Towards turnkey reproducibility

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Problem: Reproducing someone’s work can be hard

- Need to install necessary software (assume open source)
  - Takes time, expertise, patience, privileges
  - Could affect system stability
- Could wrap source in VM (virtual machine) image
  - Usually requires $\geq 300$ MB to host; big, unwieldy
  - No separation of source code & environment means no flexibility

High barrier means **people don’t run the code**

Lower hosting & time barrier by specifying environment in separate repo using configuration management software
Solution: Specify environment with configuration management software

- Config management tools specify config in text files
  - Shell scripts (simplest, fewest prepackaged features)
  - Puppet (puppetlabs.com)
  - Chef (wiki.opscode.com)
  - Fabric (http://docs.fabfile.org/en/1.5/)
  - Related: Hashdist, Blueprint, Reprozip, others...

- Instantiate config using virtualization tools
  - Serial, small parallel jobs: Vagrant (vagrantup.com) + VirtualBox (virtualbox.org)
  - StarCluster (star.mit.edu/cluster)
  - CloudFormation (aws.amazon.com/cloudformation)
  - Any other virtualization software + hardware
  - Use web services instead (like Wakari, RunMyCode)

- Idea is **flexibility**: pick & choose (even none, mix)
Example: Install Python interface for DASSL

- DASSL: differential-algebraic equation solver package in Fortran (L. Petzold)
- PyDAS: Python interface to DASSL (J. W. Allen, on GitHub)
- Example: Solve Robertson problem in IPython notebook using PyDAS
- Presentation, environment and source repos on https://github.com/goxberry (all labeled with ICERM-2012)
  - Requires Vagrant + VirtualBox
  - Vagrantfile to specify VM to create (here, Ubuntu 12.04)
  - Configuration in Puppet
  - README with directions for running software
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