Here there be dragons

The HPC Code Development Journey

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scheduler memory

user interface

libraries MPI language

testing

performance CUDA bugs

documentation licensing

OpenMP throughput compilers

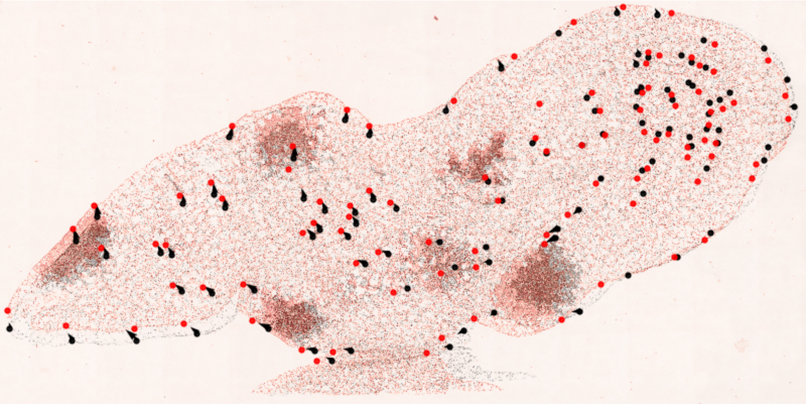
version control algorithms

What makes an application HPC?

Anything that your laptop can't do on its own...

- More compute power
- More memory
- Specialist hardware
- Large dataset storage
- Better visualisation
- etc...

A real world example — image registration



How do I write code for an HPC?

Work out what your code needs:

Large Memory - A bigger node than your laptop

- Code is fast enough, but need more memory
- No changes to "laptop code"
- Use HPC large memory nodes for larger datasets

High Throughput - Run many jobs at once

- Code is fast enough, but need to run lots
- No changes to "laptop code"
- Use HPC to run many jobs in parallel

How do I write code for an HPC?

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Work out what your code needs:

Shared Memory - Multiple cores on one node

- Code fits in a single node's memory, but needs to be faster
- Parallel algorithms for "bottlenecks" in the code
- Can often be added to existing serial code

Message Passing - Multiple cores on multiple nodes

- Need multiple nodes to fit problem in memory
- Parallelise data structures and algorithms
- Serial code usually needs a complete rewrite

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How do I write code for an HPC?

Work out what your code needs:

GPU Accelerator

- Code fits in a single node's memory, but needs to be faster
- Use 1000s of parallel threads for computation
- Needs large, parallel problems for efficient use of hardware

You can use parallel libraries to help

Low level parallel libraries

- OpenMP - Shared memory helpers for C/C++/Fortran
- MPI - MPI standard implemented by many vendors, available for many languages
- CUDA - Run many parallel threads on Nvidia GPUs
- OpenACC - OpenMP-like primitives for GPU/Intel MIC offload
- Intel TBB - threading building blocks for parallel applications

No maths in these libraries. Just tools to help you write parallel code.

But don't reinvent the wheel

Lots of higher level libraries available

- General high performance math - GSL, MKL, NAG
- Linear Algebra - LaPACK, BLAS, Intel MKL
- ODE/PDE solvers - PETSc, PVODE, FEniCS
- Scientific frameworks - PETSc, Trilinos
- Cluster computing - Dask, Hadoop, Spark
- Domain specific frameworks - Tensorflow, OpenFOAM, MFEM

Managing dependencies

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Use a dependency manager

- Give manager a list of required packages and versions
- Dependency manager coordinates installation
- Loaded using modules just like system provided software
- Install multiple versions of a library side-by-side

easybuild

Spack

Easier installation and reproducibility

- Easier installation for users
- Reproducible environment across platforms
- Easy testing of dependency versions

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Writing pFIRE

pFIRE - Image Registration Code

- Computationally intensive linear algebra
- Must scale to very large 3D images — need lots of memory!
- MPI is the best choice – look for an MPI linear algebra library

PETSc

- High performance, parallel linear algebra library
- Supports MPI or CUDA for parallelism
- High performance matrix solvers
- Lots of helpful routines for matrix and vector manipulation

Parallel linear Algebra with PETSc

```
Mat A;                                               // Create a 100000×100000 matrix called A
MatCreate(MPI_COMM_WORLD, &A);
MatSetSizes(A, PETSC_DECIDE, PETSC_DECIDE,
            100000, 100000);

Vec X, Y;                                            // Create compatible sized vectors X and Y
MatCreateVecs(A, &X, &Y);

                                                     // Insert values into the matrix and vector Y
MatSetValue(A, row, col, value, INSERT_VALUES);      // Set a matrix value
VecSetValue(Y, loc, value, INSERT_VALUES);           // Set a vector value

                                                     // Solve the equation AX = Y
KSP solver;
KSPCreate(MPI_COMM_WORLD, &solver);                  // Create Krylov solver object
KSPSetOperator(solver, A, A);
KSPSetUp(ksp);
KSPSolve(ksp, Y, X);                                 // Solve for X given M and Y
```

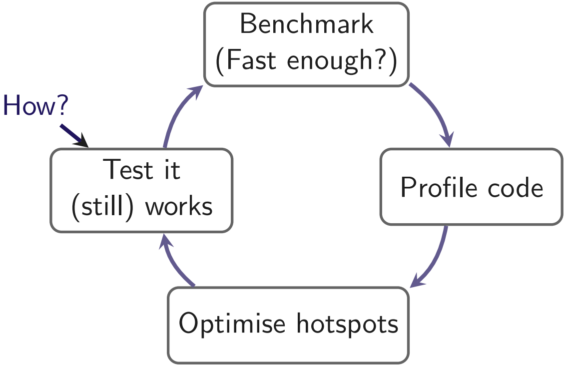
Performance and Profiling

Ignore code performance **until it works!**

- Test often
- Focus on hot spots
- Decide what is “fast enough”

Lots of tools — free and £££

- Code profilers — Slow sections
- Memory profilers — Usage and access
- MPI Profilers — Communication



Testing and Benchmarking

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Testing early and often helps catch mistakes

- Test individual functions:
  - Ensure correct output for valid input
  - Graceful failures with invalid input
- Test full program behaviour (integration tests):
  - Identify useful test cases with known results
  - Test on different machines/architectures
  - Regression tests: compare to previous versions

Lots of tools to help automate this

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Conclusions

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Writing high quality HPC code is not easy, but...

- Lots of options for applying HPC to a problem

  determine appropriate approach based on current and future needs
- Using high-level frameworks provides all the building blocks

  e.g PETSc for parallel linear algebra, Spark for big data
- Small changes can bring big gains

  parallelising just the slowest part can really help with speed
- Software development best practice helps create robust software

  regular testing finds bugs early, version control makes fixing them easier

With the right tools, *anyone* can write good HPC code

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Thank You

Useful Resources

- RSE Code Clinic

  Free 30 minute advice sessions: https://rse.shef.ac.uk/support/code-clinic/

- Best Practice Guidance

  RSE@Sheffield: https://rse.shef.ac.uk
  SSI: https://software.ac.uk

- HPC Programming

  PRACE Training: http://www.training.prace-ri.eu/
  LLNL Online Training: https://hpc.llnl.gov/training/tutorials
  GPU@Sheffield: http://gpucomputing.shef.ac.uk/
  ShARC Documentation: http://docs.hpc.shef.ac.uk/en/latest/sharc/

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