Computational Husbandry

Seth Russell - seth.russell@cuanschutz.edu

Peter DeWitt - peter.dewitt@cuanschutz.edu

SOM, Dept of Biomedical Informatics

Presentations: https://github.com/magic-lantern/Computational-Husbandry-2022

Survey: https://forms.gle/ZumeuAiWRm83ra9h9

Computational Husbandry

- Husbandry
- Homesteading
- Permaculture

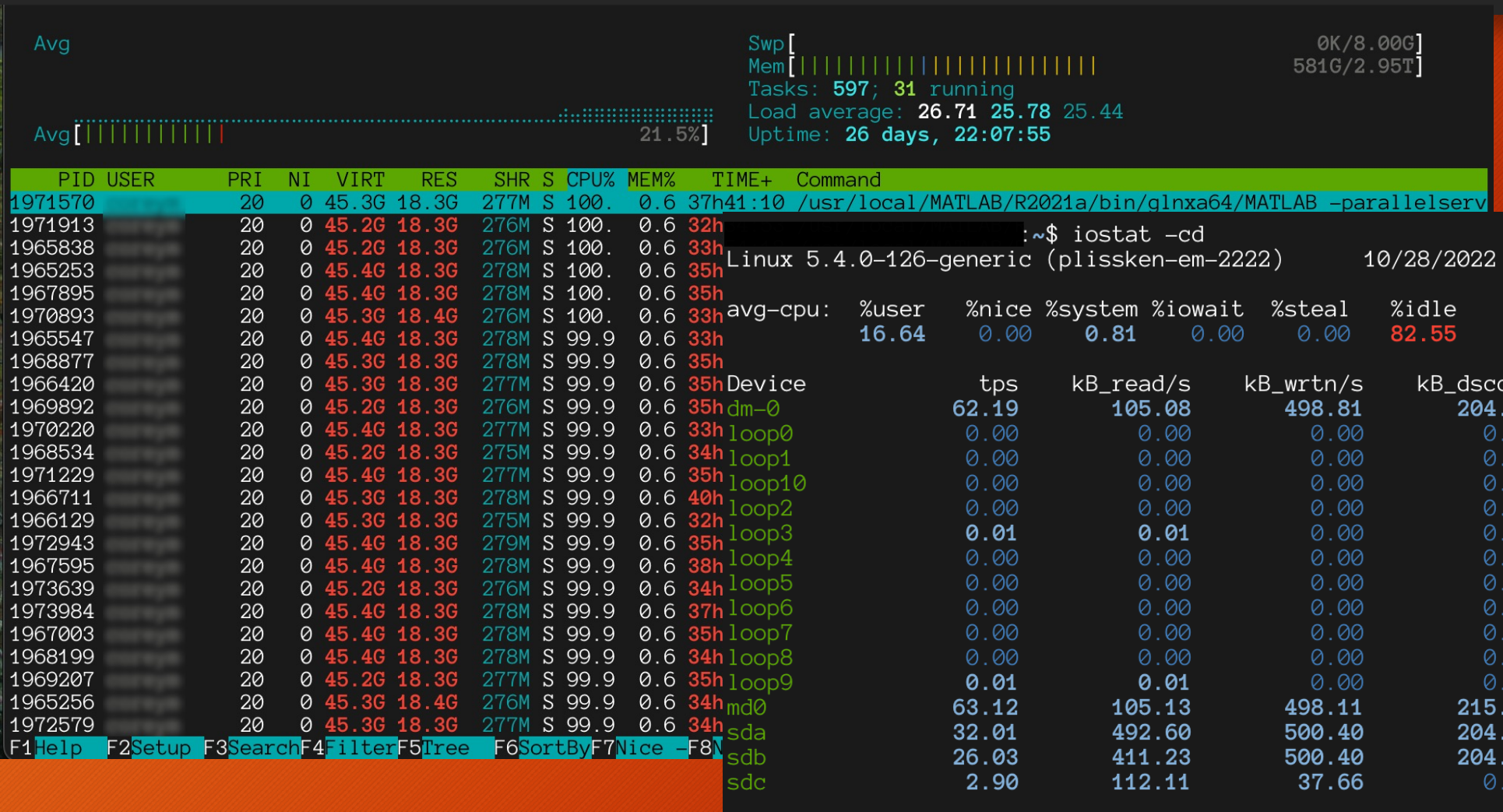
Computing Resources

- CPU – Central Processing Unit
- RAM – Random Access Memory
- Persistent Storage – Hard Disk, Solid State Drive
- GPU – Graphics Processing Unit
- Network – Communication to other machines (storage, data, programs, etc).
- Software
- Data

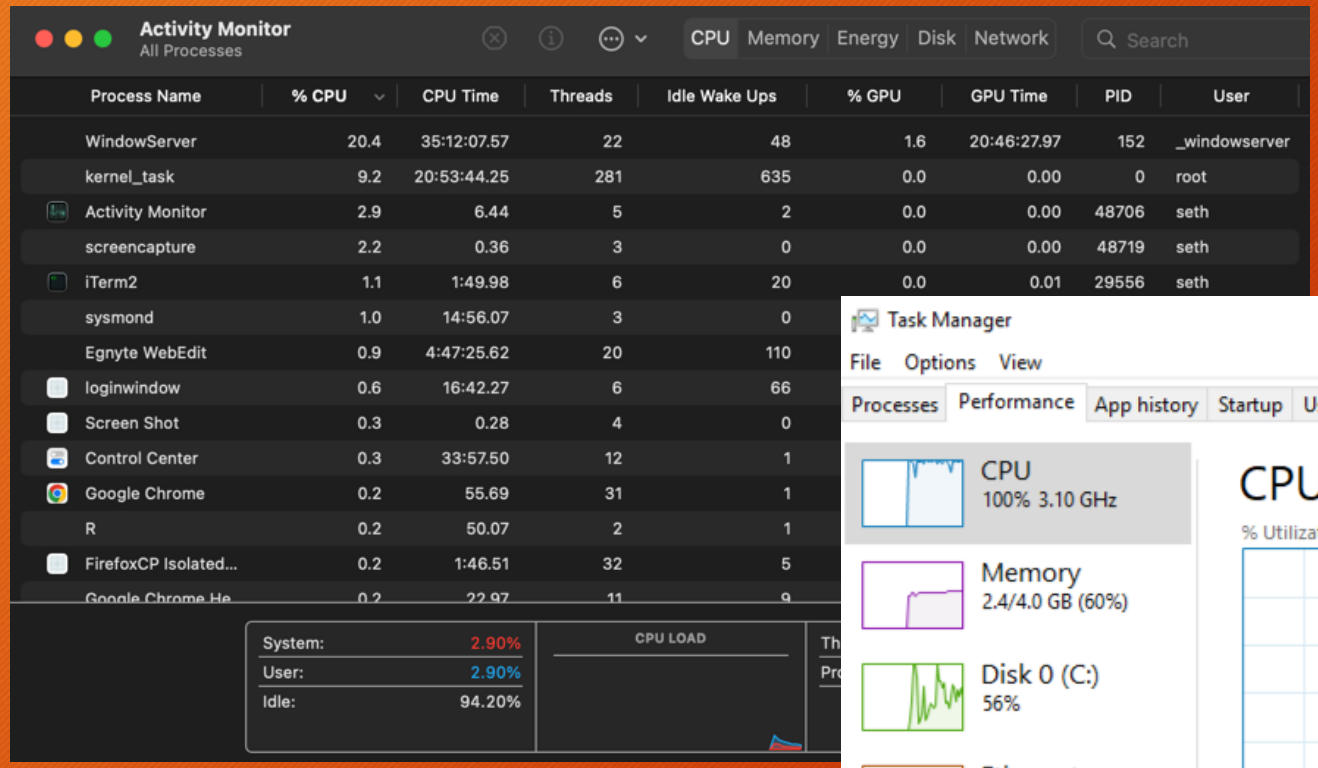
Computing Resources

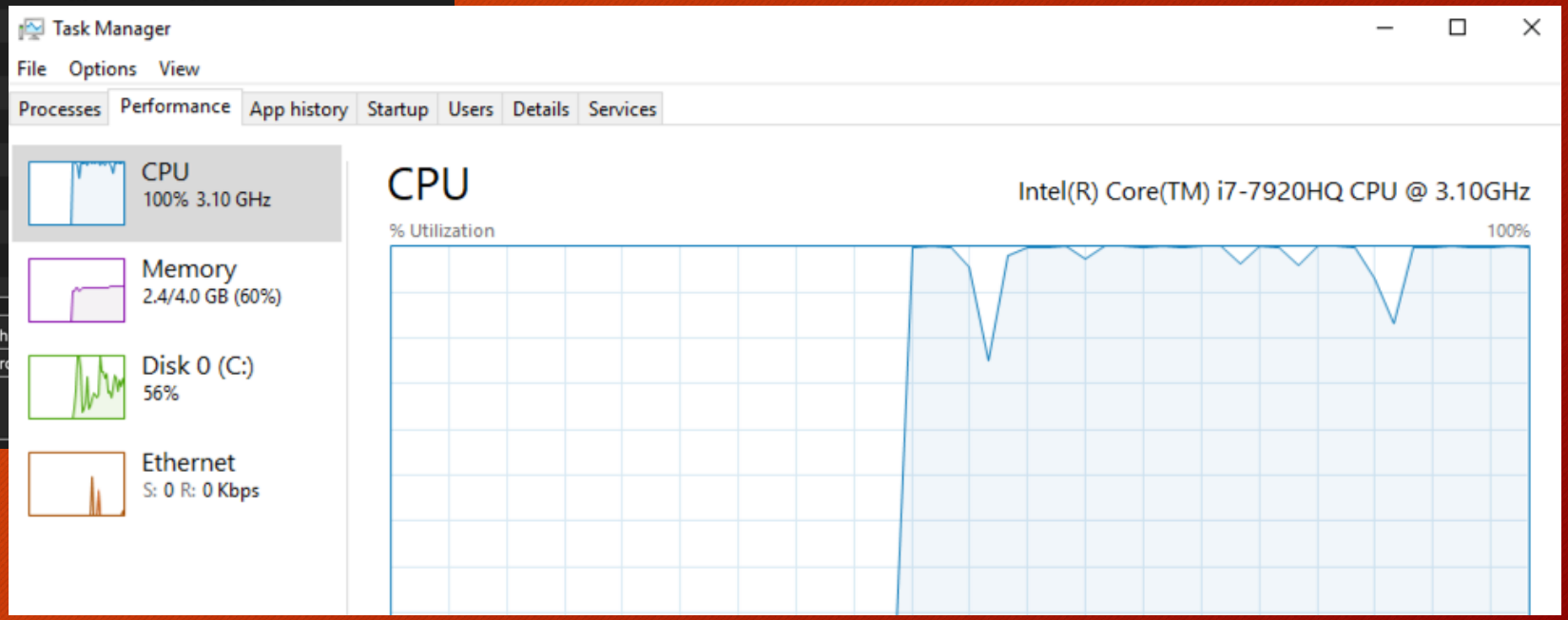
- The Operating System is the main program controlling access to and allocation of these resources. All of these are shared by all users and running programs on a system.
- The slowest/most limited resource involved controls the maximum throughput of the system.
- Networking interfaces allow the sharing of all computing resources among many people and many programs.
  - Network computing increases the complexity of software development

Measure twice, cut once



Measure twice, cut once





Computer Hardware vs the Human Brain

Line endings – aka “I've got a blank space, baby”

- MS-DOS used the two-character combination of **CRLF** to denote line endings in files, and modern Windows computers continue to use **CRLF** as their line ending to this day. Meanwhile, from its very inception, Unix used **LF** to denote line endings, ditching CRLF for consistency and simplicity. Apple originally used only **CR** for Mac Classic but eventually switched to **LF** for OS X, consistent with Unix. https://www.aleksandrhovhannisyan.com/blog/crlf-vs-lf-normalizing-line-endings-in-git/

Floating point representations vs Math

```
✓ (1/3)+(1/3)+(1/3) == 1 ···
··· True
```

```
✓ 1/10 + 1/10 + 1/10 == 3/10 ···
··· False
```

```
✓ (0.1 + 0.1 + 0.1) == 0.3 ···
··· False
```

```
✓ 0.1 + 0.1 + 0.1 ···
··· 0.30000000000000004
```

```
✓ from decimal import * ···

✓ Decimal('0.1') + Decimal('0.1') + Decimal('0.1') ···
··· Decimal('0.3')
```

```
✓ Decimal('0.1') + Decimal('0.1') + Decimal('0.1') == Decimal('0.3') ·
··· True
```

Floating point representations vs Math

https://0.30000000000000004.com/

Java	`System.out.println(.1 + .2);`	`0.30000000000000004`
	AND	AND
	`System.out.println(.1F + .2F);`	`0.3`

Java has built-in support for arbitrary-precision numbers using the BigDecimal class.

JavaScript	`console.log(.1 + .2);`	`0.30000000000000004`

The decimal.js library provides an arbitrary-precision Decimal type for JavaScript.

Julia	`.1 + .2`	`0.30000000000000004`

Julia has built-in rational numbers support and also a built-in arbitrary-precision BigFloat data type. To get the math right, `1//10 + 2//10` returns `3//10`.

K (Kona)	`0.1 + 0.2`	`0.3`

Kotlin	`println(.1 + .2)`	`0.30000000000000004`
	AND	AND
	`println(.1F + .2F)`	`0.3`

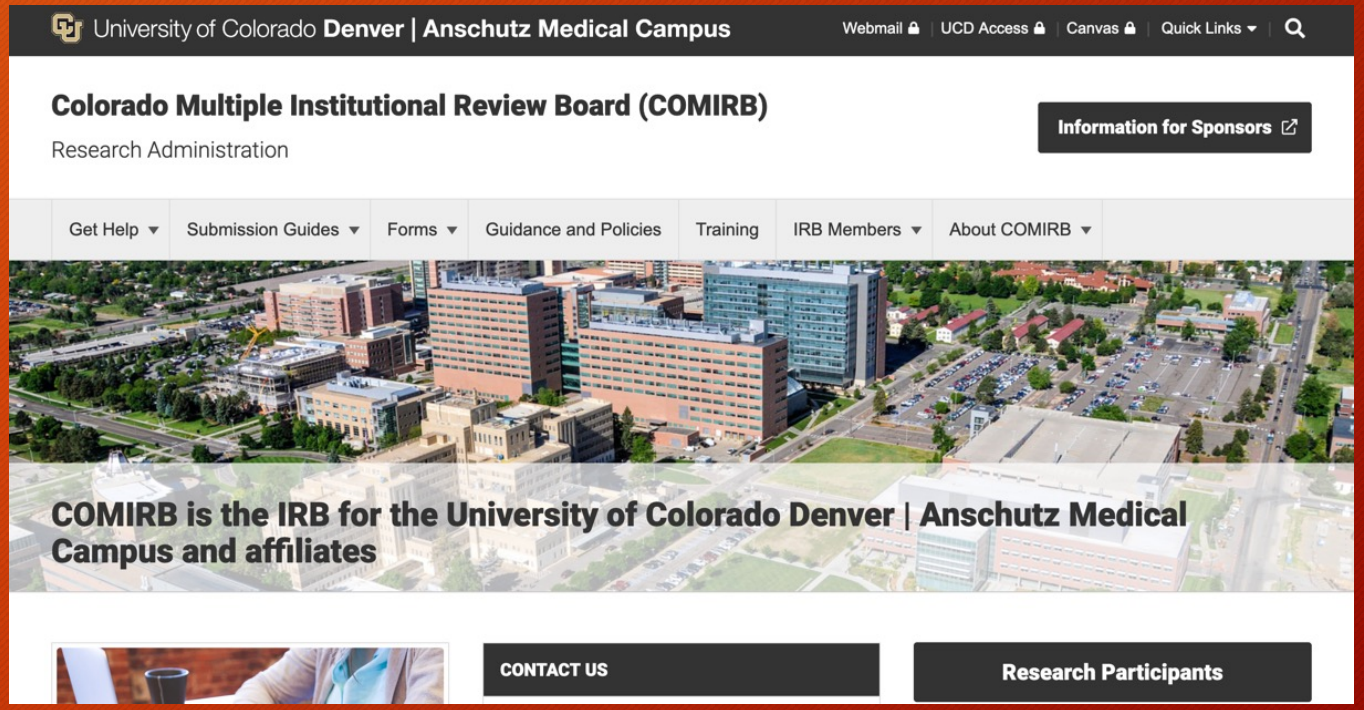
See Reference documentation.

Status check

https://cups.fast.ai/computationalhusbandry

Working with health care data

- Data Use Agreements
- Institutional Review Boards

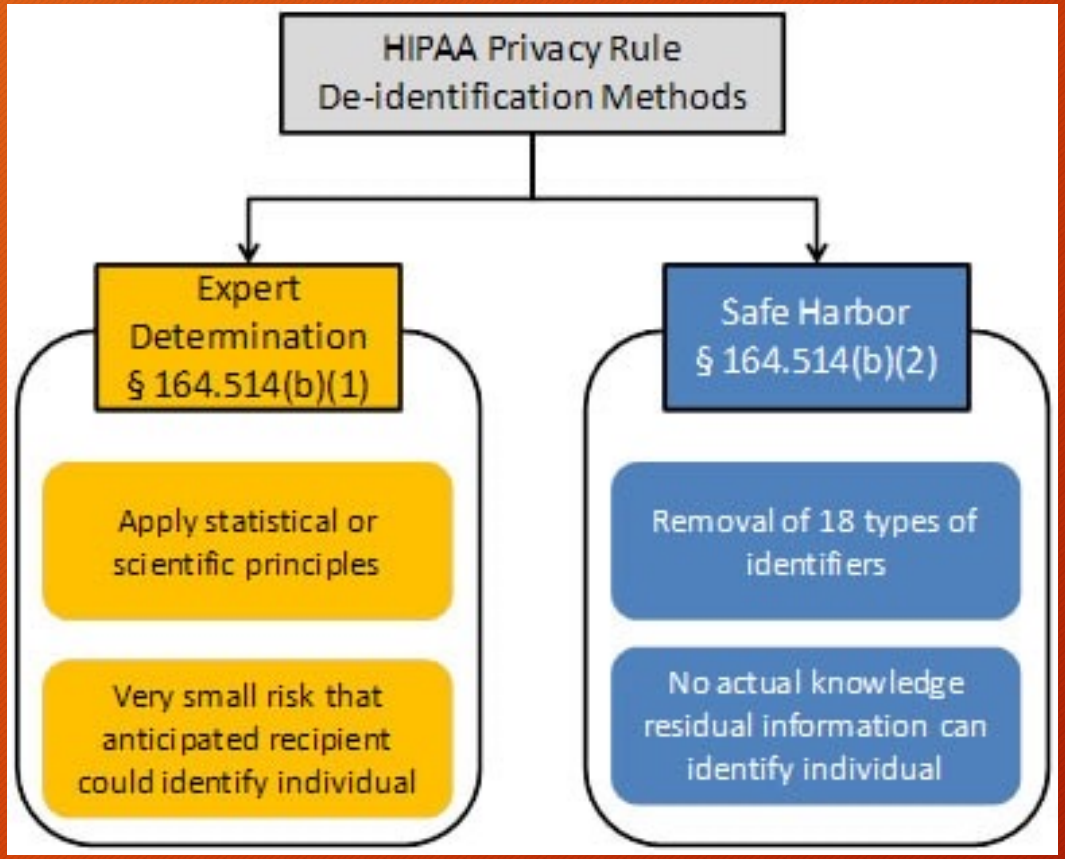


https://research.cuanschutz.edu/regulatory-compliance/home/hipaa/data-use-agreement
https://research.cuanschutz.edu/regulatory-compliance/home/hipaa/data-sharing

Working with health care data

- Health Insurance Portability and Accountability Act (HIPAA) Privacy Rule
- https://www.hhs.gov/hipaa/for-professionals/privacy/special-topics/de-identification/index.html#standard
- Protected health information is information, including demographic information, which relates to:
  - the individual's past, present, or future physical or mental health or condition,
  - the provision of health care to the individual, or
  - the past, present, or future payment for the provision of health care to the individual…

Working with health care data



Working with health care data

Safe Harbor method: Remove all of the following

(A) Names

(B) All geographic subdivisions smaller than a state, … except for the initial three digits of the ZIP code

(C) All elements of dates (except year) for dates that are directly related to an individual, including birth date, admission date, discharge date, death date, and all ages over 89 …

(D) Telephone numbers

(L) Vehicle identifiers and serial numbers, including license plate numbers

(E) Fax numbers

(M) Device identifiers and serial numbers

(F) Email addresses

(N) Web Universal Resource Locators (URLs)

(G) Social security numbers

(O) Internet Protocol (IP) addresses

(H) Medical record numbers

(P) Biometric identifiers, including finger and voice prints

(I) Health plan beneficiary numbers

(Q) Full-face photographs and any comparable images

(J) Account numbers

(R) Any other unique identifying number, characteristic, or code, except as permitted

(K) Certificate/license numbers

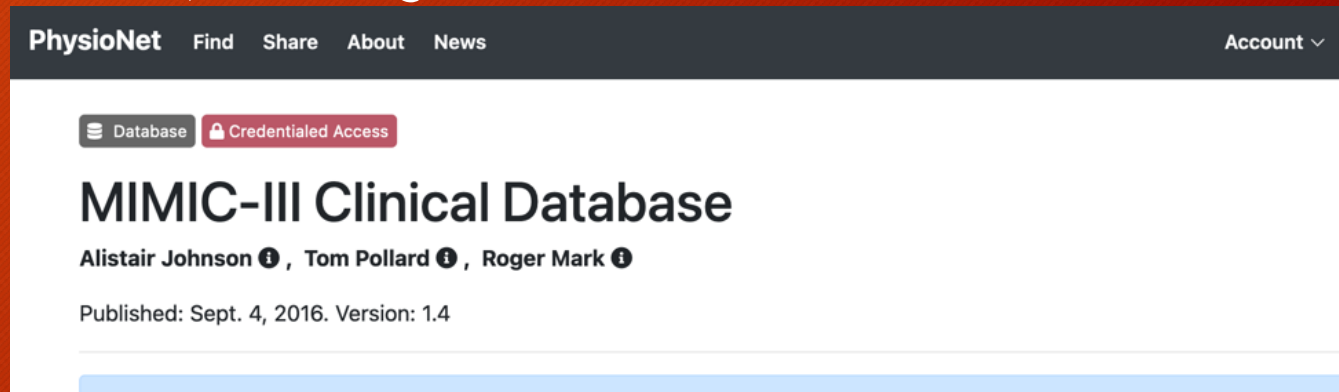
Working with health care data

Example dataset: https://physionet.org/content/mimiciii/

MIMIC-III integrates deidentified, comprehensive clinical data of patients admitted to the Beth Israel Deaconess Medical Center in Boston, Massachusetts, and makes it widely accessible to researchers internationally under a data use agreement. The open nature of the data allows clinical studies to be reproduced and improved in ways that would not otherwise be possible.

The MIMIC-III database was populated with data that had been acquired during routine hospital care, so there was no associated burden on caregivers and no interference with their workflow. Data was downloaded from several sources, including:

- archives from critical care information systems.
- hospital electronic health record databases.
- Social Security Administration Death Master File.



Working with Data – OS/Human Protections

- OS Protections
  - Firewalls
  - Access controls
  - User permissions
  - Group permissions

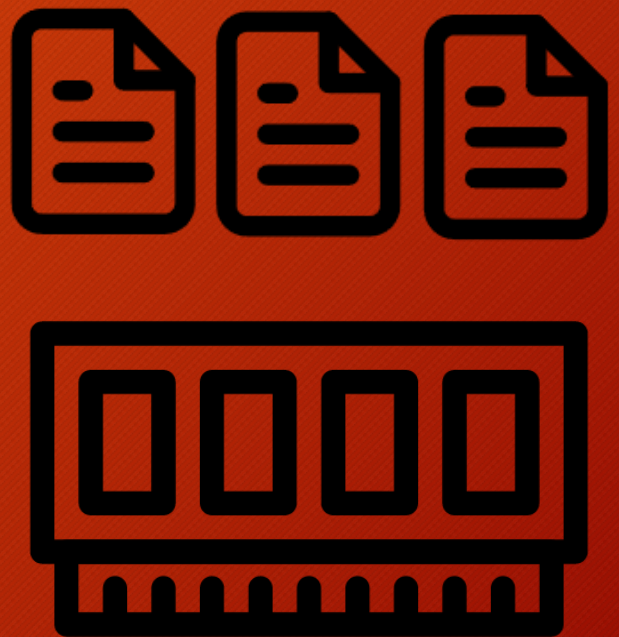
- Human Protections
  - Don’t reuse passwords
  - Don’t share passwords
  - Report problems ASAP
  - Don’t move data to other systems
  - Keep OS Software current
  - Run trusted software
  - Specific tasks are performed by specific people

Working with Data – Deep vs Shallow Copies

variable A = load_large_dataset()
B = A[colums 1 to 3]
C = A[columns 3 to 7]

A, B, C

A B C



Creating code that others can understand

I'm starting with the man in the mirror
I'm asking him to change his ways
And no message could've been any clearer
If they wanna make the world a better place
Take a look at yourself and then make a change

Glen Ballard and Siedah Garrett; Performed by Michael Jackson, Bad 1987

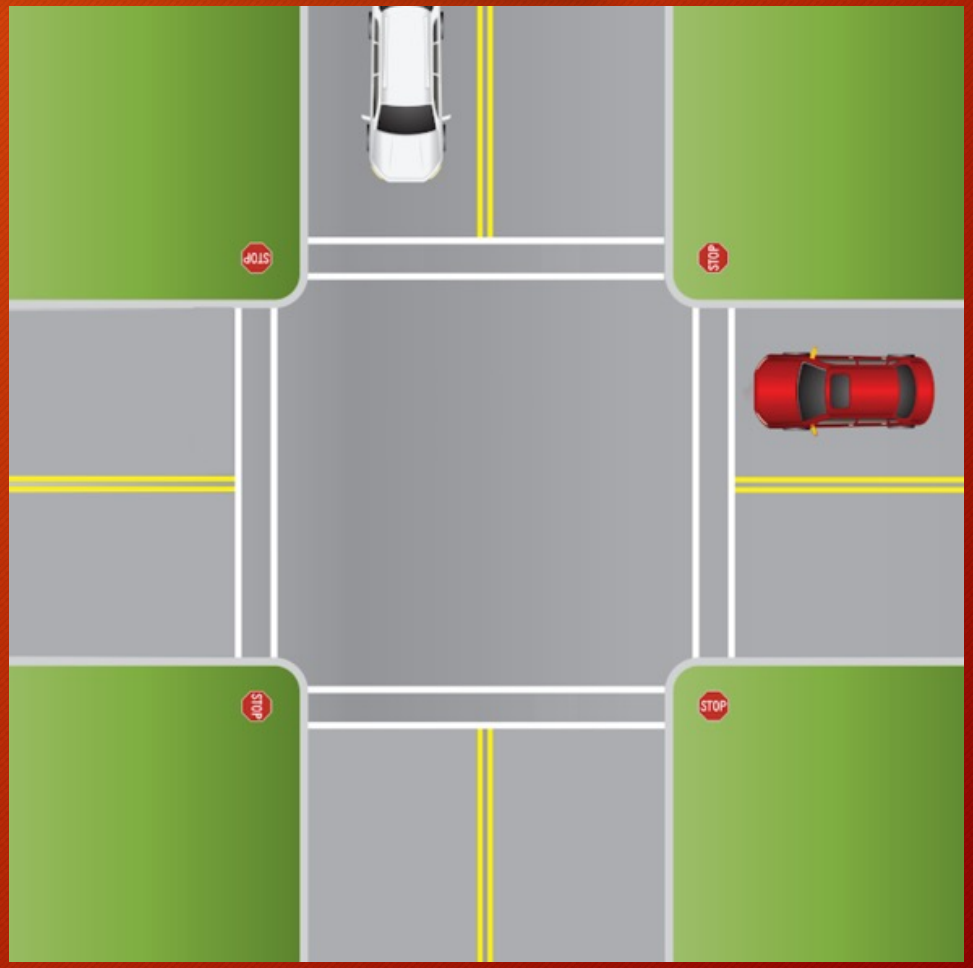
Status check

Close your browser window first if you still have it open

https://cups.fast.ai/computationalhusbandry

Project Organization

- Predictable behavior
- Versioning
- Backups
- How to build software/analysis pipeline



Project Naming Conventions

File and folder naming standards

1. Use lower case letters
2. Separate words with "_"

If the language or framework requires uppercase/camelcase or "-" separator, follow those requirements instead.

Over all structure and project specific standards should be as follows:

I. Create teams for all user groups at the Repository Level:
   a. Ex: Analytics Team, Informatics Team, teams for projects, grants, etc.
   b. All repositories for a specific team should start with the team name:
      i. EX: analytics_"project/grant name"
      ii. Use all lower case letters

II. Everyone that creates an account under the CUD2V Organization can set up a repository for their work as well, using the following naming convention:
      i. EX: name_project/grant

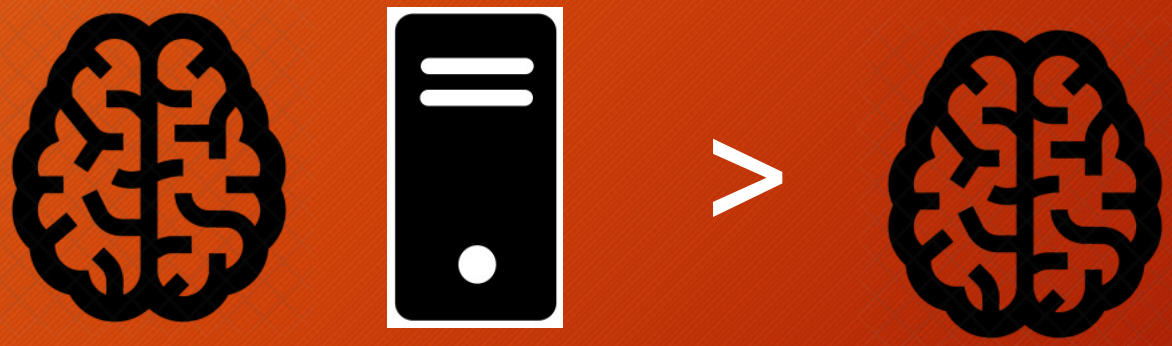
III. For each repository, follow a standard project structure. At a minimum, there needs to be:
      i. README.md
      ii. LICENSE (UC Denver Standard)
      iii. .gitignore

IV. If appropriate there should be THREE folders:
      1) Documentation
         - If documentation is not stored in the repository, a README.md file should indicate where the documentation is located.
      2) data
         - If data not stored in the repository, a README.md file should indicate where the data is located.
      3) sourcecode

Backups

- If it is important it should be backed up
- If it took a non-trivial amount of work, it should be backed up
- If it changes over time, it should be versioned
- If it is generated by software, it should NOT be backed up
- If you are not sure, back it up

Literate Programming



Literate Programming

R Markdown

```
---
title: "PCCC: An Example Using the Center for Disease Control's Multiple Cause of Death Dataset"
author:
- James Feinstein
- Seth Russell
- Tell Bennett
date: "`r Sys.Date()`"
output: rmarkdown::html_vignette
vignette: >
  %\VignetteIndexEntry{pccc-example}
  %\VignetteEngine{knitr::rmarkdown}
  %\VignetteEncoding{UTF-8}
---

```{r, include = FALSE}
knitr::opts_chunk$set(collapse = TRUE, comment = "#>")
```

Introduction
This vignette provides an example using publicly available death certificate data to illustrate how the `pccc` package generates the Complex Chronic C

To evaluate the code chunks in this example you will need to load the
following R packages.

```{r, message = FALSE}
library(pccc)
library(dplyr)
```

Accessing the Data

The Center for Disease Control maintains vital statistics including death certificate data. The publicly available death certificate data, known as th

The data documentation and instructions for direct download are available at: ftp://ftp.cdc.gov/pub/health_statistics/nchs/datasets/comparability/icd9

Preparing the Data

For this illustrative example, we have provided just 2 columns of the data for decedents <=21 years old: the ICD-9-CM underlying cause of death diagno

Here's a sample of how the file could be read and processed:

```{r, eval = FALSE}
# download and unzip file from ftp://ftp.cdc.gov/pub/health_statistics/nchs/datasets/comparability/icd9_icd10/ICD9_ICD10_comparability_public_use_ASC
# columns of interest
# start end    width description
```
```

Jupyter

https://github.com/CUD2V/kungfauxpandas/blob/master/sourcecode/python/notebooks/kfp_dork_test.ipynb

Chapter 1: The Problem

Monsters are a tricky lot. They have widely varying statistics and capabilities and many have spent centuries building up their r
adventurers from invading their spaces. The smarter varieties of monsters have retained good lawyers through the ages, and it
illegal to publish the "personal" data on any monster.

Of course, we would like to study the monsters without violating their privacy rights. KFP can help this problem!

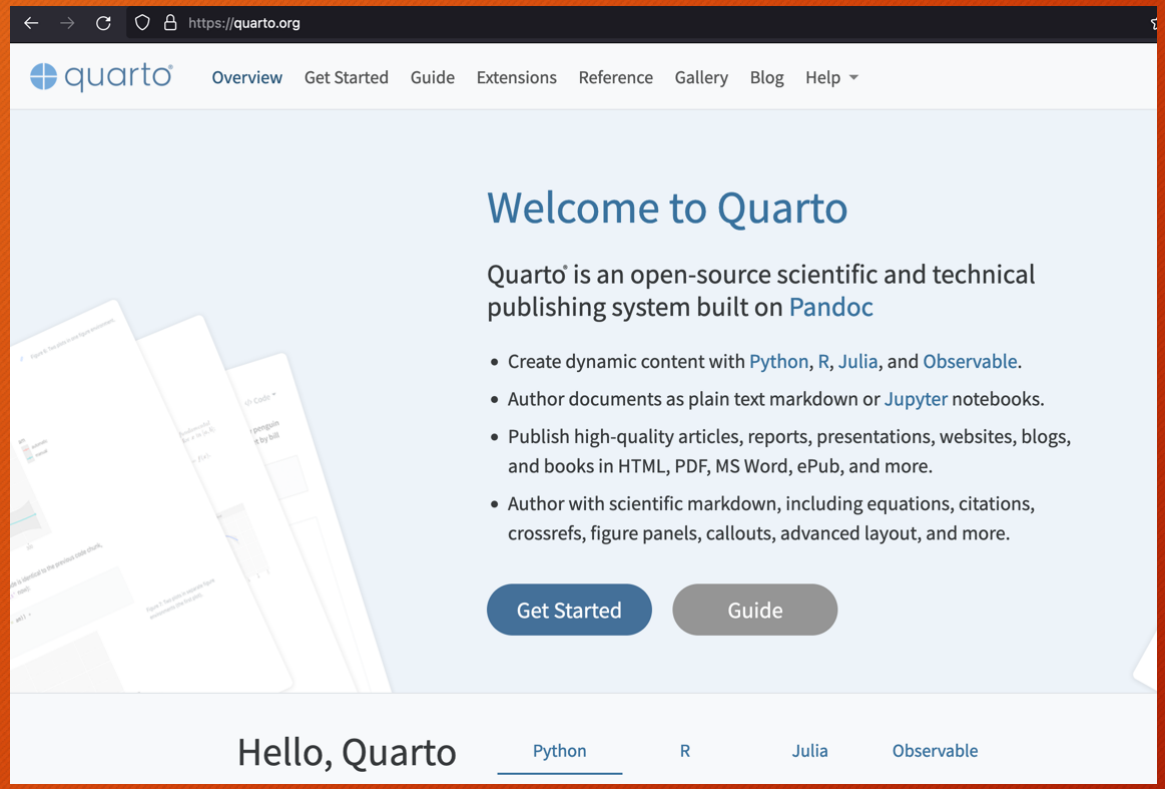
1. Generate a fake data set based on the real stuff
2. Work out all steps necessary to clean the data up
3. Code the data cleaning steps into a function
4. Re-run the data generation using the data cleaner
5. Get a clean, synthetic data set to study
6. Have a trusted agent (DM?) run your study code on the real data and deliver you the results.

In [1]:

```
import sqlite3
import pandas as pd
import numpy as np
import scipy as sp
import scipy.stats as stats
import pylab as plt
from collections import Counter
import datetime
import sys
sys.path.append('../')
sys.path.append('../../../plugins/DataSynthesizer/DataSynthesizer/')
```

Literate Programming

Quarto



https://www.rstudio.com/conference/2022/talks/literate-programming-quarto/

Meta Programming

Programs that write programs

Programs that run programs

Programs that write programs

SQL that writes SQL

```
/*      You, a year ago • Updating tables/views to create snapshot in-time …
Script to create date stamped backup of tables/views that are important to track over time

Could update this to do all tables/views in the covidmab table space or specific named
tables in a table...
*/

DECLARE datestamp STRING;
SET datestamp = (
  SELECT
    substr(table_name, 15)
  FROM
    hdccovidmab.covidemr.INFORMATION_SCHEMA.TABLES
  WHERE table_name like 'table1_patient%'
  ORDER BY table_name DESC
  LIMIT 1
);

EXECUTE IMMEDIATE "CREATE OR REPLACE TABLE hdccovidmab.covidmab.
datestamp || " AS SELECT * FROM hdccovidmab.covidmab.cd4_severit
EXECUTE IMMEDIATE "CREATE OR REPLACE TABLE hdccovidmab.covidmab
```

Bash that writes SQL

```
#!/bin/bash
# need table created in multiple schemas, so using bash
# to templatize the script
set -x
query_template=""

for dataset in full harmonized
do
  query_template+="
  CREATE OR REPLACE TABLE \`hdcekapedsepsis1.$dataset.tests_checks\` AS

  WITH m AS (
      SELECT DISTINCT
          site,
          test_name_source,
          test_name,
          biennial_admission,
          test_units
```

Programs that run programs

Make

```
TARGETS = /sepsis_data/meds_qa_qc/.split_by_med_name

all : $(TARGETS)

/sepsis_data/meds_qa_qc/meds.csv : ../build_medication_mapping_configuration.sql ../harmonize_medications.sql
	bq query < $(word 1, $^)
	bq query < $(word 2, $^)
	rm -f harmonized_medication/*.csv
	gsutil -m cp -r "gs://hdcekapedsepsis1/meds_qa_qc/harmonized_medication" .
	gsutil rm -f "gs://hdcekapedsepsis1/meds_qa_qc/harmonized_medication/*.csv"
	awk 'NR == 1' harmonized_medication/*.csv > /sepsis_data/meds_qa_qc/meds_header.csv
	awk 'FNR > 1' harmonized_medication/*.csv > $@

/sepsis_data/meds_qa_qc/.split_by_med_name : split_by_med_name.R /sepsis_data/meds_qa_qc/meds.csv
	R --vanilla -f $<
	touch $@

/sepsis_data/meds_qa_qc/meds_randomized.csv : /sepsis_data/meds_qa_qc/meds.csv
	shuf $< > $@

/sepsis_data/meds_qa_qc/meds_25pct.csv : /sepsis_data/meds_qa_qc/meds_randomized.csv
	split -n l/1/4 $< > $@

/sepsis_data/meds_qa_qc/meds_50pct.csv : /sepsis_data/meds_qa_qc/meds_randomized.csv
	split -n l/1/2 $< > $@
```

https://www.gnu.org/software/make/

Programs that run programs

Continuous Integration – Github Actions

```yaml
name: Python package

on: [push]

jobs:
  build:

    runs-on: ubuntu-latest
    strategy:
      matrix:
        python-version: ["3.7", "3.8", "3.9", "3.10"]

    steps:
      - uses: actions/checkout@v3
      - name: Set up Python ${{ matrix.python-version }}
        uses: actions/setup-python@v4
        with:
          python-version: ${{ matrix.python-version }}
```

https://docs.github.com/en/actions

Status check

Close your browser window first if you still have it open

https://cups.fast.ai/computationalhusbandry

Software Testing

It is a capital mistake to theorise before one has data. Insensibly one begins to twist facts to suit theories, instead of theories to suit facts.

A Scandal in Bohemia
Sir Arthur Conan Doyle

Software Testing – What to test

- Identify the most important or unique feature(s) of software being implemented. Software bugs are found to follow a Pareto or Zipfian distribution.
- Test data and software configuration.
- If performance is a key feature, build tests to evaluate performance.

https://www.crn.com/news/security/18821726/microsofts-ceo-80-20-rule-applies-to-bugs-not-just-features.htm

Software Testing – How to test

- Software developer develops unit tests.
- Intended user of software should perform validation/acceptance tests.
- Run all tests regularly.
- Review key algorithms with domain experts.

Software Testing – Antipatterns

- Interdependent tests — When a failure in an early test case breaks a later test, it can cause difficulty in resolution and remediation.
- Testing application performance — Creating an automated test to perform this is difficult and does not carry over well from one machine to another.
- Slow running tests— As much as possible, tests should be automated but still run quickly. If tests are slow they will not be used.
- Only test correct input—A common problem in testing is to only validate expected inputs and desired behavior. Make sure tests cover **invalid** input, **exceptions**, and similar items.

Computational Husbandry

questions?

Seth Russell - seth.russell@cuanschutz.edu

Peter DeWitt - peter.dewitt@cuanschutz.edu

SOM, Dept of Biomedical Informatics

Presentations: https://github.com/magic-lantern/Computational-Husbandry-2022

Survey: https://forms.gle/ZumeuAiWRm83ra9h9