Accelerating Python: Offloading to Intel® Xeon Phi™ (Co)processors

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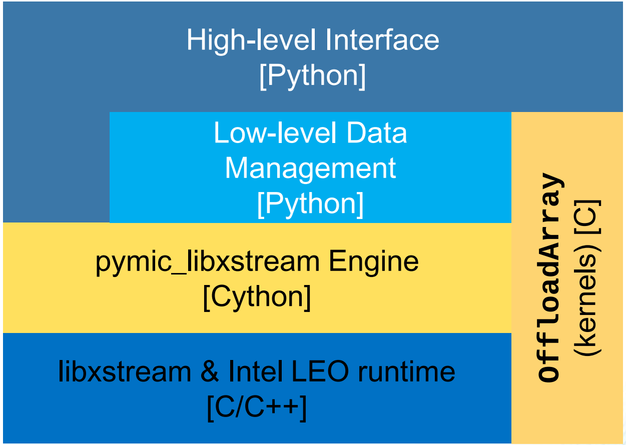
The pyMIC Offload Infrastructure

- 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
  - 3800 lines of C/C++ code;
  - 1100 lines of Python code for the main API;
  - libxstream and Intel® LEO for interfacing with MPSS

High-Level Overview

- libxstream & Intel® LEO: low-level device interaction
  - Transfer of shared libraries
  - Data transfers, kernel invocation
- C/C++ extension module
  - Low-level device management
  - Interaction with LEO
- Low-level API with memcpy-like interface, smart device pointers
- High-level API with offload arrays
- Library with internal device kernels



Example dgemm: The Host Side...

```python
import numpy as np




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.empty((m, n))

am = np.matrix(a)
bm = np.matrix(b)
cm = np.matrix(c)
cm = alpha * am * bm + beta * cm
```

```python
import pymic as mic
import numpy as np

device = mic.devices[0]
stream = device.get_default_stream()
library = 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.empty((m, n))

stream.invoke(library.dgemm_kernel,
              a, b, c,
              m, n, k, alpha, beta)
stream.sync()
```

Example dgemm: The Host Side...

- Get a device handle (numbered from 0 to n-1)
- Load native code as a shared-object library

- Invoke kernel function and pass actual arguments
- Copy-in/copy-out semantics for arrays
- Copy-in semantics for scalars

- Synchronize host and coprocessor

```python
import pymic as mic
import numpy as np

device = mic.devices[0]
stream = device.get_default_stream()
library = 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.empty((m, n))

stream.invoke(library.dgemm_kernel,
              a, b, c,
              m, n, k, alpha, beta)
stream.sync()
```

Example dgemm: The Target Side…

- Arguments are passed as C/C++ types
- All argument passing is done with pointers to actual data

- Invoke (native) dgemm kernel

```
#include <pymic_kernel.h>

#include <mkl.h>

PYMIC_KERNEL
void dgemm_kernel(const double *A, const double *B,
                  double *C,
                  const int64_t *m, const int64_t *n,
                  const int64_t *k,
                  const double *alpha, const double *beta) {
    cblas_dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
                *m, *n, *k, *alpha, A, *k, B, *n,
                *beta, C, *n);
}
```

High-level Data Structures

`OffloadDevice`

- Interaction with devices
- Loading of shared libraries

`OffloadStream`

- Invocation of kernel functions
- Buffer management

`OffloadArray`

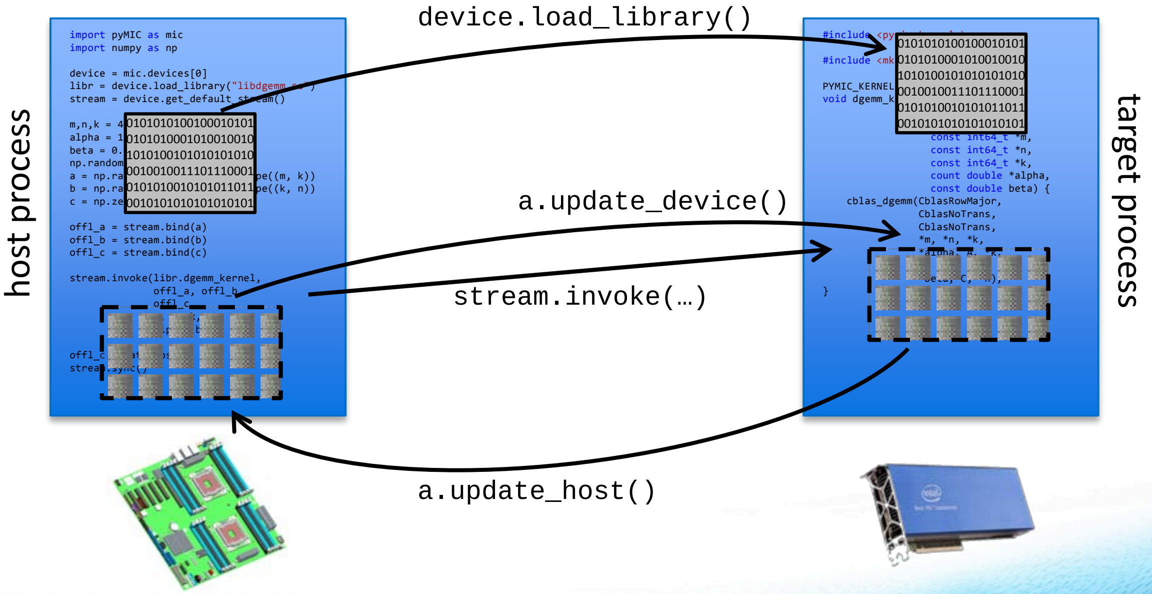
- numpy.ndarray container
- Transfer management
- Simple kernels and operators (fill, +, *)

Optimize Offloads with High-level Containers

- 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

```python
import pymic as mic
import numpy as np

device = mic.devices[0]
stream = device.get_default_stream()
library = 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 = stream.bind(a)
offl_b = stream.bind(b)
offl_c = stream.bind(c)

stream.invoke(library.dgemm_kernel,
              offl_a, offl_b, offl_c,
              m, n, k, alpha, beta)

offl_c.update_host()
stream.sync()
```

The High-level Offload Protocol



Buffer Management: Buffer Creation

```python
class OffloadStream:
  def bind(self, array, update_device=True):
    if not isinstance(array, numpy.ndarray):
      raise ValueError("only numpy.ndarray can be associated "
                       "with OffloadArray")

    # detect the order of storage for 'array'
    if array.flags.c_contiguous:
      order = "C"
    elif array.flags.f_contiguous:
      order = "F"
    else:
      raise ValueError("could not detect storage order")

    # construct and return a new OffloadArray
    bound = pymic.OffloadArray(array.shape, array.dtype, order, False,
                               device=self._device, stream=self)
    bound.array = array

    # allocate the buffer on the device (and update data)
    bound._device_ptr = self.allocate_device_memory(bound._nbytes)
    if update_device:
      bound.update_device()

    return bound
```

```python
class OffloadStream:
  def allocate_device_memory(self, nbytes, alignment=64, sticky=False):
    device = self._device_id
  if nbytes <= 0:
    raise ValueError('Cannot allocate negative amount of '
                     'memory: {0}'.format(nbytes))
  device_ptr = _pymic_impl_stream_allocate(device, self._stream_id,
                                           nbytes, alignment)
  return SmartPtr(self, device, device_ptr, sticky)
```

```cpp
unsigned char *buffer_allocate(int device,
                               libxstream_stream *stream,
                               size_t size,
                               size_t alignment) {
  void *memory = NULL;
  libxstream_mem_allocate(device, &memory, size, alignment);
  return reinterpret_cast<unsigned char *>(memory);
}
```

Buffer Management: Data Transfer

```python
class OffloadArray:
  def update_device(self):
    host_ptr = self.array.ctypes.get_data()
    s = self.stream
    s.transfer_host2device(host_ptr,
                           self._device_ptr,
                           self._nbytes)
    return None

  def update_host(self):
    host_ptr = self.array.ctypes.get_data()
    s = self.stream
    s.transfer_device2host(self._device_ptr,
                           host_ptr,
                           self._nbytes)
  return self
```

```c
void buffer_copy_to_target(int device,
                           libxstream_stream *stream,
                           unsigned char *src,
                           unsigned char *dst,
                           size_t size,
                           size_t offset_host,
                           size_t offset_device) {
  unsigned char *src_offs = src + offset_host;
  unsigned char *dst_offs = dst + offset_device;

  libxstream_memcpy_h2d(src_offs, dst_offs,
                        size, stream);
}
```

SOFTWARE AND SERVICES

The Low-level Offload Protocol

host process

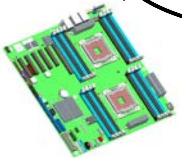
```python
import pyMIC as mic
import numpy as np

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

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 = stream.bind(a)
offl_b = stream.bind(b)
offl_c = stream.bind(c)

stream.invoke(libr.dgemm_kernel,
              offl_a, offl_b,
              offl_c,
```

stream.allocate_device_memory(…)

stream.transfer_host2device(…)

```c
#include <pymic_kernel.h>

#include <mkl.h>

PYMIC_KERNEL
void dgemm_kernel(const double *A,
                  const double *B,
                  double *C,
                  const int64_t *m,
                  const int64_t *n,
                  const int64_t *k,
                  count double *alpha,
                  const double beta) {
    cblas_dgemm(CblasRowMajor,
                CblasNoTrans,
                CblasNoTrans,
                *m, *n, *k,
}
```

target process



stream.transfer_device2host(…)

stream.deallocate_device_memory(…)

Using the Low-level API

```python
import pymic
import numpy

device = pymic.devices[0]
stream = device.get_default_stream()

a = numpy.arange(0.0, 32.0)
b = numpy.empty_like(a)

# determine size of the array in bytes and get pointer
nbytes = a.dtype.itemsize * a.size
ptr_a = a.ctypes.data
ptr_b = b.ctypes.data

# allocate buffer spaces in the target
dev_ptr_1 = stream.allocate_device_memory(nbytes)
dev_ptr_2 = stream.allocate_device_memory(nbytes)
```

```python
# transfer a into the first buffer and shuffle a bit
stream.transfer_host2device(ptr_a, dev_ptr_1,
                            nbytes/2, offset_host=0,
                            offset_device=nbytes/2)
stream.transfer_host2device(ptr_a, dev_ptr_1, nbytes/2,
                            offset_host=nbytes/2,
                            offset_device=0)
# do some more shuffling on the target
for i in xrange(0, 4):
    stream.transfer_device2device(dev_ptr_1, dev_ptr_2,
                                  nbytes/4,
                                  off_dev_src=i*(nbytes/4),
                                  off_dev_dst=(3-i)*(nbytes/4))
# transfer data back into 'b' array and shuffle even more
for i in xrange(0, 4):
    stream.transfer_device2host(dev_ptr_2, ptr_b, nbytes/4,
                                offset_device=i*(nbytes/4),
                                offset_host=(3-i)*(nbytes/4))
stream.sync()
```

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

Integration with GPAW

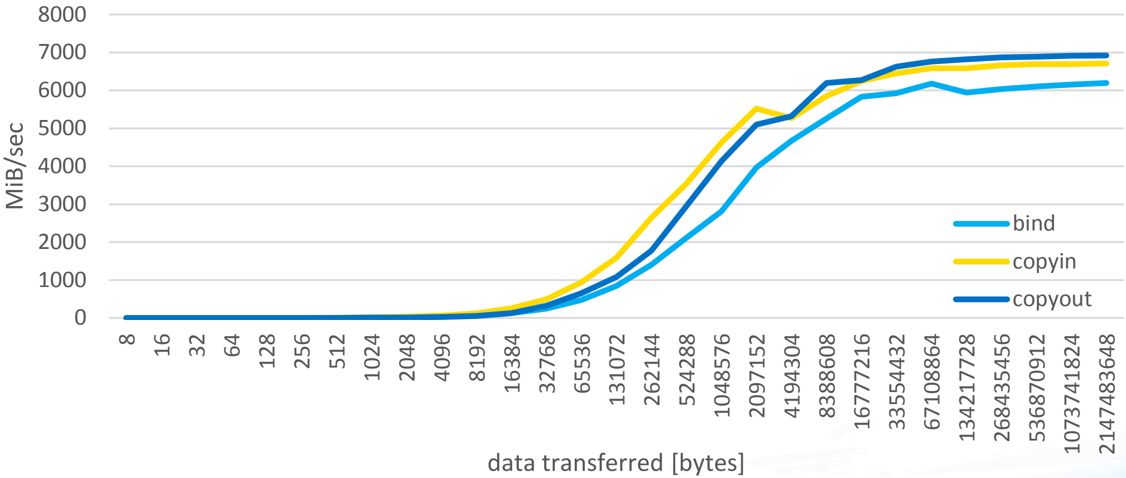
- GPAW is an open source software package for various quantum mechanical simulations at atomic scale
  - http://wiki.fysik.dtu.dk/gpaw
  - Few hundred users all over the world
- Implemented as a combination of Python and C
  - High-level algorithms in Python
  - Computational kernels in C (or in libraries)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

Integration 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]
stream = device.get_default_stream()

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

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

Performance: Bandwidth of Data Transfers



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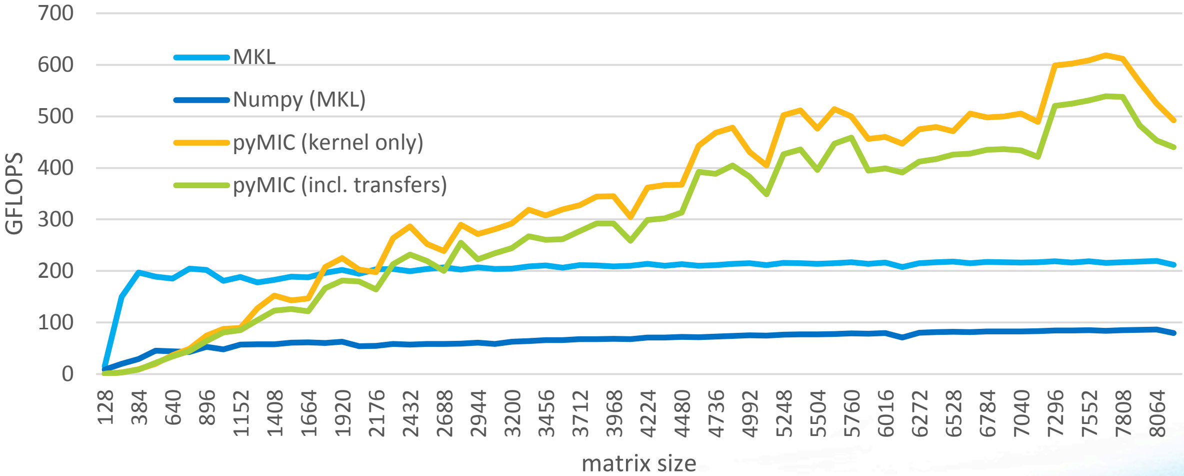
Performance: dgemm



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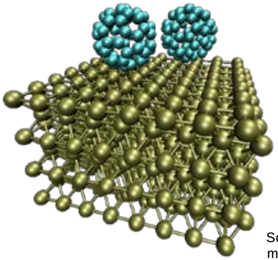
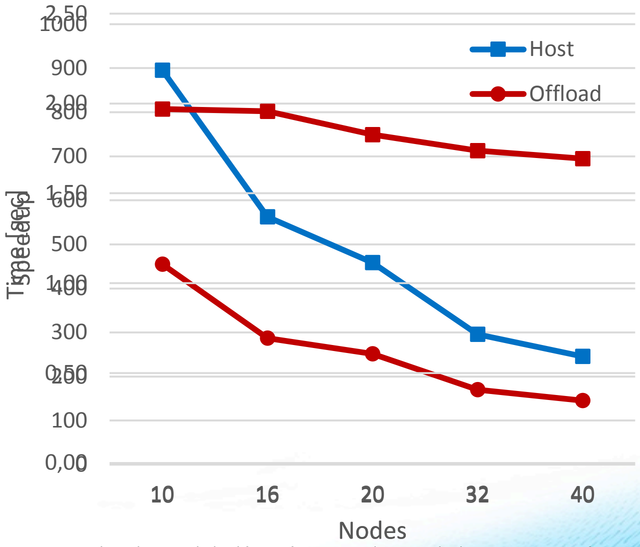
Example Application: GPAW

- Open-source software package for quantum mechanical simulations at atomic scale (http://wiki.fysik.dtu.dk/gpaw)
- Combination of Python & C
  - High-level algorithms in Python
  - Computational kernels in
  - Massively parallelized (with MPI)
  - Key operation: dgemm





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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 {C|P}ython code

- Download pyMIC at https://github.com/01org/pyMIC.
- Mailinglist at https://lists.01.org/mailman/listinfo/pymic

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