Performance, Portability, Productivity: Which two do you want?

Bryan Lawrence ’
NCAS, University of Reading
...and a cast of thousands.

Outline

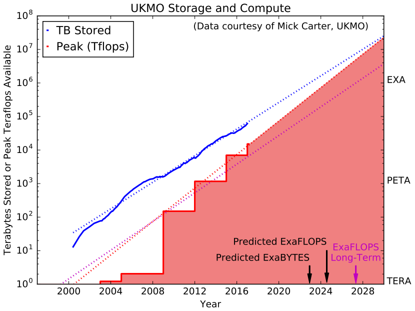
Motivation

1. Performance
2. Evolution of hardware and software
3. The Chasm - What Chasm?
    - What's in the Gap
    - Building Blocks for crossing the chasm
    - Next Steps

Summary

Long Term Trends

The long-term trend in computing requirement (over decades); compute and storage:



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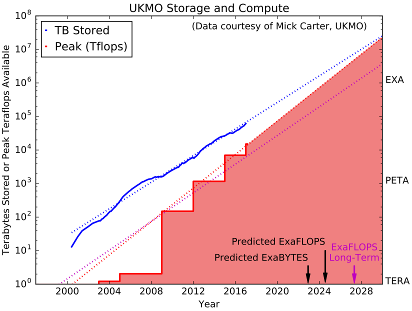
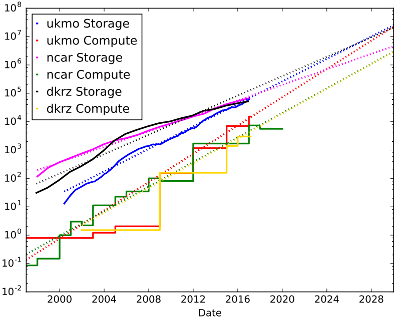




…but how do we get to exploit this new capability/capacity if it transpires?

CPMIP

Geosci. Model Dev., 10, 19?34, 2017
www.geosci-model-dev.net/10/19/2017/
doi:10.5194/gmd-10-19-2017

CPMIP: measurements of real computational performance of Earth system models in CMIP6

Balaji, Maisonnave, Zadeh, Lawrence, Biercamp, Fladrich, Aloisio, Benson, Caubel, Durachta, Foujols, Lister, Mocavero, Underwood, Wright

1. How long will the experiment take (including data transfer and post-processing)?
2. How many nodes can be efficiently used in different phases of the experiment?
3. Can/should the experiment be split up into parallel chunks (e.g., how many ensemble members should be run in parallel)? What is the best use of my (limited) allocation?
4. *How much short-term/medium-term/long-term storage (disk, tape, etc.) is needed?*
5. Are there bottlenecks in the experiment workflow, either from software or from system policies, such as queue structure and resource allocation?

CPMIP Metrics

Criteria:

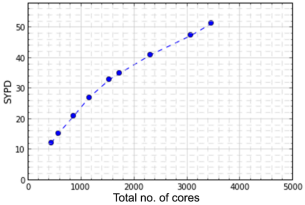
1. They are universally available from current ESMs, and applicable to any underlying numerics, as well as any underlying hardware architecture;
2. They are representative of the actual performance of the ESMs running as they would in a science setting, not under ideal conditions, or collected from representative subsets of code;
3. They measure performance across the entire lifecycle of modeling, and cover both data and computational load; and
4. They are extremely easy to collect, requiring no specialised instrumentation or software, but can be acquired in the course of routine production computing.

Metric Scope

1. Speed, of which more later ...
2. Computational cost
    2.1 based on the number of *degrees of freedom* in the model, factored into the influence of resolution and complexity;
    2.2 cost of load balancing and coupling;
3. Memory Boundedness;
4. Input/Output;
5. System policies (influence of queuing time etc)

Many of these are dependent on the **Platform**!

Speed or Throughput



Scaling behaviour of a GFD model. Model is clearly can get speed up to 50 SYPD, but in practice is often run at 35 SYPD, which maximises throughput.

Model performance can have two optimal points of interest:

1. Speed: Minimising time to solution, maximising simulated years per day or SYPD — termed S-Mode;
2. Throughput: Best use of a resource allocation (Minimizing compute hours per simulated year, or CHSY— termed T-Mode).

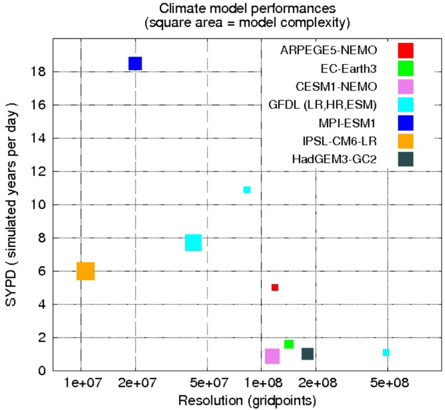
A single ESM experiment may contain both phases, e.g. spinup in S-mode, science in T-Mode.

The Metrics

Resolution	Number of gridpoints, summed over components.
Complexity	Number of prognostic variables, summed over components (NOT, the number of lines of code).
SYPD	Simulated Years Per Day (in both Speed and Throughput mode).
ASYPD	Actual SYPD measured from the start of enqueuing until the last data has reached it's destination.
CHSY	Core-Hours per simulated year.
Parallelisation	Total number of cores allocated for the job .
JPSY	Energy cost of the simulation, in Joules per simulated year.
Coupling Cost	Normalised difference between actual run time, and the sum of the individual component times, with suitable parallelisation weightings.
Memory Bloat	Ratio of actual memory size (less memory for executable code) to ideal memory size (the size of memory you'd use if you had only cone copy of your prognostic variables).
DataOutput Cost	The cost of doing I/O (compared to an I/O free run).
Data Intensity	The data produced divided by the compute used: GB/CH.

All but the first two are dependent on the platform, so there are additional metrics aimed at understanding the nature of the platform.

Comparing Performance



- Comparison for T-mode!
- Different hardware, and different complexity: complexity shown as the size of the square.
- In general the low-complexity models are AOGCMS and the high complexity models are ESMs.
- On similar hardware, we might expect to see models of similar complexity to cluster along similar resolution SYPD slopes, but we don't have similar complexity or hardware!
- Aiming to do a much more comprehensive analysis for CMIP6!

Is the new hardware fast?

Consider these two (NOAA) machines:

- c1+c2 (2014): Cray XE6 (120 320 AMD Interlagos cores rated at 3.6 GHz on a Cray Gemini fabric).
- c3 (2016): Cray XC40 (48128 Intel Haswell cores rated at 2.3 GHz but with higher clock-cycle concurrency and Cray Aries interconnnect).

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And these results

Model	Machine	Resol	SYPD	CHSY	JPSY
CM4 S	gaea/c2	1.2×10^8	4.5	16000	8.92×10^8
CM4 S	gaea/c3	1.2×10^8	10	7000	3.40×10^8
CM4 T	gaea/c2	1.2×10^8	3.5	15000	8.36×10^8
CM4 T	gaea/c3	1.2×10^8	7.5	7000	3.40×10^8

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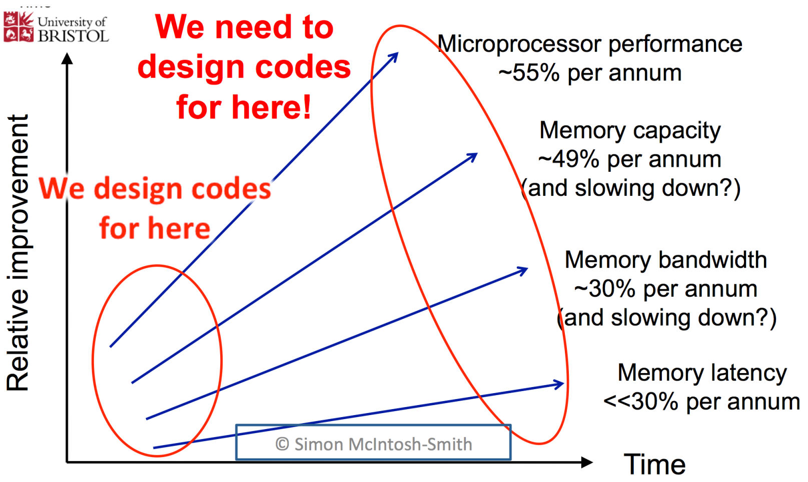
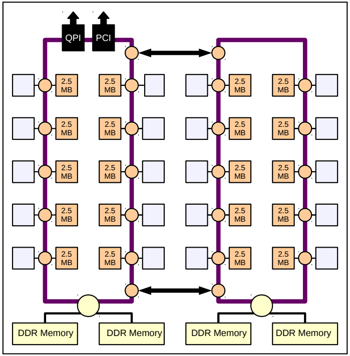
1. Core for core, the new machine shows a speedup of 2.2X, which one could not have inferred from the clock ratings (influence of *clock-cycle concurrency*).
2. However, the total number of cores has dropped by 2.5X. Thus, in aggregate, c3 provides about 87% (2.2 / 2.5) of the capacity of the older c1 and c2 partitions combined, for the GFDL workload.
   - …however, that the PF rating of c3 is considerably higher than c1 and c2 combined (1.77 PF vs. 1.12 PF).
3. Cray Cray Aries is showing a manifest increase in performance, with the same CHSY in both configurations (i.e., with different numbers of PEs) unlike Gemini.
4. There is a concrete and substantial fall in the total energy cost of simulation science!

Designing Code

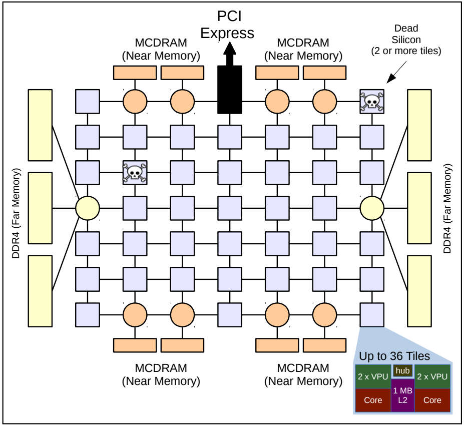


Evolving Hardware

Broadwell



KNL



Evolving Software

Requirement: Ensure model quality (the models available are meeting the advancing scientific requirements)!

Available really means models with:

1. Performance — satisfactory SYPD for affordable CHSY given real data intensity.
2. Portability — models need to run on all the relevant platforms currently in use, or likely to be in use in the foreseeable future — without excessive lead times associated with porting, and
3. Productivity — the ability to work with the codes from a scientific perspective – changing algorithms, adding processes, etc, in a reasonable period of time, and without inadvertently compromising on reliability/accuracy of code.

- To be productive, we need to be able to exploit mathematics!
- The best mathematical methods to use at any given time are going to be slaves to the nature of the hardware – which will be problematic if the hardware is changing quicker than the mathematics and its implementation!
- What is the lead time from maths to code?
- How hard is it to make that code performant?
- And will that code be portable?

Our best guess, today, is that it won't be long before you can have only any two of those! The free X86 based free lunch is over!

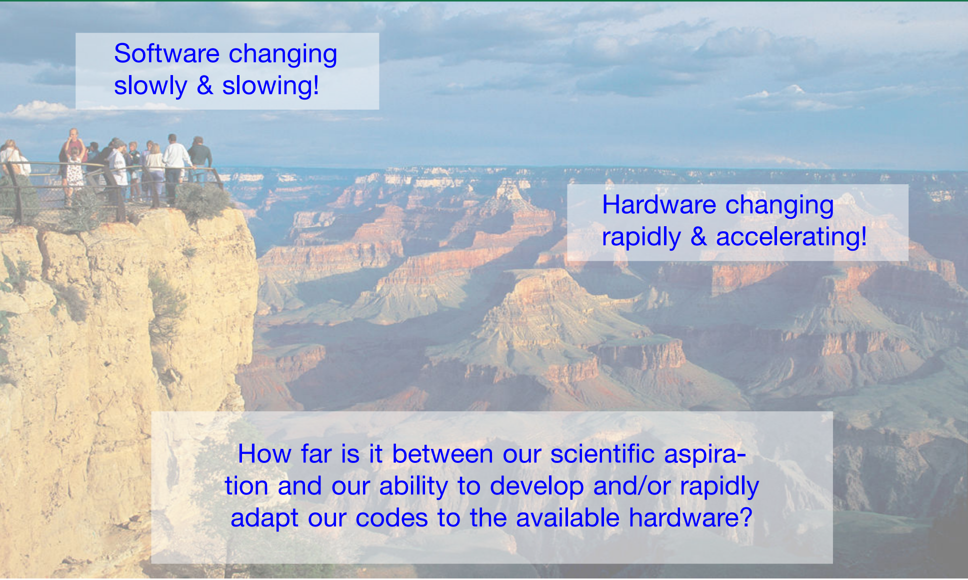
Crossing the Chasm

Crossing the Chasm: How to develop weather and climate models for next generation computers?

Lawrence, Rezny, Budich, Bauer, Behrens, Carter, Deconinck, Ford, Maynard, Mullerworth, Osuna, Porter, Serradell, Valcke, Wedi, and Wilson

Targeting GMD, submission within weeks!
IS-ENES2 Deliverable 3.2

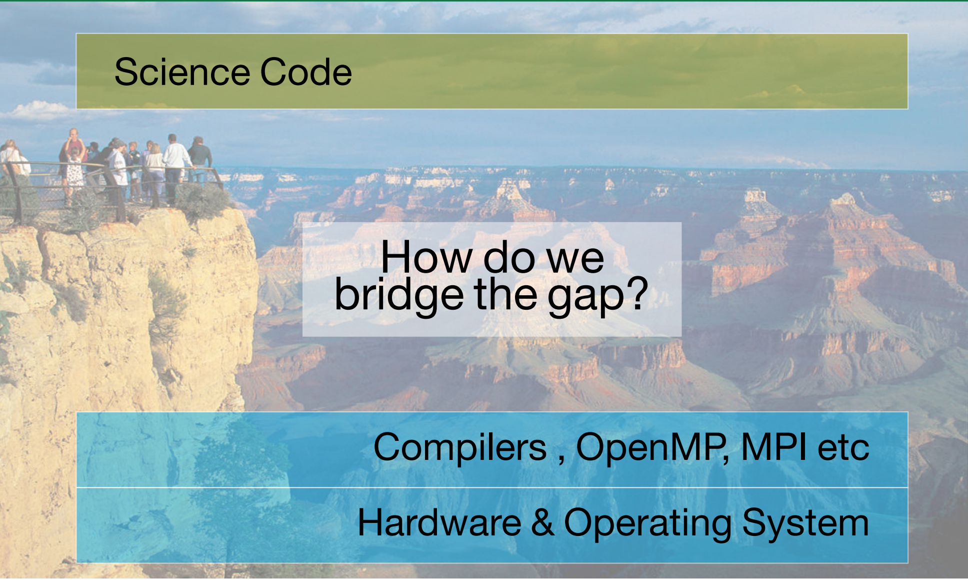
is-enes
INFRASTRUCTURE FOR THE EUROPEAN NETWORK FOR EARTH SYSTEM MODELLING



Software changing slowly & slowing!

Hardware changing rapidly & accelerating!

How far is it between our scientific aspiration and our ability to develop and/or rapidly adapt our codes to the available hardware?



Science Code

How do we bridge the gap?

Compilers , OpenMP, MPI etc

Hardware & Operating System

Too many levels of parallelism!

1. Vectorisation within a CPU or GPU core or accelerator (via the compiler, or compiler directive languages such as OpenACC),
2. Shared parallelism across CPU and accelerators/GPUs.
3. Threading providing shared memory concurrency within nodes/sockets (using a tool such as OpenMP),
4. Distributed memory concurrency across nodes, either by
    - utilising MPI (traditional "domain decomposition"); directly, or with a library, or
    - exploiting a PGAS implementation (e.g. CoArray Fortran)
5. Internal component concurrency (using, e.g. ESMF) or manually provisioned using OpenMP,
6. Concurrent coupled model components, either
    - executed independently using a coupler such as OASIS, or executed together using a framework, or
    - concurrent models running as part of a single executable ensemble
7. I/O parallellism (using an I/O server such as XIOS)

Best practice for parallelism?

Current best practice for addressing these modes of concurrency is to

1. Code for hierarchies of parallelism (loops, blocks, do- mains),
2. Use standard directives (OpenMP/OpenACC),
3. Optimise separately for many-core/GPU, and
4. Try to minimise code differences associated with architectural optimisations.

However, this is no longer seen as a successful strategy – at least on its own!

With the advent of exascale systems, entirely new programming models are likely to be necessary, with entirely new constructs such as thread pools and task-based parallelism possible.

Current Experience

Clearly lots of activity addressing these problems, including, e.g:

1. Early experiences re-coding for new processors which did effective rewrites which became orphaned because they used the left the science code owners behind (wrong language etc). (Performant, but not portable or Productive).
2. Aggressive code development and maintenance with many lines of directives with great scope for error. Opinion divided as to how easy it will be to maintain the resulting codes (productivity?)
3. Code translation: works to an extent, but require invasive changes (productivity).
4. Experiments with new programming models suggest that the developer really needs to understand the fundamental algorithms and vice versa (issues for productivity).

All these have addressed "fine-grained" parallelisation and have delivered modest results.

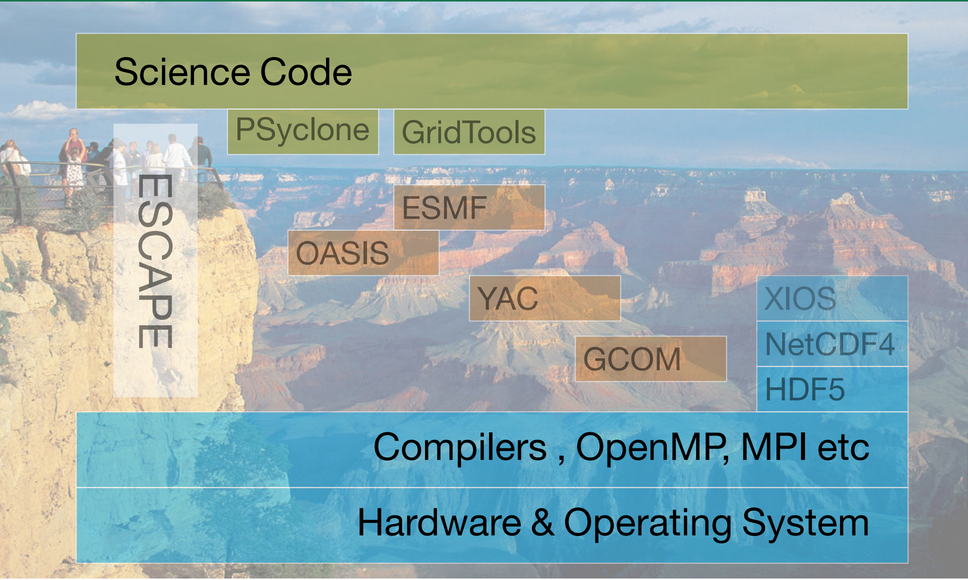
Route 1: The Massive Edifice

- No group has enough effort to do all the work needed.
- No group has **all** the relevant expertise.

Route 2: Incremental Advances

- The peril of the local minimum
- Any given span/leap may not be sufficient to cross the next gap!

Architecture for crossing?



Why and What is a DSL?

Why?

- Humans currently produce the best optimised code!
- Humans can inspect an algorithm, and exploit domain-specific knowledge to reason how to improve performance – but a compiler or generic parallelisation tool doesn't have that knowledge.
- Result: Humans better than generic tools every time, but it's big slow task and mostly not portable!

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What?

- A domain specific compiler, with a set of rules!
- Inclusive knowledge includes things like
  - Operations are performed over a mesh,
  - The same operations are typically performed independently at each mesh point/volume/element,
  - the meshes themselves typically have consistent properties.
  - …
- Let the tools exploit that knowledge, and leave a much smaller task for the humans!

DSLs in the Wild

Two major projects:

- GridTools (formerly Stella)
- PSyclone (evolved from Gung Ho)

Both are DSELs ... domain specific embedded languages.

- Embedded in C++
- Originally targeted finite difference lat-lon LAM.
- Backends (via human experts) mapped to the science description via C++ templates.

- Embedded in Fortran
- Originaly targeted finite element irregular mesh.
- A recipe of optimisations (via human experts) is used by PSyclone to produce targeted code.

In both cases the DSL approach allows mathematical experts to do their thing, while HPC experts do their thing, and the DSL provides a separation of concerns.

Whither the DSL?

- DSLs are becoming more common across disciplines.
- The Domains are more or less specific …
  - the more specific, the cleaner a domain specific separation of concerns, but the larger the technical debt (maintaining the code and the teams of experts for the backends
  - the more generic, the less the DSL can do for you, and the less the separation of concerns.

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  - the more generic, the less the DSL can do for you, and the less the separation of concerns.
- The holy grail is to add further separation of concerns inside the DSL ...e.g. can we imagine a GridTools *and a* PSyclone front end to a vendor managed intermediate DSL compiler?
  - compare with MPI: successful because vendors manage their own specific backends with a defined API that we all work with to develop our own libraries (e.g. GCOM, YAXT etc)!

Weather and Climate Dwarfs

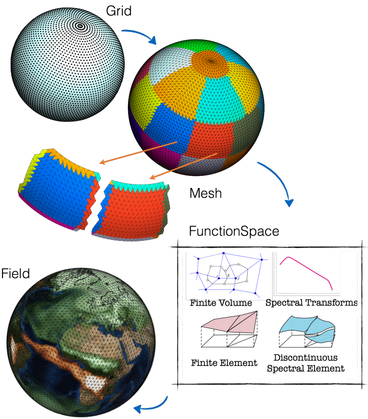
1. Flat computational profiles: select exemplar codes, ”mini-apps”, typical of key functionality, so-called dwarfs (after the Berkely Dwarfs).
2. Aim for computational performance challenges which are fundamentally different between dwarfs just like their functional separation within an Earth system model.
3. ESCAPE (Energy-efficient Scalable Algorithms 60 for Weather Prediction at Exascale; `www.hpc-escape.eu`) project is investigating this approach for weather and climate.
4. For each dwarf ESCAPE targets performance on existing and emerging processor technologies (specifically Intel Xeon, Xeon Phi and NVIDIA GPGPU and a novel technique employing optical interferometry particularly suitable for Fourier transforms), but it is also targeting programming methodologies.

ESCAPE: Dwarfs

D	Spectral Transform	Spherical harmonics based transform to facilitate semi-implicit solvers on the sphere.
D	Spectral Transform	A 2D Fourier spectral transform for regional model applications.
D	Advection	A flux-form advection algorithm for sign-preserving and conservative transport of prognostic variables and species.
I	3D Interp.	Interpolation algorithm representing a wide class of interpolation and remapping uses in NWP & Climate.
D	Elliptic Solver	An iterative solver for the 3D elliptic problem arising in semi-implicit time-stepping algorithms.
D	Advection, SLT	An implementation of the semi-Lagrangian advection algorithm.
P	Cloud MicroPx	Cloud microphysics scheme from IFS, an exemplar of a range of physical parameterisations.
P	Radiation	An exemplar radiation scheme used in regional NWP modelling.

…and more

1. No established convention or standard for layout in memory grids and meshes or how the various cell entities are associated with each cell: scope for data models and associated efficiency.
2. Exploit knowledge about data types and data movement: Improved MPI libraries
3. How best to optimise, find bottlenecks? Better use of tools for optimisation




If we work together …
…can we reduce the problem to a set of small leaps?

Science Code

Defined Interfaces and Contracts

High Level Libraries and Tools

Defined Interfaces and Contracts

Libraries and Tools

Defined Interfaces and Contracts

Low-Level Libraries and Tools

Defined Interfaces and Contracts

Compilers , OpenMP, MPI etc

Hardware & Operating System

What do we need?

- Progressing at the community level will require methods to allow the community to discuss, specify, design, develop, maintain, and document the necessary libraries and tools.
- …that is, a commonly deployed structured approach to sharing, one that maximises delivery of requirements, while minimising risk of future technical burden – the sort of approach that has delivered the MPI libraries upon which nearly all of HPC depends.
- While a fully fledged standards track is probably beyond the will of the community at this point, it is certainly possible for the community to take more steps towards joint working!

What steps can the community make now?

Begin by recognising that:

- business as usual, consisting of modest incremental steps, is unlikely to deliver the requisite next generation models,
- none of us have enough internal resource to take the leap to the next generation alone, and most importantly,
- there are library or tool projects which can be exploited, some of which may be from outside our traditional communities of collaborators.

What institutional characteristics are necessary?

They will most probably:

- Have understood the issue fully at the management level, the science level, and in the infrastructure teams,
- Be able to reward individuals for innovation in, and/or contributions to, external projects,
- Recognise the benefit of external scrutiny and contributions into their own projects,
- Have the courage to stop existing activities and pickup and use/integrate third party libraries and tools, and
- Have the ability to recognise the cost-benefit trade-off between “doing it themselves” and contributing intellectually and financially to third party solutions, and
- Be ready to apply more sophisticated and complex software engineering techniques, and encourage more computational science research.

What project characteristics are necessary?

They will:

- be open source *and* have an open development process,
- have clear goals, scope, and where appropriate, deliver stable software interfaces,
- have a mechanism to understand and respond to the timescales of collaborators (that is, some sort of governance mechanism which assimilates and responds to requirements),
- potentially be able to accumulate and spend funds to provide user-support, training, and documentation,
- be not initially disruptive of existing solutions, and ideally
- engage both the scientific community and vendors (compare with MPI where vendor implementations are often key to enhanced MPI performance).

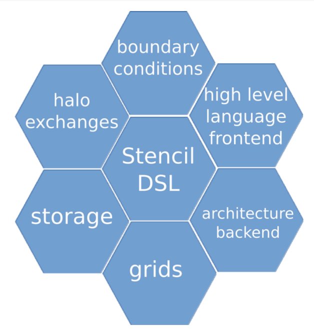
What do we need?

To work out what components exist and which can be shared. To do that we need a taxonomy. Such a taxonomy will cover at least:

- Tools for exposing mathematical algorithms for implementation on a sphere (domain specific languages),
- Tools for describing and using data models for the variables in those algorithms (including stencils for computation),
- Mathematical Libraries such as Fast Fourier and Spherical Transforms,
- Solvers which can exploit specific data models and algorithms,
- Interpolation and Regridding Libraries,
- Embedded and standalone visualisation tools,
- Exchange libraries (for problems ranging from domain halo exchanges to 3D field exchange between high level components),
- Fully fledged couplers (e.g. OASIS) and frameworks (e.g. ESMF),
- I/O servers (such as XIOS),
- Data Assimilation tools such as minimisers and adjoint compilers,
- Clock, calendar, time-stepping and event handling libraries (events such as ”do at first time step, do every three hours, etc),
- Testing Frameworks,
- Performance and Debugging tools,
- Domain specific tools for automatic code documentation.

The bottom line

Lots of pieces in play:



…and more!

Cambrian explosion in hardware means:

- Performance is tough.
- Getting all of Performance, Portability and Productivity is going to become much harder!

To get timely and manageable progress

- We are going to have to change the way we work, and work more together.
- Working together isn't going to be easy either!