Advanced Collectives

Advanced Message-Passing Programming

Reusing this material

Overview

- Motivation
- 2D gather pattern
- MPI_Gather
- Resized datatypes
- MPI_Gatherv
- Other collectives
- Summary

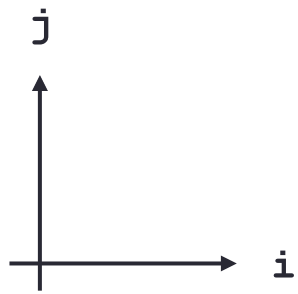
Motivation

- Collectives are a key feature of MPI
  - much simpler to use than implementing your own operations
  - much faster than a DIY approach
- Flexibility in what processes take part
  - e.g. pass a sub-communicator instead of MPI_COMM_WORLD
- However ...
  - what if your data layout does not match the collective's pattern?
  - what if your data type is not supported?
- Solutions
  - derived datatypes
  - derived datatypes + user-defined reduction operations (see later)

Canonical example

- Have a 2D array distributed across a 2D process grid
- Want to use MPI_Gather to collect data on single process
  - e.g. before performing serial controller-IO to disk
- Study this particular example in some detail
  - straightforward to generalise to other collectives
  - e.g. MPI_Scatter, MPI_Reduce, MPI_Allreduce, MPI_Alltoall, ...
- Difficulty is understanding how derived datatypes work with collectives
  - after that, relatively straightforward to apply to other cases

Canonical example (global indices)



(assume integer arrays
and C-like array storage)

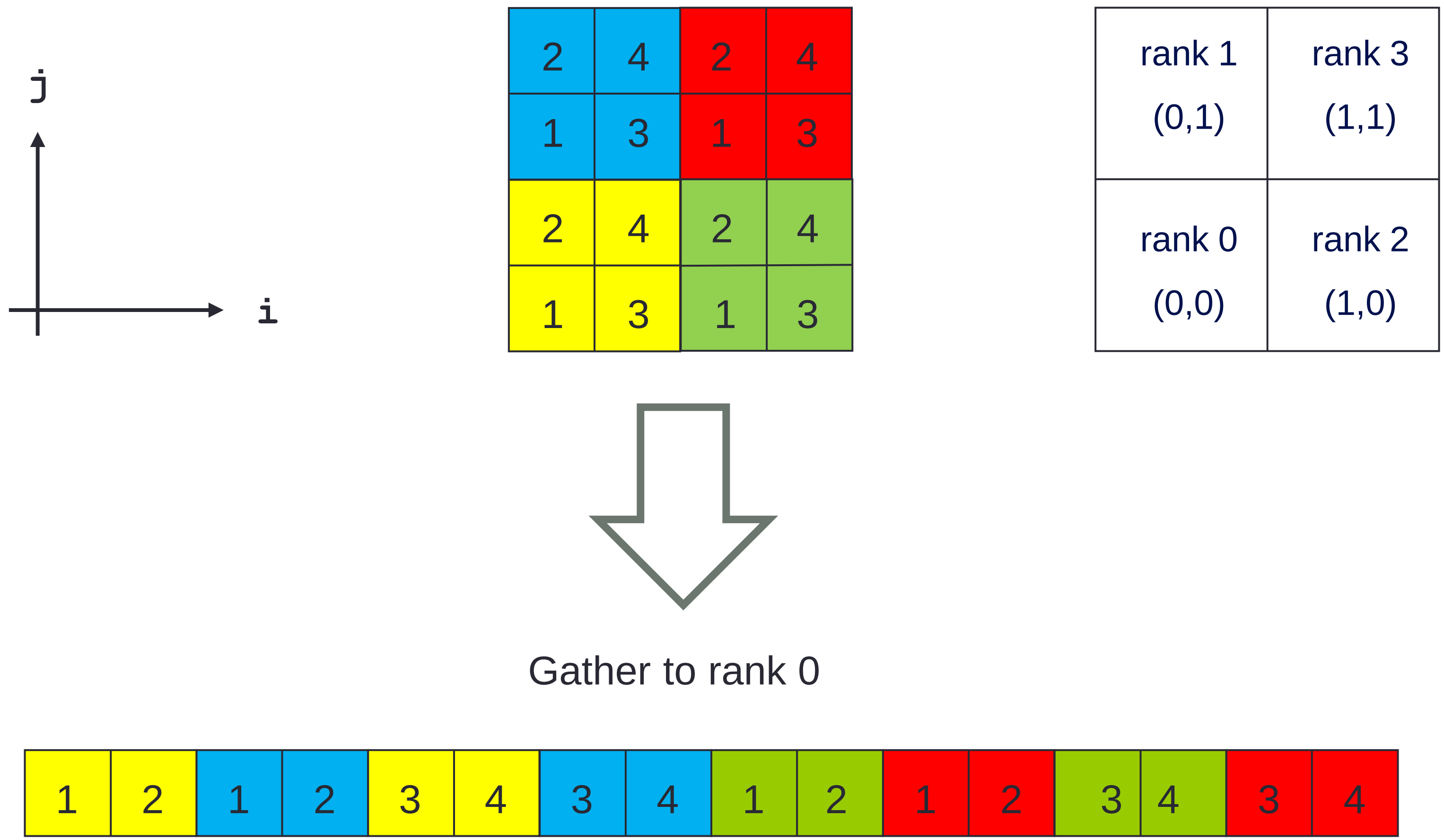
4	8	12	16
3	7	11	15
2	6	10	14
1	5	9	13

rank 1 (0,1)	rank 3 (1,1)
rank 0 (0,0)	rank 2 (1,0)

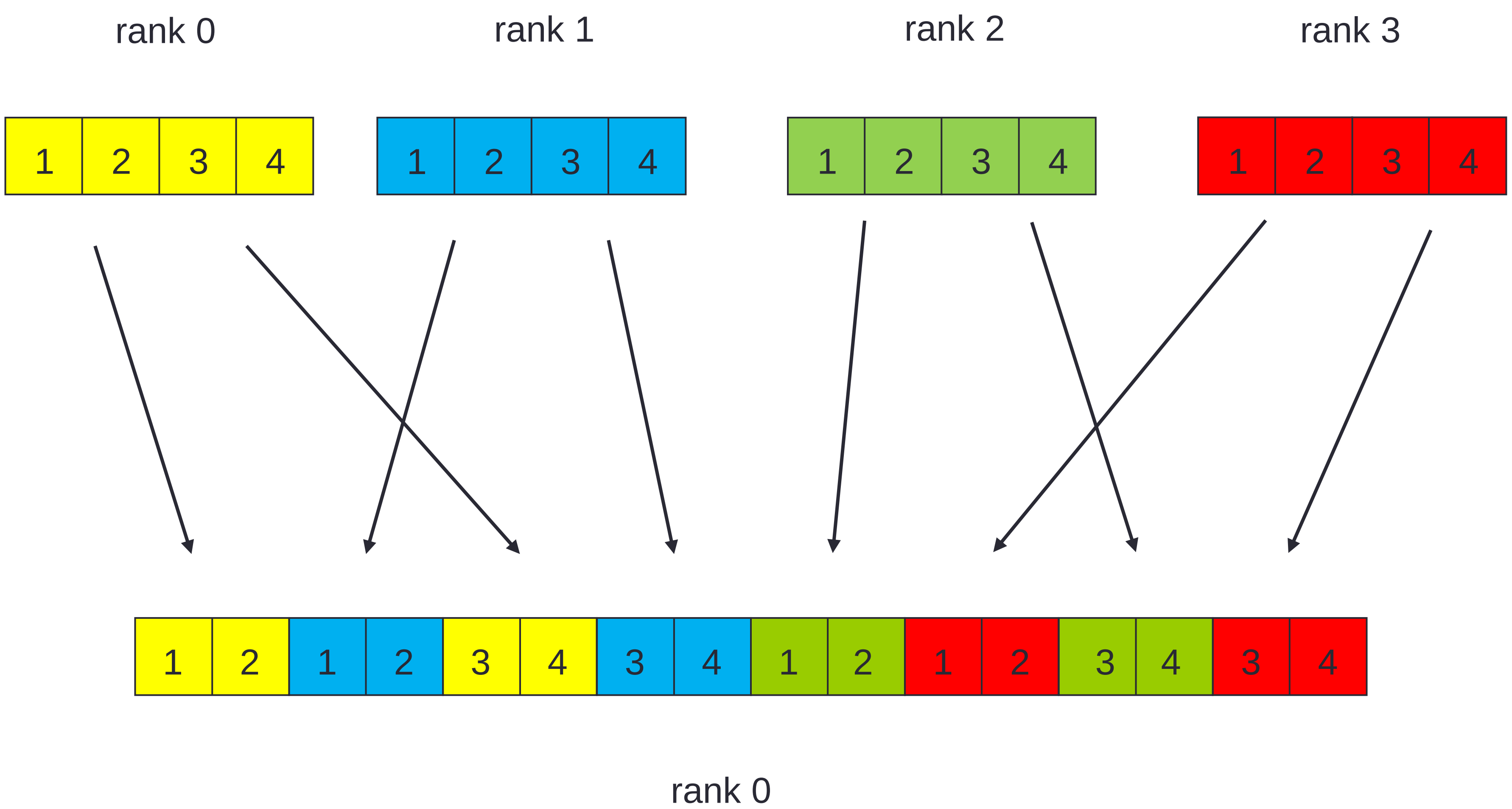
Gather to rank 0

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16

Canonical example (local indices)



Canonical example (linear buffers)



MPI_Gather (i)

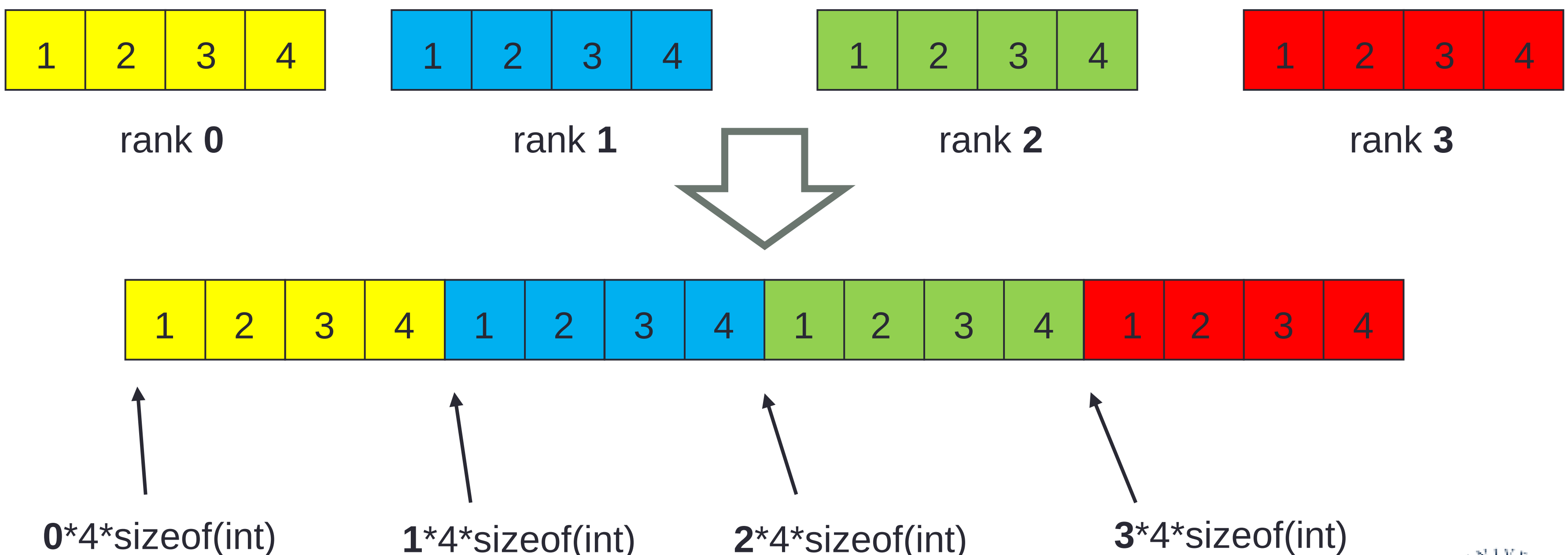
```
MPI_Gather(void *sendbuf, int sendcount, MPI_Datatype sendtype,
           void *recvbuf, int recvcount, MPI_Datatype recvtype
           int root, MPI_Comm comm)
```

```
MPI_GATHER(SENDBUF, SENDCOUNT, SENDTYPE, RECVBUF, RECVCOUNT, RECVTYPE,
           ROOT, COMM, IERROR)
```

- All processes in comm:
  - send **sendcount** items of type **sendtype** from **sendbuf** to rank **root**
- Root process only:
  - receive **recvcount** items of type **recvtype** separately from every process
  - these are received into **recvbuf** in rank order
  - ... but where exactly are they placed?

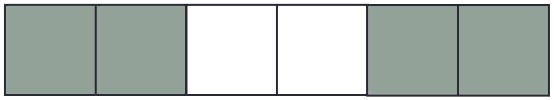
MPI_Gather (ii)

- Message from **rank** is received at (byte) displacement:
  - disp = **rank***recvcount*extent(recvtype)
  - straightforward for basic datatypes where recvtype = sendtype
    - in this case: sendtype = recvtype= MPI_INT, sendcount = recvcount = 4



First problem

- Data pattern at receive side is incorrect
  - incoming messages needs to be scattered into receive buffer
- Solution
  - specify a vector (or subarray) for recvtype
  - pattern is a 2x2 subsection of a 4x4 array



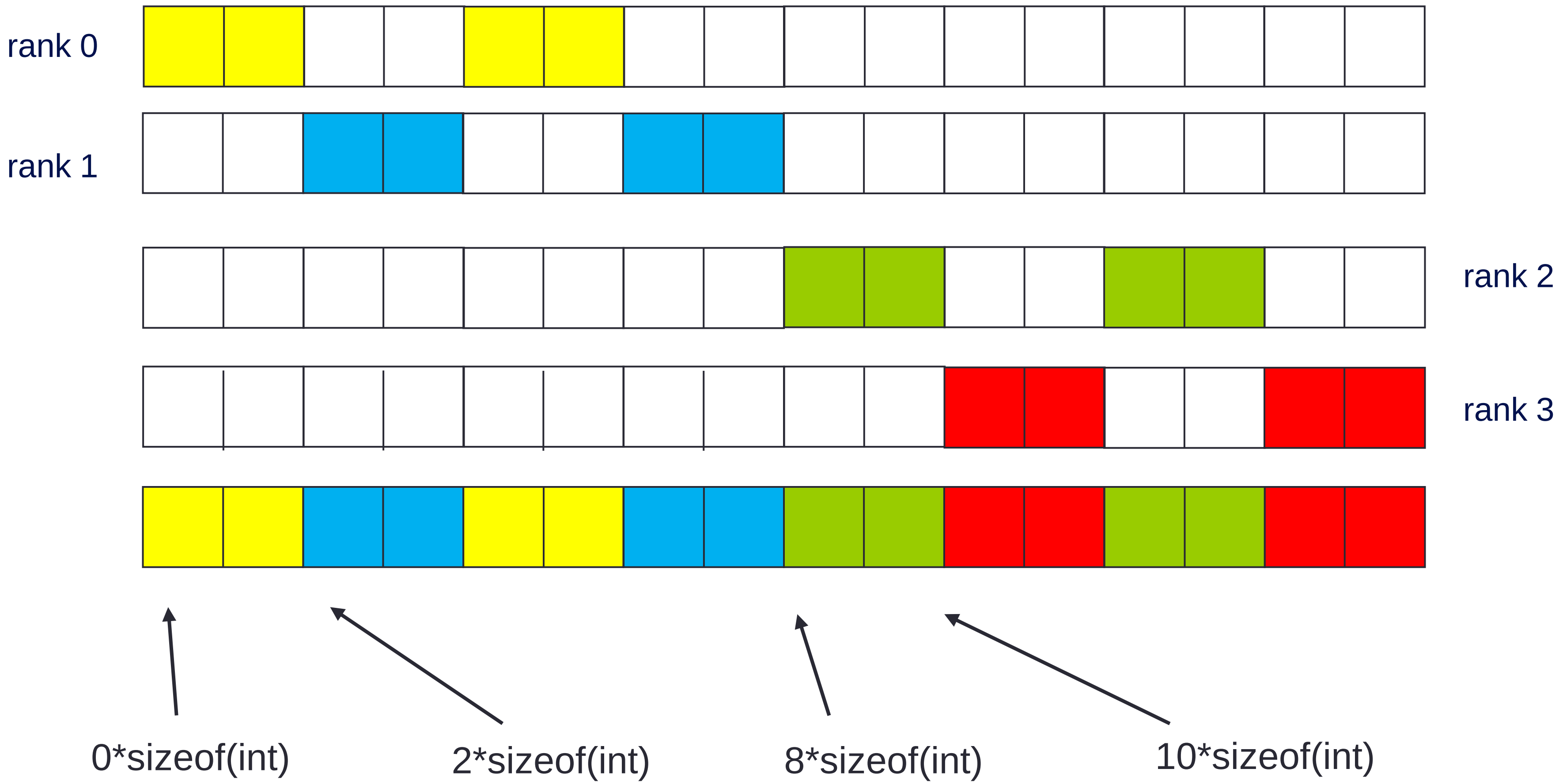
- Now: sendcount, sendtype **not equal** to recvcount, recvtype
  - sendcount=4, sendtype=MPI_INT; recvcount=1, recvtype=vector2x2
- But they are **compatible** as they both contain 4 integers

Why not subarrays?

- If we were implementing by hand, an option would be
  - every worker sends 4 integers
  - controller defines a different subarray type for each worker
  - simply issue a receive of 1 subarray type
    - specify the start of the controller's array as the receive buffer

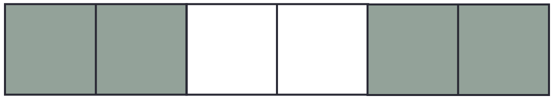
- But ...
  - MPI_Gather() only allows for a single receive type
  - need to ensure that all the displacements are correctly calculated

Required pattern



Second problem

- Displacements in receive buffer are not regular
  - counting in integers: 0, 2, 8 and 10
- Solution
  - MPI_Gatherv takes vectors of recvcounts and displacements
  - all are counted in terms of number of recvtypes
  - MPI_Gather assumes: recvcounts = 1, 1, 1, ...; displs = 0, 1, 2, 3, ...
- So what is the extent of the recvtype?



  - extent is distance from start of first to end of last element
  - MPI_Type_get_extent(vector2x2, ...) = 6 integers

Third problem

- Displacements in receive buffer are not multiples of extent
  - counting in integers, required displacements are: 0, 2, 8 and 10
  - extent of vector2x2= 6, so can only place at 0, 6, 12, 18, ...
- Solution
  - resize new datatype so it has a more useful extent, e.g. 1 integer

```
MPI_Type_create_resized(MPI_Datatype oldtype, MPI_Aint lb,
MPI_Aint extent, MPI_Datatype *newtype)
```

```
MPI_TYPE_CREATE_RESIZED(OLDTYPE, LB, EXTENT, NEWTYPE, IERR)
INTEGER OLDTYPE, NEWTYPE, IERROR
INTEGER(KIND=MPI_ADDRESS_KIND) LB, EXTENT
```

Resizing a datatype

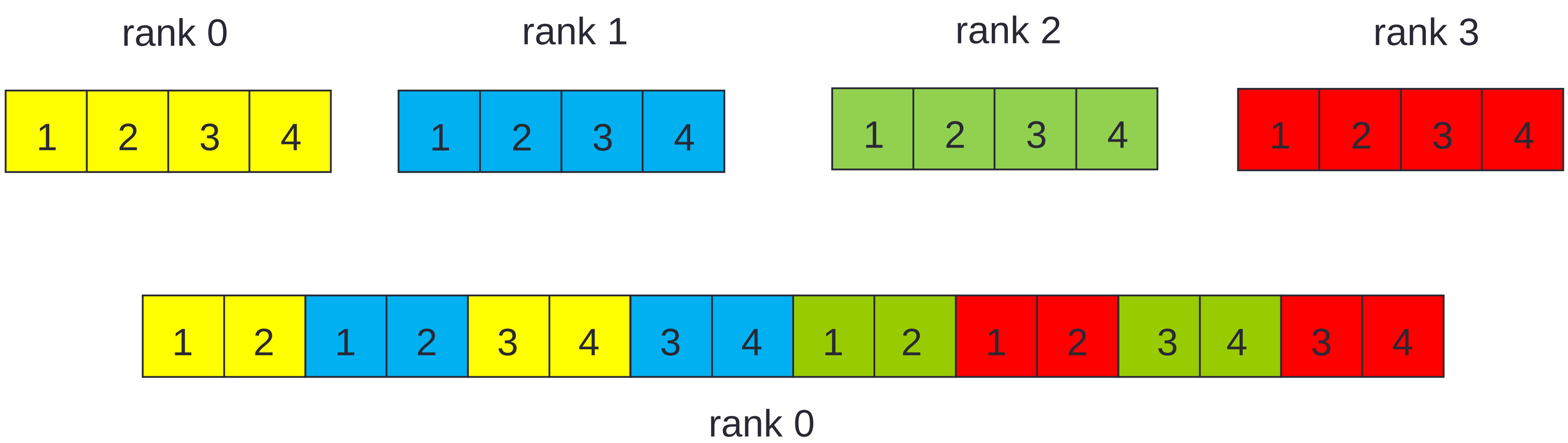
- “lower bound” specifies where datatype starts
  - e.g. create a leading gap (not needed here so lb=0)
  - lb and extent are 64-bit types: **MPI_Aint** or **MPI_ADDRESS_KIND**

```
MPI_Aint intlb, intsize, lb = 0;
MPI_Type_get_extent(MPI_INT, &intlb, &intsize);
MPI_Type_create_resized(vector2x2, lb, intsize, &vecresize);
MPI_Type_commit(&vecresize);
```

```
INTEGER(KIND=MPI_ADDRESS_KIND) :: INTLB, INTSIZE, LB=0
CALL MPI_TYPE_GET_EXTENT(MPI_INTEGER, INTLB, INTSIZE, IERR)
CALL MPI_TYPE_CREATE_RESIZED(VECTOR2x2, LB, INTSIZE,
VECRESIZE, IERR)
CALL MPI_TYPE_COMMIT(VECRESIZE, IERR)
```

MPI_Gatherv

- MPI_Gatherv(sendbuf, sendcount, sendtype, recvbuf, recvcounts, displs, recvtype, root, comm)
  - sendcount = 4, sendtype = MPI_INT
  - recvcounts = [1,1,1,1], displs = [0, 2, 8, 10], recvtype = vecresize



Other collectives

- Similar tricks can be used for scatter
  - MPI_Allgather / Allscatter also have “vector” versions

- Many scientific applications use Alltoall pattern
  - e.g. transposing a matrix between row and column decompositions
  - vector version, Alltoallv, plus derived types can ensure all data ends up directly in the correct place – avoids copy-in / copy-out
  - Alltoallv has single sendtype and recvtype, but vectors for sendcounts and sdispls as well as recvcounts and rdispls
    - all displacements in terms of extent(type) as for Gatherv
  - Even more general form MPI_Alltoallw exists
    - vectors for sendtypes and recvtypes as well as counts and disps
    - no obvious base unit for disps: Alltoallw uses **byte** displacements (yuk!)

Summary

- Technicalities of derived datatypes can be complicated
  - may have to play tricks with extents so collectives work as expected
- However, it is worth the effort!
  - MPI collectives are very highly optimised
  - naive DIY implementation will send *P* messages on *P* processes
  - optimised collectives should scale as $\log_2(P)$
  - 100 times faster on as few as 1000 processes!
- Derived types in collectives avoids ugly copy-in / copy out
  - rearrangement of data done automatically by MPI
  - MPI_Alltoall[v,w] used by many parallel scientific applications