Beyond MPI_Send: What I learned implementing MPI for halo exchange

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Slides: git.io/fNH3t

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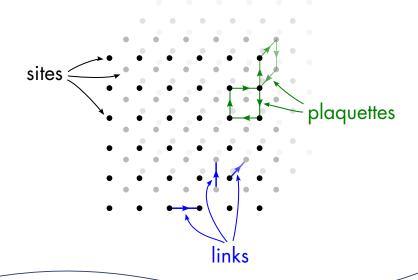
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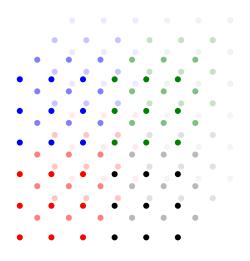
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- Three-dimensional problem; 1-3 additional d.o.f.s

3D lattice



Partitioning a 3D lattice



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- Collectives, e.g. MPI_Reduce

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- In-place reductions

TIL #2: Subarray types

Slides: ait.io/fNH3t

```
subroutine init_single_halo_type_4(direction, position, size4, &
                                   datatype, typetarget)
  integer, intent(in) :: direction, position, size4
  type(MPI_Datatype), intent(in) :: datatype
  type(MPI_Datatype), intent(out) :: typetarget
  integer, dimension(4) :: sizes, subsizes, starts
  sizes = (/ ksizex_l + 2, ksizey_l + 2, ksizet_l + 2, size4 /)
  subsizes = (/ ksizex 1, ksizey 1, ksizet 1, size4 /)
  subsizes(direction+1) = 1
  starts = (/ 1, 1, 1, 0 /)
  starts(direction+1) = position
  call MPI Type Create Subarray(4, sizes, subsizes, starts, &
                   MPI Order Fortran, datatype, typetarget)
  call MPI_Type_Commit(typetarget)
  return
end subroutine init_single_halo_type_4
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call MPI_Cart_Shift(comm, 2, 1, ip_tdn, ip_tup)
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- Gives index of processes in both directions

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- Collectives planned for MPI 3.2, e.g. MPI_AllReduce_Init

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- Test each function still gives same results as previously

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 - Store state from rank 0
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- Check that read and write still give same results

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- Include the type for MPI-IO here

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- Unit test

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- All MPI calls are wrapped with #ifdef MPI
- Check regression tests

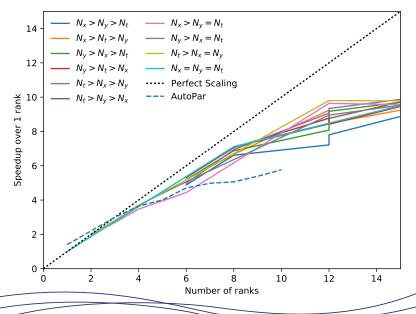
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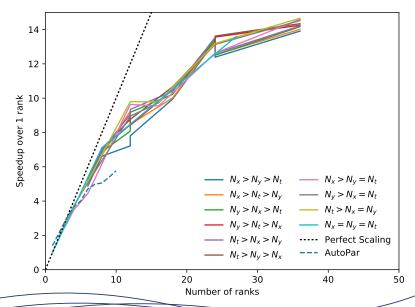
- Correlation functions: lots of extra bookkeeping
- Reading input parameters: do on rank 0 and broadcast

Performance on Hawk



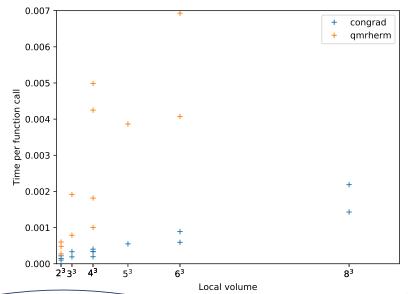
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Weak and strong scaling of a single operation



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Thanks for listening!

