Interfacing C++/CUDA with Python

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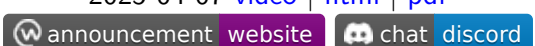
2025-04-07 video | html | pdf



History

Context

ctypes

https://docs.python.org/3/library/ctypes.html

- *Foreign Function Interface* (FFI)

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- Hack to call C/C++ functions from Python

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- *Foreign Function Interface* (FFI)
- Hack to call C/C++ functions from Python
- e.g. https://github.com/gschramm/square_array

ctypes example

```
import ctypes
lib = ctypes.CDLL("./libmy_experiment.so")

# (re)define function signature for `void myfunc(float*, size_t)`
lib.myfunc.argtypes = [ctypes.c_void_p, ctypes.c_size_t]
lib.myfunc.restype = None

input_array = np.array([1, 2, 3], dtype=np.float32)
# call function
lib.myfunc(
    input_array.ctypes.data_as(ctypes.POINTER(ctypes.c_float)),
    ctypes.c_size_t(len(input_array)))
```

CPython API

https://docs.python.org/3/c-api/intro.html

- "correct" way to call C/C++ functions from Python

CPython API example

```
#include <Python.h>
#include <numpy/arrayobject.h>

static PyObject *myfunc(PyObject *self, PyObject *args) {
  PyObject *arr = NULL;
  if (!PyArg_ParseTuple(args, "O", &arr)) return NULL;
  PyArrayObject *np_arr = PyArray_FROM_OTF(
    arr, NPY_FLOAT32, NPY_ARRAY_INOUT_ARRAY);
  float *arr_ptr = PyArray_DATA(np_arr);
  npy_intp *size = PyArray_SHAPE(np_arr);
  for (size_t i = 0; i < size[0]; ++i) arr_ptr[i] *= 2;
}
```

```c
static struct PyModuleDef my_module = {
  PyModuleDef_HEAD_INIT,
  .m_name = "my_experiment"
};
static PyMethodDef my_methods[] = {
  {"myfunc", myfunc, METH_VARARGS, "In-place modifies ndarray[float]"},
  {NULL, NULL, 0, NULL} // Sentinel
};
PyMODINIT_FUNC PyInit_spam(void) {
  import_array();
  return PyModule_Create(&my_module);
}
```

with `my_experiment.{so,dll}` in `PYTHONPATH`:

```
>>> import my_experiment
>>> help(my_experiment.myfunc)
Help on built-in function myfunc in my_experiment:

my_experiment.myfunc = myfunc(...)
    In-place modifies ndarray[float]
```

Buffer protocol

https://docs.python.org/3/c-api/buffer.html

- Subset of CPython API

Buffer protocol

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- Subset of CPython API
- Standard `struct` to expose arrays

```
float *data
size_t ndim
size_t shape[]
```

https://github.com/AMYPAD/CuVec/blob/main/cuvec/include/cuvec_cpython.cuh#L128

```
int my_buffer(PyObject *obj, Py_buffer *view, int flags) {
  view->buf = (void *)MY_GET_ARR_PTR(obj);
  view->obj = obj;
  view->len = MY_GET_ARR_SIZE(obj) * sizeof(float);
  view->readonly = 0;
  view->itemsize = sizeof(float);
  view->format = "f";
  view->ndim = MY_GET_ARR_NDIM(obj);
  view->shape = MY_GET_ARR_SHAPE(obj);
  view->strides = MY_GET_ARR_STRIDES(obj);
  view->suboffsets = NULL; view->internal = NULL;
  Py_INCREF(view->obj);
  return 0;
}
```

```c
static PyObject *myfunc(PyObject *self, PyObject *args) {
  Py_buffer *view = NULL;
  if (!PyArg_ParseTuple(args, "w*", &view)) return NULL;
  float *arr_ptr = view->buf;
  for (size_t i = 0; i < view->shape[0]; ++i) arr_ptr[i] *= 2;
  PyBuffer_Release(view);
}
```

C++ wrappers (pybind11, etc)

https://pybind11.readthedocs.io/en/stable/

- C++ templates reduce boilerplate

```cpp
#include <pybind11/pybind11.h>

void myfunc(pybind11::buffer view) {
  pybind11::buffer_info arr = view.request();
  float *ptr = arr.ptr;
  if (arr.ndim != 1) throw std::runtime_error("expected 1D array");
  for (size_t i = 0; i < arr.size; ++i) ptr[i] *= 2;
}
using namespace pybind11::literals;
PYBIND11_MODULE(my_examples, m){
  m.def("myfunc", &myfunc, "input_array"_a,
        "In-place modifies ndarray[float]");
}
```

Python interfaces

`__cuda_array_interface__`

https://numba.readthedocs.io/en/stable/cuda/cuda_array_interface.html

- Python-level equivalent of C buffer protocol

Python interfaces

`__cuda_array_interface__`

https://numba.readthedocs.io/en/stable/cuda/cuda_array_interface.html

- Python-level equivalent of C buffer protocol
- IMO a bad idea

```
@property
def __cuda_array_interface__(self) -> Dict[str, Any]:
    return {'shape': self.shape, 'typestr': numpy.dtype(self.typechar).str
            'data': (self.get_memory_address(), self.read_only), 'version'
```

`__dlpack__`

https://data-apis.org/array-api/latest/API_specification/generated/array_api.array.__dlpack__.html

https://dmlc.github.io/dlpack/latest/python_spec.html#reference-implementations

- Similar to `__cuda_array_interface__` but also handles ownership & multiple devices/streams

```
@property
def __dlpack__(self, copy=False, max_version: tuple[int]=None,
    stream: int=None, dl_device: tuple[int]=None
):
    dl_tensor = DLTensor(data=self.addr, device=dl_device, ndim=self.ndim,
        dtype=DLDataType.from_dtype(self.dtype),
        shape=ctypes.cast(self.shape, ctypes.POINTER(ctypes.c_int64)),
        strides=None, byte_offset=0)

    managed_tensor = DLManagedTensor(dl_tensor=dl_tensor, manager_ctx=0,
        deleter=DLTensorDeleter(lambda addr: None))
    return pythonapi.PyCapsule_New(ctypes.byref(managed_tensor), b'dltensor
```

CUDA Unified Memory

Host (CPU) vs Device (GPU)

```
#include <cuda_runtime.h>
int N = ...;
float cpu_data[N];
for (int i = 0; i < N; ++i) data[i] = ...;

float *gpu_data;
cudaMalloc(&gpu_data, sizeof(float) * N);
cudaMemcpy(gpu_data, cpu_data, sizeof(float) * N, cudaMemcpyHostToDevice);
mykernel<<<1, N>>>(gpu_data, N);
cudaDeviceSynchronize();
cudaMemcpy(cpu_data, gpu_data, sizeof(float) * N, cudaMemcpyDeviceToHost);
cudaDeviceSynchronize();
cudaFree(gpu_data);
```

Unified Memory

```
#include <cuda_runtime.h>
int N = ...;
float *data;
cudaMallocManaged(&data, sizeof(float) * N);
for (int i = 0; i < N; ++i) data[i] = ...;

mykernel<<<1, N>>>(data, N);
cudaDeviceSynchronize();
```

CuVec

https://amypad.github.io/CuVec/

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  - `std::vector<T>::data()`
  - `std::vector<T>::size()`

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- `std::vector<T, {malloc, free}>` → `std::vector<T, {cudaMallocManaged, cudaFree}>`
  - `std::vector<T>::data()`
  - `std::vector<T>::size()`
  - `std::vector<T>::resize()`

CuVec in Python

- Buffer protocol to expose to Python

CuVec in Python

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- Inherit from `numpy.ndarray`

NiftyPET

Case Study

- NumPy arrays

Case Study

- NumPy arrays
  - CPython API

Case Study

- NumPy arrays
  - CPython API
    - CUDA: cudaMalloc, memcpyH2D, kernel, memcpyD2H, cudaFree

CuVec

- CuVec arrays
  - CPython API
    - CUDA: kernel, sync

NumCu

https://amypad.github.io/NumCu/

Minimal Python/C++/CUDA library using `CuVec`'s CPython buffer protocol.

Bonus

Packaging

- `pip install`

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- `pyproject.toml::build-system`

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Packaging

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- `requires = [cmake, scikit-build-core, pybind11, ...]`
- `cmake`
- install `*.{py,so,dll}`

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