Progress in Numerical Methods at ECMWF

EWGLAM / SRNWP October 2016

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N.P. Wedi, P. Bauer

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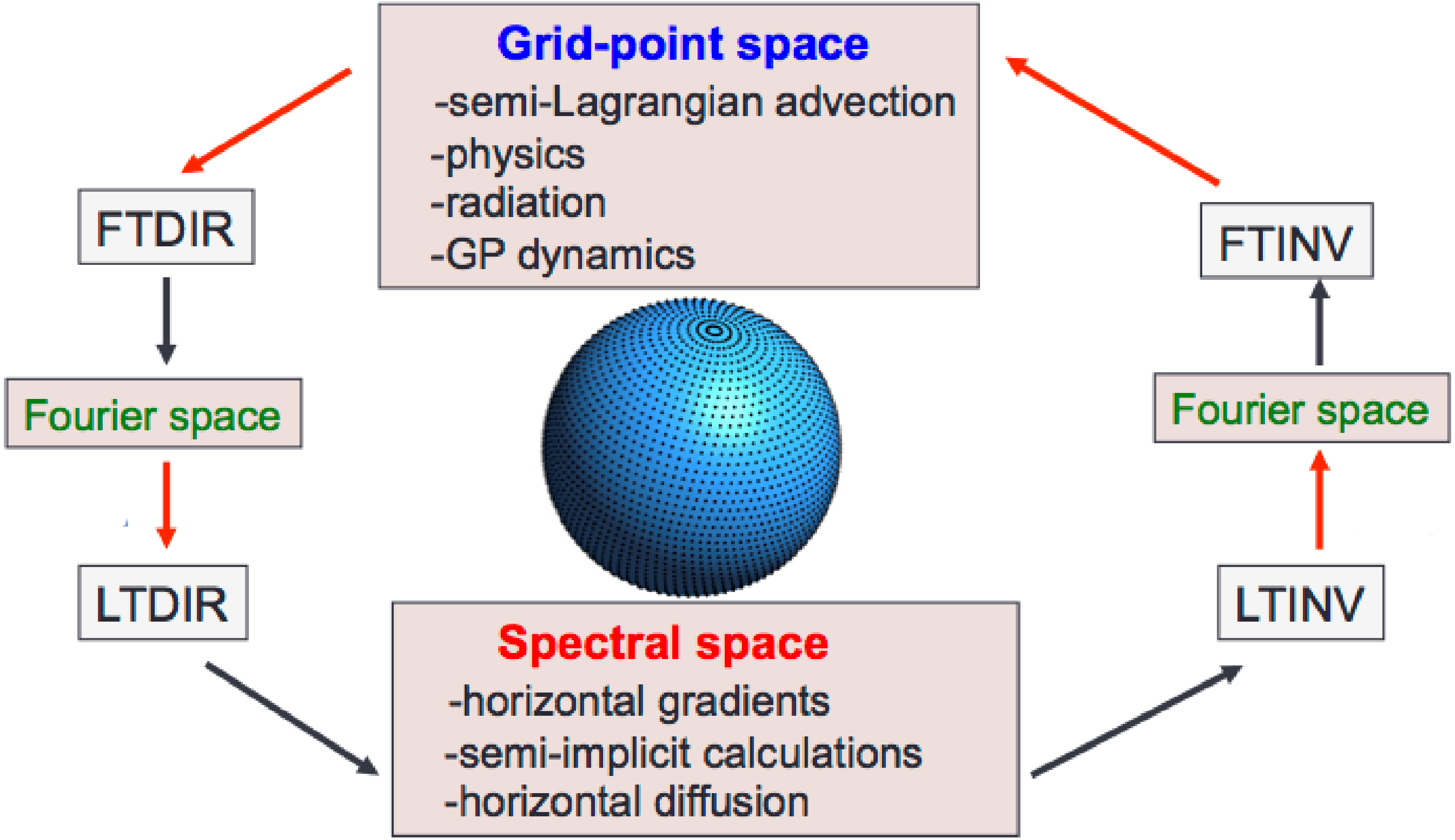
IFS

Semi-Implicit Semi-Lagrangian Spectral Transform dynamical core

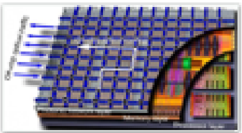


global spectral transform model

COMPUTATIONAL COSTS ON CURRENT HARDWARE

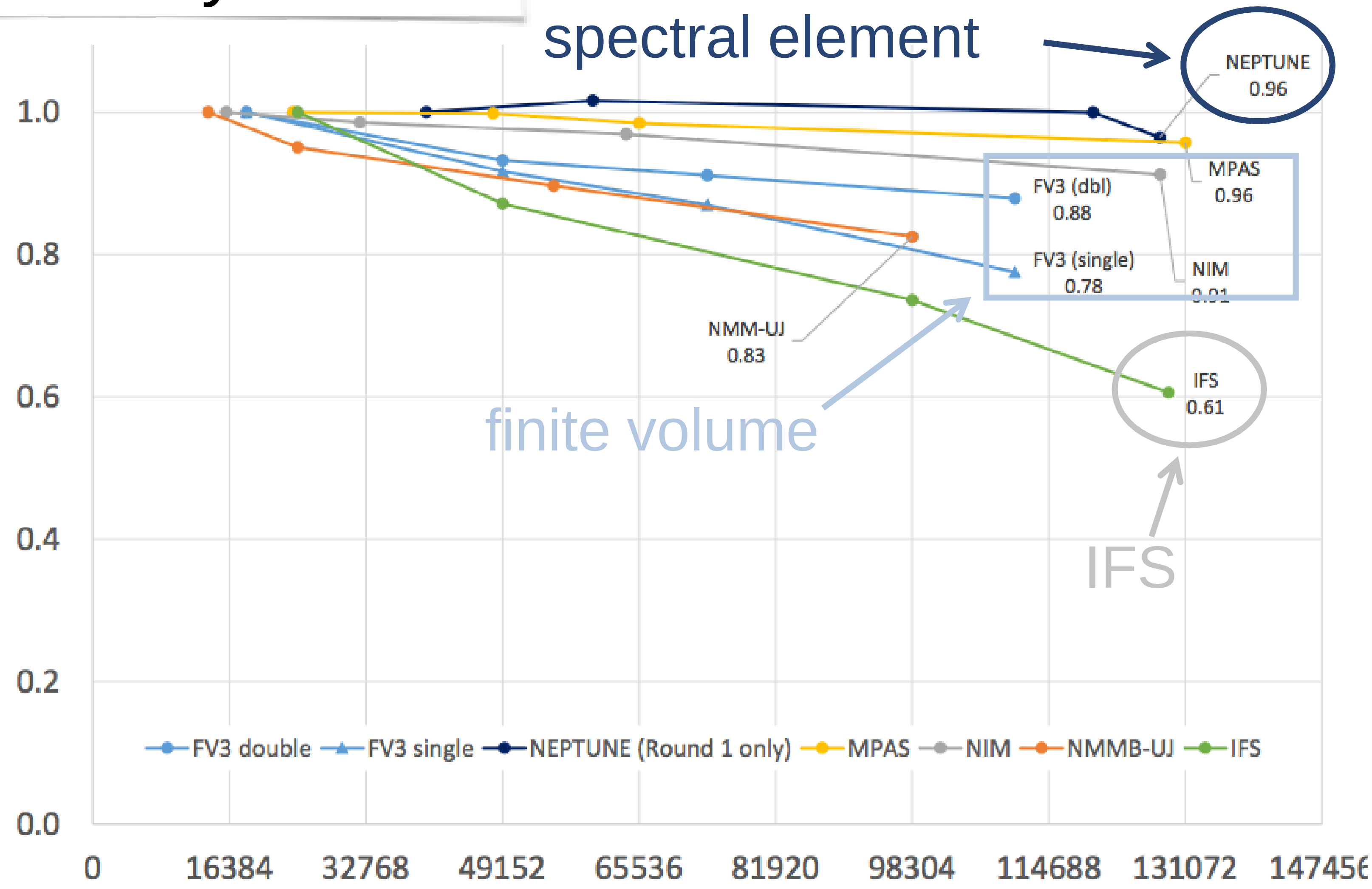
Resolution $[km]$	Prognostic variables	Vertical levels	Grid points $[\times 10^6]$	computational cost factor	time-step $[s]$
18	10	91	1.661	1	720
9	10	137	6.60	10	450
5	10	200	16.072	64	240
2.5	~20	200	64.14	1018	120
1.3	~20	200	256.28	8139	60
0.65	~20	200	1026.56	65200	30

HORIZONTAL RESOLUTION



EMERGING HARDWARE?

Strong scalability at 3km



Michalakes et al. NGGPS AVEC Report, 2015

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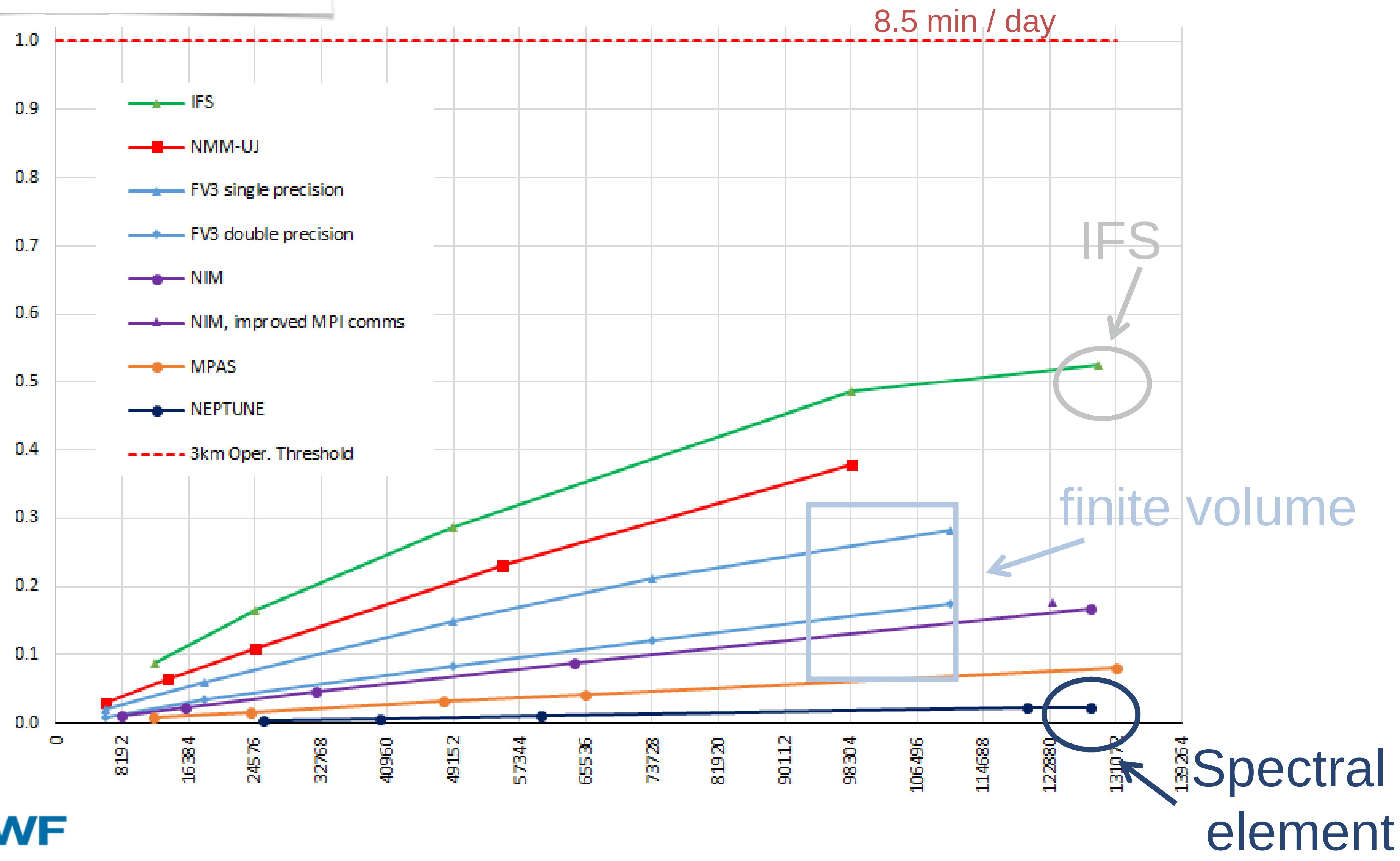
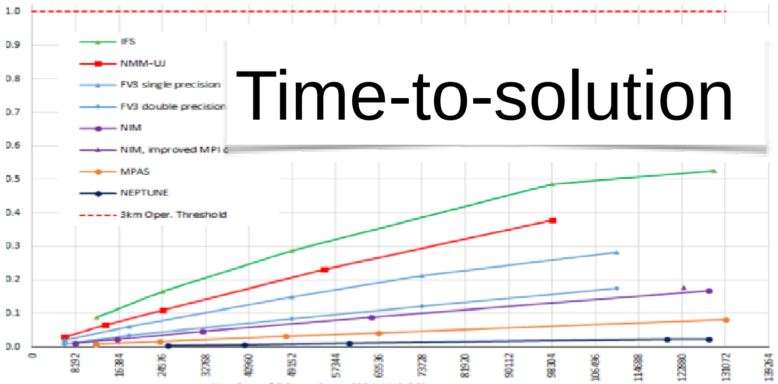
Time-to-solution



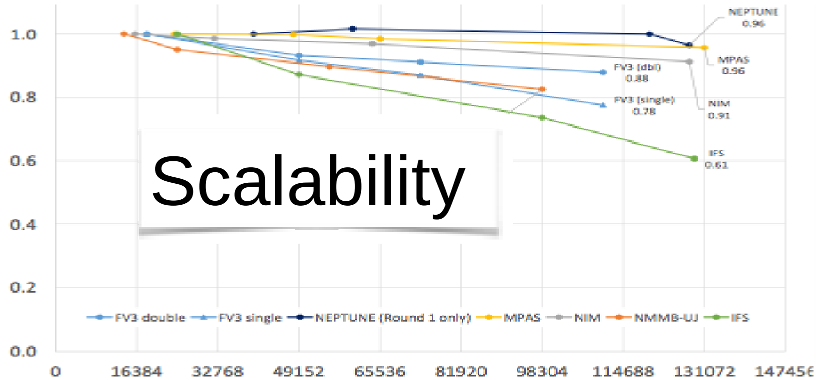
The Challenge

Two (possibly) competing factors

Time-to-solution

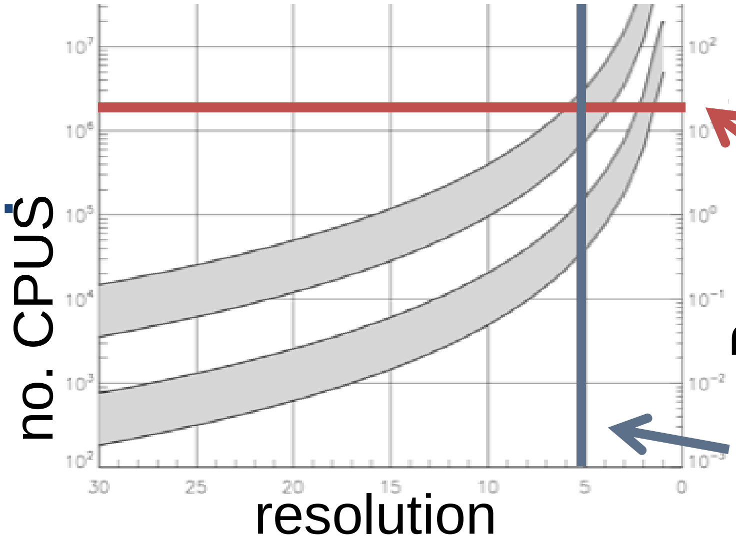


Scalability



and a constraint…

Energy-to-solution



Hard limit for HPC ~ 20MW?

< 5km resolution

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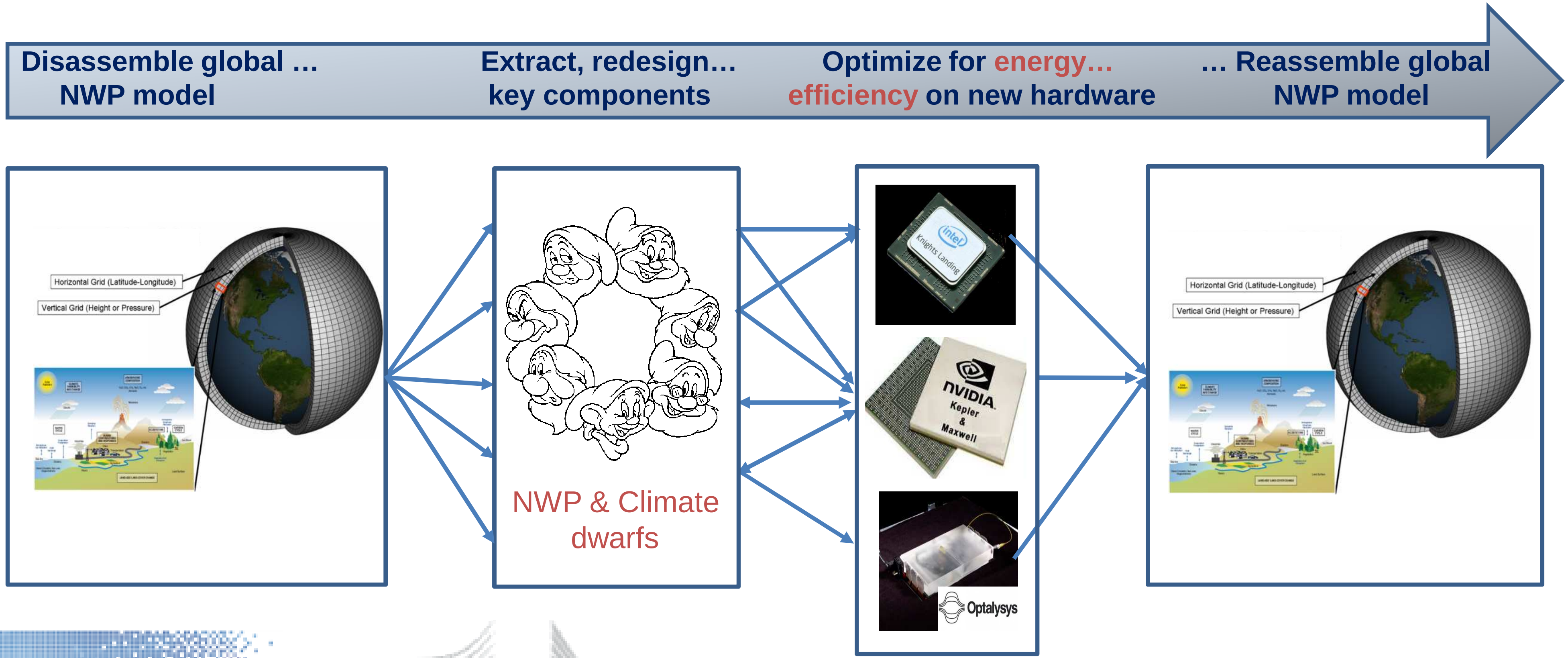
Outline

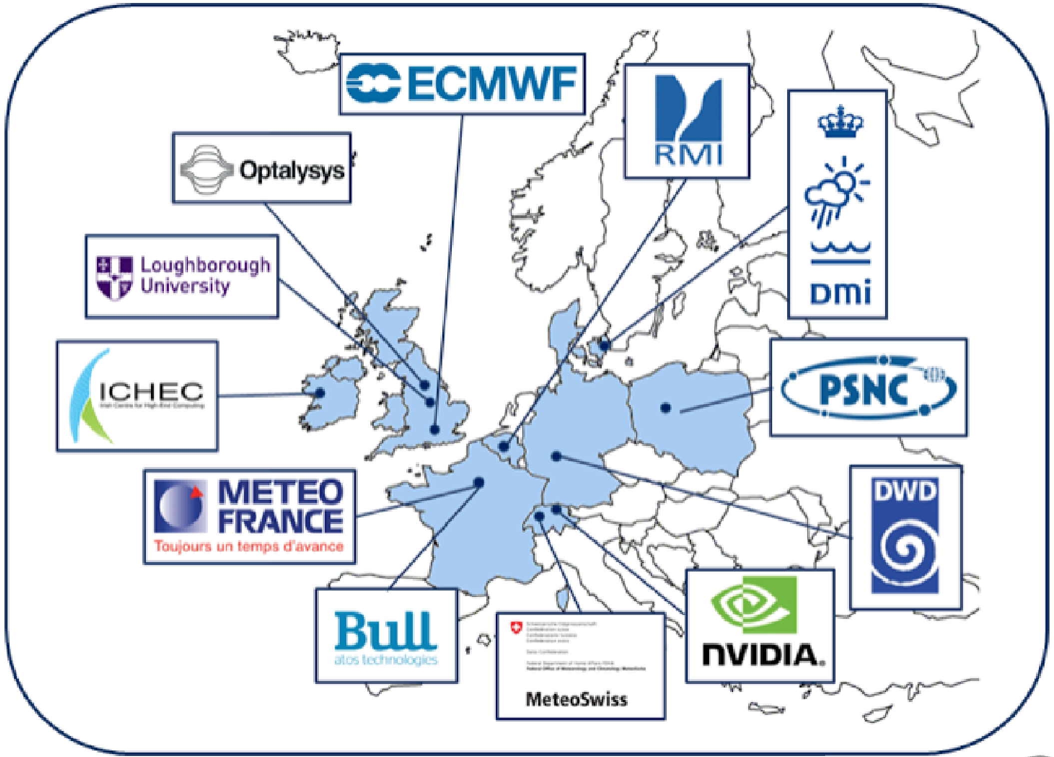
- ESCAPE
- Atlas
- PantaRhei - FVM

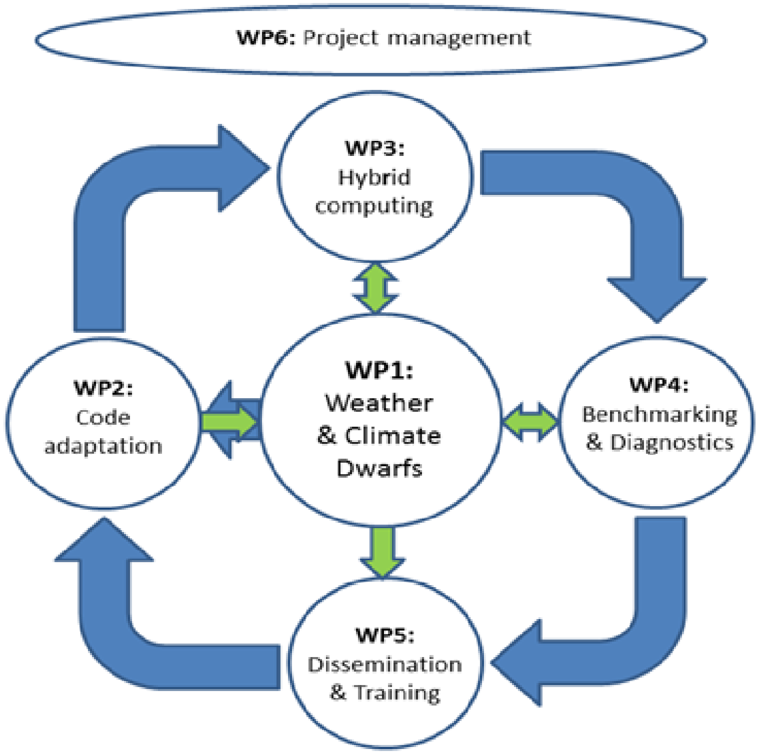
ESCAPE: Energy efficient SCalable Algorithms for weather Prediction at Exascale

www.hpc-escape.eu



First dissemination workshop:
18-29 October, Elsinor, Denmark





Dynamics

Advection (SL)
Elliptic solver (GCR)
Spectral transform (SH+biFFT)

Physical parameterisation

Cloud Microphysics (CloudSC)
Radiation

ECMWF

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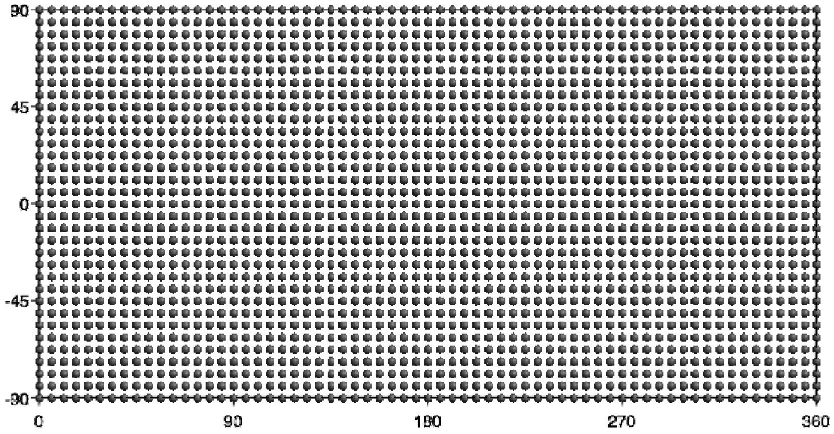
“Atlas, a library for NWP and climate modelling”
Deconinck et al. 2016, in preparation

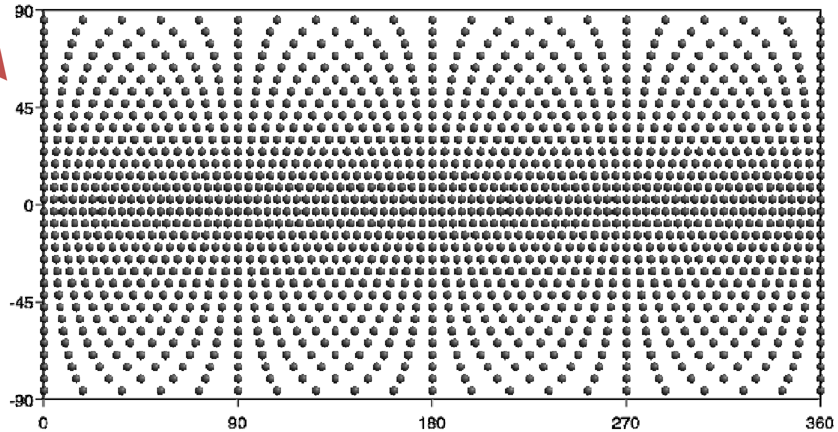
Atlas underlies many ESCAPE dwarfs and new numerical developments

A flexible parallel framework for

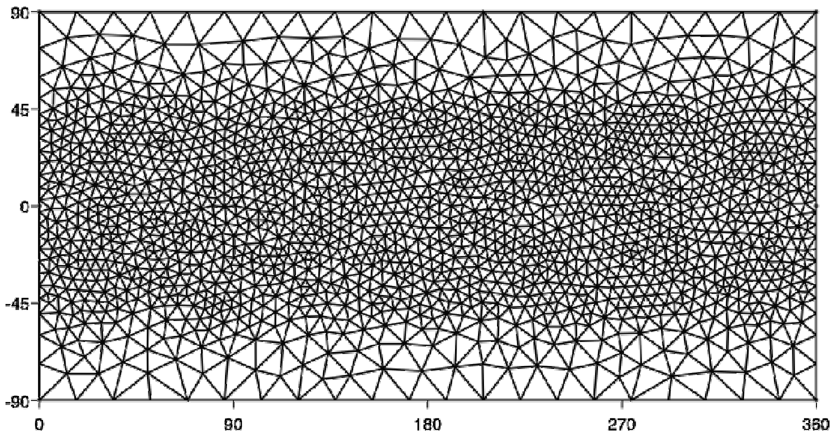
- structured grids
- unstructured hybrid meshes



Regular
Lat-Lon
(L32)



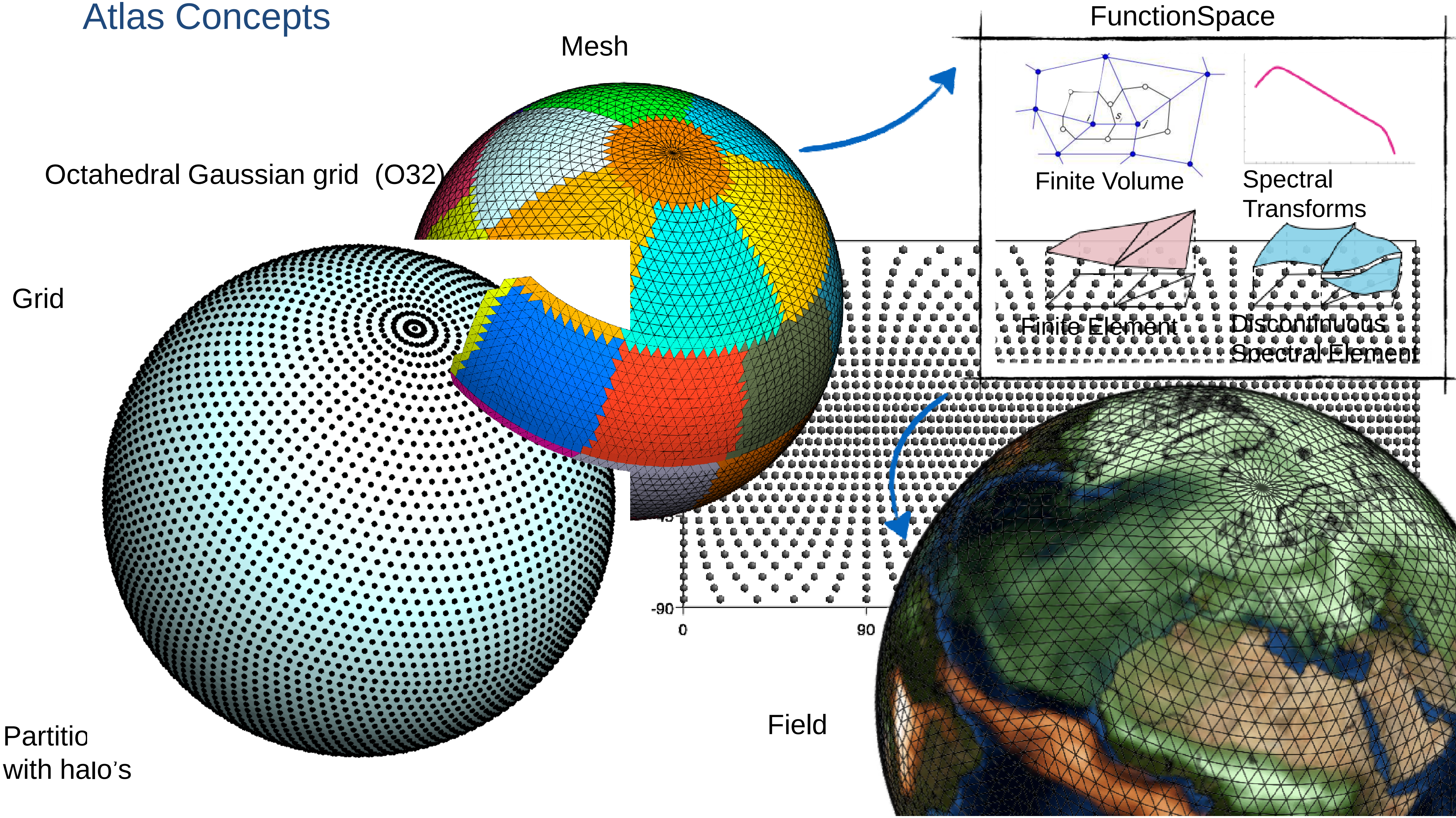
Octahedral
Gaussian
(O32)



Unstructured
mesh

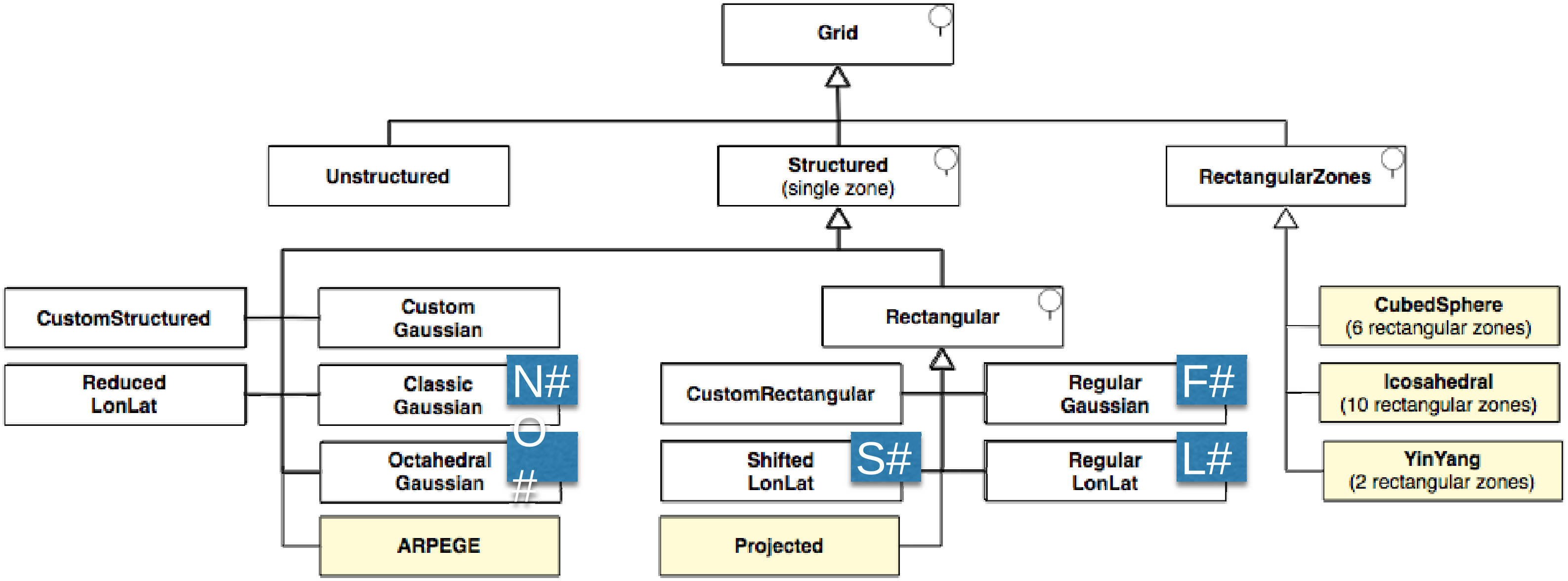
- Parallel mesh generation
- Mathematical operators
- C++ / Fortran

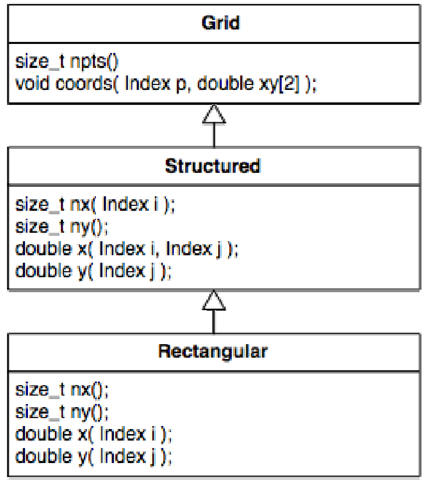
Atlas Concepts

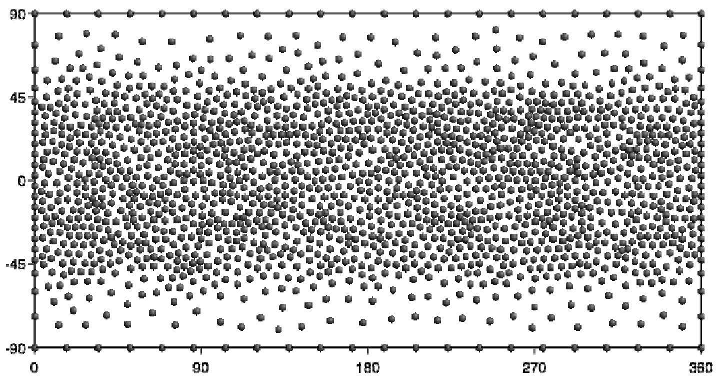


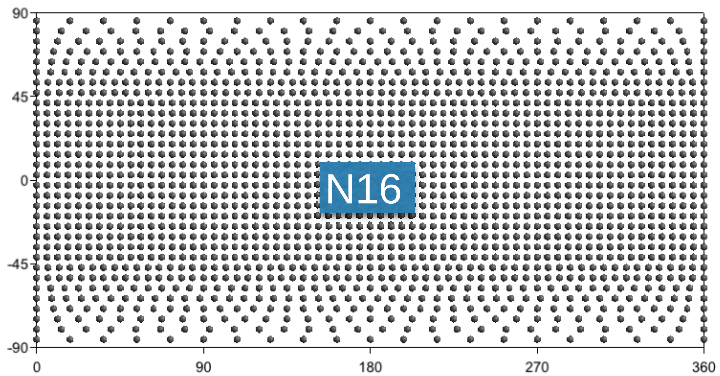
Atlas classifies grids

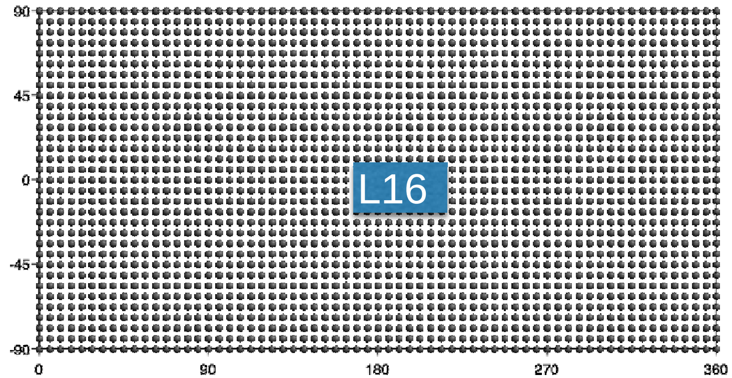
ESCAPE collaboration (RMI)



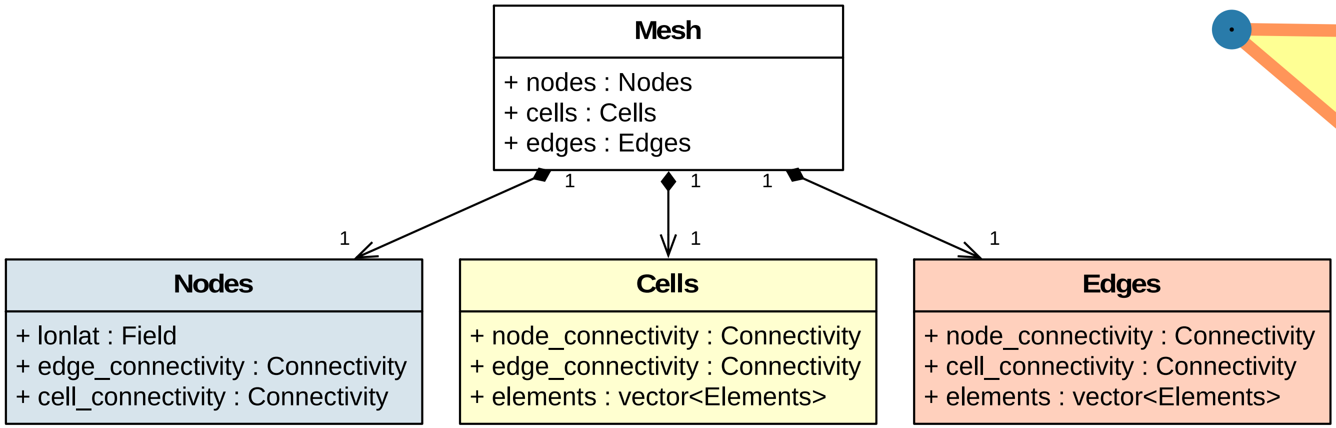




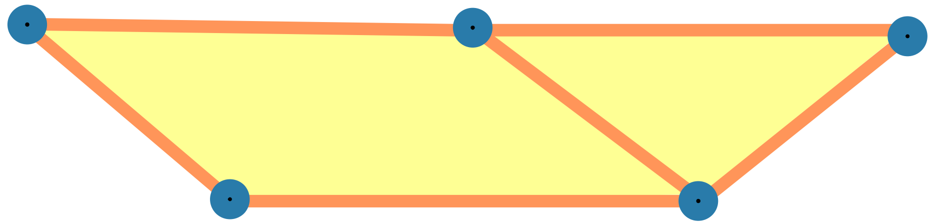




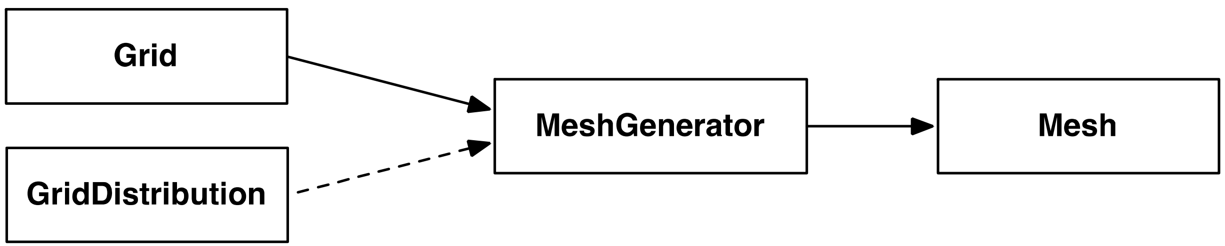
Atlas and unstructured meshes

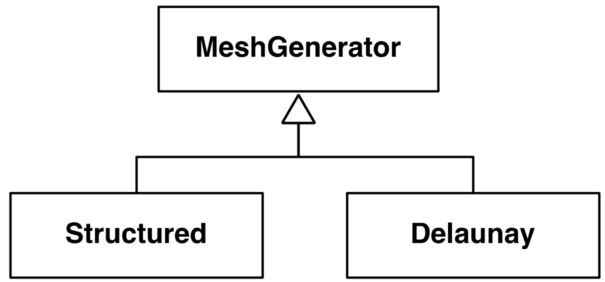


unstructured hybrid mesh of 2 elements

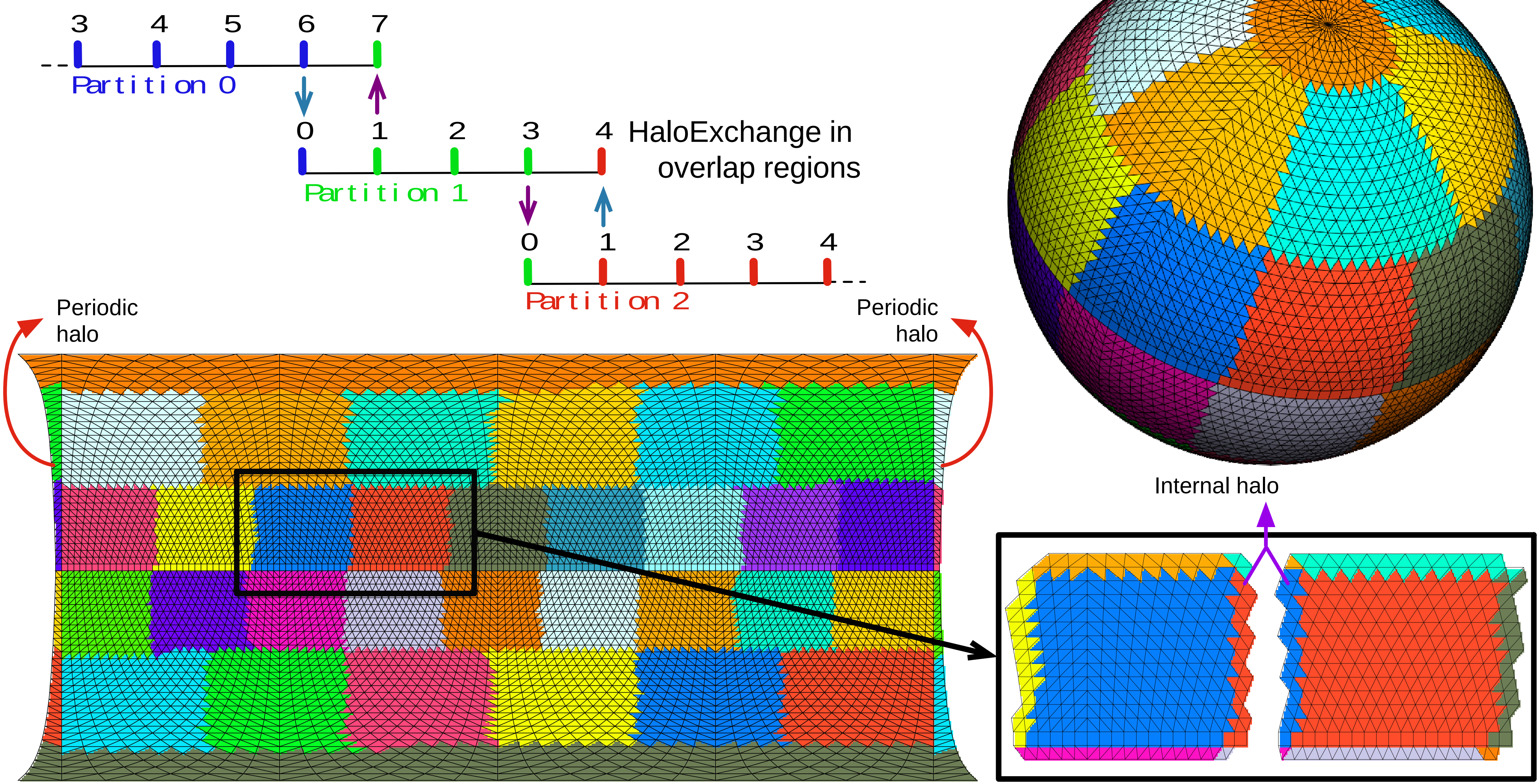


Mesh generation



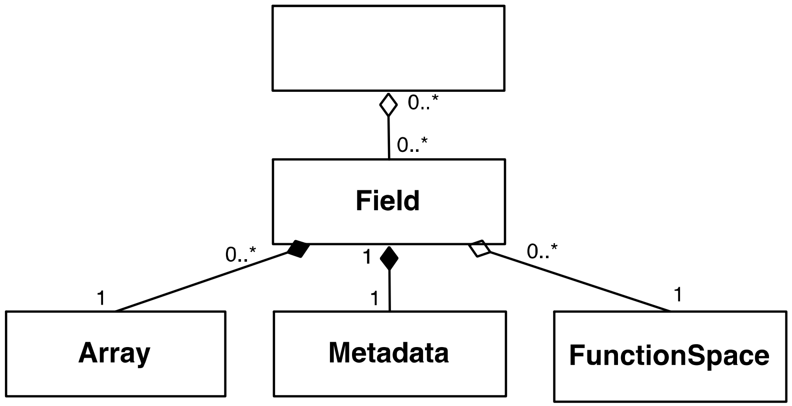


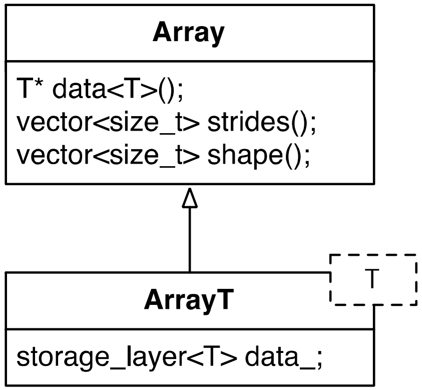
Atlas parallelisation



Field, FieldSet, Array, Metadata

- Array contains the actual memory
- Field contains Array and Metadata
- Fields can be grouped in FieldSets.



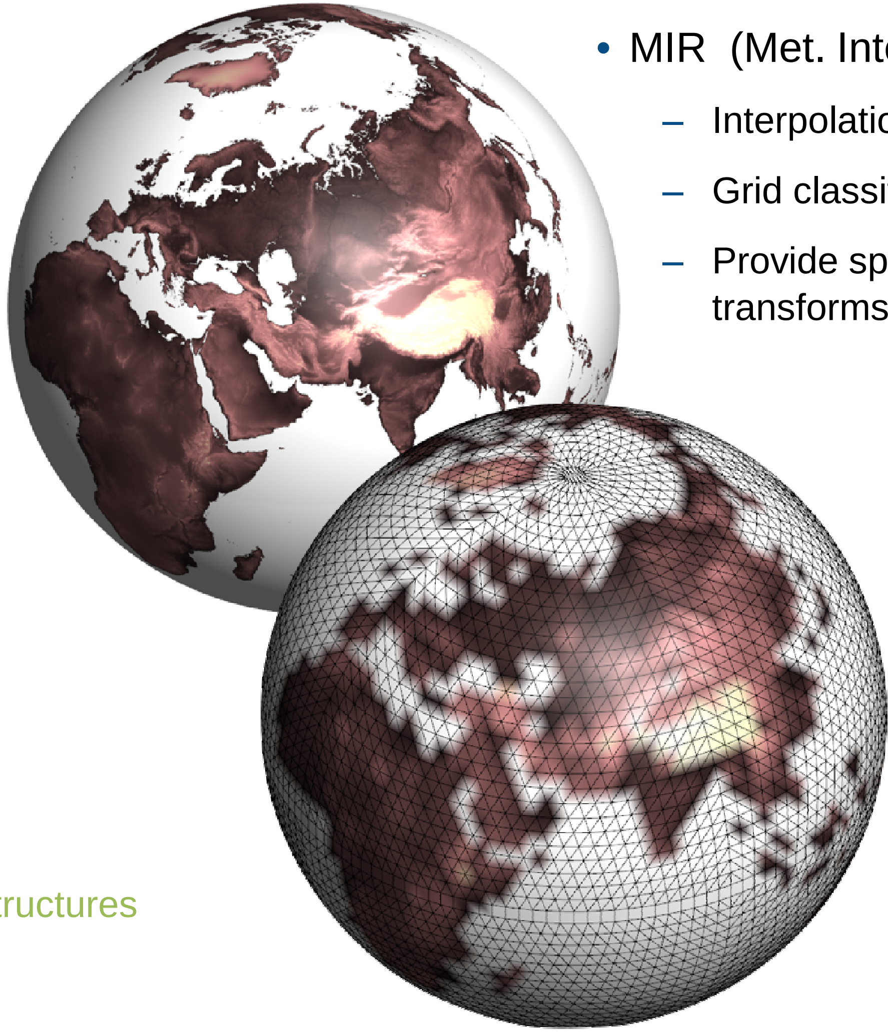


Atlas not the solution, but enabling

- ESCAPE dwarfs
  - Object Oriented data structures
  - LAM grids
  - GPU aware memory storage

- IFS
  - Grid-point derivatives
  - Parallel interpolations
  - Object Oriented data structures

- FVM
  - Object Oriented data structures
  - Parallelisation



- MIR (Met. Interpol. & Regrid.
  - Interpolation
  - Grid classifications
  - Provide spectral transforms

  - MARS
  - MetView
  - PRODGEN

Outline

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- PantaRhei - FVM

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Volume 314, 1 June 2016, Pages 287–304

A finite-volume module for simulating global all-scale atmospheric flows

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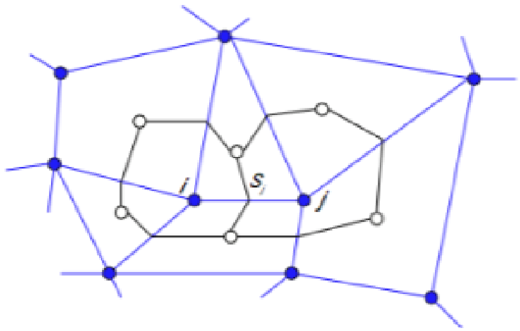
FVM : Finite Volume Module

Horizontally Unstructured Median-Dual Edge-based Finite Volume scheme

Szmelter and Smolarkiewicz (2010, JCP)

MPDATA (cf. EULAG)

- Non-oscillatory forward-in-time scheme, capable of accomodating a wide range of scales and conservation problems
- Unstructured meshes allow irregular spatial resolution and enhancement of polar regions.

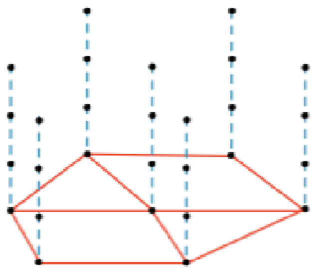


$$\int_{\Omega} \nabla \cdot \mathbf{A} = \int_{\partial\Omega} \mathbf{A} \cdot \mathbf{n} = \frac{1}{\mathcal{V}_i} \sum_{j=1}^{l(i)} A_j^{\perp} S_j$$

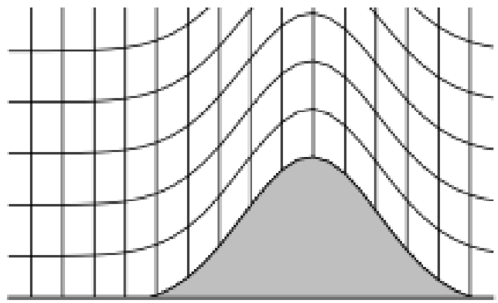
- Generalised curvilinear coords
- Compressible Euler eqns.
- 2-time-level semi-implicit integration scheme with 3d implicit acoustic, buoyant and rotational modes

Vertically structured Finite Volume

- Finite-Difference / structured Finite-Volume operators
- Structured treatment of vertical direction discounts cost of horizontal indirect addressing
- Empowers direct preconditioning of complex elliptic boundary value problems

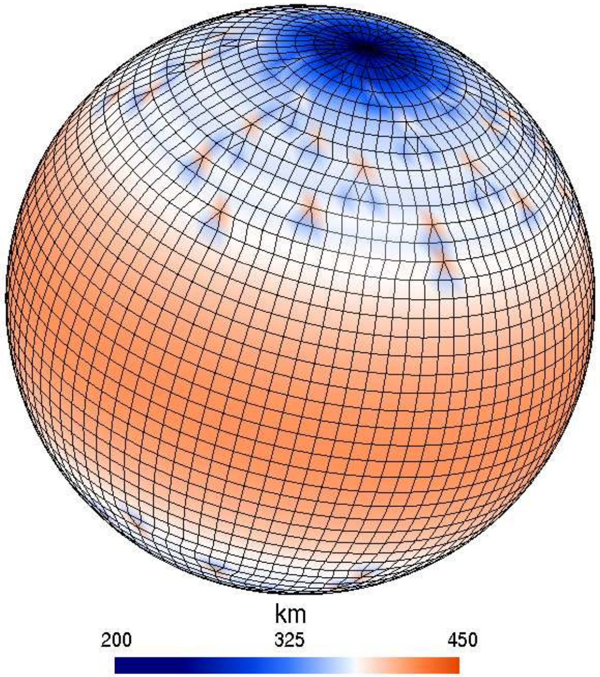


- Terrain following height based

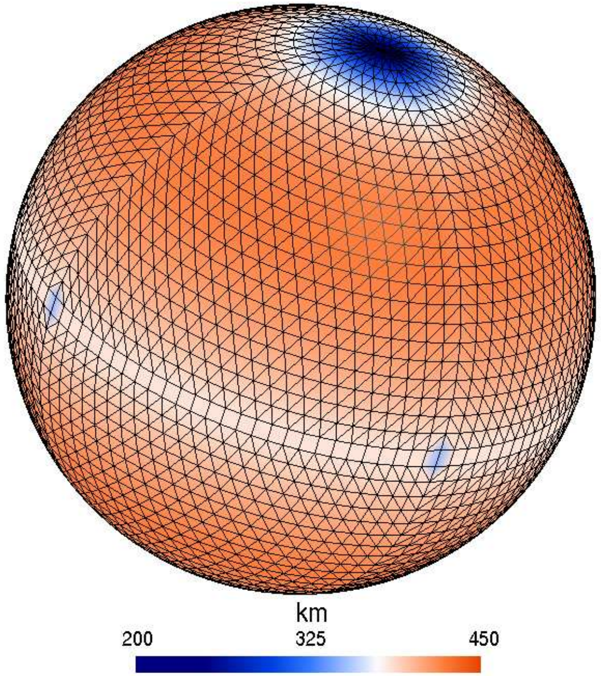


Unstructured mesh but … based on IFS reduced Gaussian grids

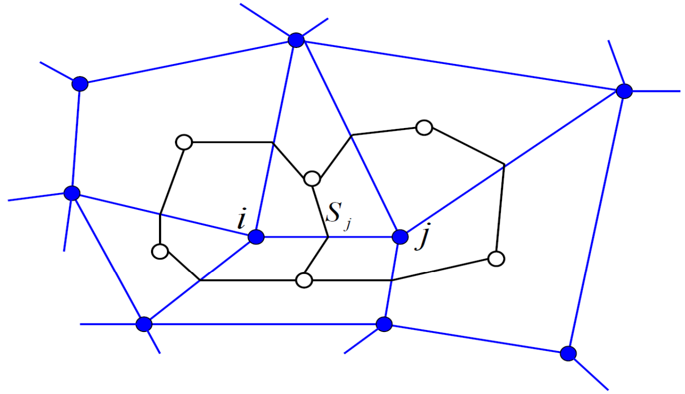
- Compatibility with IFS, (direct exchange of collocated quantities)
- Spectral transforms easy for analysis
- Visualisation / Post-processing tools



Mesh of N24 grid



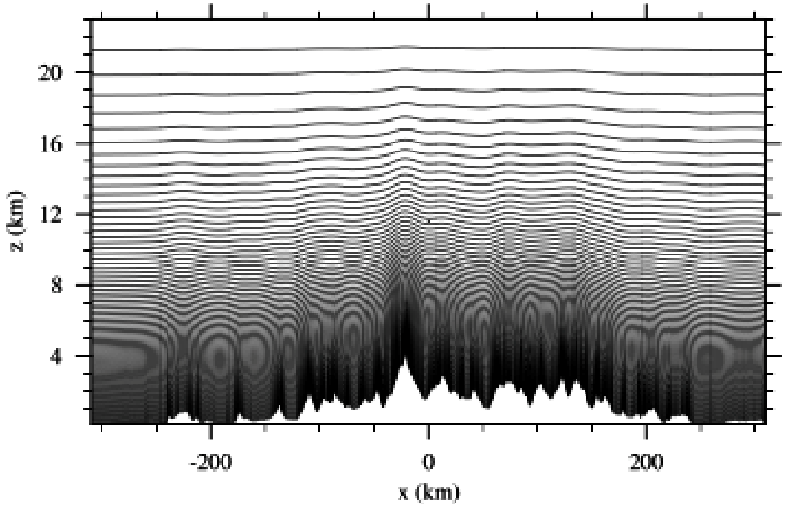
Mesh of O24 grid



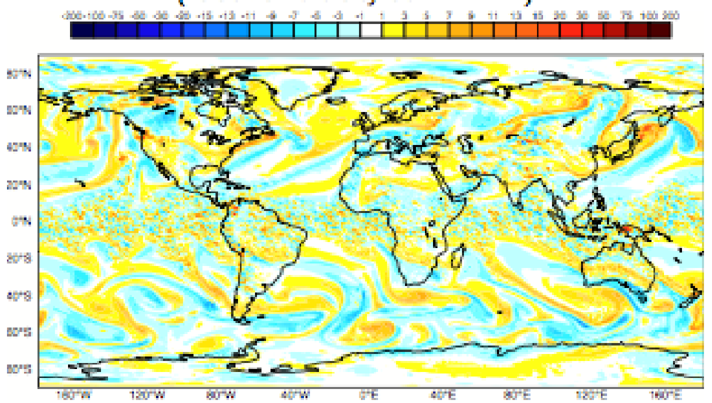
Octahedral grid (right) improves quality for idealised case studies

Key features and results: steep orography

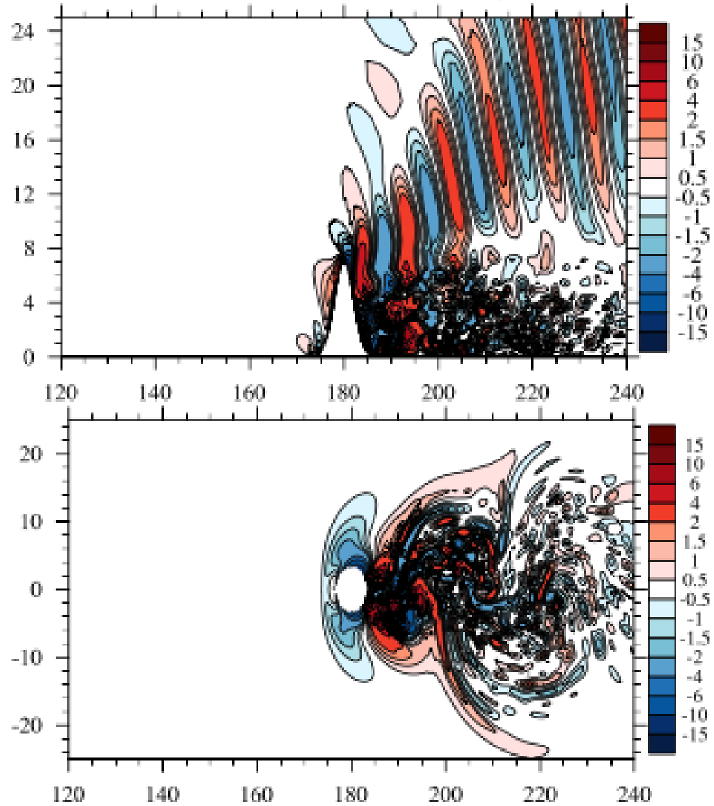
Generalised terrain-following vertical coordinate



Held-Suarez benchmark N640 (16 km) with realistic IFS orography at day 90
(relative vorticity at z=2 km)



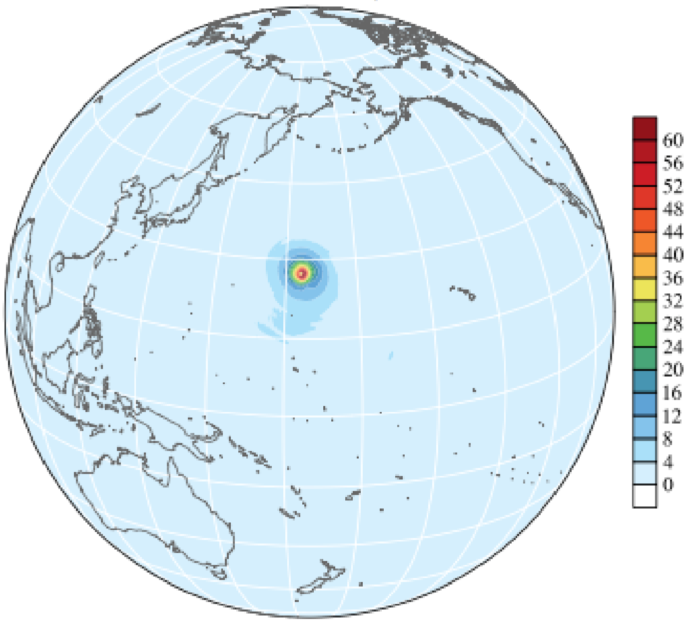
stratified flow past steep orography with maximum slope $\sim 70^{\circ}$ on small planet
(vertical velocity in m/s, lon-height section at lat=0, lon-lat section at z=2 km)

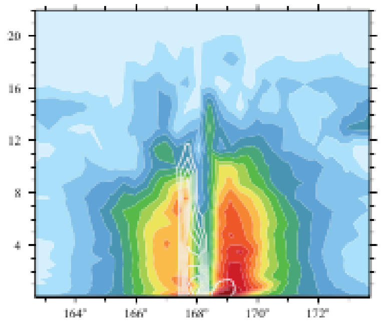


$\Rightarrow$ robust and efficient handling of steep orography

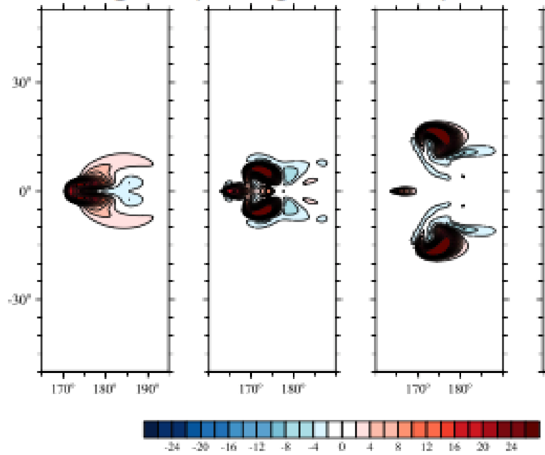
Key features and results: Dynamical Core Model Intercomparison Project 2016

Tropical cyclone with FVM at day 10 ($\Delta_h = 0.25^\circ$):

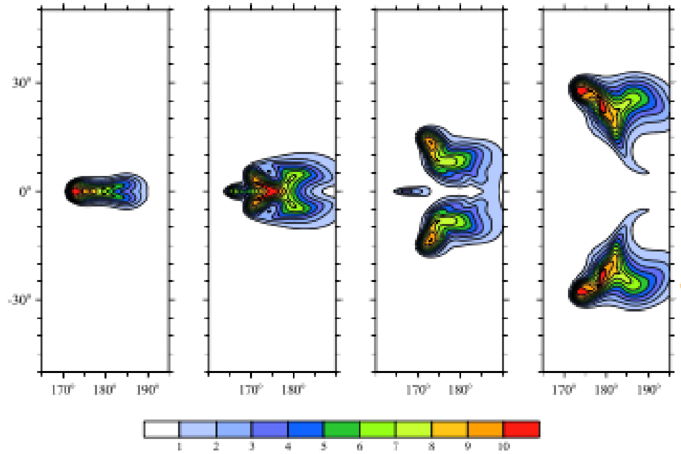




Supercell evolution (0.5, 1, 1.5, 2h) with FVM at 500 m grid spacing on small planet:



Vertical velocity (m/s) at 5 km

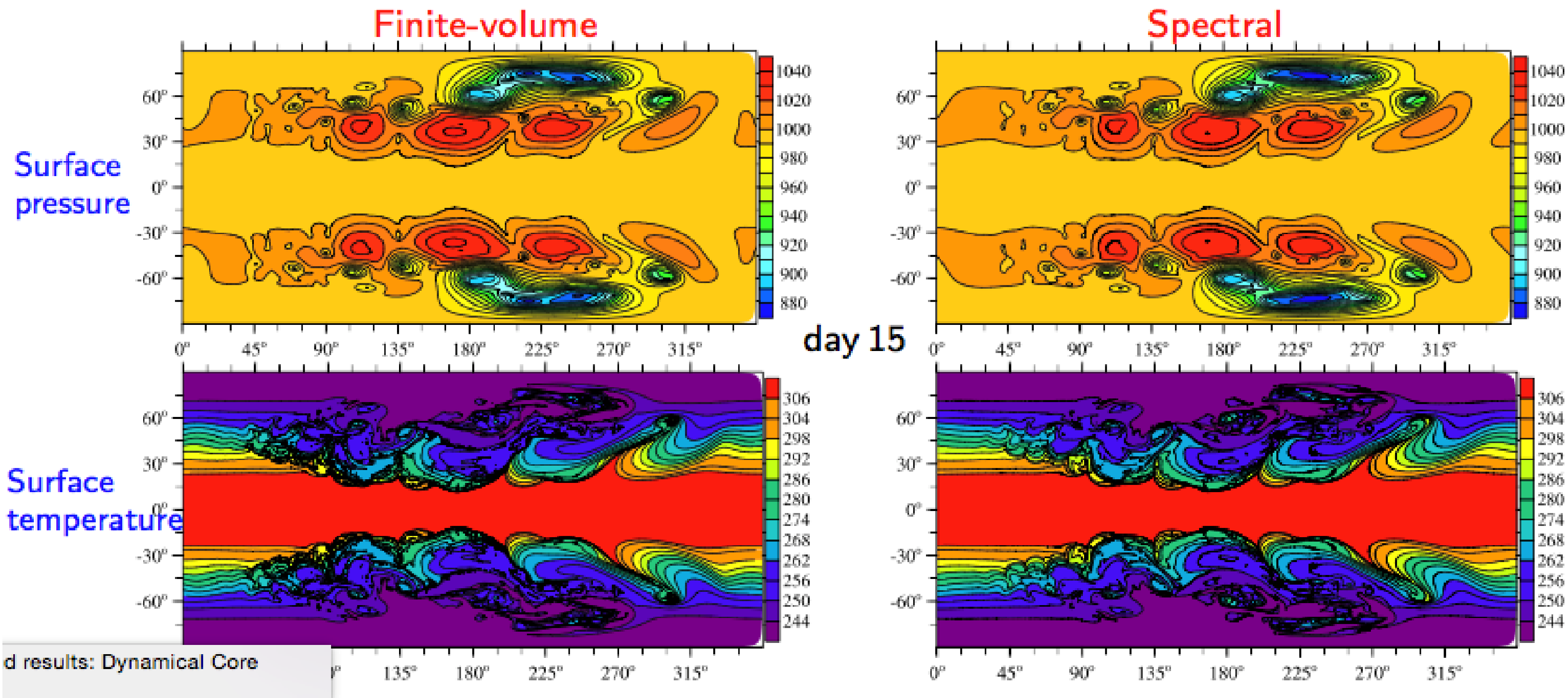


Rainwater (g/kg) at 5 km

→ FVM with simplified cloud microphysics and PBL parametrisations

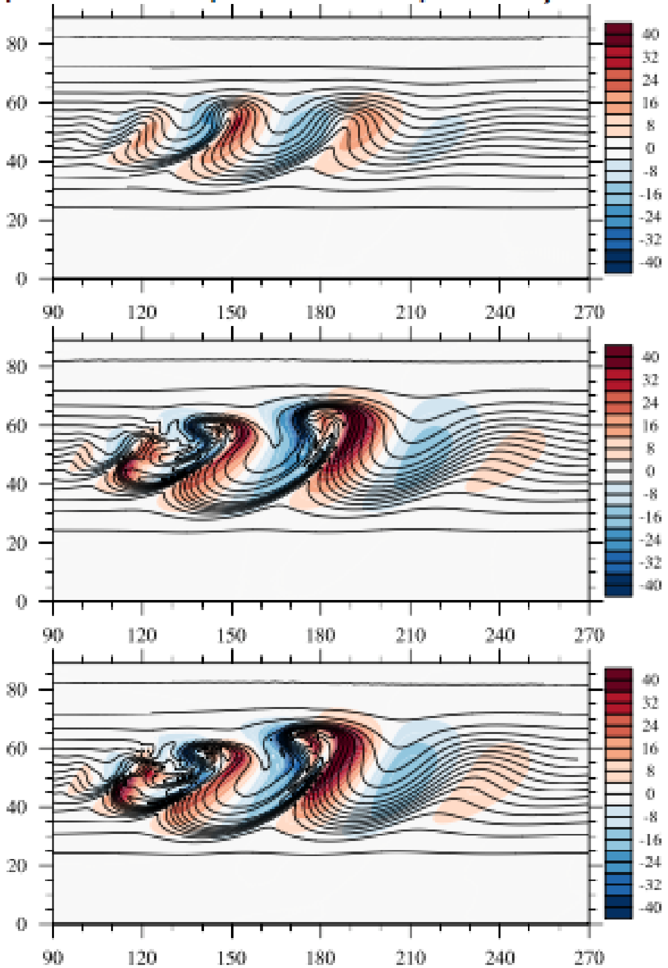
Key features and results: Comparison FVM with spectral IFS (matching gridpoints)

Dry baroclinic instability, FVM (O640) versus the spectral IFS (T_{co}639):



Options for 3D governing equations in FVM

Baroclinic instability (Jablonowski and Williamson, 2006) with FVM (from top: anelastic, pseudo-incompressible, compressible)



→ Generic nonhydrostatic formulation with consistent options:

- ⋆ fully compressible Euler equations (default)
- ⋆ pseudo-incompressible (Durran, JAS 1989)
- ⋆ anelastic (Lipps and Hemler, JAS 1982)

$$\frac{\partial \mathcal{G}\varrho}{\partial t} + \nabla \cdot (\mathbf{v}\mathcal{G}\varrho) = 0$$

$$\frac{\partial \mathcal{G}\varrho\mathbf{u}}{\partial t} + \nabla\cdot(\mathbf{v}\mathcal{G}\varrho\mathbf{u}) = -\mathcal{G}\varrho\left(\Theta\tilde{\mathbf{G}}\nabla\varphi' + \mathbf{g}\Upsilon_B\frac{\theta'}{\theta_b} + \mathbf{f}\times(\mathbf{u} - \Upsilon_C\mathbf{u}_a) + \mathbf{M}\right)$$

$$\frac{\partial \mathcal{G}\varrho\theta'}{\partial t} + \nabla \cdot \left(\mathbf{v}\mathcal{G}\varrho\theta'\right) = -\mathcal{G}\varrho\left(\tilde{\mathbf{G}}^T\mathbf{u}\cdot\nabla\theta_a\right)$$

with optional coefficients:

$$\varrho := \left[\rho(\mathbf{x},t),\ \rho_b\frac{\theta_b(z)}{\theta_0},\ \rho_b(z)\right], \quad \varphi' := \left[c_p\theta_0\pi',\ c_p\theta_0\pi',\ c_p\theta_b\pi'\right]$$

$$\Theta := \left[\frac{\theta}{\theta_0}, \frac{\theta}{\theta_0}, 1\right], \ \Upsilon_B := \left[\frac{\theta_b(z)}{\theta_a(\mathbf{x})}, \frac{\theta_b(z)}{\theta_a(\mathbf{x})}, 1\right], \ \Upsilon_C := \left[\frac{\theta}{\theta_a(\mathbf{x})}, \frac{\theta}{\theta_a(\mathbf{x})}, 1\right]$$

Final remarks

- High level of optimization in ECMWF's IFS spectral transforms

... the global spectral transform method is not dead, but need to prepare to

- *Increase* the flexibility in discretization choices (and/or hybrid solution procedures)
- *Develop* alternative algorithms and methods that reduce data movement, as well as communication and synchronization
- *Add* numerical and structural (code) flexibility in the effor towards full Earth-System complexity

ESCAPE

- FVM with compressible NH equations. agreement with spectral IFS

Thank you for your attention

Progress in Numerical Methods at ECMWF

EWGLAM / SRNWP October 2016

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