Exploring reproducible scientific computing using Vagrant, Ansible, and Anaconda.

Bret Davidson

NCSU Libraries

go.ncsu.edu/dsvil-sb

Agenda

- Open science as problem space
- Open science at NC State
- Scholar's Backpack

Open Science: what is it?

- Open Access
- Open Data
- Open Notebooks
- Open Source

Open Science is a return to first principles of scientific practice.

PHILOSOPHICAL TRANSACTIONS:

GIVING SOME

ACCOMPT

OF THE PRESENT

Undertakings, Studies, and Labours

OF THE

INGENIOUS

IN MANY

CONSIDERABLE PARTS

OF THE

WORLD.

Vol I.

For *Anno* 1665, and 1666.

In the *SAVOY*,

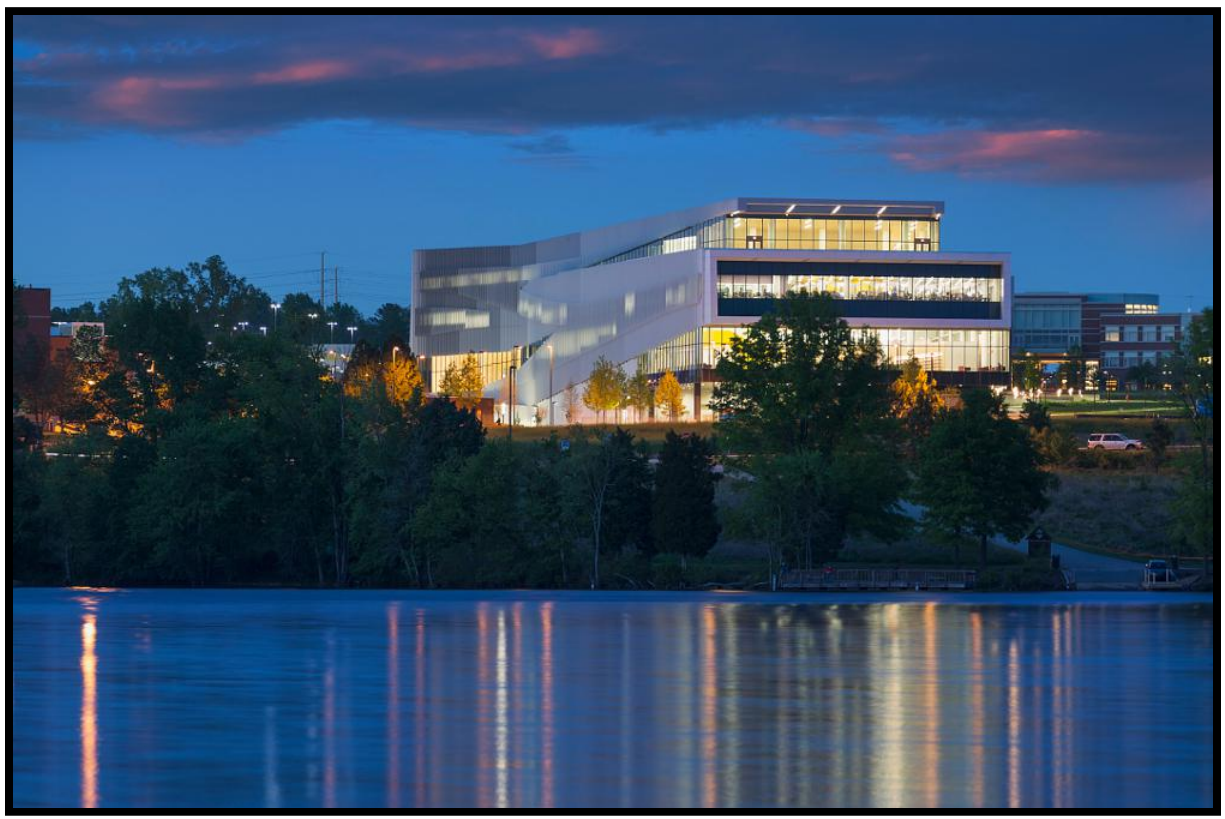
Printed by *T. N.* for *John Martyn* at the Bell, a little without *Temple-Bar*, and *James Allestry* in *Duck-Lane*, Printers to the *Royal Society*.

Nullius in Verba

"Take nobody's word for it."

Open Science can increase reproducibility.

Why Libraries?



Aligns with core library values

- information access
- open peer review
- community-based knowledge creation
- the preservation and dissemination of research
- libraries are champions of open (open source; open data)

The NCSU Libraries' **Open Science Initiative**

Goals

- explore open science practice at NCSU
- better understand researcher needs in context

Open Science Unconference

Follow-up Informal Interviews

- Modern Research Skills Gap
- Insufficient Incentives


NCSU LIBRARIES
SUMMER of OPEN SCIENCE


NCSU LIBRARIES
FIND
GET HELP
SERVICES
LIBRARIES
ABOUT
Search books, articles, journals,
ASK US | MY ACCOUNT | HOURS | FAQ | LOG OUT | CHAT NOW
EVENTS
All Events & Exhibits
All Workshops
Events Calendar
Exhibits
EVENT SERIES
Coffee & Viz
Summer of Open Science
Fabulous Faculty
Amazing Alumni
Stellar Students
AV Geeks at the Hunt Library
Read Smart
Making Space
WORKSHOPS
All Workshops
Visualization Workshops
Makerspace Workshops
Research Workshops
Digital Media Workshops
MAY
S M T W T F S
1 2 3 4 5 6 7
8 9 10 11 12 13 14
15 16 17 18 19 20 21
22 23 24 25 26 27 28
29 30 31
Summer of Open Science Event Series
The NCSU Libraries Summer of Open Science is a series of workshops and meetups that support modern research practice through hands on skill building.
Researchers are increasingly using digital tools in a complex, increasingly open, scholarly ecosystem. This has created a technical skills gap for experienced and novice researchers alike. The Summer of Open Science is designed to address this skills gap.
NCSU LIBRARIES
SUMMER of OPEN SCIENCE
INTRODUCTION TO THE COMMAND LINE INTERFACE
May 19, 2016
2:00 PM to 4:00 PM
At the D.H. Hill Makerspace, D. H. Hill Library
WEB SCRAPING WITH PYTHON
May 25, 2016
2:00 PM to 5:00 PM
At the D.H. Hill Makerspace, D. H. Hill Library
UNDERSTAND AND BUILD YOUR SCHOLARLY IDENTITY
Jun 2, 2016
10:00 AM to 12:00 PM
At the Multimedia Seminar Center, D. H. Hill Library
SCIENTIFIC COMPUTING WITH PYTHON AND RASPBERRY PI
Jun 7, 2016
2:00 PM to 5:00 PM
At the D.H. Hill Makerspace, D. H. Hill Library
BUILD YOUR SCHOLARLY WEBSITE THE EASY WAY
Jun 10, 2016
10:00 AM to 12:00 PM

Goals

- Hands on skill building
- Provide networking opportunities
- Increase visibility of library spaces & services

Skills

- Scholarly identity creation
- Scientific computing
- Building a website
- Data harvesting
- Code collaboration

The Planning Team

Representation from broad range of departments.

Ekatarina [Eka] Grguric (Project Lead)
NCSU Libraries Fellow, Digital Libraries Initiatives / User Experience

Lauren Di Monte (Project Manager)
NCSU Libraries Fellow, User Experience / Administration

Alison Blaine (Content Development)
NCSU Libraries Fellow, Digital Libraries Initiatives / Research & Information Services

Bret Davidson (Technical Lead)
Digital Technologies Development Librarian, Digital Libraries Initiatives

Jennifer Garrett (Community Development)
Research Librarian for Mgmt, Education, and Social Sciences, Research & Information Services

Summer of Open Science

- Workshops
  - Intro to the Command Line Interface
  - Web Scraping with Python
  - Understand and Build Your Scholarly Identity
  - Scientific Computing with Python & Raspberry Pi
  - Build Your Scholarly Website the Easy Way

- Events
  - Meetups
  - End-of-Summer Showcase

Instructors

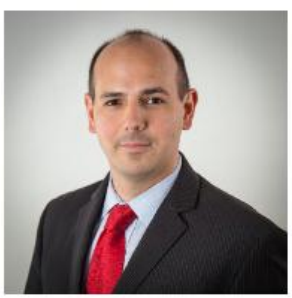
Brittany Johnson

Eka Grguric

Lauren DiMonte

Alison Blaine

Madison Sullivan



Will Cross

Todd Stoffer

Scientific Computing with Python & Raspberry Pi

40 person waiting list

Interdisciplinary Need:
over 40 departments across ~16 colleges

Takeaways

- Libraries are well positioned to fill gaps in the curriculum
- "Open Science" attracted a range of disciplines
- High demand for introductory skill training, particularly coding
- Interest in interdisciplinary research sharing
- Summer presents interesting opportunities and challenges

Virtual Environments for Reproducible Computing

Technical workshops are ripe for disaster.

What could go wrong?

- Images reset overnight
- Improper permissions
- Network connectivity issues
- Language Versions
- Missing packages

Instructor Challenges

- Inconsistent user environments
- Inconsistent course materials
- Provisioning is time consuming
- Difficult to collaborate

Student Challenges

- Data types and structures
- Module system
- Control Structures
- Exception Handling
- Working with file system
- Retrieve a web page with Requests
- Parse content with Beautiful Soup
- Generate a word cloud with matplotlib

Computing Tasks
vs.
Computing Environments

Rise of Scholarly Code

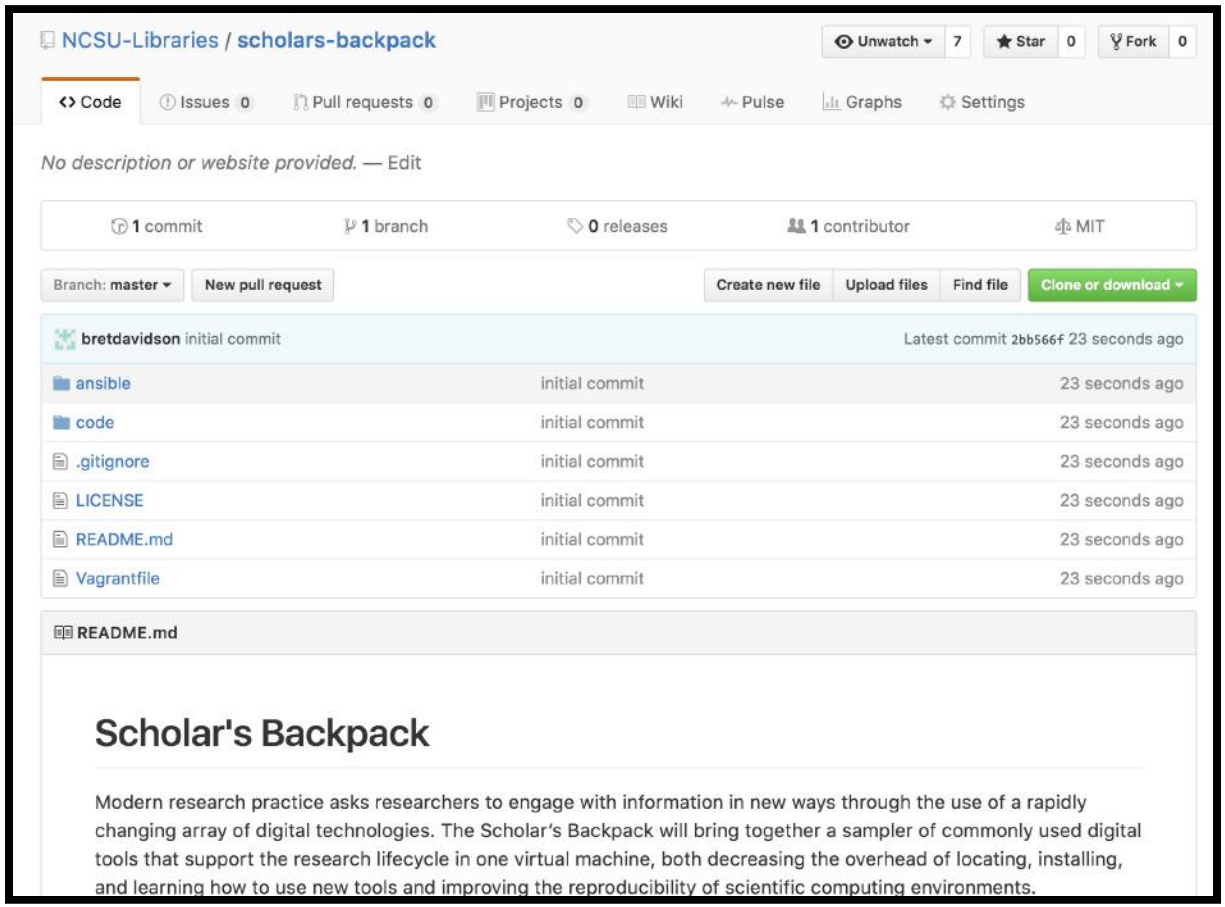
Researcher Needs

- Consistency across lab environments
- Ability to see results of code
- Consistency across time
- Ease of collaboration

Many Options

- Custom Operating System Images
- Custom Distributions, e.g. Anaconda
- Interactive Environments, e.g. Jupyter

github.com/NCSU-Libraries/scholars-backpack



Our Approach

- Vagrant for managing operating system
- Ansible for provisioning and configuration
- Anaconda for managing environments and packages
- Workshop specific resources

Easy!

1. Install Vagrant
2. Install VirtualBox
3. Clone project repo
4. `vagrant up`
5. `vagrant ssh`
6. Execute code!

This is reproducible computing!

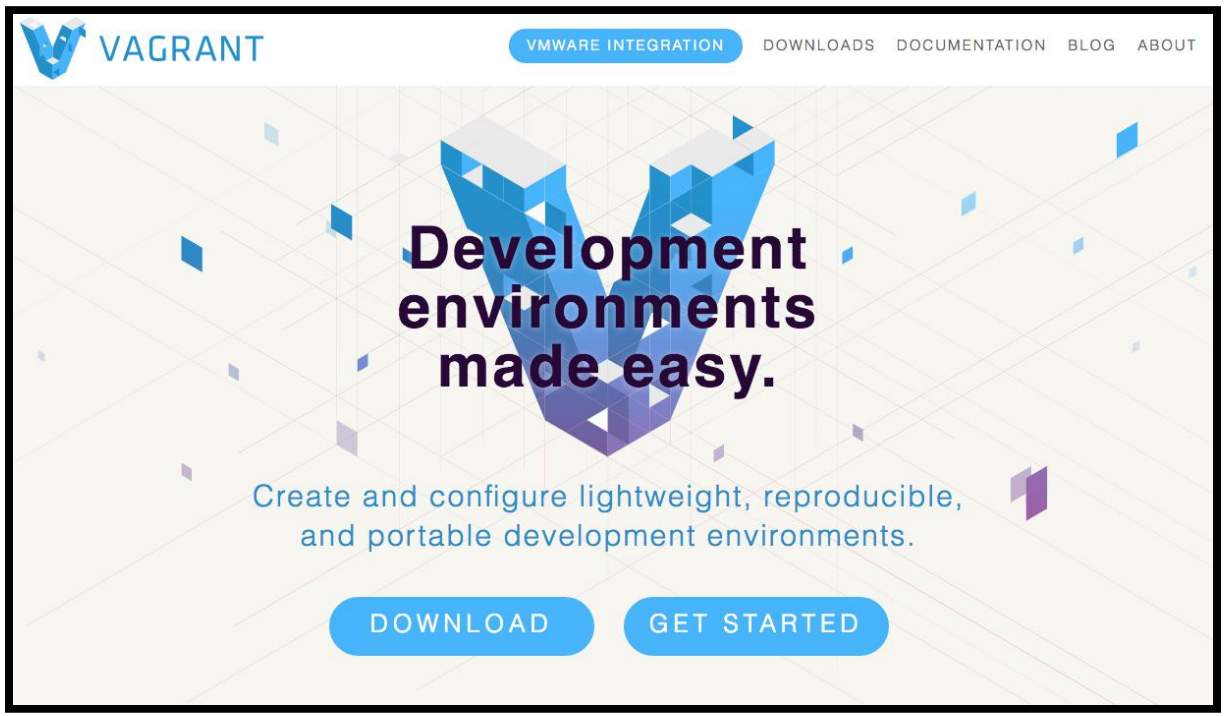
Benefits

- Consistent environment user to user
- Single target for course materials
- Faster provisioning for new workshops
- Repeatable course to course

Features

- Python
- R and R Studio
- Jupyter Notebook Server
- Example Notebooks
- Accessible from web browser

Vagrant


VAGRANT
VMWARE INTEGRATION
DOWNLOADS
DOCUMENTATION
BLOG
ABOUT
Development environments made easy.
Create and configure lightweight, reproducible, and portable development environments.
DOWNLOAD
GET STARTED

Create and configure lightweight, **reproducible**, and portable development environments.

Usage

- Easy installation through binary package
- Flexible configuration via **text-based configuration file**
- Single command: `vagrant up`

Ansible

"Automation engine" for provisioning and configuration management.

Provisioning

"Installation!"

Configuration Management

"Establish and maintain **consistency** of an environment."

Provisioning

- Anaconda
- Python & R
- Software packages
- Jupyter Notebooks
- etc.

Configuration

- Start Jupyter notebook server
- Set environment variables
- Set default login directory

Anaconda

ANACONDA
Leading Open Data Science Platform
Powered by Python

ANACONDA MAKES...

DATA SCIENCE TEAMS HAPPIER

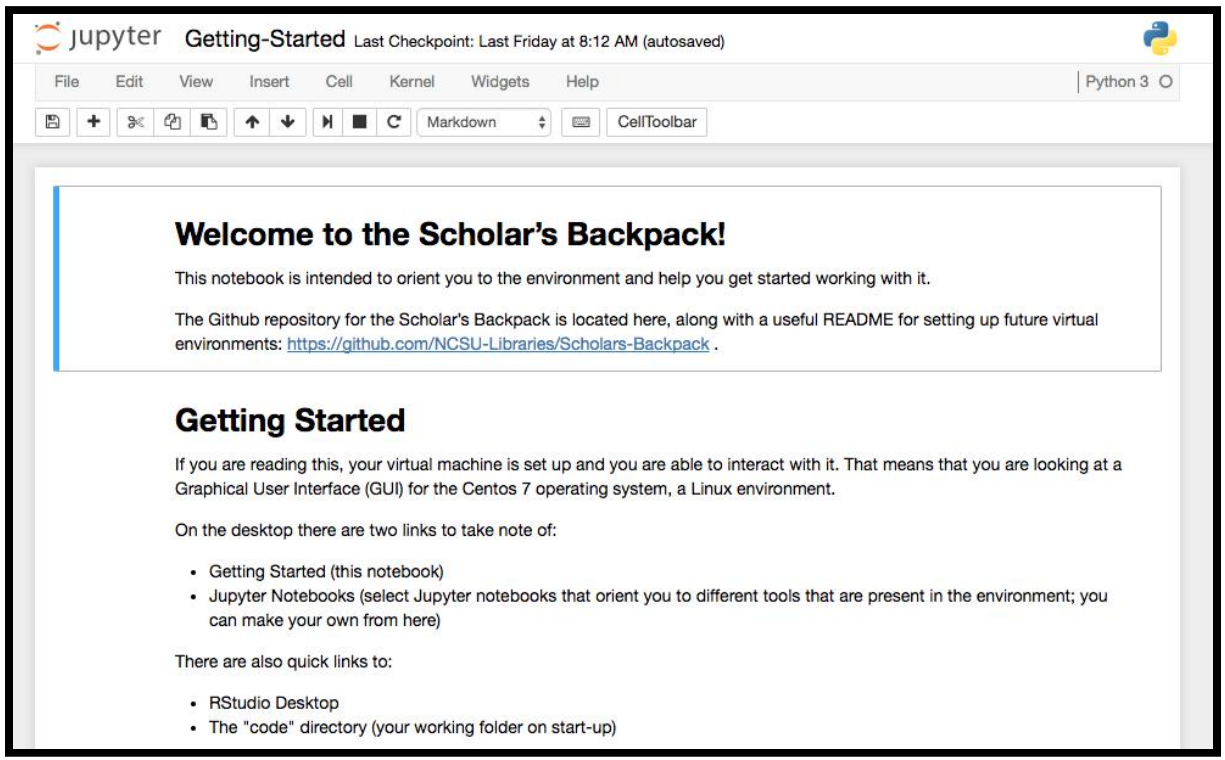
That means better and more results

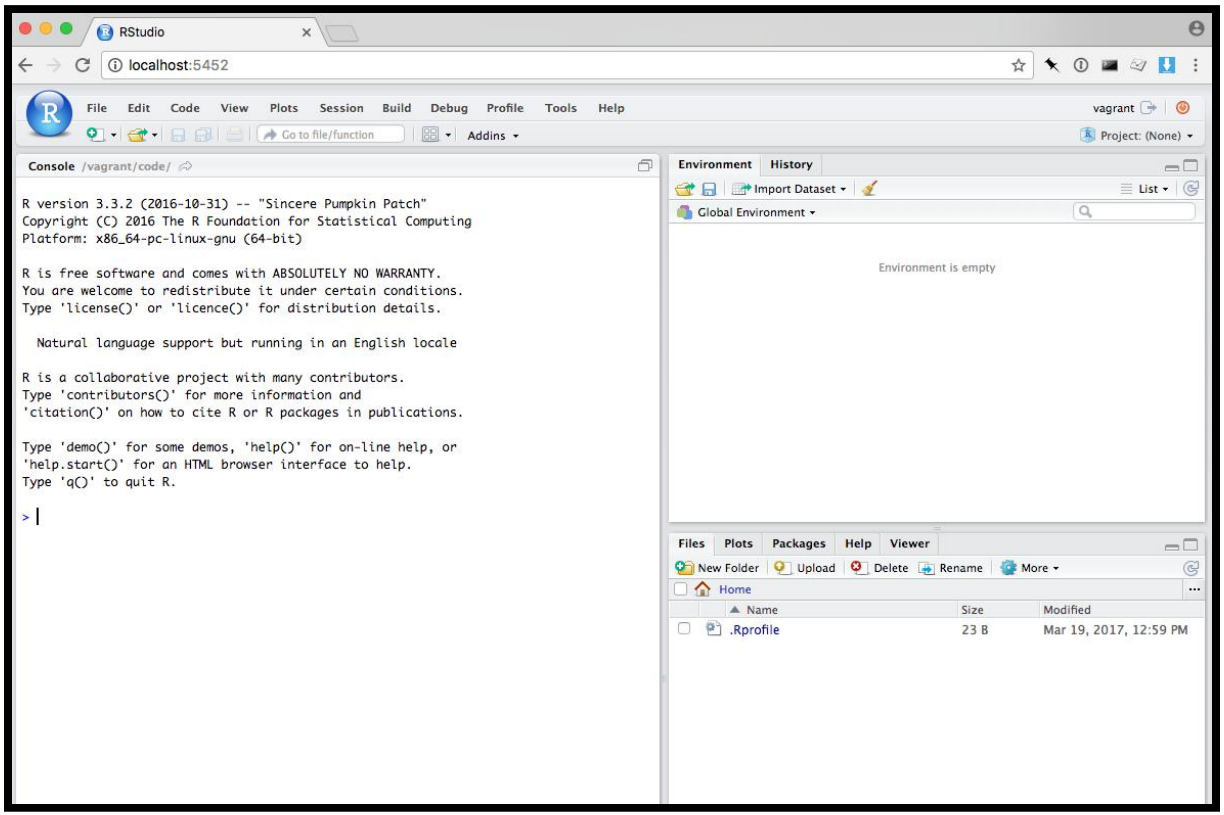
Python Packages

astropy, beautifulsoup4, conda, flask, jupyter, matplotlib, numpy, nltk, pandas, pillow, pip, pytest, qt, requests, scipy, scikit-learn, seaborn, sqlite, etc.

R Packages

r, essentials, formatr, ggplot2, irkernel, knitr, kernsmooth, maps, markdown, mass, matrix, nnet, rbokeh, recommended, spatial, tidyr, etc.


jupyter Getting-Started Last Checkpoint: Last Friday at 8:12 AM (autosaved)
File Edit View Insert Cell Kernel Widgets Help
Python 3
Markdown
CellToolbar
Welcome to the Scholar's Backpack!
This notebook is intended to orient you to the environment and help you get started working with it.
The Github repository for the Scholar's Backpack is located here, along with a useful README for setting up future virtual environments: https://github.com/NCSU-Libraries/Scholars-Backpack .
Getting Started
If you are reading this, your virtual machine is set up and you are able to interact with it. That means that you are looking at a Graphical User Interface (GUI) for the Centos 7 operating system, a Linux environment.
On the desktop there are two links to take note of:
Getting Started (this notebook)
Jupyter Notebooks (select Jupyter notebooks that orient you to different tools that are present in the environment; you can make your own from here)
There are also quick links to:
RStudio Desktop
The "code" directory (your working folder on start-up)


RStudio
localhost:5452
File Edit Code View Plots Session Build Debug Profile Tools Help
vagrant
Go to file/function
Addins
Project: (None)
Console /vagrant/code/
R version 3.3.2 (2016-10-31) -- "Sincere Pumpkin Patch"
Copyright (C) 2016 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)
R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.
Natural language support but running in an English locale
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.
>
Environment History
Import Dataset
List
Global Environment
Environment is empty
Files Plots Packages Help Viewer
New Folder
Upload
Delete
Rename
More
Home
Name
Size
Modified
.Rprofile
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Mar 19, 2017, 12:59 PM

Future Work

- Docker containers for portability
- Embedded use in curriculum
- Additional open source contributions

Summary

Open Science represents a new framework for research and provides an opportunity for libraries to engage researchers in new ways.

NCSU Libraries has done workshops and outreach around this framework and there is evidence of strong interest across disciplines.

We are redeploying existing technical resources and cutting edge technology in ways that used to be difficult or impossible.

This approach has helped us identify a new leadership role for libraries in open research support.

Thanks!

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github.com/NCSU-Libraries/scholars-backpack

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