Numerical Libraries

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Overview

- Modular programming:
  - What is it?
  - How do we implement it?
  - Examples
- Libraries
- Module systems
- Scientific libraries
- Examples using GSL and cuFFT

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Don't reinvent the wheel!

Modular programming

Motivation

- Scientific software can be very large and complex, with lots of subtleties.
- Interactions grow as (number of lines of code)^2.
- You're either recoding the same thing, or are copy-pasting from elsewhere increasing the chance of mistakes.

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- Take a step back and look at what you want to achieve from a top-level perspective.
- Design the interface (header files in C++, interface in Fortran).
- Implementation is separate (ideally separate file).
- Enforce boundaries. **Avoid global variables!** Use namespaces where needed (C++).

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Advantages

- Modules can be unit tested individually.
- Rebuilding software becomes much more efficient.
- Modifying code is much easier and version control is more powerful.

Compilation and linking

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- Lets look at an example: `app.cpp/app.f90` contains the main program and we want to link against `alibrary.cpp/alibrary.h/alibraryf.f90/alibraryf.mod` which are a C++ and f90 module.

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```
g++ -g -O2 -c -o app.o app.cpp
g++ -g -O2 -c -o alibrary.o alibrary.cpp
g++ -g app.o alibrary.o -o cppapp

gfortran -g -O2 -c -o app.o app.f90
gfortran -g -O2 -c -o alibraryf.o alibraryf.f90
gfortran -g app.o alibraryf.o -o f90app
```

(by the way, please use `make` or `cmake` in real life).

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gfortran -g -O2 -c -o alibraryf.o alibraryf.f90
gfortran -g app.o alibraryf.o -o f90app
```

(by the way, please use `make` or `cmake` in real life).

- What if we wanted to use our alibrary in another project called newapp, without recompiling `alibrary.cpp` or `alibraryf.f90`?

From modular programming to libraries

From modular programming to libraries

- Copy .o and .h to separate directories:

```
alibrary.h      -> /base/include/alibrary.h
alibraryf.mod   -> /base/include/alibraryf.mod
alibrary.o      -> /base/lib/alibrary.o
alibraryf.o     -> /base/lib/alibraryf.o
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```

- Must let compiler know where they are:
  - Add `-I` flag for include directories.
  - Absolute path for object file *(only for now!)*.

```
g++ -g -O2 -I/base/include -c -o newapp.o newapp.cpp
g++ -g -o newapp newapp.o /base/lib/alibrary.o

gfortran -g -O2 -I/base/include -c -o newf90app.o newf90app.f90
gfortran -g -o newf90app newf90app.o /base/lib/alibraryf.o
```

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Linux: library filenames start with `lib` and end in `.a` or `.so`.

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g++ -g -o cppapp cppapp.o /base/lib/libalibrary.a
gfortran -g -o f90app f90app.o /base/lib/alibraryf.a
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Instead of giving the explict path in linker command, we should specify:

- the path to the library's object using the `-L` option
- the object code using `-lNAME` (with a lower case letter `-l`)
- libraries should come after the object files that use them.

```
g++ -g -L/base/lib -o cppapp cppapp.o -lalibrary
gfortran -g -L/base/lib -o f90app f90app.o -lalibraryf
```

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  (Note: the `-lNAME` flag is still needed to specify the name of the library)
- If you compile your own libraries in non-standard locations, you do need `-I` and `-L` options (as well as the `-lNAME` clause).

Example: MPI

```
$ mpicc -show
gcc -I/opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/include
 -L/opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/lib/release
 -L/opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/lib
 -Xlinker --enable-new-dtags -Xlinker -rpath -Xlinker
 /opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/lib/release
 -Xlinker -rpath -Xlinker /opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/lib
 -lmpifort -lmpi -lrt -lpthread -Xlinker --enable-new-dtags -ldl
```

```
$ mpifc -show
gfortran -I/opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/include/gfortran/4.8.0
 -I/opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/include
 -L/opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/lib/release
 -L/opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/lib
 -Xlinker --enable-new-dtags -Xlinker -rpath -Xlinker
 /opt/intel/compilers_and_libraries_2019.3.199/linux/mpi/intel64/lib/release
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Software modules

Software modules are a very common way to make software available on shared supercomputers.

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$ module avail
------------------------------ /opt/modulefiles ------------------------------
abaqus/2016          abyss/2.0.2                      anaconda/4.2.0-3.5.2
abaqus/2017          AI/anaconda2-5.1.0_gpu           anaconda2/5.1.0
Abinit/7.10.5        AI/anaconda3-5.1.0_gpu           anaconda2/5.2.0
Abinit/8.0.8b        AI/anaconda3-5.1.0_gpu.2018-08   anaconda3/2019.03
Abinit/8.4.3         AIPS/31DEC16                     anaconda3/5.1.0
abyss/1.5.2          allpaths-lg/52488                anaconda3/5.2.0(default)
...
```

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For example, if you want to load the OpenBLAS library try `module avail openblas` and `module help openblas` (and `module spider openblas` for systems using lmod).

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Must first do a `module load MODULE` before compiling and before running.

Installing libraries from source

What to do when your package manager does not have the library, or it's not in the software module stack, and you do not have permission to install packages in the system paths?

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Compile from source code with a "base" or "prefix" directory.

Common installation procedure (but read documentation!):

```
$ ./configure --prefix=<BASE>
$ make
$ make install
```

```
$ cmake -DCMAKE_INSTALL_PREFIX=<BASE> ....
$ make
$ make install
```

You choose the <BASE>, but it should be a directory that you have write permission to, e.g., a subdirectory of your **$HOME**.

Using libraries that are not in standard directories

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- Alternatively, you can omit these by setting some linux environment variables:

```
export CPATH="$CPATH:<BASE>/include"                # compiler looks here for include files
export LIBRARY_PATH="$LIBRARY_PATH:<BASE>/lib"      # and here for library files
export LD_LIBRARY_PATH="$LD_LIBRARY_PATH:<BASE>/lib" # runtime linker looks here
```

  You either enter these commands on the linux prompt before compiling, or, to set these automatically when you log in, add these lines to the `.bashrc` file in your home folder.

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- The last one (`LD_LIBRARY_PATH`) may be necessary to run the application, even when it was successfully built and linked already.
- If the library installs binary applications (i.e. commands) as well, you'll also need to set

```
export PATH="$PATH:<BASE>/bin"     # linux shell looks for executables here
```

2

So many libraries, so little time...

Some libraries for scientific computing (CPU)

BLAS interface for libraries for basic linear algebra operations. C C++ Fortran

LAPACK Linear solvers, eigenvalue problems, SVD, factorization. C C++ Fortran Python

ScaLAPACK Distributed version of LAPACK. C C++ Fortran

ARPACK-NG and SLEPc Eigenvalue problems. C C++ Fortran

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Eigen Matrices, vectors, numerical solvers, ... C++

FFTW Fourier and related transforms. C C++ Fortran

HDF5 and NetCDF Portable data model, library, and file formats. C C++ Fortran

GSL Numerical analysis library. C C++

PETSc Scalable (parallel) solution of partial differential equations. C C++ Fortran

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GSL Numerical analysis library. C C++

PETSc Scalable (parallel) solution of partial differential equations. C C++ Fortran

Armadillo Matrix and vector maths similar to MATLAB. C++

Blaze Dense and sparse arithmetic. C++

Dlib Machine learning algorithms and tools. C++

Mlpack Machine learning algorithms. C++ Python

Trilinos algorithms etc. for the solution of large-scale, complex multi-physics engineering and scientific problems. C C++

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Some libraries for scientific computing (GPU)

cuBLAS / rocBLAS GPU-accelerated BLAS implementations

cuSOLVER / rocSOLVER$^{(\beta)}$ / MAGMA GPU-accelerated LAPACK-like libraries

cuSPARSE / rocSPARSE GPU-accelerated sparse matrix libraries

cuFFT / rocFFT GPU-accelerated Fast Fourier Transforms libraries

cuRAND / rocRAND Random number generation on the GPU

NPP (CUDA) Performance primitives for image & video processing

Thrust GPU-accelerated STL-like library (parallel algorithms)

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Some libraries for scientific computing (Python)

NumPy Faster arrays for Python. Mind all the lessons from the HPC Python programming session!

SciPy Provides many user-friendly and efficient numerical routines such as routines for numerical integration and optimization.

Numba JIT compilation of a subset of Python and NumPy code into fast machine code.

Pandas Tabular data manipulation and analysis.

scikit-learn (sklearn) Machine Learning in Python. Simple and efficient tools for data mining and data analysis.

TensorFlow & PyTorch Neural nets/deep learning libraries.

Stan, PyMC Statistical modelling, data analysis, and Bayesian predictions.

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Example: GNU Scientific Library (GSL)

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Is a C library containing many useful scientific routines, such as:

- Root finding
- Minimization
- Sorting
- Integration, differentiation, interpolation, approximation
- Statistics, histograms, fitting

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- Minimization
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- Integration, differentiation, interpolation, approximation
- Statistics, histograms, fitting
- Monte Carlo integration, simulated annealing
- ODEs
- Polynomials, permutations
- Special functions
- Vectors, matrices

Note: C library means we'll likely need to deal with some pointers and casts.

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GSL root finding example (`gslrx.cpp`)

Suppose we want to find where $f(x) = a\cos(\sin(v + wx)) + bx - cx^2$ is zero.

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```
#include <iostream>
#include <gsl/gsl_roots.h>
#include <gsl/gsl_errno.h>

struct Params {double v, w, a, b, c;};

double examplefunction(double x, void* param){
 auto [v, w, a, b, c] = *(Params*)param;
 return a*cos(sin(v+w*x))+b*x-c*x*x;
}

int main() {
 double x_lo = -4.0;
 double x_hi =  5.0;
 Params args = {0.3, 2./3., 2., 1./1.3, 1/30.};
 gsl_root_fsolver* solver;
 solver = gsl_root_fsolver_alloc(
              gsl_root_fsolver_brent);
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```
 gsl_function fwrapper;
 fwrapper.function = examplefunction;
 fwrapper.params = &args;
 gsl_root_fsolver_set(solver,&fwrapper,x_lo,x_hi);

 std::cout << "iter lower upper root err\n";
 int status, iter = 0;
 do {
  gsl_root_fsolver_iterate(solver);
  double x_rt = gsl_root_fsolver_root(solver);
  double x_lo = gsl_root_fsolver_x_lower(solver);
  double x_hi = gsl_root_fsolver_x_upper(solver);
  std::cout << iter++ <<" "<< x_lo <<" "<< x_hi
            <<" "<< x_rt <<" "<<x_hi-x_lo<<"\n";
  status=gsl_root_test_interval(x_lo,x_hi,0,1e-8);
 } while (status==GSL_CONTINUE and iter < 100);
 gsl_root_fsolver_free(solver);
}
```

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Output

```
$ ./gslrx
iter lower      upper     root      err
0    -4         -1.27657  -1.27657  2.72343
1    -1.95919   -1.27657  -1.95919  0.682622
2    -1.75011   -1.27657  -1.75011  0.473542
3    -1.75011   -1.74893  -1.74893  0.001179
```

Compilation and linkage

- Lots of `gsl...` stuff.
- The rest is just wrappers, setting up parameters and calling the appropriate functions.
- There are pointers and typecasts, because we're dealing with a C library.
- How to compile on the command line?
- GSL root finding documentation: https://www.gnu.org/software/gsl/doc/html/roots.html

```
module load gcc
g++ gslrx.cpp -o gslrx -lgsl -lgslcblas
```

1. When using software modules, you don't need the -I and -L options.
2. GSL is usually a module (not on Bridges2).

Output

```
$ ./gslrx
iter lower      upper    root       err
0    -4         -1.27657 -1.27657   2.72343
1    -1.95919   -1.27657 -1.95919   0.682622
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```

4

Using a C or C++ library in Python

But I only like Python!

No problem! Most numerical libraries have a Python ***API***.

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If not, you can create your own wrapper using PyBind11, ctypes, SWIG or f2py for Fortran code.

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Lets look at an example using PyBind11

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PyBind11 example

Suppose we want to use cuFFT to calculate a Fourier transform, but in Python.

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We first write a function in C++ that wraps the library call

Then use *PyBind11* to create a Python "package", which we can import and use like any other.

PyBind11 example

Suppose we want to use cuFFT to calculate a Fourier transform, but in Python.

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Then use *PyBind11* to create a Python "package", which we can import and use like any other.

Note: GPU-based FFT functionality (via cuFFT or otherwise) is provided by some packages on PyPI already.

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PyBind11 example (pycufft.cu)

This is the wrapper, defining a C++ function, that calls the cuFFT C function.

```
#include <complex>
#include <cufft.h>
#include <vector>

std::vector<std::complex<float>>
 fft(const std::vector<float>& signal)
{
 const size_t size = signal.size();
 float *signal_d;
 cudaMalloc((void**)&signal_d,
  size*sizeof(float));
 cudaMemcpy(signal_d, signal.data(),
  size*sizeof(float), cudaMemcpyHostToDevice);
 float2 *result_d;
 cudaMalloc((void**)&result_d,
  (size/2+1)*sizeof(float2));
 cufftHandle plan;
 cufftPlan1d(&plan, size, CUFFT_R2C, 1);
 cufftExecR2C(plan, (cufftReal*)signal_d,
  (cufftComplex*)result_d);
```

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 cufftExecR2C(plan, (cufftReal*)signal_d,
  (cufftComplex*)result_d);
 std::vector<std::complex<float>>
  result(size/2+1);
 cudaMemcpy(result.data(), result_d,
  (size/2+1)*sizeof(float2),
  cudaMemcpyDeviceToHost);
 cudaFree(signal_d);
 cudaFree(result_d);
 cufftDestroy(plan);
 return result;
}

#include <pybind11/pybind11.h>
#include <pybind11/stl.h>
#include <pybind11/complex.h>
PYBIND11_MODULE(pycufft, m) {
    m.doc() = "cuFFT wrapper";
    m.def("fft", &fft, "docstring");
}
```

PyBind11 example (`pycufft_example.py`)

This is an example of a Python script using our wrapped library.

```
import pycufft, numpy as np
w0    = 5   # rad/s
t_max = 20  # s
n     = 2048
t = np.linspace(0, t_max, n)
x = np.sin(w0*t)
result = pycufft.fft(x)
mag = np.abs(result)
w_recovered = mag.argmax() * 2*np.pi/t_max
print(f'Recovered angular frequency: {w_recovered} rad/s')
```

Note that the return type of our wrapped function is a list, we can ask PyBind11 to return a NumPy array, but that doesn't fit on one slide

PyBind11 example (how to use on Bridges2)

(1) Copy code for Python session if you haven't done so already:

```
cp -r /jet/home/rzon/hpcpycode ~
```

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```
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```

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```
source ~/hpcpycode/activate
```

(3) Load the CUDA module and compile the shared object file:

```
module load cuda
nvcc -O3 -shared -std=c++17 -Xcompiler="-Wall -fPIC" \
 $(python3 -m pybind11 --includes) pycufft.cu \
 -o pycufft.cpython-38-x86_64-linux-gnu.so -lcufft
```

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```

(4) Try running the script:

```
srun --partition=GPU-shared --gres=gpu:v100-32:1 \
 --time=00:01:00 python pycufft_example.py
```

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Final remarks

- "Do not reinvent the wheel", i.e. reuse libraries already developed.

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Final remarks

- "Do not reinvent the wheel", i.e. reuse libraries already developed.
- Use **mature** libraries, well-known in the corresponding field/community. They have been developed, maintained, debugged, tested, optimised and are really good at the task(s) in question.

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Final remarks

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- Use **mature** libraries, well-known in the corresponding field/community. They have been developed, maintained, debugged, tested, optimised and are really good at the task(s) in question.
- Libraries are a cornerstone element in modularity and professional sofware development.

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- Use **mature** libraries, well-known in the corresponding field/community. They have been developed, maintained, debugged, tested, optimised and are really good at the task(s) in question.
- Libraries are a cornerstone element in modularity and professional sofware development.
- Consider including further elements of software engineering, such as, automation (via `make` or `cmake`) of compilation and linking – helps with compilation flags and cross-platform developments.

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