Open science: How libraries can support modern research practice

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Supporting the modern research skillset: The summer of open science

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NCSU Libraries

bretdavidson.github.io/dlf-2016

Agenda

- Open science as problem space
- Open science as modern research practice
- Open science at NC State
- Vagrant, Ansible, & Python

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."

Only **6 out of 53** "landmark" cancer studies could be reproduced.

Nature, www.nature.com/nature/journal/v483/n7391/full/483531a.html

How Science Goes Wrong

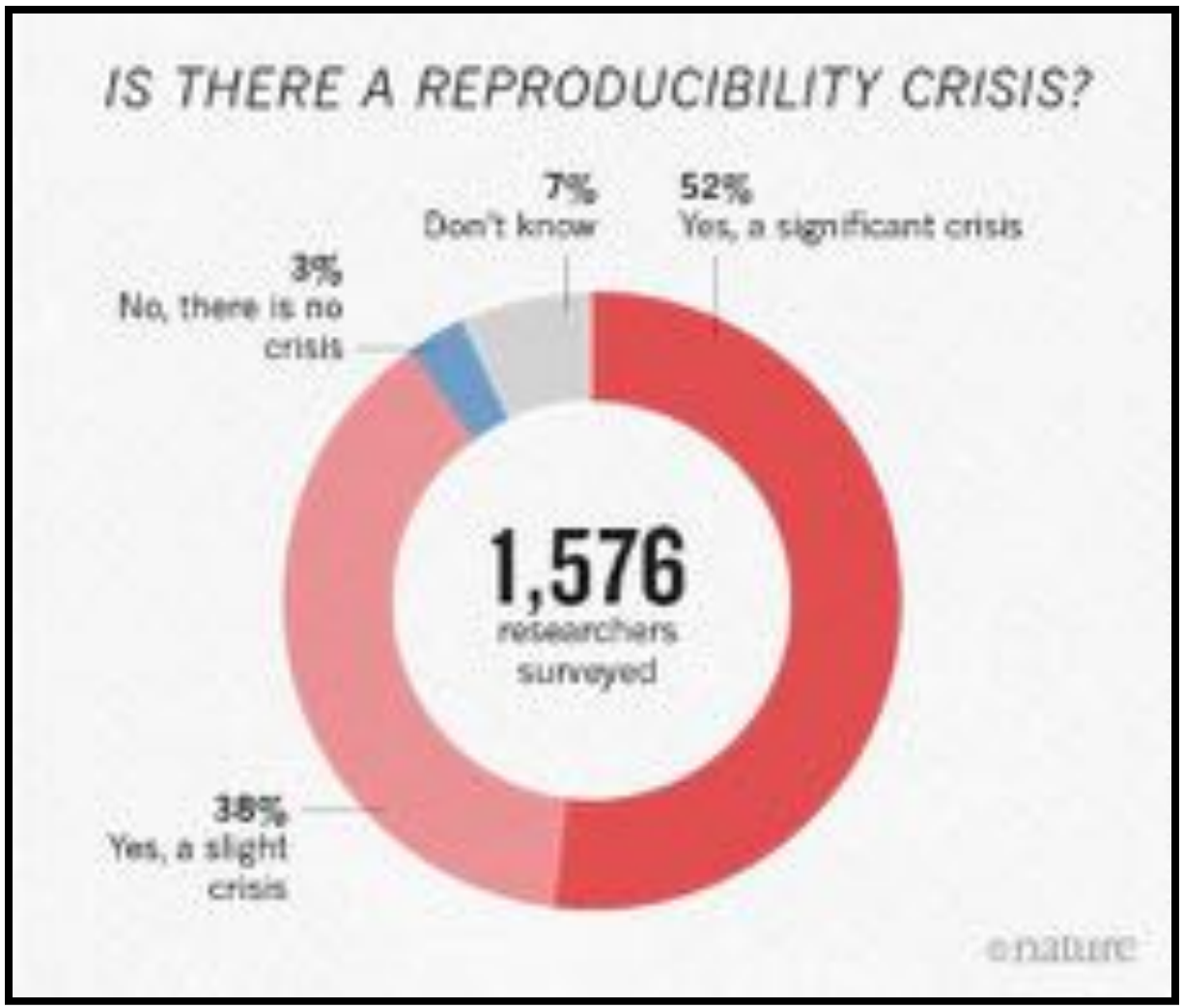
"Too much trusting, not enough verifying."

Economist, www.economist.com/news/leaders/21588069-scientific-research-has-changed-world-now-it-needs-change-itself-how-science-goes-wrong

Reproducibility Crisis

Empirical estimates suggest most published medical research is true.

arXiv, arxiv.org/abs/1301.3718



Nature, www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970

Open Science can increase reproducibility.

What is Open Science?

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

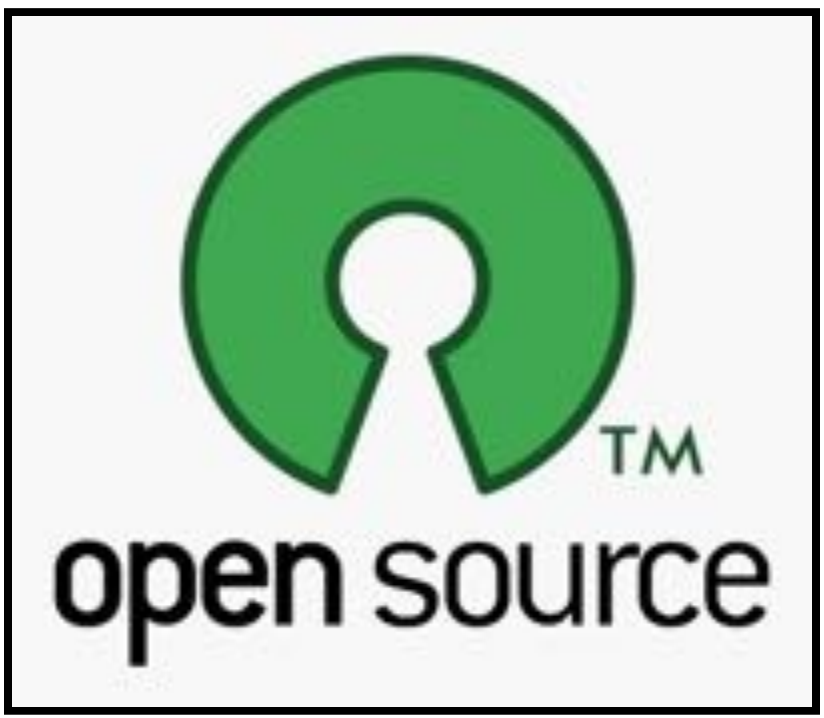
Open Science is a return to first principles of scientific practice.

Open practices require new skillsets.

The way that research is carried out.

The way that research is disseminated.

How digital technologies are affecting the practice of science.


TM
open source


open science

Paul David

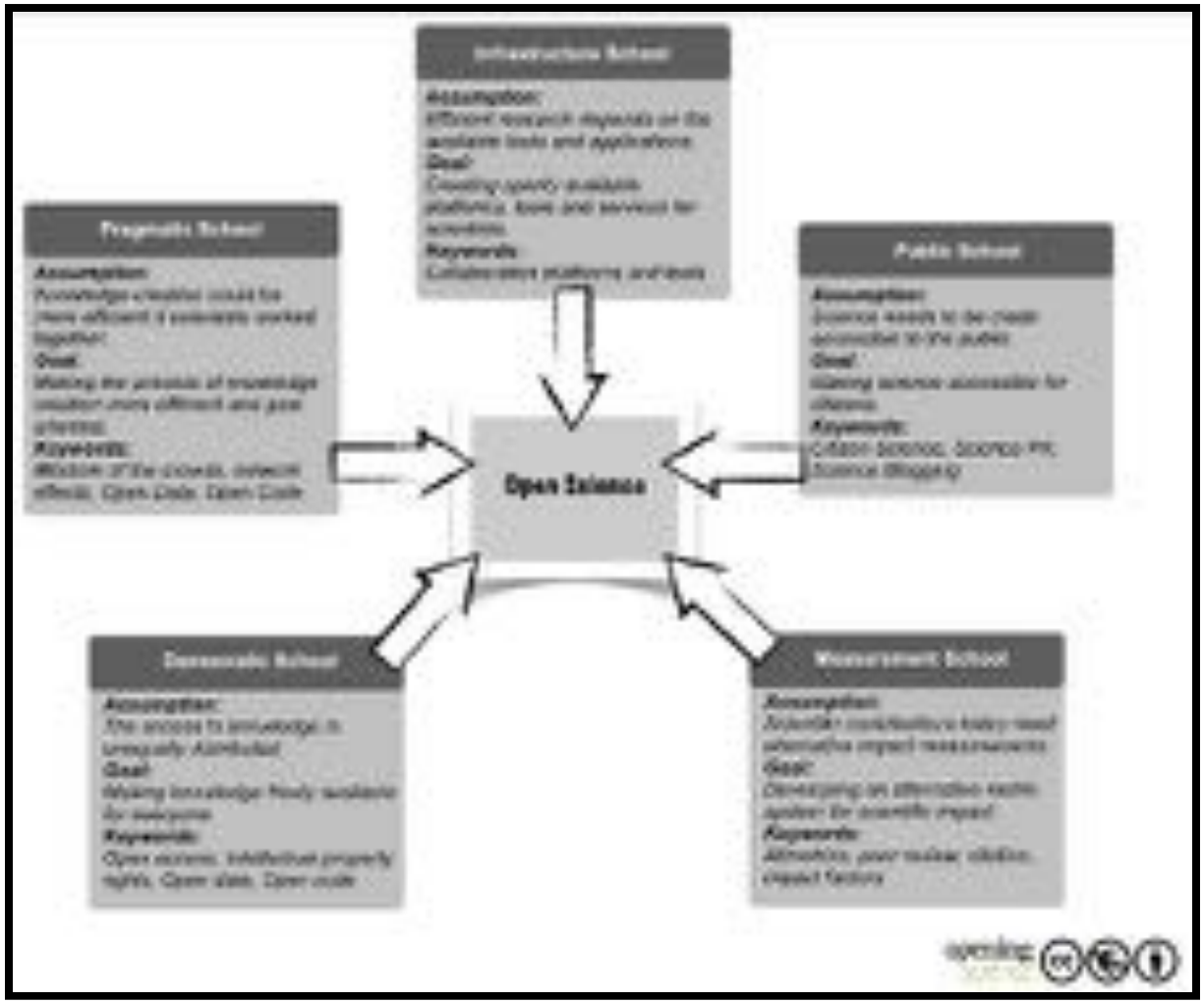
Economist / Historian

The Knowledge Economy

Five schools of thought

by Sönke Bartling & Sascha Friesike

Editors, http://book.openingscience.org/



The Five Schools of Thought

Infrastructure

tech. architecture

Public

accessibility of knowledge creation + citizen science

Measurement

alt. impact measurement

Democratic

access to knowledge

Pragmatic

collaborative research

Recent Events


REUTERS
In cancer science, many "discoveries" don't hold up

Is the evidence for austerity based on an Excel spreadsheet error?

THE CONVERSATION

Students Reveal How They Broke the Lead Contamination Case in Flint, Mich.


F1000Research
Open drug discovery for the Zika virus [version 1; referees awaiting peer review]
Abstract
Open Peer Review

Why Libraries?

Aligns with core library values

- information access
- peer review
- community-based knowledge creation
- the preservation and dissemination of research

Libraries are champions of open source

Libraries

are about

supporting their users

Academic Libraries

are about

supporting research practice

Ongoing disruption by digital technologies in modern research practice

Hypothetical Open Science Workflow

101 Innovations in Scholarly Communication,
https://innoscholcomm.silk.co/

Policy Shifts in support of open

Ecosystem of Support for Modern Research Practice at NCSU Libraries

Research Support

Ask Us

CHANCELLOR'S FACULTY EXCELLENCE PROGRAM

SUBJECT SPECIALISTS


Visualization Workshops
NOV
18
DEC
2
DEC
2
DEC
5

Makerspace

D. H. HILL LIBRARY

A D + T creation and collaboration space

JAMES B. HUNT JR. LIBRARY

3D Printing services and more


WOLFPACK
CITIZEN
SCIENCE
CHALLENGE

The NCSU Libraries' **Open Science Initiative**

Goals

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

We took a non-prescriptive **user-centered** approach.

Creating opportunities for communication.

Open Science Unconference

Follow-up Informal Interviews

Modern Research Skills Gap
Insufficient Incentives


NCSU LIBRARIES
SUMMER of OPEN SCIENCE


Summer of Open Science Event Series
SUMMER
OPEN SCIENCE

Goals

- Support modern research practice through 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

Tools

- Open source software
- Virtual machines

The Planning Team

(Representation from Digital Library Initiatives, Makerspace, Research & Information Services, Libraries Fellows)

- **Ekatarina [Eka] Grguric (Project Lead)**
- **Lauren Di Monte (Project Manager)**
- **Alison Blaine (Content Development)**
- **Bret Davidson (Technical Lead)**
- **Jennifer Garrett (Community Development)**

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

Workshop Goals

- Skills for introductory-level users
- Hands-on practice
- Provide resources and opportunities for going deeper

Workshop Structure

- Brief presentation with contextual overview
- Activities
- Roving instruction support and live demo from instructor
- Instruction handouts to allow for work at own pace

Introduction to the Command Line Interface

Definitions

go.ncsu.edu/...

In-Workshop Logistics

- Shared materials folder on Google Drive
- Laptops provided via a laptop cart
- Evaluation forms for feedback
- At least 2 instructors

Instructors

Brittany Johnson

Eka Grguric

Lauren DiMonte

Alison Blaine

Madison Sullivan

Will Cross

Todd Stuffer

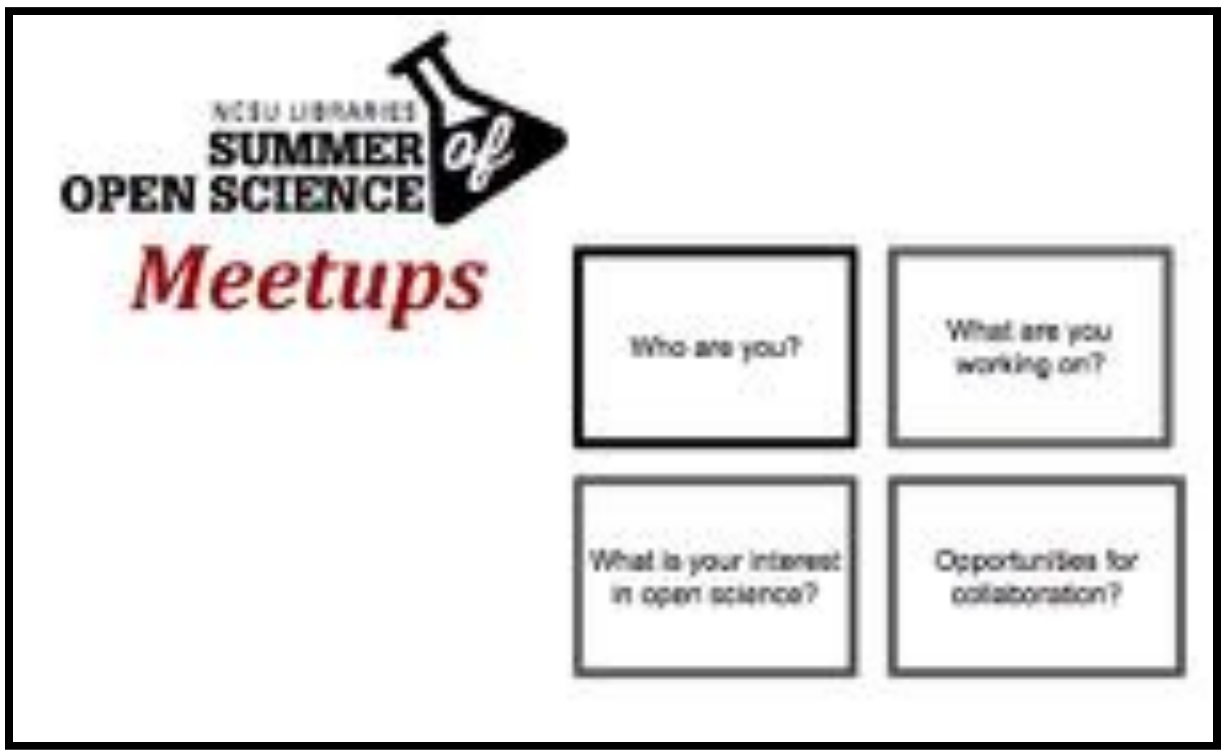
Marketing

- Slide on library front page linking to event website with logo
- Emails to various listservs
- E-board advertisements on campus
- Press release

Scientific Computing with Python & Raspberry Pi:

40 person waitlist

Meetups



- Monthly informal networking and discussion
- Held at a coffee shop on campus
- Rich conversations, although small numbers

Final Showcase

- Food & mingling
- Lightning talks
  - Agriculture and Accidents: Digital Learning in Summer 2016
  - Modeling Individual Developer Concept Knowledge Using Public Git Repositories
  - SciBridge: Bringing together African and U.S. scientists

Takeaways

Interdisciplinary Need:
over 40 departments across ~16 colleges

Takeaways

- "Open Science" attracted non-scientists as well as scientists
- High demand for introductory coding skills (Python)
- Interest among graduate students for opportunities for interdisciplinary research sharing
- Summer presents interesting opportunities and challenges

Web Scraping with Python

Technical workshops are ripe for disaster.

What could go wrong?

- OS images reset overnight
- Improper permissions
- Network connectivity issues
- Python 2 vs Python 3
- Missing packages

This is not theoretical!

Image courtesy of Tumblr, animisensa

Instructor Challenges

- Consistency across user environments
- Consistency of course materials
- Time to provision computing environments
- Ease of collaboration

Student Challenges

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

Many Options

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

Our Approach

- Vagrant for managing OS
- Ansible for provisioning and configuration
- Course or lab specific packages and 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!

github.com/NCSU-Libraries/python-vagrant

Benefits

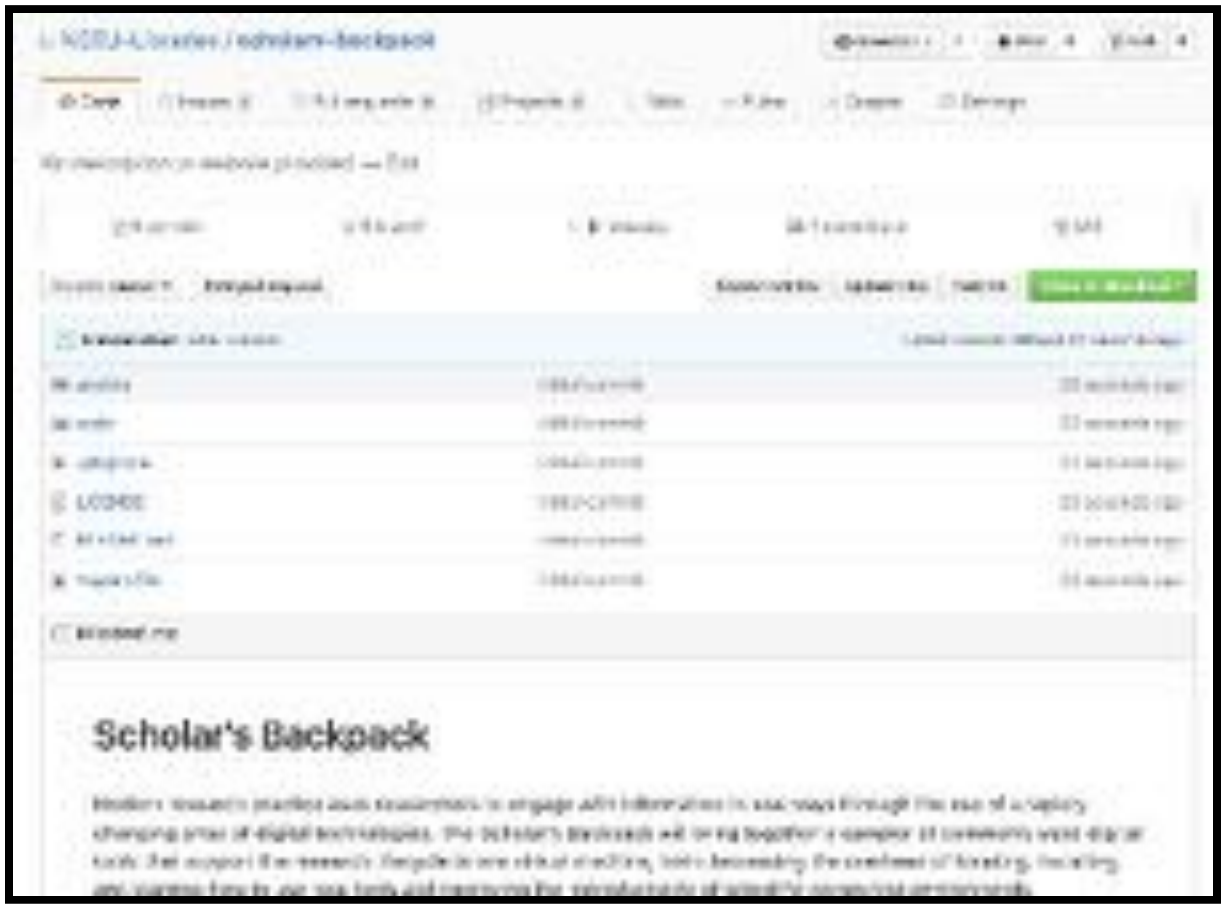
- Consistent environment user to user
- Single target for course materials
- Faster provisioniong for new workshops
- Reproducible

Rise of Scholarly Code

Researcher Challenges

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

github.com/NCSU-Libraries/scholars-backpack



Features

- Python 3
- Jupyter Notebook Server
- R and R Studio
- Example Notebooks

Benefits

- Decrease overhead
- Improve reproducibility
- Encourage collaboration

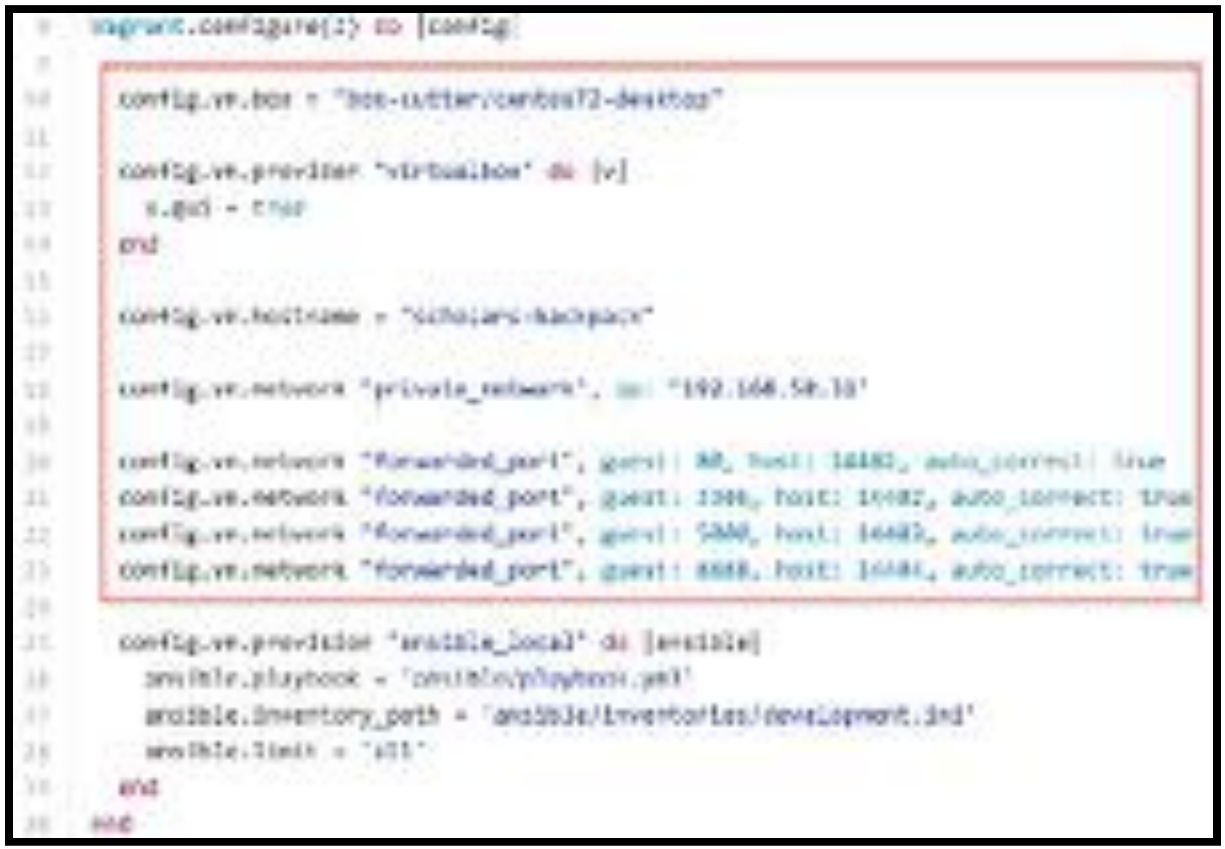
Vagrant


VAGRANT
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 file**.
- Single command: `vagrant up`


Vagrant.configure(2) do |config|
config.vm.box = "box-cutter/centos72-desktop"
config.vm.provider "virtualbox" do |v|
v.gui = true
end
config.vm.hostname = "scholars-backpack"
config.vm.network "private_network", ip: "192.168.50.10"
config.vm.network "forwarded_port", guest: 80, host: 10101, auto_correct: true
config.vm.network "forwarded_port", guest: 3306, host: 10102, auto_correct: true
config.vm.network "forwarded_port", guest: 5000, host: 10103, auto_correct: true
config.vm.network "forwarded_port", guest: 8888, host: 10104, auto_correct: true
config.vm.provision "ansible_local" do |ansible|
ansible.playbook = 'ansible/playbook.yml'
ansible.inventory_path = 'ansible/inventories/development.ini'
ansible.limit = 'all'
end
end


Vagrant.configure(2) do |config|
config.vm.box = "bento/centos72-desktop"
config.vm.provider "virtualbox" do |v|
v.gui = true
end
config.vm.hostname = "scholars-backpack"
config.vm.network "private_network", ip: "192.168.50.10"
config.vm.network "forwarded_port", guest: 80, host: 18181, auto_correct: true
config.vm.network "forwarded_port", guest: 3306, host: 13307, auto_correct: true
config.vm.network "forwarded_port", guest: 5000, host: 14481, auto_correct: true
config.vm.network "forwarded_port", guest: 8888, host: 14181, auto_correct: true
config.vm.provision "ansible_local" do |ansible|
ansible.playbook = 'ansible/playbook.yml'
ansible.inventory_path = 'ansible/inventories/development.ini'
ansible.limit = 'all'
end
end

Ansible

"Automation engine" for provisioning and configuration management.

Provisioning

"To make something available."

Installation!

Configuration Management

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

playbook.yml

```yaml
---
- hosts: scholars-backpack
  gather_facts: yes
  become: yes
  become_method: sudo
  become_user: root
  vars:
    project_name: "scholars-backback"
  roles:
    - role: basic-setup
    - role: python
    - role: jupyter
    - role: r
    - role: desktop
  handlers:
    - include: handlers/handlers.yml
```

```yaml
---
- name: install epel-release
  yum:
    name: epel-release
    state: present
- name: install required packages using yum
  yum:
    pkg: "{{item}}"
    state: present
    update_cache: yes
  with_items:
    - firefox
    - git-core
    - vim
    - curl
```

```
50  - name: set default vagrant ssh directory
51    lineinfile: dest=/home/vagrant/.bashrc line="cd /vagrant/code"
52    tags:
53      - set_default_dir
54  - name: set $DISPLAY environment variable
55    lineinfile: dest=/home/vagrant/.bashrc line="export DISPLAY=:0.0"
```

Future Work

Richer Environment

- Broader scientific computing
- Improved adherance to best practices
- Docker containers for portability

Embedded Use

- Curricular use
- Laboratory use

Summary

Emphasis on reproducibility has ignited a shift toward new practices.

With these new practices come new requirements for researchers.

Reproducible and portable computing environments are critical for future success.

Tools like Vagrant and Ansible can help researchers develop the scientific environments they need to be productive.

Thanks!

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github.com/NCSU-Libraries/scholars-backpack