Approaches to Developing Performance Portable Scientific Software

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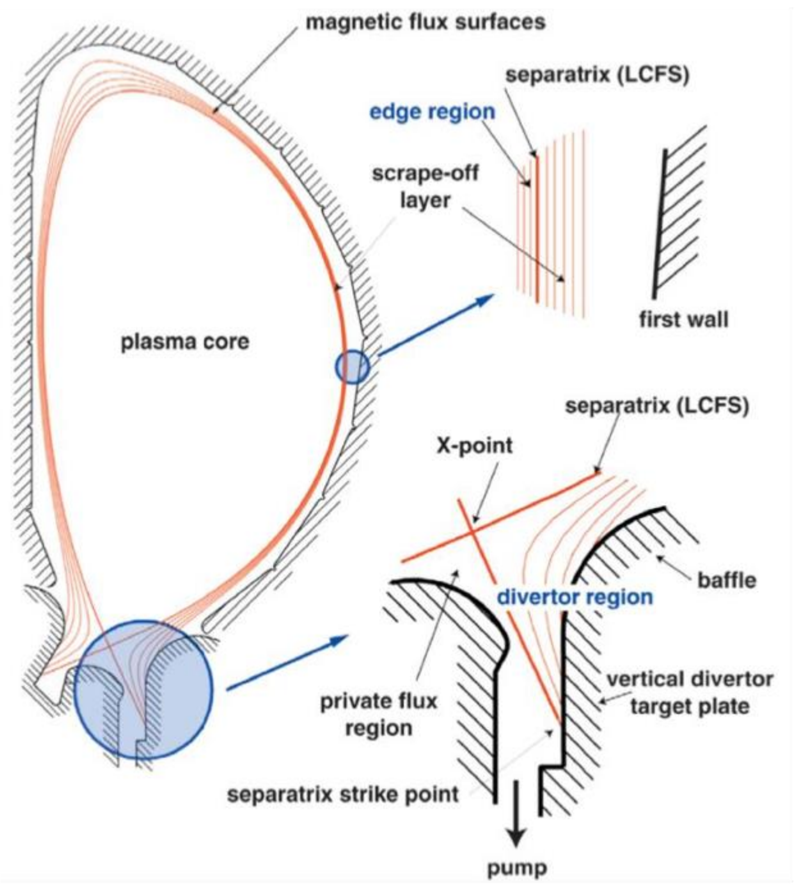
Context

Project NEPTUNE (NEutrals & Plasma TUrbulence Numerics for the Exascale)

- ***Fusion Modelling System*** **use case of ExCALIBUR**
- **Develop software to make efficient use of current Petascale and future Exascale hardware**
  - **in order to draw insights from ITER**
  - **to guide and optimise the design of the UK demonstration nuclear fusion power plant STEP**
- **Initial focus on the edge and divertor regions**
- **Our work is on investigating approaches to developing a *performance portable* code**



Challenges in Developing Modern Parallel Applications

Pre- and Post-Exascale Hardware

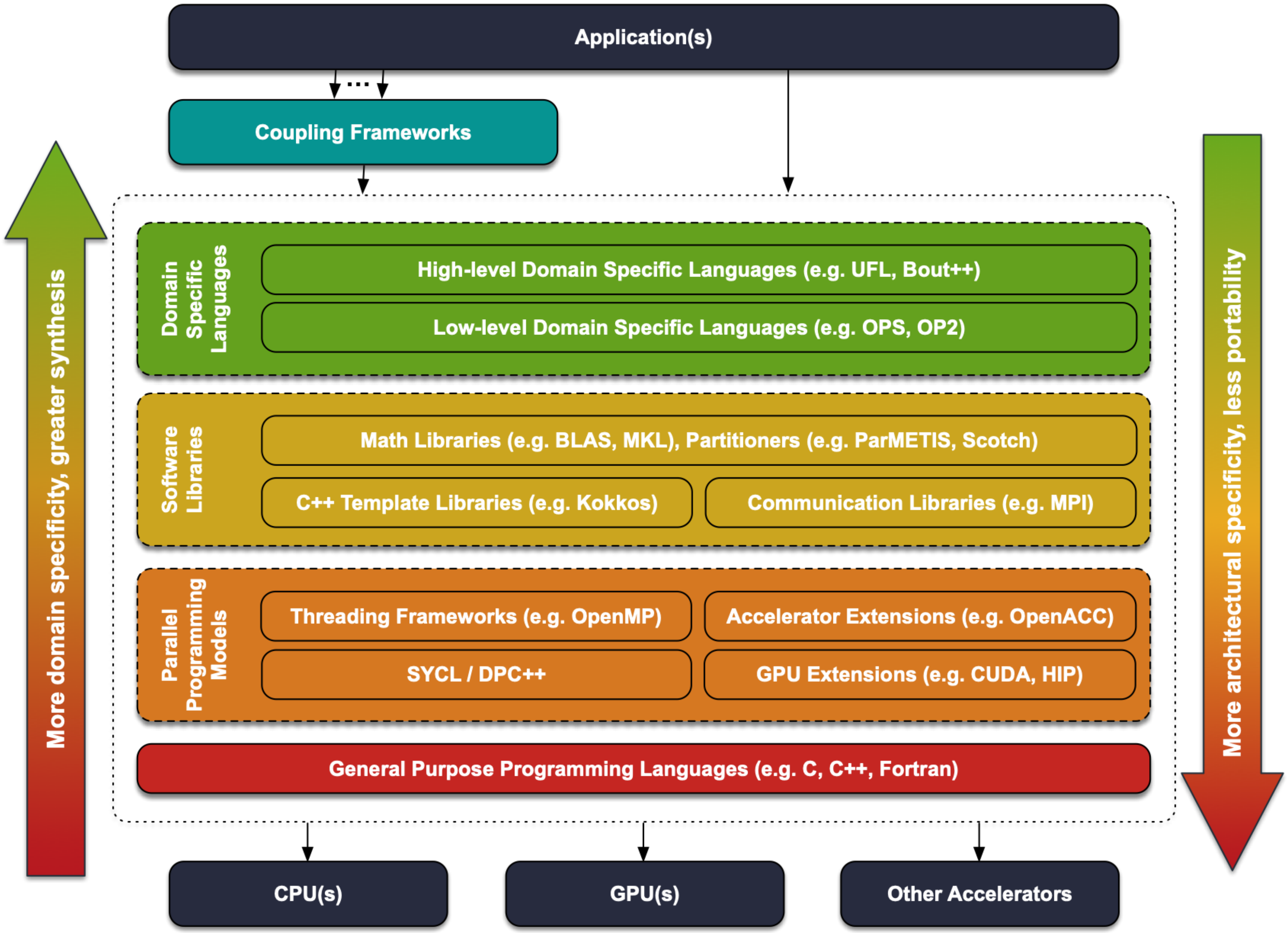
- All pre- and post-Exascale systems will be (or are) heterogenous (… except Fugaku)
- Most of the FLOP/s will be provided by GPU accelerators
  - NVIDIA Hopper
  - AMD Instinct
  - Intel Xe
- Most systems will use x86_64 hosts from Intel and AMD
  (+ perhaps some NVIDIA Grace)

Challenges in Developing Modern Parallel Applications

Developing Applications for Exascale

- How do we achieve *Performance*, *Portability*, and *Productivity* on Exascale systems?
- MPI+*X* likely for Exascale systems
  - MPI for inter-node
  - *X* for intra-node and accelerators

Challenges in Developing Modern Parallel Applications



- Review has focussed on
  - Programming languages
  - Parallel programming models
  - Software libraries
  - Domain specific languages
  - Coupling frameworks
- Assessment of 3Ps

General Purpose Programming Languages

Traditional programming languages with established history in scientific computing

- Fortran and C/C++ dominate HPC
  - Fortran codes account >50% ARCHER2 time, C/C++ >30%
- Python not traditionally "HPC", but often a glue language
- Julia promising with some "best-in-class" libraries

Considerations:

- Languages very prescriptive, optimisation may reduce portability and maintainability
- Multiple code paths may be required, duplicating development and maintenance
- Parallelism typically explicit, significantly increasing complexity

Parallel Programming Models

Extensions providing parallelism on- and off-node, or to accelerators

- **Loop-level parallelism often achieved with OpenMP**
- **MPI is de facto standard for distributed memory parallelism**
  - **Alternatives include Co-array Fortran, UPC**
- **Task-level parallelism available in OpenMP, or Charm++, LEGION, etc.**
- **Extensions targeting accelerators**
  - **CUDA, ROCm/HIP, SYCL/DPC++, OpenCL, OpenACC, OCCA**

Considerations:

- **Open standards sometimes lag hardware development**
- **Complete implementations of standards sometimes slow**
- **Low-level control over parallelism may lead to code specialisation**

Software Libraries

Scientific and mathematical libraries, and libraries that facilitate data- and task-parallelism

- Mathematical libraries provide common mathematical routines
  - Most based on BLAS, LAPACK, FFTW, optimised by vendors (e.g. MKL)
- Data libraries provide partitioning, data structures
  - Common examples include PETSc, METIS, Scotch
- C++ template libraries as parallel programming models
  - Kokkos, RAJA, Thrust

Considerations:

- Standard interfaces restrict use, but encourages vendor optimisation
- Library functions often work in lock-step, restricting fusing of operations
- Template libraries restrict use to modern C++
- Templates can increase compilation time and obfuscate errors
- But, platform specific code can be easily integrated into templated code

Domain Specific Languages

Languages and libraries limited to a particular application or algorithmic domain

- Sacrificing generality perhaps makes it feasible to achieve all 3 *P*s
- Low-level DSLs focus on parallel computation patterns
  - Mesh-based DSLs: Halide, YASK, OP-DSLs, PSyclone
  - Particle-based DSLs: PPML, PPME, OpenFPM, PPMD
- High-level DSLs focus on specific numerical methods
  - Finite differences, finite volume, finite element: FEniCS, Firedrake, ExaStencils, Bout++

Considerations:

- Debugging may be more difficult because of hidden layers
- Extensibility and customisability requires additional expertise
- There may be escape hatches, but this breaks the abstraction

Coupling Frameworks

Libraries acting as interfaces to enable communication between applications

- **Multiscale problems require different models that can interact (e.g. fluid and particle models)**
- **Typically flexible and lightweight**
  - **Minimal effect on performance and portability**
- **Examples include preCICE, CWIPI, MUI**

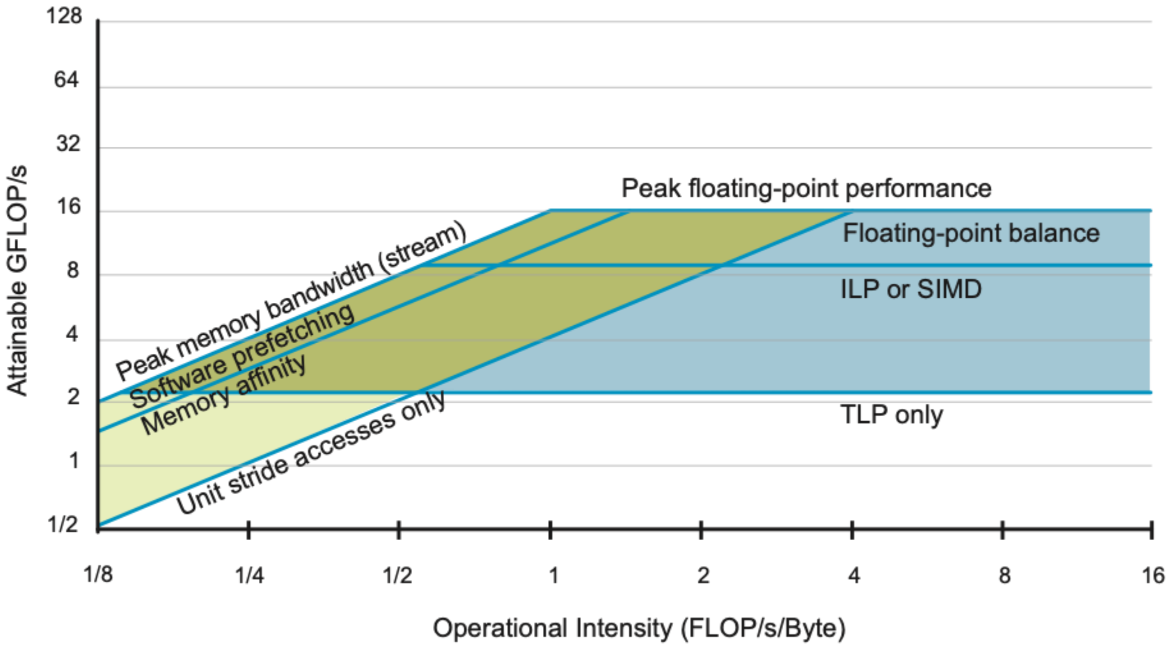
Considerations:

- **Performance of communication and coupling numerics**
- **Ease of use (and minimal intrusion)**

Evaluating Performance, Portability and Productivity

Metrics and heuristics for measuring the 3 *Ps*

- **Performance typically measured by metrics or proxies for "time-to-science"**
  - **Runtime, FLOP/s, Memory bandwidth, Energy, etc.**
- **Roofline model [1] helps us reason about performance compared to potential**



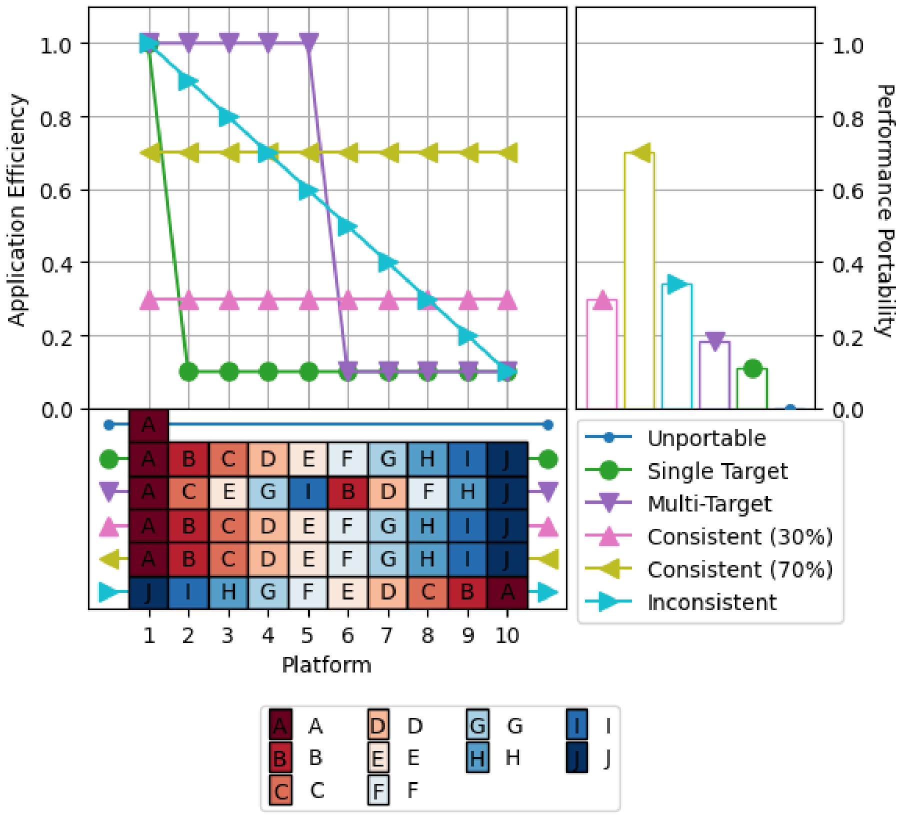
[1] S. Williams, A. Waterman, D. Patterson, Roofline: An Insightful Visual Performance Model for Multicore Architectures, Commun. ACM 52 (2009) 65–76.

Evaluating Performance, Portability and Productivity

Metrics and heuristics for measuring the 3 *Ps*

- **Although portability is a binary measure, we care about *portable performance***
- **One such metric and visual heuristic from Pennycook et al. [2] and Sewall et al. [3]**

$$\Phi(a,p,H) = \begin{cases} \dfrac{|H|}{\sum_{i \in H} \dfrac{1}{e_i(a,p)}} & \text{if } i \text{ is supported } \forall i \in H \\ 0 & \text{otherwise} \end{cases}$$



[2] S.J. Pennycook, J.D. Sewall, and V.W. Lee. Implications of a metric for performance portability. Future Generation Computer Systems, 92:947 –958, 2019.
[3] J.D. Sewall, S.J. Pennycook, D. Jacobsen, T. Deakin, and S. McIntosh-Smith. Interpreting and visualizing performance portability metrics. In 2020 P3HPC Workshop, pages 14–24, 2020.

Evaluating Performance, Portability and Productivity

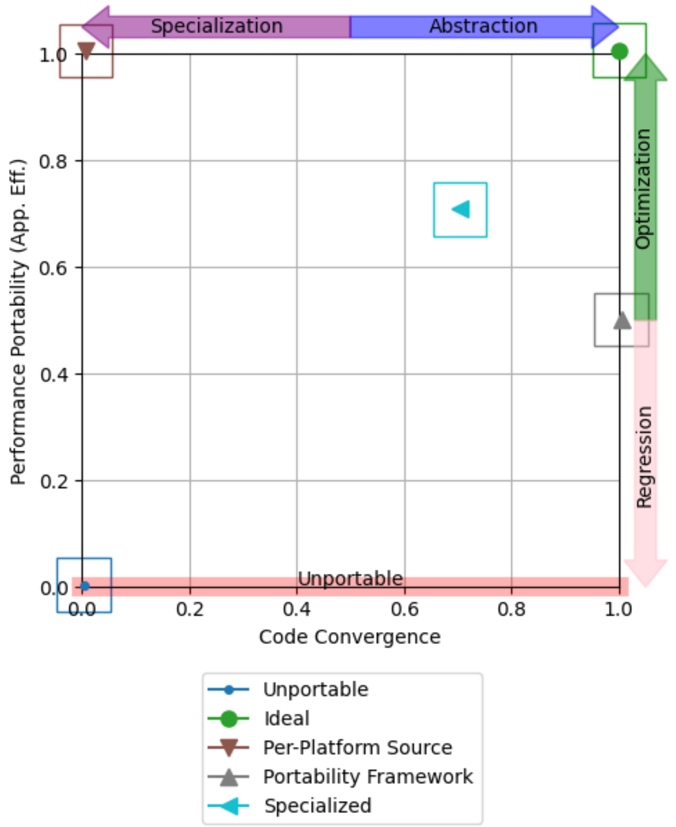
Metrics and heuristics for measuring the 3 *Ps*

- **Developer productivity is perhaps the most difficult to assess objectively**
  - **Proxies: LoC, Dev time, Code complexity**
- **Harrell et al. [4] propose Code Divergence**

$$\mathrm{CD}(a,p,H) = \binom{|H|}{2}^{-1} \sum_{\{i,j\}\in H\times H} d_{i,j}(a,p)$$

$$d_{i,j}(a,p) = 1 - \frac{|c_i(a,p) \cap c_j(a,p)|}{|c_i(a,p) \cup c_j(a,p)|}$$

- **Can be combined with *Performance Portability* on a Navigation Chart [5]**



[4] S. L. Harrell, J. Kitson, R. Bird, S. J. Pennycook, J. Sewall, D. Jacobsen, D. N. Asanza, A. Hsu, H. C. Carrillo, H. Kim, R. Robey, Effective performance portability, in: 2018 IEEE/ACM International Workshop on Performance, Portability and Productivity in HPC (P3HPC), 2018, pp. 24–36
[5] S. J. Pennycook, J. D. Sewall, D. W. Jacobsen, T. Deakin, S. McIntosh-Smith, Navigating Performance, Portability, and Productivity, Computing in Science & Engineering 23 (2021) 28–38

Summary

- New simulation software likely to employ software and DSLs at many different levels of software development stack
    - High-level DSLs for users to express equations directly
    - Low-level DSLs and programming models targeting different architectures
- Targeting high performance, portability and productivity from a single code base is challenging!
- There are a number of metrics, tools and visual heuristics to guide developers and measure success

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