Towards Energy Efficient Numerical Weather Prediction

Scalable Algorithms and Approaches

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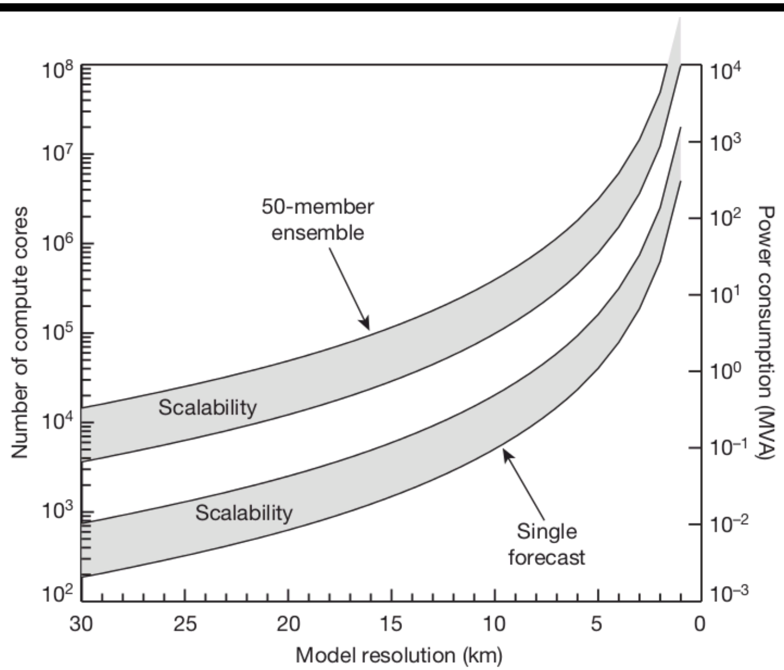
Future Comput./resource requirements & Challenges

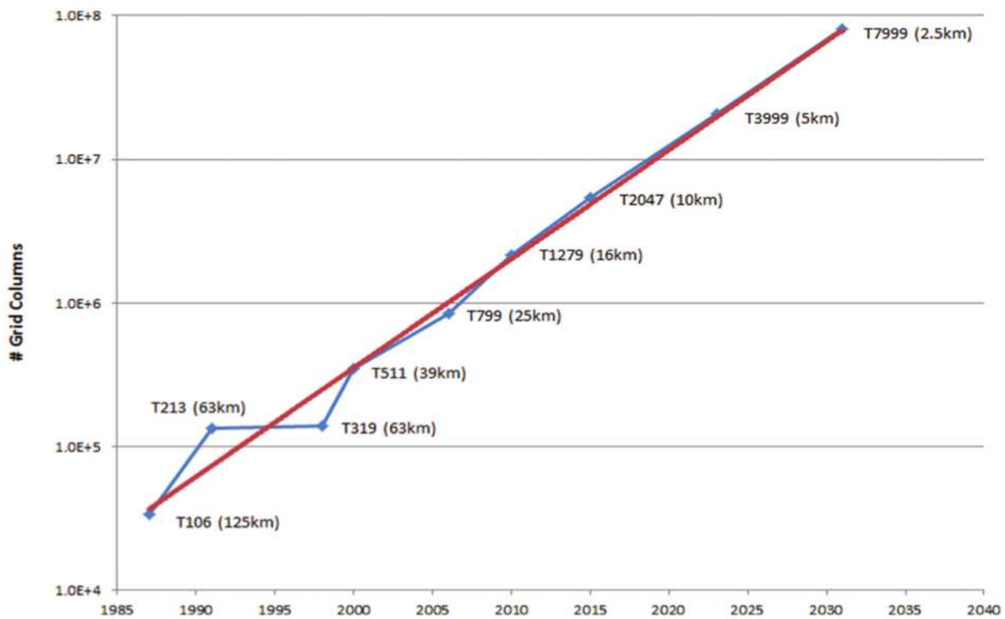


- Upper limit for affordable power at about 20 MVA
- Enhance parallelism & scalability of NWP (achieve time-to-solution gains on MPP)
- Change of paradigm needed: hardware, design of codes, numerical methods,& data movement (efficiency)

. *Nature*, P. Bauer et.al (2015)

- ECMWF could expect to be running a T7999 (2.5 km) global forecast model by 2030
- IFS model may continue to use the spectral transform method
- Adaptation to diff. programming model (coarrays)

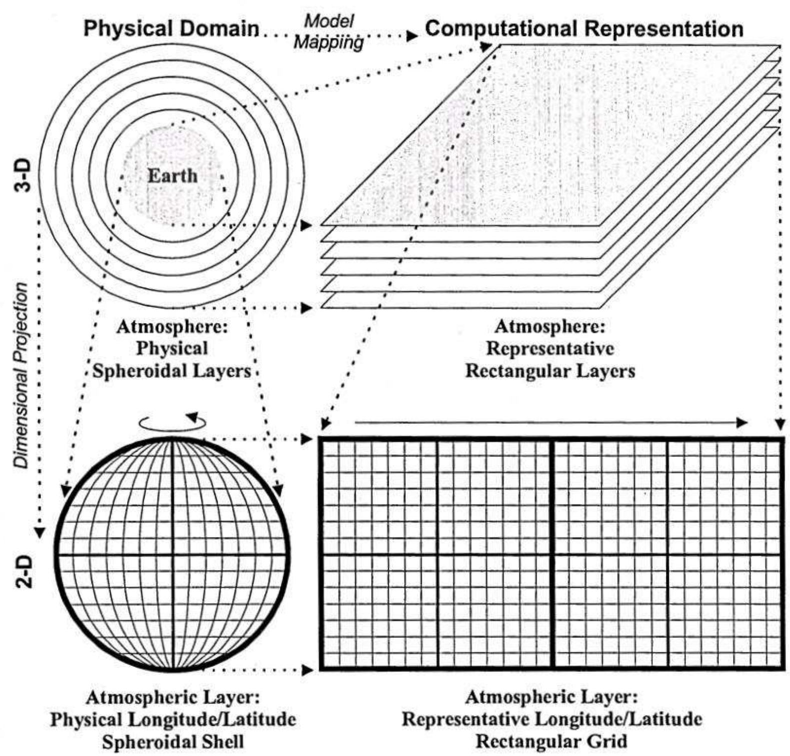
. *IJHPCA*, G. Mozdzynski et.al (2015)



NWP: Atmosphere, Model, Computation

A quantitative forecast of weather (or climate) based on model over a prescribed domain

- A *system of coupled PDEs* and other equations *dynamic* & *thermodynamic* processes in the Earth's atmosphere
  - Conservation laws (momentum, energy, mass) & Equation of state (ρ, P, T)
  - Fluid motion (relative to the Earth's rotation)



courtesy: Ray Melton PhD thesis (2003)

- Discretize, spatial & temporal derivatives $\Rightarrow$ a set of algebraic equations
- Suitable discretization; coord.: ($\lambda,\ \mu,\ z$), time integration schemes
- Constraint: relative sizes of the space grid, time step & wind speed (Courant-Fedrichs-Lewy criteria)
- Boundary/Initial cond. & param.
- Fluid velocity $\mathbf{V} \equiv (u,\ v,\ w)$, pressure, density, temperature, humidity

. *Climate modeling for Scientists and Engineers*, J. B. Drake (2014)

Shallow Water Equation (Model)

SWM: **Two dimensional model of atmospheric fluid dynamics**, captures the essential math. & comput. complexity of the meteorogical primitive equations (atmospheric flow). SWE on a sphere $\Leftrightarrow$ conservation of *momentum* & *mass*.

$$\frac{d\mathbf{V}}{dt} = -f\mathbf{k} \times \mathbf{V} - \nabla\Phi$$

$$\frac{d\Phi}{dt} = -\Phi\nabla \cdot \mathbf{V}$$

$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla$

$\nabla = \frac{\mathbf{i}}{a(1-\mu^2)} \frac{\partial}{\partial \lambda} + \frac{\mathbf{j}}{a} \frac{\partial}{\partial \mu}$

- $\mathbf{V} = u\mathbf{i} + v\mathbf{j}$, velocity on the sphere
- $\mathbf{i}, \mathbf{j}, \mathbf{k}$: unit vectors on sphere
- f: Coriolis force
- Φ: geopotential
- a: radius of sphere
- λ: longitude
- ϕ: latitude, $\mu = \sin\phi$

- **Spectral Transform method:** equations are solved in terms of the vorticity η and the horizontal divergence δ
- $\eta = f + \mathbf{k} \cdot (\nabla \times \mathbf{V}), \delta = \nabla \cdot \mathbf{V}$
- To avoid singularity in velocity at poles, transform $(U,\ V) = \mathbf{V}\cos\phi$
- Equations for *time evolution of scalar fields* $\eta,\ \delta,\ \Phi$, along with transformation $(U,\ V) \Rightarrow (\psi,\ \chi)$, relating $\eta \Leftrightarrow \psi$ & $\delta \Leftrightarrow \chi$ (via differential equations)

. *NCAR technical note*, J. J. Hack and R. Jacob (1992)

Spectral Transform method

The spectral representation of the scalar field variable $\xi(\lambda,\ \mu)$ is represented by a truncated series expansion in terms of spherical harmonic functions $[P_n^m(\mu)e^{im\lambda}]$ as below,

$$\xi(\lambda,\ \mu) = \sum_{m=-M}^{M} \sum_{n=|m|}^{N(m)} \xi_n^m P_n^m(\mu)e^{im\lambda}$$

$$\xi_n^m = \int_{-1}^{1} \left[\frac{1}{2\pi} \int_0^{2\pi} \xi(\lambda,\ \mu)e^{-im\lambda} d\lambda \right] P_n^m(\mu)d\mu$$

$$\equiv \int_{-1}^{1} \xi^m(\mu) P_n^m(\mu) d\mu = \sum_{j=1}^{J} \xi^m(\mu_j) P_n^m(\mu_j)\, w_j$$

- λ_i: longitude, $i \in [1:I]$
- ϕ: lat. $\mu_j = \sin\phi_j,\ j \in [1:J]$
- m: wave number/Fourier mode
- $P_n^m(\mu)$: assoc. Legendre func.

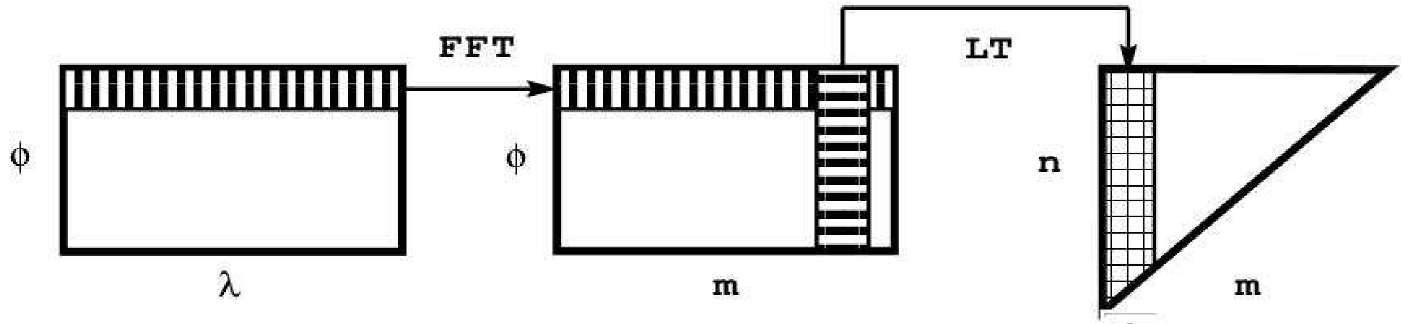
$$\xi^m(\mu) = \frac{1}{I} \sum_{i=1}^{I} \xi(\lambda_i,\ \mu)e^{-im\lambda_i}$$

- Grid: longitude (evenly spaced grid), latitude (Gaussian grid)
- M: the highest Fourier wavenumber (cut-off) included (East-West representation)
- $N(m)$: the highest degree of the associated Legendre functions (North-South rep.)
- Triangular trunc. $(m,\ n)$: $N(m) = M$; $I \times J$ long.-lat. grid: $I \geq 3M + 1$, $I = 2J$
- Physical qtys.: real, $\xi_n^{-m} = [\xi_n^m]^*$, reduces comput./storage (only coeff. $+$ve modes)
- TM, "M" $\equiv$ horizontal resolution; T85 $\Rightarrow M = 85,\ I = 256,\ J = 128$

. *NCAR technical note*, J. J. Hack and R. Jacob (1992)

Spectral Transform method (contd.)

- Spectral Transform (spherical harmonics transform) is a Fourier transform in longitude (evenly spaced grid) **followed by** a Legendre transform in latitude (Gaussian grid).
- $I \times J$: $(\lambda_i,\ \mu_j)$; $i \in [1:I], j \in [1:J]$; $N(m) = M$; $I \geq 3M+1, I = 2J$



Physical space **Fourier space** **Spectral space**

$$\text{Forward transform:} \quad (\lambda_i,\ \mu_j) \overset{\text{FT}}{\Longrightarrow} (m,\ \mu_j) \overset{\text{LT}}{\Longrightarrow} (m,\ n)$$

$$\text{Inverse transform:} \quad (\lambda_i,\ \mu_j) \overset{\text{IFT}}{\Longleftarrow} (m,\ \mu_j) \overset{\text{ILT}}{\Longleftarrow} (m,\ n)$$

- Computations are performed in both the *physical* space and *spectral* space
- Physical quantities & non-linear terms comput. performed in the **physical** space
- Time stepping is performed in **spectral** space
- At each time step, the data is transformed across the two spaces

. *SIAM Rev. Sc. Comp.*, I. T. Foster and P. H. Worley (1997)

Spec. Trans. meth. for SWM: Practical outlook

$\{\mathbf{V},\ \Phi\} \Rightarrow \{\eta,\ \delta,\ \Phi\}$; Compute *time evolution of scalar fields* $\eta,\ \delta,\ \Phi$, physical quantities

At each time step:

1. Inverse Transform the fields from spectral space to physical space
2. Compute physical quantities like U, V (Inv. Trans. of expressions computed using spectral quantities)
3. Compute non-linear terms in physical space and Forward Transform to spectral space
4. Time integration (step) of spectral quantities; $\eta_n^m,\ \delta_n^m,\ \Phi_n^m$

Computation Complexity

- Fourier transform (FFT): $\mathcal{O}[N^2 \log N]$
- Legendre transform: $\mathcal{O}[N^3]$
- For inc. horizontal resol., the LT is expensive (computation) [$N_{\text{spec}} \sim N^2$ spec. pts.]

Communication

- Spectral to physical space transform & vice versa require global comm. at every time step (expensive on massively parallel computers, scalability)
- Need to look at communication avoiding approach

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MWR, I. T. Foster et.al (1992)

Spec. Trans. meth.: Computational efforts

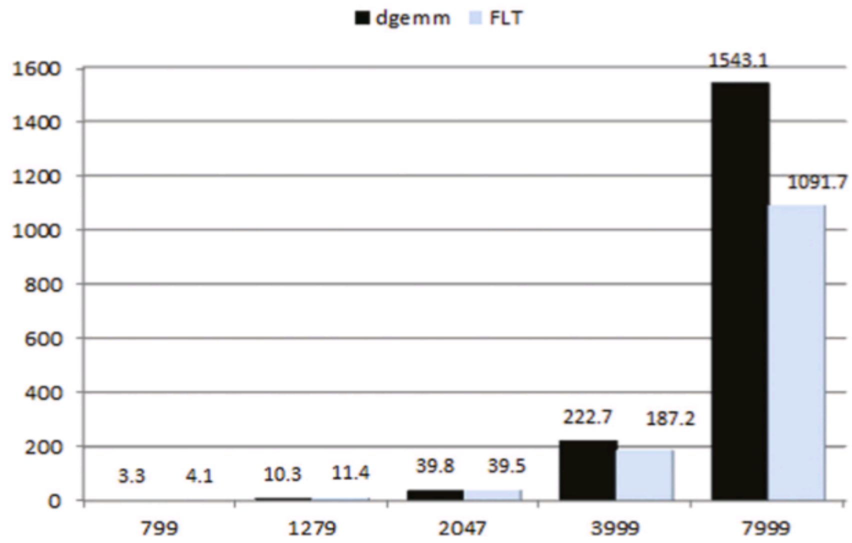
- *To reduce the computation workload* (use of math. & reduction of physical grid points).
  - Use of *reduced Gaussian grid* (30% few points) in computing FT, and the **number of waves** retained, *progressively reduced for Gaussian latitudes towards poles*.
  - **Reduced spectral transformation**: reduced Gaussian grid (both FT & comput. non-linear terms) & reduced spectral summations (save time on LT up to 50%).
  - NCEP seasonal forecast global spectral model (Compared computation: full grid transform, reduced grid, & reduced spectral transform for 1-month integration)

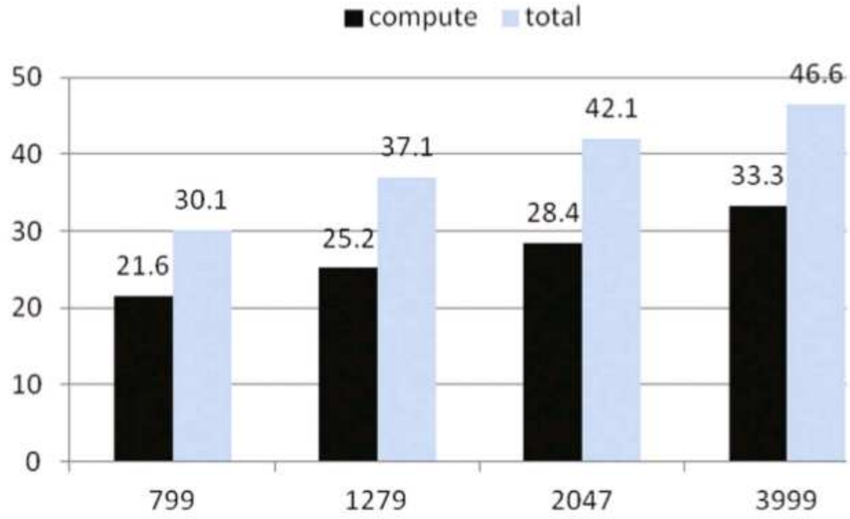
  . *MWR*, H. -M. Juang (2004)
- Global models (spectral transform) are used by NCEP, JMA, & ECMWF for forecasting (elegant treatment of the spherical problem $\Rightarrow$ quest to improve efficiency)

  . *JMSJ*, D. L. Williamson (2007)
- With **Fast Legendre transform**: $\mathcal{O}[N^2 \log^3 N]$. ECMWF forecasting efforts (IFS) have benefitted immensely by **FLT**
- (T7999 $\approx$ 2.5 km horizontal resolution was possible !!) longitude-latitude grid; $I \times J$: $23998 \times 11999 \approx 10^8$ points

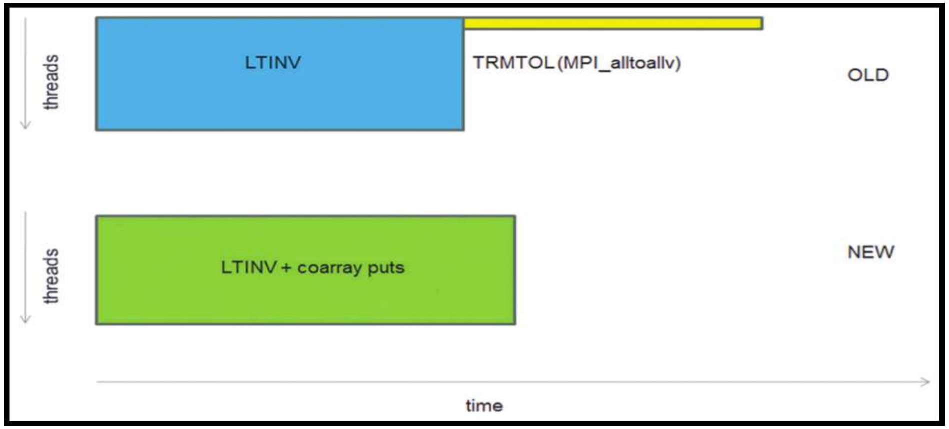
  . *MWR*, N. P. Wedi et.al (2013)

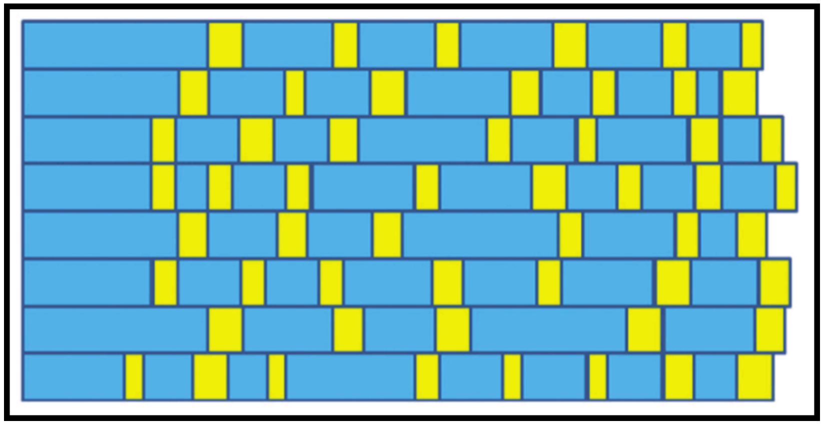
Spec. Trans. meth.: Computational efforts (contd.)





Av. wall-clock time for **LT** [millisec.] & Rel. cost comput. (IFS spec. tran.) for diff. model resol.

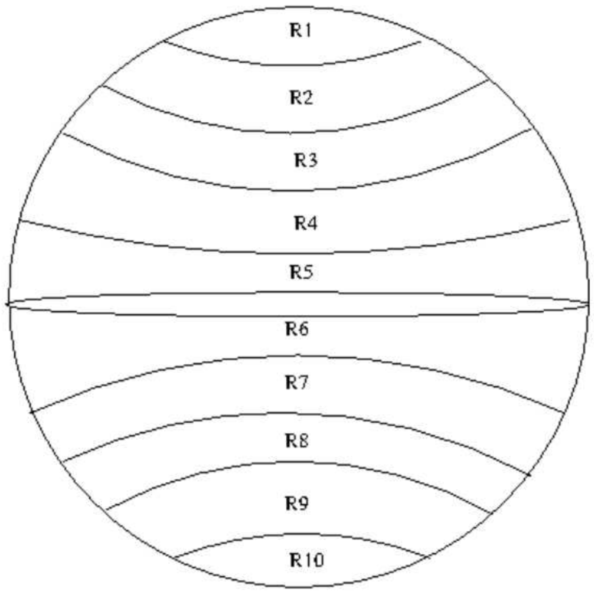




– Transposition are communication intensive: **Fourier**⇔**Spectral** & **Physical**⇔**Fourier**

– PGAS: **ILT** & **S**⇒**F** transpose overlapped; Overlap in time for **8** OpenMP threads
. *IJHPCA*, G. Mozdzynski et.al (2015)

Spectral Transform method: Comm. avoiding algo.



- Replace single-domain global spectral method by multi-domain spectral method (local harmonic expan.)
- Schwarz Domain Decomposition: subdomains; polar caps, latitudinal bands
- Construct spectral transform (subdomain): local Fourier basis (tailored for sperical geometry) + Sub-spherical harmonics (polar cap & spherical band)
- Kernel to be developed will be tested for shallow water model
- Solve PDEs on the subdomains with appropriate boundary conditions to obtain local solution $\Rightarrow$ "Construct" global solution from local solutions (comput. & comm.)
  - Computations over sub-domain can be performed across several processing elements for each domain independently
  - Communication overhead is reduced considerably in comparison to single domain spectral method (comm. required across a subset of the processing elemnts only)
  - Still ride on the advantages of the spectral transform w.r.t the treatment of the spherical geometry

. *C-DAC Technical Note*, S. Janakiraman (2017)

Petascale/Exascale approaches to NWP

Grid-point methods (Discretization on a cubed sphere)

- 1.63 PFlops global shallow water model on Tianhe-2 based on stencil computation over cubed sphere mesh using Xeon Phi accelerators along with Xeon within the power envelope of 17.8 MW [W. Xue et.al, IPDPS (2014)]
- Shallow water equation solver on heterogeneous architecture (GPU, Xeon Phi, FPGA) based on stencil over cubed sphere mesh [H. Fu et.al, PLOS One (2017)]

Spectral element dynamical core

- Redesigning CAM-SE for Peta-Scale climate modeling performance and ultra-high resolution on Sunway TaihuLight [H. Fu et. al, SC (2017)]
  - Sustainable double-precision performance of 3.3 PFlops for a 750 m global simulation across 10,075,000 cores

ESCAPE Project

- ESCAPE: Energy-efficient Scalable Algorithms for weather Prediction at Exascale
  - Focus on weather and climate dwarfs
  - New algorithms and programming models
  - Use of GPUs, Xeon Phi and photonics technology for computation

. `http://www.hpc-escape.eu/home`

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Thank You

for your attention

Cubed sphere mesh