 - resources: Tools: R Stud...

<https://hpc2.org/tools/rstudiotool/session/1123>

Google



Most Visited ▾ Getting Started

Disable ▾ Cookies ▾ CSS ▾ Forms ▾ Images ▾ Information ▾ Miscellaneous ▾ Outline ▾ Resize ▾ Tools ▾ View Source ▾



Improved Simulation Through Collaboration

Jeanette Sperhac (jsperhac)

[Logout](#)[My Account](#)

16 New Messages

 Search

Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory

HOME USER INFO ACCOUNTS SOFTWARE ABOUT RESEARCH GROUPS

You are here: [Home](#) » [resources](#) » [Tools](#) » [R Studio Tool](#) » [Session: 1123 "R Studio Tool"](#)

HELP! (?)

Rstudio session:
Terminate
Suspend

[X Terminate](#)[Keep for later](#)

R Studio Tool

File Edit Code View Plots Session Project Build Tools Help

Go to file/function

Project: (None)

plot-extravaganza-mtcars.R x

ggplot2-examp >

```
1 # plot examples from statmethods.net
2 # using mtcars dataset
3 # 3 May 2013
4 # JMS
5
6
7 # pch controls point selection
8 # col controls point color
9 plot(mtcars$wt, mtcars$mpg, xlab="Vehicle Weight (lb/100 miles)", ylab="Vehicle MPG, miles/gallon"
10      , pch=8, col="darkblue")
11 abline(lm(mtcars$mpg~mtcars$wt), col="red")
12 title("Regression of Vehicle MPG on Weight")
13
14
15 # ----- Histograms -----
16
```

1:1 (Top Level) ▾ R Script ▾

Workspace History

Import Dataset

Files Plots Packages Help

New Folder Delete Rename More

Home

	Name	Size	Modified
	.Rhistory	1.4 KB	May 13, 2013, 4:28 PM
	apps		
	checkSubmit		

hpc2 - resources: Tools: R Stud...

<https://hpc2.org/tools/rstudiotool/session/1123>

Google



Most Visited ▾ Getting Started

Disable Cookies CSS Forms Images Information Miscellaneous Outline Resize Tools View Source

```
6  
7 # pch controls point selection  
8 # col controls point color  
9 plot(mtcars$wt, mtcars$mpg, xlab="Veh  
10      ylab="Vehicle MPG, miles/gallon"  
11      pch=8, col="darkblue")  
12 abline(lm(mtcars$mpg~mtcars$wt), col=  
13 title("Regression of Vehicle MPG on W  
14  
15 # ----- Histograms -----  
16
```

1:1 f (Top Level) R Script

Console ~/ ↻

distribution details.

R is a collaborative project with many contributors.

Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.

Type 'q()' to quit R.

> |

Storage (manage)

0% of 0GB

Files Plots Packages Help

New Folder

Delete

Rename

More

 Home

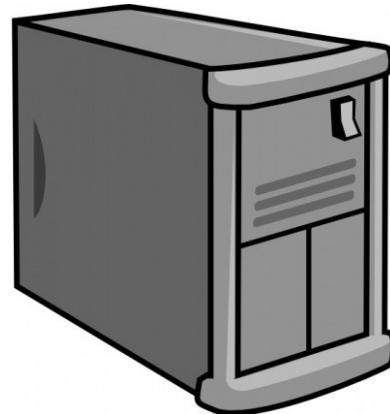
Name	Size	Modified
.Rhistory	1.4 KB	May 13, 2013, 4:28 PM
apps		
checkSubmit		
data		
possum.RData	2.6 KB	May 13, 2013, 11:26 AM
R		

Rstudio window:
Pop out
Refresh
Expand



New Window

GitHub



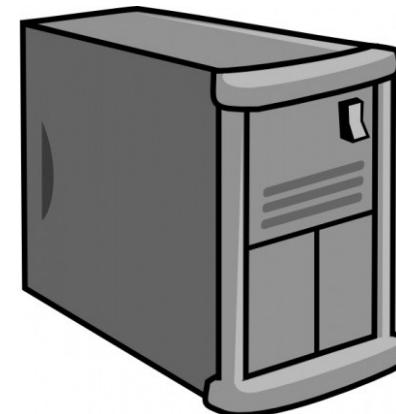
GitHub server

View files

Pull files and data

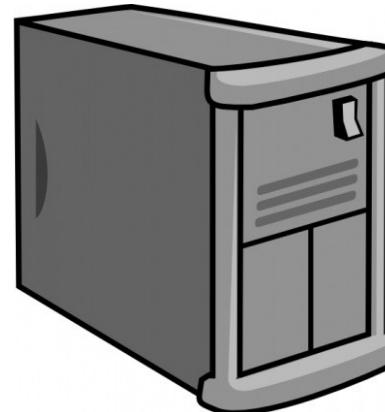


Student workstation



hpc2 server

Workshop Files and Data: GitHub

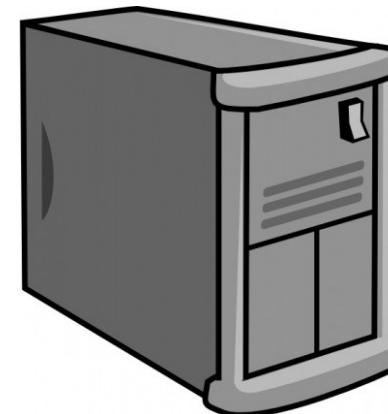


GitHub server

Pull R source files
Create RStudio project

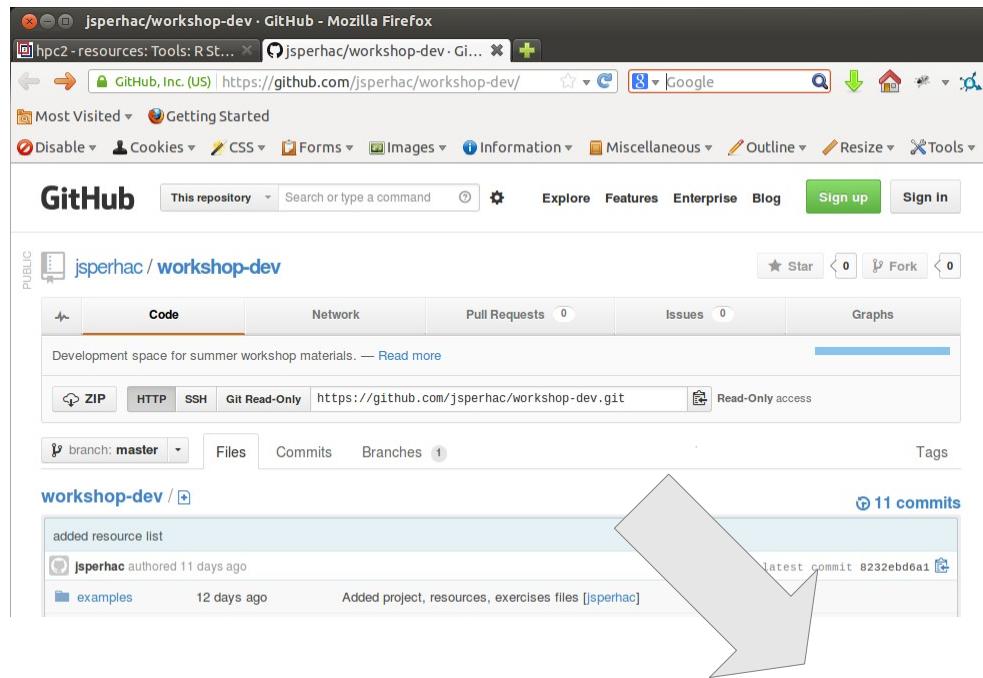


Student workstation

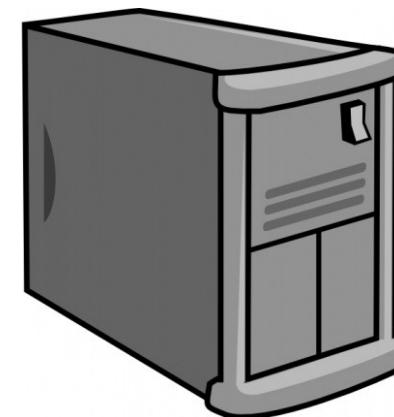


hpc2 server

Workshop Files and Data: GitHub



Student workstation

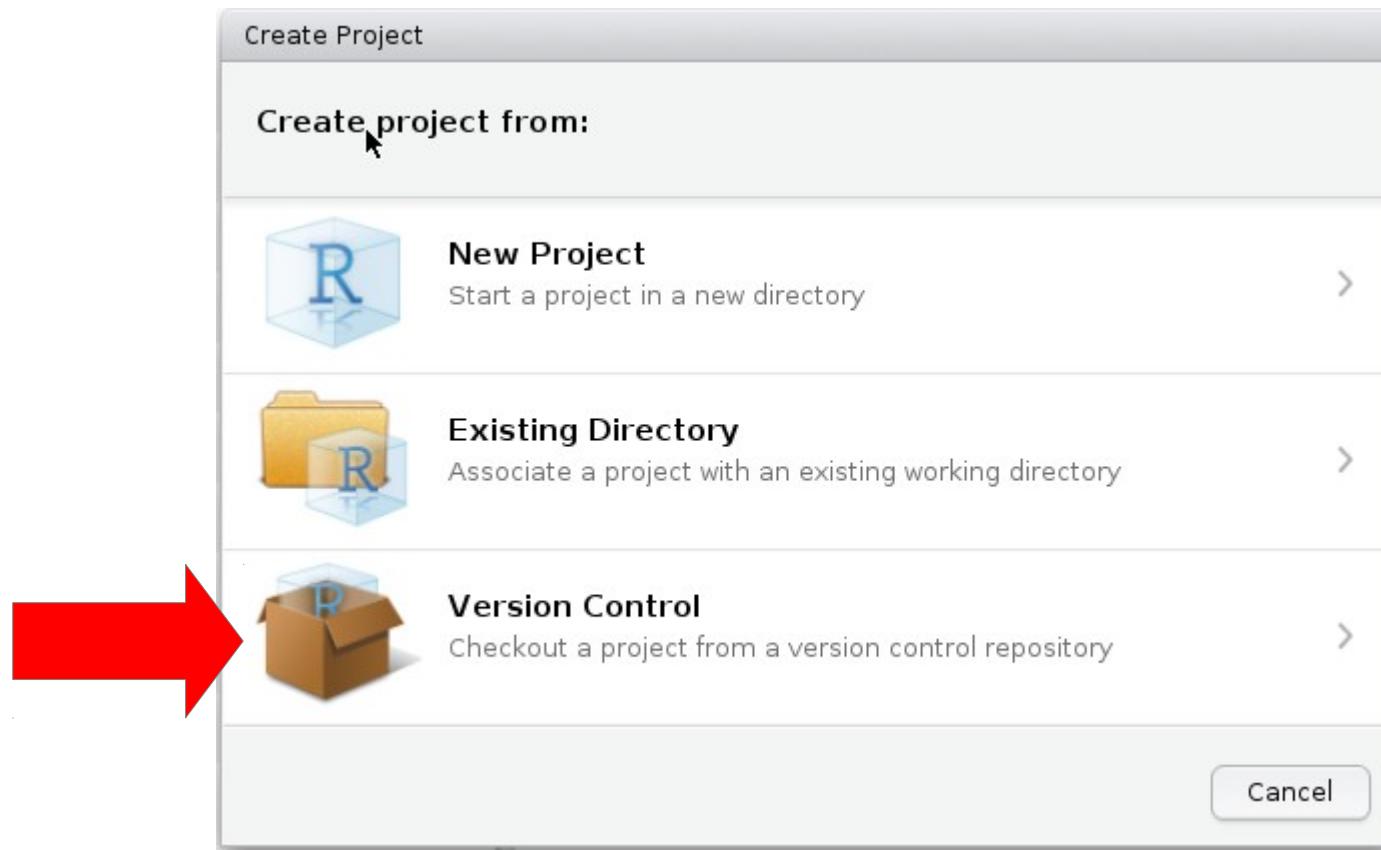


hpc2 server

Create project in RStudio

1. In the RStudio menu:

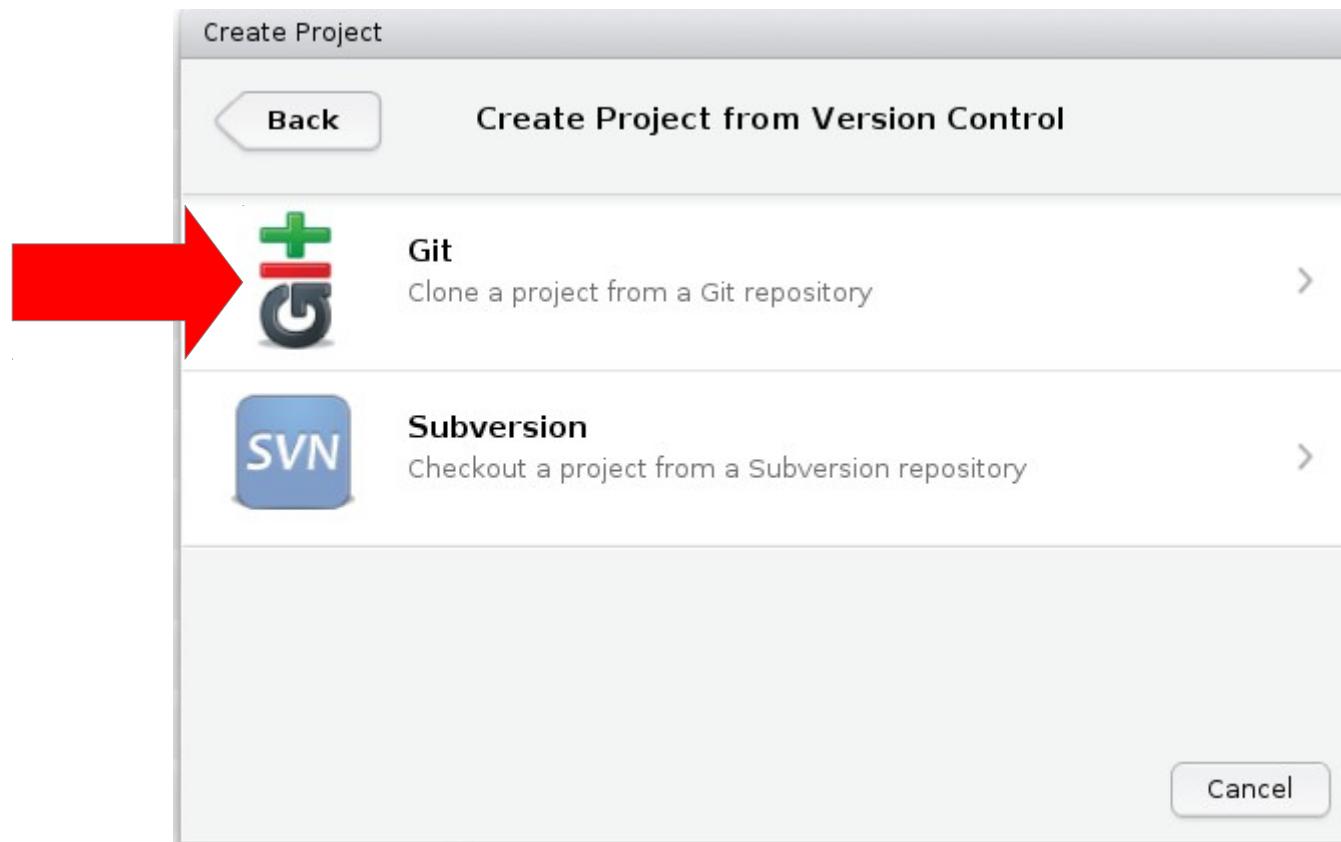
- Select Project: Create Project
- Select Version Control



Create project in RStudio

2. In RStudio:

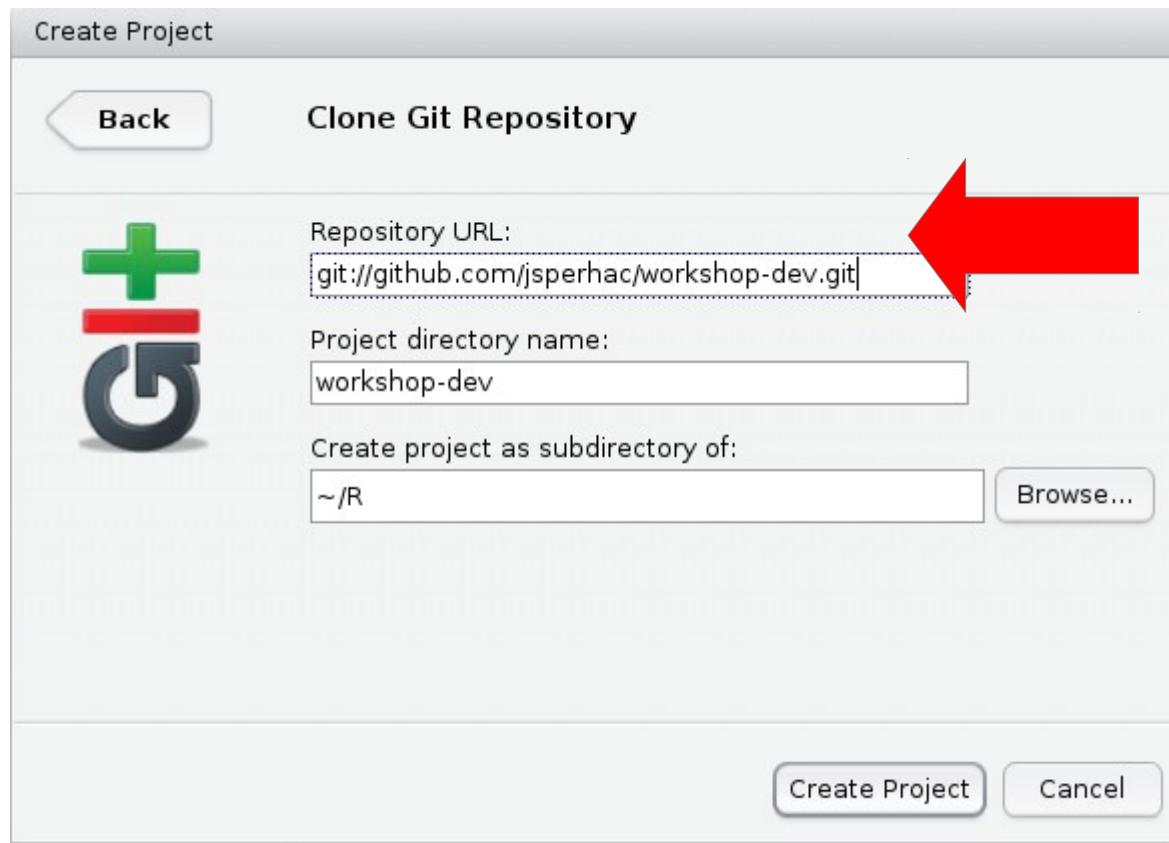
Next, select Git



Create project in RStudio

3. In RStudio:

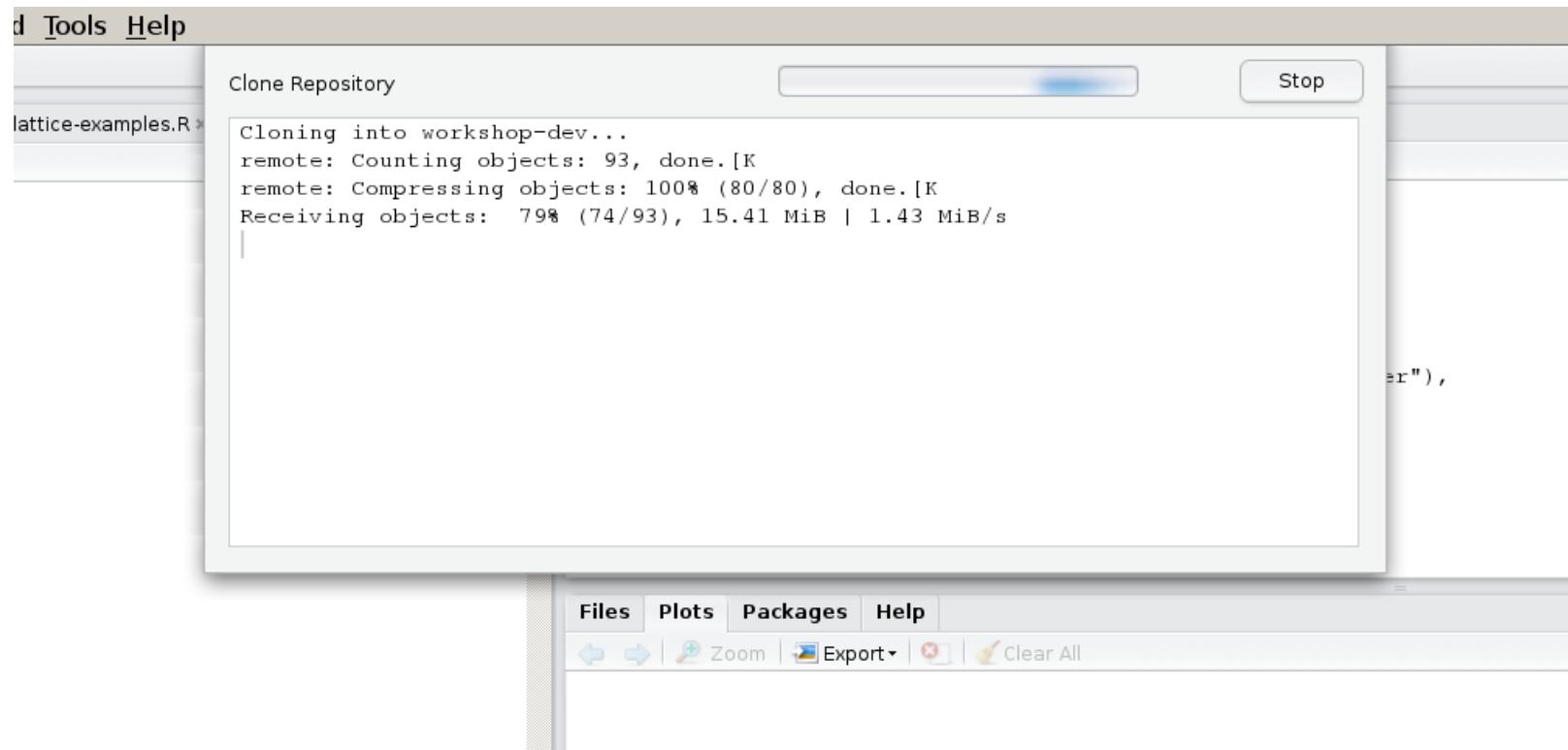
- Type the Repository URL as shown
- Use a unique project directory name



git://github.com/jsperhac/workshop-dev.git

Create project in RStudio

4. RStudio copies the files from GitHub to your home directory on hpc2.

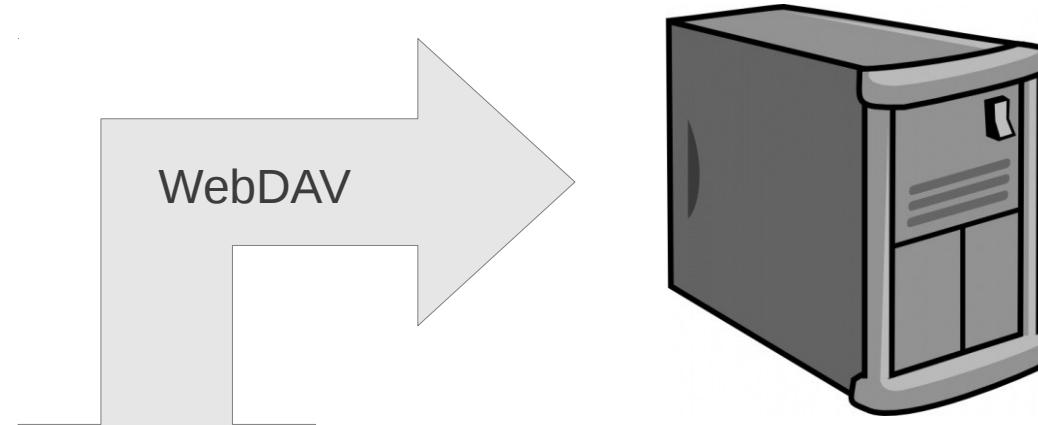




Create project in RStudio

- Selecting the project sets the working directory
- Your RStudio project contains directories:
 - examples
 - exercises
 - project
 - resources

File transfer

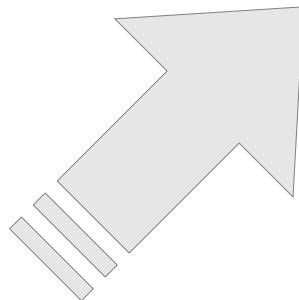


Student workstation

You'll need file transfer for adding graphics files to your presentation slides

File transfer: WebDAV

Home folder



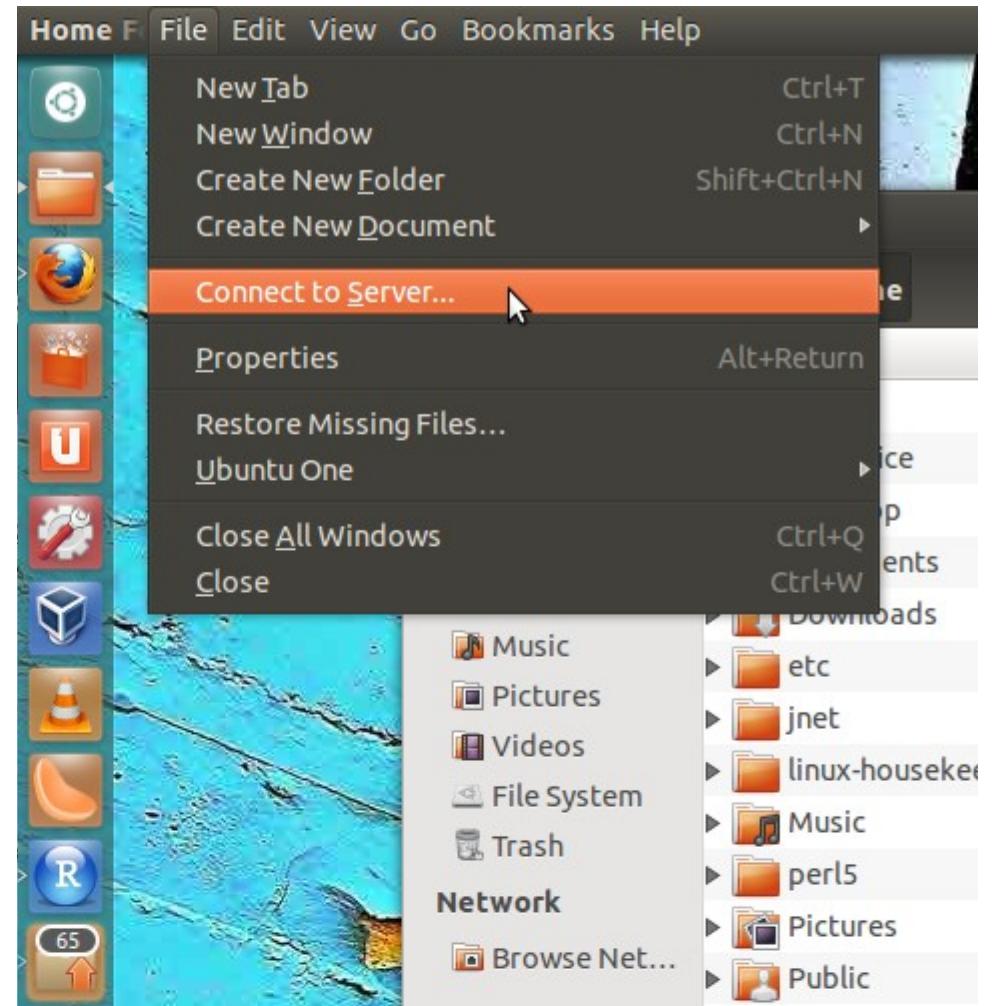
Student workstation

File transfer: WebDAV

File: Connect to Server...



Student workstation

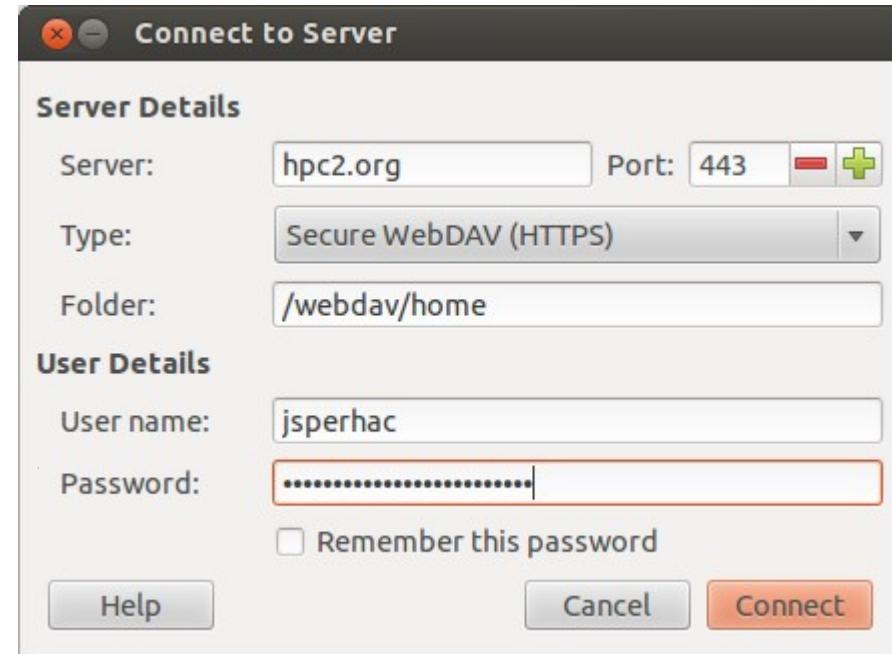


File transfer: WebDAV

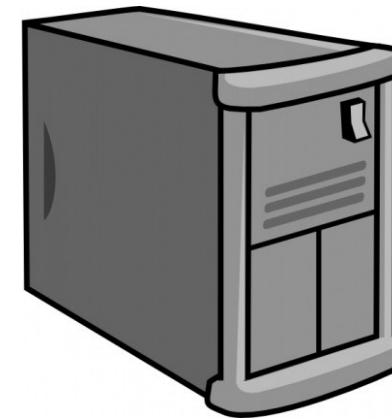
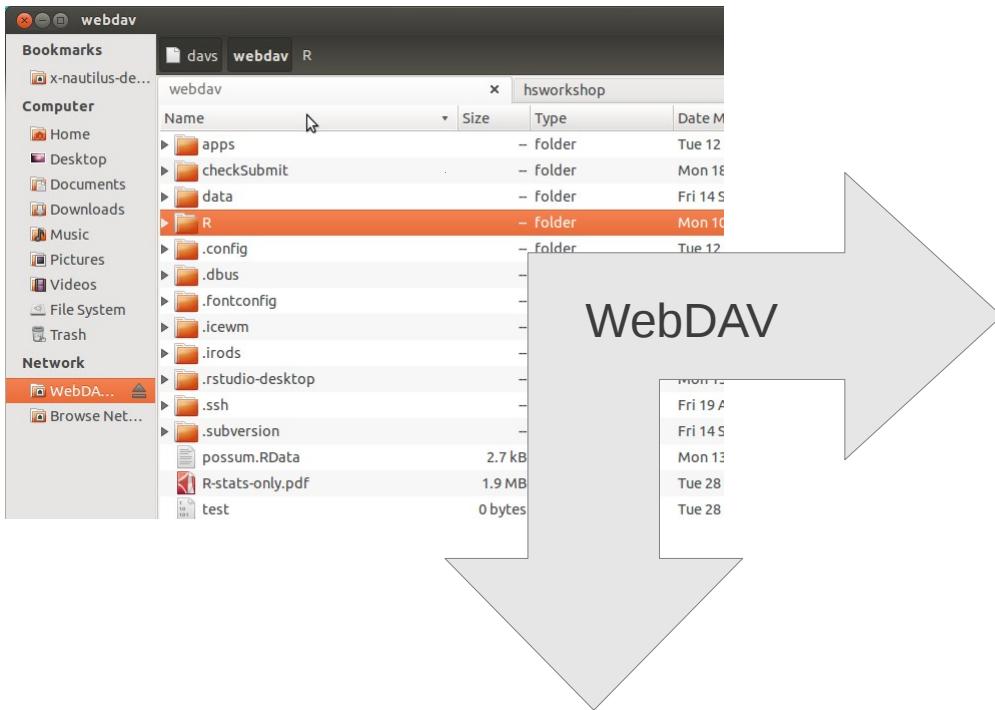
Use your hpc2 user credentials



Student workstation



File transfer



hpc2 server



Student workstation