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Special Cases: Licenses, Interpreted Languages, and Containers for DHTC

Wednesday morning, 10:45 am

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Expanding Our Horizons

- Previously, we were using simple, open source code that could be easily compiled or built.
- This presentation discusses some special cases:
  - Licensed software
  - Running interpreted languages
  - Using containers

LICENSING

Licensing

- Many scientific softwares are licensed.
- Licenses are restrictive, particularly for high-throughput computing

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License Variations

- Per machine or 'single-install’
- Per *running* instance of the software (per “job”)
- Per username / user
- Via a license server
  - can support 1 - 1000s of concurrently running processes (“seats”)

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Licensing implications for DHTC

- Per machine or 'single-install': can’t be used for DHTC
- Per job: restrictive, limits the number of jobs you can have running, how do you access licenses from execute servers?
- Username: restrictive, could only run jobs on one system where your jobs run as *your username*

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Approaches

- Seek out open source alternatives
  - Python or R packages that emulate specific software behavior
  - If you can’t replace entire workflow, substitute free software where you can
- License-free workarounds (Matlab)
- Choose the least restrictive license possible

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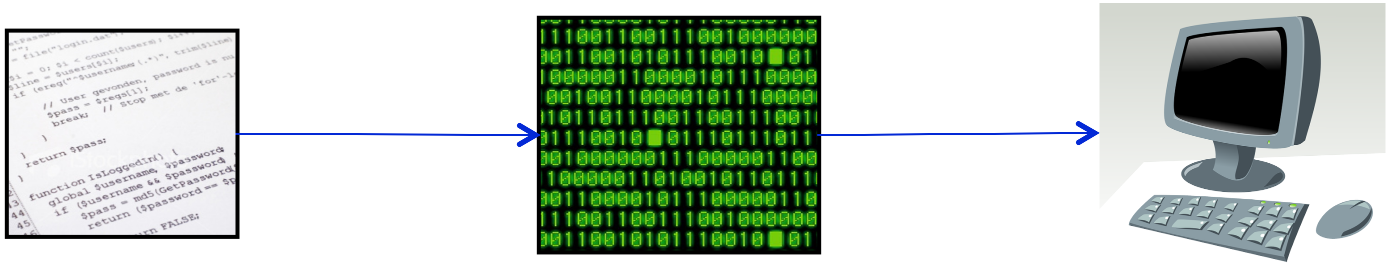
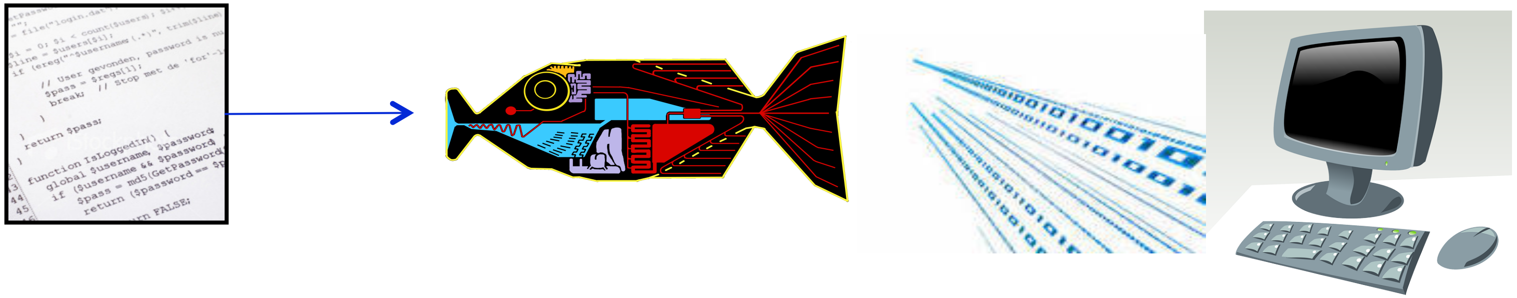
INTERPRETED LANGUAGES

Interpreted code

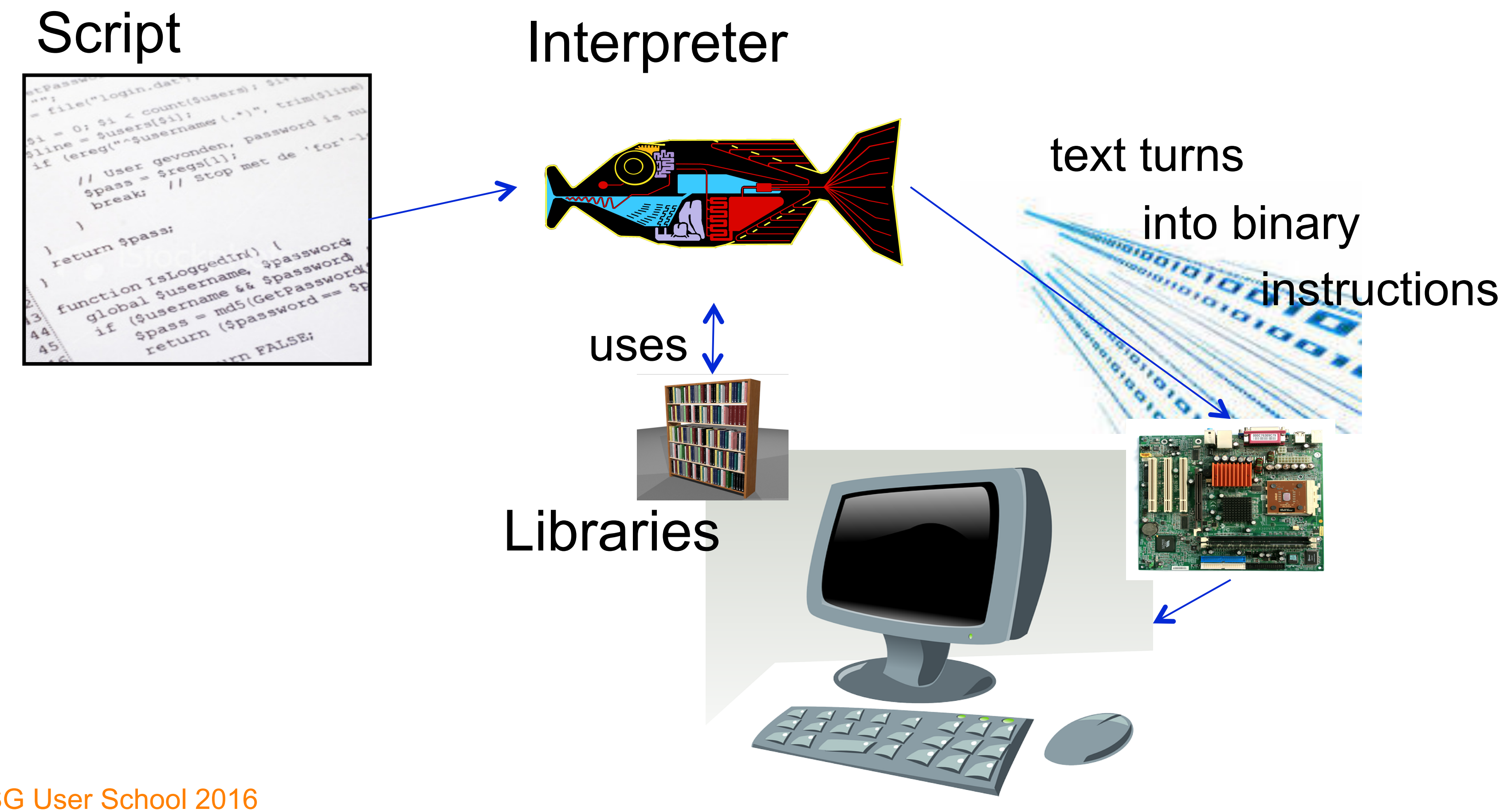
- Instead of being compiled and then run…



- …interpreted languages are translated into binary code "on the fly"



Interpretation



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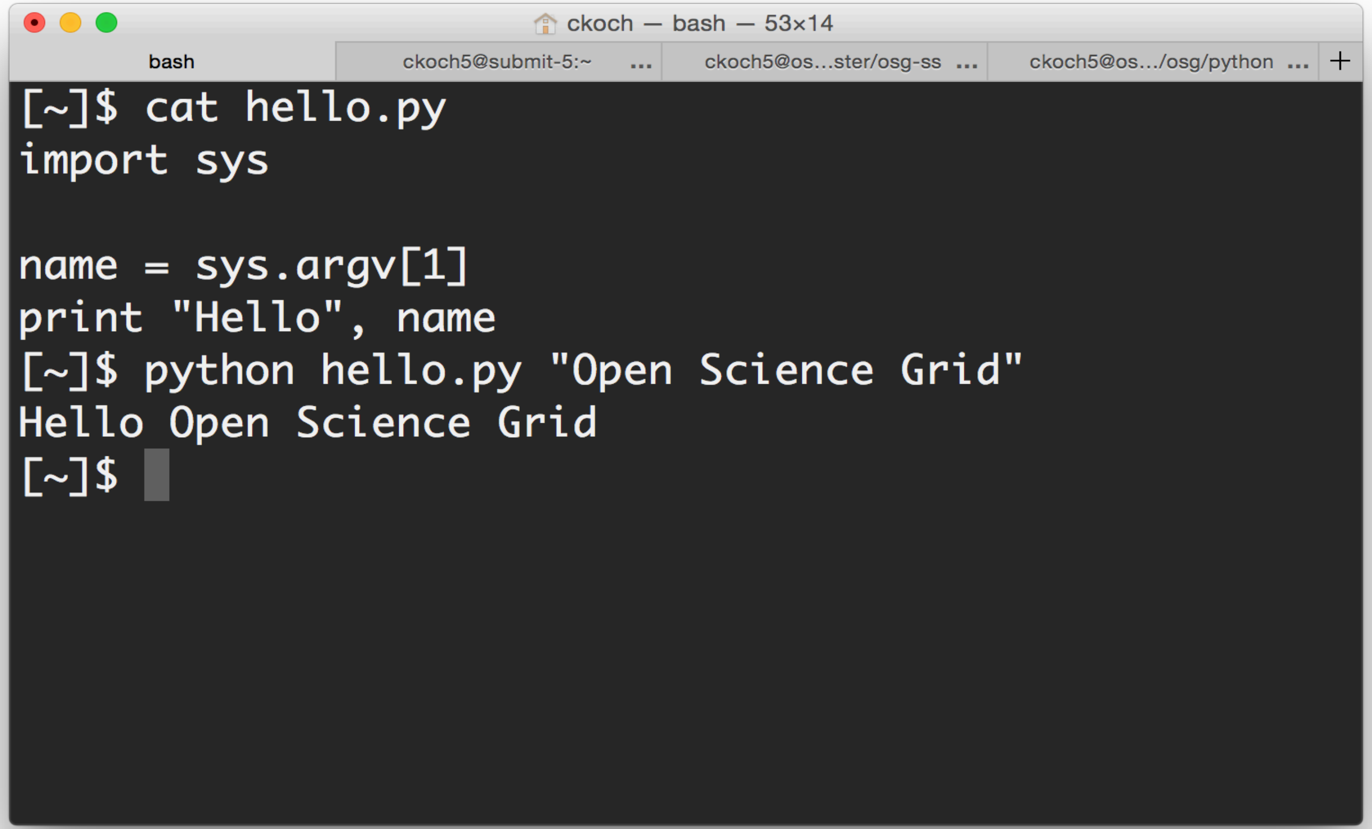
On the command line



```
[~]$ cat hello.py
import sys

name = sys.argv[1]
print "Hello", name
[~]$ python hello.py "Open Science Grid"
Hello Open Science Grid
[~]$
```

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Common interpreted languages*

- Python
- R
- Julia
- Ruby
- Matlab
- Perl
- Javascript

*Note: the line between interpreted/compiled languages can be fuzzy. Many languages support both options, with one method being more common.

Running interpreted code in jobs

General procedure

- Need to bring along interpreter and script
- Use a wrapper script as the executable
- Wrapper script will:
  - “Install” the interpreter
  - Run the script using the local installation

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Python on DHTC

1. Create a portable Python installation (optional)
2. Bring along:
   - pre-built installation OR Python source code
   - your Python code
3. Use a wrapper script to:
   - unpack pre-built install OR install from source
   - run your Python script

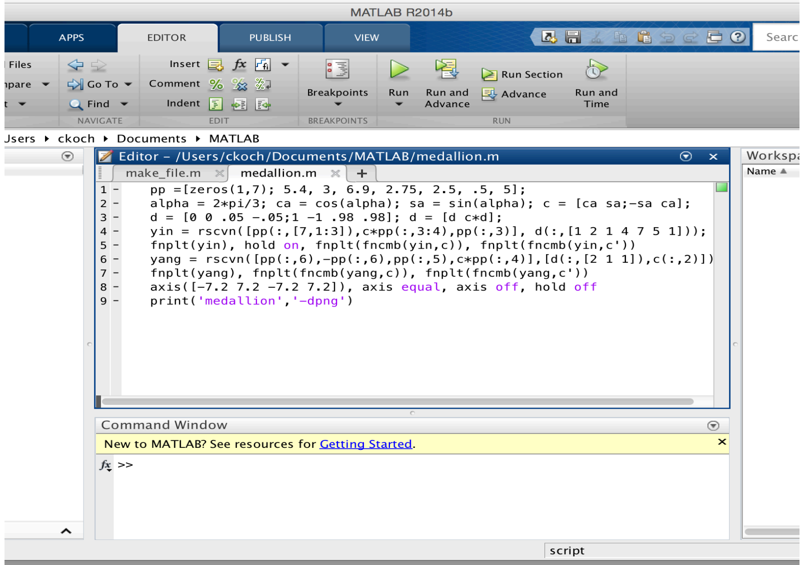
Matlab

- Wait a minute…isn't Matlab licensed?
- Yes, when interpreted on your computer using a normal Matlab installation.
- However, Matlab code can also be compiled.
- Once compiled, the code can be run without a license using a (free) set of files called the Matlab runtime (which acts like the interpreter).

Matlab contrast

Running Matlab on your computer

Uses license per instance



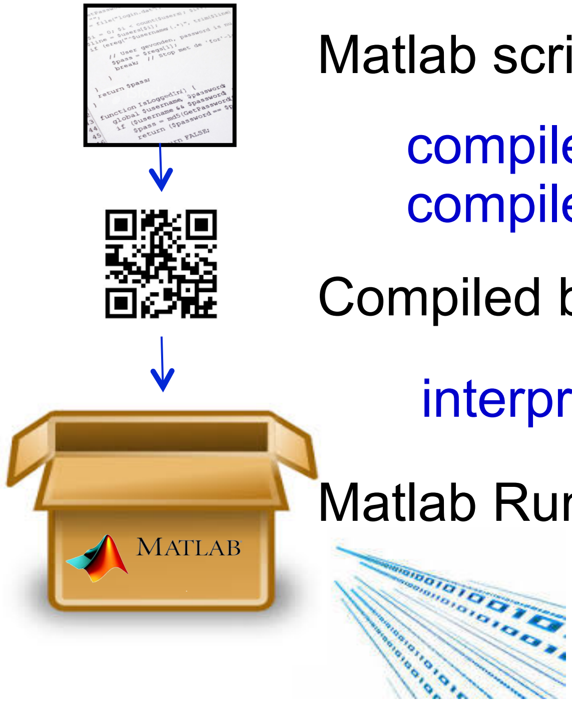
```
pp =[zeros(1,7); 5.4, 3, 6.9, 2.75, 2.5, .5, 5];
alpha = 2*pi/3; ca = cos(alpha); sa = sin(alpha); c = [ca sa;-sa ca];
d = [0 0 .05 -.05;1 -1 .98 .98]; d = [d c*d];
yin = rscvn([pp(:,[7,1:3]),c*pp(:,3:4),pp(:,3)], d(:,[1 2 1 4 7 5 1]));
fnplt(yin), hold on, fnplt(fncmb(yin,c)), fnplt(fncmb(yin,c'))
yang = rscvn([pp(:,6),-pp(:,6),pp(:,5),c*pp(:,4)],[d(:,[2 1 1]),c(:,2)])
fnplt(yang), fnplt(fncmb(yang,c)), fnplt(fncmb(yang,c'))
axis([-7.2 7.2 -7.2 7.2]), axis equal, axis off, hold off
print('medallion','-dpng')
```

New to MATLAB? See resources for Getting Started.

```
>>
```

Running Matlab on DHTC

Uses license once, runs many instances for free



Matlab script(s)

compiled w/ Matlab compiler (uses license)

Compiled binary

interpreted by

Matlab Runtime (free)

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Matlab on DHTC

1. Compile Matlab code using the Matlab compiler (mcc)
   - requires a license
2. Prepare a copy of the Matlab runtime
   - download for free from Mathworks
3. Write a script that “installs” the runtime
   - The Matlab compiler actually writes most of this script for you
4. Use the runtime install to run the compiled Matlab code

CONTAINERS

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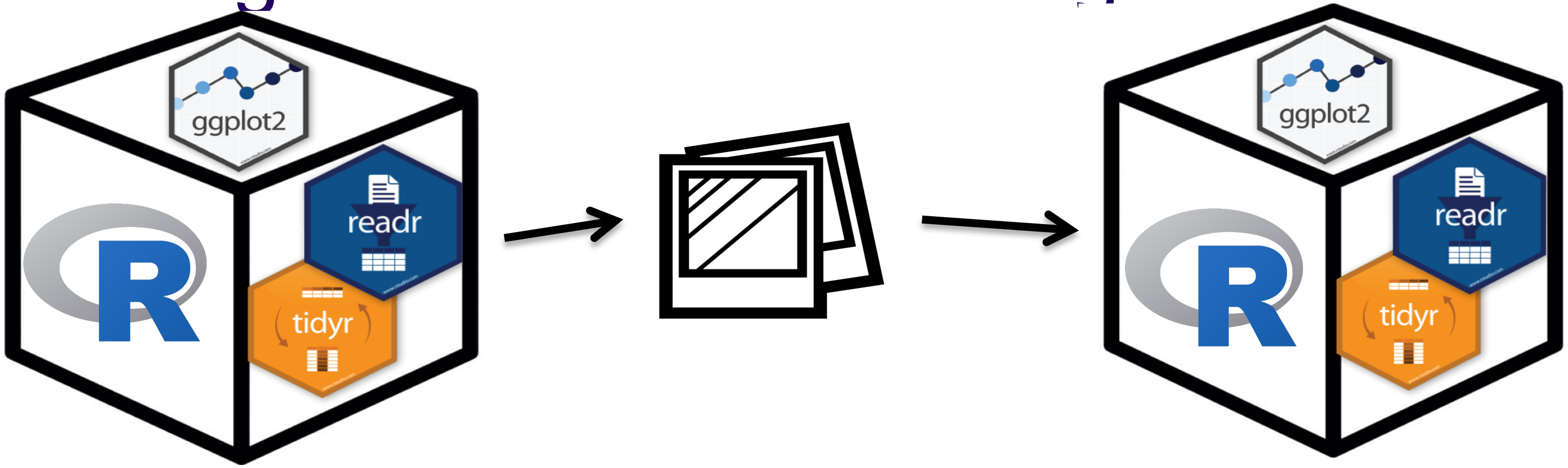
Containers

- Containers are a tool for capturing an entire job “environment” (software, libraries, operating system) into an “image” that can be used again.



polaroid photos by Nick Bluth from the Noun Project

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Using Containers in DHTC

- Two common container systems:

Docker

https://www.docker.com/

Singularity

http://singularity.lbl.gov/

- Requirements:
  - Underlying container system needs to be installed on the computers where your job runs
  - Permissions on that system allow the use of containers

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Container Workflow

1. Create a container or find one online
   - DockerHub: https://hub.docker.com/
   - SingularityHub: https://singularity-hub.org/faq
2. Place container into public or private registry
3. Create a customized script/submit file that fetches/uses the container
   - Docker: Use HTCondor’s docker universe
   - Singularity: Wrapper script

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Conclusion

To use any software in a DHTC system:

1. Create environment/software package
   - download pre-compiled code, compile your own, build your own, create/find a container
2. Write a script to set up the environment when the job runs
3. Account for all dependencies, files, and requirements in the submit file

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Exercises

- Running Matlab Jobs
  - Exercise 1.6
- Running Python Jobs
  - Exercise 1.7: Pre-building Python and using that installation
  - Exercise 1.8: Writing a script that installs Python with every job
- Half of the room should start with Matlab, the other with Python

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Questions?

- Now: Hands-on Exercises
  - 11:15am-12:15pm
- Next:
  - 12:15-1:15pm: Lunch
  - 1:15 onward: free time