PyMAGMA: A Python Library for MAGMA

• • •

Delario Nance, Jr. (Davidson College)
Mentors: Stanimire Tomov (UTK) and Kwai Wong (UTK)
Research Assistant: Julian Halloy (UTK)

Presentation Outline

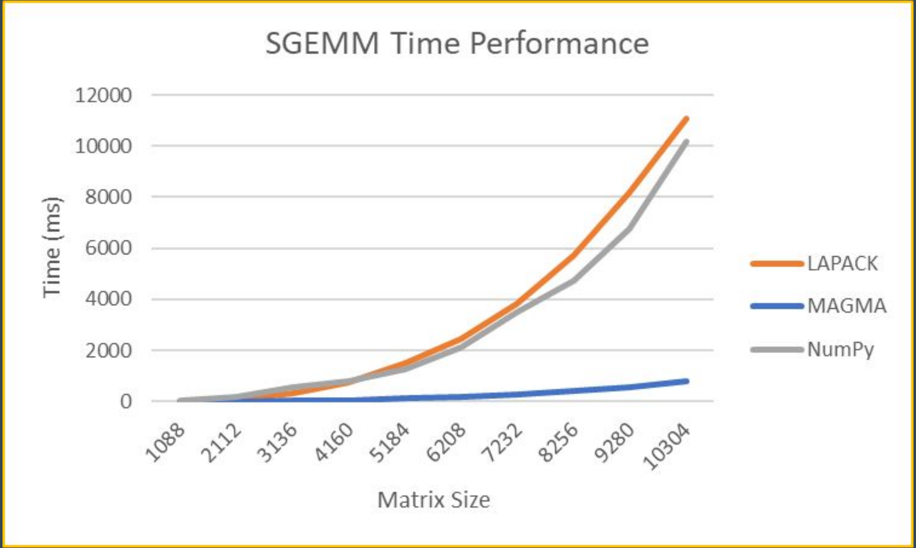
1) Background
2) SWIG Workflow
3) Creating PyMAGMA
4) Extending PyMAGMA
5) Performing SGEMM with PyMAGMA
6) Conclusion and Future Work

Background

What is MAGMA?

- Stands for “Matrix Algebra on GPU and Multicore Architectures”
- A large package of C++ functions optimized for running linear algebra operations on GPUs
    - LAPACK and NumPy are linear algebra packages whose code only runs on CPUs

Comparing the times taken by LAPACK, MAGMA, and NumPy to perform SGEMM (C = -AB + C)



GPU Model: NVIDIA GeForce GTX 1650 SUPER
CPU Model: Intel(R) Xeon(R) CPU X5650

C++ vs. Python

C++

- Code is ran very quickly
- Syntax can be difficult for new programmers to understand

Printing “Hello REU” in C++

```cpp
#include <iostream>
using namespace std;

int main()
{
    cout << "Hello REU \n";
    return 0;
}
```

Python

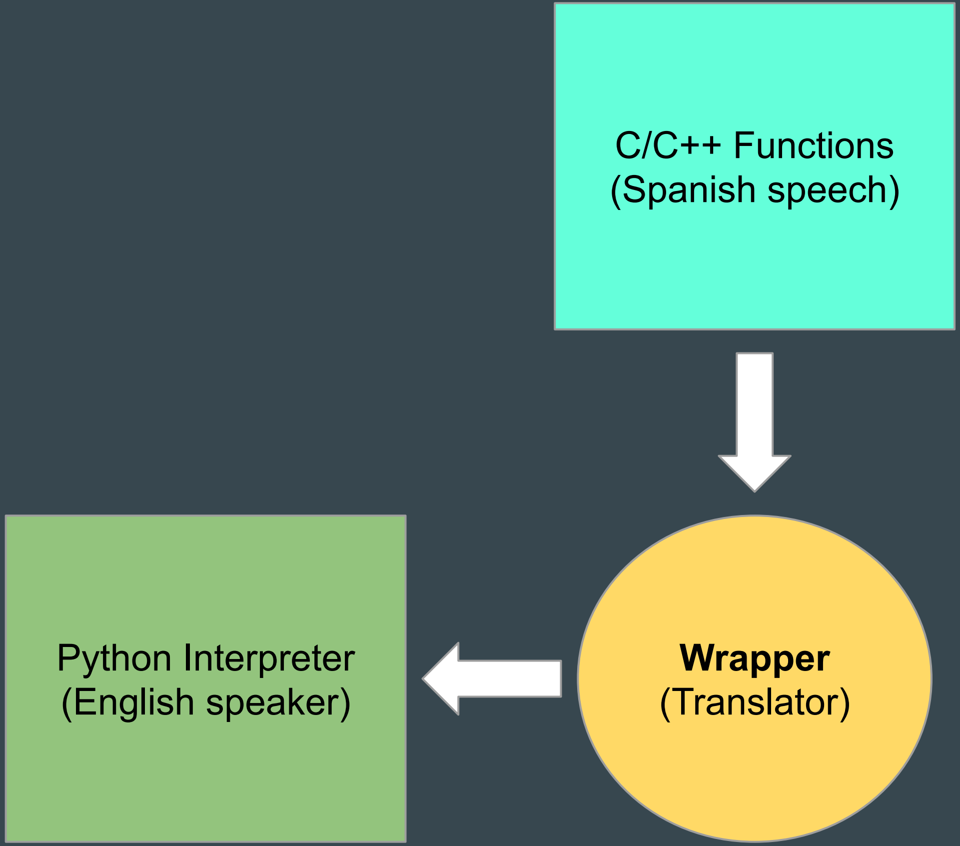
- Code is ran relatively slowly
- Syntax is often easy to understand

Printing “Hello REU” in Python

```python
print("Hello REU")
```

What is SWIG?

- Stands for “Simplified Wrapper and Interface Generator”
- A tool for interfacing C/C++ code with high-level programming languages (e.g., Python)
- Works by generating three files
  - Wrapper file - translates C/C++ functions to the target language
  - Shared library - contains the original C/C++ functions and wrapper code
  - Import file - lets users import the shared library into the target language



C/C++ Functions
(Spanish speech)

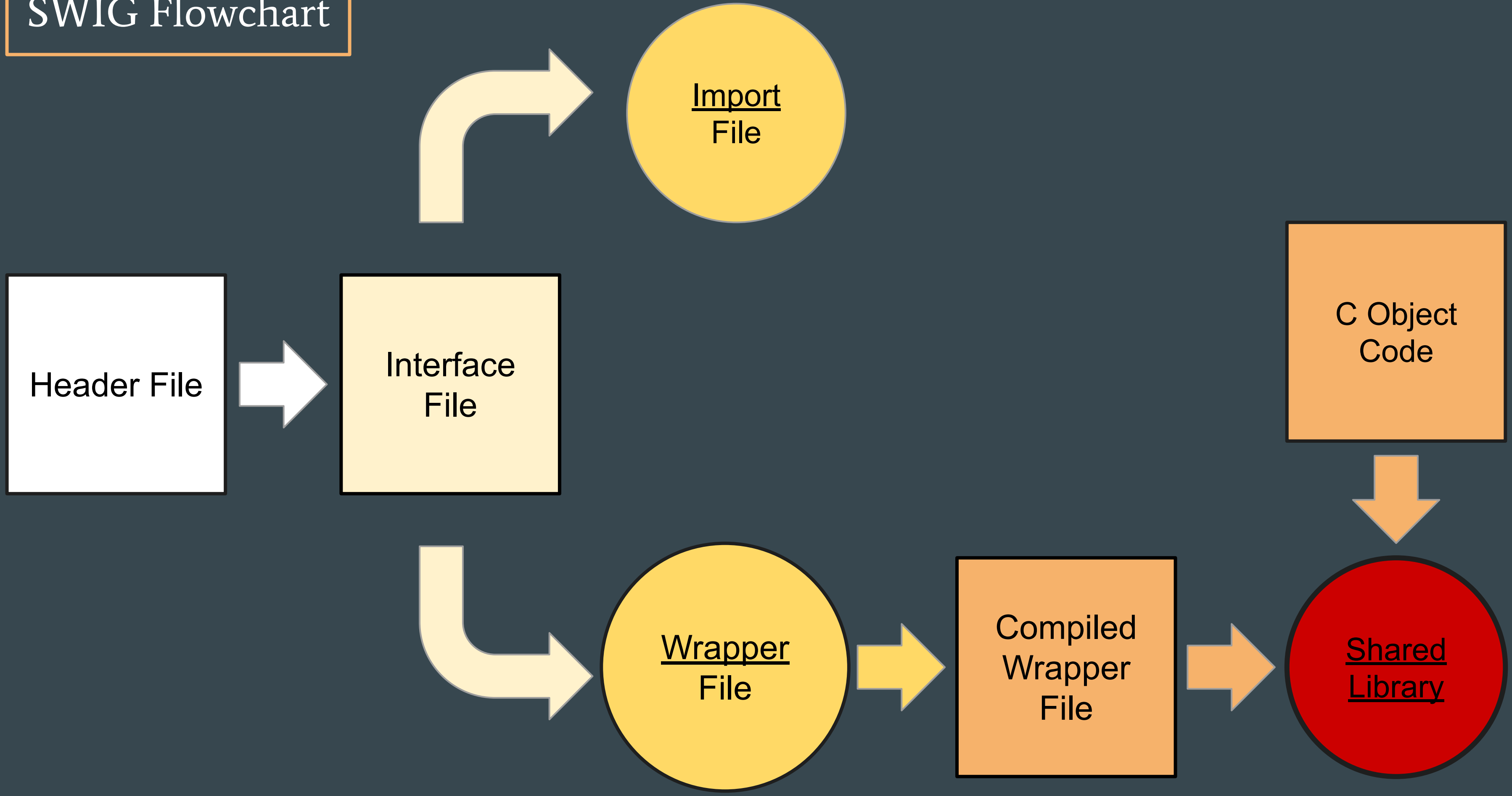
Wrapper
(Translator)

Python Interpreter
(English speaker)

A real-life analogy of SWIG’s wrapper code

SWIG Workflow

SWIG Flowchart



Header File

Interface File

Import File

Wrapper File

Compiled Wrapper File

C Object Code

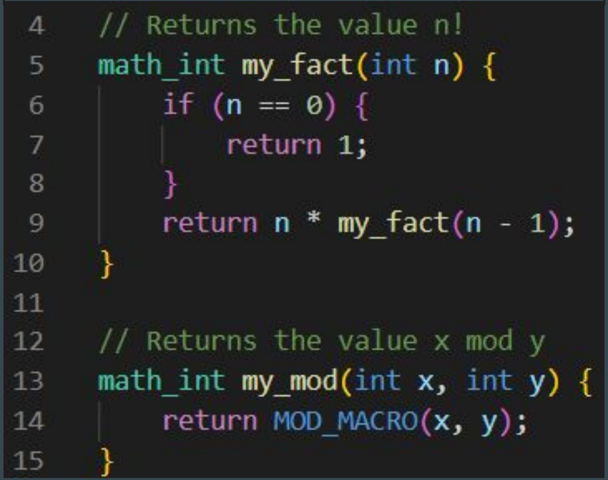
Shared Library

File 1: Header File (.h)

Header File

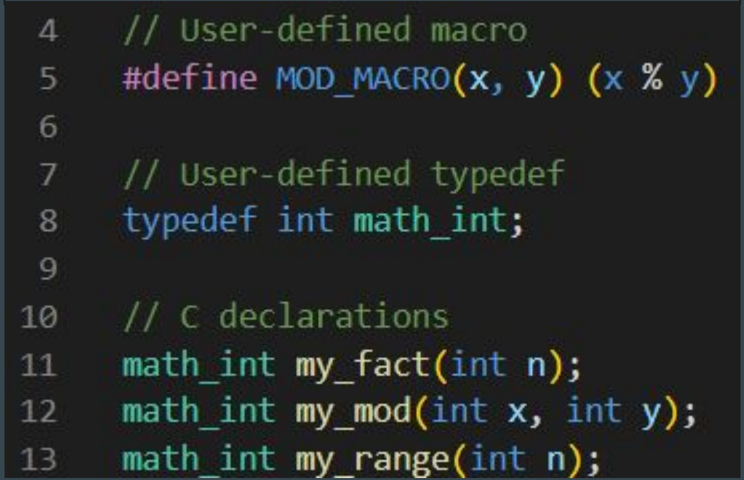
- First, the user must choose which C functions to interface with Python
- Each of the C functions should be declared in a file known as the “header file”
- By editing the header file, the user can easily extend the Python interface

Sample C functions to interface



```c
// Returns the value n!
math_int my_fact(int n) {
    if (n == 0) {
        return 1;
    }
    return n * my_fact(n - 1);
}

// Returns the value x mod y
math_int my_mod(int x, int y) {
    return MOD_MACRO(x, y);
}
```

Header file for the chosen C functions



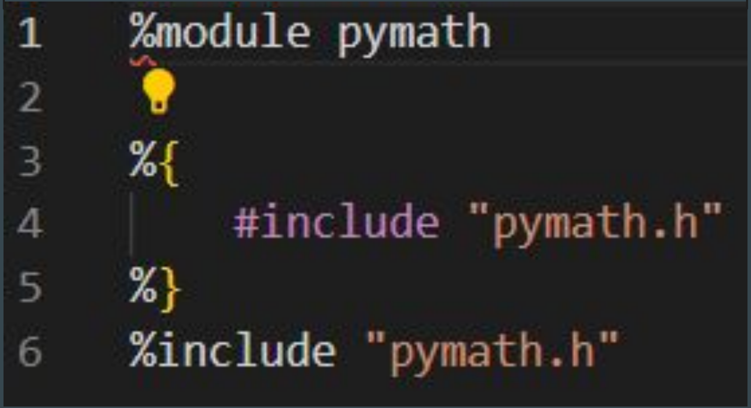
```c
// User-defined macro
#define MOD_MACRO(x, y) (x % y)

// User-defined typedef
typedef int math_int;

// C declarations
math_int my_fact(int n);
math_int my_mod(int x, int y);
math_int my_range(int n);
```

File 2: Interface File (.i)

Header File → Interface File

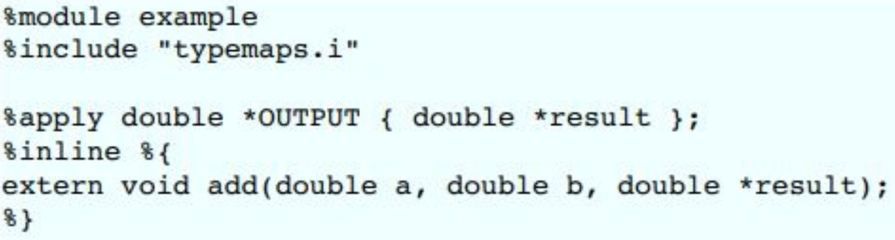
- Must contain the name of the Python library to create **(Line 1)**
- Usually contains two “include” statements for the previously created header file **(Lines 4 and 6)**
- Where users can insert typemaps to give SWIG directions on how to handle specific C-to-Python type conversions

Interface File for the PyMath Library



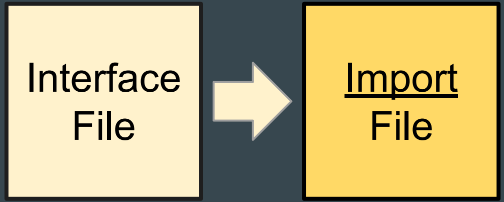
```
1    %module pymath
2
3    %{
4        #include "pymath.h"
5    %}
6    %include "pymath.h"
```

Example of a SWIG Typemap



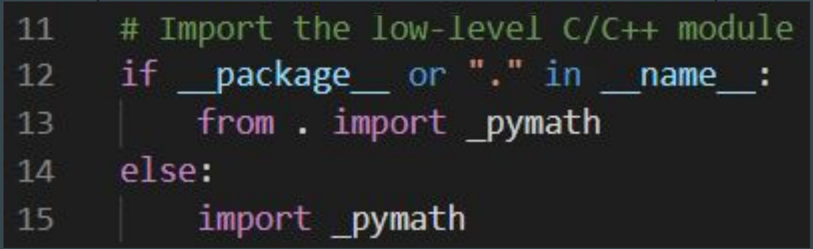
```
%module example
%include "typemaps.i"

%apply double *OUTPUT { double *result };
%inline %{
extern void add(double a, double b, double *result);
%}
```

FIle 3a: Import File (.py)



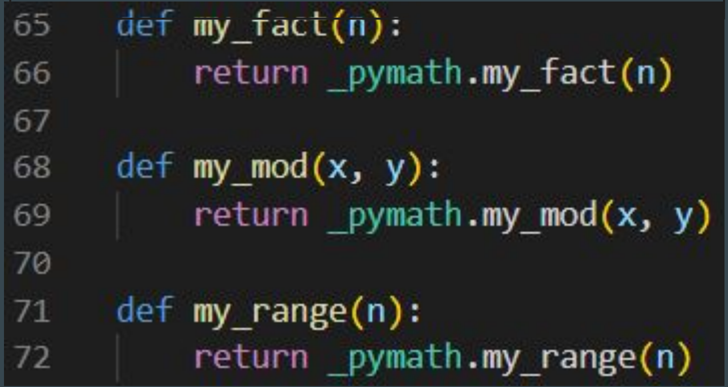
- The “payment” in our real-life analogy
- Lets users import the library of C code into Python after it is created (Line 15)
- Contains a Python function for each C function which was declared in the header file (Lines 65-72)

The Python import command for importing the Python library



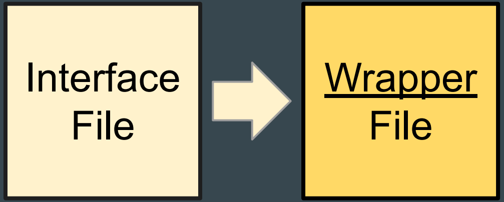
```
11    # Import the low-level C/C++ module
12    if __package__ or "." in __name__:
13        from . import _pymath
14    else:
15        import _pymath
```

The Python functions which users will call to use the C functions



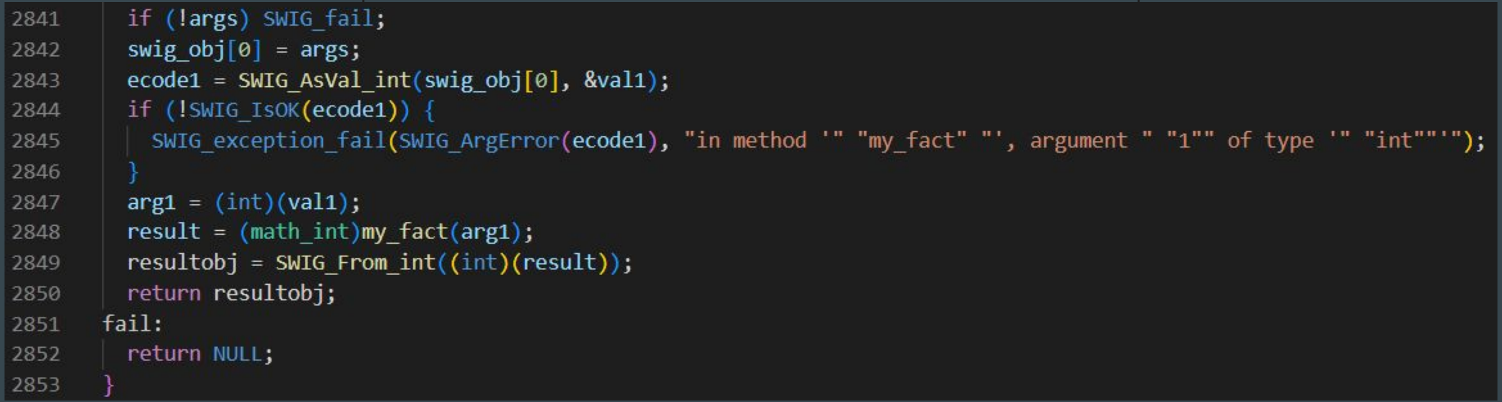
```
65    def my_fact(n):
66        return _pymath.my_fact(n)
67
68    def my_mod(x, y):
69        return _pymath.my_mod(x, y)
70
71    def my_range(n):
72        return _pymath.my_range(n)
```

FIle 3b: Wrapper File (_wrap.c)



- The "translator" in our real-life analogy
- Contains the "wrapper" code which will translate our chosen C functions to the Python interpreter
- Incorporates any typemaps which the user enforced in the interface file (.i)

Wrapper code for the *my_fact()* function

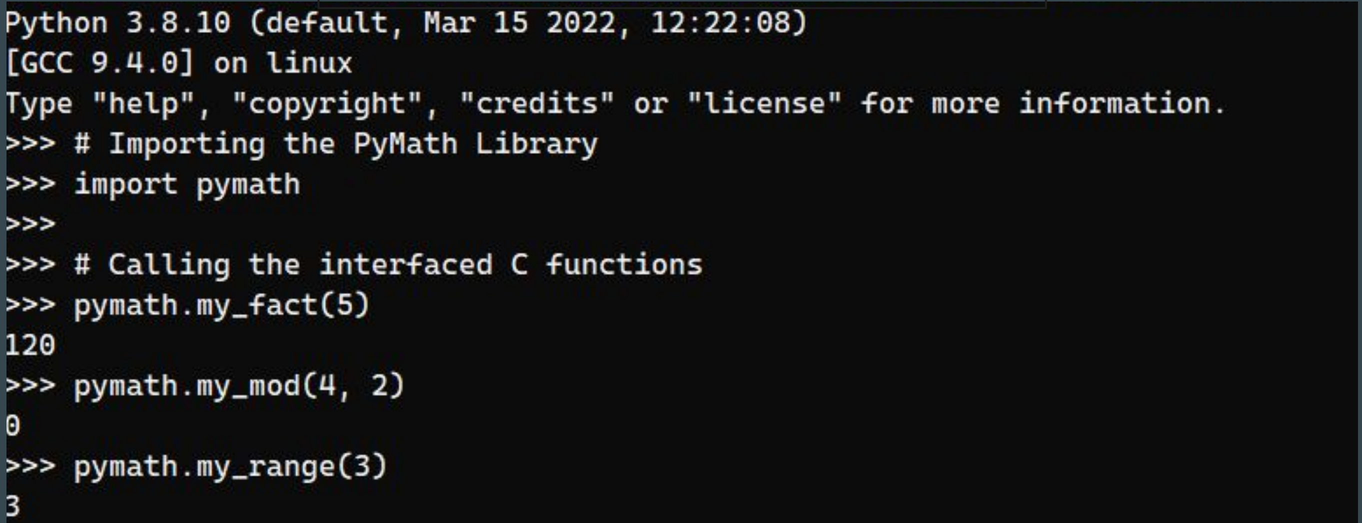


```
  if (!args) SWIG_fail;
  swig_obj[0] = args;
  ecode1 = SWIG_AsVal_int(swig_obj[0], &val1);
  if (!SWIG_IsOK(ecode1)) {
    SWIG_exception_fail(SWIG_ArgError(ecode1), "in method '" "my_fact" "', argument " "1"" of type '" "int""'");
  }
  arg1 = (int)(val1);
  result = (math_int)my_fact(arg1);
  resultobj = SWIG_From_int((int)(result));
  return resultobj;
fail:
  return NULL;
}
```

File 4: Shared Library (.so)

- The library of C functions which users will import into Python
- Contains the compiled wrapper code and object code for the C functions

Using the PyMath library in Python



```
Python 3.8.10 (default, Mar 15 2022, 12:22:08)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> # Importing the PyMath Library
>>> import pymath
>>>
>>> # Calling the interfaced C functions
>>> pymath.my_fact(5)
120
>>> pymath.my_mod(4, 2)
0
>>> pymath.my_range(3)
3
```

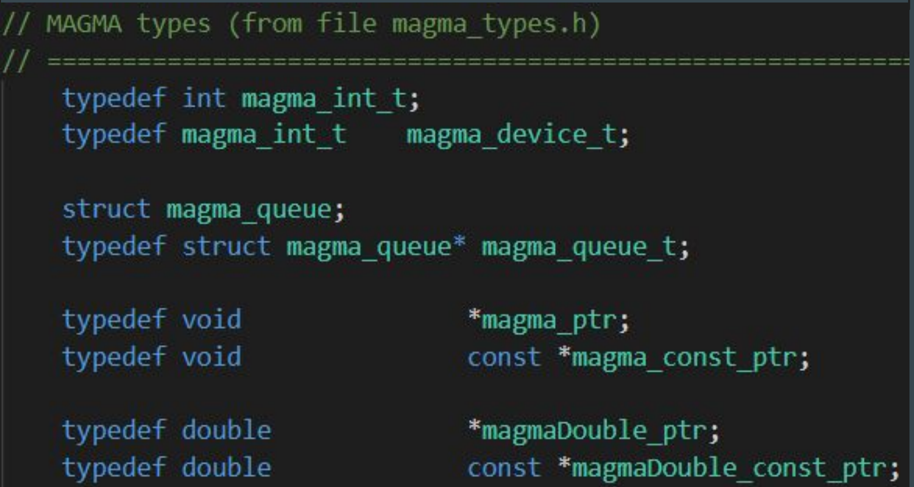
Creating PyMAGMA

Header File (*pymagma.h*)

Header File

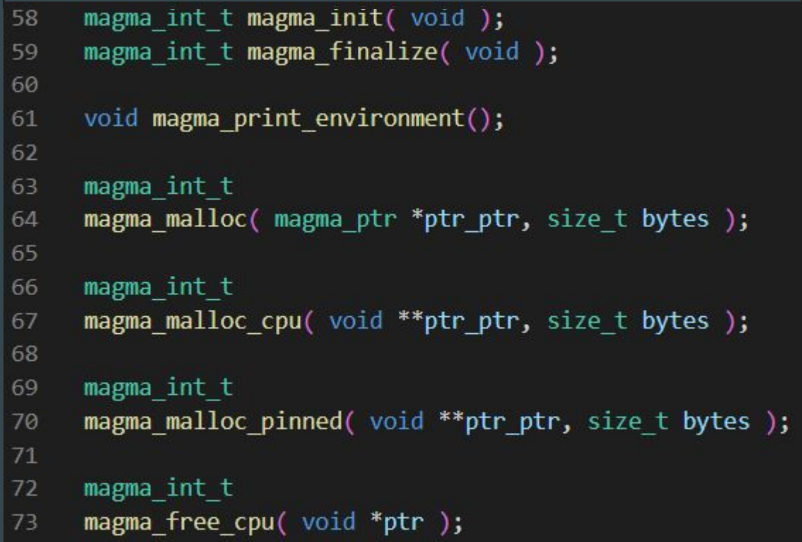
- ➢ Contained typedefs and declarations for the MAGMA functions which we wanted to use in Python
- ➢ Previous Errors
  - ○ *‘Magma_trans_t was not declared in this scope’*

Example Typedefs for MAGMA Functions



```
// MAGMA types (from file magma_types.h)
// ===============================================================
   typedef int magma_int_t;
   typedef magma_int_t    magma_device_t;

   struct magma_queue;
   typedef struct magma_queue* magma_queue_t;

   typedef void               *magma_ptr;
   typedef void               const *magma_const_ptr;

   typedef double             *magmaDouble_ptr;
   typedef double             const *magmaDouble_const_ptr;
```

Example C++ declarations from MAGMA

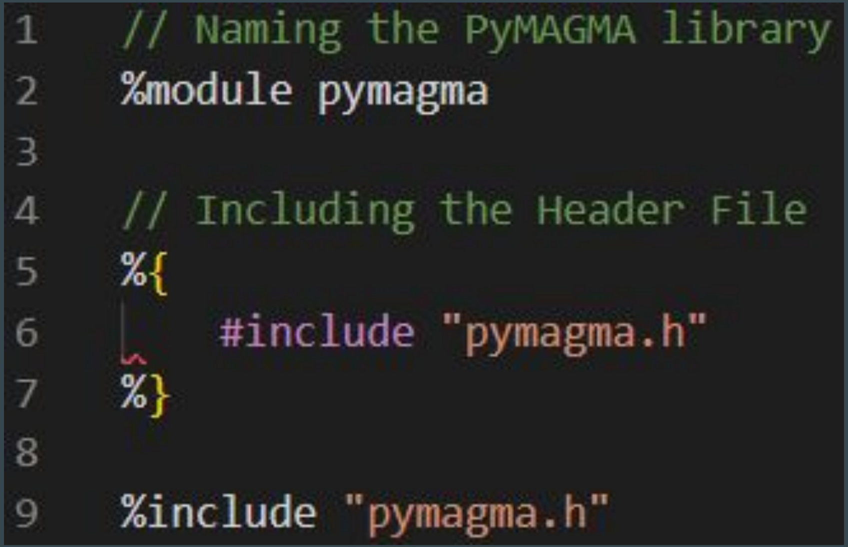


```
magma_int_t magma_init( void );
magma_int_t magma_finalize( void );

void magma_print_environment();

magma_int_t
magma_malloc( magma_ptr *ptr_ptr, size_t bytes );

magma_int_t
magma_malloc_cpu( void **ptr_ptr, size_t bytes );

magma_int_t
magma_malloc_pinned( void **ptr_ptr, size_t bytes );

magma_int_t
magma_free_cpu( void *ptr );
```

Interface File (*pymagma.i*)

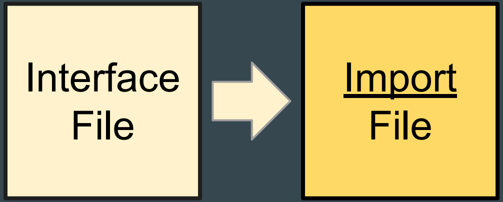
Header File → Interface File

- Where we specified the name of the library we were creating (PyMAGMA)
- Contains two include statements for the py*magma.h* header file



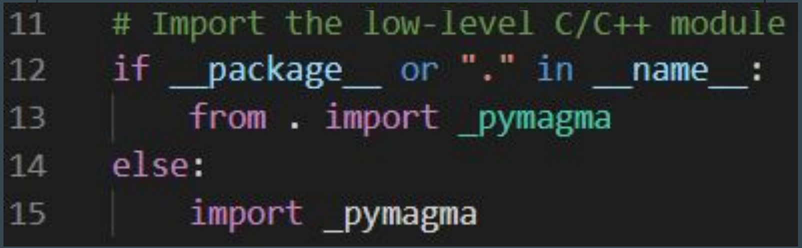
```
// Naming the PyMAGMA library
%module pymagma

// Including the Header File
%{
    #include "pymagma.h"
%}

%include "pymagma.h"
```

Import File (*pymagma.py*)



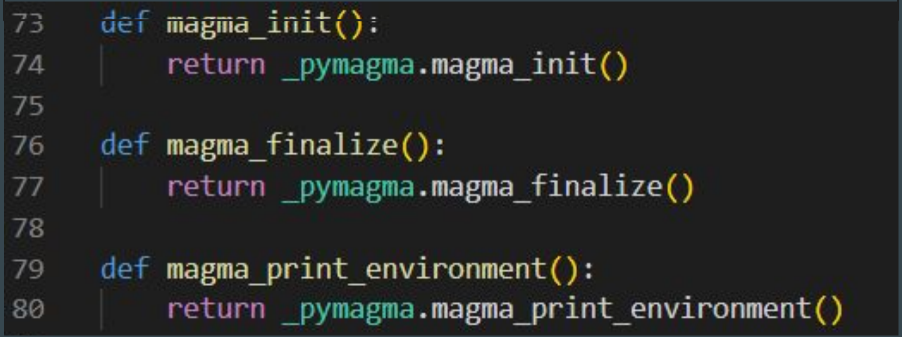
- Contained the Python statement for importing the PyMAGMA library into Python once it was built (Line 15)
- Included Python functions for calling the C++ code from MAGMA (Lines 73-80)
- Created with the command `swig -DSWIG_NO_CPLUSPLUS_CAST -c++ -python pymagma.i`

The Python import statements



```
11   # Import the low-level C/C++ module
12   if __package__ or "." in __name__:
13       from . import _pymagma
14   else:
15       import _pymagma
```

Python functions which call MAGMA functions in the PyMAGMA library



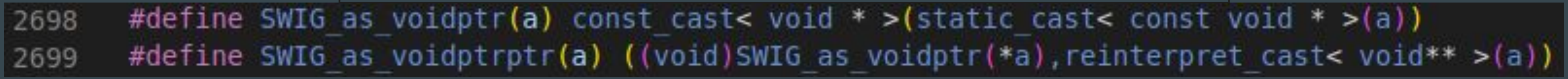
```
73   def magma_init():
74       return _pymagma.magma_init()
75
76   def magma_finalize():
77       return _pymagma.magma_finalize()
78
79   def magma_print_environment():
80       return _pymagma.magma_print_environment()
```

Wrapper File (*pymagma_wrap.cxx*)

Interface File → Wrapper File

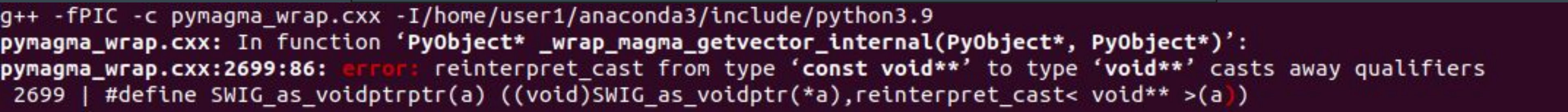
- Contained the wrapper code for translating the MAGMA functions to the Python interpreter
- Created with the command `swig -DSWIG_NO_CPLUSPLUS_CAST -c++ -python pymagma.i`
- Previous errors
    - *reinterpret_cast from type 'const void**'...*

Wrapper Code Source of Error



```
2698    #define SWIG_as_voidptr(a) const_cast< void * >(static_cast< const void * >(a))
2699    #define SWIG_as_voidptrptr(a) ((void)SWIG_as_voidptr(*a),reinterpret_cast< void** >(a))
```

Compilation Error

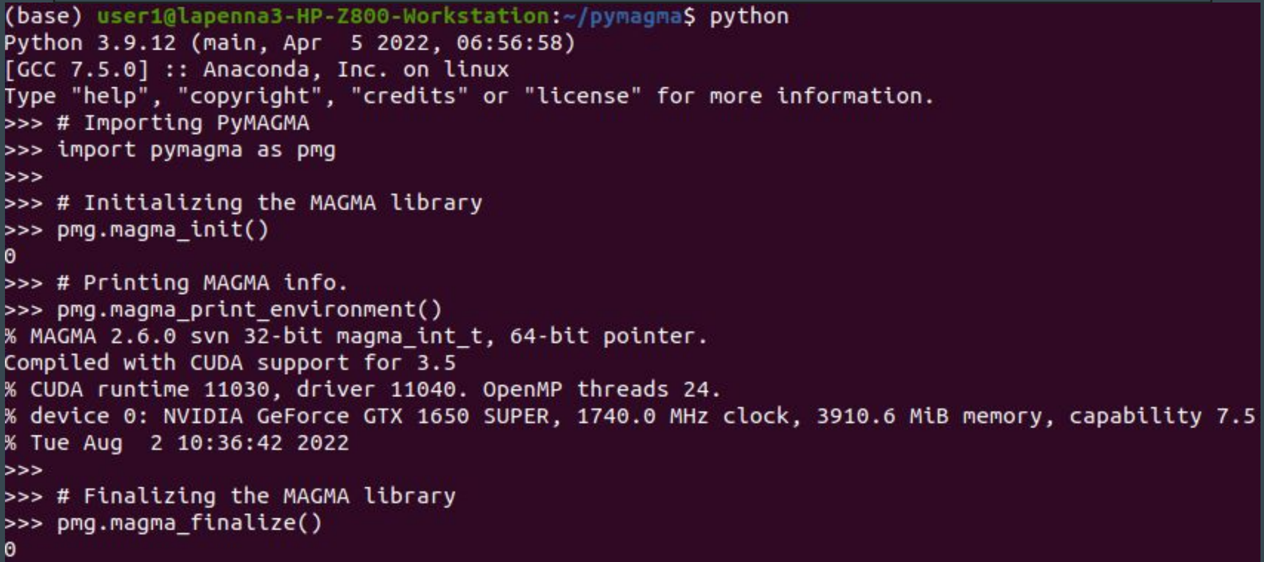


```
g++ -fPIC -c pymagma_wrap.cxx -I/home/user1/anaconda3/include/python3.9
pymagma_wrap.cxx: In function ‘PyObject* _wrap_magma_getvector_internal(PyObject*, PyObject*)’:
pymagma_wrap.cxx:2699:86: error: reinterpret_cast from type ‘const void**’ to type ‘void**’ casts away qualifiers
 2699 | #define SWIG_as_voidptrptr(a) ((void)SWIG_as_voidptr(*a),reinterpret_cast< void** >(a))
```

Shared Library (*_pymagma.so*)

- Created with the command `ld -shared /home/user1/magma/lib/libmagma.so pymagma_wrap.o -o _pymagma.so`

Using three MAGMA functions in Python with PyMAGMA



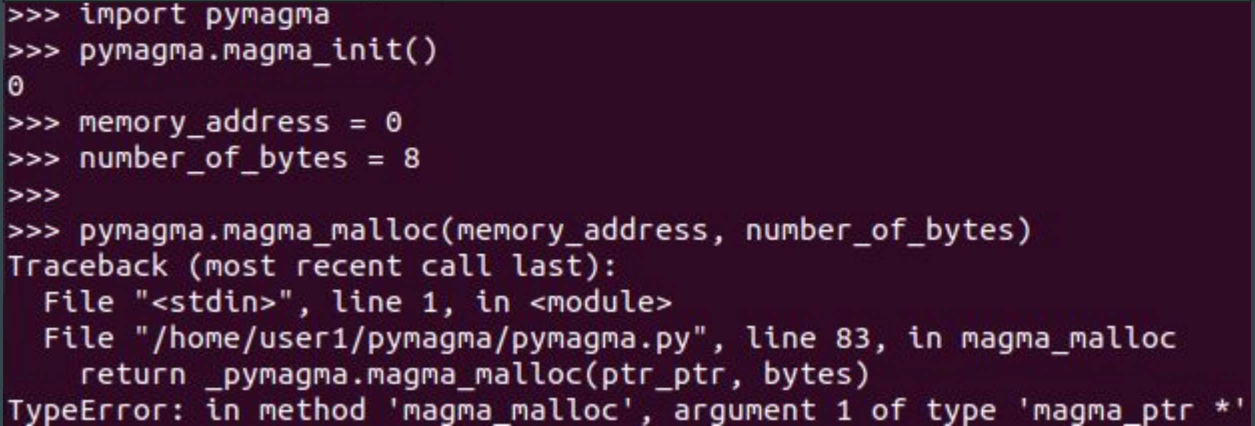
```
(base) user1@lapenna3-HP-Z800-Workstation:~/pymagma$ python
Python 3.9.12 (main, Apr  5 2022, 06:56:58)
[GCC 7.5.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> # Importing PyMAGMA
>>> import pymagma as pmg
>>>
>>> # Initializing the MAGMA library
>>> pmg.magma_init()
0
>>> # Printing MAGMA info.
>>> pmg.magma_print_environment()
% MAGMA 2.6.0 svn 32-bit magma_int_t, 64-bit pointer.
Compiled with CUDA support for 3.5
% CUDA runtime 11030, driver 11040. OpenMP threads 24.
% device 0: NVIDIA GeForce GTX 1650 SUPER, 1740.0 MHz clock, 3910.6 MiB memory, capability 7.5
% Tue Aug  2 10:36:42 2022
>>>
>>> # Finalizing the MAGMA library
>>> pmg.magma_finalize()
0
```

Extending PyMAGMA

Pointer Error

- Many C++ functions in MAGMA require pointer types as arguments, but Python users cannot normally create pointers in Python!
- How do we resolve this *pointer* error???

Trying to call the *magma_malloc()*, which expects a pointer argument, through PyMAGMA



```
>>> import pymagma
>>> pymagma.magma_init()
0
>>> memory_address = 0
>>> number_of_bytes = 8
>>>
>>> pymagma.magma_malloc(memory_address, number_of_bytes)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
  File "/home/user1/pymagma/pymagma.py", line 83, in magma_malloc
    return _pymagma.magma_malloc(ptr_ptr, bytes)
TypeError: in method 'magma_malloc', argument 1 of type 'magma_ptr *'
```

We create new “pointerless” functions in PyMAGMA which call their “pointer” counterparts!

pymagma_malloc_cpu()

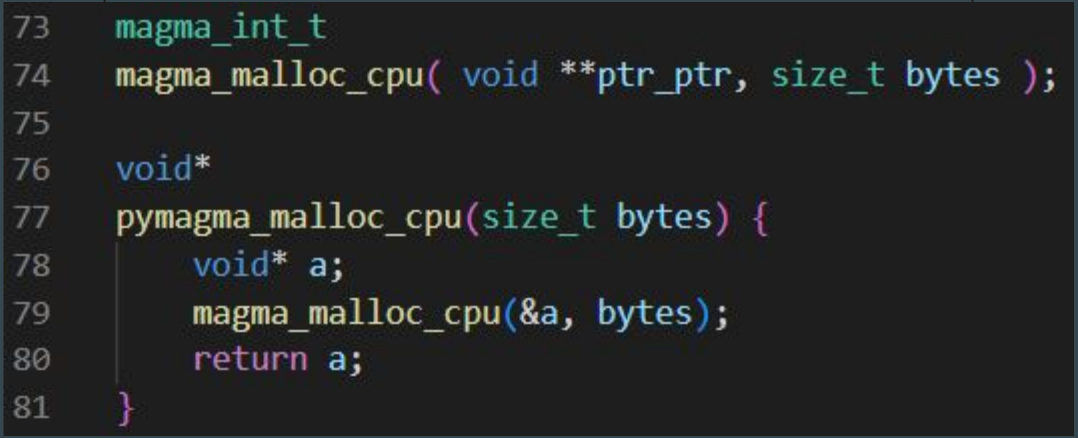
Base Address 824	Address 825	Address 826	Address 827	Address 828

- ➢ Purpose
  - ○ Dynamically allocates a user-specified number of bytes for a block of CPU memory
- ➢ Returns
  - ○ The base address of the allocated block of CPU memory

Additional Added Functions:

- *pymagma_malloc()*
- *pymagma_free()*
- *pymagma_malloc_pinned()*
- *pymagma_free_pinned()*
- *pymagma_queue_create()*
- *pymagma_queue_destroy()*
- *pymagma_queue_sync()*

The definition for *pymagma_malloc_cpu()*



```
magma_int_t
magma_malloc_cpu( void **ptr_ptr, size_t bytes );

void*
pymagma_malloc_cpu(size_t bytes) {
    void* a;
    magma_malloc_cpu(&a, bytes);
    return a;
}
```

pymagma_sarray_cpu()

$$\begin{pmatrix} \qquad & \qquad \\ & \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

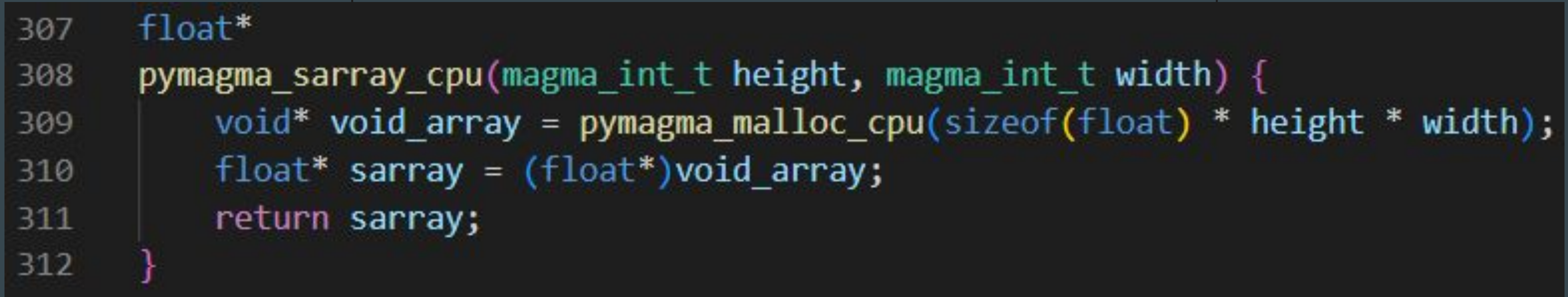
Purpose:

- Creates a matrix of floats by dynamically allocating a *height x width* block of memory for floats on the CPU

Returns:

- The base address of the allocated block of memory

The definition for *pymagma_sarray_cpu()*



```
float*
pymagma_sarray_cpu(magma_int_t height, magma_int_t width) {
    void* void_array = pymagma_malloc_cpu(sizeof(float) * height * width);
    float* sarray = (float*)void_array;
    return sarray;
}
```

pymagma_sset_cpu()

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Rightarrow \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

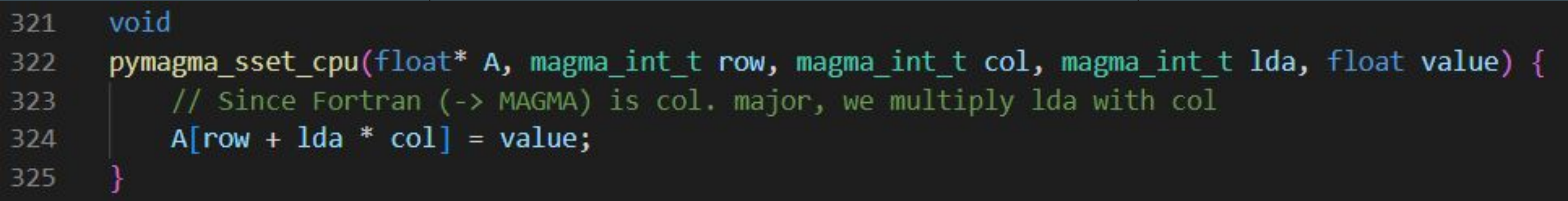
Purpose:

- Changes the value at a given position in a matrix of floats on the CPU

Returns:

- N/A

The definition for *pymagma_sset_cpu()*



```c
void
pymagma_sset_cpu(float* A, magma_int_t row, magma_int_t col, magma_int_t lda, float value) {
    // Since Fortran (-> MAGMA) is col. major, we multiply lda with col
    A[row + lda * col] = value;
}
```

pymagma_sprint_cpu()

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

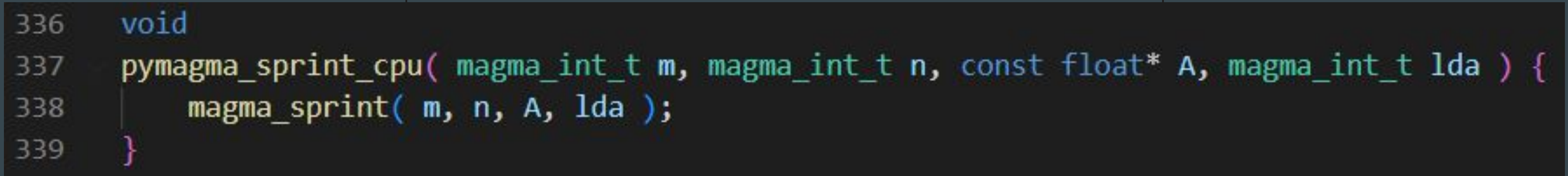
Purpose:

- Prints an array of floats stored on the CPU

Returns:

- N/A

The definition for *pymagma_sprint_cpu()*



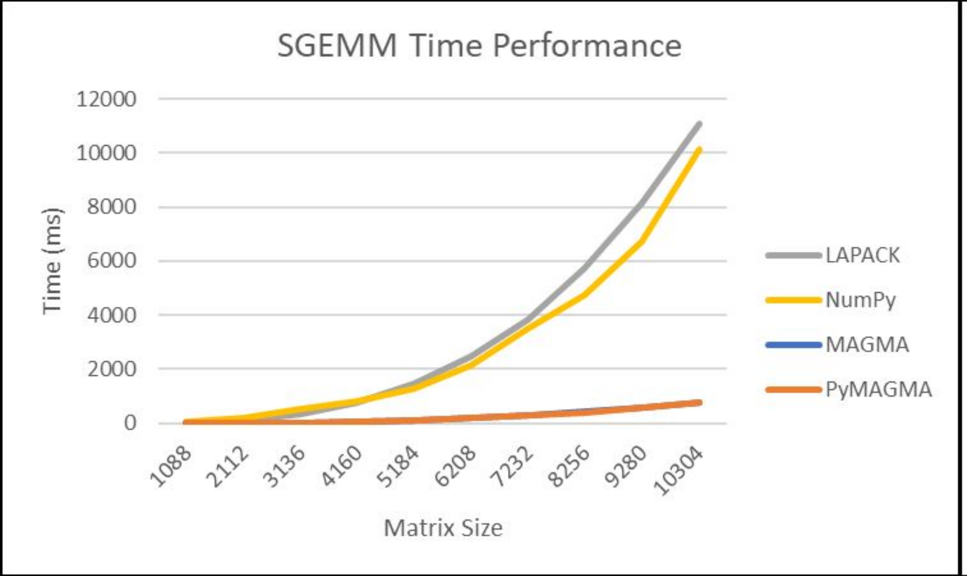
```
void
pymagma_sprint_cpu( magma_int_t m, magma_int_t n, const float* A, magma_int_t lda ) {
    magma_sprint( m, n, A, lda );
}
```

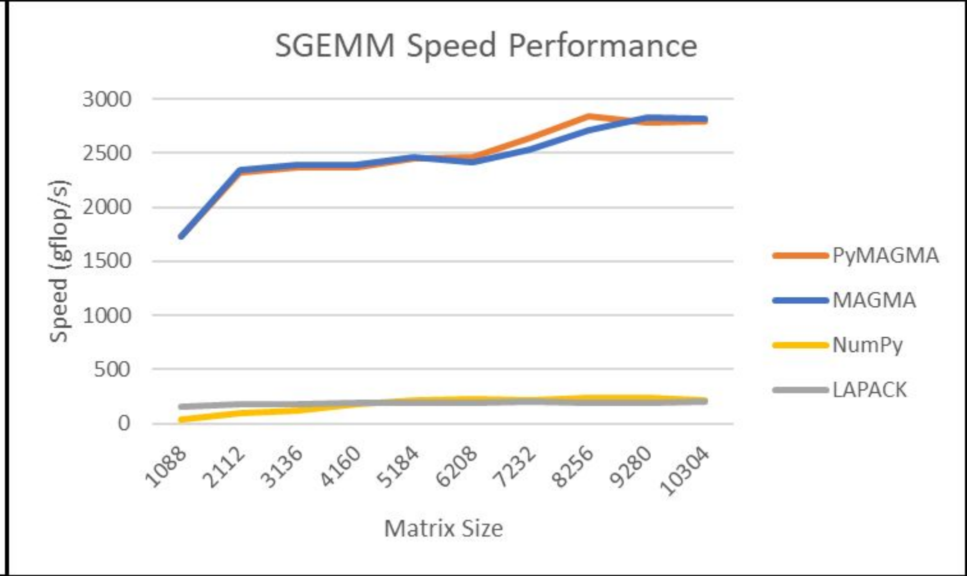
Performing SGEMM with PyMAGMA

SGEMM Performance (C = -AB + C)

Takeaways:

- ➢ PyMAGMA performs SGEMM with a similar time and speed to MAGMA
- ➢ Like MAGMA, PyMAGMA performs faster than LAPACK and NumPy





Conclusion and Future Work

Conclusion

- We successfully used SWIG to build PyMAGMA, an interface through which currently ~34 functions in MAGMA can be used with Python
- We learned that PyMAGMA can perform SGEMM with similar speeds to MAGMA
- We learned that we can easily add functions to PyMAGMA by adding their declaration/definition to py*magma.h*

Future Work

- Research how SWIG typemaps can be used to direct SWIG in how to wrap pointer arguments
- Research how to use SWIG with foreign data types (e.g., NumPy arrays)

Acknowledgments and References

Acknowledgments

- National Science Foundation (NSF)
- Innovative Computing Laboratory (ICL)
- National Institute of Computational Sciences (NICS)

References

- Stanimire Tomov, Jack Dongarra, Marc Baboulin, “Towards dense linear algebra for hybrid GPU accelerated manycore systems,” Parallel Computing, Volume 36, Issues 5-6, 2010, Pages 232-240, ISSN 0167-8191
- LAPACK - Linear Algebra PACKage (2022, April 12). Retrieved from https://netlib.org/lapack/.
- PEP 8 — the Style Guide for Python Code. Retrieved from https://pep8.org/
- PyTorch. Retrieved from https://pytorch.org/.
- SWIG-4.0 Documentation [PDF file]. Retrieved from https://swig.org/Doc4.0/SWIGDocumentation.pdf.
- Welcome to SWIG. (2019, April 18). Retrieved from https://swig.org/.