Extending the Cppyy support in Numba

Progress Update

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cppyy

Numba

RECAP

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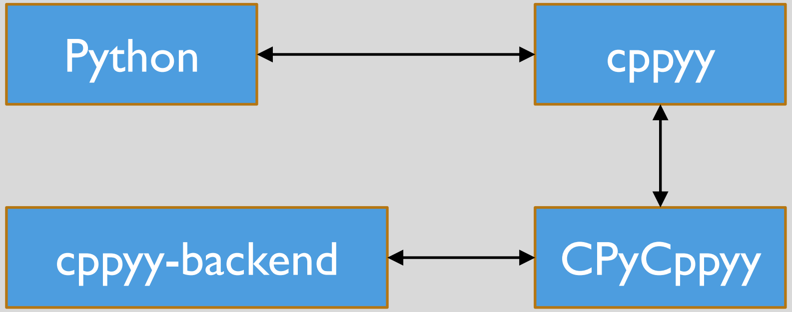
- **Cppyy**:
  An automatic, run-time, Python-C++ bindings generator
- **Cling**
  is used in Cppyy's backend since an interactive C++ interpreter provides a runtime exec approach to C++ code

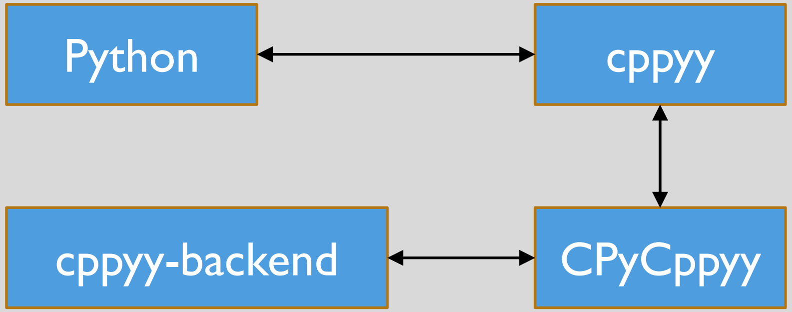



```
cppyy.cppdef(r"""\
struct MyNumbaData03 {
    MyNumbaData03(int64_t i1, int64_t i2) : fField1(i1), fField2(i2) {}
    int64_t fField1;
    int64_t fField2;
};""")
```

```
@numba.jit(nopython=True)
def go_fast(a, d):
    trace = 0.0
    for i in range(a.shape[0]):
        trace += d.fField1 + d.fField2
    return a + trace
```

INTRODUCTION

- **Cppyy**:
  An automatic, run-time, Python-C++ bindings generator
- **Cling**
  is used in backend since an interactive C++ interpreter provides a runtime exec approach to C++ code



WHY USE NUMBA?

- **Numba**
  JIT compiler that translates Python and NumPy code into fast machine code.
- The compute time overhead while switching between languages accumulates in loops with cppyy objects.

```
def go_slow(a):
    trace = 0.0
    for i in range(a.shape[0]):
        trace += cppyy.gbl.tanh(a[i, i])
    return a + trace

@numba.njit
def go_fast(a):
    trace = 0.0
    for i in range(a.shape[0]):
        trace += cppyy.gbl.tanh(a[i, i])
    return a + trace
```

- Numba optimizes the loop and compiles it into machine code which crosses the language barrier only once

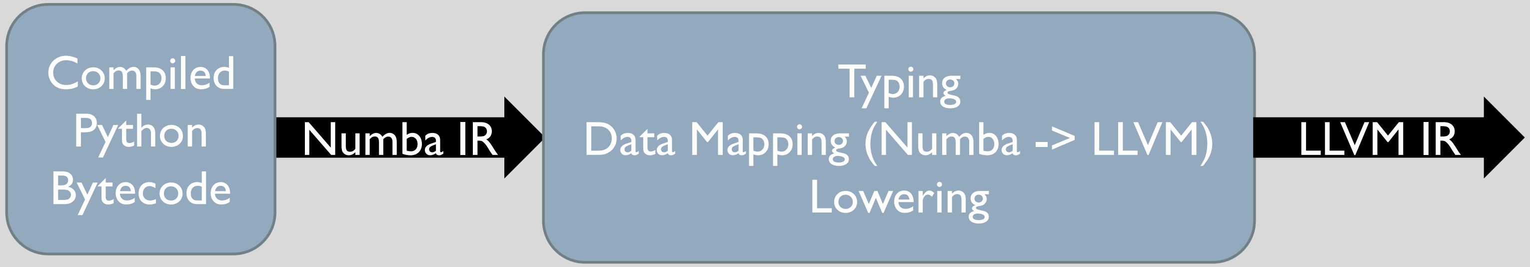
```
x = np.arange(10000, dtype=np.float64).reshape(100, 100)
run_jit_test(x)

✓ 0.1s

Numba disabled = 0.10824203491210938 ms
Numba typeinfer in dispatcher: array(float64, 2d, C)
Numba njit enabled = 0.007867813110351562 ms
```

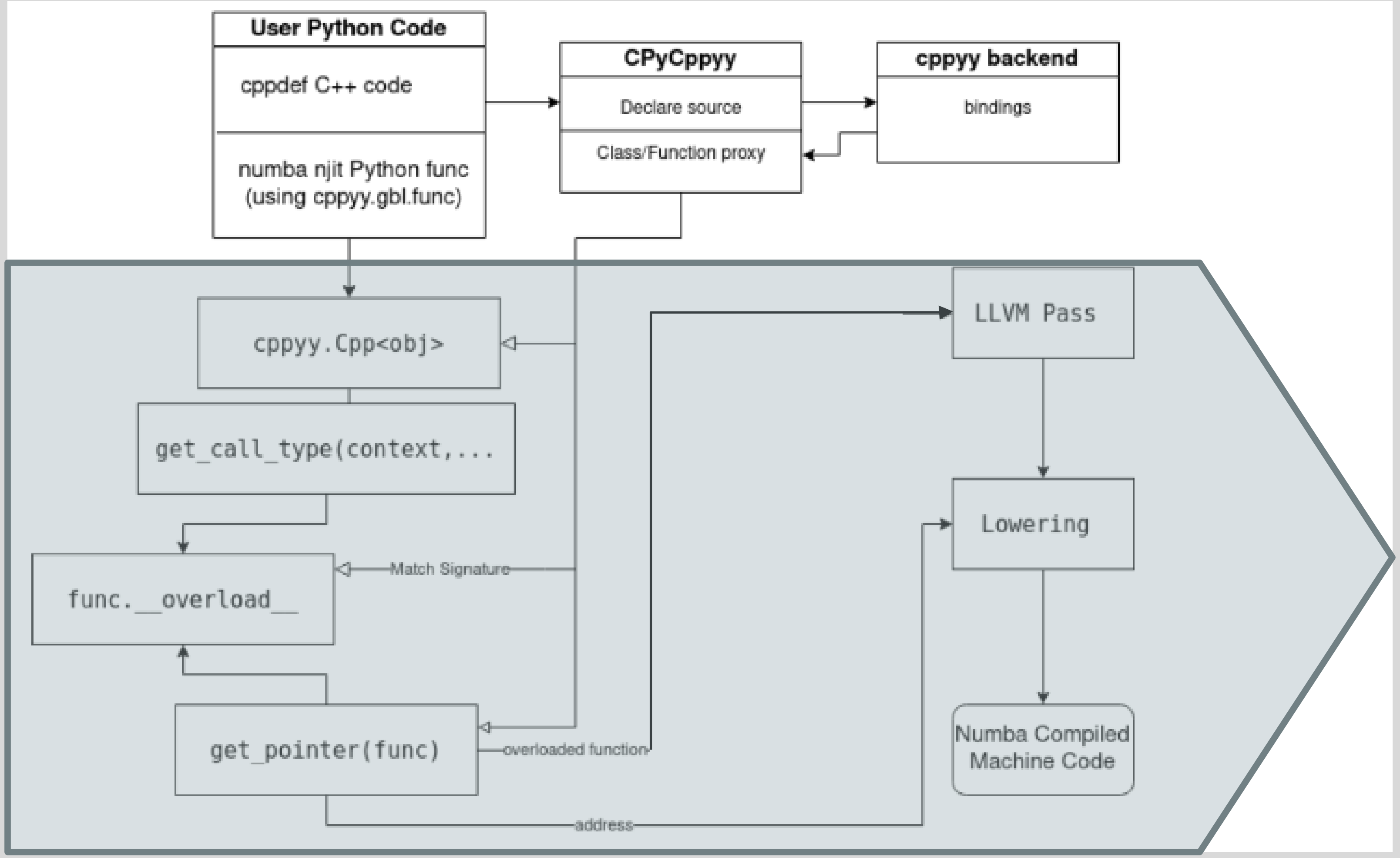
NUMBA PIPELINE

- **Typing**
  Numba core has a type inference algorithm which assigns a nb_type for a variable
- **Lowering**
  Numba lowers high-level Python operations into low-level LLVM code.
  Exploits typing to map to LLVM type
- **Boxing and unboxing**
  convert PyObject* 's into native values, and vice-versa.



We utilise the runtime numba compilation process to lower C++ code cppdef'ed in Python
How? →

NUMBA LOW LEVEL EXTENSION API



CPPYY NUMBA SUPPORT
cppyy/numba_ext.py

STATUS

Currently, the following functionality has been added to Cppyy's numba extension:

- Extended typing and non type template definition support [Test 9]
- nJIT function pointers to C++ functions that return a reference type [Test 10]
- nJIT support for pointers and reference types to builtins and std::vectors [Test 11- 13]
- Successful typing and overload matching for Eigen templated classes [Test 14]

POINTER AND REFERENCE TYPE SUPPORT

- The Numba extension now supports njitting ref types, const refs and pointers to C++ methods/functions
- The results are reflected directly on the python side using the ctypes interface that provides a "pointer-like" behaviour that can be emulated in Python

```
cppyy.cppdef("""
  namespace RefTest {
    class Box{
      public:
        long a;
        long *b;
        long *c;
        Box(long i, long& j, long& k){
        a = i;
        b = &j;
        c = &k;
        }

        void swap_ref(long &a, long &b) {
            long temp = a;
            a = b;
            b = temp;
         }

        void inc(long* value) {
         (*value)++;
         }
      };
    }
  """)
```

```
ns = cppyy.gbl.RefTest
assert ns.Box.__dict__['a'].__cpp_reflex__(cppyy.reflex.TYPE) == 'long'
assert ns.Box.__dict__['b'].__cpp_reflex__(cppyy.reflex.TYPE) == 'long*'

@numba.njit()
def inc_b(d, k):
    for i in range(k):
        d.inc(d.b)

@numba.njit()
def inc_c(d, k):
    for i in range(k):
        d.inc(d.c)

x = random.randint(1, 5000)
y = random.randint(1, 5000)
z = random.randint(1, 5000)
b = ctypes.c_long(y)
c = ctypes.c_long(z)
```

```
d = ns.Box(x, b, c)
k = 5000
```

Here the members of Box class are initialized via pass-by-ref

```
x = 2856
y = 1896
```

```
inc_b(d, k)
inc_c(d, k)

assert b.value == y + k
assert c.value == z + k
```

Args :
CppClass(Box)
int64

Result:
d.b, d.c are incremented through *pointers*

POINTER AND REFERENCE TYPE SUPPORT

The "pointer" like behavior is especially useful in cases like these

```
cppyy.cppdef("""
  namespace RefTest {
      class Box{
          public:
              long a;
              long *b;
              long *c;
              Box(long i, long& j, long& k){
              a = i;
              b = &j;
              c = &k;
              }

              void swap_ref(long &a, long &b) {
                  long temp = a;
                  a = b;
                  b = temp;
               }

              void inc(long* value) {
               (*value)++;
               }
          };
      }
  """)
```

x, b = 2856
y, c = 1893

```
inc_b(d, k)
inc_c(d, k)

assert b.value == y + k
assert c.value == z + k
```

b = 7856,
c = 6893

Now we call a swap by ref function which causes b and c to automatically swap on the python side

b = 7856,
c = 6893

```
d.swap_ref(d.b, d.c)

assert b.value == z + k
assert c.value == y + k
```

b = 6893,
c = 7856

POINTER AND REFERENCE TYPE SUPPORT

The fact that Numba lowers cppyy calls using C++ pointers to LLVM IR opens the avenue of significant speedups

```
label 0:
    d = arg(0, name=d)                          ['d']
    k = arg(1, name=k)                          ['k']
    $2load_global.0 = global(range: <class 'range'>) ['$2load_global.0']
    $6call_function.2 = call $2load_global.0(k, func=$2load_global.0, args=[Var(k, test_numba.py:433)], kws=(), vararg=None, varkwarg=None, t
    $8get_iter.3 = getiter(value=$6call_function.2) ['$6call_function.2', '$8get_iter.3']
    $phi10.0 = $8get_iter.3                     ['$8get_iter.3', '$phi10.0']
    jump 10                                     []
label 10:
    $10for_iter.1 = iternext(value=$phi10.0) ['$10for_iter.1', '$phi10.0']
    $10for_iter.2 = pair_first(value=$10for_iter.1) ['$10for_iter.1', '$10for_iter.2']
    $10for_iter.3 = pair_second(value=$10for_iter.1) ['$10for_iter.1', '$10for_iter.3']
    $phi12.1 = $10for_iter.2                    ['$10for_iter.2', '$phi12.1']
    branch $10for_iter.3, 12, 28                ['$10for_iter.3']
label 12:
    i = $phi12.1                                ['$phi12.1', 'i']
    $16load_method.3 = getattr(value=d, attr=inc) ['$16load_method.3', 'd']
    $20load_attr.5 = getattr(value=d, attr=c) ['$20load_attr.5', 'd']
    $22call_method.6 = call $16load_method.3($20load_attr.5, func=$16load_method.3, args=[Var($20load_attr.5, test_numba.py:434)], kws=(), va
    jump 10                                     []
label 28:
    $const28.0 = const(NoneType, None)          ['$const28.0']
    $30return_value.1 = cast(value=$const28.0) ['$30return_value.1', '$const28.0']
    return $30return_value.1                    ['$30return_value.1']

Numba Base Function pointer call funcptr:  %".135" = bitcast i8* %".134" to i8* (i8*, i64*)*
Numba Base Function pointer call args:  [<ir.CastInstr '.128' of type 'i8*', opname 'bitcast', operands [<ir.LoadInstr '.127' of type '{i64,
```

STD::VECTOR<>* AND NUMPY ARRAYS

We can explore those speedups by also adding pointer and reference support to std::vector objects

This is achieved by constructing IR Pointer Types to Array and Vector Types, that point to cppyy.gbl.std.vector() objects linked to numpy arrays for initialization

```
cppyy.cppdef("""
template<typename T>
std::vector<T> make_vector(const std::vector<T>& v, std::vector<T> l) {
    std::vector<T> u(l);
    u.insert(u.end(), v.begin(), v.end());
    return u;
}
    namespace RefTest {
        class BoxVector{
            public:
                std::vector<long>* a;

                BoxVector() : a(new std::vector<long>()) {}
                BoxVector(std::vector<long>* i) : a(i){}

                void square_vec(){
                for (auto& num : *a) {
                    num = num * num;
                 }
                }

                 void add_2_vec(long k){
                for (auto& num : *a) {
                    num = num + k;
                 }
                }

                 void append_vector(const std::vector<long>& value) {
                    *a = make_vector(value, *a);
                 }
               };
            }
    """)
```

```
a = np.random.randint(1, 100, size=10000, dtype=np.int64)
b = np.random.randint(1, 4, size=10, dtype=np.int64)

x = cppyy.gbl.std.vector['long'](a.flatten())
y = cppyy.gbl.std.vector['long'](b.flatten())
```

```
Aaron Jomy
@numba.njit()
def square_vec_fast(d):
    for i in range(5):
        d.square_vec()

Aaron Jomy
@numba.njit()
def square_vec_slow(x):
    for i in range(5):
        x = np.square(x)
    return x
```

```
Aaron Jomy
@numba.njit()
def add_vec_fast(d):
    for i in range(10000):
        d.add_2_vec(i)

Aaron Jomy
@numba.njit()
def add_vec_slow(x):
    for i in range(10000):
        x = x + i
    return x
```

```
t0 = time.time()
square_vec_fast(ns.BoxVector(y))
time_square_njit = time.time() - t0
```

Here the members of the BoxVector class are initialized via pass-by-ref within the python function call

STD::VECTOR<>* AND NUMPY ARRAYS

Initial benchmarks with Numpy-C++ equivalent functions for the same operations:

```
t0 = time.time()
add_vec_fast(ns.BoxVector(x))
time_add_njit = time.time() - t0

t0 = time.time()
square_vec_fast(ns.BoxVector(y))
time_square_njit = time.time() - t0
```

```
assert (np.array(y) == np_square_res).all()
assert (np.array(x) == np_add_res).all()
```

Directly access the result since the Numba obtains the cling address to the cppyy.gbl.std.vector

Njitted Cppyy function
Standard loop over numpy function

```
njit execution time: 20.38860321044922
numpy execution time: 77.96597480773926
njit execution time: 0.058174133300078125
numpy execution time: 0.2288818359375
```

Njitted Cppyy function
Njitted Numpy function

```
cppyy execution time: 17.93956756591797
numpy execution time: 368.68953704833984
cppyy execution time: 0.042438507080078125
numpy execution time: 291.74327850341797
```

STD::VECTOR<>* AND NUMPY ARRAYS

Exploring vectorization speedups with a dot product operation

```
cppyy.cppdef("""
namespace RefTest {
    class DotVector{
        private:
            std::vector<long>* a;
            std::vector<long>* b;

        public:
            long g = 0;
            long *res = &g;
            DotVector(std::vector<long>* i, std::vector<long>* j) : a(i), b(j) {}

            long dot_product(const std::vector<long>& vec1, const std::vector<long>& vec2) {
                                long result = 0;
                                for (size_t i = 0; i < vec1.size(); ++i) {
                                    result += vec1[i] * vec2[i];
                                }
                                return result;
            }
        };
    }""")
```

Initialising using pointers
Running the dot product through pass-by-ref

STD::VECTOR<>* AND NUMPY ARRAYS

Exploring vectorization speedups with a dot product operation

```
cppyy.cppdef("""
namespace RefTest {
    class DotVector{
        private:
            std::vector<long>* a;
            std::vector<long>* b;

        public:
            long g = 0;
            long *res = &g;
            DotVector(std::vector<long>* i, std::vector<long>* j) : a(i), b(j) {}

            long self_dot_product() {
                long result = 0;
                size_t size = a->size();  // Cache the vector size
                const long* data_a = a->data();
                const long* data_b = b->data();

                for (size_t i = 0; i < size; ++i) {
                    result += data_a[i] * data_b[i];
                }
                return result;
            }
```

Even faster dot product by using the DotVector datamembers which are in turn std::vector pointers

STD::VECTOR<>* AND NUMPY ARRAYS

Exploring vectorization speedups with a dot product operation

```python
# Aaron Jomy
@numba.njit()
def dot_product_fast(d):
    res = 0
    for i in range(10000):
        res += d.self_dot_product()
    return res
# Aaron Jomy
def np_dot_product(x, y):
    res = 0
    for i in range(10000):
        res += np.dot(x, y)
    return res
```

```python
x = cppyy.gbl.std.vector['long'](a.flatten())
y = cppyy.gbl.std.vector['long'](b.flatten())
d = ns.DotVector(x, y)
dot_product_fast(d)
res = 0

t0 = time.time()
njit_res = dot_product_fast(d)
time_njit = time.time() - t0

res = 0
t0 = time.time()
res = np_dot_product(x, y)
time_np = time.time() - t0
```

SOME BENCHMARK TRENDS

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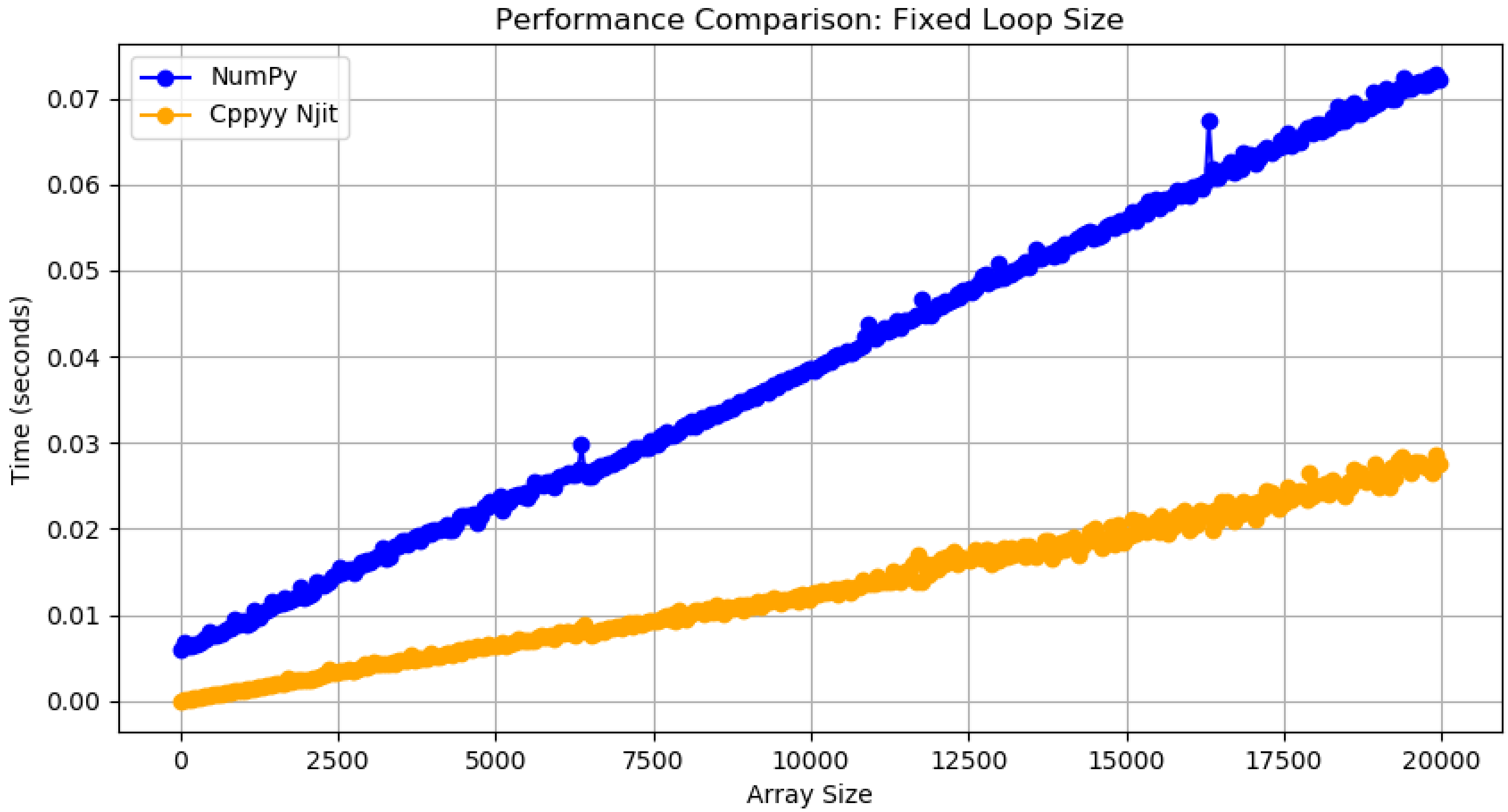

CURRENT STATUS WITH EIGEN

Templated class args like Eigen are resolved to cpp types and successfully matches the CPPOverloads in those cases

The Eigen numba typeinfer is refactored into the C++ expression and handled in numba2cpp

Able to handle the templated class Eigen::Matrix< Scalar_, Rows_, Cols_, Options_, MaxRows_, MaxCols_ > using Eigen::Dynamic
so the dispatcher typeinfer is CppClass(Eigen::Matrix<double,-1,-1,0,-1,-1>)

```
# Define the templated function that takes Eigen objects
cppyy.cppdef('''
template<typename T>
T multiply_scalar(T value, int64_t scalar) {
    return value * scalar;
}
''')
```

```
Return type: <class cppyy.gbl.Eigen.Matrix<float,3,1,0,3,1> at 0x73d66d0>
VAL: <class cppyy.gbl.Eigen.Matrix<float,3,1,0,3,1> at 0x73d66d0> type: <class 'Matrix<float,3,1,0,3,1>_meta'>
```

```
> c = {_UnboxContext: 3} _UnboxContext(context=<numba.core.cpu.CPUContext obj
> obj = {LoadInstr} %".21" = load i8*, i8** %".5"
> self = {PythonAPI} <numba.core.pythonapi.PythonAPI object at 0x7fdf9591ad30>
> typ = {ImplClassType} CppClass(Eigen::Matrix<float,3,1,0,3,1>)
```

Thank You!

Aaron Jomy