



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

Wednesday morning, 10:45 am

Christina Koch (ckoch5@wisc.edu)

Research Computing Facilitator

University of Wisconsin - Madison

Expanding Our Horizons

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



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LICENSING

Licensing

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

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”)

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*

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



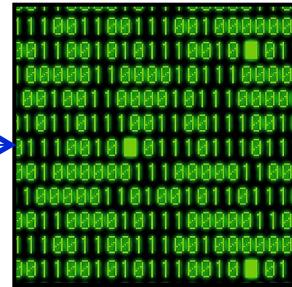
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INTERPRETED LANGUAGES

Interpreted code

- Instead of being compiled and then run...

```
1 //pass
2 // - file("login.dat")
3 $i = 0; $i < count($users); $i++
4 $line = $users[$i];
5 if (eregi("username(.*)", $line))
6 {
7     // User gevonden, password is nu
8     // opgeslagen in $pass
9     $pass = $reg[$i];
10    break; // stop met de 'for'-loop
11 }
12 return $pass;
13
14 function IsLoggedIn()
15 {
16     Global $username, $password;
17     if ($username == $password)
18         $pass = md5($password);
19     return ($password == $pass);
20     $i = FALSE;
21 }
```

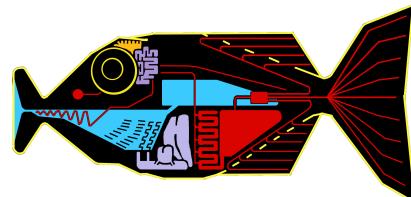


```
1110011001110010000000
10110010101110010101
0000001100001011100000
0010011000010111000000
1101101110011001110011
01110010101110110111
101000000111000001100
1000001101001011011111
101100001011100000110
1110011001110010000000
10110010101110010101
```



- ...interpreted languages are translated into binary code “on the fly”

```
1 //pass
2 // - file("login.dat")
3 $i = 0; $i < count($users); $i++
4 $line = $users[$i];
5 if (eregi("username(.*)", $line))
6 {
7     // User gevonden, password is nu
8     // opgeslagen in $pass
9     $pass = $reg[$i];
10    break; // stop met de 'for'-loop
11 }
12 return $pass;
13
14 function IsLoggedIn()
15 {
16     Global $username, $password;
17     if ($username == $password)
18         $pass = md5($password);
19     return ($password == $pass);
20     $i = FALSE;
21 }
```

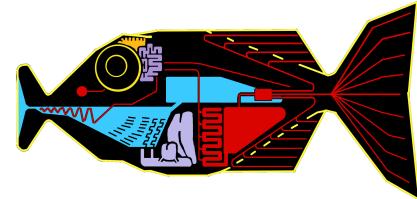


Interpretation

Script

```
1 if($pass == null) {
2     $pass = '';
3     $file = file("login.dat");
4     $i = 0; $i < count($users); $i++;
5     $line = $users[$i];
6     if (ereg("^\$username(.*)", trim($line))
7         $pass = $regs[1];
8     break; // Stop met de 'for'-loop
9 }
10 return $pass;
11 }
12 function IsLoggedIn() {
13     global $username, $password;
14     if ($username != $password)
15         $pass = md5(GetPassword());
16     return ($pass == $password);
17     return FALSE;
18 }
```

Interpreter



text turns
into binary
instructions

uses



Libraries





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On the command line

A screenshot of a macOS terminal window titled "ckoch — bash — 53x14". The window has three tabs: "bash", "ckoch5@submit-5:~" (selected), and "ckoch5@os...ster/osg-ss" and "ckoch5@os.../osg/python". The terminal displays the following text:

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

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

The terminal window has a dark background and light-colored text. The cursor is visible at the end of the last line.

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

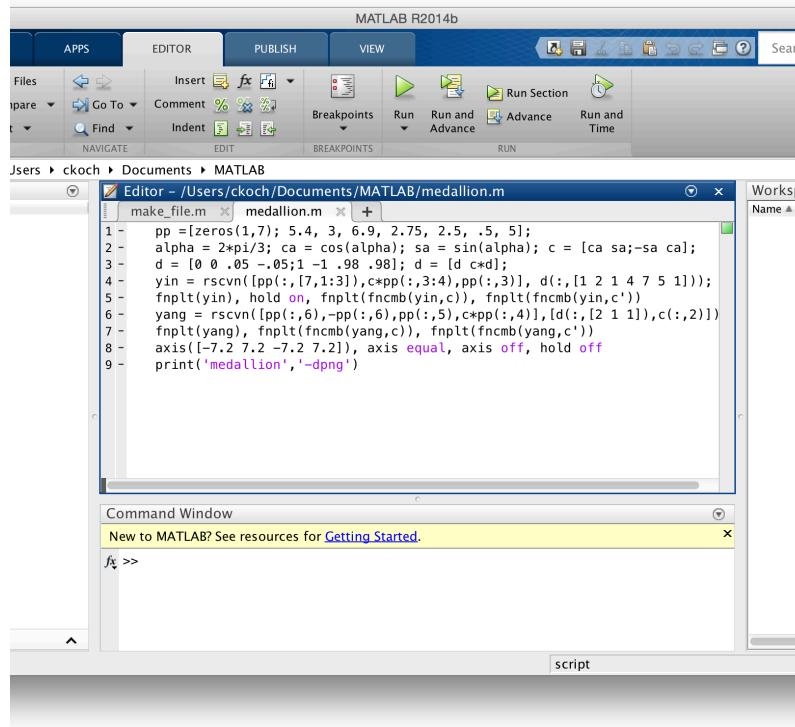
- Need to bring along interpreter and script
- Use a wrapper script as the executable
- Wrapper script will:
 - “Install” the interpreter
 - Run the script using the local installation

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



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)



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

Interpreted Languages

- Matlab is still being compiled before running
- What about programs like Python or R that aren't usually compiled?

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

(Similar to Exercise 1.4 this morning, will also work for R)



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CONTAINERS

Containers

- Containers are a tool for capturing an entire job “environment” (software, libraries, operating system) into an “image” that can be used again.
- Two common container systems:
 - Docker: <https://www.docker.com/>
 - Singularity: <http://singularity.lbl.gov/>

Using Containers in DHTC

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

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

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

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

Questions?

- Feel free to contact me:
 - ckoch5@wisc.edu
- Now: Hands-on Exercises
 - 11:00am-12:15pm
- Next:
 - 12:15-1:15pm: Lunch
 - 1:15 onward: free time