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Running operational Canadian NWP models and assimilation systems on next-generation supercomputers

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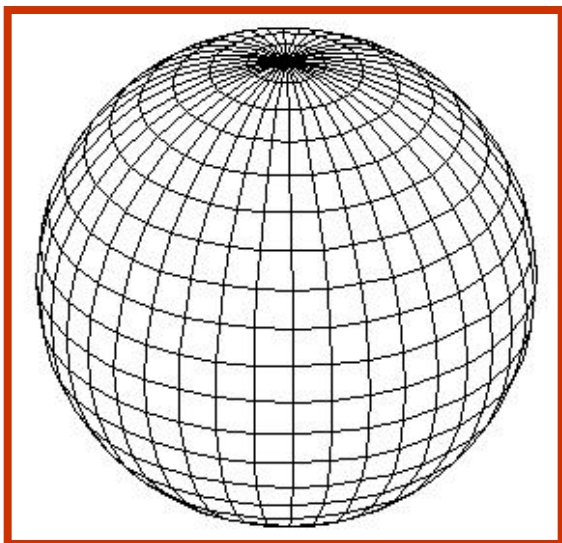
Meteorological Research Division

Scalability Workshop
ECMWF, Reading, UK
April 14-15, 2014



The GEM model

1. Grid point lat/lon model
2. Finite differences on an Arakawa-C grid
3. Semi-Lagrangian (poles are an issue)
4. Implicit time discretization
 1. Direct solver (Nk 2D horizontal elliptic problems)
 2. Full 3D iterative solver based on FGMRES
5. Global uniform, Yin-Yang and LAM configurations
6. Hybrid MPI/OpenMP
 1. Halo exchanges
 2. Array transposes for elliptic problems
7. PE block partitioning for I/O

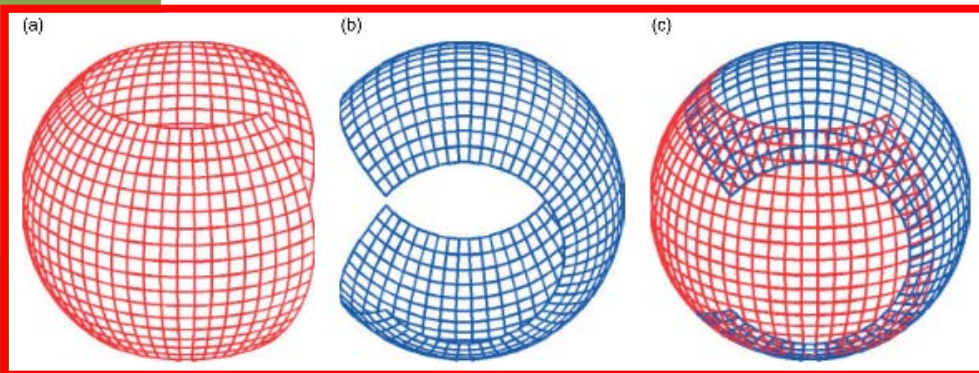
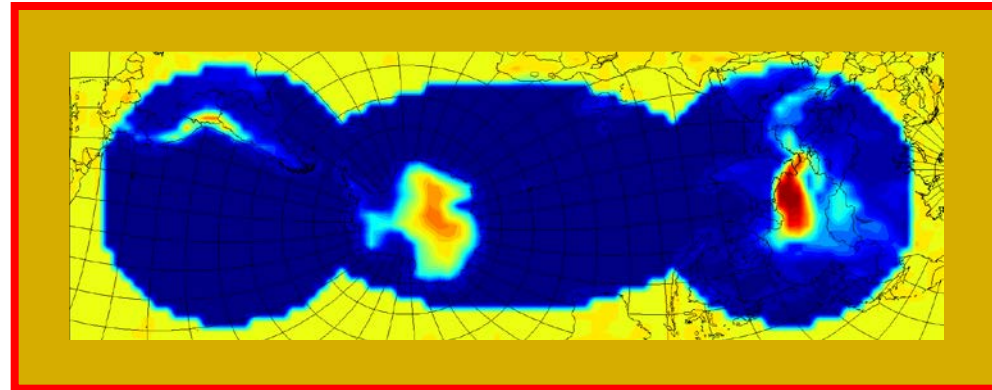
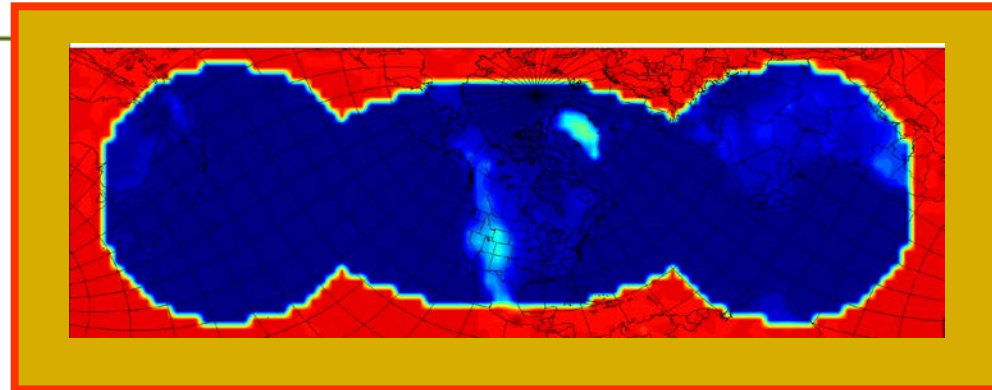


Global uniform grid:

- 1) a challenge for DM implementation
- 2) many more elliptic problems to solve due to implicit horizontal diffusion (transposes)
- 3) semi-Lagrangian near the poles
- 4) current DM implementation will not scale

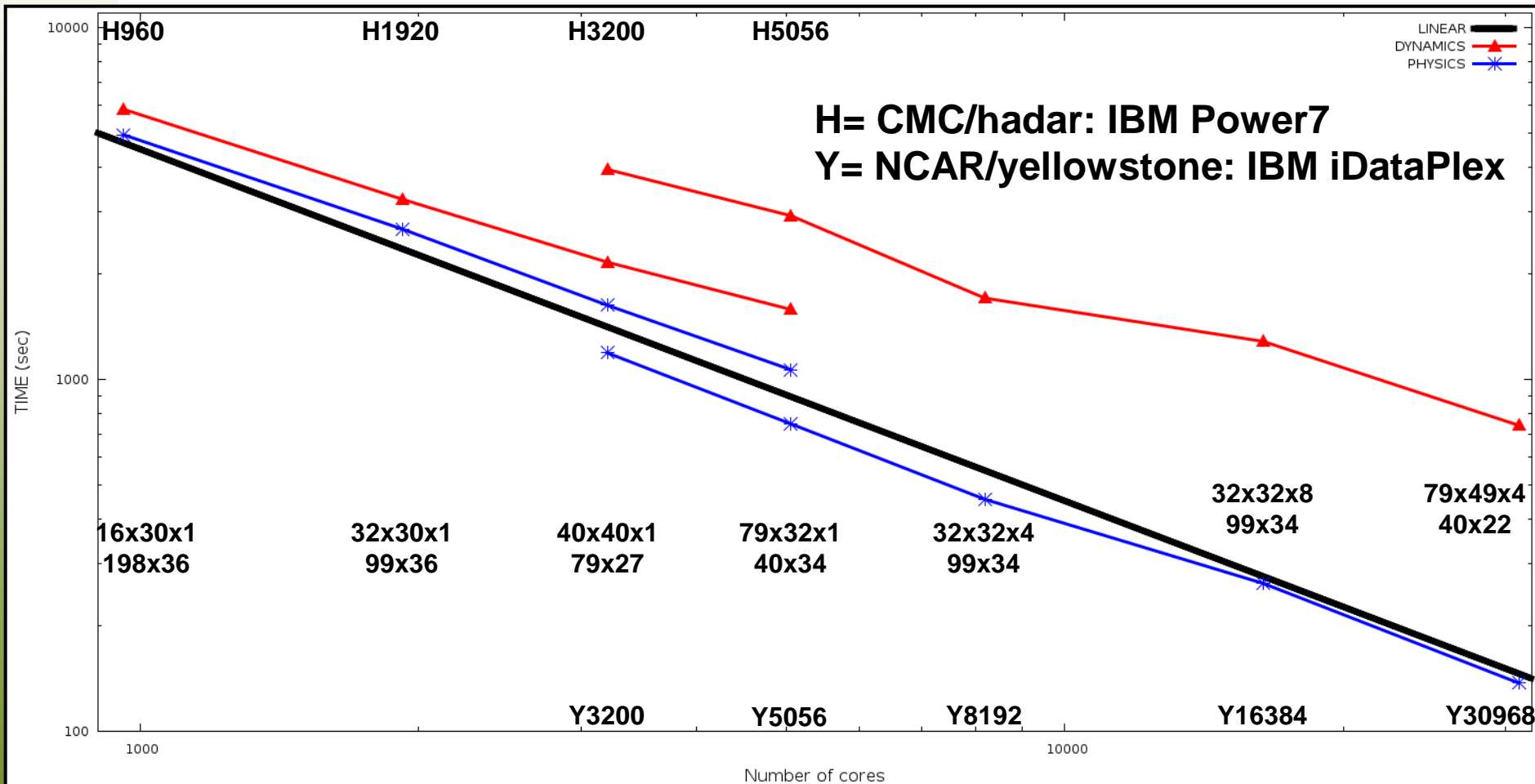
Yin-Yang grid configuration

- Implemented as 2 LAMs communicating at boundaries
- Optimized Schwarz iterative method for solving the elliptic problem.
- Scales a whole lot better
- Operational implementation due in spring 2015
- Communications are an issue
- Exchanging a Global Uniform scalability problem (poles) by another scalability problem



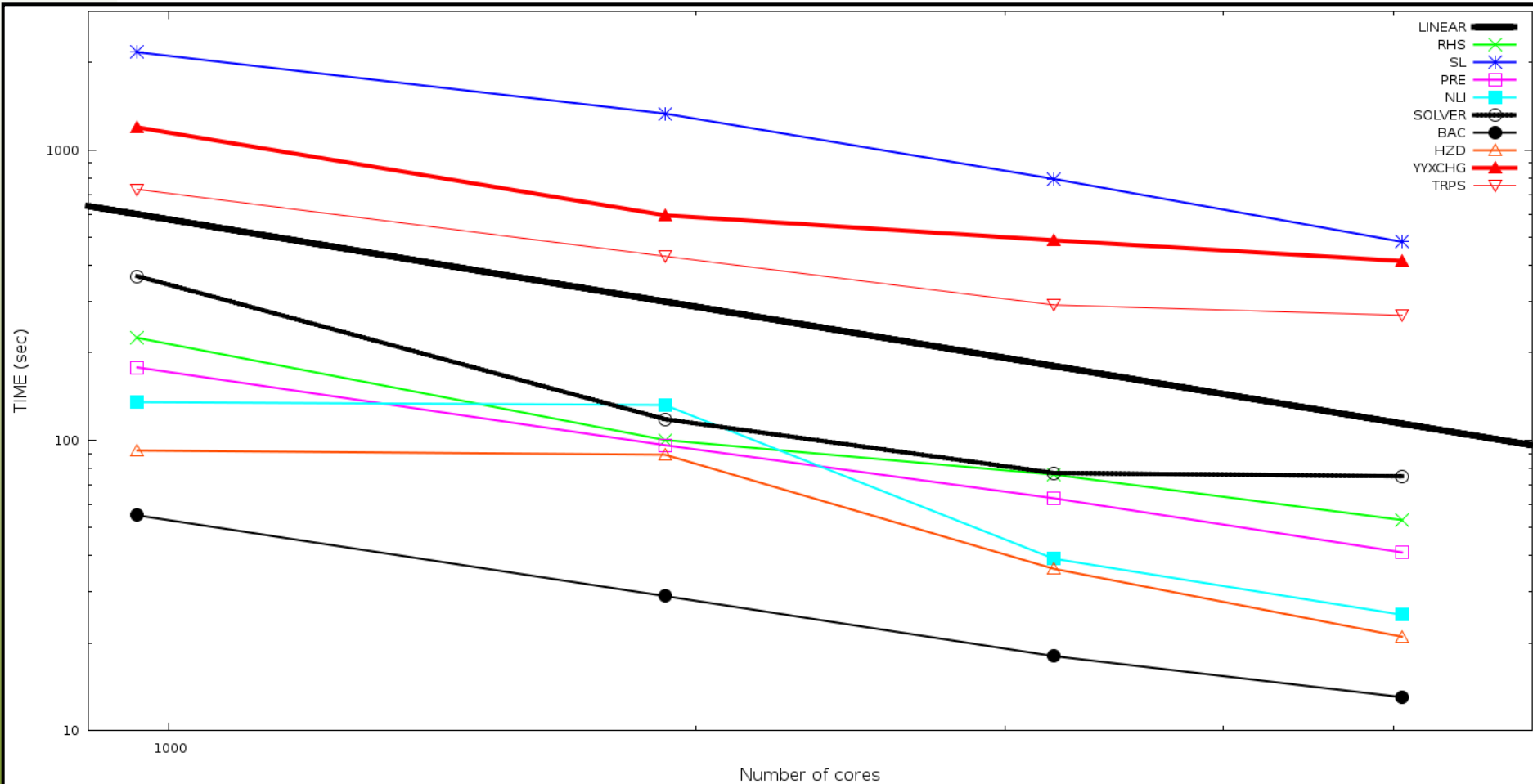
Yin-Yang 10 km scalability

Ni=3160, Nj=1078, Nk=158



Yin-Yang 10 km scalability

Dynamics components



The future of GEM

- Yin-Yang 2km on order 100K cores is already feasible on P7 processors or similar
- Yin-Yang exchanges will need work
- Using GPUs capabilities is on the table
- Improve Omp scalability
- Re-partition MPI sub-domain (bni,bnj,ni,nj,nk)
- Export SL interpolations to reduce halo size
- Processor mapping to reduce the need to communicate through the switch
- Partition NK
- MIMD approach for I/O





Investigating scalability and accuracy on an icosahedral geodesic grid

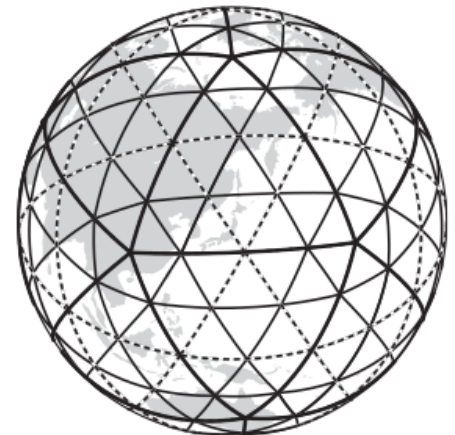
Spatial discretization: finite volume method on
icosahedral geodesic grid

Time discretization: exponential integration methods which
resolve high frequencies to the required level of
tolerance without severe time step restriction

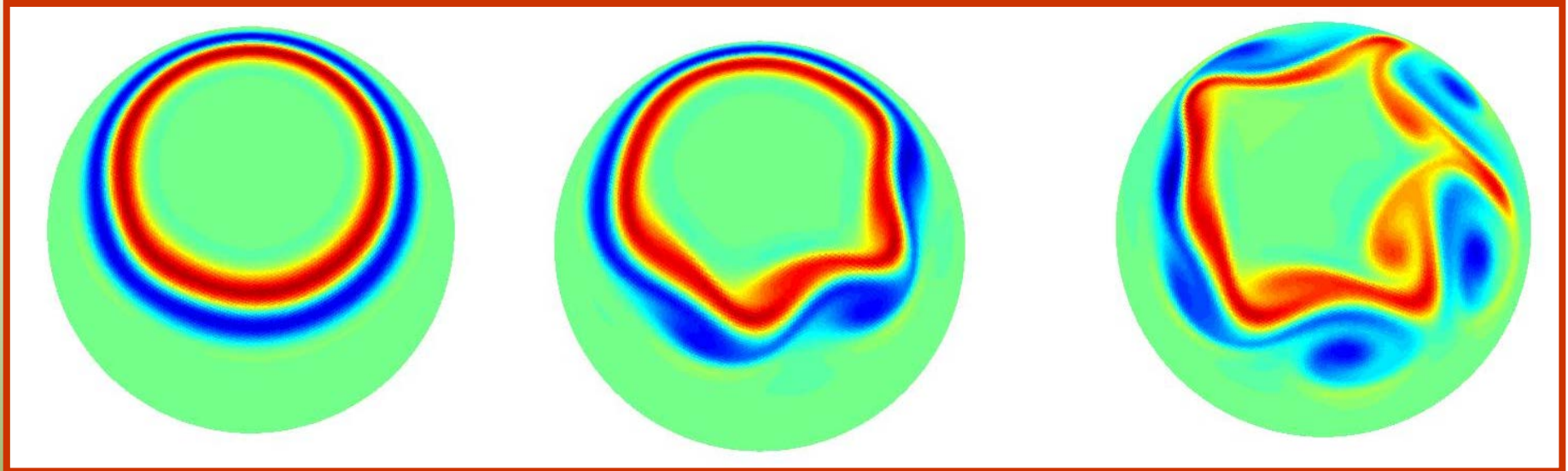
Shallow water implementation already shows
great scalability

Vertical coordinates:
Generalized quasi-Lagrangian with
conservative monotonic remapping

SPHERICAL GEODESIC
OR ICOSAHEDRAL GRID



Unstable jet, icosahedral grid number 6, $dx = 112$ km, $dt = 7200$ sec (typically 30 sec)



Pudykiewicz (2006), J. Comp. Phys., 213, pp 358-390

Pudykiewicz J. (2011), J. Comp. Phys., 230, pp 1956--1991

Qaddouri A., J. et al. (2012), Q. J. Roy. Met. Soc., 138, pp 989--1003

Clancy C., Pudykiewicz J. (2013), Tellus A, vol. 65



Ensemble-Variational Assimilation: EnVar

- EnVar will replace 4D-Var at Environment Canada in 2014 for both global and regional deterministic prediction systems
- EnVar uses a **variational assimilation approach** in combination with the already available **4D ensemble covariances** from the EnKF
- By using 4D ensembles, EnVar performs a 4D analysis without need of tangent-linear/adjoint of forecast model
- Consequently, it is **more computationally efficient** and **easier to maintain/adapt** than 4D-Var:
 - EnVar: ~10 min, 320 cores, 50km grid spacing
 - 4D-Var: ~1hr, 640 cores, 100km grid spacing
- Future improvements to EnKF will benefit both ensemble and deterministic forecasts → **incentive to increase overall effort on EnKF development**
- EnKF scalability examined by Houtekamer et al. (2014, MWR)

EnVar formulation

- In 4D-Var the 3D analysis increment is evolved in time using the TL/AD forecast model (here included in \mathbf{H}_{4D}):

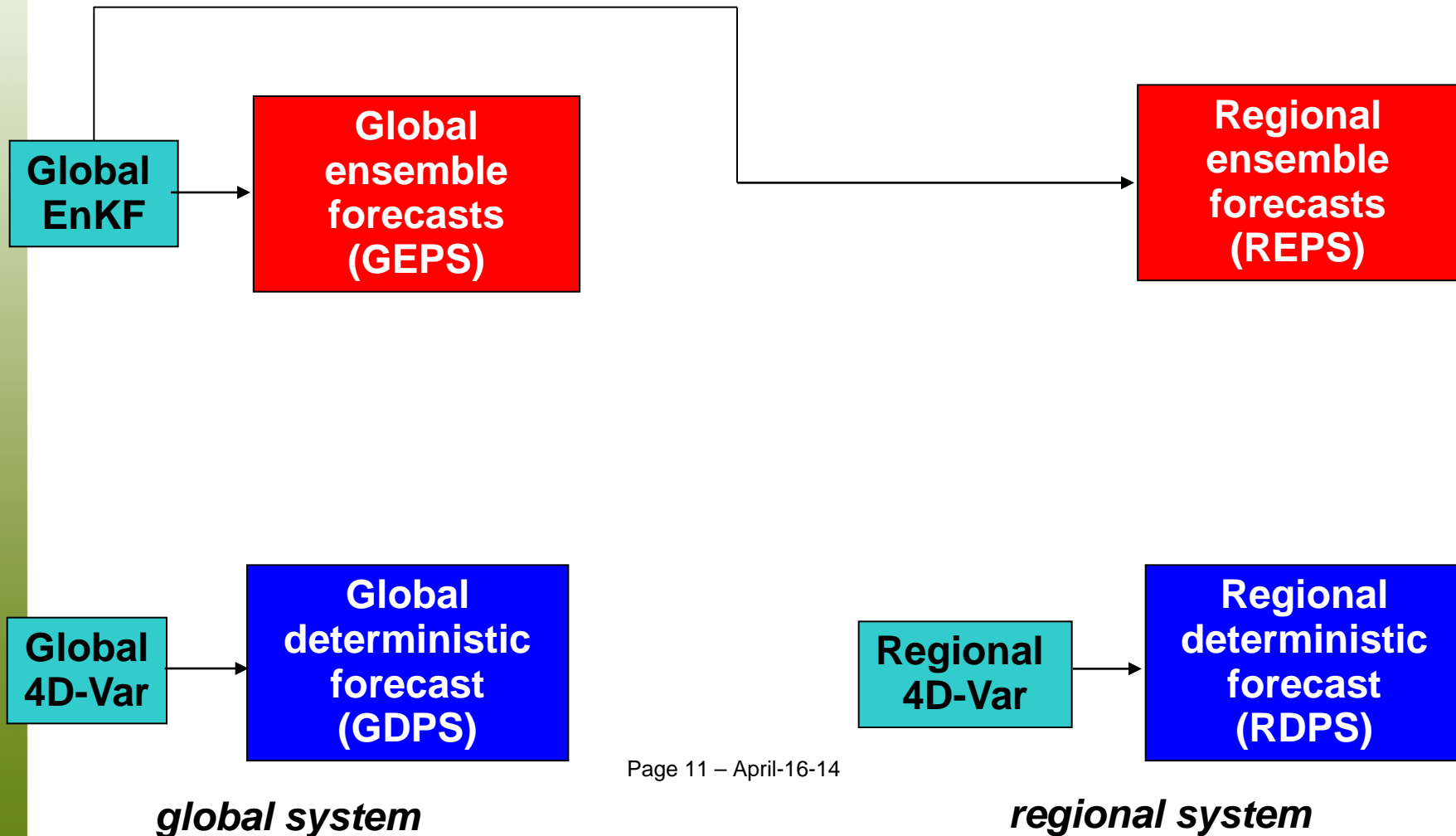
$$J(\Delta\mathbf{x}) = \frac{1}{2} (H_{4D}[\mathbf{x}_b] + \mathbf{H}_{4D}\Delta\mathbf{x} - \mathbf{y})^T \mathbf{R}^{-1} (H_{4D}[\mathbf{x}_b] + \mathbf{H}_{4D}\Delta\mathbf{x} - \mathbf{y}) + \frac{1}{2} \Delta\mathbf{x}^T \mathbf{B}^{-1} \Delta\mathbf{x}$$

- In EnVar the background-error covariances and increment are explicitly 4-dimensional, resulting in cost function:

$$J(\Delta\mathbf{x}_{4D}) = \frac{1}{2} (H_{4D}[\mathbf{x}_b] + \mathbf{H}\Delta\mathbf{x}_{4D} - \mathbf{y})^T \mathbf{R}^{-1} (H_{4D}[\mathbf{x}_b] + \mathbf{H}\Delta\mathbf{x}_{4D} - \mathbf{y}) + \frac{1}{2} \Delta\mathbf{x}_{4D}^T \mathbf{B}_{4D}^{-1} \Delta\mathbf{x}_{4D}$$

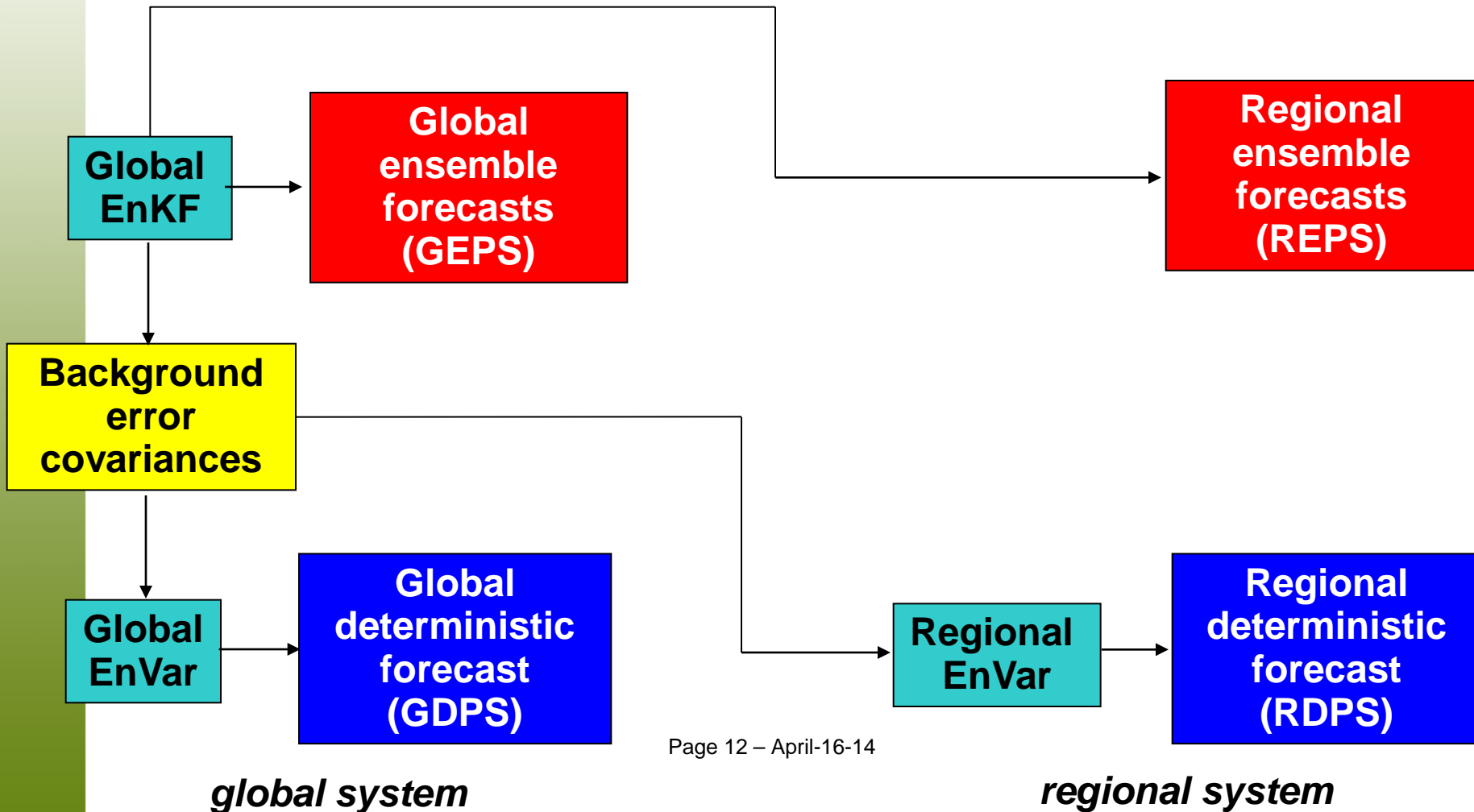
2013-2017: Toward a Reorganization of the NWP Suites at Environment Canada

Current operational systems



2013-2017: Toward a Reorganization of the NWP Suites at Environment Canada

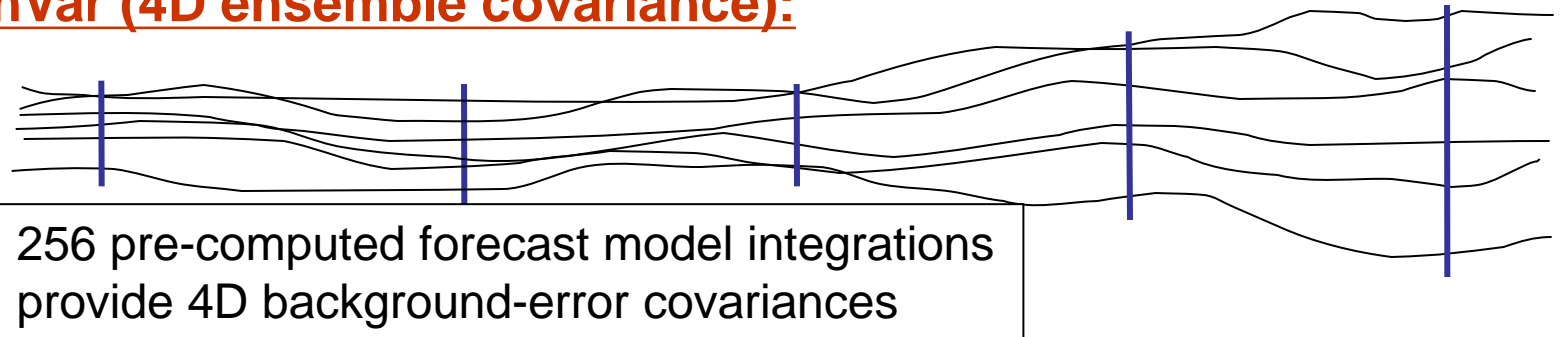
2014 implementation: 4D-Var replaced by EnVar



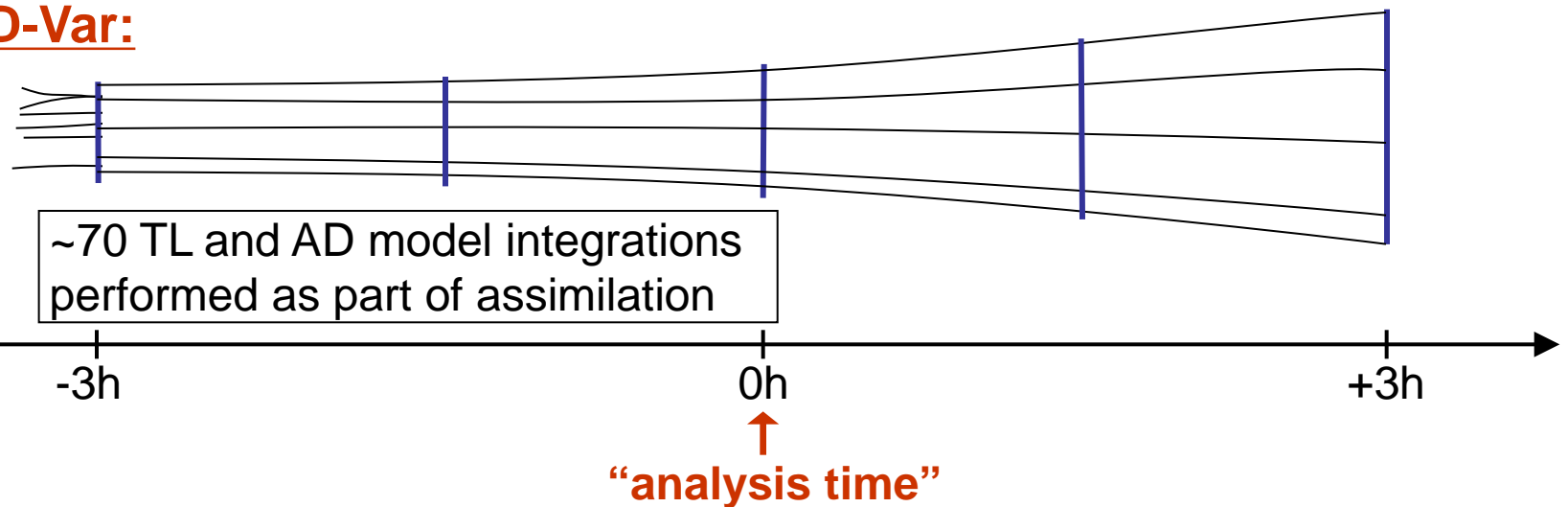
4D error covariances

Temporal covariance evolution

EnVar (4D ensemble covariance):



4D-Var:



Spatial covariance localization in EnVar

(Buehner 2005, Lorenc 2003)

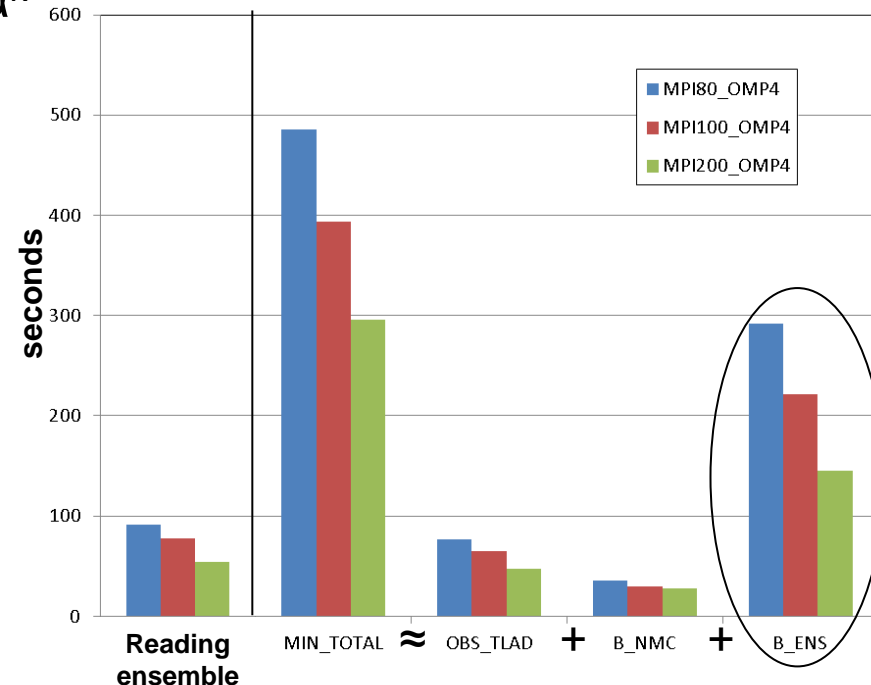
- Complexity of 4D-Var is replaced by relatively simple use of 4D ensemble covariances to compute analysis increment and gradient during each iteration of the cost function minimization
- If the spatial localization function is horizontally homogeneous and isotropic, then spectral approach is efficient (for global lat-lon system):
$$\Delta \mathbf{x}_{4D} = \sum_k \mathbf{e}_{4D}^k \circ (\mathbf{L}^{1/2} \boldsymbol{\xi}^k) = \sum_k \mathbf{e}_{4D}^k \circ (\mathbf{S}^{-1} \mathbf{L}_v^{1/2} \mathcal{L}_h^{1/2} \boldsymbol{\xi}^k)$$

where:

- \mathbf{e}_{4D}^k is the k th 4D ensemble deviation
 - $\boldsymbol{\xi}^k$ is corresponding control vector
 - \mathbf{S}^{-1} is the inverse spectral transform
 - $\mathcal{L}_h = \mathbf{S} \mathbf{L}_h \mathbf{S}^T$ is the diagonal spectral horizontal localization matrix
- Equivalent to using sqrt of localized sample covariance matrix:
$$\mathbf{L} \circ [\sum_k \mathbf{e}^k (\mathbf{e}^k)^T]$$

Scalability of EnVar

- Computation and I/O must be highly parallel, \mathbf{e}_{4D}^k is large:
 - 256 members, 7 times, 4 vars, 800x400x75L \rightarrow ~640GB
- Calculation of analysis increment (and adjoint) currently about 1/2 of overall cost of minimization: $\Delta \mathbf{x}_{4D} = \sum_k \mathbf{e}_{4D}^k \circ (\mathbf{S}^{-1} \mathbf{L}_v^{1/2} \mathcal{L}_h^{1/2} \boldsymbol{\xi}^k)$
- Currently, Schur product is the most expensive (and simplest) step, but scales perfectly: $\Delta \mathbf{x}_{4D} = \sum_k \mathbf{e}_{4D}^k \circ \boldsymbol{\alpha}^k$
- Spectral transform is next most expensive, involves a global transpose: $\boldsymbol{\alpha}^k = \mathbf{S}^{-1} \mathbf{L}_v^{1/2} \mathcal{L}_h^{1/2} \boldsymbol{\xi}^k$
- Currently only 1D decomposition:
 - $\boldsymbol{\xi}^k$: split by ens member (256)
 - $\Delta \mathbf{x}$: split by latitude (400)
- Improved scalability requires 2D decomposition (3D transposition strategy) \rightarrow under development



END



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