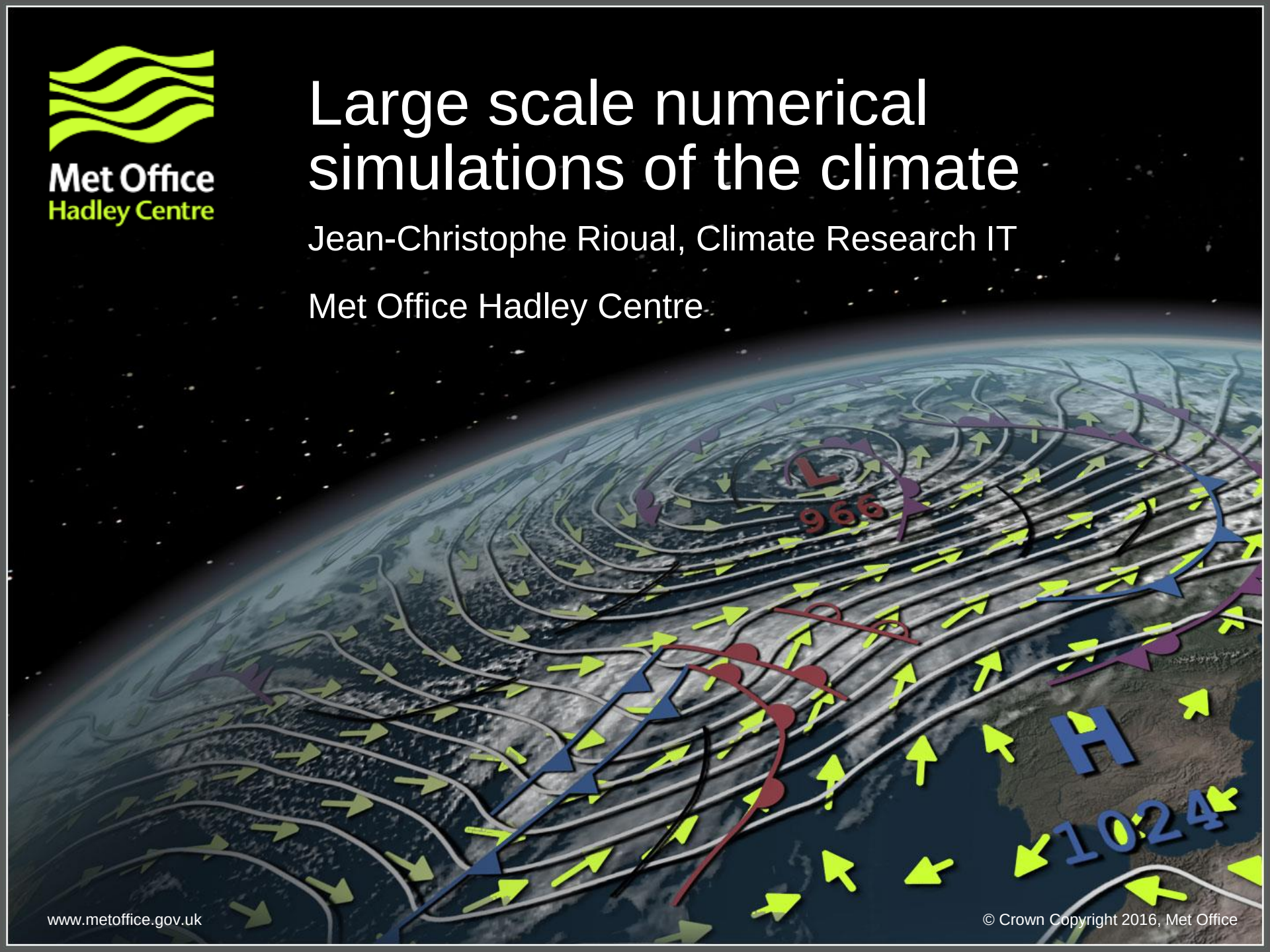
Large scale numerical simulations of the climate

Jean-Christophe Rioual, Climate Research IT

Met Office Hadley Centre



www.metoffice.gov.uk

Met Office HQ locations

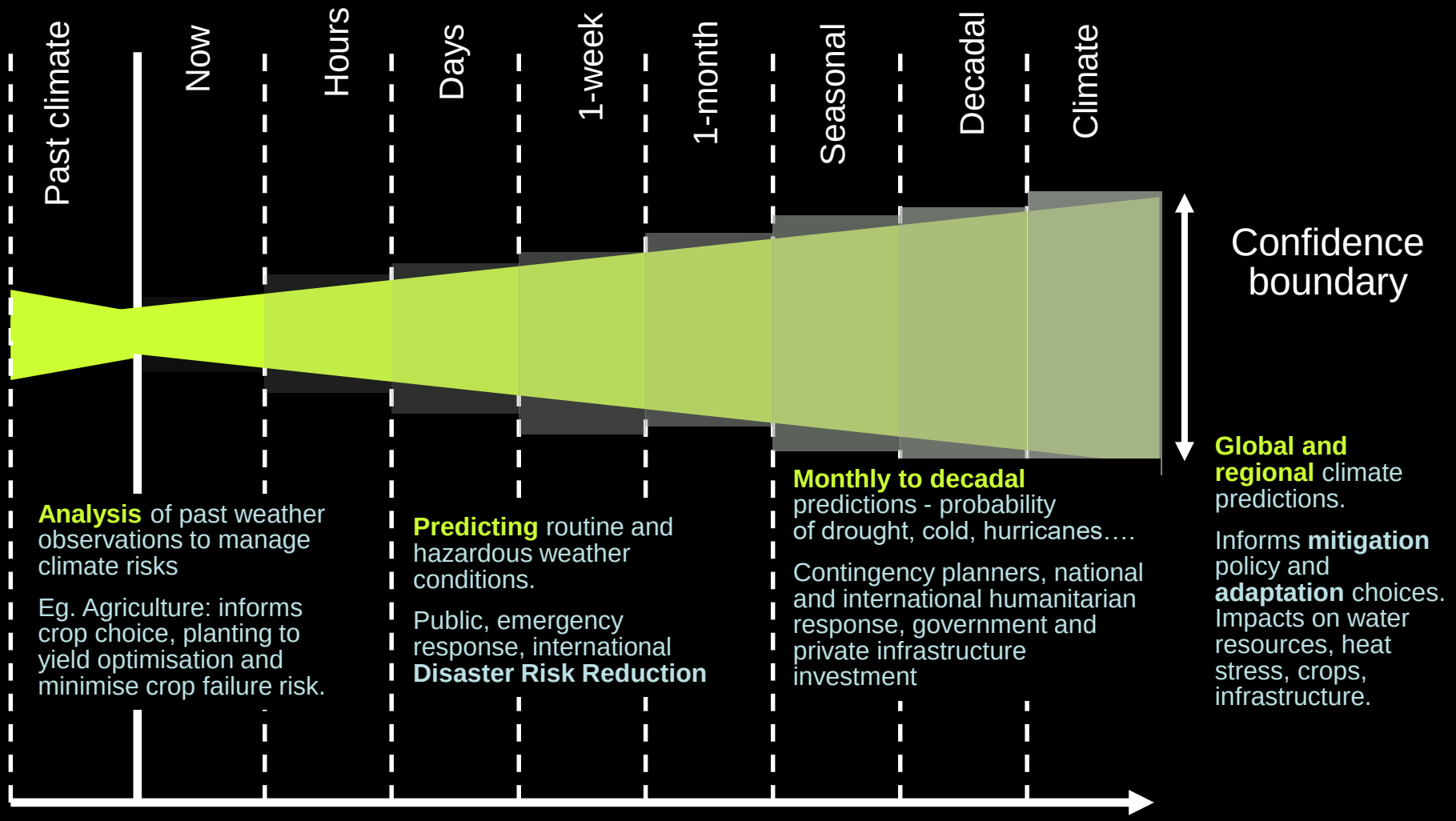
Exeter, Devon

Basic facts

Turnover	~£208m (approx 16% Commercial)
People	~2000 Staff ~1400 at Exeter HQ
Locations	~50 manned locations ~Many more unmanned observing sites ~inc 5 permanent and 2 Mobile Met Unit overseas sites
Working areas	37% Forecasting & Observations 28% Science & Research 16% Technology (IT) 12% Commercial and Government Business 7% Corporate Services

Predictions across all timescales

Global coupled modelling on all timescales



Computing - Yesterday

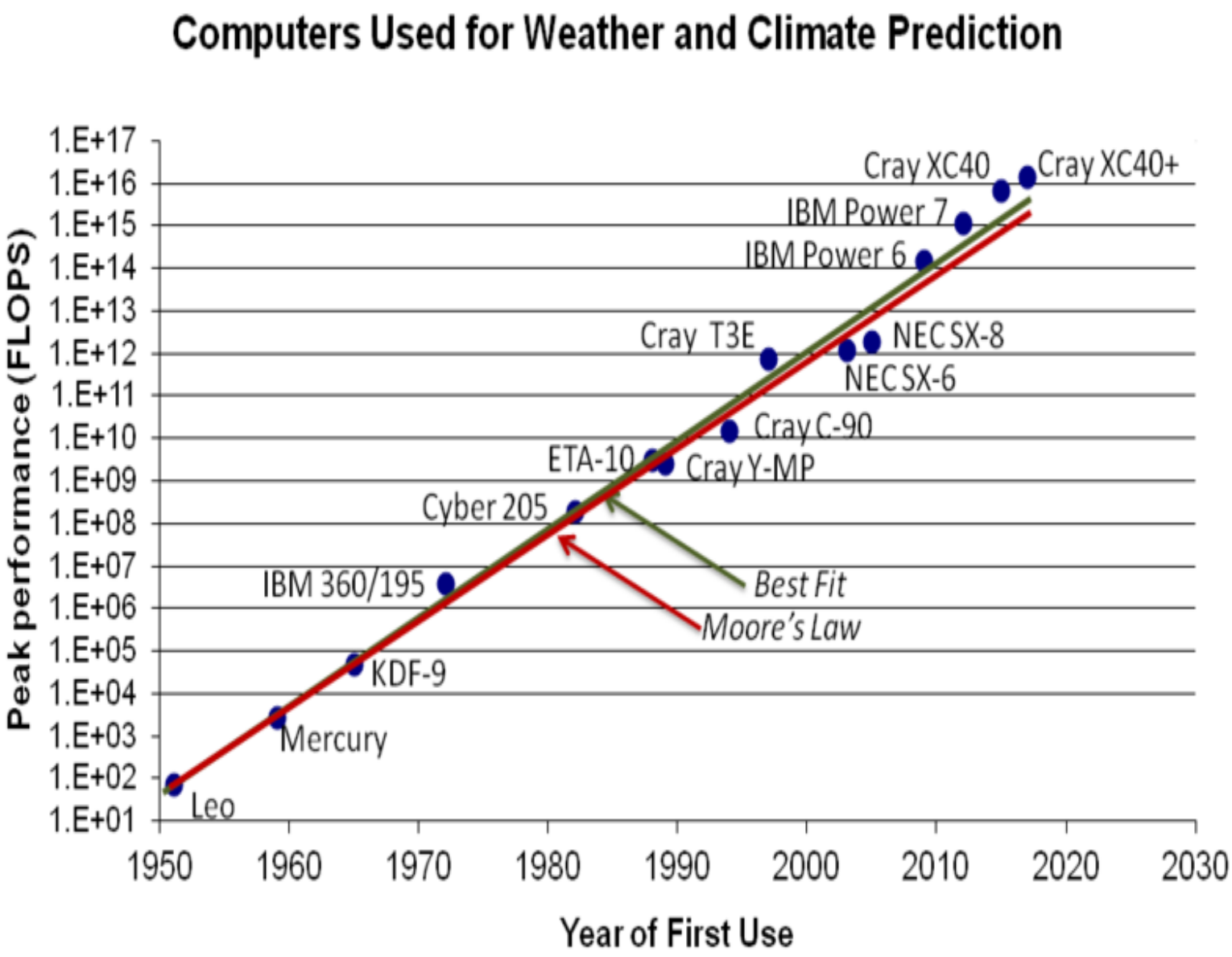
Lewis Fry Richardson
1922

~64000 human ‘computers’

Computing - Yesterday

- 1959
- Ferranti Mercury
- 30000 FLOPS

Met Office
Hadley Centre



Computing - Today

Computing - Today

Cray XC40

- Intel Broadwell processors
- 2 sockets, 36 cores per node
- 128GB RAM per node
- Proprietary interconnect *Aries*

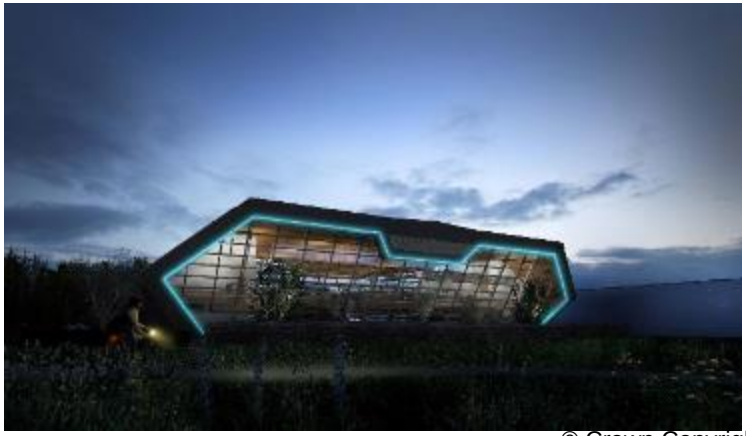
Cray XC40

Operational Clusters

- NWP
- 2 x 2492 nodes (redundancy)
- 6 PB Lustre FS
- Met Office network

Research Cluster

- Research
- 6720 nodes
- 12 PB Lustre FS
- Shared Facility
- Largest research HPC for climate/weather (11 Top500)



Unified Model

Met Office Atmospheric Simulation Model

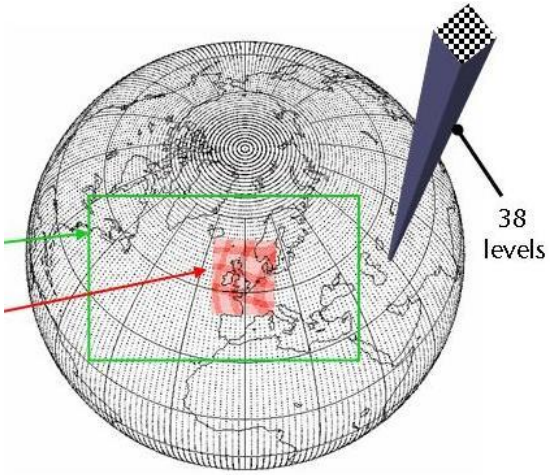
- Numerical Weather Prediction *and* Climate Modelling
- General Circulation Model
- ~1 million LOC
- 4 releases a year
- 100+ active developers per release
- Worldwide user community

Unified Model

Components

Dynamical Core - ENDgame

- Equations of motion on a sphere
- Finite Differences
- 3D Latitude-Longitude rectangular grid
- MPP code – 2D domain decomposition
- MPI + OpenMP



Unified Model

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- MPP code – 2D domain decomposition
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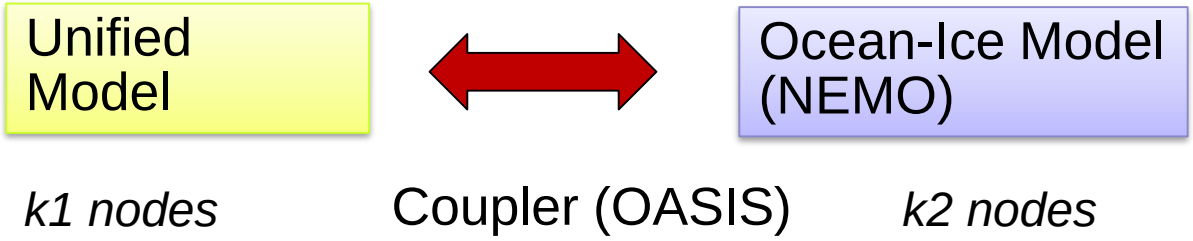
Physical parametrisations

- Not fully resolved
- Convection, Clouds
- Column-based

Subsystems

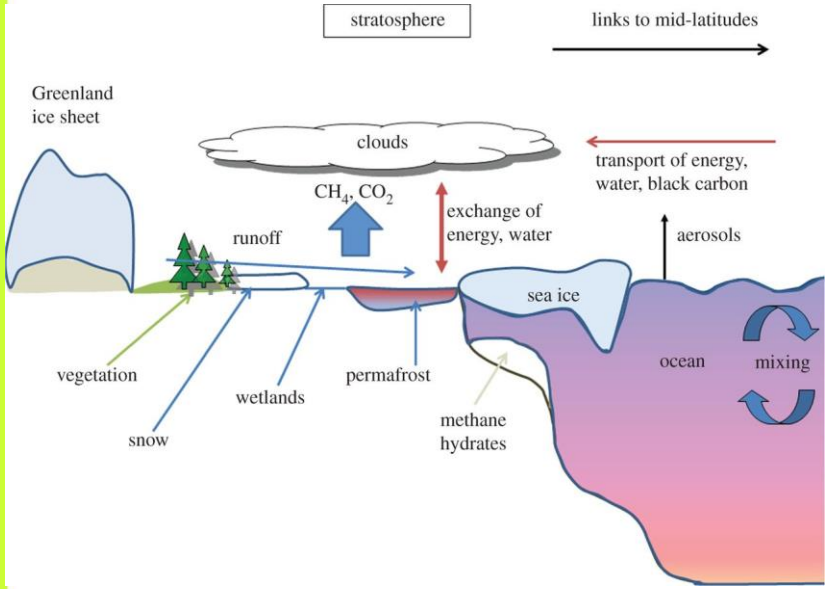
- Land surface
- Chemistry

Coupled Models



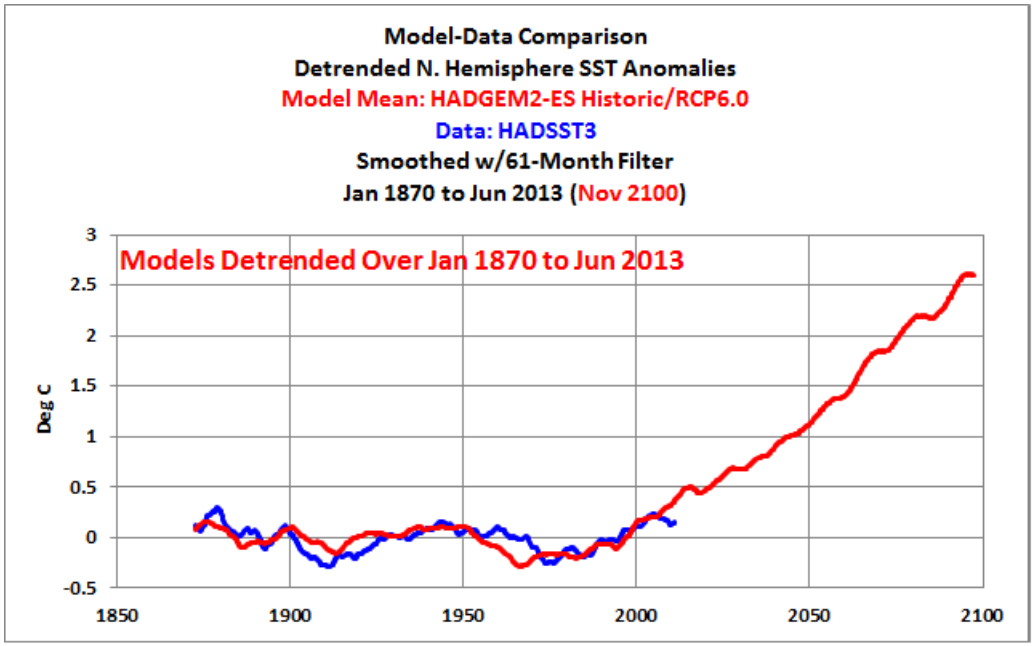
- Particularly important on climatic timescales
- Met Office HadGEM3 model

Climate Models



- Complexity
- Feedback loops

Climate Models Numerics

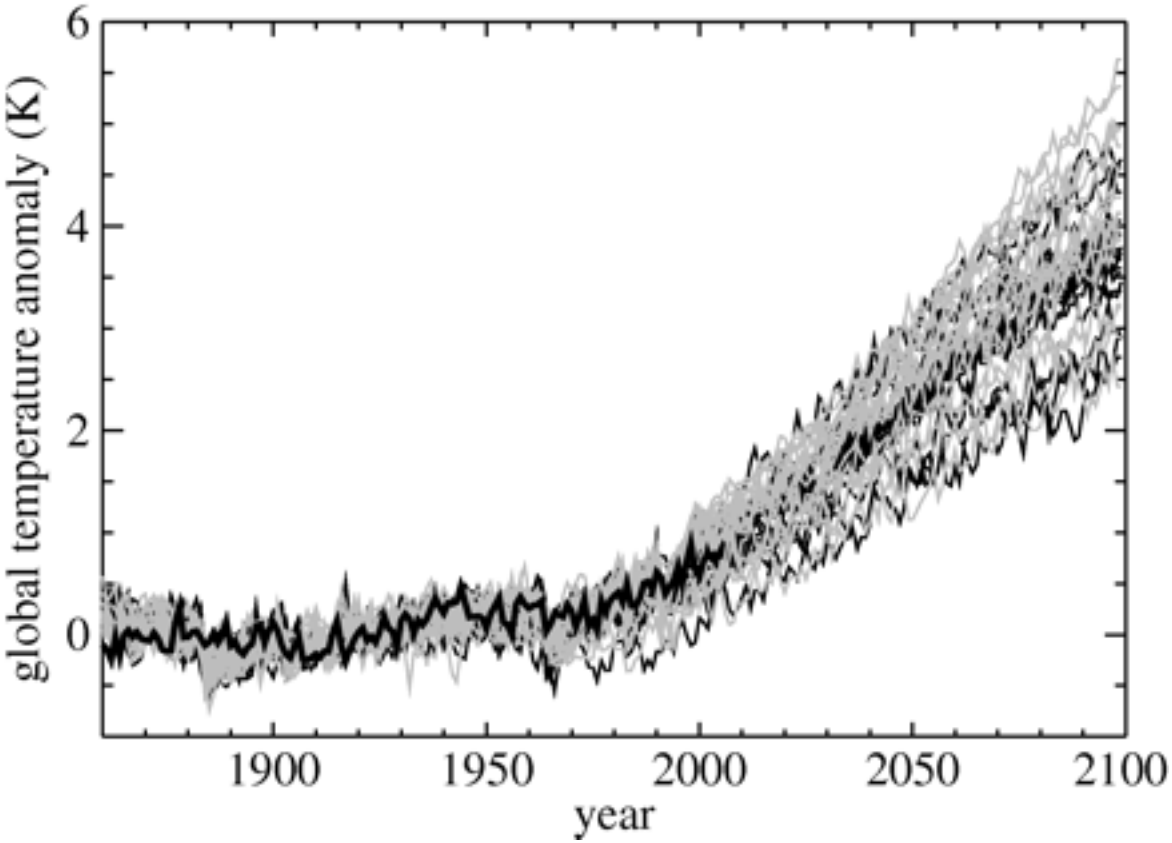


Bob Tisdale

- Validated until present day
- No reference solution past present day
- Societal demand for accuracy

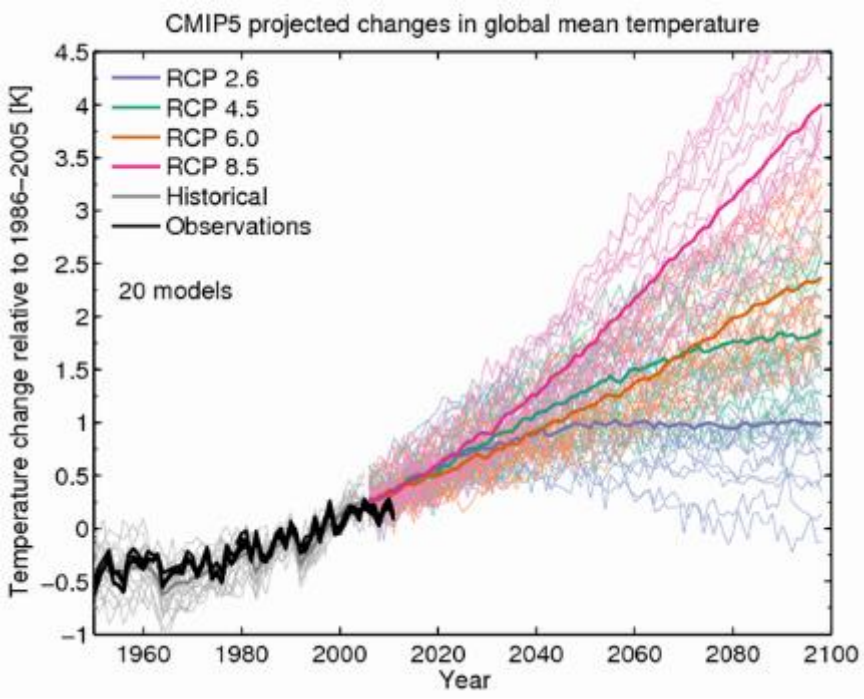
Ensemble systems

- Perturbed initial conditions of the model



Ensemble systems

- *Better : ensemble of ensembles*
- Intercomparison of models
- Specific model biases compensated

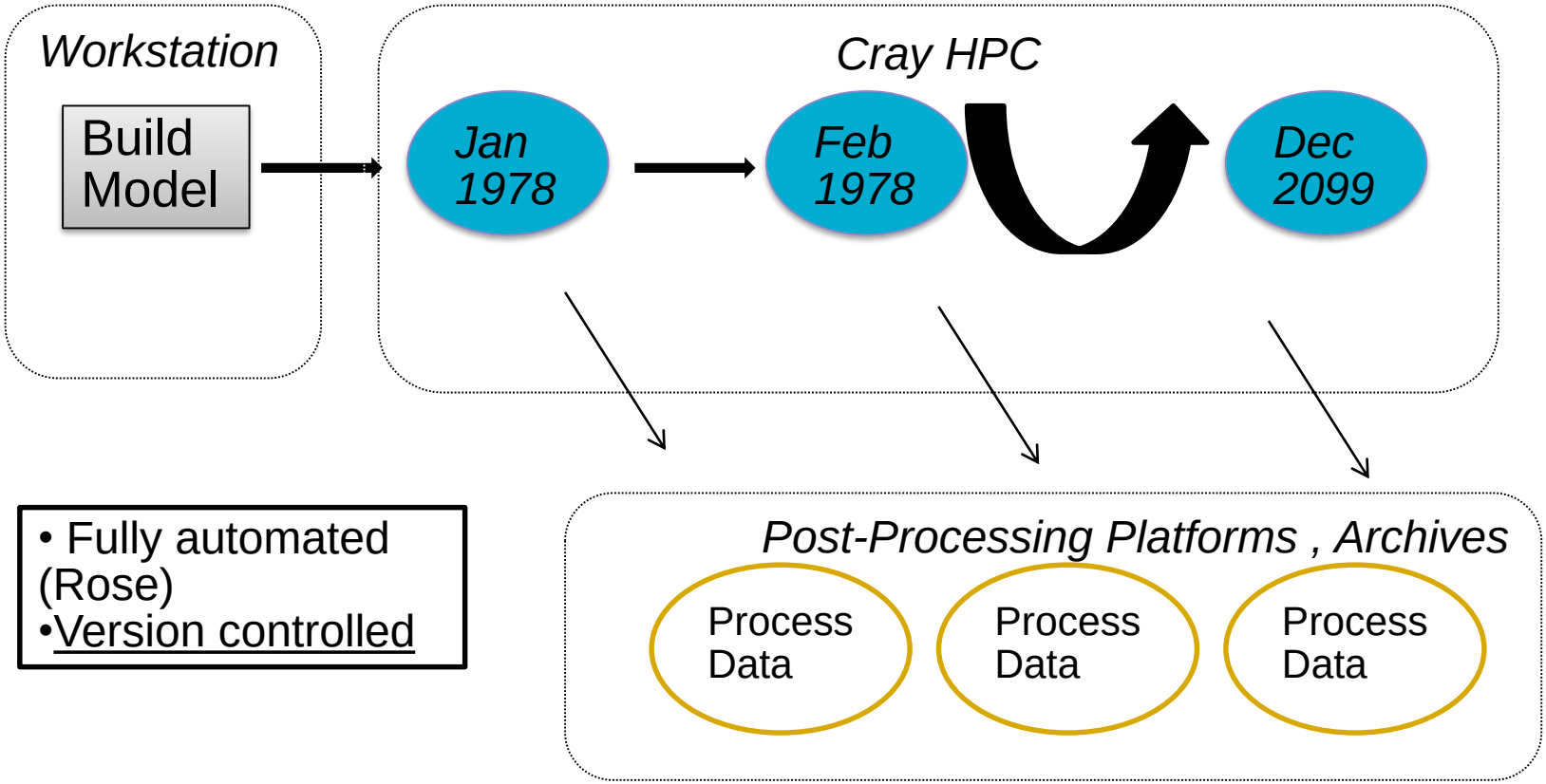


Worldwide
Coordinated
Numerical
Simulation Campaigns

CMIP6

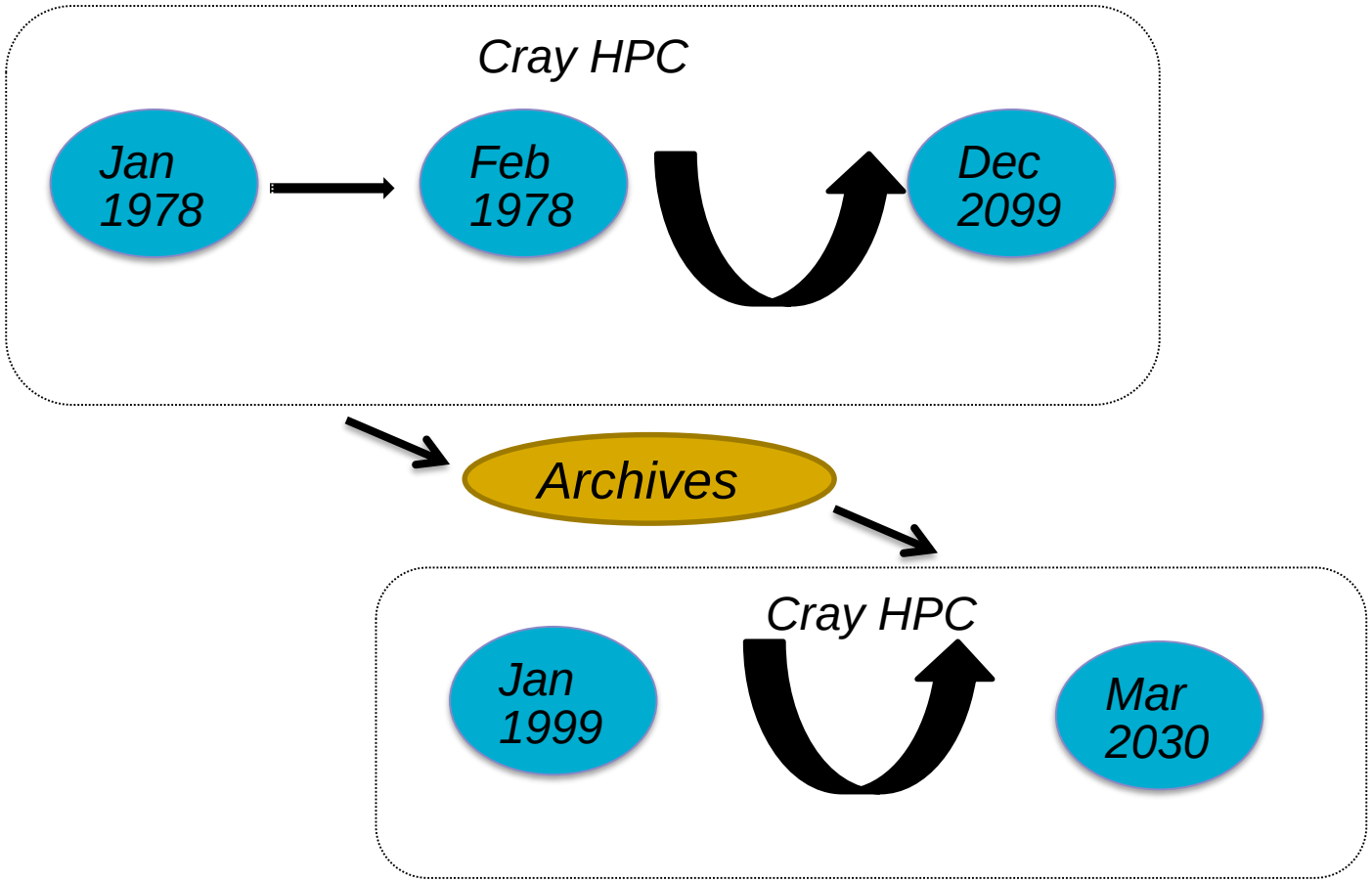
- Organised by World Climate Research Program
- 5 years organisation
- Complex experimental apparatus
- Results analysed in time for IPCC AR6 in 2023
- Data hosted in ESGF database ~20+ Pbytes
- Billions of core hours

Workflows



- Fully automated (Rose)
- Version controlled

Numerical Reproducibility



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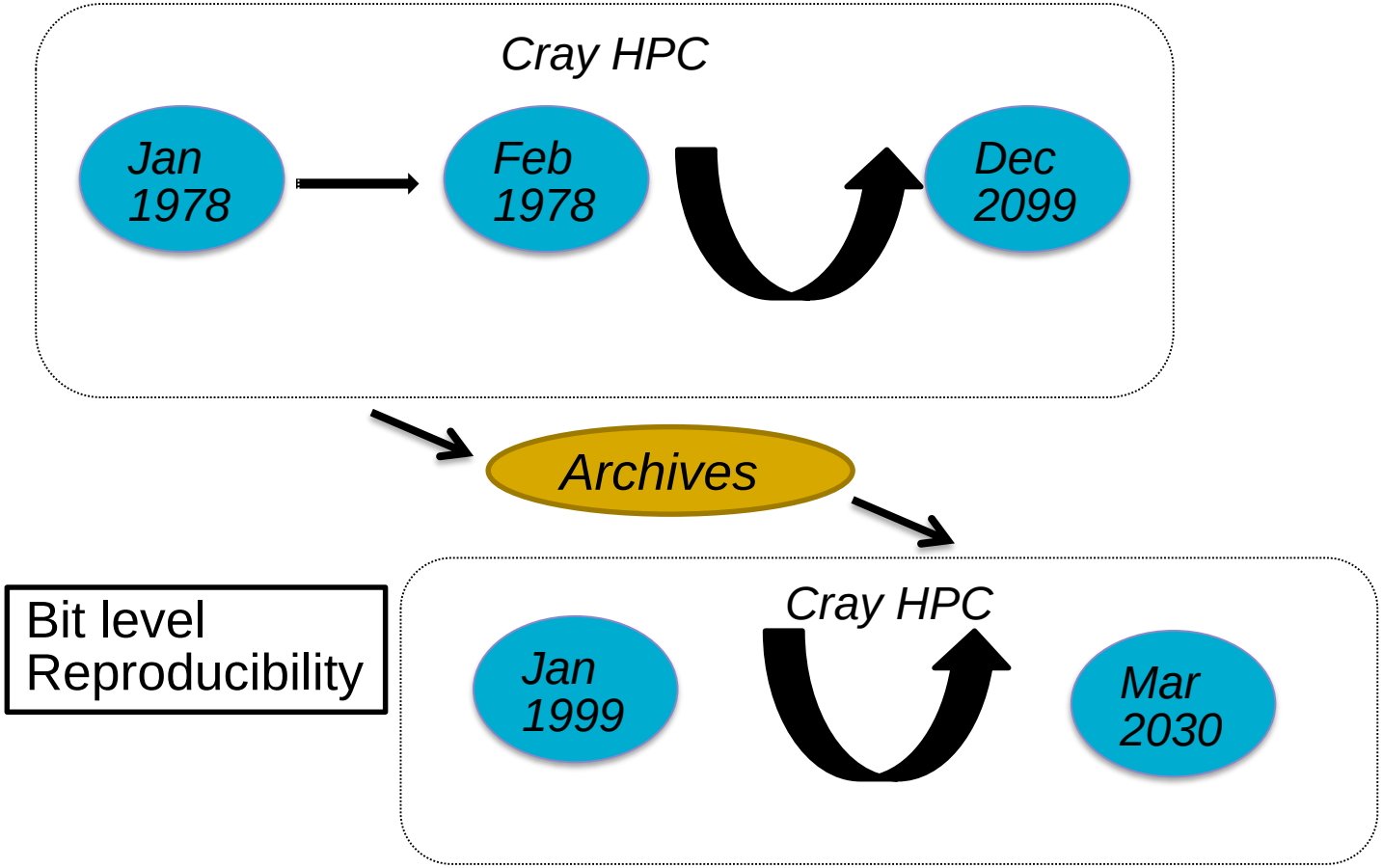

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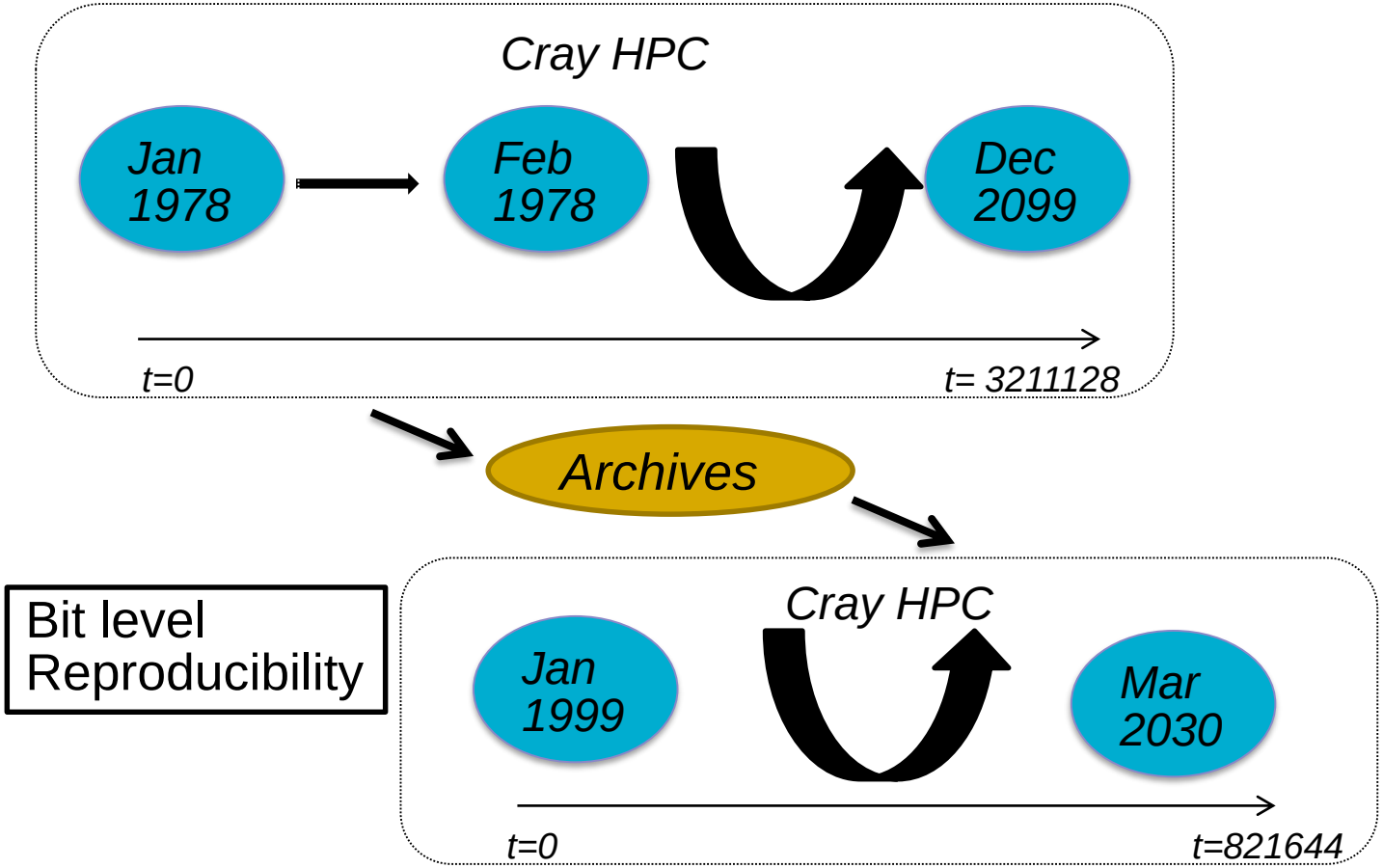

Bit level Reproducibility

Numerical reproducibility

Good Coding

```
use timestep, only : current_timestep
use submodel, only : initialise, integrate

if (current_timestep().eq.0) then
    call initialise()
else
    call integrate(current_timestep())
end if
```

Numerical reproducibility

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```
use timestep, only : current_timestep
use submodel, only : initialise, integrate

if (current_timestep().eq.0) then
    call initialise()
else
    call integrate(current_timestep())
end if
```

Bad/Lazy Coding

```
use my_favorite_module
logical first_call = .true.

if (first_call) then
    call interpolate(a,a_grid)
    first_call=.false.
end if
call do_stuff(a)
```

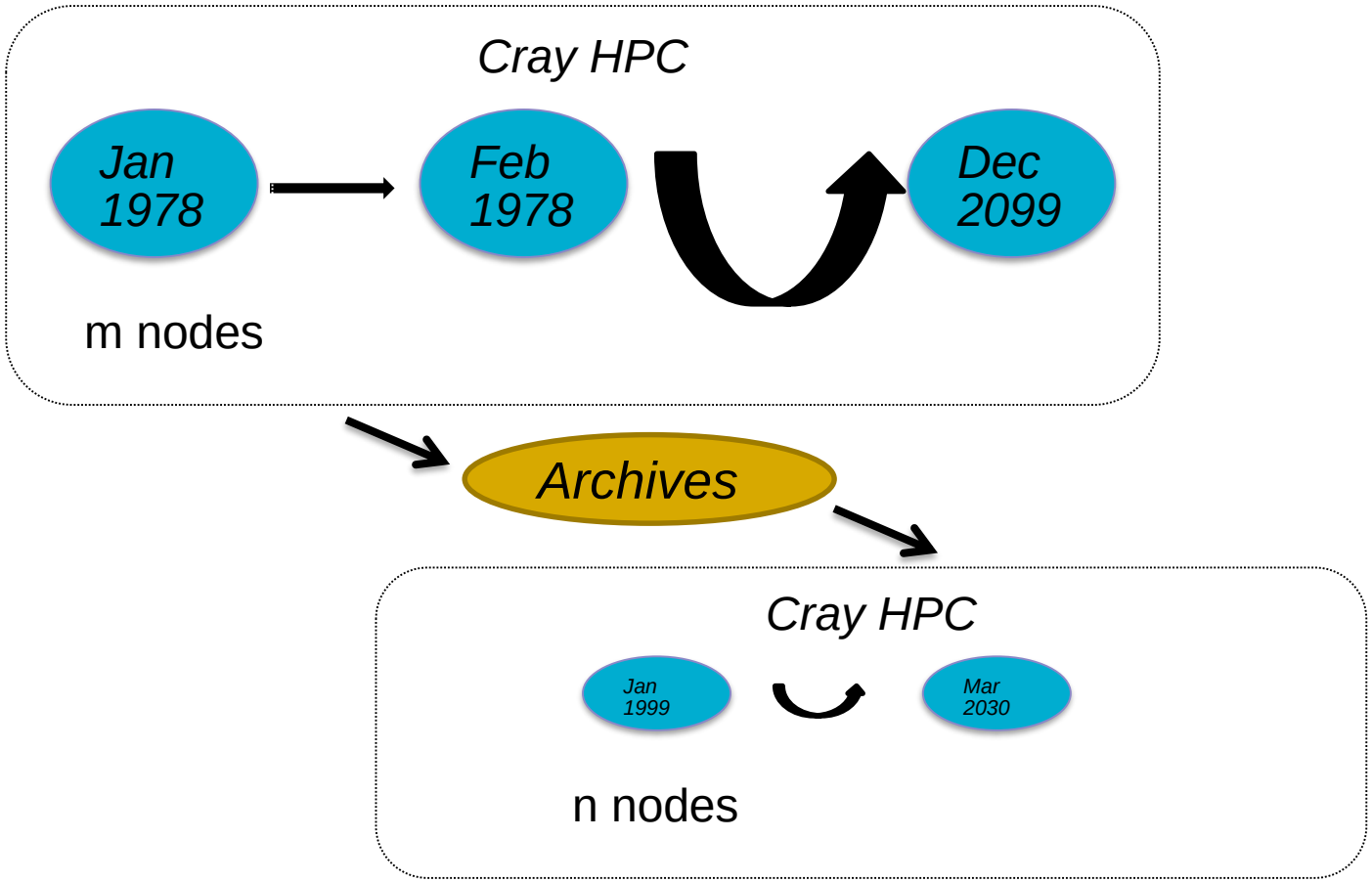
Quality Assurance

- *is important*
- Coding Standards
- Code reviews
- Unit tests
- Version Control

- Investment
- But can save a lot of time

(and computing resources)

Numerical Reproducibility



Bit Reproducibility

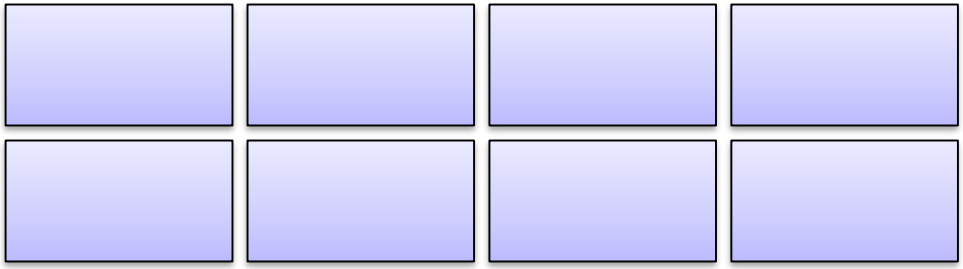
Across domain decompositions

m x n vs n x m vs k x l

All numerical computations are local except
- Halos Exchange
- Global Sums (Iterative Linear Solvers)

Bit reproducible global sums

Original implementation



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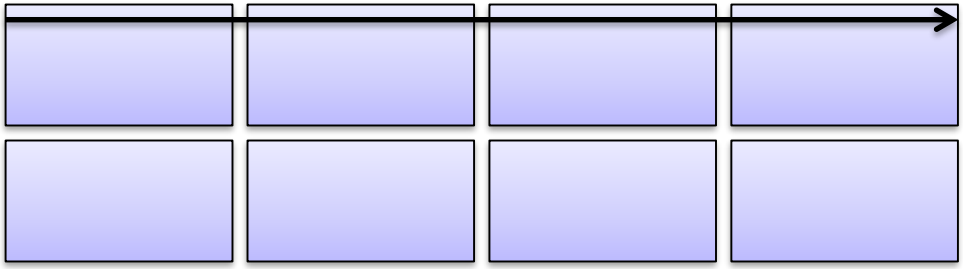

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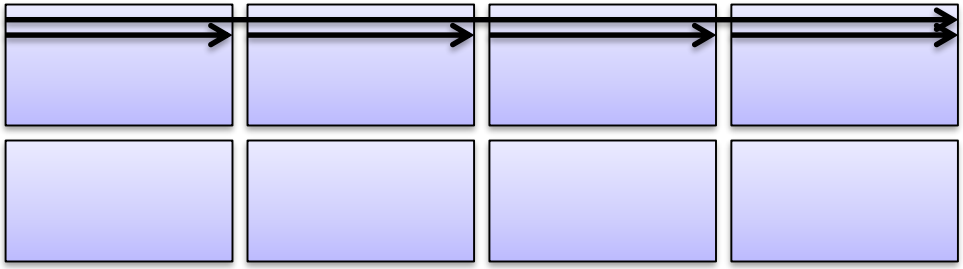

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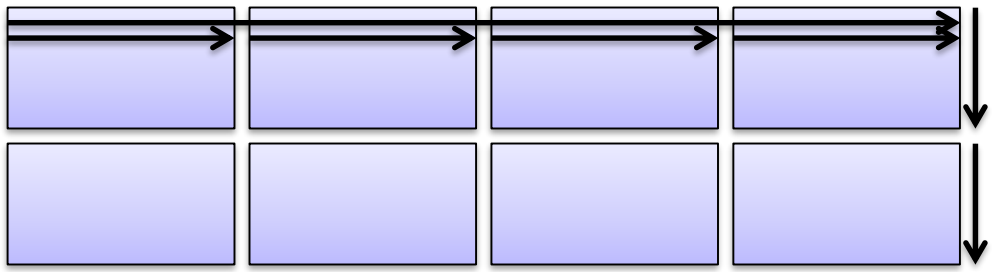
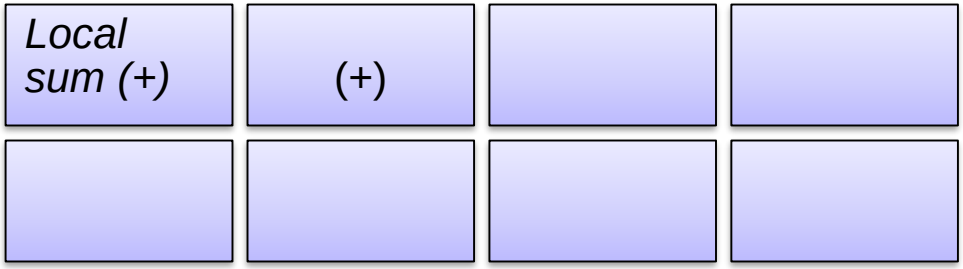


Bit reproducible global sums

New implementation



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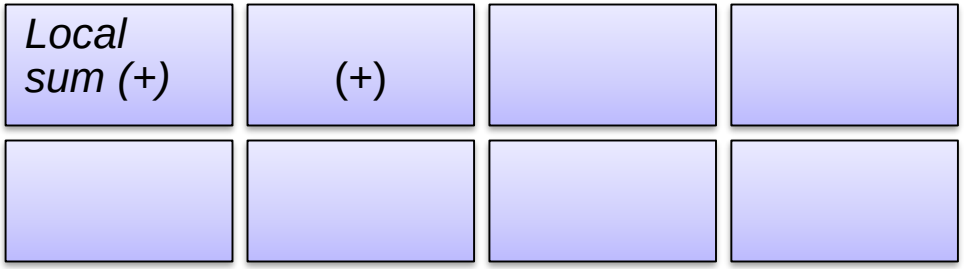

- Double-Double (complex) precision
- Knuth, D.H Bailey

Bit reproducible global sums

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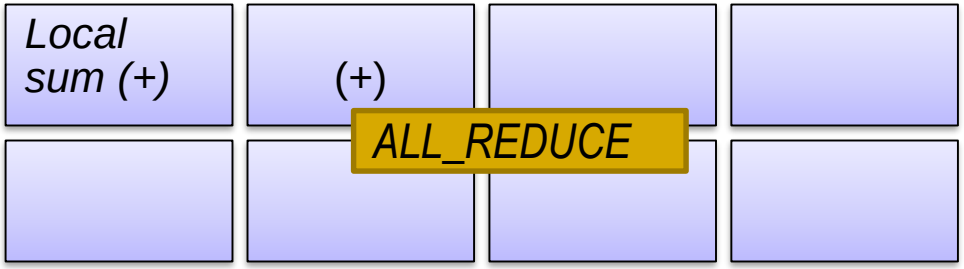

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- MPI_ALLREDUCE
- Double-Double Operator

Bit reproducible global sums

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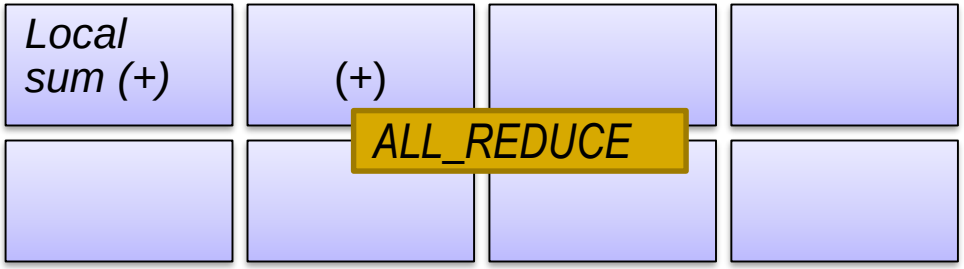

- Double-Double (complex) precision
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- MPI_ALLREDUCE
- Double-Double Operator

Cores	Double	Double-Double
896	2264 s	2186 s

Bit reproducible global sums

- Do we really need this ?
- *It is a <u>proxy</u> for good quality code (QA)*
- Coarse grained *Unit Test*

Using single precision

Always use double precision? … No.

Understanding the error
Accuracy of Krylov subspace solver – BiCGStab
Iterative solver, it improves the answer each iteration

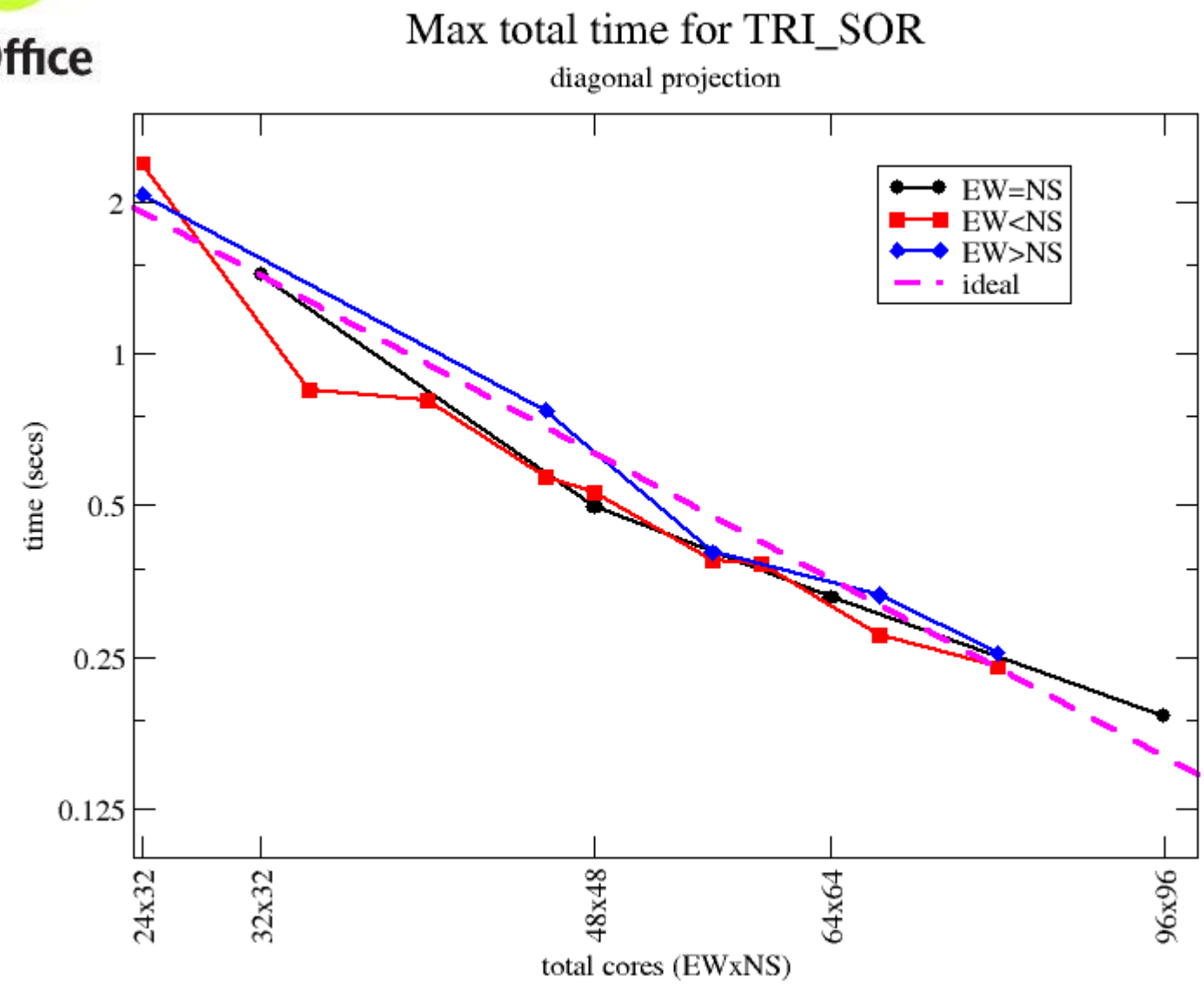
$$\|\vec{r}_k\| = \|\vec{b} - A\vec{v}_k\| < \epsilon$$

In our model $\varepsilon < 10^{-3}$ answer is *good enough*
What precision is needed to satisfy this?
Single precision is good enough

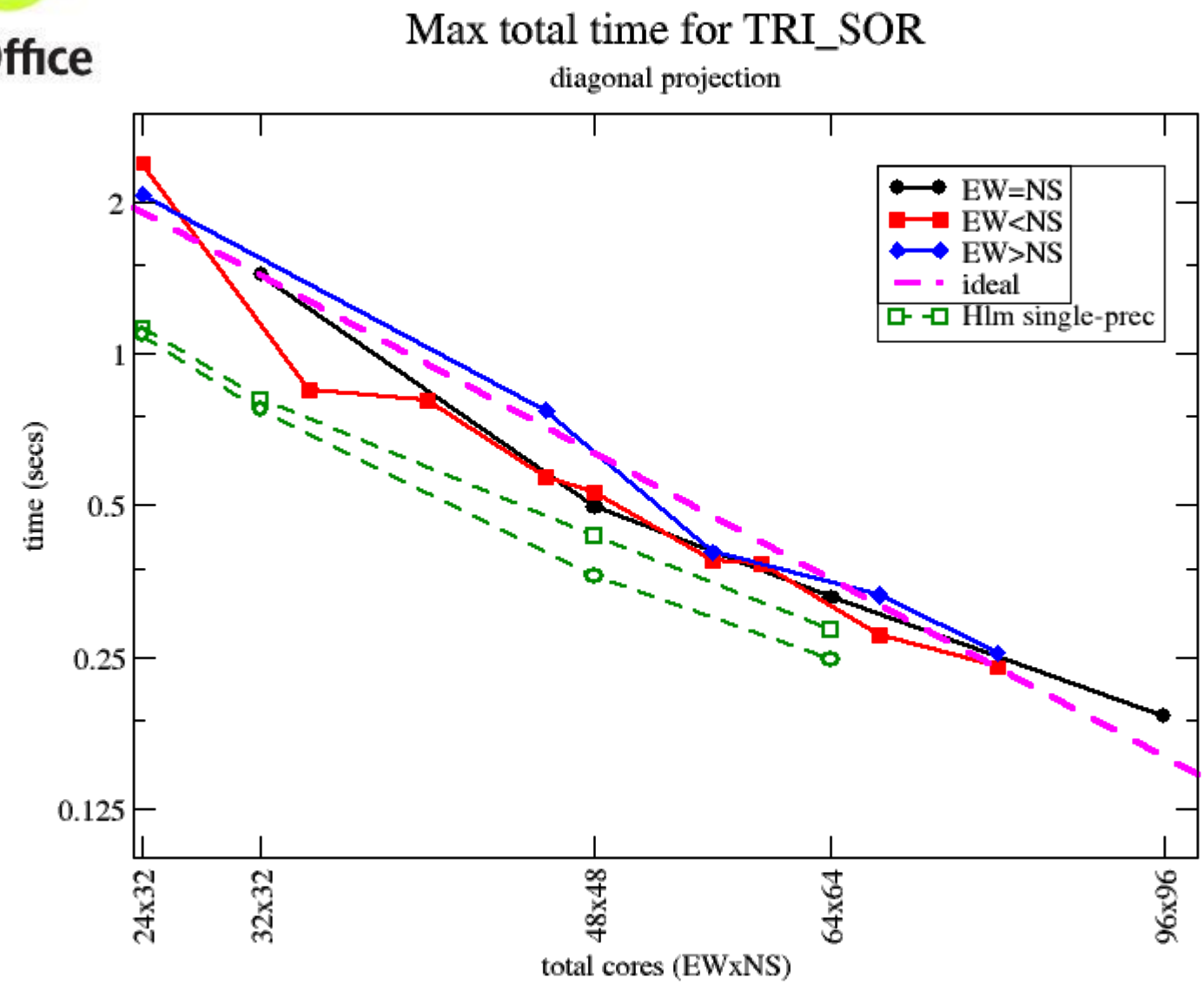
Modern FPU single prec operation is not significantly faster than double
Single prec words are half the size of double prec words
Compute values of A in double precision
Store them in single precision
Doubles the effectiveness of cache

Courtesy Dr C. Maynard

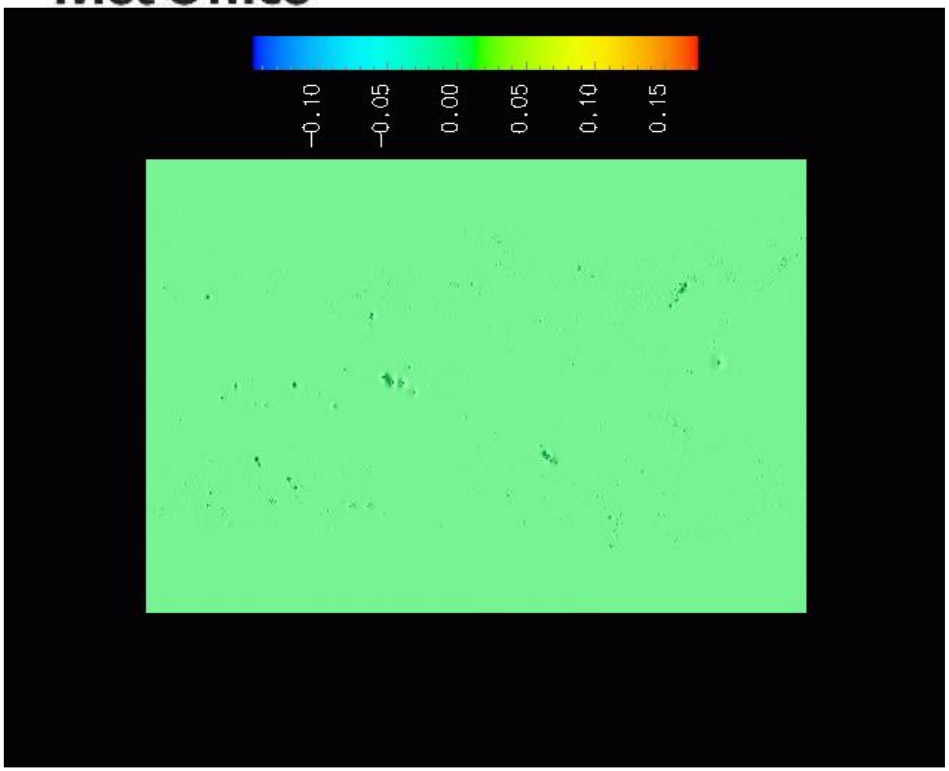
ENDGame



ENDGame



Accuracy of answers



After 5 time-steps, level 10 biggest differences

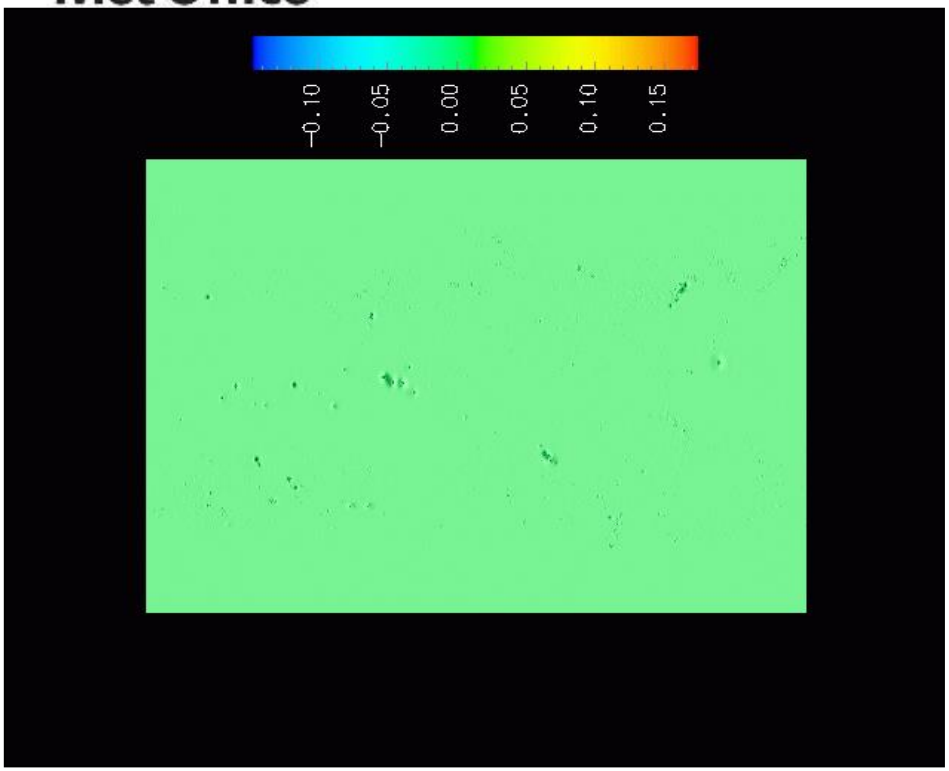
$$f = (\xi_{64} - \xi_{32}) \times 10^{-4}$$

$$\xi = \text{exner} = \left(\frac{p}{p_0}\right)^k$$

24x32 EWxNS Proc
1024x769x70 grid

Plot by T. Allen

Accuracy of answers



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N512 6 time-steps (s)	64 bit	32 bit	Speed-up
EG_SL_HELMHOLZ	3.884	2.836	1.4
EG_BICGSTAB	2.876	1.809	1.6
TRI_SOR	2.075	1.124	1.8

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Plot by T. Allen

Single precision physics

- Precision required by subscale phenomena ?
- Less obvious answer than for Krylov solver
- Ongoing research work
- but careful assessment required

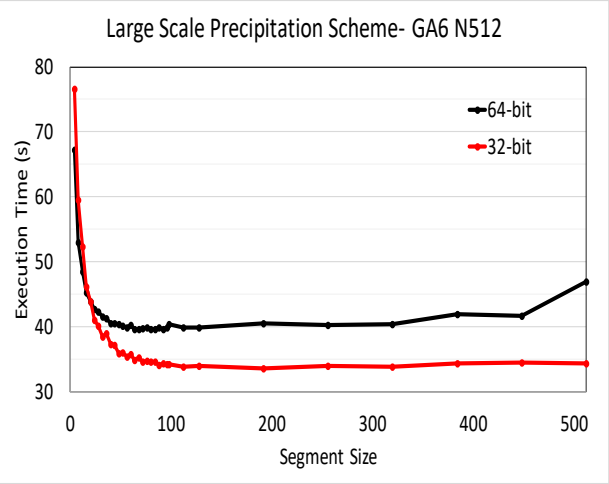
32-bit LS-Precip: Early Results

Build-time selection of scheme precision

Minimal effect on model evolution

Retune segment size to aid cache blocking

Modest speedup. More understanding required.



richard.gilham@metoffice.gov.uk

32-bit GW-Drag: Early Results

Same implementation approach as LS-Precip

- Very different experience

Technically much easier, but…

…minimal performance gain at 32-bit

…big change in model evolution at 32-bit

- Cause still under investigation

Future Architectures

- We are not tied to a particular architecture
- Have changed in the past (vector to MPP)
- Engagement with new technologies

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- HPC Tier 2 system *Isambard*
- Cray inc
- Met Office
- GW4 Universities

Cardiff, Bristol, Bath, Exeter

Future Architectures

- **Phase 1**
- 8x1 Intel Xeon Phi nodes
- 4x2 NVIDIA Pascal GPUs
- Infiniband connection

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- **Phase 1**
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- **Phase 2**
- + "10000+" ARMv8 cores

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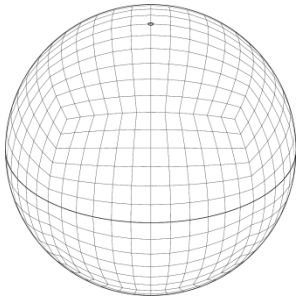
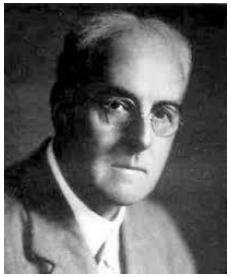
Performance Portability

- Unified Model
- Fortran90 + MPI + OpenMP
- 25 years development
- CUDA, Open ACC difficult to implement



- New LFRic model
- Complete rewrite
- Finite elements



- Opportunity
- Modern Programming Paradigms
- Python generating F2003 code (PsyKAI) / STFC
- Architecture Agnostic
- Will be used for 20+ years

Met Office
Hadley Centre

Summary

- Insatiable computing demands
- Numerical reproducibility important
- (Some) flexibility on precision
- Involvement with new architectures
- and new programming paradigms

Thank You !

Questions ?

jean-christophe.rioual@metoffice.gov.uk

Met Office
Hadley Centre