

Eric Pitman Summer Workshop in Computational Science



0. Workshop environment

Jeanette Sperhac

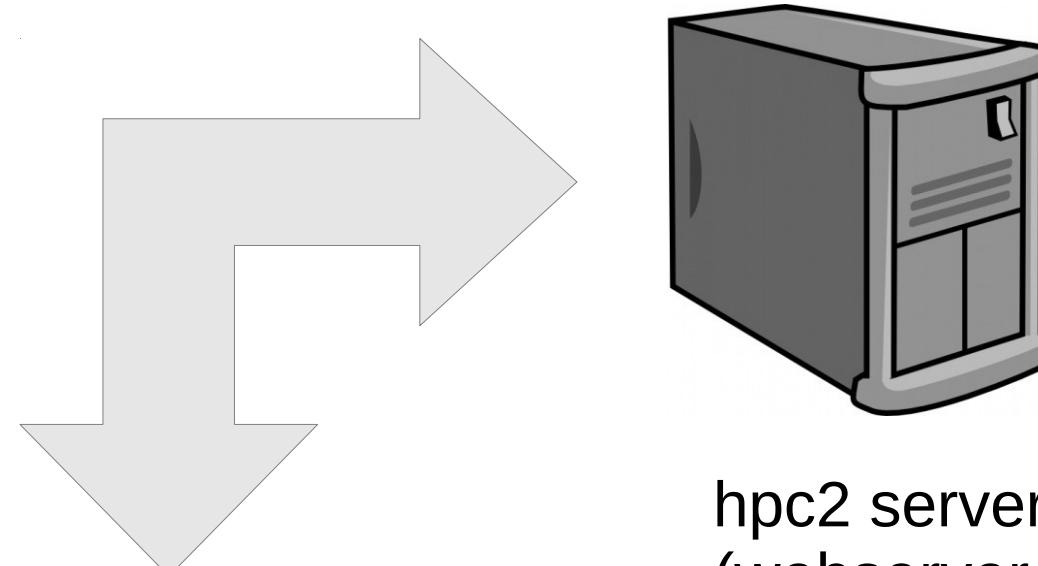
Intro to



0. Workshop environment: set up on hpc2.org

- Register on hpc2.org
- Starting the RStudio tool
- Setting up RStudio Projects: GitHub
- File transfer: using WebDAV

Workshop Computing Environment



Student workstation
(Firefox browser)

hpc2 server
(webserver, RStudio)

You
are
here!

Register on hpc2.org

You must have an email address...

1. On hpc2.org website, click Login link
2. On Login form, click Create One link
3. In Create New Account page:
 - a) Choose username and password; specify email address; submit
4. Click link on confirmation email; sign in

Login link on hpc2.org

A screenshot of a web browser displaying the hpc2.org website. A large red arrow points from the top right towards the 'Tools' menu item in the browser's toolbar. The browser's address bar shows the URL <https://hpc2.org>. The website header includes the 'hpc' logo with a '2' icon, the tagline 'Improved Simulation Through Collaboration', and links for 'Login' and 'Register'. Below the header is a navigation menu with 'HOME' selected. On the left, a sidebar features a section titled 'The NY State High Performance Computing Consortium' with text about the partnership and four menu items: 'GETTING STARTED', 'COMPUTING SOFTWARE' (which is highlighted in blue), 'RESEARCH HIGHLIGHTS', and 'DOCUMENTATION AND TRAINING'. To the right is a 3D visualization of a fire plume simulation, showing a complex, turbulent flow field with color-coded temperature or density gradients.

https://hpc2.org

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hpc 2

Improved Simulation Through Collaboration

>Login | Register | RSS

Search

HOME USER INFO ACCOUNTS SOFTWARE ABOUT RESEARCH GROUPS HELP! ?

The NY State High Performance Computing Consortium

HPC² is a partnership between NYSERNet and supercomputing centers at RPI, Stony Brook, Brookhaven, and SUNY Buffalo. Our goal is to increase New York State's competitiveness and foster economic development by providing industry and academic institutions with high performance computing resources, including staff with expertise in modeling and simulation. Account access and a variety of open source software is available through this portal.

▶ GETTING STARTED

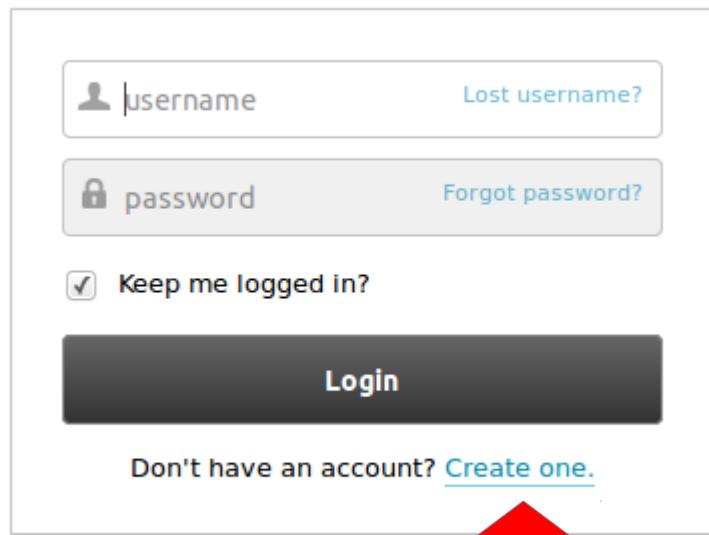
▶ COMPUTING SOFTWARE

▶ RESEARCH HIGHLIGHTS

▶ DOCUMENTATION AND TRAINING

Fire Plume Modeling P. E. DesJardins, University at Buffalo

Click “Create One”



Pick a login name and password

The screenshot shows a web browser window with the following details:

- Address Bar:** https://hpc2.org/register
- Toolbar:** Includes icons for Back, Forward, Stop, Refresh, Home, and various search and download functions.
- Menu Bar:** Most Visited, Getting Started, Disable, Cookies, CSS, Forms, Images, Information, Miscellaneous, Outline, Resize, Tools, View Source.
- Header:**
 - hpc** logo with a red square icon containing a '2'.
 - Text: Improved Simulation Through Collaboration
 - Links: Login, Register, Search bar.
 - Text: Rensselaer Polytechnic Institute • Stony Brook University • University at Buffalo • Brookhaven National Laboratory • NYSERNet
- Navigation Bar:** HOME, USER INFO, ACCOUNTS, SOFTWARE, ABOUT, RESEARCH GROUPS, HELP! ?
- Breadcrumbs:** You are here: Home » Register
- Section:** Create New Account
- Login Information Form:**
 - User Login: required (text input field)
 - Description: Combination of lowercase letters and numbers. No spaces or punctuation.
 - Password: required (text input field)
 - Confirm Password: required (text input field)
 - Strength: (text input field)
- Text on the right:** Usernames 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

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

[Login](#) | [Register](#) | [!\[\]\(89d1e09f668245d223896beda39443bd_img.jpg\)](#)

Search

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

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Jeanette Sperhac (jsperhac) Logout My Account 16 New Messages

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HOME USER INFO ACCOUNTS SOFTWARE ABOUT RESEARCH GROUPS HELP! ?

Dashboard

My Account

Getting Started

Computing Software

Browse All Software and Materials

Wish List

Support

Machine Status

Knowledge Base

Profile

Account

Groups

Contributions

Points

Usage

Favorites

Messages 60

Personalize Dashboard

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

Storage (manage) 0% of 0GB

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

My Account (jsperhac)

Dashboard

My Groups

My Contributions

My Messages

Resources

https://hpc2.org/members/myaccount

A large red arrow points from the left towards the "Dashboard" link in the top navigation bar. A second large red arrow points from the bottom towards the "R Studio Tool" entry in the "My Tools" section.

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Improved Simulation Through Collaboration

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

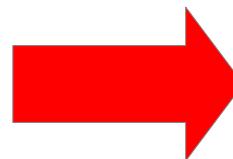
You are here: Home » Tools » R Studio Tool » About

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)

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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>

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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



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

1:1 (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

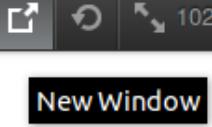
Files Plots Packages Help

New Folder Delete Rename More

Home

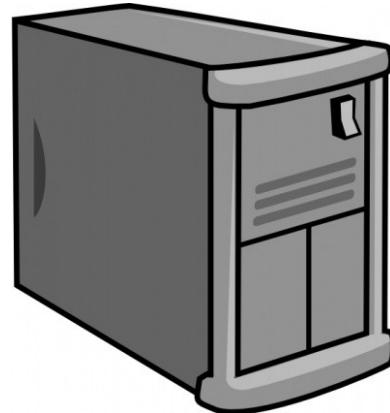
Name	Size	Modified
.Rhistory	1.4 KB	May 13, 2013, 4:28 PM
apps		
checkSubmit		
data		
possum.RData	2.6 KB	May 13, 2013, 11:26 AM
R		

RStudio window:
Pop out
Refresh
Expand



1024 x 768

GitHub



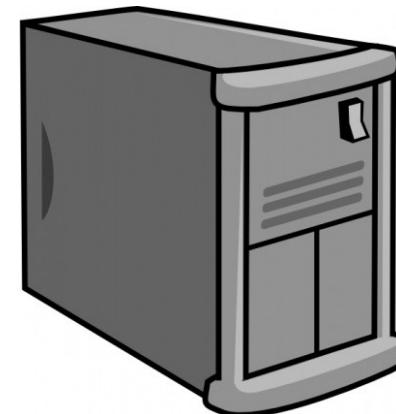
GitHub server

View files

Pull files and data

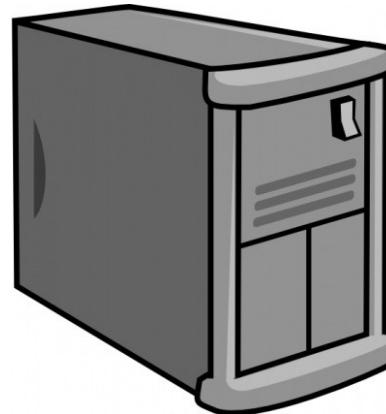


Student workstation



hpc2 server

Workshop Files and Data: GitHub

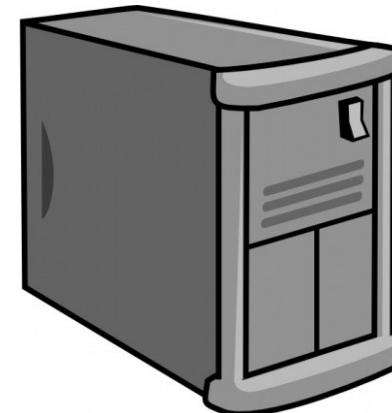


GitHub server

Pull R source files
Create RStudio project

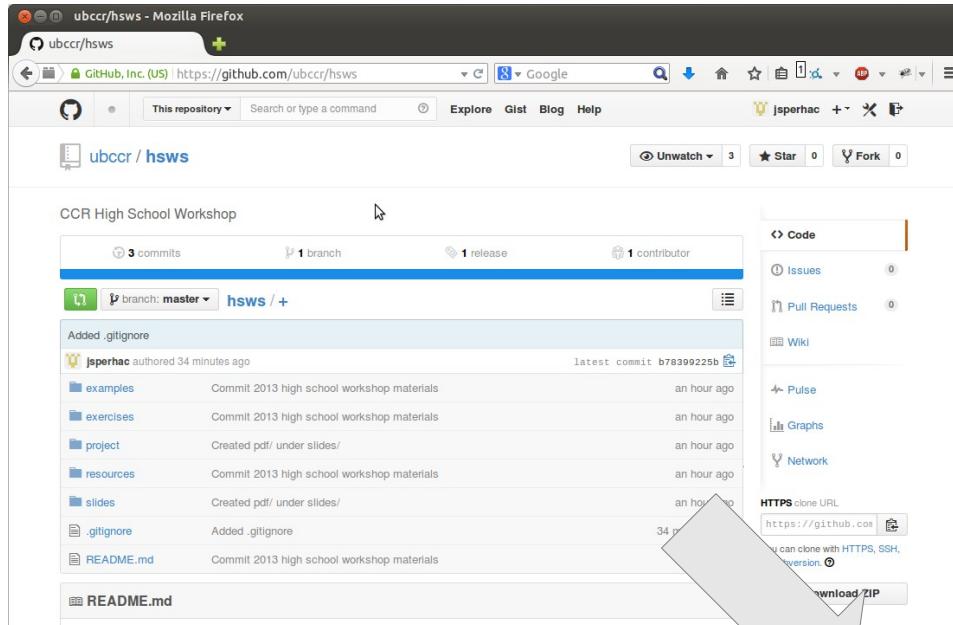


Student workstation

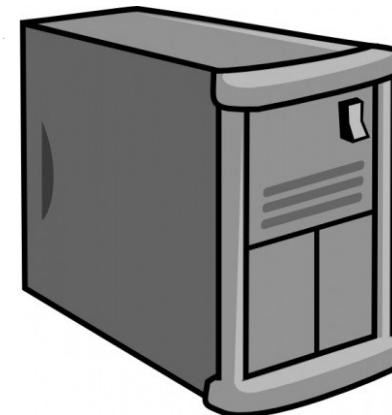


hpc2 server

Workshop Files and Data: GitHub



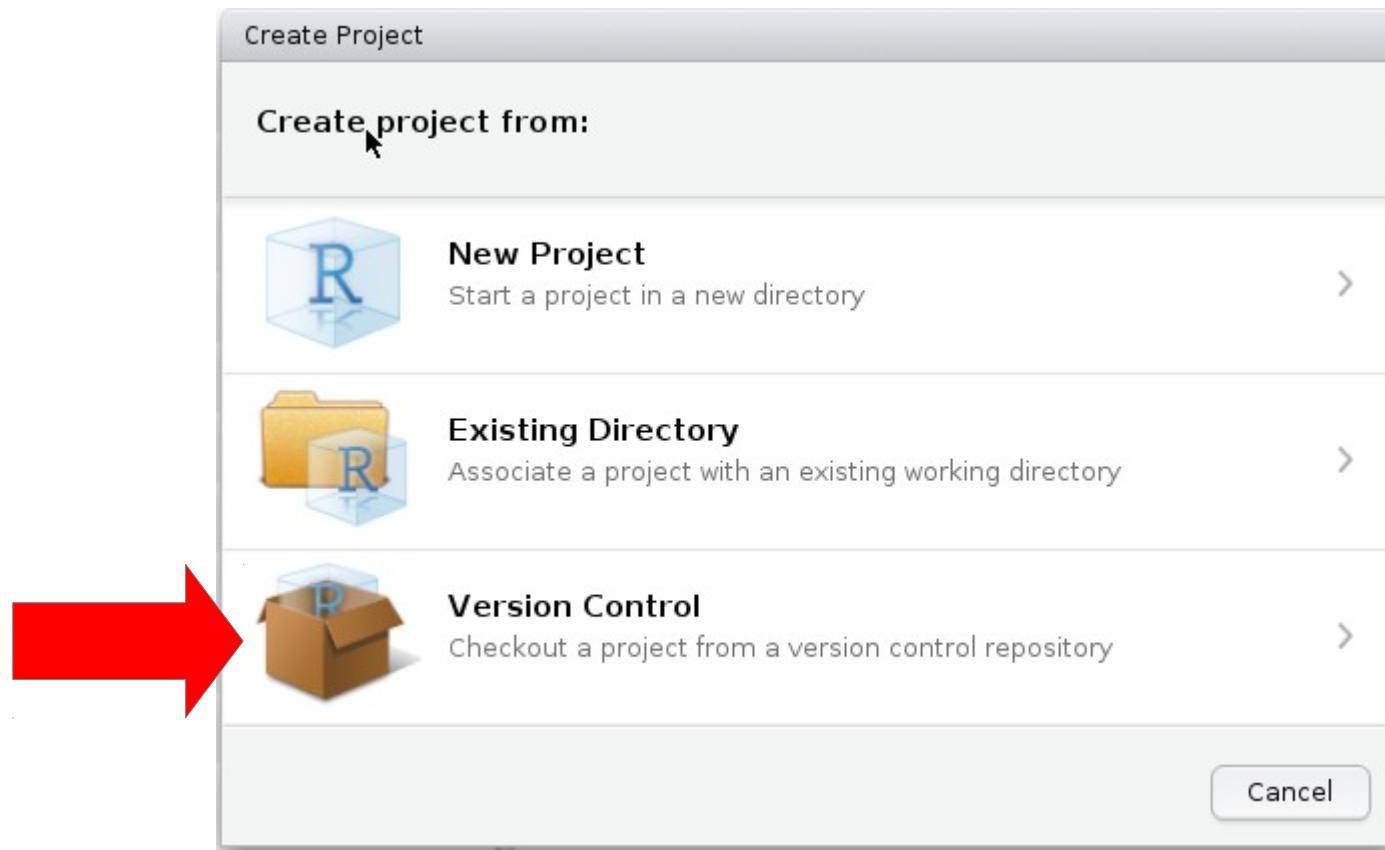
Student workstation



hpc2 server

Create Project in RStudio

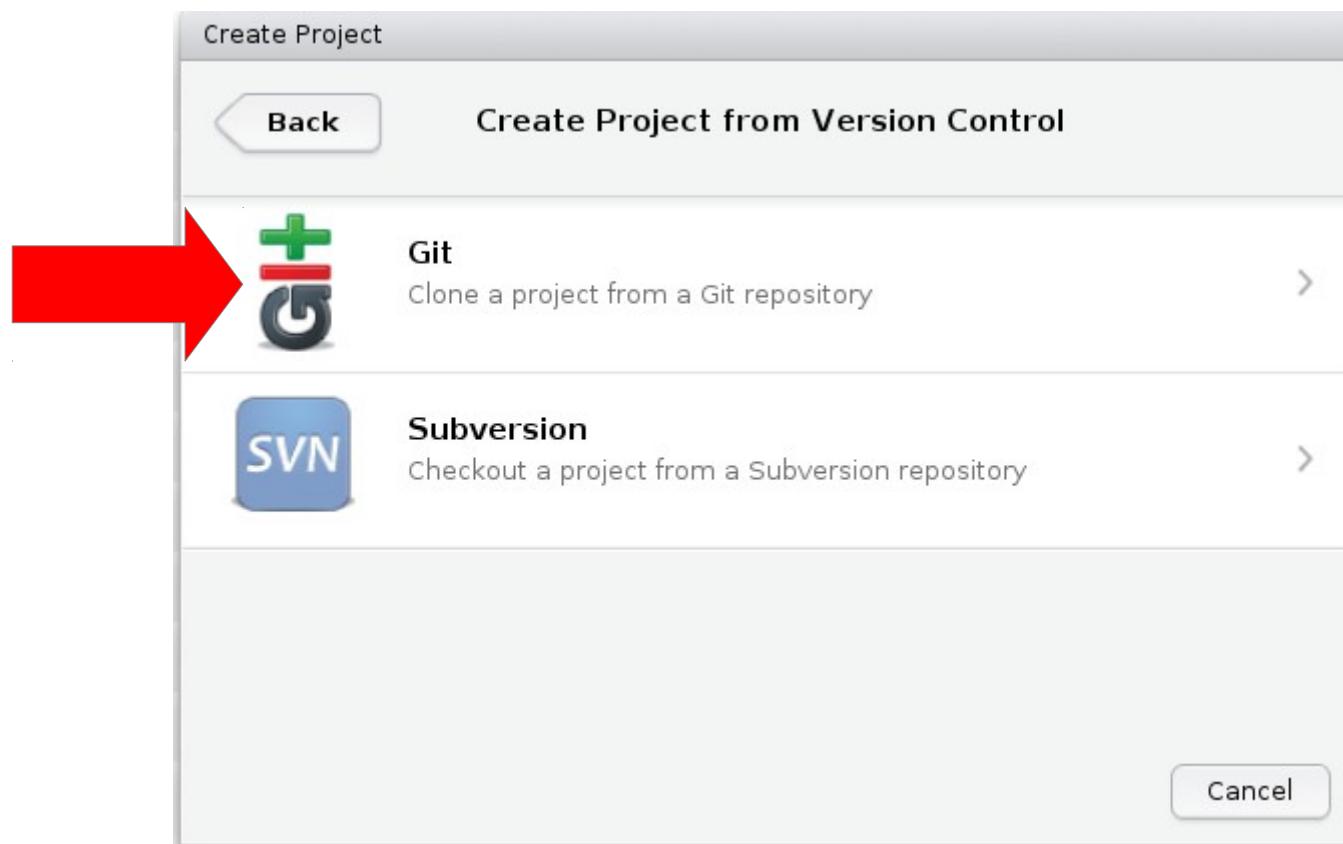
1. In the RStudio menu:
 - Select Project: Create Project
 - Select Version Control



Create Project in RStudio

2. In RStudio:

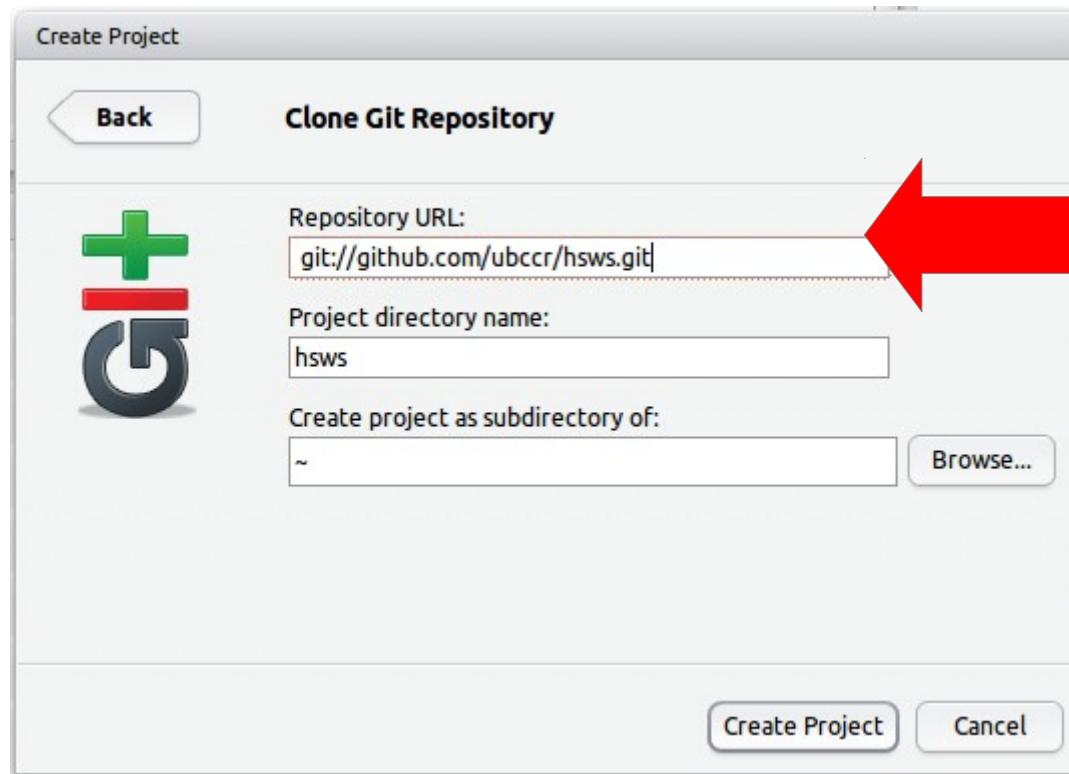
Next, select Git



Create Project in RStudio

3. In RStudio:

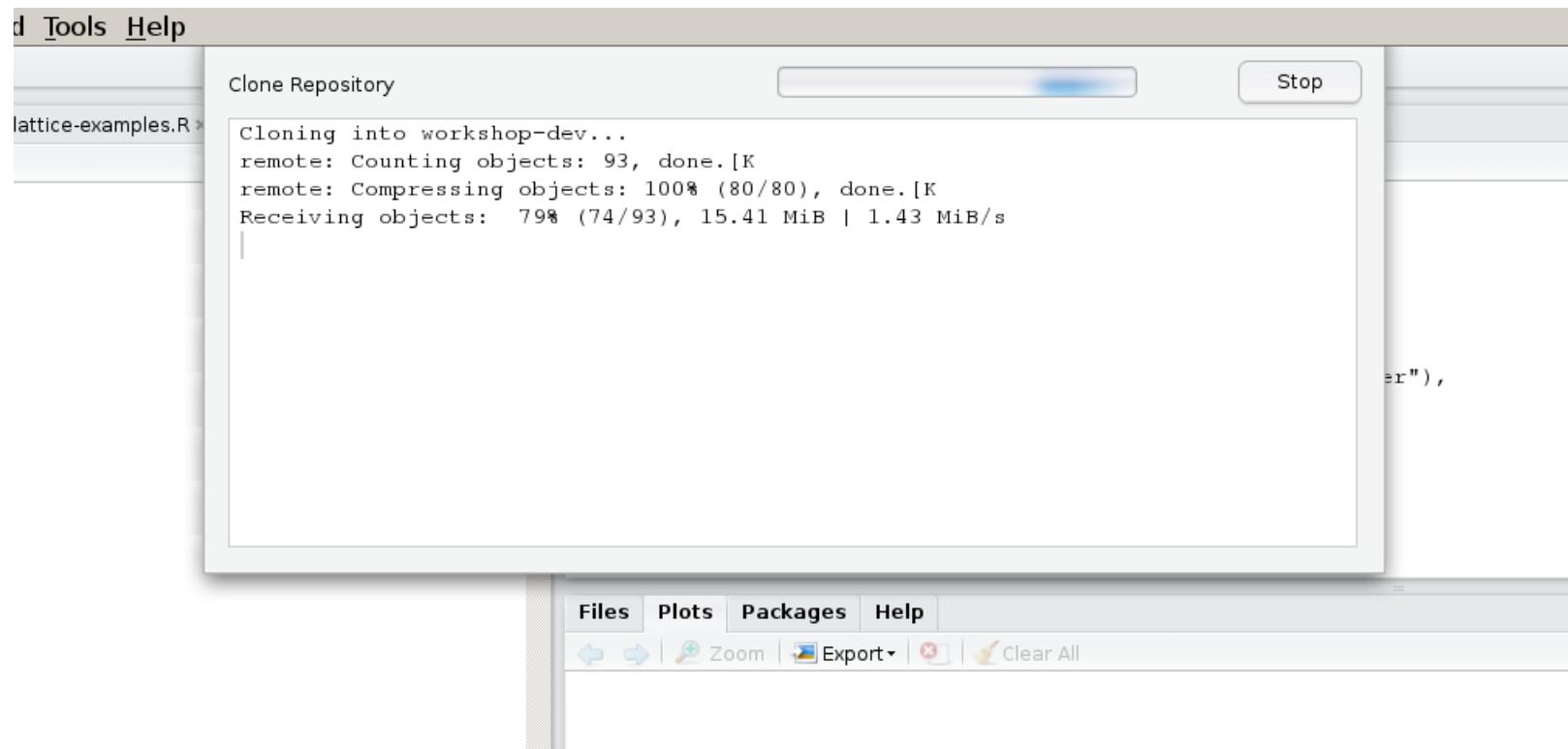
- Type the Repository URL as shown
- Use a unique project directory name



git://github.com/ubccr/hsws.git

Create Project in RStudio

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

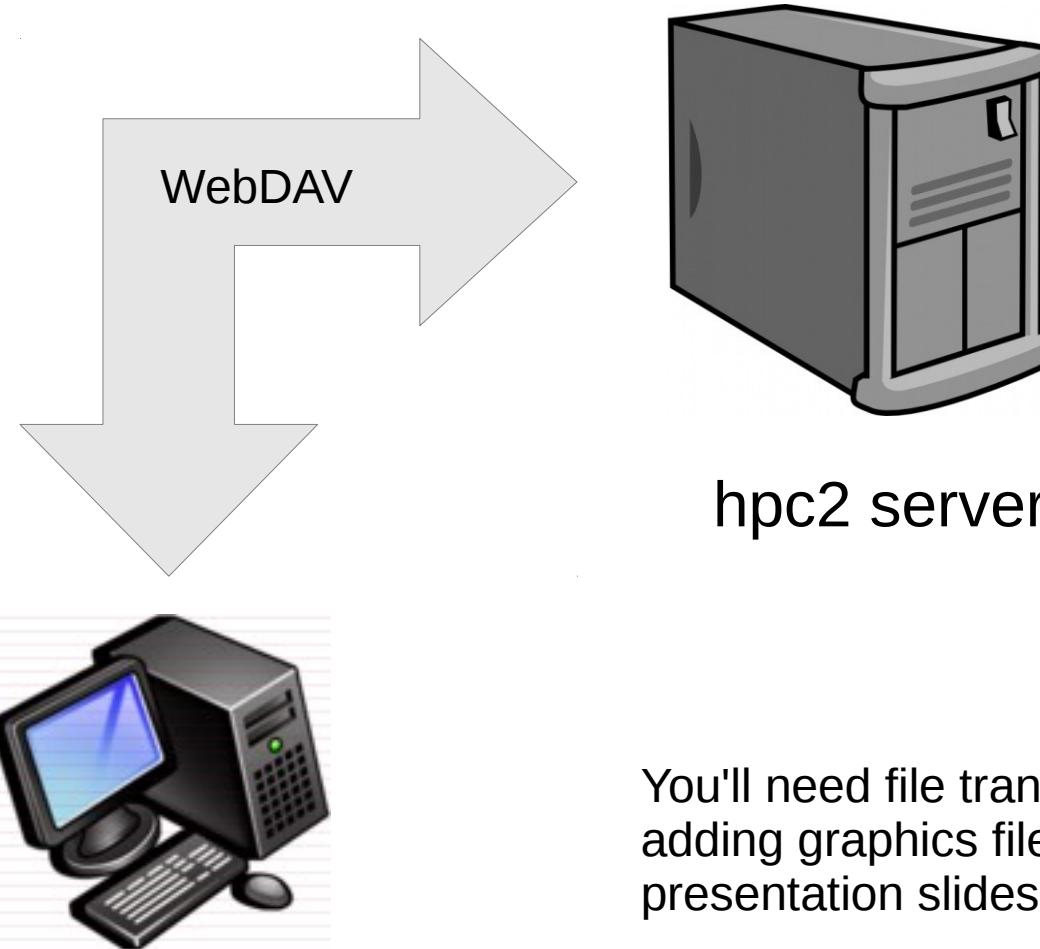




Create Project in RStudio

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

File Transfer

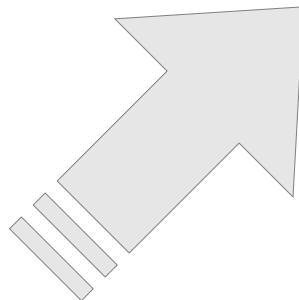


Student workstation

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

File Transfer: WebDAV

Home folder



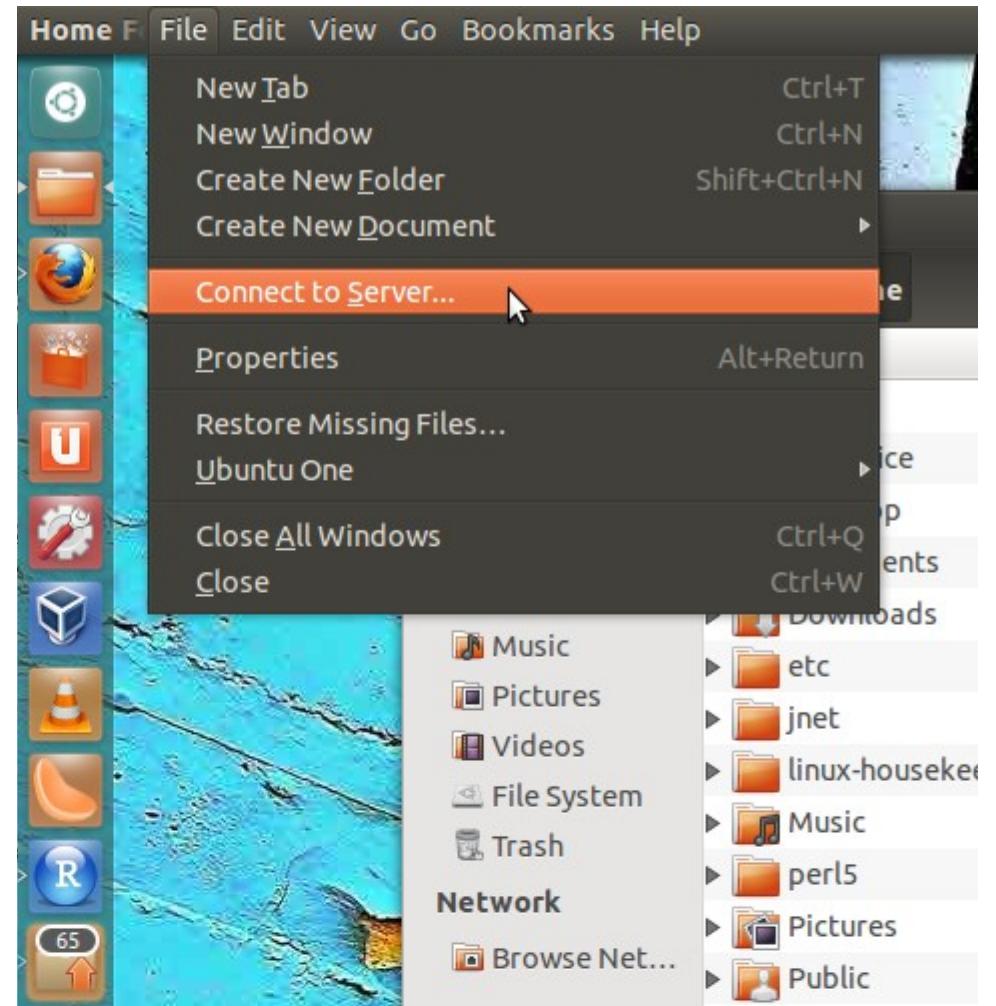
Student workstation

File Transfer: WebDAV

File: Connect to Server...



Student workstation

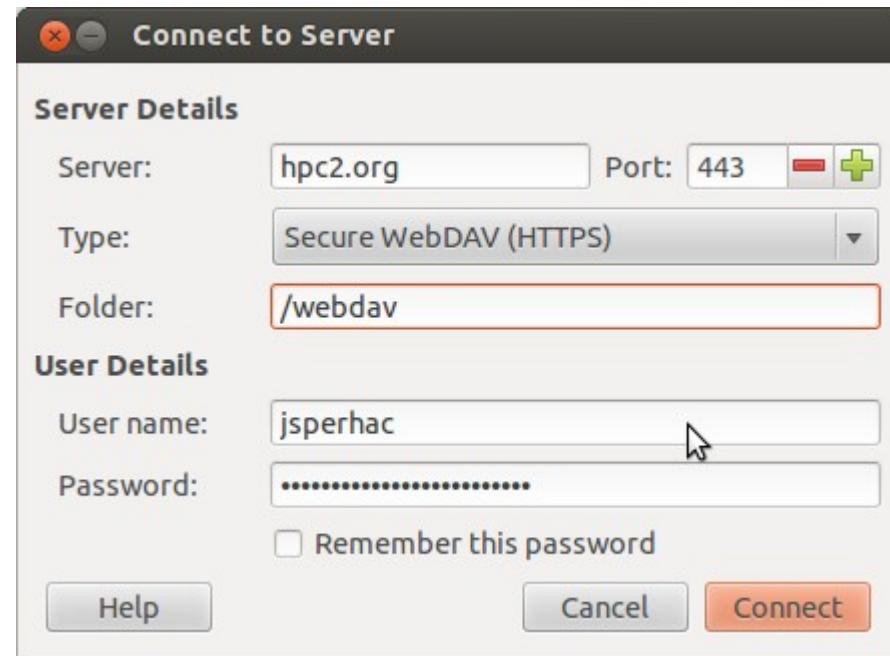


File Transfer: WebDAV

Use your hpc2 user credentials

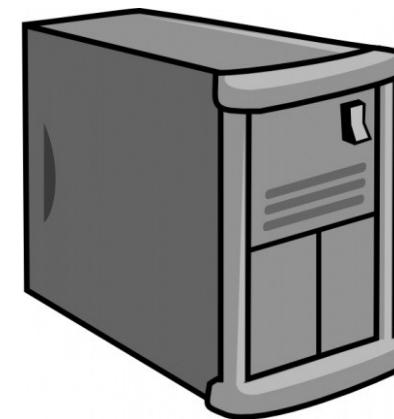
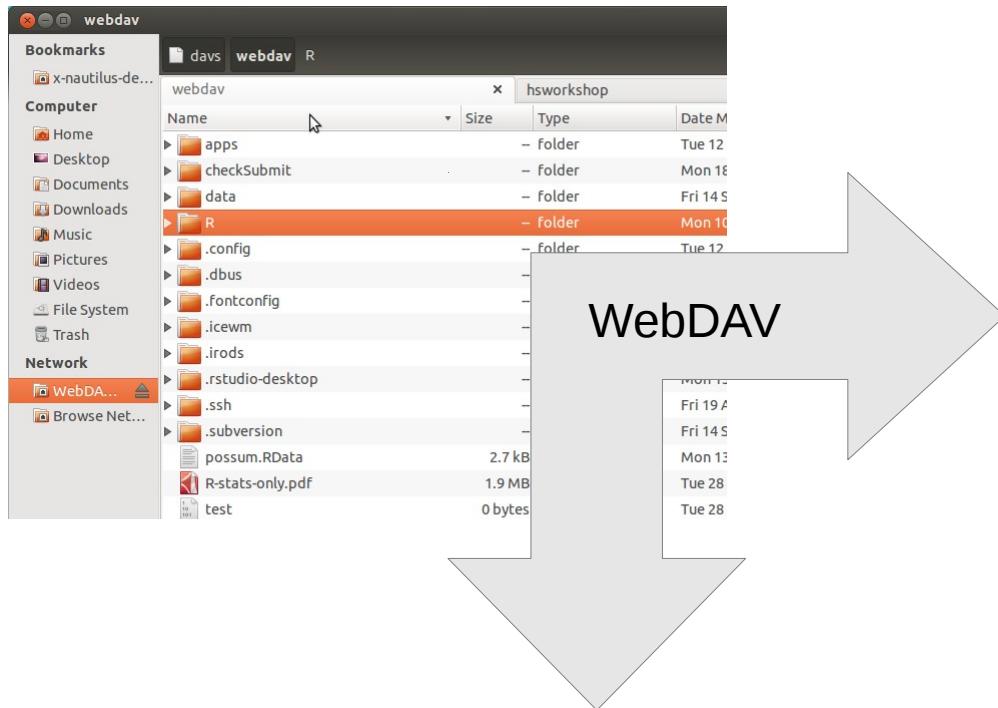


Student workstation



Server: hpc2.org
Type: Secure WebDAV
Folder: /webdav

File Transfer



hpc2 server



Student workstation