Intro to Docker Containers for Reproducible Research in Computational Science

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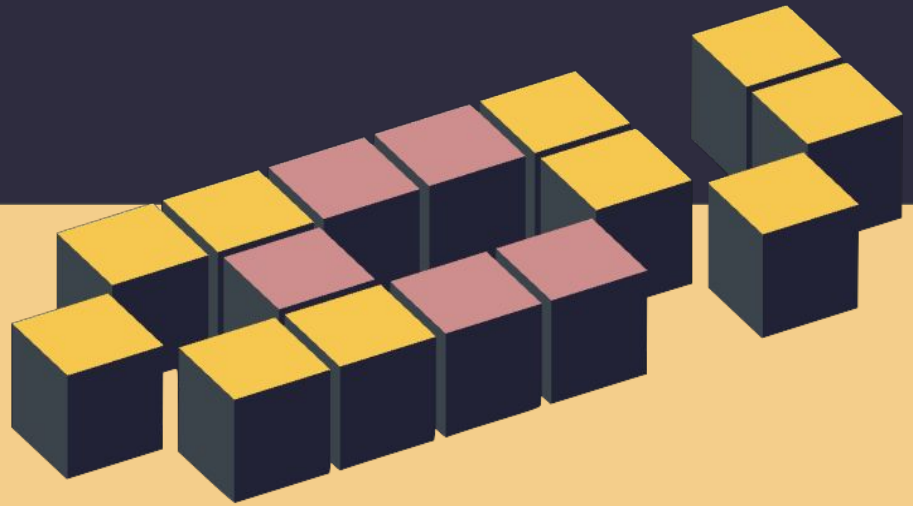
Outline

1. About CCV
2. Crisis of reproducibility
3. Improving reproducibility
4. Containers 101
    a. What is Docker?
5. Example
    a. “Hello, world!”
    b. Fibonacci
    c. Interactive
    d. Using host GPU



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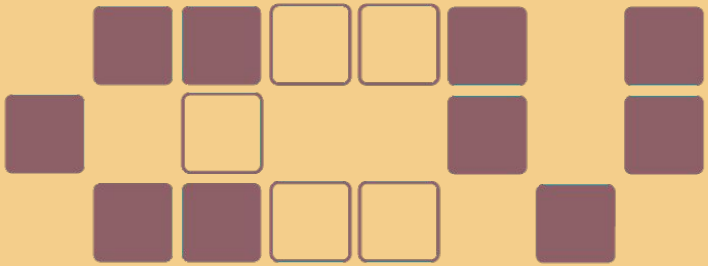

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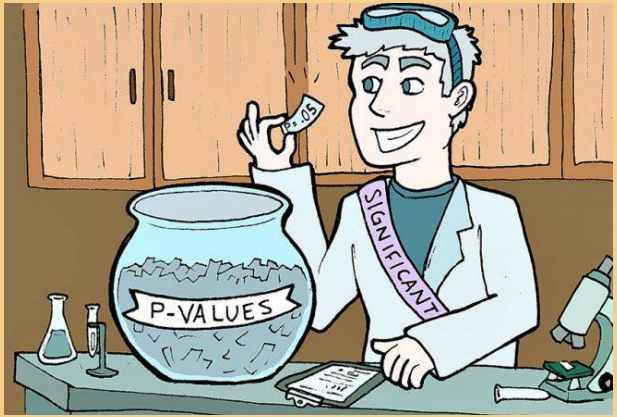
Crisis of Reproducibility

1. Ioannadis (2005)
   a. "*Why Most Published Research Findings Are False*"
      i. "*p*-hacking"
      ii. Hypothesizing-after-the-fact
      iii. Small studies with low power
2. Misaligned Incentives in Academia
   a. "*Publish or perish!*"
   b. Priority of "Oh, wow!" findings
   c. Dis-incentives for replication studies



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How do we Improve Reproducibility?

1. Use free, open-source software
2. Make code public
3. Share data (F.A.I.R.)
    a. Findable, Accessible, Interoperable, Reusable
4. Share entire compute environment
    a. Code, 3rd-party libraries, runtime env
        i. Use containers!!

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What is a Container?

1. Container is a virtualized environments
2. Similar to VMs (i.e., virtual machines)
    a. Containers have less performance overhead
3. Container Software
    a. Docker
    b. Singularity
    c. Linux-VServer

docker

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Docker

1. Container engine for Windows, macOS, and Linux
2. Easy-to-use
3. Can use host's GPUs
4. Free (as in beer and speech)!!!

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Live Demo

Code available here:

https://github.com/brown-ccv/docker-reprod-research

Any questions?

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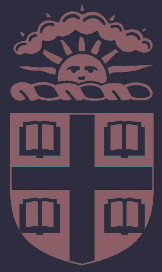

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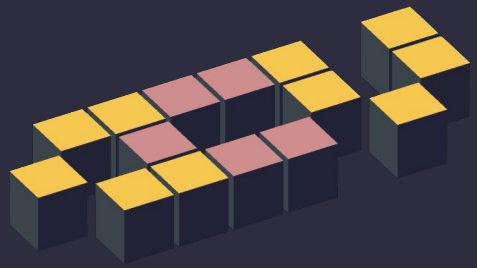

Thank you!!!

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