Implementing MPI RMA in the ONETEP DFT code

Chris Brady, Heather Ratcliffe
University of Warwick

ONETEP

Warwick RSE

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Background

- ONETEP is a linear scaling density functional theory code
  - Calculate electronic structure for sets of atoms
- Conventional DFT codes scale as $O(N^3)$
- ONETEP reduces this to O(N) by localising orbitals and truncating the density matrix
  - This means that it has electron density and local effective potential defined in boxes that have to be either deposited to or extracted from an underlying grid

Background

- ONETEP is a OpenMP threaded MPI code using MPI_THREAD_SERIALIZED level multithread support
  - Performance is **much** worse with MPI_THREAD_MULTIPLE - not worth considering
- MPI decomposition is **NOT** simple domain decomposition
  - A given rank is responsible for a given section of the underlying grid but not necessarily the boxes that overlap that section of the grid

Background

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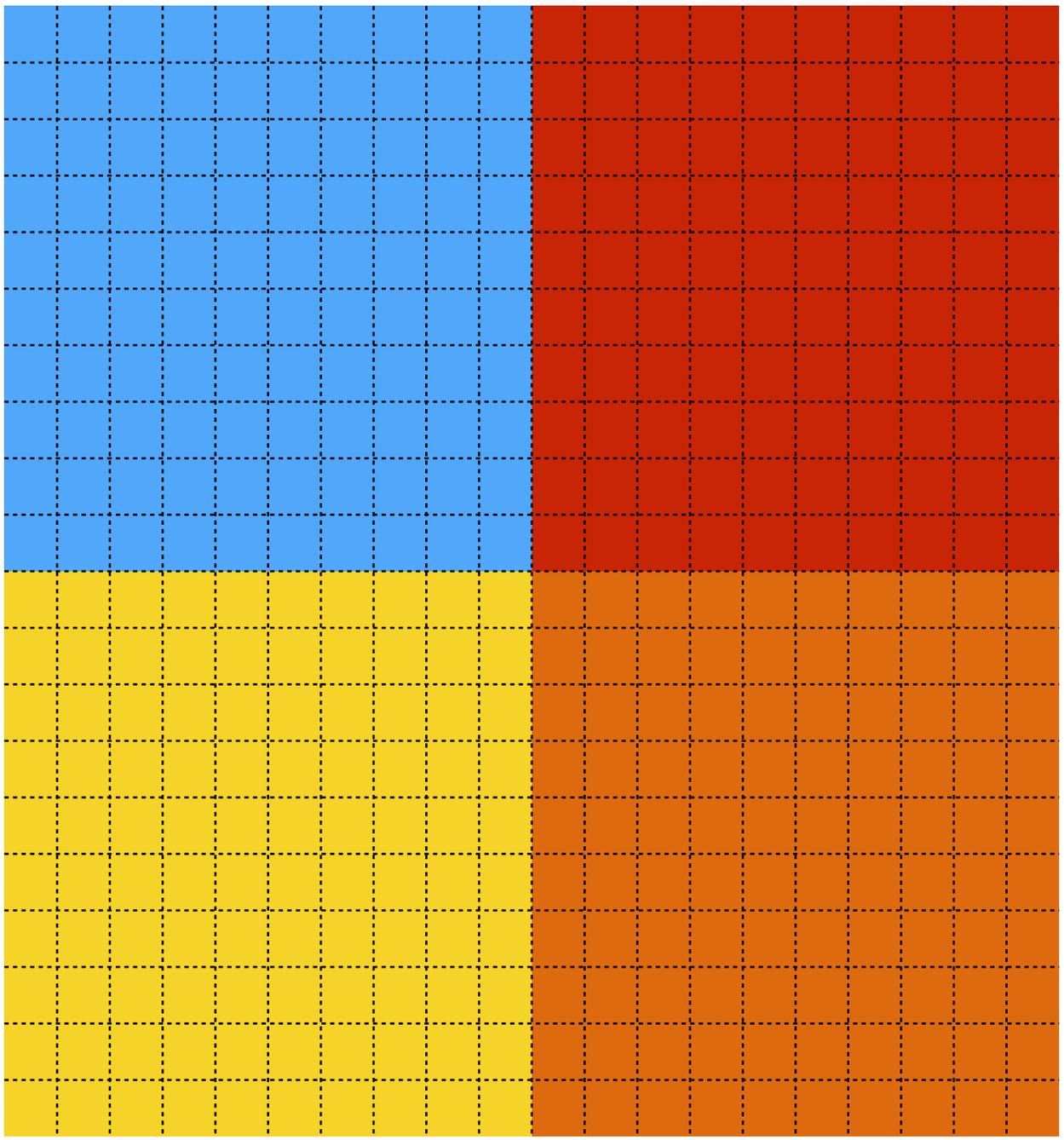
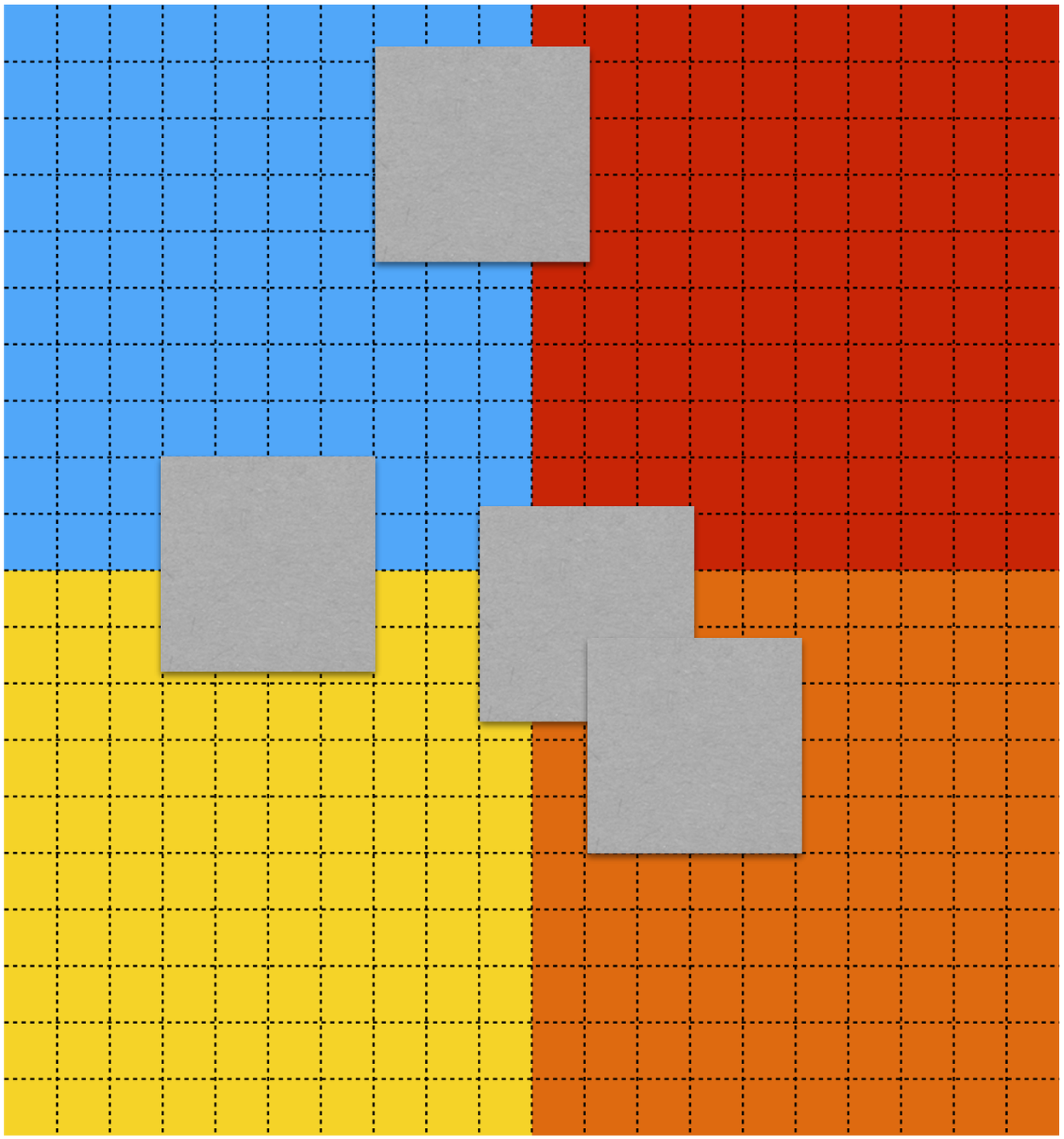


ONETEP
Is actually 3D!

Background



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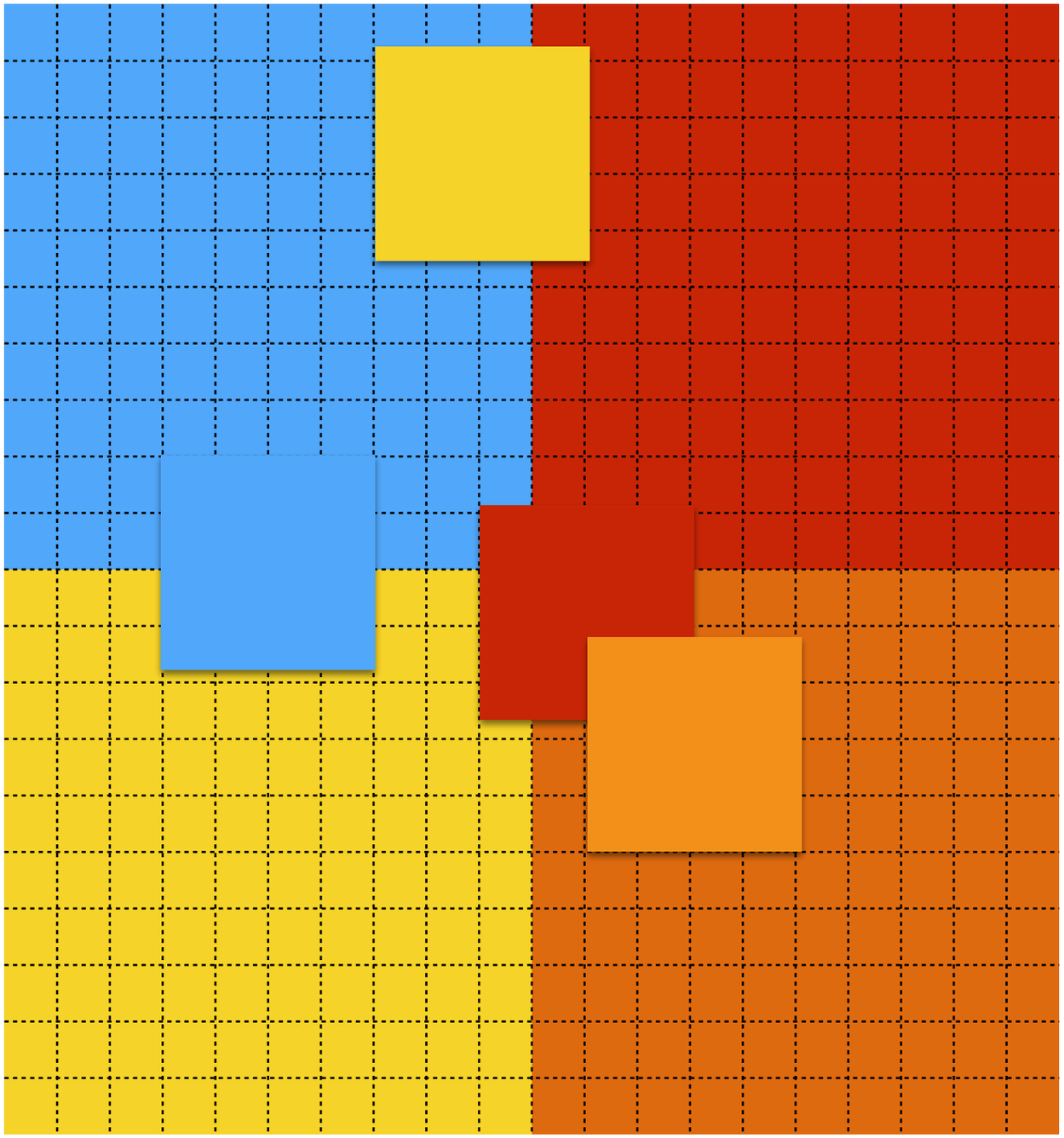


Deposition

- First consider depositing density to the grid
- The density is not simply stored for each box but is calculated just before it is deposited
  - Each box is calculated in a separate thread
- In an OpenMP critical section the actual deposition occurs

Deposition

- All ranks call MPI_Alltoall to describe the part of their current box that they are going to deposit on each other rank
- All ranks then simply loop over all ranks and send and receive the parts of the boxes that are needed by or sent from each other rank
- Received box parts are then added to the underlying grid using local stores
    - Box parts that are on local ranks are accumulated by a local store
- Introduces artificial synchronisation - different ranks only need to synchronise because of the two sided communications.
    - Because of OpenMP critical section threads are blocked as well

RMA Addition

- Performance at high thread counts per rank was limited at high rank count
- The idea of using RMA was to remove the necessity to synchronise across ranks that is enforced by the call to MPI_Alltoall and hence reduce the time in an OpenMP critical section
- The code could also be simplified by using MPI_Accumulate, removing the need for separate transmit and store semantics
- I am thinking here only as an application programmer, I'm not thinking at all about what would be a major annoyance to implement for an MPI library
    - If you spot that I am describing any misunderstandings of the MPI standard, please let me know!

Initial Approach

- The grid to be accumulated to is not a fixed piece of memory so a new window is created every time the density is to be accumulated (and freed at the end)

- The destination array is not updated except by calls to MPI_Accumulate until the window is freed so first thought is that I can use MPI_Win_fence to start the epochs immediately after window is created (and end it before MPI_Win_free is called)

  - Have to reuse the source buffer to MPI_Accumulate so can't do that

  - Would be nice to have source lifetime control in MPI RMA without having to use MPI_Win_lock and MPI_Win_flush_local

Initial Approach

- Would have been nice to be able to have multiple calls to MPI_Win_start/MPI_Win_complete for a single call to MPI_Win_post/MPI_Win_wait

- Instead do MPI_Win_lock_all immediately after MPI_Win_create and MPI_Win_unlock_all immediately before MPI_Win_free

  - Every processor has to (potentially) communicate with every other processor, hence lock_all

Initial Approach

- Actual transfer of the data involves working out the overlap between the source box and the grid domain of every rank
  - If there is an overlap between the source box and a given rank then types for source and destination are created and MPI_Accumulate is called with MPI_SUM operation
- MPI_Win_flush_all_local is called after the loop over ranks to ensure that the source array can be reused
- All individual MPI commands are placed in OpenMP critical sections

Problem

- This worked and gave the same answer as the conventional comms version

- There was an unexpected problem as the problem scaled up
  - Code started to be killed for excessive memory use

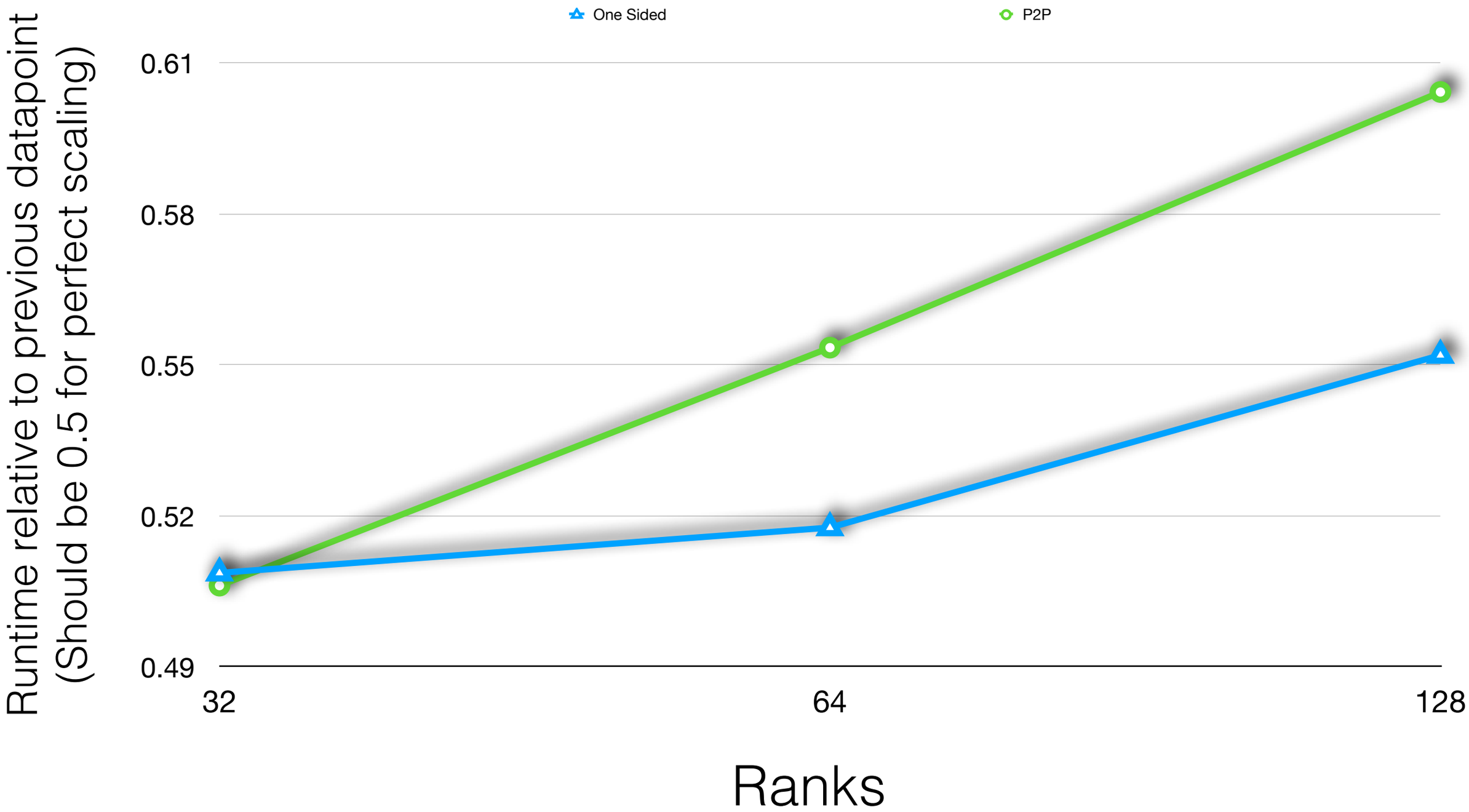
- Turns out that both the OpenMPI and Cray MPI implementations were dealing with my calls to MPI_Win_flush_all_local by copying the input buffer

  - Would be nice to have an option to set a buffer to this and have it block until the buffer has space rather than crashing

Solution

- Tried to replace with call to MPI_Win_flush_all
- Doesn’t actually seem to change behaviour
- So had to switch to another approach
- Switched across to calling MPI_Win_lock as soon as start trying to deposit a box and MPI_Win_unlock once you have finished
- Now have to return to putting the whole deposition of a given box into a critical section
    - Limits performance improvement a bit

Scaling over three doublings



128 Threads per Rank

Strange result

- This is an implementation issue but…
  - Under both Cray and OpenMPI there is a very strange result
  - Scaling of the code is better than with the two sided implementation
  - Actual speed is slower when the code is running with > 1 thread per rank
  - Slowdown is actually at the end of the OpenMP end parallel section (actually inside pthread_join)
    - Not sure why?

Conclusions

- MPI RMA works and does improve scaling
- Current MPI RMA interface isn't natural idiom for this type of problem
  - Would be nice to have more control over local completion in active target synchronisation modes
  - Would be **really** be good to have some way of avoiding local completion in passive target synchronisation modes from causing memory usage growth and that to be specified by standard rather than implementation dependent