

Deploying Community Codes

Joshua Alexander
University of Oklahoma – IT/OSCER
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What are Community Codes?

- Designed for use with UNIX-like operating systems (mostly)
- Used for computationally intensive scientific analysis
- Open Source (free ... sort of)
- Any programming language
- Written by Scientists & Engineers for Scientists & Engineers

What are Community Codes?

- **Numerical Libraries**
 - Matrix Operations
 - Fast Fourier Transforms
 - Linear Algebra
 - ODE & PDE
- **Scientific Software**
 - Weather Forecasting
 - Molecular Dynamics
 - Ab Initio Chemistry
 - Bioinformatics & Genomics
- **Visualization Software**
 - Climate/Weather Tracking
 - Molecular Rendering
 - Star Formation

Community Code: Languages

- Fortran
- C, C++, Obj-C
- Java
- Python
- Perl
- Outliers
 - Visual Basic
 - Cobol
 - Pascal

Community Code Examples

- **Numerical Libraries**

- Fastest Fourier Transform in the West (FFTW)
- Goto Basic Linear Algebra Subprograms (GotoBLAS)
- Linear Algebra PACKage (LAPACK)

- **Scientific Software**

- The Weather and Research Forecasting model (WRF)
- GRONingen MACHine for Chemical Simulations (GROMACS)
- NWChem: Open Source High-Performance Computational Chemistry
- Basic Local Alignment Search Tool (BLAST)

- **Visualization Software**

- Weather and Climate Toolkit (WCT)
- Avogadro
- Astronomical Image Processing System (AIPS)



Identifying Your Use Case

What am I trying to accomplish?

- **From the user perspective:**
 - I am a computational chemist
 - Need the following software
 - GROMACS
 - NWChem
 - TOWHEE
 - LAMMPS
 - How do I install them?
 - Do it yourself
 - Ask the System Administrators

What am I trying to accomplish?

- **From the System Administrator perspective:**
 - I have a user who is a computational chemist
 - They have requested the following software be made available on the system
 - GROMACS
 - NWChem
 - TOWHEE
 - LAMMPS
 - How popular are these applications?
 - Are there other users of these applications?
 - How to maintain version control?
 - How will the user interactive with the applications?

Scenario: Single-User System

- You are the System Administrator
- You are the user
- Do it yourself

Scenario: Multi-user system

- **You are the user**
 - Download, compile & install the applications in your user space
- **You are the System Administrator**
 - Download, compile & install the applications in the requesting user's space
 - Download, compile & install the applications in a system wide space
 - Will this affect other users?
 - Will this be manageable with future updates/releases?
 - How will this user or future users of these applications interact with said applications?



Deploying The Software

Some Assumptions

- System is a UNIX-like operating system
- If you are the user:
 - Have some experience with UNIX-like operating systems
 - Limited access to system resources (no root privileges)
- If you are the System Administrator:
 - Unlimited access to system resources (i.e. have root privileges)

First Steps: Finding the Application

- Ask the requester
 - Is there a link for downloading
 - Is it on physical media (e.g. CD/DVD/Bluray, USB or External Harddrive)
- Ask colleagues
- Ask <insert your favorite search engine here>

First Steps: Read Available Documentation

- Installation Instructions
 - Online
 - Included PDFs, text files or other
- Prerequisites
- End User Licensing Agreement (EULA)
- User Manual

First Steps: Determine the Path Forward

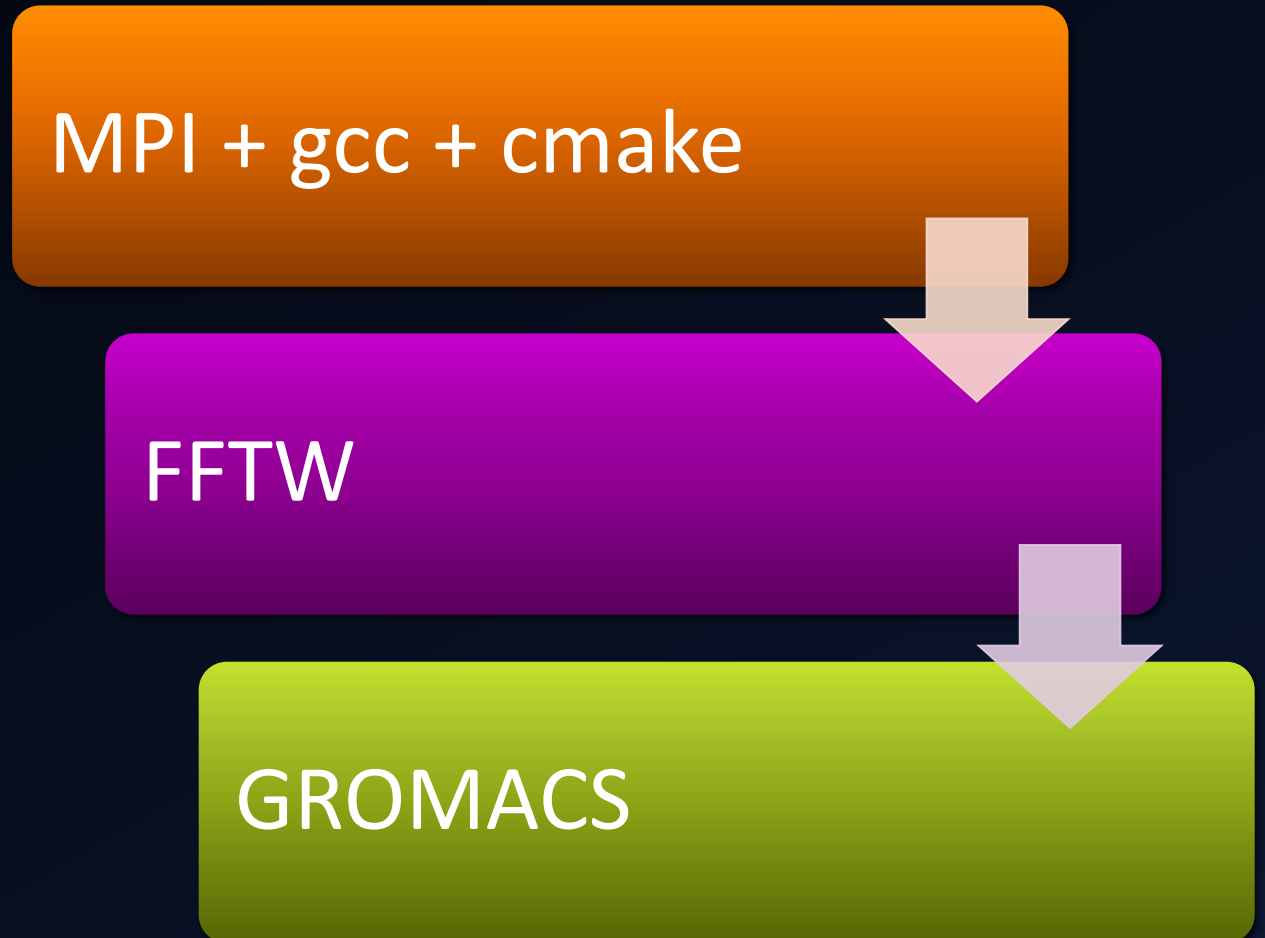
- If I am the user:
 - Limited options which makes the decisions much easier
 - Install in my /home directory
- If I am the System Administrator
 - Lots of options but which one is best
 - Who are the users?
 - How will the applications be managed?

Example Application: GROMACS

- Where to get it:
 - [GROMACS Website](#)
- Documentation says it has dependencies:
 - cmake 2.8.8 or greater
 - gcc 4.7 or greater
 - MPI
 - FFTW (latest) or MKL
- Optional components
 - GPU support
 - Several others

Possible Workflow

- Install MPI + gcc + cmake
 - Most systems already have gcc & cmake installed
- Install FFTW (or MKL)
- Install GROMACS





Live Demo

A close-up, artistic photograph of a glass filled with a golden-brown liquid, possibly whiskey or cognac. The glass is partially filled, and the liquid has a rich, warm hue. The background is softly blurred, showing hints of a white surface and a light-colored wall, creating a clean and elegant atmosphere. The lighting is soft, highlighting the texture of the glass and the clarity of the liquid.

**Thank you.
Questions?**