The Impact of the Changing Nature of Computing on Climate Science

Bryan Lawrence & a cast of thousands

NCAS &
University of Reading: Departments of Meteorology and Computer Science

UoR, 21 Jan 2020

Outline

- An introduction to climate modelling …
- and the data handling workflow.
- The JASMIN super data computer, and some examples of JASMIN cloud usage.
- The end of Moore's Law
- What next? Maths, computer science, and some of our research directions.

The reality of climate change

A little more than 1C global warming is not manifesting as slightly nicer summers and slightly warmer winters!

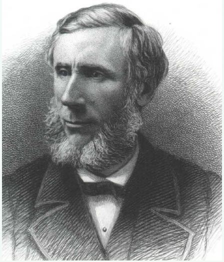
The Greenhouse Effect: How did we get here?

Not a new idea: Arrhenius **1896**

On the Influence of Carbonic Acid in the Air upon the Temperature of the Ground, Philosophical Magazine and Journal of Science, 1896: Doubling atmospheric carbon dioxide will lead to an increase in surface temperatures of 5–6K.

Building on Tyndall, c **1859**

The Earth's atmosphere is warmer than it should be (in terms of the radiative heat input from the sun).



Tyndall explained the heat in the Earth's atmosphere in terms of the capacities of the various gases in the air to absorb radiant heat, in the form of infrared radiation (from the earth radiating outward).

We have not wasted the following hundred years

IPCC reports

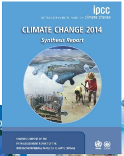
Five assessment reports *(1990, 1995, 2001, 2007, 2013-14)*

1992 supplementary report and 1994 special report

Nine special reports *(1997, 1999, 2000, 2005, 2011, 2012)*

Guidelines for national GHG inventories, good practice guidance *(1995, 2006, 2013)*

Six technical papers *(1996-2008)*



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IPCC reports

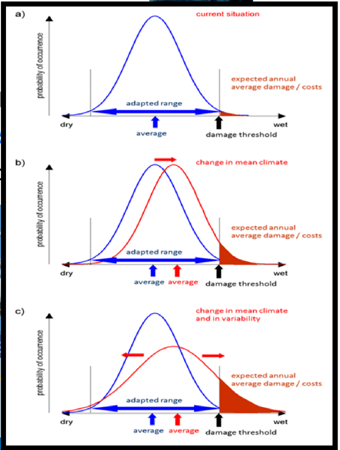
Five assessment reports *(1990, 1995, 2001,*

1992 ... 1994 special

..., 2000, 200...

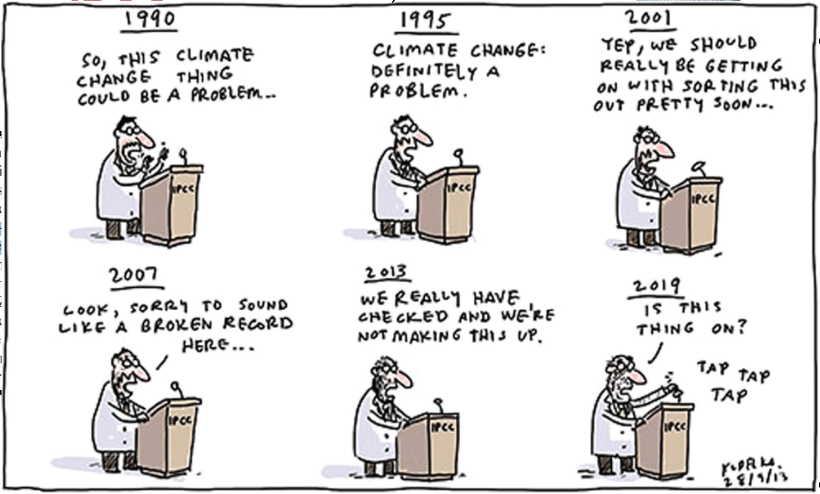
...entories, goo...

An increase in fire danger in Australia is likely to be associated with a reduced interval between fires, increased fire intensity, a decrease in fire extinguishments and faster fire spread (Tapper, 2000; Williams et al., 2001; Cary, 2002). In south-east Australia, the frequency of very high and extreme fire danger days is likely to rise 4-25% by 2020 and 15-70% by 2050 (Hennessy et al., 2006). By the 2080s, 10-50% more days with very high and extreme fire danger are likely in eastern areas of New Zealand, the Bay of Plenty, Wellington and Nelson regions (Pearce et al., 2005), with increases of up to 60% in some western areas. In both Australia and New Zealand, the fire season length is likely to be extended, with the window of opportunity for controlled burning shifting toward winter.



We have not wasted the following hundred years

John Kudelka, kudelka.com.au



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We want to simulate our world

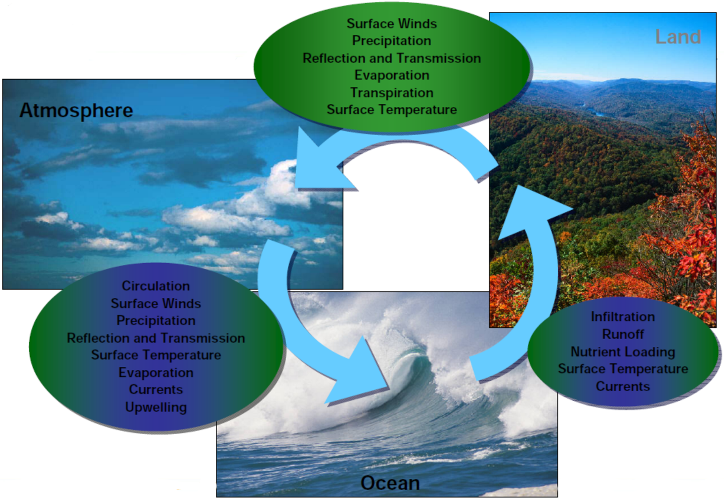


Image: from J. Lafeuille, 2006

Basic Fluid Equations (for the atmosphere)

State Variables:
u, v, w — wind
Π — Exner function (non-dimensional pressure)
Θ — Potential temperature

Coordinates:
r, ϕ, λ — radial position, latitude, longitude

Things that cause change:
$\frac{D}{Dt}$ — time derivative following motion
S — External Forcing (radiative heating etc)

Newton's second law

$$\frac{D_r u}{Dt} - \frac{uv\tan\phi}{r} - 2\Omega\sin\phi v + \frac{c_{pd}\theta}{r\cos\phi}\frac{\partial\Pi}{\partial\lambda} = -\left(\frac{uw}{r} + 2\Omega\cos\phi w\right) + S^u$$

$$\frac{D_r v}{Dt} + \frac{u^2\tan\phi}{r} + 2\Omega\sin\phi u + \frac{c_{pd}\theta}{r}\frac{\partial\Pi}{\partial\phi} = -\left(\frac{vw}{r}\right) + S^v$$

$$\frac{D_r w}{Dt} + c_{pd}\theta\frac{\partial\Pi}{\partial r} + \frac{\partial\Pi}{\partial r} = \left(\frac{u^2 + v^2}{r}\right) + 2\Omega\cos\phi u + S^w$$

mass continuity

$$\frac{D_r}{Dt}\left(\rho_d r^2\cos\phi\right) + \rho_d r^2\cos\phi\left[\frac{\partial}{\partial\lambda}\left(\frac{u}{r\cos\phi}\right) + \frac{\partial}{\partial\phi}\left(\frac{v}{r}\right) + \frac{\partial w}{\partial r}\right] = 0$$

thermodynamics

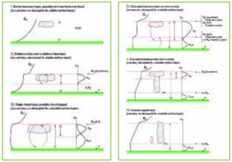
$$\frac{D_r\theta}{Dt} = S^\theta$$

Objective is given knowledge of the external forcing S and the state (u, v, w, Π, Θ) at time t, to advance knowledge of the state variables to time $t + \Delta t$, where Δt is the **timestep**.

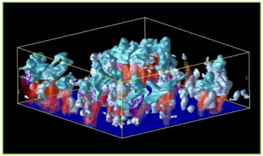
Many of the forcing terms come from parameterisations

Slide Images from Slingo, 2013

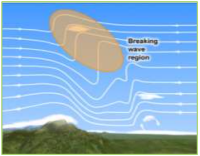
Boundary layer turbulence and mixing



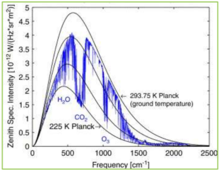
Cumulus convection



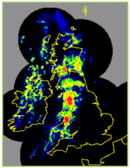
Effects of mountains



Radiation



Precipitation

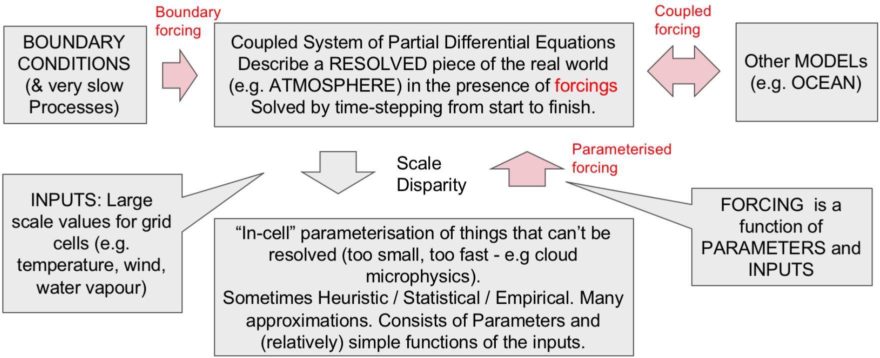


Clouds and microphysics

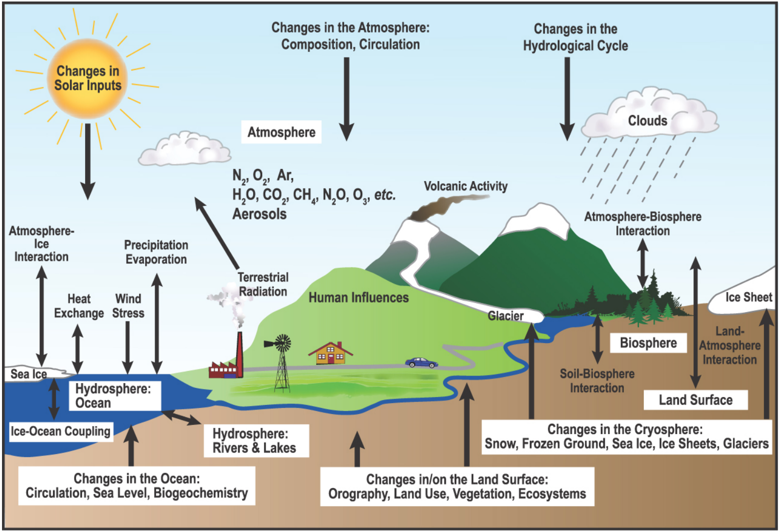
Atmospheric composition

Many sub-grid scale processes which have to be parameterised (that is, approximated, and their "grid-scale" affect is represented by functions of the grid-scale variables and some knowledge of the sub-grid, e.g. orography).

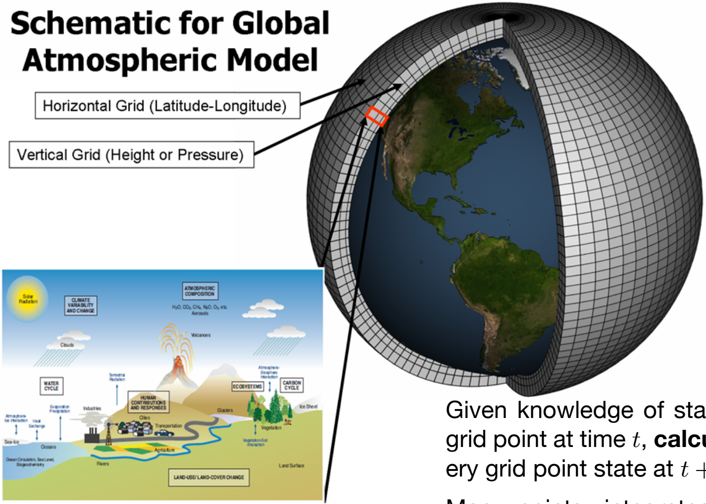
One slide introduction to numerical modelling



beyond the fluid atmosphere - Adding more processes



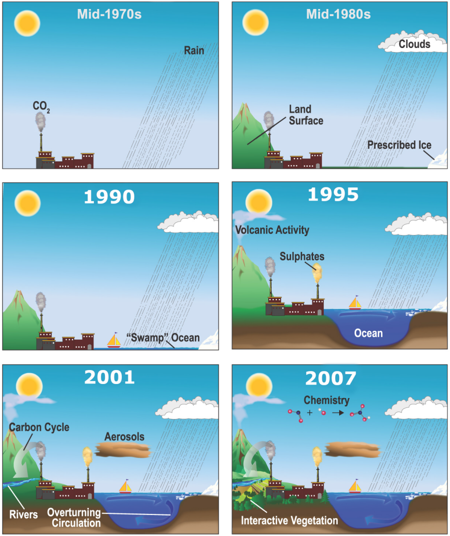
Everything is solved on a grid



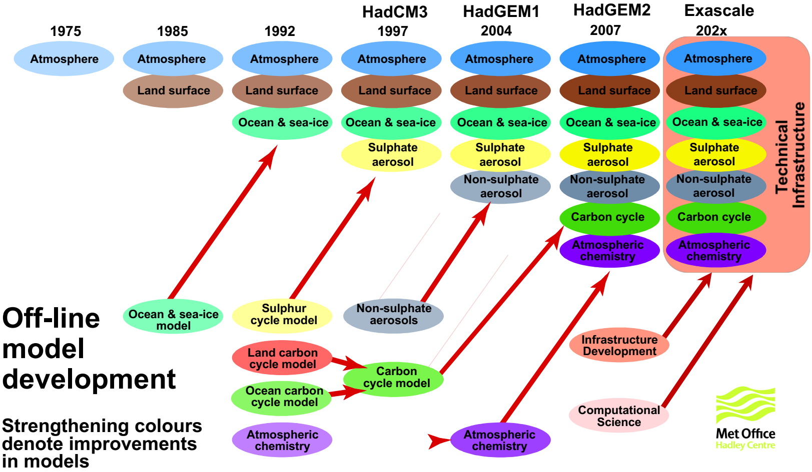
Given knowledge of state at every grid point at time t, **calculate** at every grid point state at $t + \Delta t$.

Many points, integrated for years with timestep of *o(minutes)*!

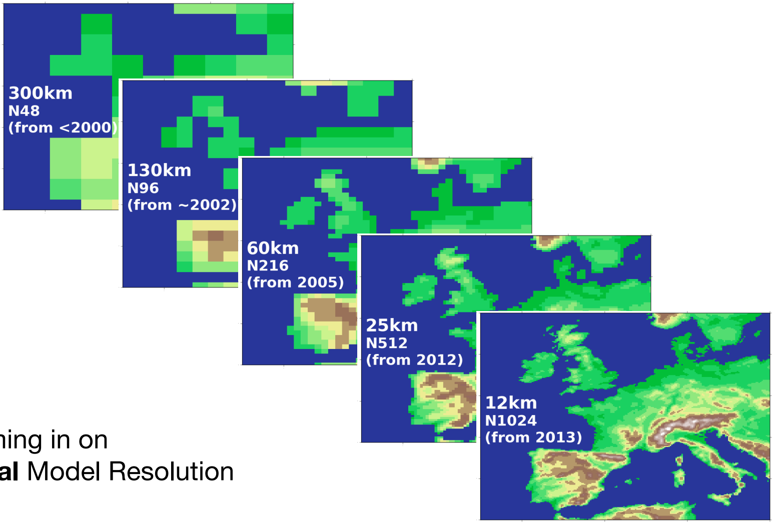
The Changing World in Climate Models



Evolution of Complexity

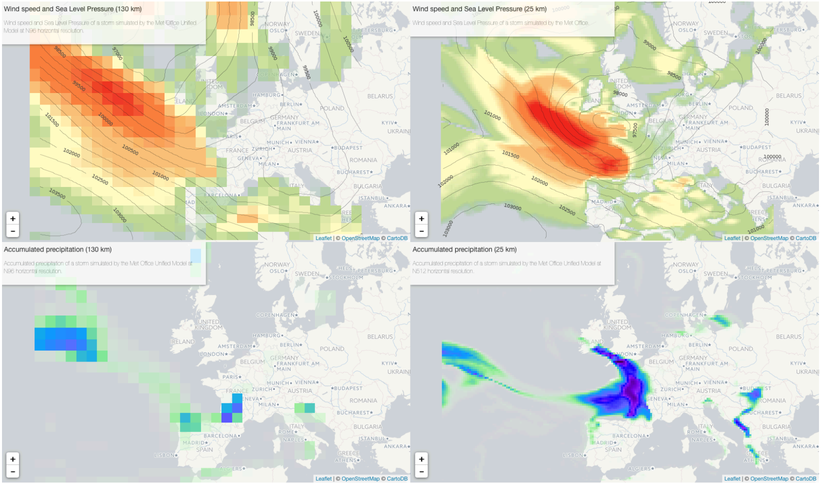


The Evolution of Resolution: A better global microscope!



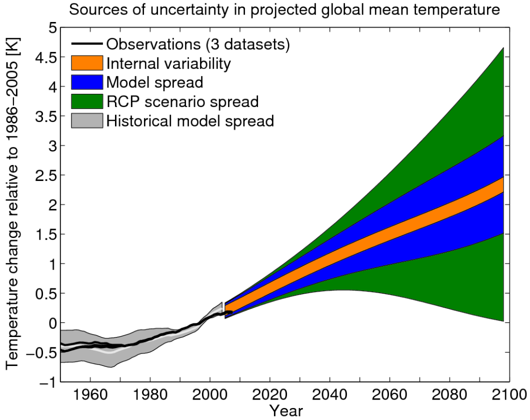
Zooming in on
Global Model Resolution

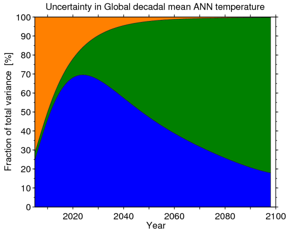
The influence of resolutioon on simulations of extratropical cyclones

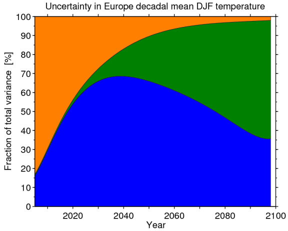


As simulated by the Met Office
https://uip.primavera-h2020.eu/storymaps/extra-tropical-cyclones

Global Climate Simulation Uncertainty as expressed in AR5





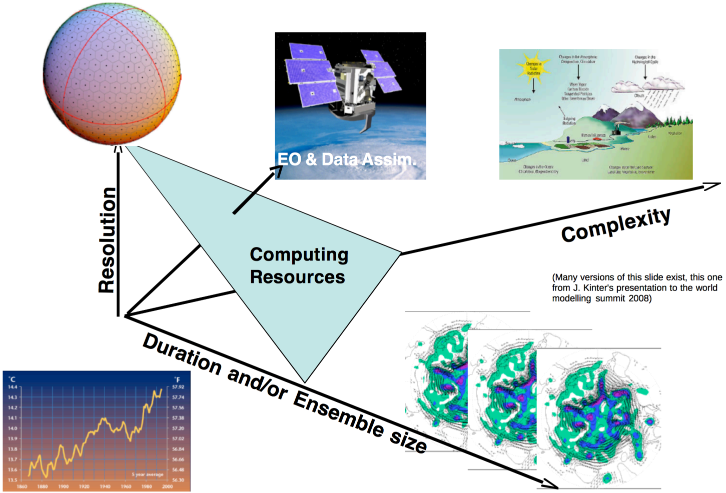


For the global big picture: model uncertainty is not the biggest problem: humanity chooses the pathway!

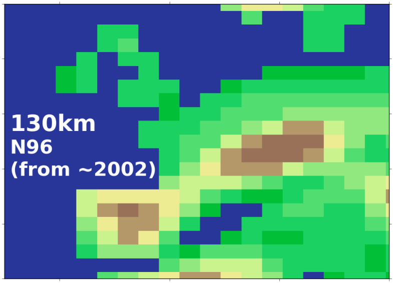
Source: Kirtman et.al., 2013: Near-term Climate Change: Projections and Predictability. In: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F. et.al. (eds.)]. Cambridge University Press.

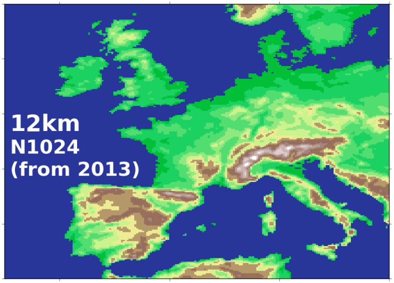
Models are more uncertain at regional scales.

Give me more computing?



A modest (?) step …





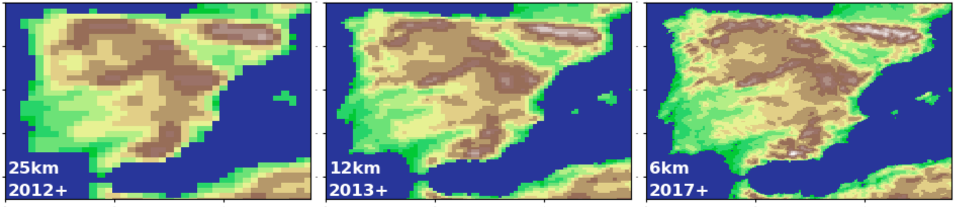
One "field-year" — 26 GB

1 field, 1 year, 6 hourly, 80 levels
1 x 1440 x 80 x 148 x 192

One "field-year" — >6 TB

1 field, 1 year, 6 hourly, 180 levels
1 x 1440 x 180 x 1536 x 2048

Volume — the reality of global 1km grids



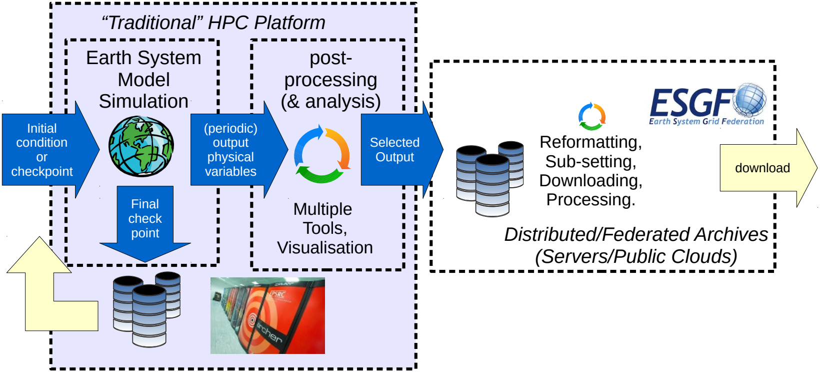
What about 1km? That's the current European Network for Earth System Modelling (ENES) goal!

Consider N13256 (1.01km, 26512x19884)):

- 1 field, 1 year, 6 hourly, 180 levels
- 1 x 1440 x 180 x 26512 x 19884 = 1.09 PB
- 760 seconds to read one 760 GB (xy) grid at 1 GB/s
- but it's worse that that: 10 variables hourly, > 220 TB/day!

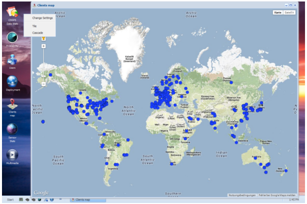
Can no longer consider serial diagnostics, and even parallelised is a challenge for the I/O system!

How we used to do it: from supercomputer to download



The consequences of data at scale — download doesn't work!

Earth System Grid Experience



Slide content courtesy of Stephan Kindermann, DKRZ and IS-ENES2

Started with **Individual End Users**

- Limited resources (bandwidth, storage)

Moved to **Organised User Groups**

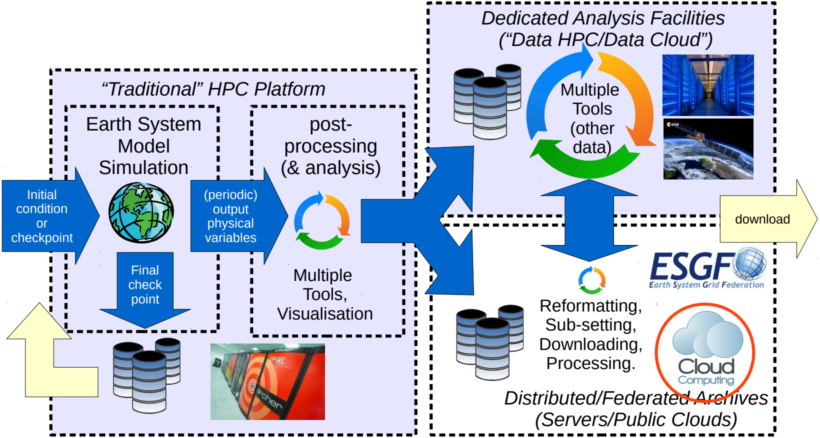
- Organize a local cache of files
- Most of the group don't access ESGF, but access cache.

Then **Data Centre Services**

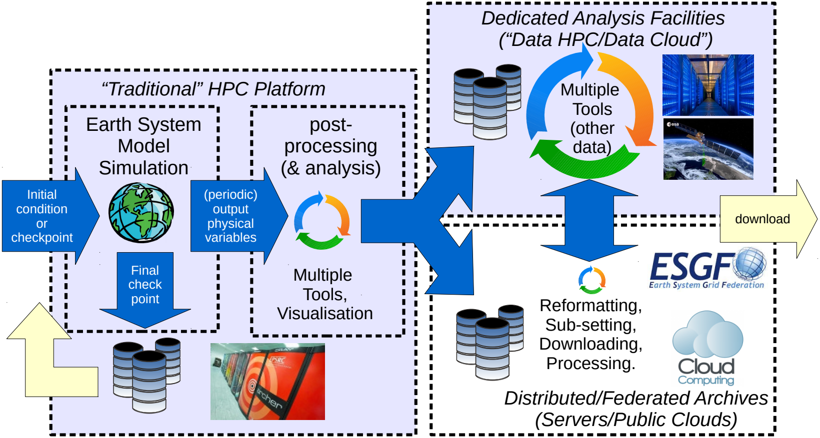
- Provide access to a replica cache
- May also provide compute by data
- CEDA, DKRZ, etc

Trend from download at home, to exploit a cache, to exploit a managed cache with compute!

Many different supercomputing environments

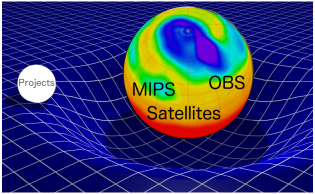


Many different supercomputing environments



Multiple Roles, at least:
Model Developer, Model Tinkerer, Runner, Expert Data Analyst, Service Provider, Data Manager, Data User

JASMIN — 4 steps in exploiting data gravity to deliver a data commons



1. Provide and populate a managed data environment with key datasets (the "archive").
2. Encourage and facilitate the bringing of data and/or computation alongside/to the archive!

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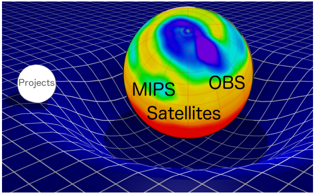
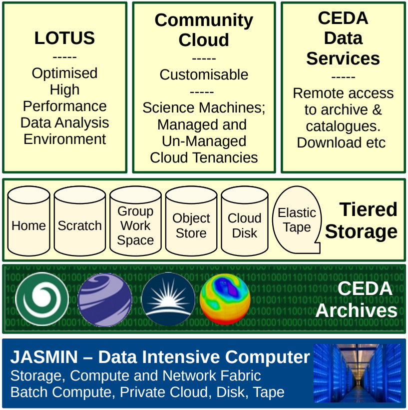
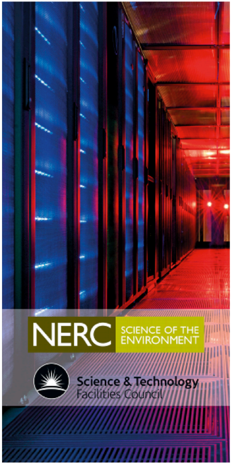
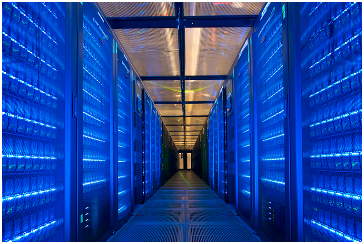


1. Provide and populate a managed data environment with key datasets (the "archive").
2. Encourage and facilitate the bringing of data and/or computation alongside/to the archive!
3. Provide a state-of-the art storage and computational environment
4. Provide FLEXIBLE methods of exploiting the computational environment.



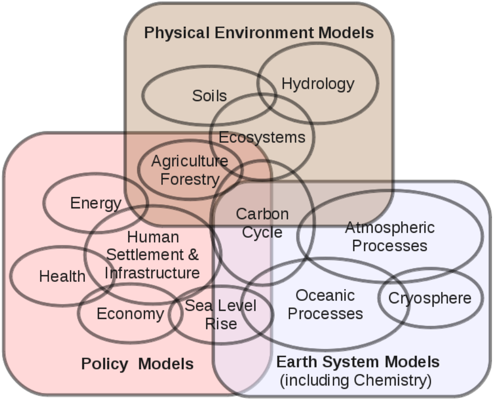
JASMIN: A Data Intensive Computing System





- Customised Fast Network.
- 44 PB Disk Storage.
- Tape Robot and “Elastic Tape Service”.
- 12000 compute cores:
  The “Lotus” batch cluster; hosted compute; cloud.
- Some high memory nodes. Some GPU systems from Q2 2019.

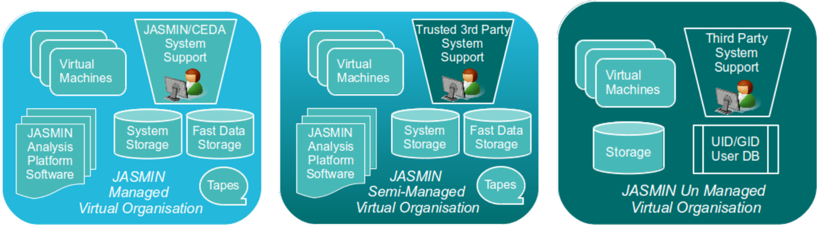
Communities



Many interacting communities, each with their own software, compute environments, observations etc.

Figure adapted from Moss et al, 2010

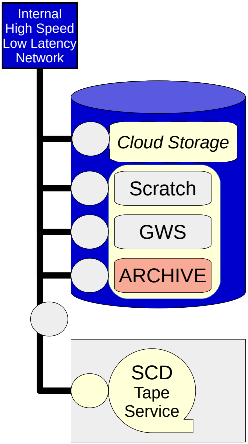
Virtual Compute and Virtual Organisations



Platform as a Service $\longrightarrow$ Infrastructure as a Service

Example: NCAS as as a big organisation can run a semi-managed virtual organisation (with multiple group work spaces), but large groups within NCAS can themselves setup a virtual organisation to run their own clusters in the un-managed environment.

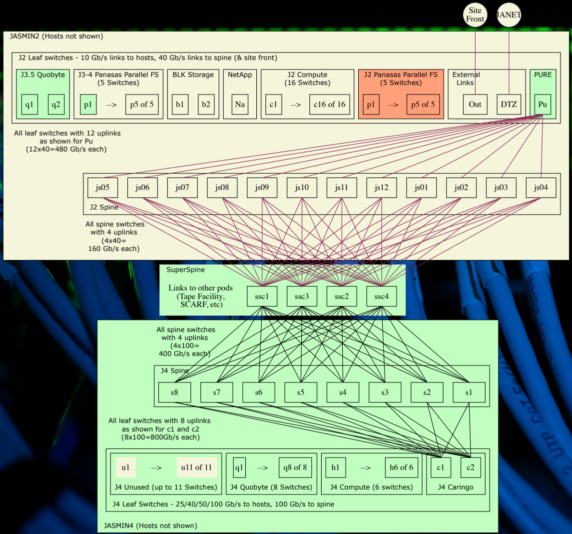
JASMIN Tiered Storage Requirements



There is not one storage system to rule them all

- Tape is (relatively) cheap. Tape is faster than you think. But tape latency is bad.
- Filesystems come with constraints: bandwidth, reliability, scalability, consistency, access control issues. You can't have it all!
- Cloud Storage:
  - Block storage: build their own file systems.
  - Object Storage: Scalable, simple, flexible access control.
- Shared file system requirements:
  - Scratch: fast, but trade-off between fast for large volume, and fast for small files.
  - Group Work Spaces: Community shared storage; not necessarily high performance.
  - Archive: long-term persistent, shared access, reliable.

JASMIN Internal Network



- Pod design with five layer CLOS network connecting pods via a superspine.
- Some blocking into the superspine.
- Evolving:
  - JASMIN 2 injection bandwidth into superspine ≈ 2 Tbit/s;
  - JASMIN 4 $>$6 Tbit/s.
- More pods possible.
- Designed by Jonathan Churchill, STFC, Inspired by Facebook.

Uncommon (and inappropriate?) software solutions

Multiple tools

Contrast between two very types of workflow:

- Build Once: Many analysis tasks are build once, use once, throwaway. No room for optimisation (or MPI). *Need efficient libraries.*
- Repeatable: "build", "run", "move", "reduce/reformat", "analyse". *Much room for automation.*.

What to use? Plethora of architectures and tools out there

APACHE Spark DASK Pandas

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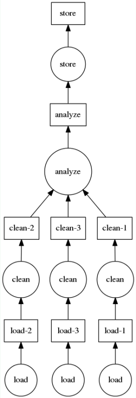
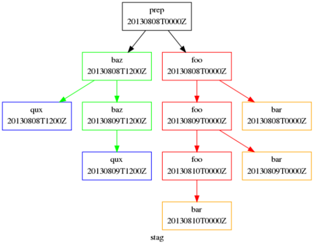
Spark DASK Pandas

Exploiting Concurrency

Whatever tools, need to get used to generating, understanding, and exploiting concurrency in more complicated ways:

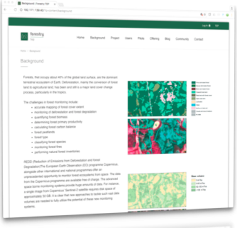




Much to do to harness tools to accelerate workflows!

(These two examples: dask, and cylc, representing bespoke analysis and scheduling, reduction and proliferation.)

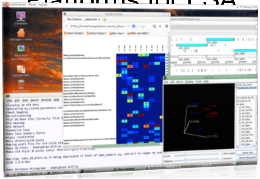
Virtual Research Environments on JASMIN hosted cloud



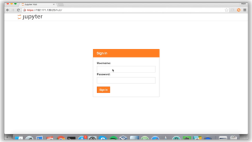
Thematic Exploitation Platforms for ESA

CCI Open Data Portal for ESA

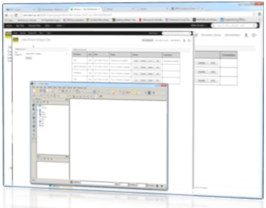
MAJIC interface to JULES model



EOS Cloud — Desktop-as-a-Service for Environmental

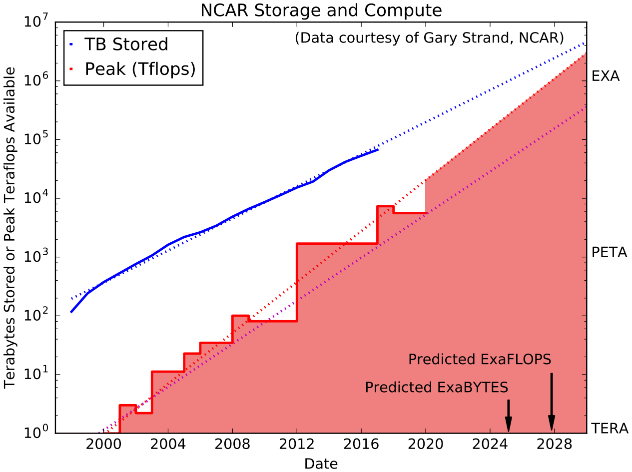


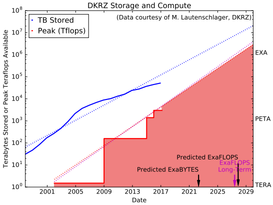
Hosted Ipython Notebooks

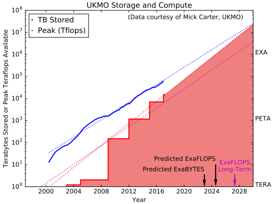


NERC Environmental

History has given us exponential compute linked to exponential data …

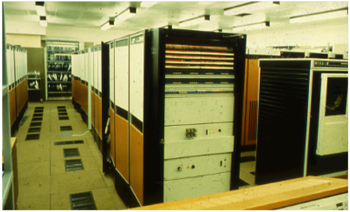






Faster Compute

1981: ICL Dist.Array.Proc. (20 MFlops)



2014: Archer (then 1.4 PFlops)

Faster Compute

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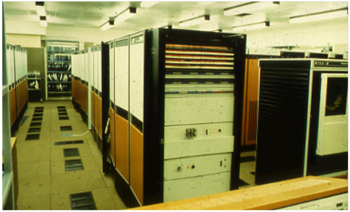
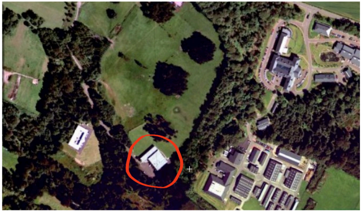


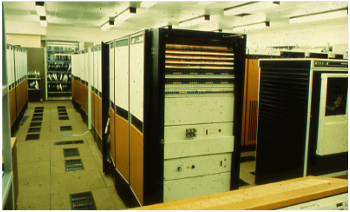
2014: Archer (then 1.4 PFlops)

EPCC Advanced Computing Facility, 2014



Faster Compute

1981: ICL Dist.Array.Proc. (20 MFlops)



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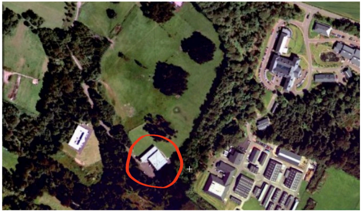


2014: Archer (then 1.4 PFlops)

From 1981, without Moore's Law

Slide content courtesy of Arthur Trew: archer | epcc |

Moore's Law and Friends

Moore's Law

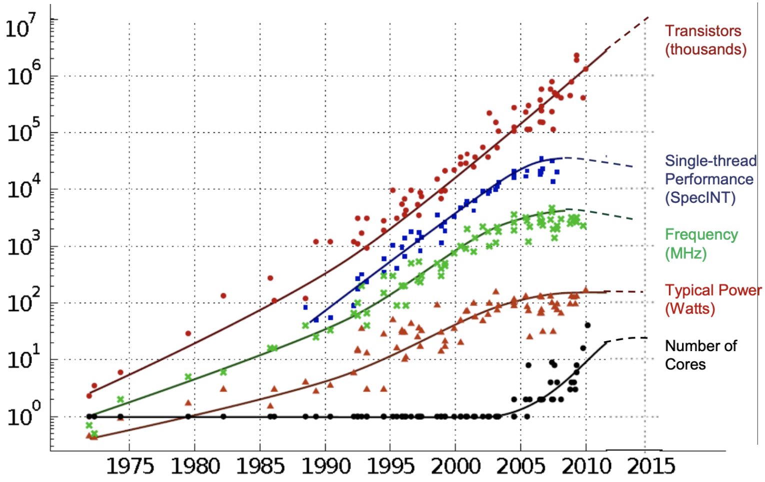
More often misquoted and misunderstood:

- Original, Moore, 1965: The complexity for minimum component costs has increased at a rate of roughly a factor of two per year.
- House (Intel) modified it to note that: The changes would cause computer performance to double every 18 months
- Moore (Modified 1975): The number of transistors in a dense integrated circuit doubles about every two years

Dennard Scaling

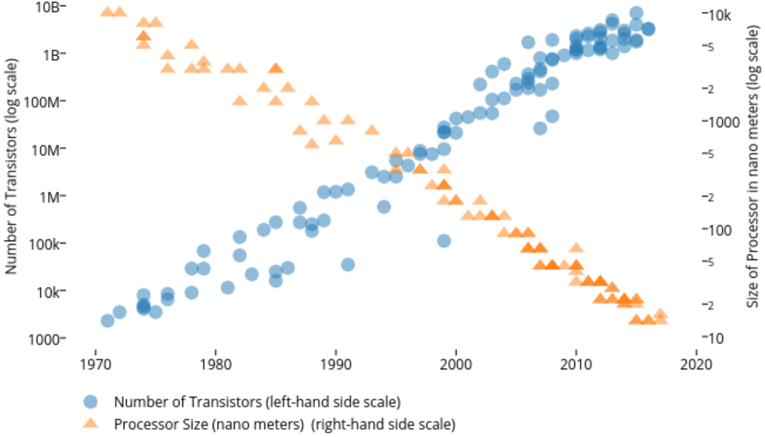
- The performance per watt of computing is growing exponentially at roughly the same rate (doubling every two years).
- (Increasing clock frequency as circuits get smaller, but this stopped working around 2006, too much power too small, means meltdown!)

The end of Dennard Scaling



Original data collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond and C. Batten

Moores's Law



https://www.yaabot.com/31345/quantum-computing-neural-chips-moores-law-future-computing/

Moore's 2nd Law aka Rock's Law

- The cost of a semiconductor chip fabrication plant doubles every four years.
- Noyce, 1977: "…further miniaturization is less likely to be limited by the laws of physics than by the laws of economics."


The Register®
Biting the hand that feeds IT

NTRE SOFTWARE SECURITY DEVOPS BUSINESS PERSONAL TECH SCIENCE

Personal Tech

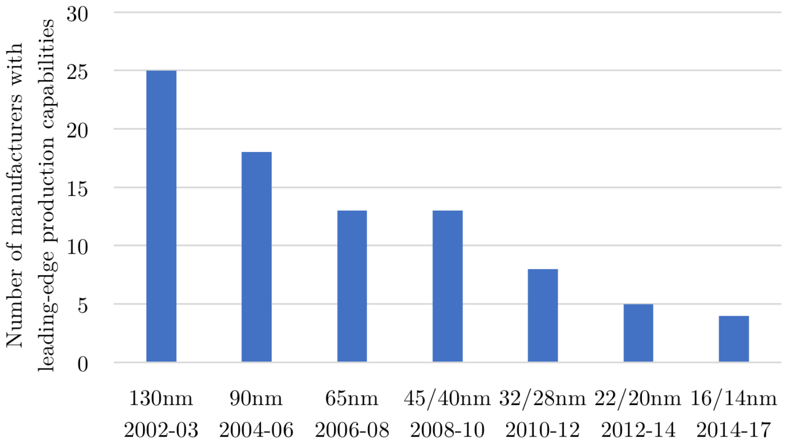
GlobalFoundries scuttles 7nm chip plans claiming no demand

AMD promptly dumps it and hires TSMC for next-gen chips

By Shaun Nichols in San Francisco 27 Aug 2018 at 23:55 18 SHARE ▲

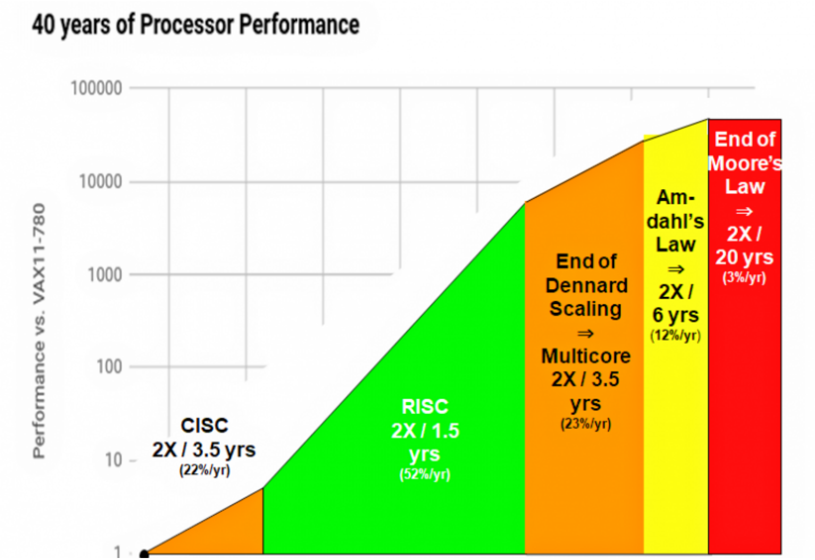
- …to shift resources (including R&D) to the 14 and 12nm efforts where …most of their chip customers …are planning to stay with the current-gen architectures and squeeze performance out by other means.

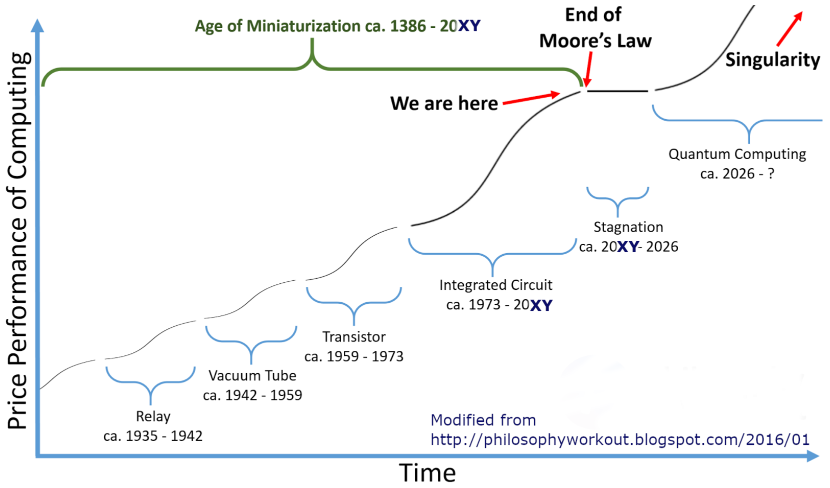
- 7nm is expensive, it's cheaper and easier to improve the performance and density of 12nm, and hardware accelerators and custom chips …



https://www.nextplatform.com/2019/02/05/the-era-of-general-purpose-computers-is-ending/

The Evolving Moore's Law




Age of Miniaturization ca. 1386 - 20XY
End of Moore's Law
Singularity
We are here
Quantum Computing ca. 2026 - ?
Stagnation ca. 20XY- 2026
Integrated Circuit ca. 1973 - 20XY
Transistor ca. 1959 - 1973
Vacuum Tube ca. 1942 - 1959
Relay ca. 1935 - 1942
Price Performance of Computing
Time
Modified from
http://philosophyworkout.blogspot.com/2016/01

What now then?

No more advances for free on the back of computer hardware improvements and relatively little pain! Need to "resort" to

Maths

Algorithms

Customised Hardware

Software Solutions for performance, portability, and productivity.

(Avoidance and Sharing)

No more free lunch, a very different modelling world!

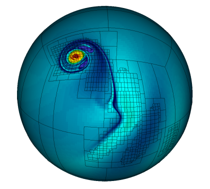
No time to talk about maths and algorithms …these, and more!

Parallel Time-Stepping

$$\mathbf{X}_{t+1}(x, y, z, t) = f(\mathbf{X}_{t-1}, \mathbf{X}_t)$$

The function f could involve several steps (iterates) *carried out in parallel*.

Adaptive Grids

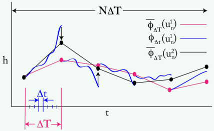


Machine Learning: Optimisation

Using AI/ML to

- Pre-condition solvers.
- Optimise/tune parameters

Parallel in Time Methods



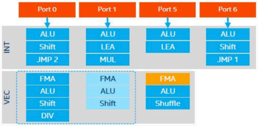
Variable Precision

Not all variables need the same precision (number of bits) in calculation, or in output.

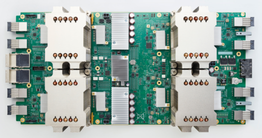
Machine Learning: Emulators

Replace slow “exact” (stationary?) parameterisations with fast “learnt” emulators.

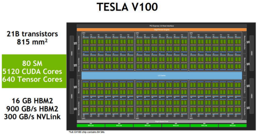
From decades of the same to a Cambrian Explosion



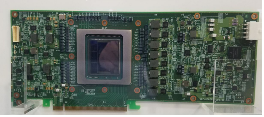
Vector Processors on Intel Zeon



Google's Tensor Programming Unit



GPUs from NVIDIA and AMD



Vector Processing Units from NEC

Server chips based on ARM designs

FPGA from many sources

The end of Moore's Law means more specialisation: all with very different programming models!

Too many levels of parallelism

- Vector Units (on chip)
- Parallelism Across Cores
- Shared Memory Concurrency
- Distributed Memory
- Numerical Method Concurrency
- Internal Component Concurrency
- Coupled Component Concurrency
- I/O and Diagnostic Parallelism
- (Storage System Parallelism)

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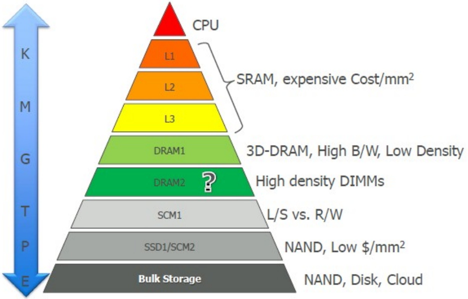

Nearly everything is processor/system dependent!
(except green layers on left).

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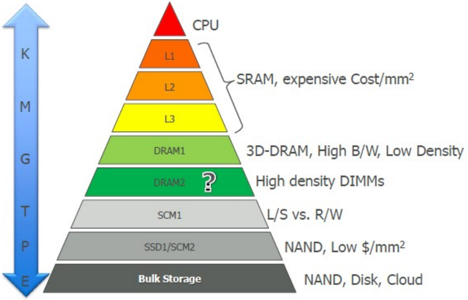

Nearly everything is processor/system dependent!
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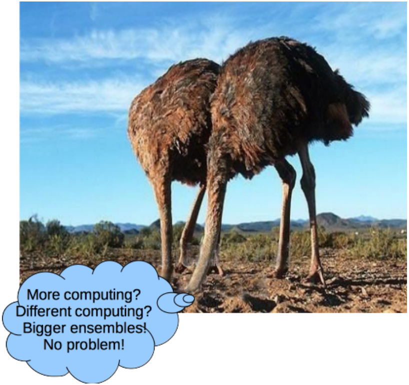
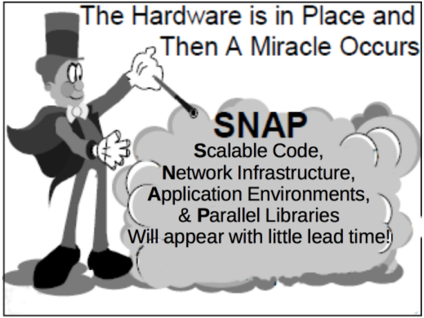
Entirely new programming models are likely to be necessary, with entirely new* constructs such as thread pools and task-based parallelism possible. Memory handling will be crucial!

* New in this context!

What about software?





Some people have a very naive idea about the relationship between the hardware and the software!

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

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

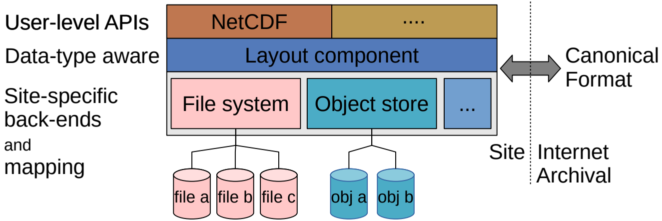
Lawrence, Rezny, Budich, Bauer, Behrens, Carter, Deconinck, Ford, Maynard, Mullerworth, Osuna, Porter, Serradell, Valcke, Wedi, and Wilson

https://doi.org/10.5194/gmd-11-1799-2018

IS-ENES2 Deliverable 3.2

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

Earth System Data Middleware



Key Concepts

- Applications work through existing application interfaces (currently: NetCDF library)
- Middleware utilizes layout component to make placement decisions
- Data is then written/read efficiently avoiding file system limitations (e.g. consistency constraints)
- Potential for deploying with an active storage management system.

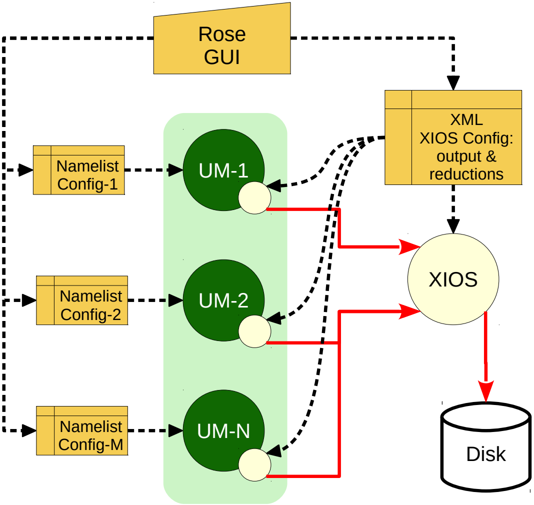
Work in Progress: In-Flight Parallel Data Analysis

An ensemble is a set of simulations running different instances of the same numerical experiment. We do this to get information about uncertainty.

Dealing with too much ensemble data

Instead of writing out all ensemble members and doing all the analysis later:

- Calculate ensemble statistics on the fly.
- Only write out some ensemble members.
- (Which ones? A tale for another day, see Daniel Galea's Ph.D work.)



Cole, Lawrence, Lister, Meursdesoif, Nash, Weiland

Summary

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There is a lot for Computer Scientists to do!
aces.cs.reading.ac.uk

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