Communicating NumPy arrays

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Overview

- Numpy and buffer-like object
- Blocking communication
- Nonblocking communication
- Collective communication

Numpy and buffer-like object

NumPy

- Powerful N-dimensional arrays
- Optimized for performance
- Easy to use
- Open source

NumPy

```
>>> import numpy as np

>>> a = np.arange(16.).reshape(4,4)
>>> a
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])
```

NumPy

```
>>> import numpy as np

>>> a = np.arange(16.).reshape(4,4)
>>> a
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])

>>> b = a.T
>>> b
array([[ 0.,  4.,  8., 12.],
       [ 1.,  5.,  9., 13.],
       [ 2.,  6., 10., 14.],
       [ 3.,  7., 11., 15.]])
```

NumPy

```
>>> import numpy as np

>>> a = np.arange(16.).reshape(4,4)
>>> a
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])

>>> c = a[0:2, 0:2]
>>> c
array([[0., 1.],
       [4., 5.]])
```

NumPy

```
>>> import numpy as np

>>> a = np.arange(16.).reshape(4,4)
>>> a
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])

>>> d = a[:,1].reshape(2,2)
>>> d
array([[ 1.,  5.],
       [ 9., 13.]])
```

NumPy

```
>>> import numpy as np

>>> a = np.arange(16.).reshape(4,4)
>>> a
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])

>>> np.matmul(a, a.T)
array([[ 14.,  38.,  62.,  86.],
       [ 38., 126., 214., 302.],
       [ 62., 214., 366., 518.],
       [ 86., 302., 518., 734.]])
```

NumPy with mpi4py

- Numpy arrays can be communicated by the all-lowercase methods like send, recv, bcast, etc.

- For best efficiency Numpy arrays can be communicated as **buffer-like objects**, using method with a leading uppercase letter.

  - Send, Recv
  - Isend, Irecv
  - Bcast, Reduce
  - Scatterv, Gatherv (more useful than Scatter/Gather)

Numpy array as buffer-like objects

- communication is fast
  - close to the speed of MPI communication in C

- less flexible
  - memory of the receiving buffer needs to be allocated
  - size of the sending buffer should not exceed that of the receiving buffer
  - mpi4py expects the buffer-like objects to have contiguous memory

Contiguous or non-contiguous?

```
>>> import numpy as np

>>> a = np.arange(16.).reshape(4,4)
>>> a
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])
```

Contiguous or non-contiguous?

```
>>> import numpy as np

>>> a = np.arange(16.).reshape(4,4)
>>> a
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])

>>> a.flags
  C_CONTIGUOUS : True
  F_CONTIGUOUS : False
  OWNDATA : False
  …
```

Contiguous or non-contiguous?

```
>>> b = a.T
>>> b.flags
  C_CONTIGUOUS : False
  F_CONTIGUOUS : True
  OWNDATA : False
  ...
```

Contiguous or non-contiguous?

```
>>> b = a.T
>>> b.flags
  C_CONTIGUOUS : False
  F_CONTIGUOUS : True
  OWNDATA : False
  ...

>>> b[0,0] = 99.0
>>> b
array([[99.,  4.,  8., 12.],
       [ 1.,  5.,  9., 13.],
       [ 2.,  6., 10., 14.],
       [ 3.,  7., 11., 15.]])
```

Contiguous or non-contiguous?

```
>>> b = a.T
>>> b.flags
  C_CONTIGUOUS : False
  F_CONTIGUOUS : True
  OWNDATA : False
  ...

>>> b[0,0] = 99.0
>>> b
array([[99.,  4.,  8., 12.],
       [ 1.,  5.,  9., 13.],
       [ 2.,  6., 10., 14.],
       [ 3.,  7., 11., 15.]])
>>> a
array([[99.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])
```

Contiguous or non-contiguous?

```
>>> a
array([[99.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])
```

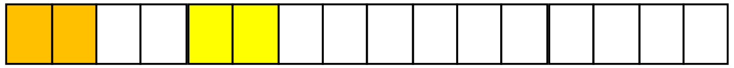
Contiguous or non-contiguous?

```
>>> a
array([[99.,  1.,  2.,  3.],
      [ 4.,  5.,  6.,  7.],
      [ 8.,  9., 10., 11.],
      [12., 13., 14., 15.]])

>>> c = a[0:2, 0:2]
>>> c
array([[99.,  1.],
      [ 4.,  5.]])

>>> c.flags
  C_CONTIGUOUS : False
  F_CONTIGUOUS : False
  OWNDATA : False
```

Contiguous or non-contiguous?

```
>>> a
array([[99.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])
```

```
>>> c = a[0:2, 0:2]
>>> c
array([[99.,  1.],
       [ 4.,  5.]])
```



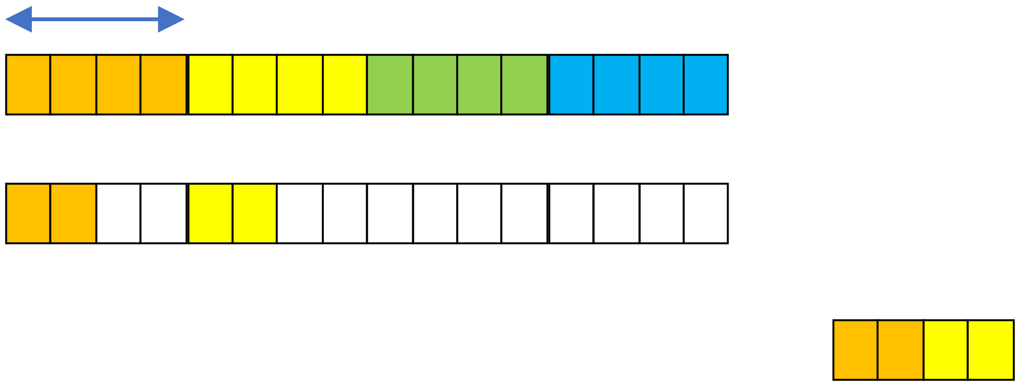
```
>>> c.flags
  C_CONTIGUOUS : False
  F_CONTIGUOUS : False
  OWNDATA : False
```

Contiguous or non-contiguous?

```
>>> d = c.copy()
>>> d.flags
  C_CONTIGUOUS : True
  F_CONTIGUOUS : False
  OWNDATA : True
  ...
```

Contiguous or non-contiguous?

```
>>> d = c.copy()
>>> d.flags
  C_CONTIGUOUS : True
  F_CONTIGUOUS : False
  OWNDATA : True
  ...

>>> a.strides
(32, 8)
>>> c.strides
(32, 8)
>>> d.strides
(16, 8)
```



Use NumPy array as buffer-like object

- The array itself, or a list or tuple with
  - 2 or 3 elements
  - 4 elements for the vector variants (Scatterv, Gatherv)

  - data
  - [data, MPI.DOUBLE]
  - [data, n, MPI.DOUBLE]
  - [data, count, displ, MPI.DOUBLE]

Blocking send/recv

Send / Recv

- Syntax
  - comm.Send(obj, dest=dest, tag=tag)
  - comm.Recv(obj, source=source, tag=rag)

- Note
  - obj needs to be created prior to the communication
  - size of obj needs to be known before hand

Send / Recv

- example

```python
import numpy as np
from mpi4py import MPI


comm = MPI.COMM_WORLD

if comm.rank == 0:
    data = np.arange(4.)
    for i in range(1, comm.size):
        comm.Send(data, dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data)
else:
    data = np.zeros(4)
    comm.Recv(data, source=0, tag=comm.rank)
    print(f"Process {comm.rank} received data:", data)
```

Send / Recv

- output

```
Process 0 sent data: [0. 1. 2. 3.]
Process 0 sent data: [0. 1. 2. 3.]
Process 0 sent data: [0. 1. 2. 3.]
Process 1 received data: [0. 1. 2. 3.]
Process 2 received data: [0. 1. 2. 3.]
Process 3 received data: [0. 1. 2. 3.]
```

Send / Recv

- question
  - If the size of the numpy array is only known on the master process (rank 0), how do we send it to other processes (rank > 0)?

Send / Recv

- question
  - If the size of the numpy array is only known on the master process (rank 0), how do we send it to other processes (rank > 0)?

- solution
  - need to send the size of the array first

- exercise
  - rewrite the above example assuming that the size of array is not known on the non-master nodes (rank > 0).
  - for sending an integer you may use the all-lowercase send

Send / Recv

- exercise
  - what will happen if you try to send an array with non-contiguous memory?

  - hint: this is how to create a simple array with non-contiguous memory

```
data = np.arange(12.)[::2]
```

Send / Recv

- exercise
  - what will happen if the receiving buffer is ***larger*** than the sent array?

```
if comm.rank == 0:
    data = np.arange(4.)
    for i in range(1, comm.size):
        comm.Send(data, dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data)
else:
    data = np.zeros(6)
    comm.Recv(data, source=0, tag=comm.rank)
    print(f"Process {comm.rank} received data:", data)
```

Send / Recv

- exercise
  - what will happen if the receiving buffer is ***smaller*** than the sent array?

```
if comm.rank == 0:
    data = np.arange(4.)
    for i in range(1, comm.size):
        comm.Send(data, dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data)
else:
    data = np.zeros(3)
    comm.Recv(data, source=0, tag=comm.rank)
    print(f"Process {comm.rank} received data:", data)
```

Send / Recv

- best practice: check status

```
if comm.rank == 0:
    data = np.arange(4.)
    for i in range(1, comm.size):
        comm.Send(data, dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data)
else:
    data = np.zeros(3)
    status = MPI.Status()
    comm.Recv(data, source=0, tag=comm.rank, status=status)
    if status.error:
        MPI.COMM_WORLD.Abort(status.error)
    print(f"Process {comm.rank} received data:", data)
```

Send / Recv with buffer size

- use [data, n, MPI.DOUBLE] to specify the buffer

```
if comm.rank == 0:
    data = np.arange(4.)
    for i in range(1, comm.size):
        comm.Send([data, 2, MPI.DOUBLE], dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data[:2])
else:
    data = np.zeros(4)
    status = MPI.Status()
    comm.Recv([data, 2, MPI.DOUBLE], source=0, tag=comm.rank, status=status)
    if status.error:
        MPI.COMM_WORLD.Abort(status.error)
    print(f"Process {comm.rank} received data:", data[:2])
```

Send / Recv with buffer size

- use [data, n, MPI.DOUBLE] to specify the buffer

```
if comm.rank == 0:
    data = np.arange(4.)
    for i in range(1, comm.size):
        comm.Send([data, 2, MPI.DOUBLE], dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data[:2])
else:
    data = np.zeros(4)
    status = MPI.Status()
    comm.Recv([data, 2, MPI.DOUBLE], source=0, tag=comm.rank, status=status)
    if status.error:
        MPI.COMM_WORLD.Abort(status.error)
    print(f"Process {comm.rank} received data:", data[:2])
```

- NOTE: The size of buffer should never be larger than the size of the Numpy array.

Send / Recv with buffer size

- use array slicing

```
if comm.rank == 0:
    data = np.arange(10)
    for i in range(1, comm.size):
        comm.Send(data[2:6], dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data)
else:
    data = np.zeros(10)
    status = MPI.Status()
    comm.Recv(data[2:6], source=0, tag=comm.rank), status=status)
    if status.error:
        MPI.COMM_WORLD.Abort(status.error)
    print(f"Process {comm.rank} received data:", data[:2])
```

Send / Recv with 2D array

- exercise
  - Send / Recv 2D array

```
if comm.rank == 0:
    data = np.arange(16).reshape(4, 4)
    for i in range(1, comm.size):
        comm.Send(data[2:6], dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data)
else:
    data = np.zeros(16).reshape(4, 4)
    status = MPI.Status()
    comm.Recv(data[2:6], source=0, tag=comm.rank, status=status)
    if status.error:
        MPI.COMM_WORLD.Abort(status.error)
    print(f"Process {comm.rank} received data:", data[:2])
```

  - Will it work if the receiving buffer is a 1D array?

Send / Recv with 2D array

- exercise
  - What will happen if we send a 2D array with .T (transpose)?

```
if comm.rank == 0:
    data = np.arange(16).reshape(4, 4).T
    for i in range(1, comm.size):
        comm.Send(data[2:6], dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data)
else:
    data = np.zeros(16).reshape(4, 4)
    status = MPI.Status()
    comm.Recv(data[2:6], source=0, tag=comm.rank, status=status)
    if status.error:
        MPI.COMM_WORLD.Abort(status.error)
    print(f"Process {comm.rank} received data:", data[:2])
```

Send / Recv with 2D array

- exercise
  - What will happen if we send a 2D array with .T.copy() (copy of transpose)?

```
if comm.rank == 0:
    data = np.arange(16).reshape(4, 4).T.copy()
    for i in range(1, comm.size):
        comm.Send(data[2:6], dest=i, tag=i)
        print(f"Process {comm.rank} sent data:", data)
else:
    data = np.zeros(16).reshape(4, 4)
    status = MPI.Status()
    comm.Recv(data[2:6], source=0, tag=comm.rank, status=status)
    if status.error:
        MPI.COMM_WORLD.Abort(status.error)
    print(f"Process {comm.rank} received data:", data[:2])
```

Non-blocking send/recv

Isend / Irecv

- Syntax
  - comm.Isend(obj, dest=dest, tag=tag)
  - comm.Irecv(obj, source=source, tag=rag)

- Note
  - obj needs to be created prior to the communication
  - size of obj needs to be known before hand
  - A Request object is returned by Isend / Irecv
  - Use Wait method of the Request object
  - No Status involved

Isend / Irecv

- example

```python
from mpi4py import MPI
import numpy as np


comm = MPI.COMM_WORLD


if comm.rank == 0:
    data = np.arange(4.)
    reqs = []
    for i in range(1, comm.size):
        reqs.append(comm.Isend(data, dest=i, tag=i))
    for req in reqs:
        req.wait()
        print(f'Process {comm.rank} sent data:', data)
else:
    data = np.zeros(4)
    req = comm.Irecv(data, source=0, tag=comm.rank)
    req.wait()
    print(f'Process {comm.rank} received data:', data)
```

Isend / Irecv

- example

```
from mpi4py import MPI
import numpy as np


comm = MPI.COMM_WORLD


if comm.rank == 0:
    data = np.arange(4.)
    reqs = []
    for i in range(1, comm.size):
        reqs.append(comm.Isend(data, dest=i, tag=i))
    for req in reqs:
        req.wait()
        print(f'Process {comm.rank} sent data:', data)
else:
    data = np.zeros(4)
    req = comm.Irecv(data, source=0, tag=comm.rank)
    req.wait()
    print(f'Process {comm.rank} received data:', data)
```

Isend / Irecv

- example

```
from mpi4py import MPI
import numpy as np


comm = MPI.COMM_WORLD


if comm.rank == 0:
    data = np.arange(4.)
    reqs = [comm.Isend(data, dest=i, tag=i) for i in range(1, comm.size)]
    for req in reqs:
        req.wait()
        print(f'Process {comm.rank} sent data:', data)
else:
    data = np.zeros(4)
    req = comm.Irecv(data, source=0, tag=comm.rank)
    req.wait()
    print(f'Process {comm.rank} received data:', data)
```

Isend / Irecv

- exercise:
  - what if the size of the receiving buffer is larger than the sent array?
  - what if the size of the receiving buffer is smaller than the sent array?
  - send a 2D array
    - without transpose
    - with .T
    - with .T.copy()

Collectives

Bcast

- Syntax
  - comm.Bcast(obj, root=root)

- Note
  - obj needs to be created prior to the communication
  - size of obj needs to be known before hand
  - root can be non-zero (source of communication)

Bcast

```
from mpi4py import MPI
import numpy as np

comm = MPI.COMM_WORLD

if comm.rank == 0:
    data = np.arange(4.0)
else:
    data = np.zeros(4)

comm.Bcast(data, root=0)

print(f'Process {comm.rank} has data:', data)
```

Bcast

- exercise
  - what will happen if the size of the receiving buffer is ***larger***?
  - what will happen if the size of the receiving buffer is ***smaller***?

Scatterv

- vector variant of Scatter

- Syntax
  - comm.Scatterv([sendbuf, count, displ, mpi_dtype], recvbuf, root=root)

- Note
  - count is count per rank
  - displ by default calculated from count
  - recvbuf needs to be created prior to the communication
  - size of recvbuf needs to be known beforehand

Scatterv

- determine count

```
base, rem = divmod(sendbuf.size, nprocs)

# count: the size of each sub-task
count = np.full(shape=comm.size, fill_value=base))
displ[:rem] += 1
```

Scatterv

- determine count

```
base, rem = divmod(sendbuf.size, nprocs)

# count: the size of each sub-task
count = np.full(shape=comm.size, fill_value=base))
displ[:rem] += 1
```

- sendbuf.size = 15; comm.size = 4
  - base = 3; rem = 3
  - count = np.array([4, 4, 4, 3])

Scatterv

- determine count

```
base, rem = divmod(sendbuf.size, nprocs)

# count: the size of each sub-task
count = np.full(shape=comm.size, fill_value=base))
displ[:rem] += 1
```

- sendbuf.size = 15; comm.size = 4
  - base = 3; rem = 3
  - count = np.array([4, 4, 4, 3])

0	1	2	3	rank 0
4	5	6	7	rank 1
8	9	10	11	rank 2
12	13	14		rank 3

Scatterv

```
from mpi4py import MPI
import numpy as np

comm = MPI.COMM_WORLD
```

Scatterv

```
if comm.rank == 0:
    sendbuf = np.arange(15.0)

    # count: the size of each sub-task
    base, rem = divmod(sendbuf.size, comm.size)
    count = np.full(shape=comm.size, base=rem)
    count[:rem] += 1

else:
    sendbuf = None

    # initialize count on worker processes
    count = np.zeros(comm.size, dtype=int)
```

Scatterv

```
# broadcast count
comm.Bcast(count, root=0)

# initialize recvbuf on all processes
recvbuf = np.zeros(count[comm.rank])

comm.Scatterv([sendbuf, count], recvbuf, root=0)

print(f'After Scatterv, process {comm.rank} has data:', recvbuf)
```

Scatterv

- output

```
After Scatterv, process 0 has data: [0. 1. 2. 3.]
After Scatterv, process 2 has data: [ 8.  9. 10. 11.]
After Scatterv, process 1 has data: [4. 5. 6. 7.]
After Scatterv, process 3 has data: [12. 13. 14.]
```

Gatherv

- vector variant of Gather
- Syntax
  - comm.Gatherv(sendbuf, [recvbuf, count, displ, mpi_dtype], root=root)
- Note
  - count is count per rank
  - displ by default calculated from count
  - recvbuf needs to be created prior to the communication
  - size of recvbuf needs to be known before hand

Gatherv

- continue with the Scatterv code

```
sendbuf2 = recvbuf
recvbuf2 = np.zeros(count.sum())

comm.Gatherv(sendbuf2, [recvbuf2, count], root=0)

if comm.rank == 0:
    print('After Gatherv, process 0 has data:', recvbuf2)
```

Gatherv

- output

```
After Gatherv, process 0 has data:
[ 0.  1.  2.  3.  4.  5.  6.  7.  8.  9. 10. 11. 12. 13. 14.]
```

Reduce

- Syntax
  - comm.Reduce(sendbuf, recvbuf, op=op, root=root)

- Note
  - default op is MPI.SUM
  - root can be non-zero (target of Reduce)

Reduce

- continue with the Scatterv code

```
partial_sum = np.zeros(1)
partial_sum[0] = sum(recvbuf)
print(f'Partial sum on process {comm.rank} is:', partial_sum[0])

total_sum = np.zeros(1)
comm.Reduce(partial_sum, total_sum, op=MPI.SUM, root=0)

if comm.rank == 0:
    print('After Reduce, total sum on process 0 is:', total_sum[0])
```

Reduce

- output

```
Partial sum on process 3 is: 39.0
Partial sum on process 1 is: 22.0
Partial sum on process 2 is: 38.0
Partial sum on process 0 is: 6.0
After Reduce, total sum on process 0 is: 105.0
```

Reduce

- exercise
  - Use Reduce to compute the sum of numpy arrays

Reduce

```
from mpi4py import MPI
import numpy as np

comm = MPI.COMM_WORLD

partial = np.arange(10.) * comm.rank
print(f'Before Reduce, partial on process {comm.rank} is:', partial)

total = np.zeros(10)
comm.Reduce(partial, total, op=MPI.SUM, root=0)
if comm.rank == 0:
    print(f'After Reduce, total on process {comm.rank} is:', total)
```

Reduce

```
Before Reduce, partial on process 0 is: [0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
Before Reduce, partial on process 2 is: [ 0.  2.  4.  6.  8. 10. 12. 14. 16. 18.]
Before Reduce, partial on process 1 is: [0. 1. 2. 3. 4. 5. 6. 7. 8. 9.]
Before Reduce, partial on process 3 is: [ 0.  3.  6.  9. 12. 15. 18. 21. 24. 27.]
After Reduce, total on process 0 is: [ 0.  6. 12. 18. 24. 30. 36. 42. 48. 54.]
```

Summary

Numpy array as buffer-like object in mpi4py

- fast communication
- less flexible code (need to deal with memory)
- blocking and nonblocking communication
    - Send, Recv, Isend, Irecv
- collective communication
    - Bcast, Scatterv, Gatherv, Reduce