pyMIC: A Python* Offload Module for the Intel® Xeon Phi™ Coprocessor

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Python in HPC

- Python has gained a lot of interest throughout the HPC community (and others):
  - IPython
  - Numpy / SciPy
  - Pandas

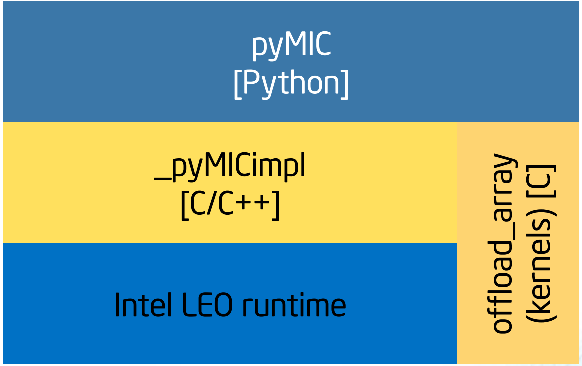
- Intel® Xeon Phi™ Coprocessor is an interesting target to speed-up processing of Python codes

The pyMIC Offload Infrastructure

- Design principles (pyMIC's 4 "K"s)
  - Keep usage simple
  - Keep the API slim
  - Keep the code fast
  - Keep control in a programmer's hand
- pyMIC facts
  - 650 lines of C/C++ code; Intel® LEO for interfacing with MPSS
  - 450 lines of Python code for the main API

High-Level Overview

- Intel® LEO: low-level device interaction
  - Transfer of shared libraries
  - Data transfers
  - Code invocation
- C/C++ extension module
  - Low-level device management
  - Interaction with LEO
- Slim Python API to hide implementation details
- Library with internal device kernels



Key Data Structures

`offload_device`

- Interaction with devices
- Loading of shared libraries
- Invocation of kernel functions
- Buffer management

`offload_array`

- numpy.ndarray container
- Device buffers
- Transfer management
- Simple kernels and operators (zeros, +, *)

Example dgemm: The Host Side…

- Get a device handle (numbered from 0 to n-1)
- Load native code as a shared-object library
- Use bind to create an offload buffer for host data
- Invoke kernel function and pass actual arguments
- Update host data from the device buffer

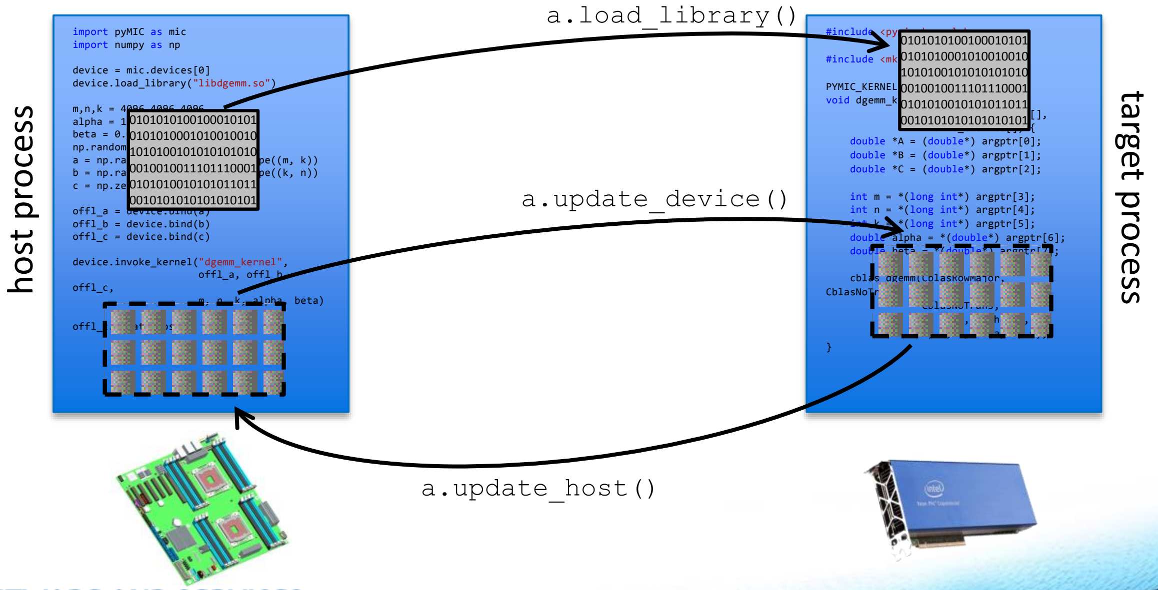
```
import pyMIC as mic
import numpy as np

device = mic.devices[0]
device.load_library("libdgemm.so")

m,n,k = 4096,4096,4096
alpha = 1.0
beta = 0.0
np.random.seed(10)
a = np.random.random(m*k).reshape((m, k))
b = np.random.random(k*n).reshape((k, n))
c = np.zeros((m, n))

offl_a = device.bind(a)
offl_b = device.bind(b)
offl_c = device.bind(c)

device.invoke_kernel("dgemm_kernel",
                     offl_a, offl_b, offl_c,
                     m, n, k, alpha, beta)

offl_c.update_host()
```

Example `dgemm`: The Target Side

- Retrieve array pointer by casting `argptr` to target type
- Retrieve scalar arguments by casting and dereferencing
- Invoke (native) dgemm kernel

```
#include <pymic_kernel.h>

#include <mkl.h>

PYMIC_KERNEL
void dgemm_kernel(int argc, uintptr_t argptr[], size_t sizes[]) {
    double *A = (double*) argptr[0];
    double *B = (double*) argptr[1];
    double *C = (double*) argptr[2];

    int m = *(long int*) argptr[3];
    int n = *(long int*) argptr[4];
    int k = *(long int*) argptr[5];
    double alpha = *(double*) argptr[6];
    double beta = *(double*) argptr[7];

    cblas_dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
                m, n, k, alpha, A, k, B, n, beta, C, n);
}
```

The Offload Protocol



Buffer Management: Buffer Creation

```python
class offload_device:
  def bind(self, array, update_device=True):
    if not isinstance(array, np.ndarray):
      raise ValueError("...")

    # construct a new offload_array
    ass = offload_array(array.shape, array.dtype,
                        order)
    ass.array = array

    if update_device:
      # allocate & copy
      self._copy_to_target(ass.array)
    else:
      # only allocate
      self._buffer_allocate(ass.array)

    return ass
```

```c
void buffer_allocate(int device, char* data,
                     size_t size) {
    uintptr_t host_ptr = (uintptr_t) data;
    uintptr_t dev = 0;
#pragma offload target(mic:device) \
      out(dev_ptr) \
      nocopy(data:length(size) \
             align(64) alloc_if(1) free_if(0))
    {
        dev_ptr = (uintptr_t) data;
    }
    buffers[device][host_ptr] = dev_ptr;
}
```

Buffer Management: Data Transfer

```python
class offload_device:
  def _buffer_update_on_target(self,
                                 *arrays):
    if len(arrays) == 0:
      raise
         ValueError("no argument")
    if type(arrays[0]) == tuple:
      arrays = arrays[0]
    for array in arrays:
      nbytes = int(array.nbytes)
      _pymic_impl_buffer_update_on_target(
        self.map_dev_id(), array, nbytes)
    return None
```

```c
void buffer_update_on_target(int device,
                             char* data,
                             size_t size)
{
    uintptr_t host_ptr =
        reinterpret_cast<uintptr_t>(data);
#pragma offload target(mic:device) \
        in(data:length(size) \
          align(64)
          alloc_if(0) free_if(0))
    {
        // do nothing
    }
}
```

Example: Singular Value Decomposition

- Treat picture as 2D matrix
- Decompose matrix:

$$M = U \times \Sigma \times V^T$$

- Ignore some singular values
- Effectively compresses images

Example: Singular Value Decomposition

Host code

```
import numpy as np
import pyMIC as mic
from PIL import Image

def compute_svd(image):
    mtx = np.asarray(image.getdata(band=0),
                     float)
    mtx.shape = (image.size[1], image.size[0])
    mtx = np.matrix(mtx)
    return np.linalg.svd(mtx)

def reconstruct_image(U, sigma, V):
    reconstructed = U * sigma * V
    image = Image.fromarray(reconstructed)
    return image
```

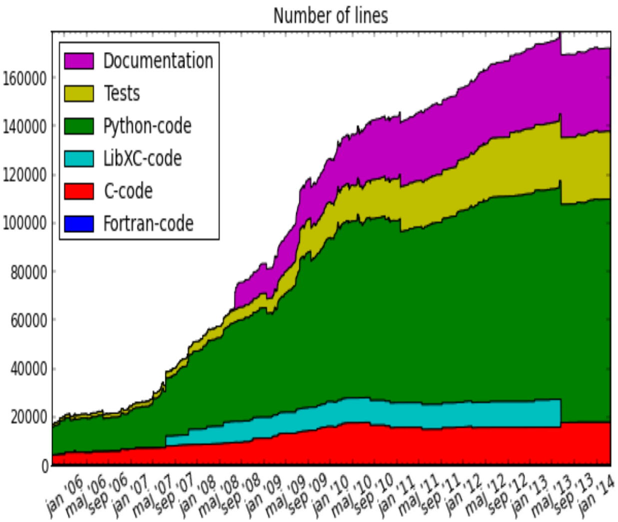
Host code, cont'd

```
def reconstruct_image_dgemm(U, sigma, V):
    offl_tmp    = device.empty((U.shape[0], U.shape[1]),
                               dtype=float, update_host=False)
    offl_res    = device.empty((U.shape[0], V.shape[1]),
                               dtype=float, update_host=False)
    offl_U      = device.bind(U)
    offl_sigma  = device.bind(sigma)
    offl_V      = device.bind(V)
    alpha, beta = 1.0, 0.0
    m, k, n = U.shape[0], U.shape[1], sigma.shape[1]
    device.invoke_kernel("dgemm_kernel",
                         offl_U, offl_sigma, offl_tmp,
                         m, n, k, alpha, beta)
    m, k, n = offl_tmp.shape[0], offl_tmp.shape[1], V.shape[1]
    device.invoke_kernel("dgemm_kernel",
                         offl_tmp, offl_V, offl_res,
                         m, n, k, alpha, beta)
    image = Image.fromarray(offl_res.update_host().array)
    return image
```

Integration with GPAW

- GPAW is an open source software package for various quantum mechanical simulations at atomic scale
  - http://wiki.fysik.dtu.dk/gpaw
  - Few hundred users all over the world
- Implemented as a combination of Python and C
  - High-level algorithms in Python
  - Computational kernels in C (or in libraries)
  - Massively parallelized (with MPI)
  - Key operation: matrix-matrix multiplication

Integration with GPAW



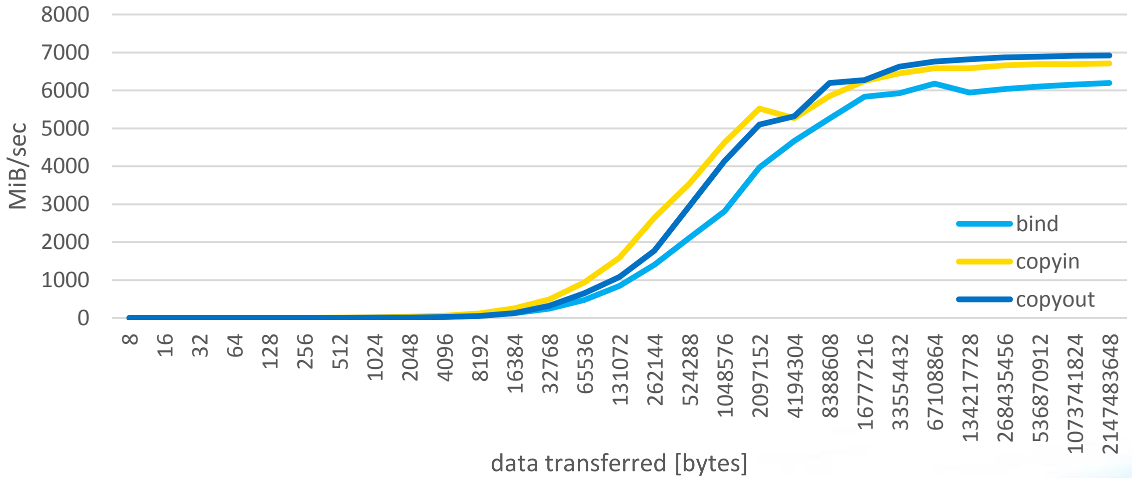
- Control the flow of large data (NumPy arrays) in Python level
- Offload heavy computations to coprocessor

Integration in GPAW

```
from gpaw.grid_descriptor
   import GridDescriptor

gpts = (64, 64, 64)
nbands = 512
cell = (8.23, 8.23, 8.23)
gd = GridDescriptor(gpts, cell)

psit_nG = gd.zeros(nbands, mic=True)
vt_G = gd.zeros(mic=True)
# Initialize psit_nG and vt_G
htpsit_nG = gd.zeros(nbands, mic=True)

for n in range(nbands):
    htpsit_nG[n] = vt_G * psit_nG[n]

H_nn = gd.integrate(psit_nG, htpsit_ng)
```

```
import pyMIC as mic

device = mic.devices[0]

...
    def zeros(self, n=(), dtype=float,
              mic=False):

        array = self._new_array(n, dtype)
        if mic:
            return device.bind(array)
        else:
            return array
```

Performance: Bandwidth of Data Transfers



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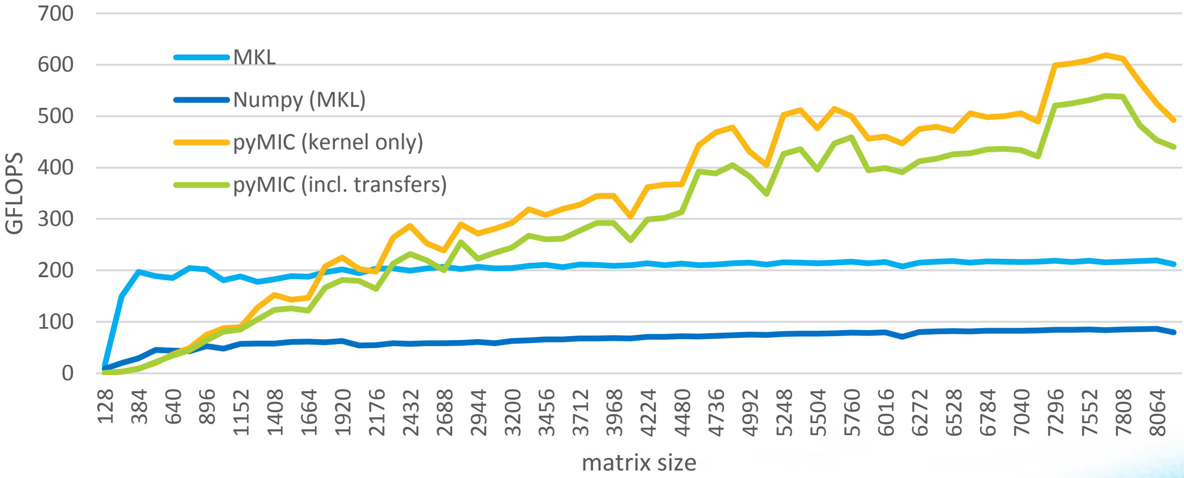
Performance: dgemm



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Performance: GPAW integrate and rotate

Matrix size	integrate			rotate		
	Xeon	Xeon Phi	S	Xeon	Xeon Phi	S
n=256, $G=48^3$	0.10	0.11	0.91x	0.10	0.04	2.50x
n=256, $G=64^3$	0.25	0.25	1.00x	0.26	0.10	2.60x
n=256, $G=86^3$	0.61	0.55	1.11x	0.55	0.17	3.24x
n=256, $G=96^3$	0.78	0.79	0.99x	1.59	0.31	5.13x
n=512, $G=48^3$	0.30	0.12	2.50x	0.35	0.11	3.18x
n=512, $G=64^3$	0.74	0.27	2.74x	0.91	0.28	3.25x
n=512, $G=86^3$	1.75	0.57	3.07x	1.89	0.50	3.70x
n=512, $G=96^3$	2.53	0.97	2.61x	6.28	0.92	6.83x

Summary & Future Work

- pyMIC
  - A slim, easy-to-use offload interface for Python
  - Native kernels on the target devices
  - Almost negligible extra overhead for Python integration
- Future versions will likely bring:
  - Offloading of full Python code
  - Asynchronous offloading and data transfers
- Download pyMIC at https://github.com/01org/pyMIC.
- Mailinglist at https://lists.01.org/mailman/listinfo/pymic

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