NATIVE MODE PORTING CASE STUDY

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Native mode porting

- Porting large FORTRAN codes
  - No code changes
  - Re-compile
  - Add linking to MKL
- MPI parallelised code
  - Some hybrid or OpenMP (small numbers of threads)
- Native mode to reduce code modifications required

GS2

- Flux-tube gyrokinetic code
  - Initial value code
  - Solves the gyrokinetic equations for perturbed distribution functions together with Maxwell's equations for the turbulent electric and magnetic fields
  - Linear (fully implicit) and Non-linear (dealiased pseudo-spectral) collisional and field terms
  - 5D space – 3 spatial, 2 velocity
  - Different species of charged particles
- Advancement of time in Fourier space
- Non-linear term calculated in position space
  - Requires FFTs
  - FFTs only in two spatial dimensions perpendicular to the magnetic field
- Heavily dominated by MPI time at scale
  - Especially with collisions

New hybrid implementation

- Funneled communication model
- OpenMP done at a high level in the code
- Single parallel region per time step
  - Better can be achieved (single parallel region per run)
- Some code excluded but computationally expensive code all hybridised

MPI processes	OpenMP threads	Execution time (seconds)
192	1	16.54
96	2	18.34
64	3	16.46
48	4	30.86
32	6	28.3

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Port to Xeon Phi

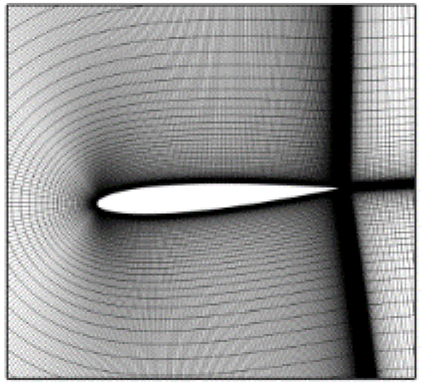
- Pure MPI code performance:
  - ARCHER (2x12 core Xeon E5-2697, 16 MPI processes): 3.08 minutes
  - Host (2x8 core Xeon E5-2650, 16 MPI processes): 4.64 minutes
  - 1 Phi (176 MPI processes): 7.34 minutes
  - 1 Phi (235 MPI processes): 6.77 minutes
  - 2 Phis (352 MPI processes): 47.71 minutes
- Hybrid code performance
  - 1 Phi (80 MPI processes, 3 threads each): 7.95 minutes
  - 1 Phi (120 MPI processes, 2 threads each): 7.07 minutes

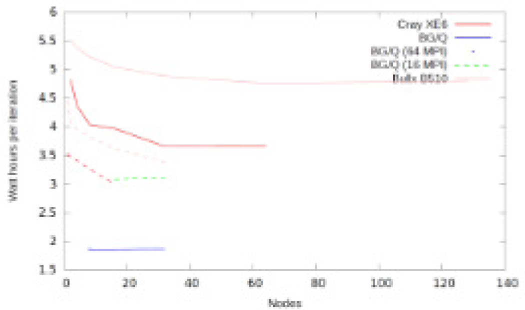
Complex number optimisation

- Much of GS2 uses FORTRAN Complex numbers
  - However, often imaginary and real parts are treated separately
  - Can affect vectorisation performance
- Work underway to replace with separate arrays
  - Initial performance numbers demonstrate performance improvement on Xeon Phi
  - 2-3% for a single routine when using separate arrays

COSA

- Fluid dynamics code
  - Harmonic balance (frequency domain approach)
  - Unsteady navier-stokes solver
  - Optimise performance of turbo-machinery like problems
  - Multi-grid, multi-level, multi-block code
  - Parallelised with MPI and with MPI+OpenMP





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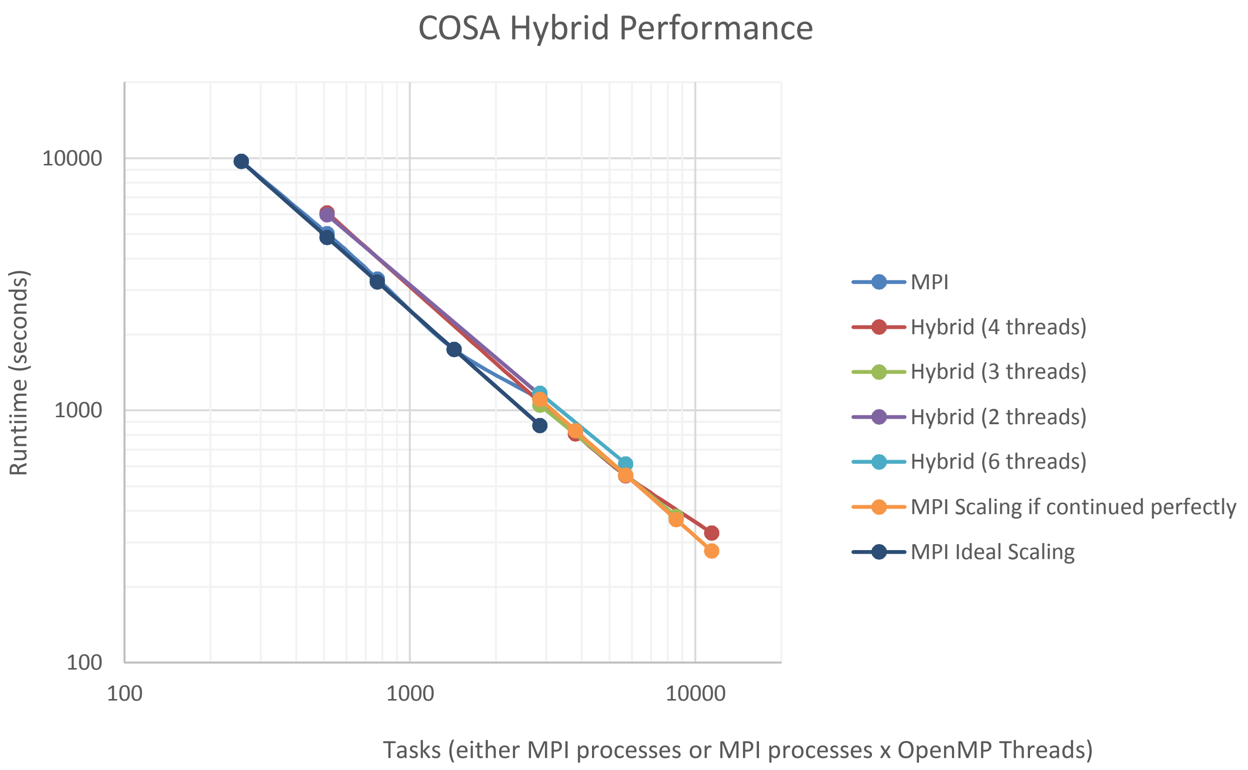
COSA Hybrid Performance
Runtiime (seconds)
10000
1000
100
100
1000
10000
Tasks (either MPI processes or MPI processes x OpenMP Threads)
MPI
Hybrid (4 threads)
Hybrid (3 threads)
Hybrid (2 threads)
Hybrid (6 threads)
MPI Scaling if continued perfectly
MPI Ideal Scaling

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Xeon Phi Performance

Configuration	Number of hardware elements	Occupancy	Runtime (s)
8 MPI processes	1/2	8/16	2105.71
16 MPI processes	2/2	16/16	1272.54
64 MPI processes	1/2	64/240	3874.45
64 MPI processes 3 OpenMP threads	1/2	192/240	2963.58
118 MPI processes 4 OpenMP threads	2/2	472/480	2118.05
128 MPI processes 3 OpenMP threads	2/2	384/480	1759.30

- Hardware:
  - 2 x Xeon Sandy Bridge 8-core E5-2650 2.00GHz
  - 2 x Xeon Phi 5110P 60-core 1.05GHz
- Test case
  - 256 blocks
  - Maximum 7 OpenMP threads

Serial optimisations

- Manual removal of floating point loop invariants divisions

```
do ipde = 1,4
      fac1 = fact * vol(i,j)/dt
end do


recip = 1.0d / dt
do ipde = 1,4
      fact1 = fact * vol(i,j) * recip
end do
```

- Provides ~15% speedup so far on Xeon Phi
  - No real benefit noticed on host
  - Changes the results

I/O

- Identified that reading input is now significant overhead for this code
  - Output is done using MPI-I/O, reading is done serially
  - File locking overhead grows with process count
  - Large cases ~GB input files
- Parallelised reading data
  - Reduce file locking and serial parts of the code
- One or two orders of magnitude improvement in performance at large process counts
  - 1 minute down to 5 seconds

Future work

Configuration	Number of hardware elements	Occupancy	Runtime (s)
8 MPI processes	1/2	8/16	2105.71
16 MPI processes	2/2	16/16	1272.54
128 MPI processes	1/2	128/240	1903.51
64 MPI processes 3 OpenMP threads	1/2	192/240	2214.56
128 MPI processes 3 OpenMP threads	2/2	384/480	1503.45

- Further serial optimisation
  - Cache blocking
- 3D version of the code now developed
  - Porting optimised and hybrid version to this

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