Profiling MPI code to identify bottlenecks

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Slides: git.io/fAV4t

MPI

- 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
- Initialise program with `MPI_Init`, finish with `MPI_Finalize`
- Point-to-point send and receive with `MPI_Send`, `MPI_Recv`
- **I**mmediate (non-blocking) versions: `MPI_Isend`, `MPI_Irecv`
- Point-to-all operations with `MPI_Bcast`
- Collectives, e.g. `MPI_Reduce`

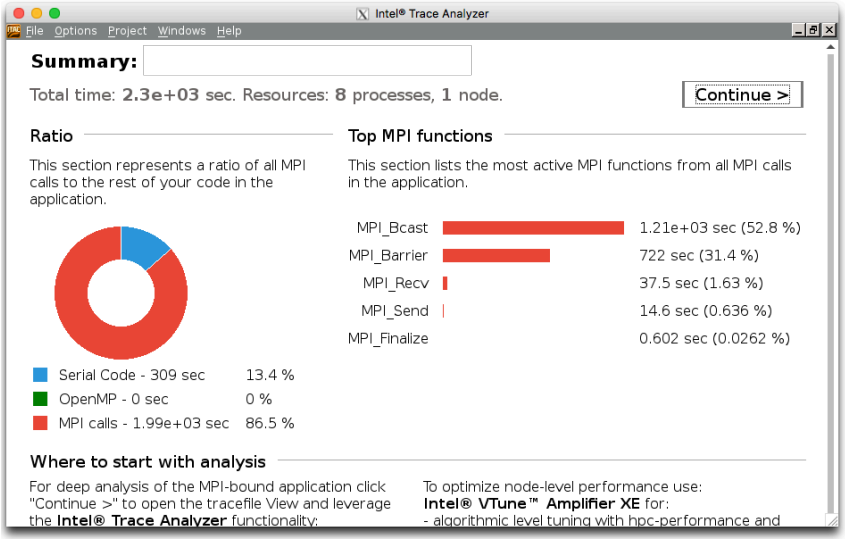
Profiling MPI

- 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



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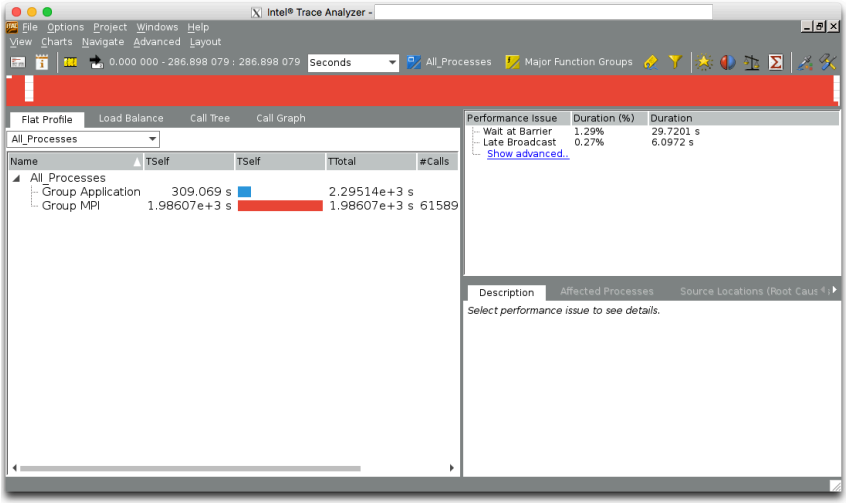
Whole application timeline



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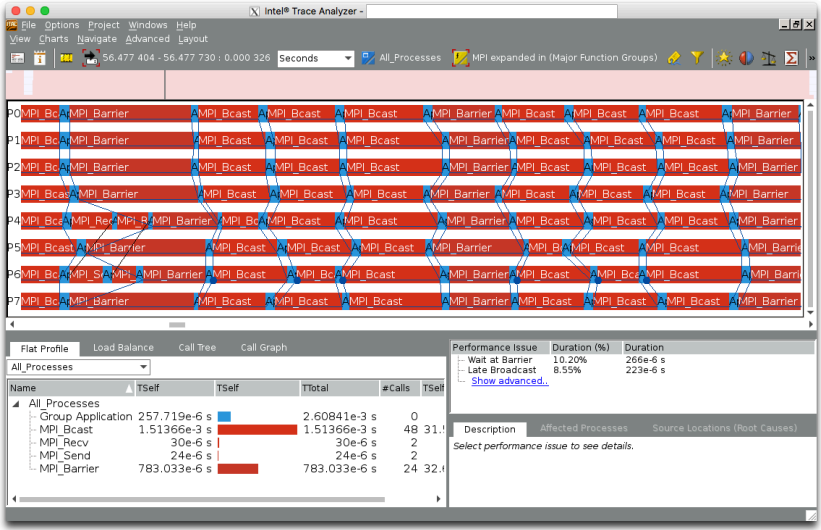
Detailed timeline



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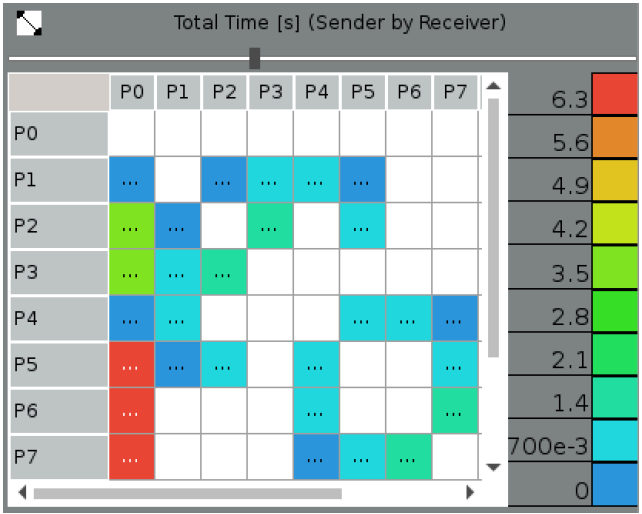
Message pattern



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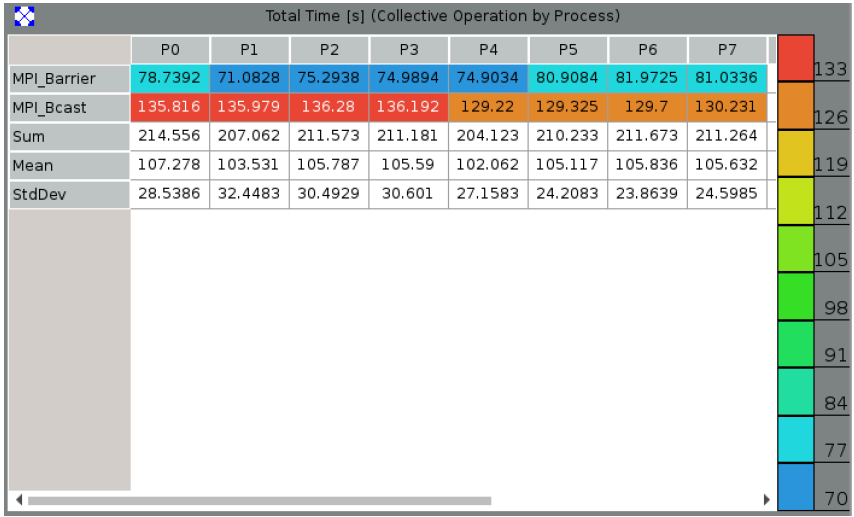
Reductions summary



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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 * 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 = (/ ksizex_l + 2, ksizey_l + 2, ksizet_l + 2, 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
```

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!

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