

Profiling MPI code to identify bottlenecks

Ed Bennett

@QuantumofEd



Swansea University
Prifysgol Abertawe

@SwanseaUni



SUPERCOMPUTING WALES
UWCHGYFRIFIADURA CYMRU

@SuperCompWales



@sa2c_swansea

Supercomputing Wales Swansea Symposium, 2018-09-13

Slides: git.io/fAV4t

MPI, briefly

- MPI: **M**essage **P**assing **I**nterface
- Born in 1991, now at version 3.1
- Single Program Multiple Data model
 - Same program runs multiple times (on one or more nodes)
 - 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.)

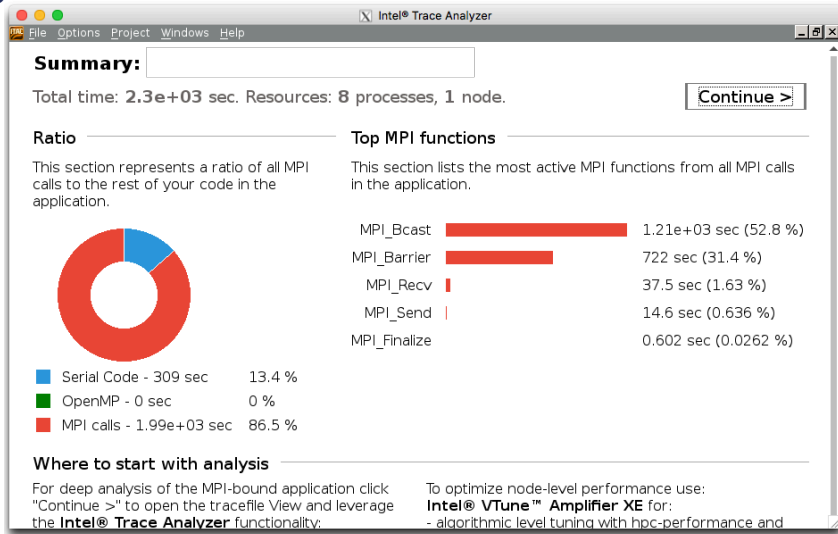
Profiling MPI

- Intel MPI provides profiling tools

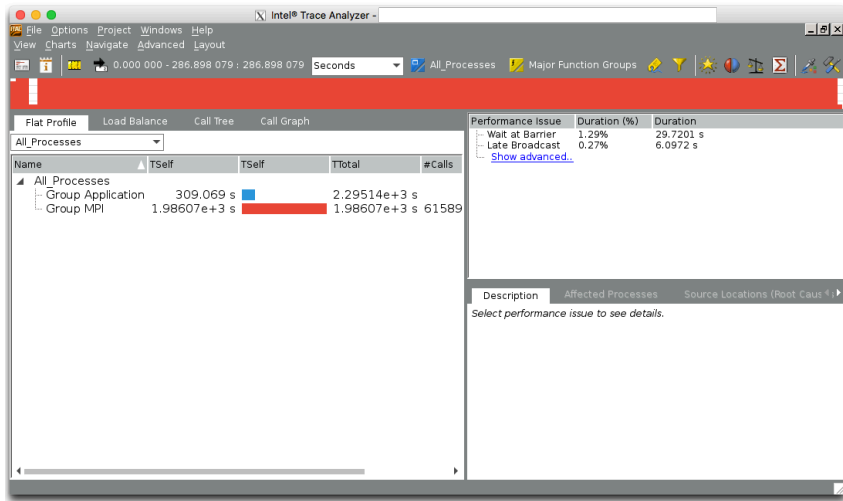
```
source /apps/compilers/intel/2018.3/itac_2018/bin/itacvars.sh  
mpirun -trace [my_application]
```

- Output can be *large*, so choose a small problem size
- Visualise the results with traceanalyzer

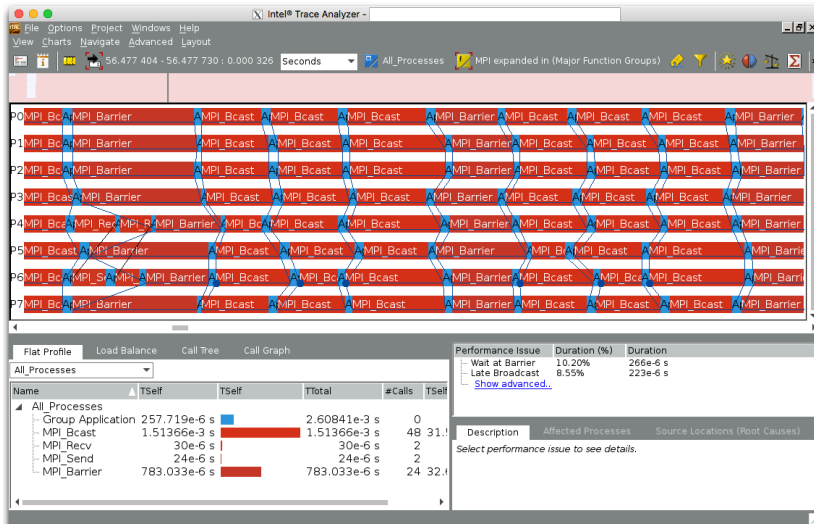
Summary view



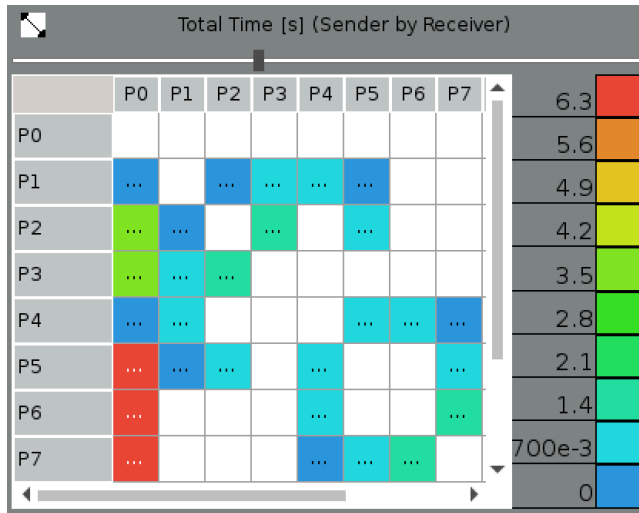
Whole application timeline



Detailed timeline



Message pattern



Reductions summary

Total Time [s] (Collective Operation by Process)									
	P0	P1	P2	P3	P4	P5	P6	P7	
MPI_Barrier	78.7392	71.0828	75.2938	74.9894	74.9034	80.9084	81.9725	81.0336	133
MPI_Bcast	135.816	135.979	136.28	136.192	129.22	129.325	129.7	130.231	126
Sum	214.556	207.062	211.573	211.181	204.123	210.233	211.673	211.264	119
Mean	107.278	103.531	105.787	105.59	102.062	105.117	105.836	105.632	112
StdDev	28.5386	32.4483	30.4929	30.601	27.1583	24.2083	23.8639	24.5985	105
									98
									91
									84
									77
									70

Ways forward

- 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

TIL #1: MPI-IO

- 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 * ksize_x_l * ksize_y_l * ksize_z_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 = (/ ksize_x_l + 2, ksize_y_l + 2, ksize_z_l + 2, size4 /)
  subsizes = (/ ksize_x_l, ksize_y_l, ksize_z_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
```

Persistent MPI communications

- 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!



Slides: git.io/fAV4t