Profiling MPI code to identify bottlenecks

Ed Bennett

@QuantumofEd







Supercomputing Wales Swansea Symposium, 2018-09-13

Slides: git.io/fAV4t

MPI: Message Passing Interface

- MPI: Message Passing Interface
- Born in 1991, now at version 3.1

- MPI: Message Passing Interface
- Born in 1991, now at version 3.1
- Single Program Multiple Data model

- MPI: Message Passing Interface
- Born in 1991, now at version 3.1
- Single Program Multiple Data model
 - Same program runs multiple times (on one or more nodes)

- MPI: Message Passing Interface
- Born in 1991, now at version 3.1
- Single Program Multiple Data model
 - Same program runs multiple times (on one or more nodes)
 - Distributed memory

- MPI: Message Passing Interface
- Born in 1991, now at version 3.1
- Single Program Multiple Data model
 - Same program runs multiple times (on one or more nodes)
 - Distributed memory
 - Communication is explicit

- MPI: Message Passing Interface
- Born in 1991, now at version 3.1
- Single Program Multiple Data model
 - Same program runs multiple times (on one or more nodes)
 - Distributed memory
 - Communication is explicit
- Point-to-point send and receive

- MPI: Message Passing Interface
- Born in 1991, now at version 3.1
- Single Program Multiple Data model
 - Same program runs multiple times (on one or more nodes)
 - Distributed memory
 - Communication is explicit
- Point-to-point send and receive
- Immediate (non-blocking) versions

- MPI: Message Passing Interface
- Born in 1991, now at version 3.1
- Single Program Multiple Data model
 - Same program runs multiple times (on one or more nodes)
 - Distributed memory
 - Communication is explicit
- Point-to-point send and receive
- Immediate (non-blocking) versions
- Point-to-all (broadcast) operations

- MPI: Message Passing Interface
- Born in 1991, now at version 3.1
- Single Program Multiple Data model
 - Same program runs multiple times (on one or more nodes)
 - Distributed memory
 - Communication is explicit
- Point-to-point send and receive
- Immediate (non-blocking) versions
- Point-to-all (broadcast) operations
- Collectives, e.g. reductions (sums, maxima, minima, etc.)

Profiling MPI

• Intel MPI provides profiling tools source /apps/compilers/intel/2018.3/itac_2018/bin/itacvars.sh mpirun -trace [my_application]

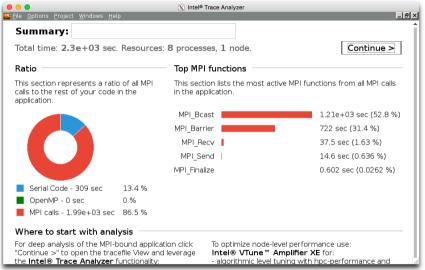
Profiling MPI

- Intel MPI provides profiling tools source /apps/compilers/intel/2018.3/itac_2018/bin/itacvars.sh mpirun -trace [my_application]
- Output can be large, so choose a small problem size

Profiling MPI

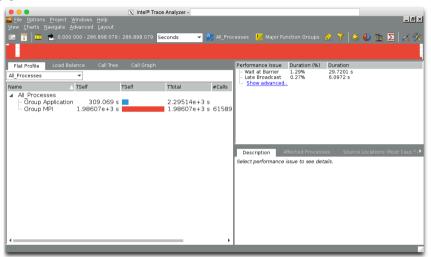
- Intel MPI provides profiling tools
 source /apps/compilers/intel/2018.3/itac_2018/bin/itacvars.sh
 mpirun -trace [my_application]
- Output can be large, so choose a small problem size
- Visualise the results with traceanalyzer

Summary view



Slides: ait.io/fAV4t

Whole application timeline



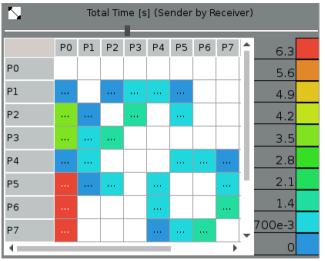
Slides: git.io/fAV4t

Detailed timeline



Slides: git.io/fAV4t

Message pattern



Reductions summary



Slides: git.io/fAV4t

• We found that:

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time
 - Communications are scattered throughout the program

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time
 - Communications are scattered throughout the program
 - Very small amounts of compute between each communication

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time
 - Communications are scattered throughout the program
 - Very small amounts of compute between each communication
 - Coordinator-worker pattern

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time
 - Communications are scattered throughout the program
 - Very small amounts of compute between each communication
 - Coordinator-worker pattern
 - Some minor load balancing concerns

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time
 - Communications are scattered throughout the program
 - Very small amounts of compute between each communication
 - Coordinator-worker pattern
 - Some minor load balancing concerns
- Things to think about

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time
 - Communications are scattered throughout the program
 - Very small amounts of compute between each communication
 - Coordinator-worker pattern
 - Some minor load balancing concerns
- Things to think about
 - Can we use a peer-to-peer pattern instead?

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time
 - Communications are scattered throughout the program
 - Very small amounts of compute between each communication
 - Coordinator-worker pattern
 - Some minor load balancing concerns
- Things to think about
 - Can we use a peer-to-peer pattern instead?
 - Can we increase the amount of work between communications?

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time
 - Communications are scattered throughout the program
 - Very small amounts of compute between each communication
 - Coordinator-worker pattern
 - Some minor load balancing concerns
- Things to think about
 - Can we use a peer-to-peer pattern instead?
 - Can we increase the amount of work between communications?
 - Is the direction we're parallelising appropriate?

- We found that:
 - MPI_Barrier and MPI_Bcast taking up a lot of time
 - Communications are scattered throughout the program
 - Very small amounts of compute between each communication
 - Coordinator-worker pattern
 - Some minor load balancing concerns
- Things to think about
 - Can we use a peer-to-peer pattern instead?
 - Can we increase the amount of work between communications?
 - Is the direction we're parallelising appropriate?
- If that fails, consider more advanced MPI features

• Avoid channelling all I/O through a single rank/node

- Avoid channelling all I/O through a single rank/node
- Higher performance for reading and writing data

- Avoid channelling all I/O through a single rank/node
- Higher performance for reading and writing data
- Works really well with subarray types

- Avoid channelling all I/O through a single rank/node
- Higher performance for reading and writing data
- Works really well with subarray types

- Avoid channelling all I/O through a single rank/node
- Higher performance for reading and writing data
- Works really well with subarray types

```
call MPI_File_Open(comm, 'con', MPI_Mode_Rdonly, &
MPI_Info_Null, mpi_fh)
call MPI_File_Set_View(mpi_fh, 0_8, MPI_Real, mpiio_type, &
"native", MPI_Info_Null)
call MPI_File_Read_All(mpi_fh, theta, &
3 * ksizex_l * ksizey_l * ksizet_l, &
MPI_Real, status)
call MPI File Close(mpi fh)
```

Subarray types

```
subroutine init single halo type 4(direction, position, size4, datatype, typet)
  integer, intent(in) :: direction, position, size4
  type(MPI_Datatype), intent(in) :: datatype
  type(MPI_Datatype), intent(out) :: typet
  integer. dimension(4) :: sizes, subsizes, starts
  sizes = (/ \text{ ksizex } 1 + 2, \text{ ksizey } 1 + 2, \text{ ksizet } 1 + 2, \text{ size4} /)
  subsizes = (/ ksizex_l, ksizey_l, ksizet_l, 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, typet)
  call MPI_Type_Commit(typet)
  return
end subroutine init_single_halo_type_4
```

• Each MPI_Send/MPI_Recv pair has an overhead

- Each MPI_Send/MPI_Recv pair has an overhead
- For a tight loop, this wastes time

- Each MPI_Send/MPI_Recv pair has an overhead
- For a tight loop, this wastes time
- Instead, use MPI_Send_Init/MPI_Recv_Init outside the loop

- Each MPI_Send/MPI_Recv pair has an overhead
- For a tight loop, this wastes time
- Instead, use MPI_Send_Init/MPI_Recv_Init outside the loop
- MPI_Start/MPI_StartAll inside

- Each MPI Send/MPI Recv pair has an overhead
- For a tight loop, this wastes time
- Instead, use MPI_Send_Init/MPI_Recv_Init outside the loop
- MPI_Start/MPI_StartAll inside
- Also need MPI_Wait/MPI_WaitAll

- Each MPI Send/MPI Recv pair has an overhead
- For a tight loop, this wastes time
- Instead, use MPI_Send_Init/MPI_Recv_Init outside the loop
- MPI_Start/MPI_StartAll inside
- Also need MPI_Wait/MPI_WaitAll
- Speedup achieved will depend on architecture/communications fabric combination

- Each MPI Send/MPI Recv pair has an overhead
- For a tight loop, this wastes time
- Instead, use MPI_Send_Init/MPI_Recv_Init outside the loop
- MPI_Start/MPI_StartAll inside
- Also need MPI Wait/MPI WaitAll
- Speedup achieved will depend on architecture/communications fabric combination
- Collectives planned for MPI 3.2, e.g. MPI AllReduce Init

Thanks for listening!

