Spectral Transform

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Overview

10 minutes	• Fourier transform • Spectral transform
30 minutes	• hands-on exercises
20 minutes	• aliasing • parallelization • performance
rest	• time for questions

IFS (Integrated Forecast System)

technology applied at ECMWF for
the last 40 years

- spectral transform
- semi-Lagrangian
- semi-implicit

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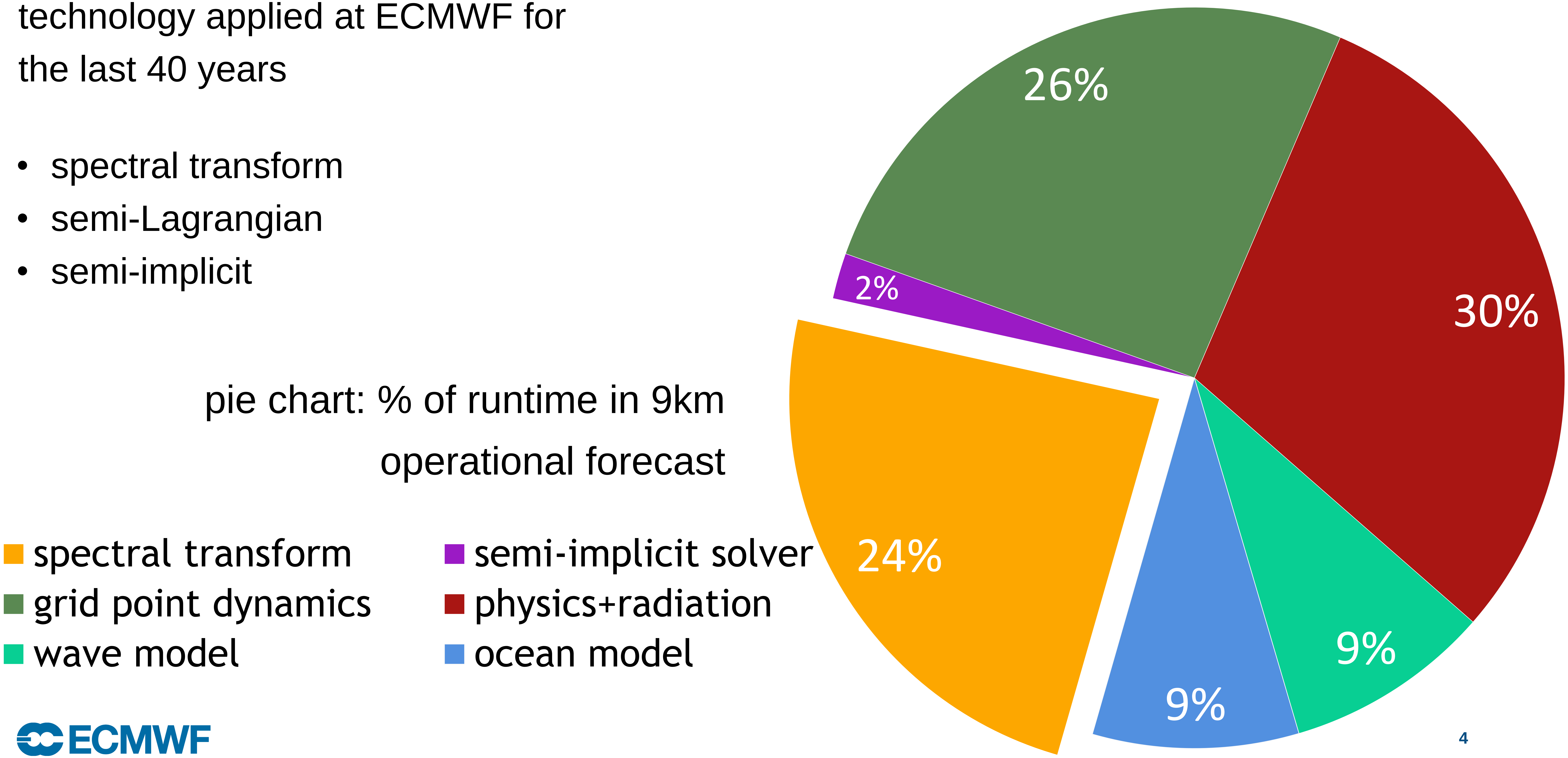
pie chart: % of runtime in 9km operational forecast



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IFS (Integrated Forecast System)

technology applied at ECMWF for the last 40 years

- spectral transform
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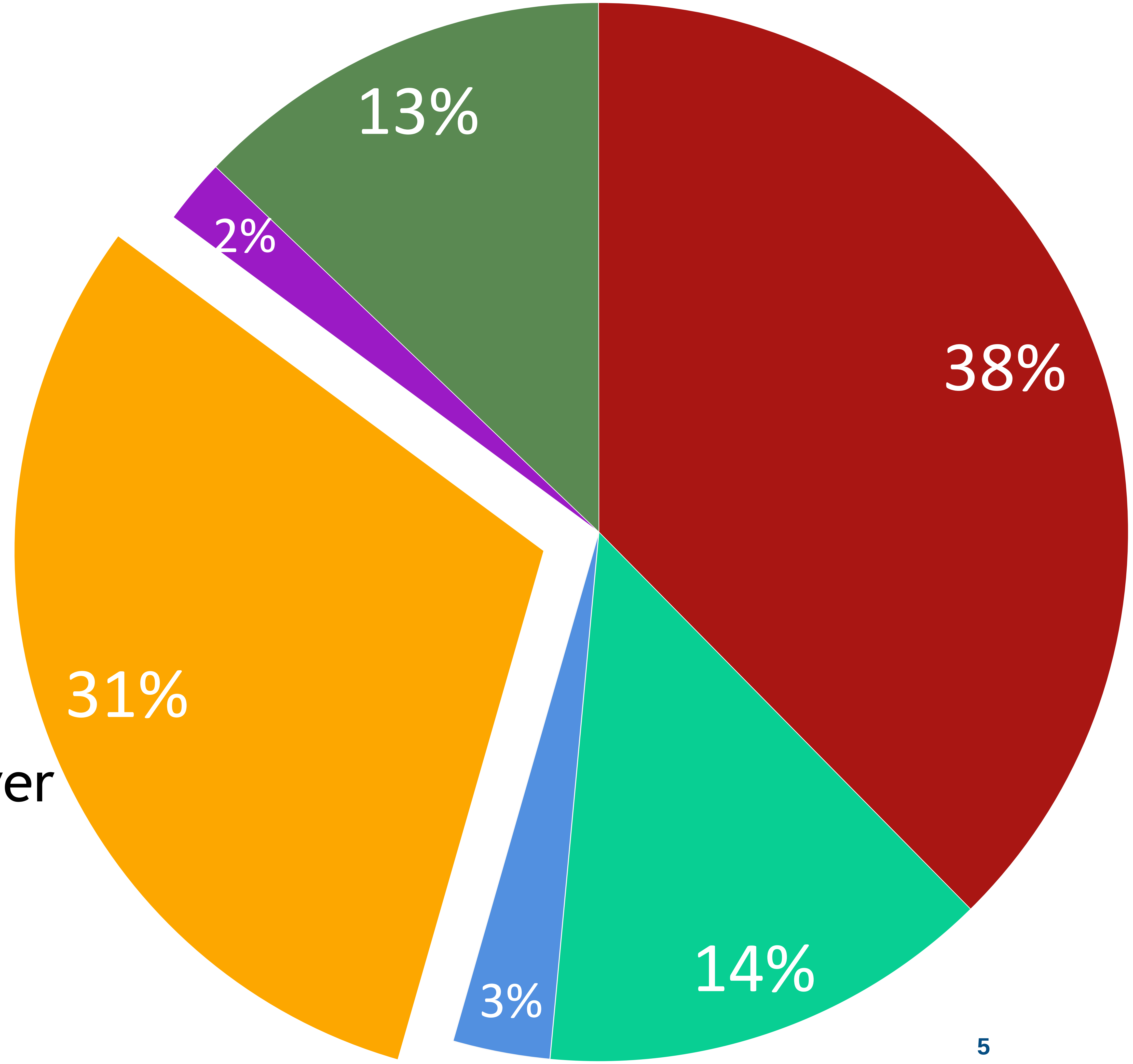
pie chart: % of runtime in 5km forecast (future operational)



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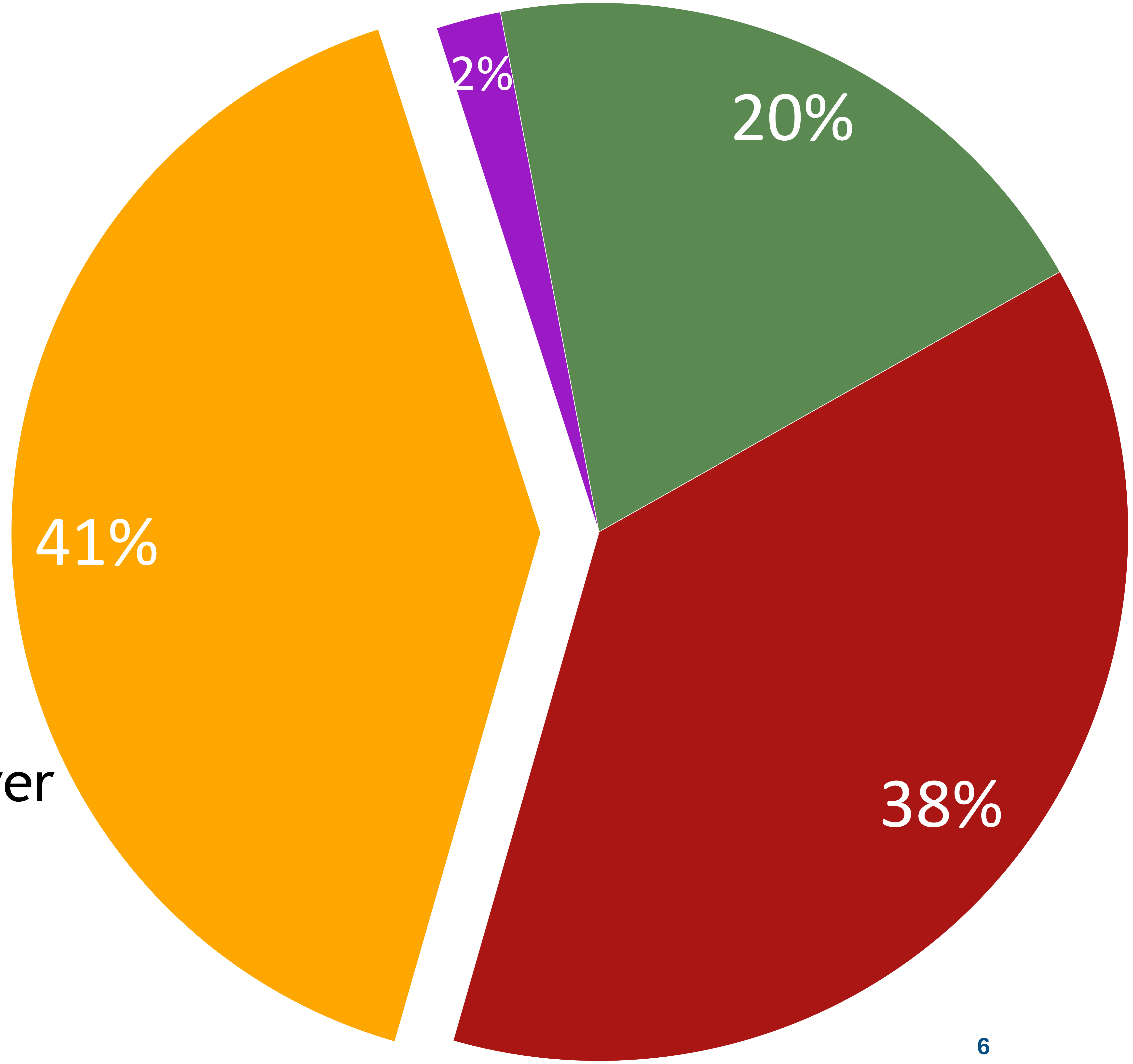
IFS (Integrated Forecast System)

technology applied at ECMWF for the last 40 years

- spectral transform
- semi-Lagrangian
- semi-implicit

pie chart: % of runtime in 1.25km forecast (experiment, no ocean)



- spectral transform
- semi-implicit solver
- grid point dynamics
- physics+radiation
- wave model
- ocean model

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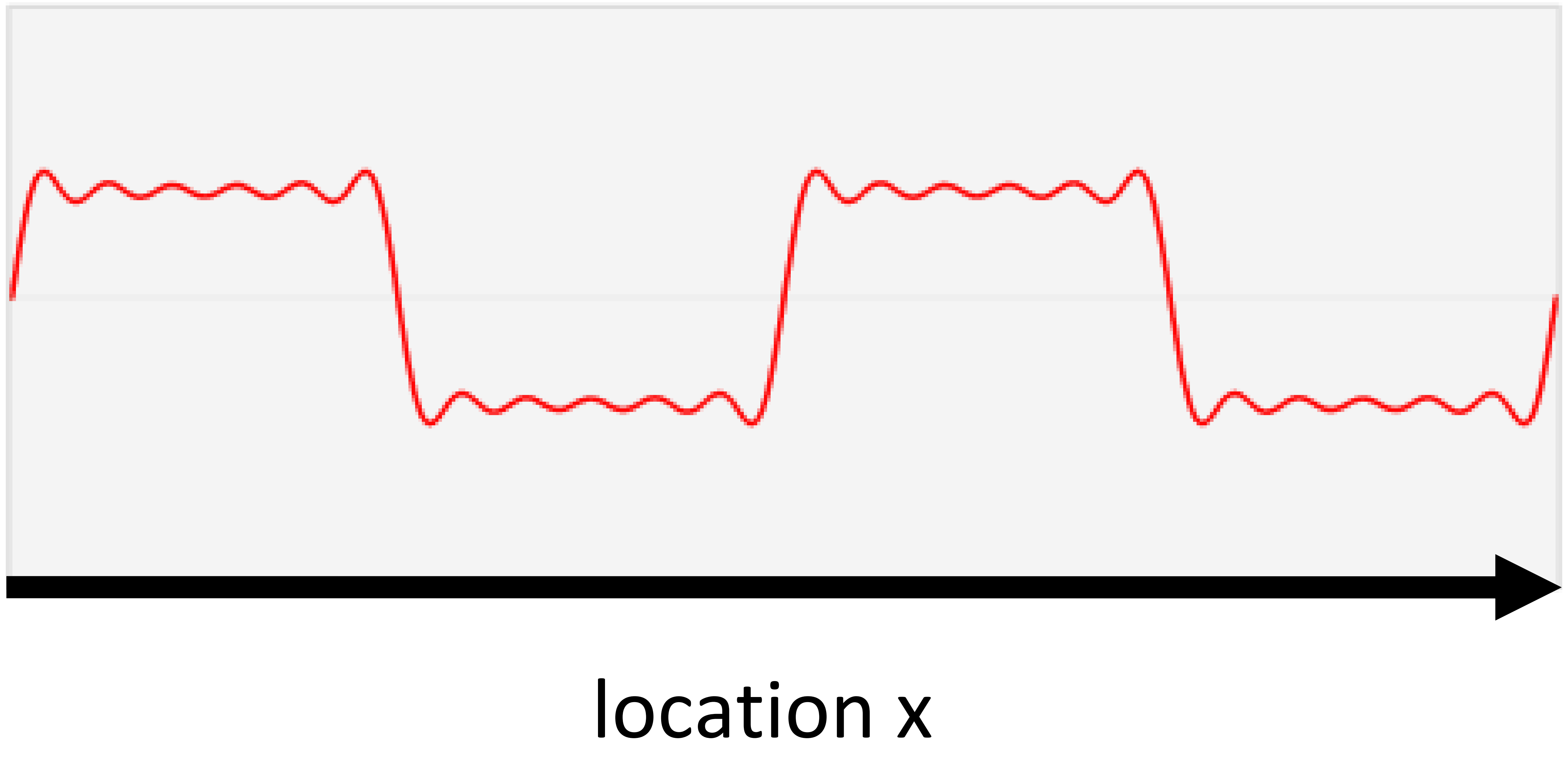
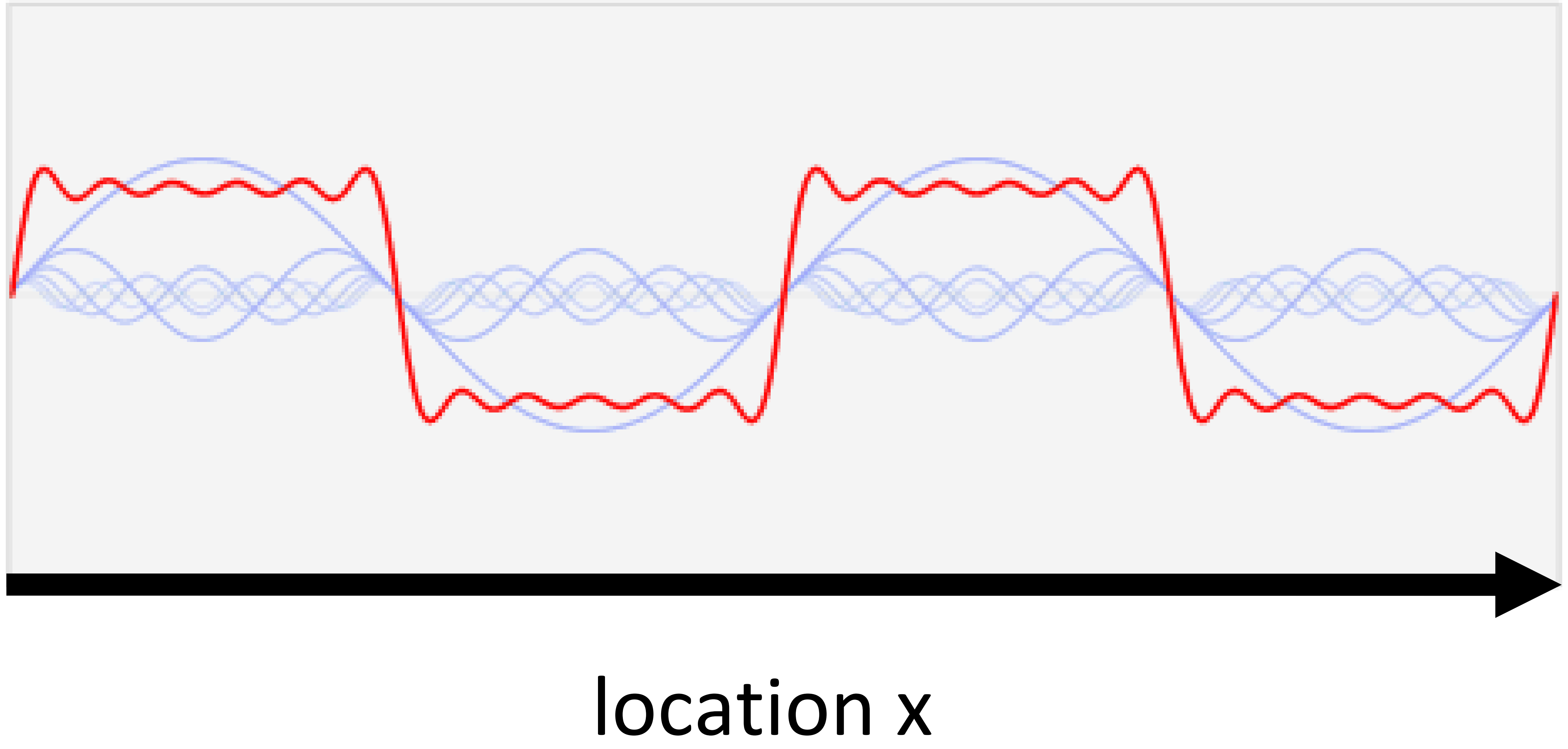
Fourier transform

Fourier transform = Spectral transform in 1D



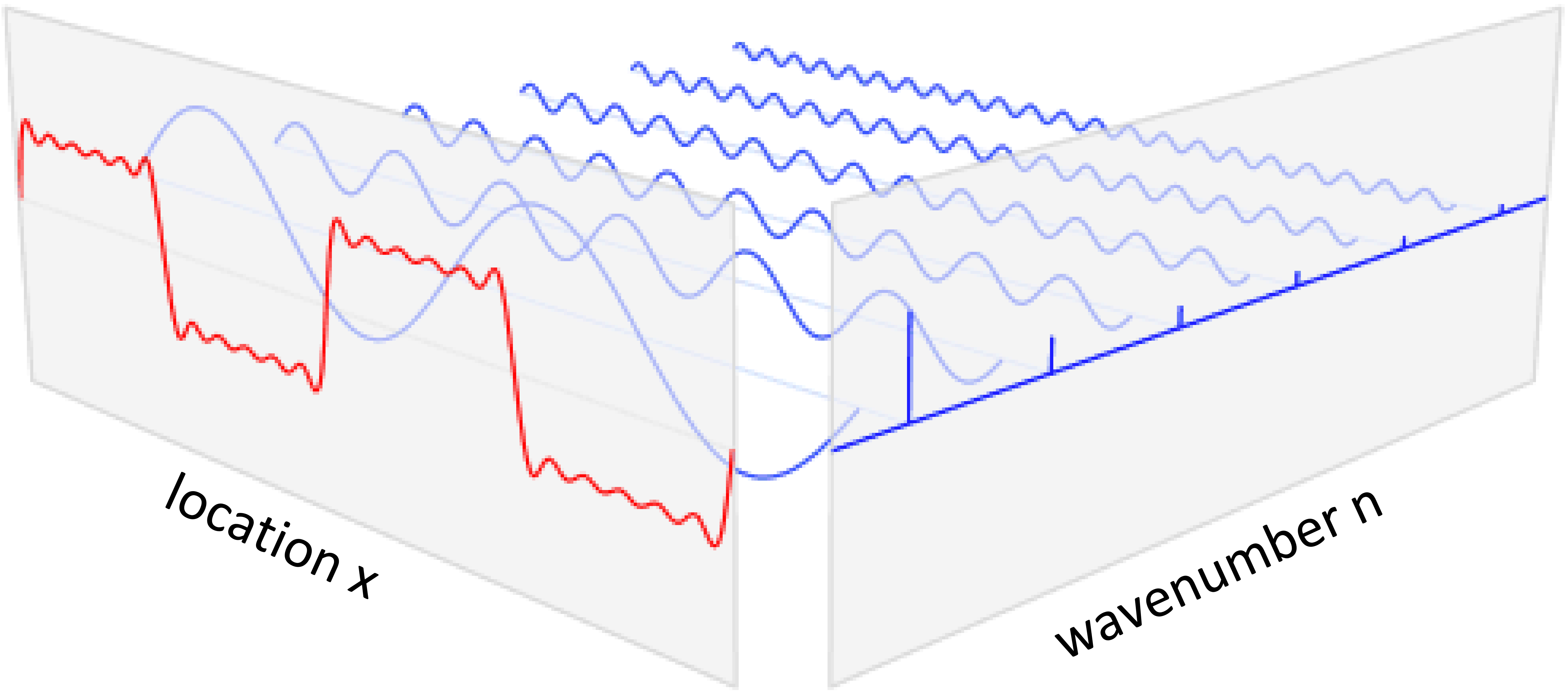
Fourier transform

Fourier transform = Spectral transform in 1D



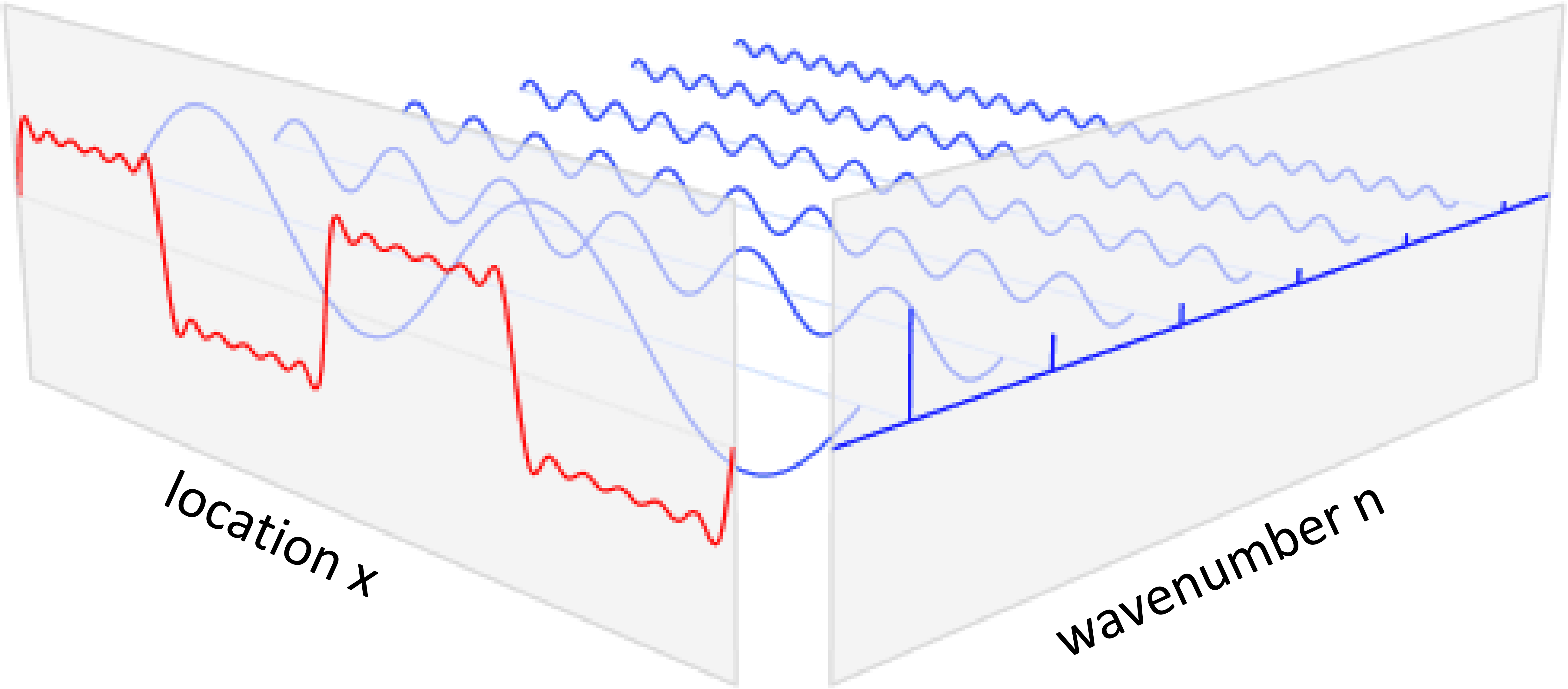
Fourier transform

Fourier transform = Spectral transform in 1D



grid point space **Fourier space**

Fourier transform



function in grid point space

Fourier coefficients

$$f(x) = \sum_n f_n \cdot \mathrm{e}^{-2\pi \mathrm{i}\, n\, x}$$

Fourier transform

function in grid point space

Fourier coefficients

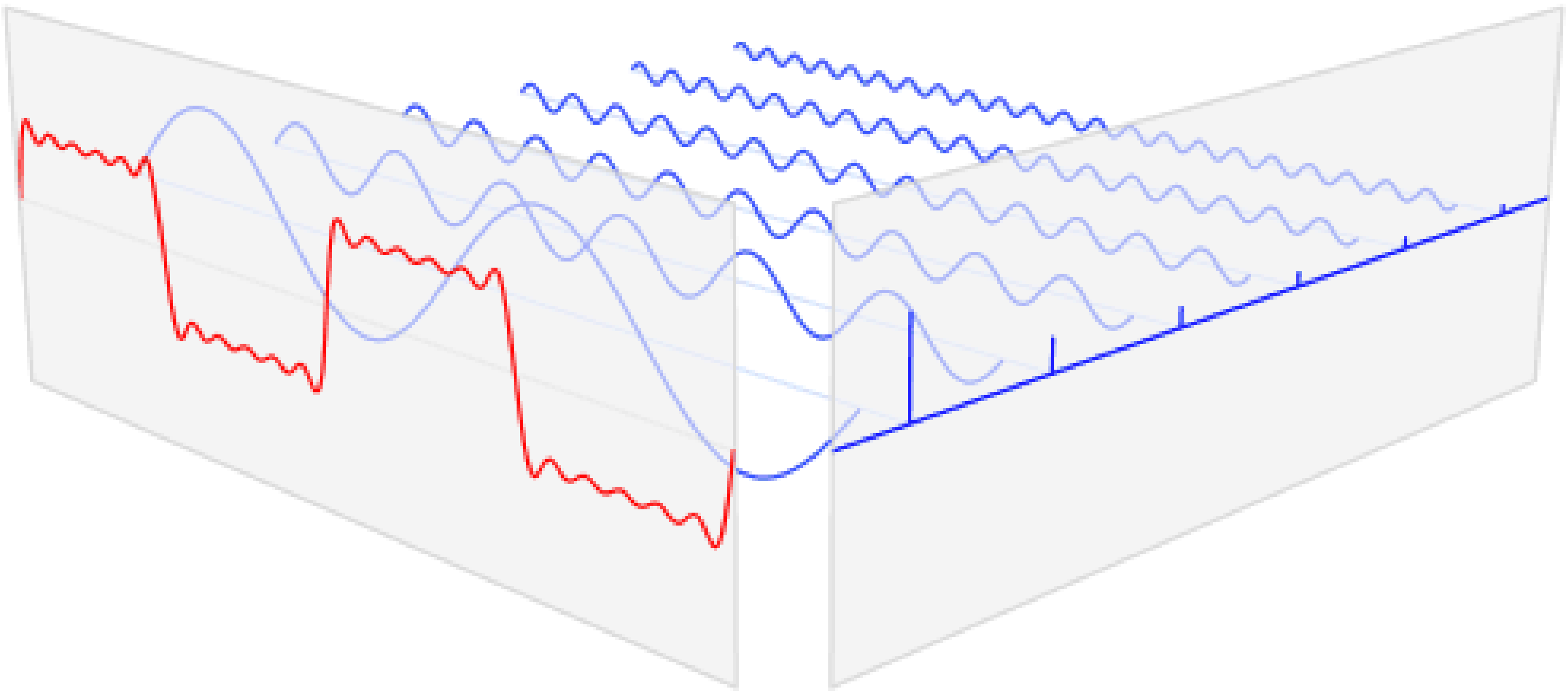
$$f(x) = \sum_n f_n \cdot \mathrm{e}^{-2\pi \mathrm{i}\, n\, x}$$

differentiation

simple multiplication

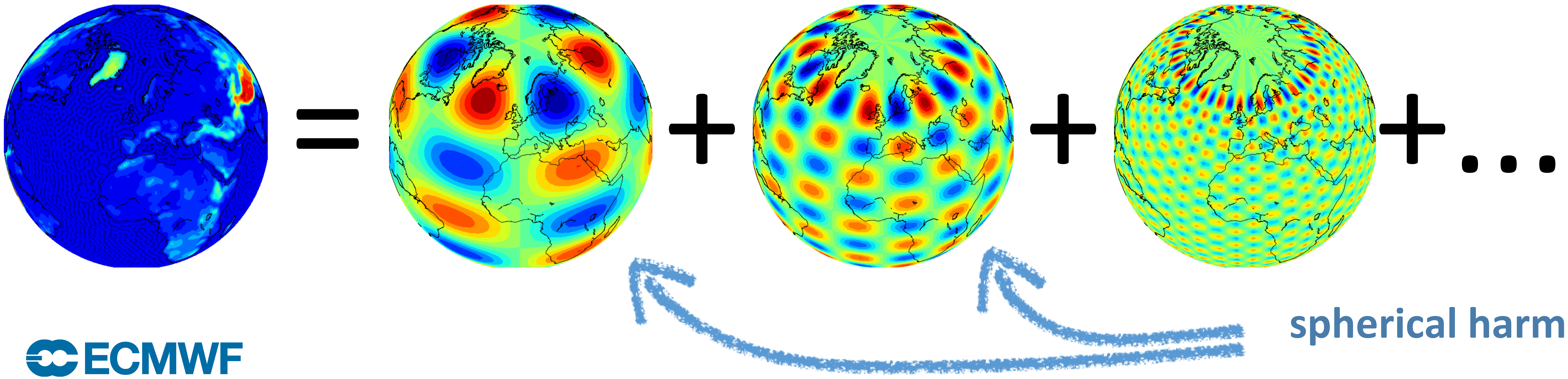
$$\frac{\mathrm{d}f(x)}{\mathrm{dx}} = \sum_n (-2\pi \mathrm{i}\, n\, f_n) \cdot \mathrm{e}^{-2\pi \mathrm{i}\, n\, x}$$

on the sphere: spectral transform



grid point space

spectral space



spherical harmonics

on the sphere: spectral transform

Spectral coefficients

Spherical harmonics

Latitude

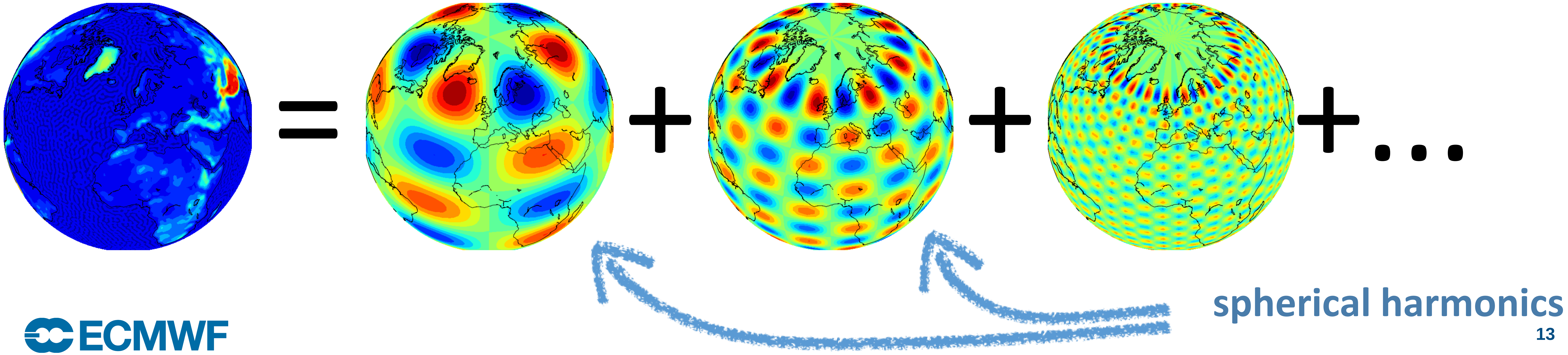
Longitude

Grid point variable

$$f(\phi,\lambda) = \Re\left(\sum_{m=0}^{M}\sum_{n=m}^{M} f_{m,n}\, Y_n^m(\phi,\lambda)\right)$$

m: zonal wavenumber
n: total wavenumber
M: truncation

grid point space **spectral space**



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on the sphere: spectral transform

Spectral coefficients

Spherical harmonics

Latitude

Longitude

Grid point variable

$$f(\phi, \lambda) = \Re\left(\sum_{m=0}^{M}\sum_{n=m}^{M} f_{m,n}\, Y_n^m(\phi, \lambda)\right)$$

m: zonal wavenumber
n: total wavenumber
M: truncation

Legendre polynomials

$$f(\phi, \lambda) = \Re\left(\sum_{m=0}^{M} \mathrm{e}^{im\lambda} \underbrace{\sum_{n=m}^{M} f_{m,n} P_n^m(\phi)}_{\text{Legendre transform}}\right)$$

Legendre transform

Fourier transform

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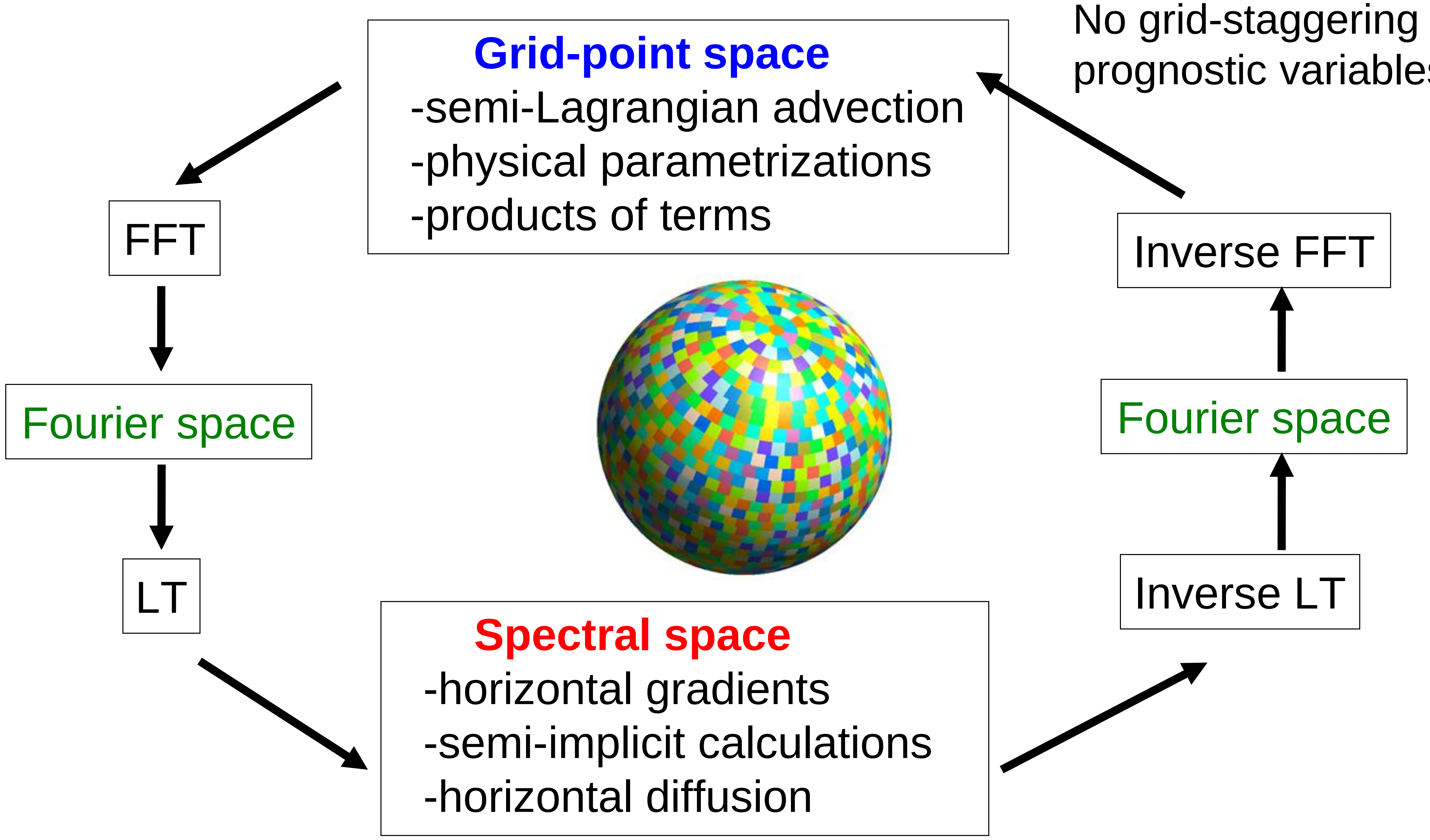
time step in IFS



No grid-staggering of prognostic variables

FFT: Fast Fourier Transform, LT: Legendre Transform

hands-on session

for everyone: interactive web-app about spectral transform

open in a browser: anmrde.github.io/spectral

optional: Python course

open in Jupyterlab in your browser: /NMcourse/spectral/solution.ipynb

Exercises are getting more difficult. Feel free to skip exercises as you want. The full Python course is designed to fill 20 hours.

files: exercises.ipynb: Python notebook with exercises
solution.ipynb: notebook including sample solutions

ECMWF Jupyterhub (16GB of RAM) or personal Linux computer:
https://github.com/anmrde/spectral/tree/master/jupyter

aliasing

Issue: multiplication of two variables produces shorter waves than grid can handle

aliasing

wave generated in spectral space

Issue: multiplication of two variables produces shorter waves than grid can handle

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aliasing

Issue: multiplication of two variables produces shorter waves than grid can handle

aliasing

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aliasing

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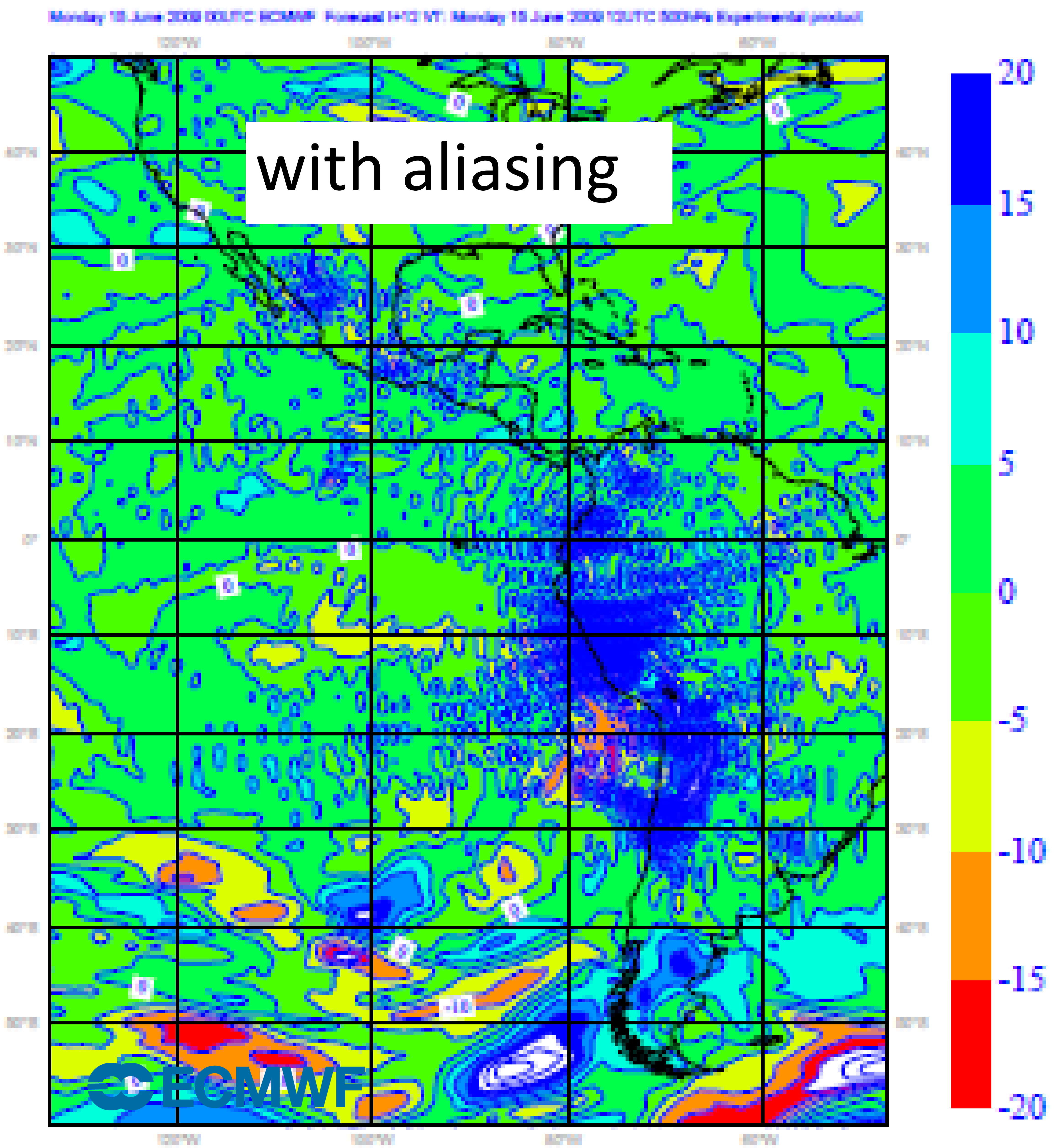
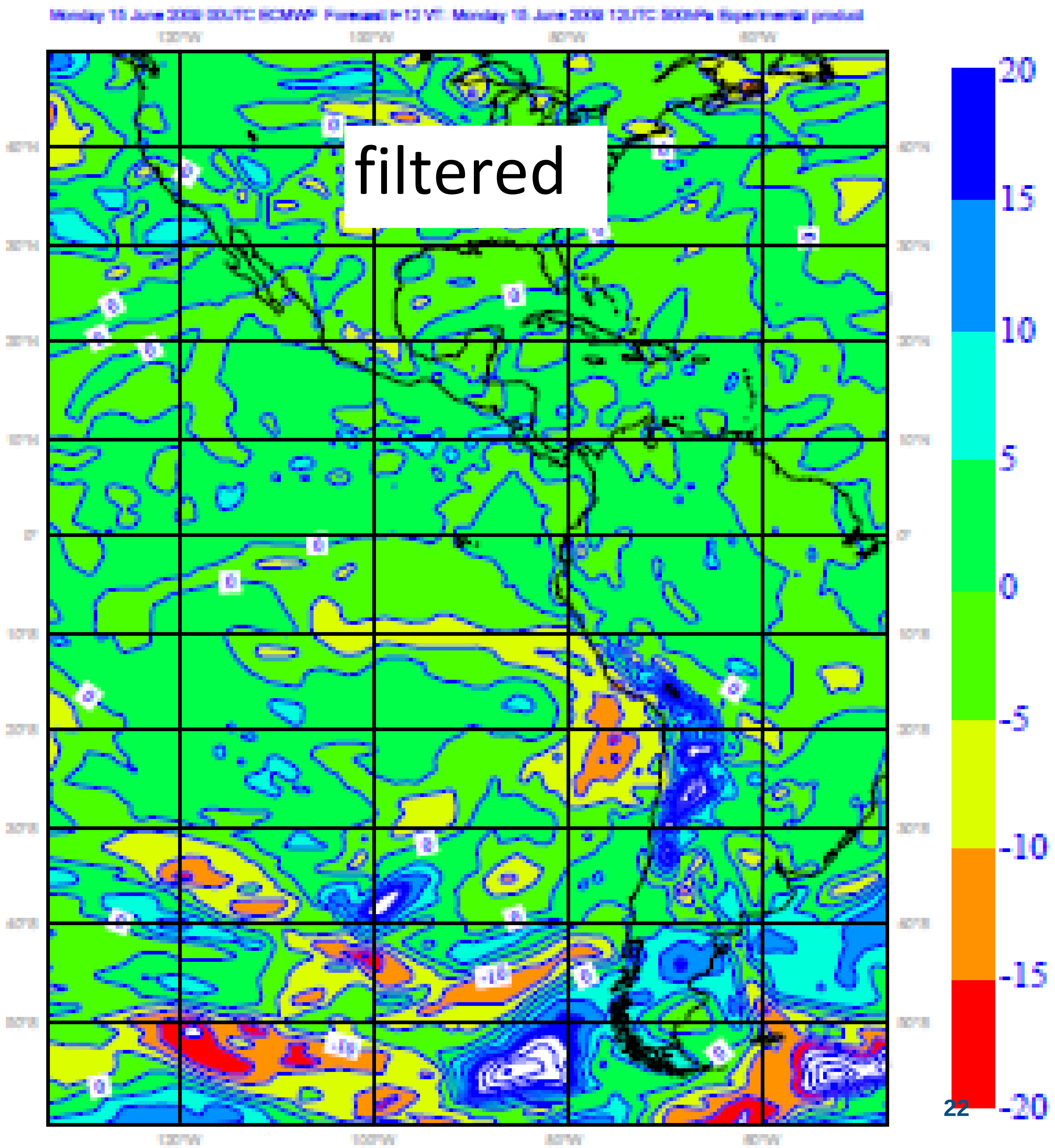
aliasing example

500hPa adiabatic zonal wind tendencies (T159)

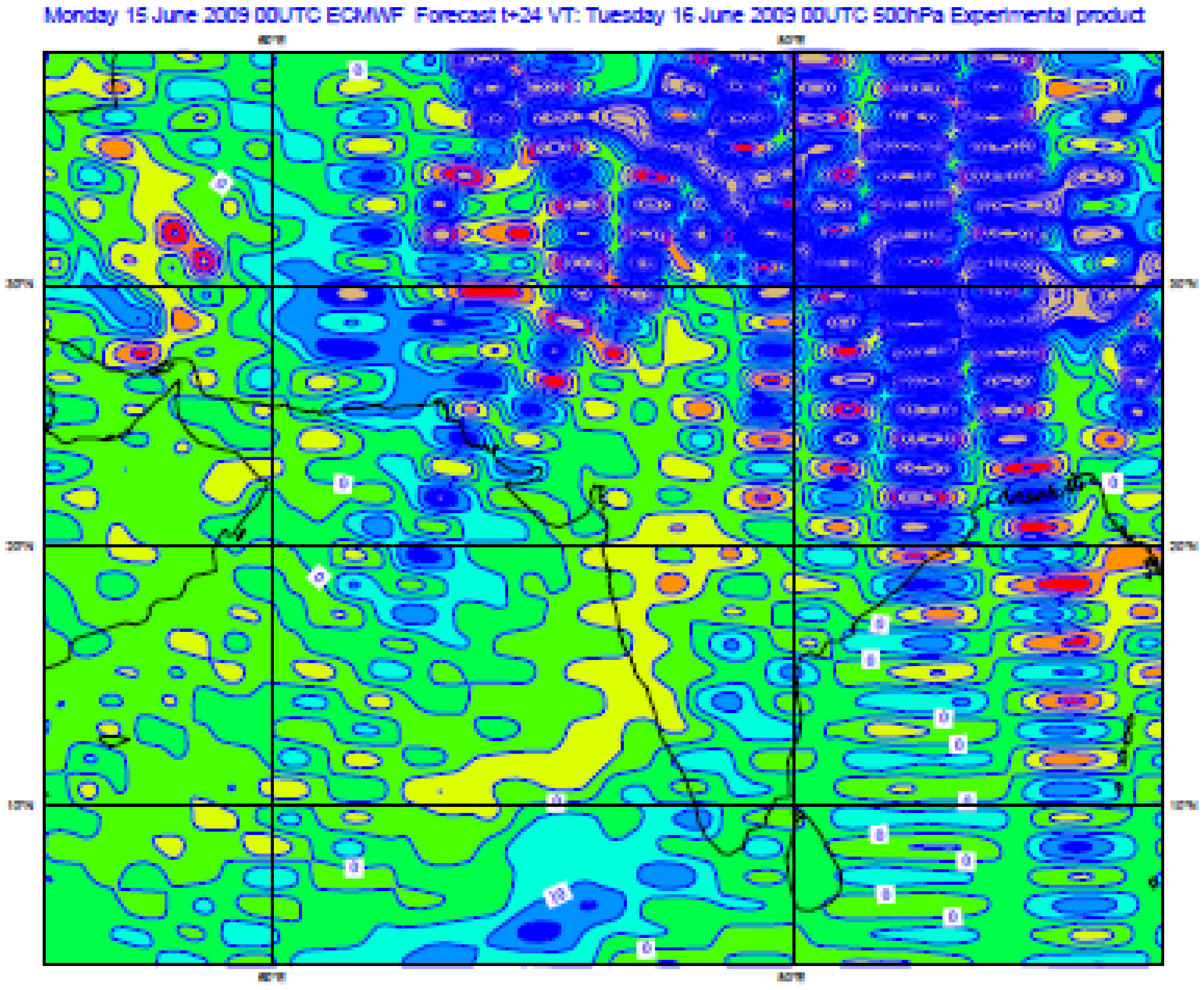




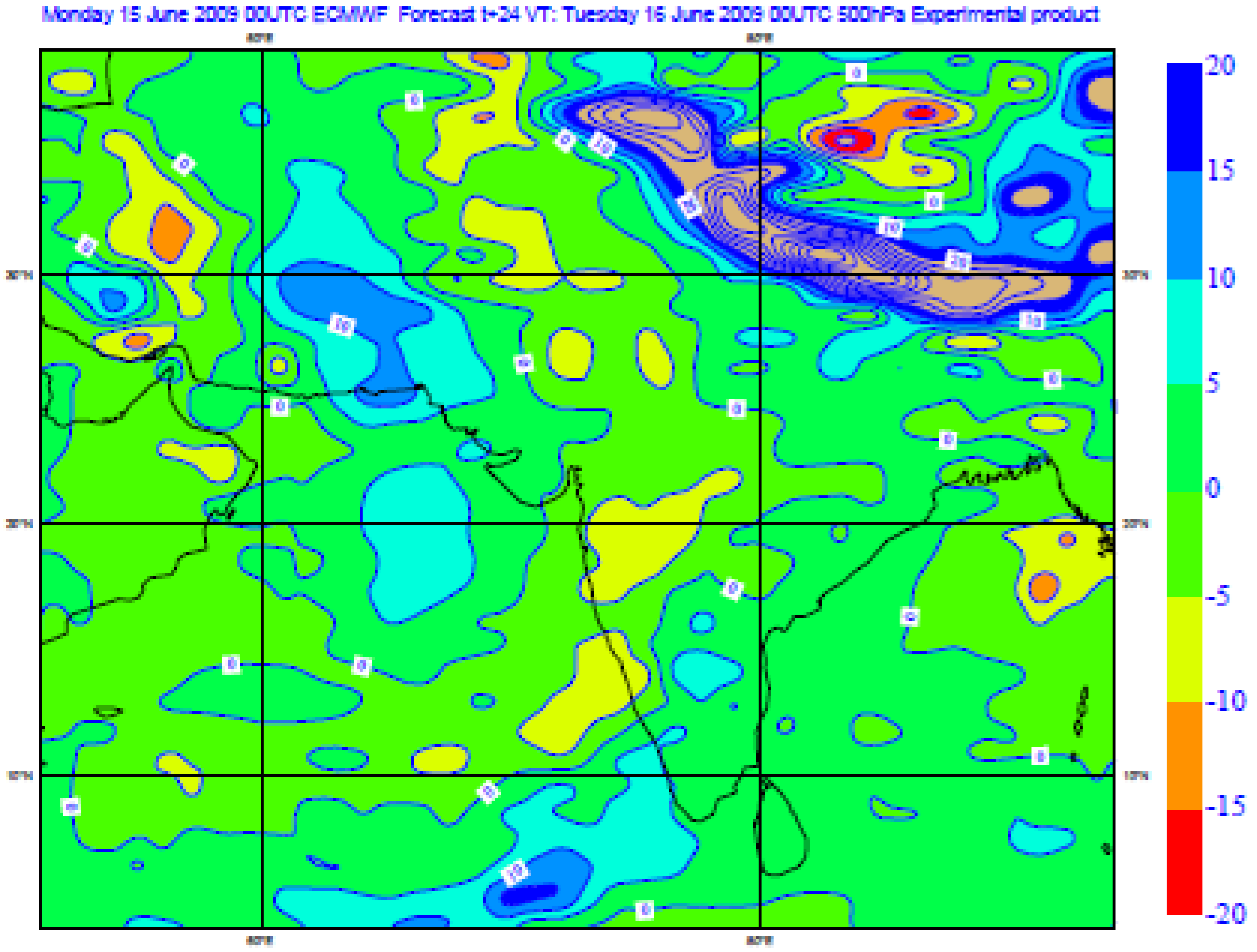
aliasing example

500hPa adiabatic meridional wind tendencies (T159)

with aliasing

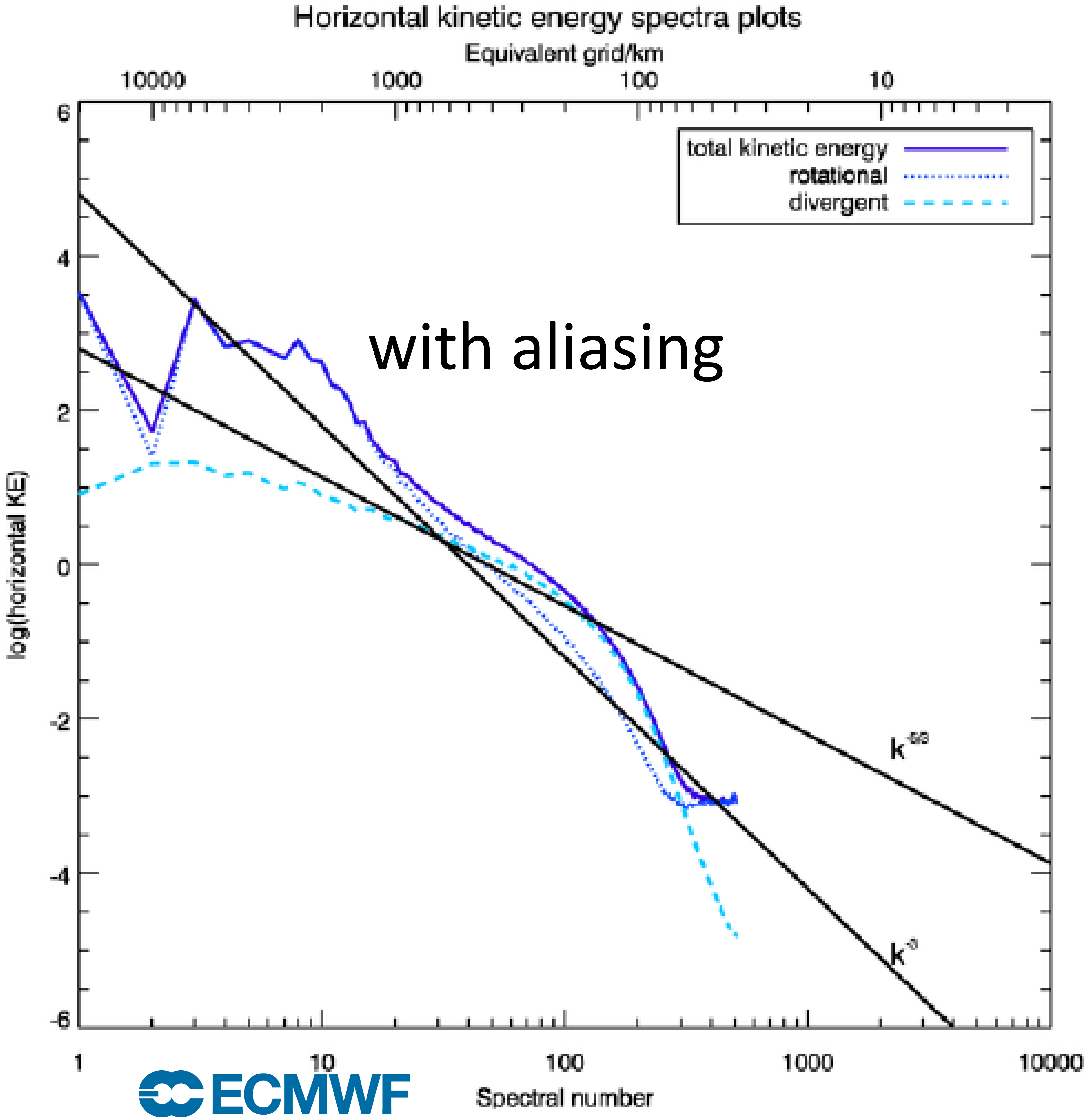


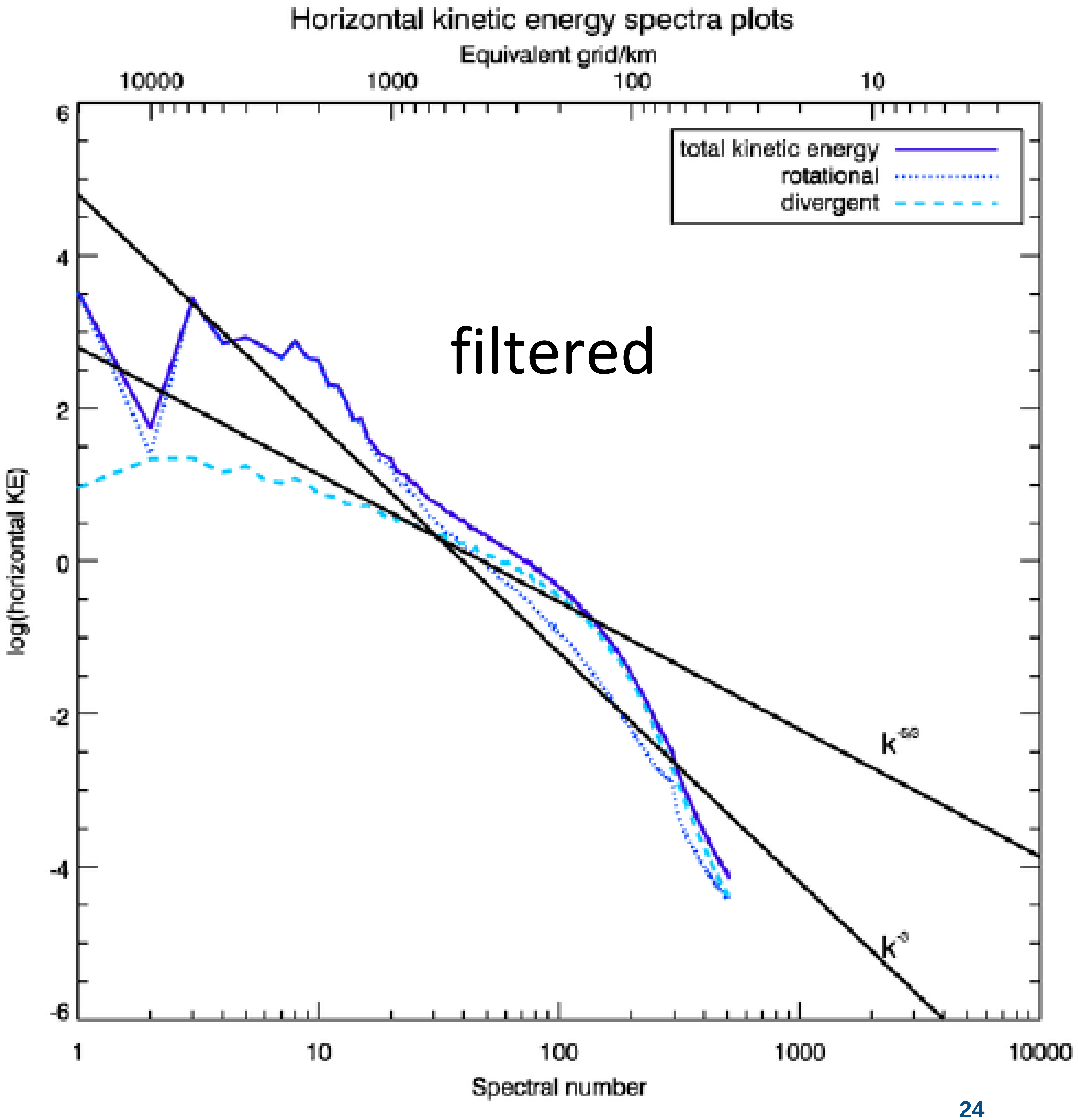
filtered



aliasing example

kinetic energy spectra, 100 hPa





alternatives to using a filter

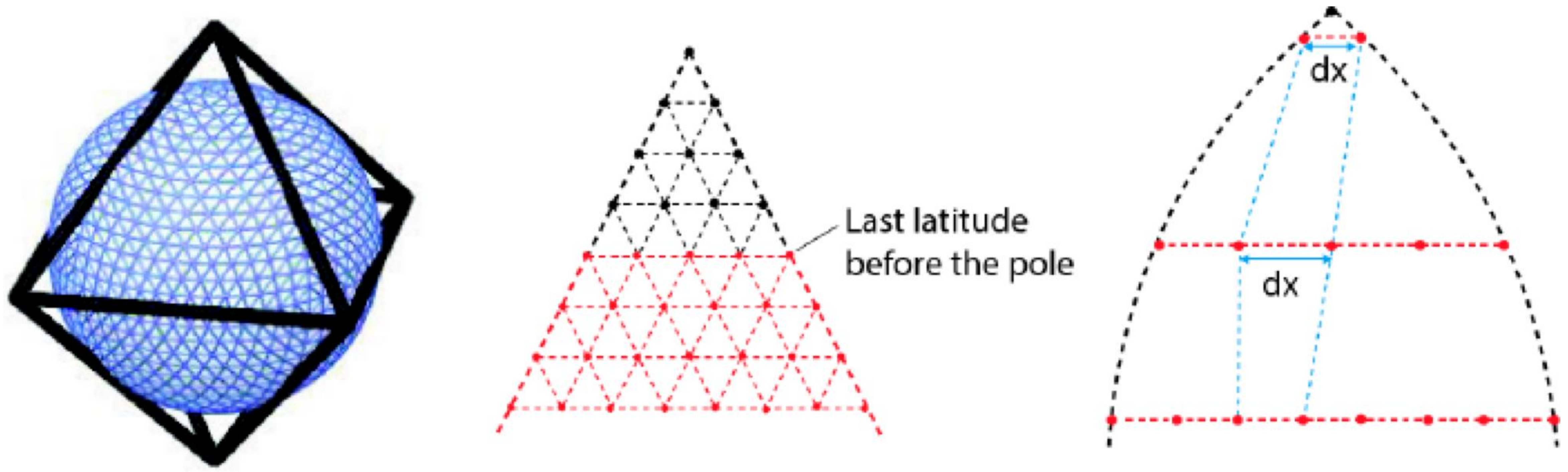
Idea: use more grid points than spectral coefficients

Orszag, 1971:

2N+1 gridpoints to N waves : linear grid	~ 1-2 Δ
3N+1 gridpoints to N waves : quadratic grid	~ 2-3 Δ
4N+1 gridpoints to N waves : cubic grid	~ 3-4 Δ
	Spatial filter range

(Wedi, 2014)

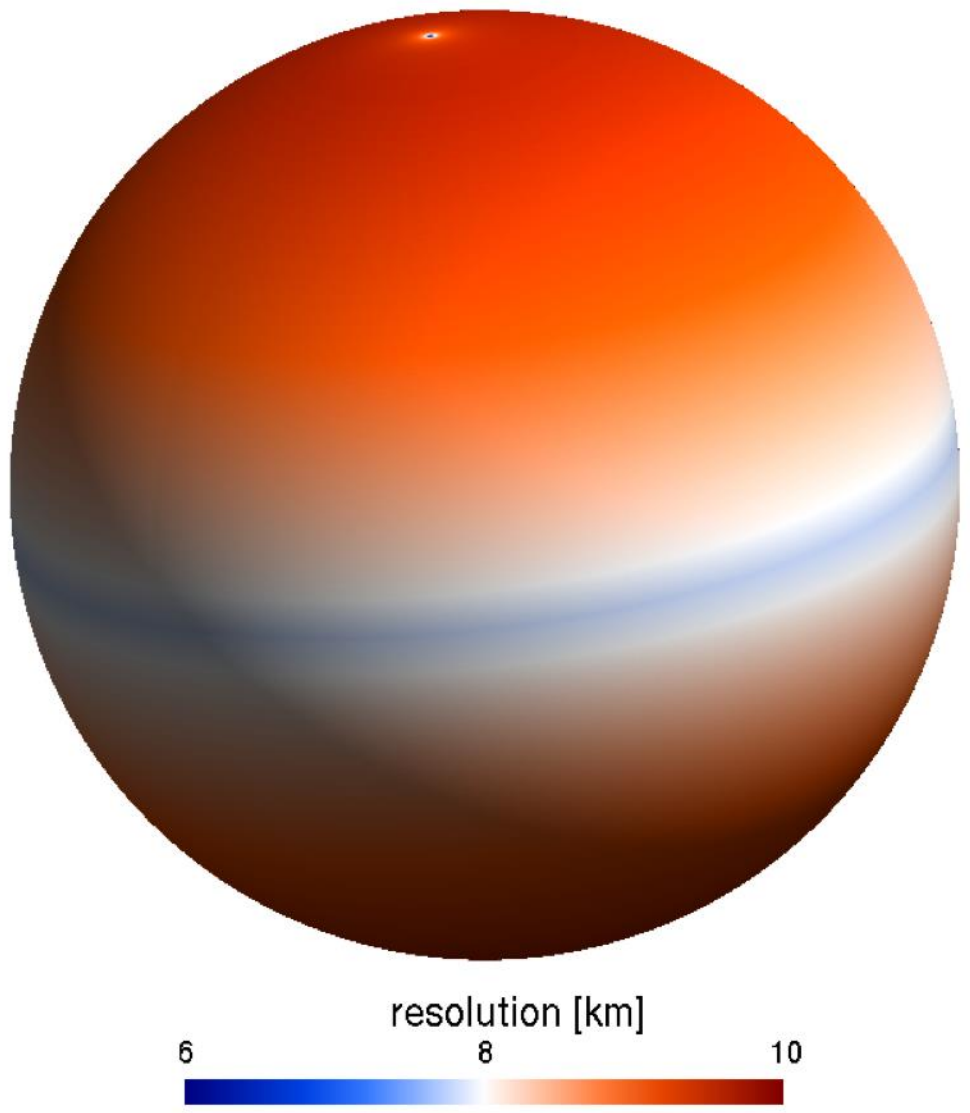
Cubic octahedral (Gaussian) grid of IFS



- No aliasing in nonlinear products
- Improved accuracy and mass conservation compared with linear grid
- Efficiency and scalability for large size problems: high grid-point resolution for a given spectral truncation i.e. expensive transforms become a smaller fraction of total computations

Collignon projection on the sphere: Number of points at latitude line i = 4 × i + 16, i = 1, . . . ,2N

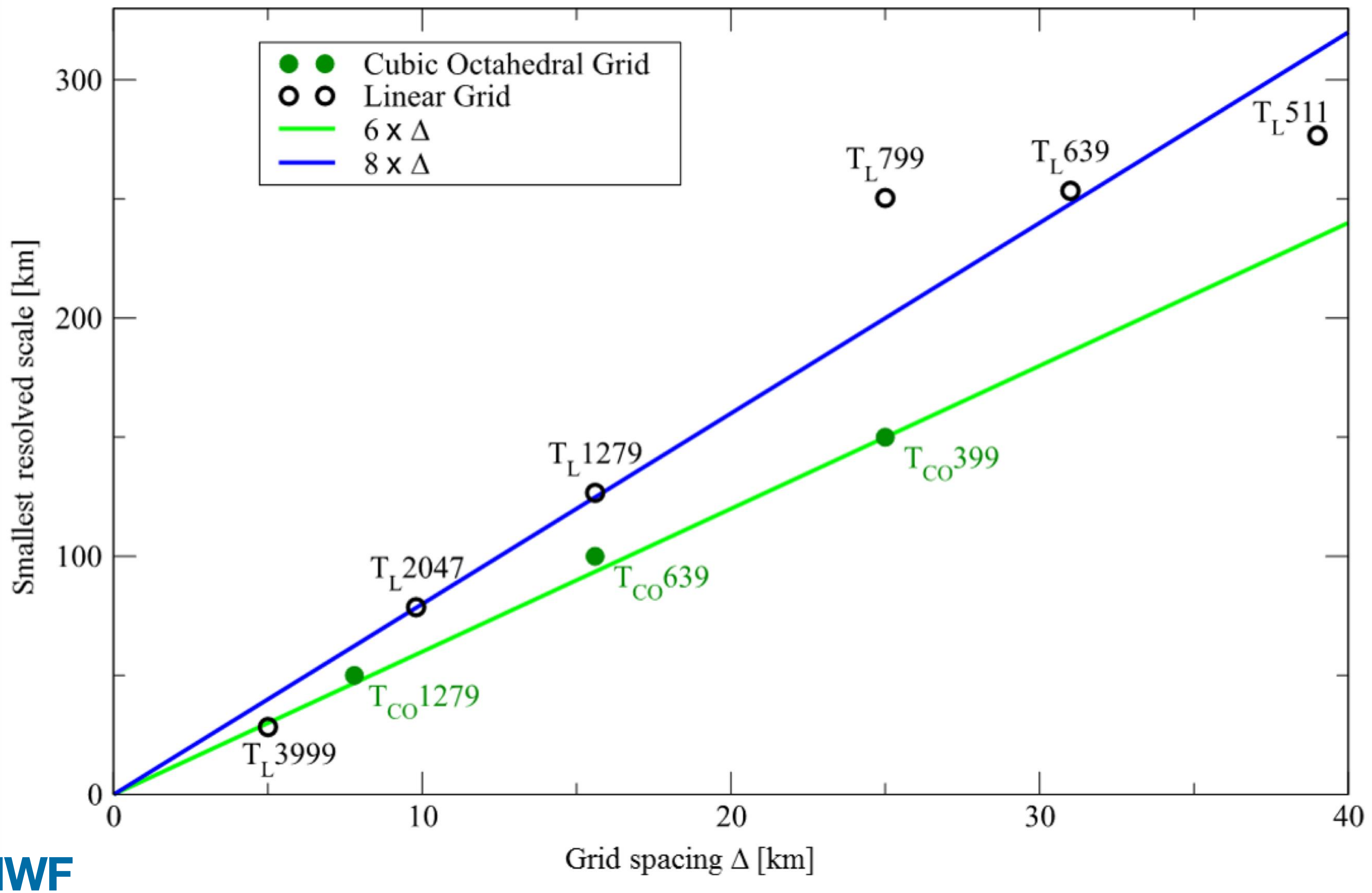
Variation of grid-point resolution with latitude



For a given spectral triangular truncation N the cubic reduced octahedral Gaussian grid has:

- 2N points between pole and equator which coincide with Gaussian latitudes
- 4N+16 east-west points along the equator
- 4N(N+9) points in total

effective resolution
of linear and cubic grids (Abdalla et al. 2013)



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inverse spectral transform

spectral data: $\mathbf{D}(f, \mathrm{i}, n, m)$

fastest index left (column-major order like in Fortran)

fields (variables, height levels)

real and imaginary part

wave numbers
m=0,…,N; n=0,…,N-m
(N: truncation)

inverse spectral transform

spectral data: $\mathbf{D}(f, \mathrm{i}, n, m)$

m=0,…,N; n=0,…,N-m

even n

odd n

for each m:

$\mathbf{D}_{e,m}(f, \mathrm{i}, n)$

$\mathbf{D}_{o,m}(f, \mathrm{i}, n)$

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inverse spectral transform

spectral data: $\mathbf{D}(f, \mathrm{i}, n, m)$

m=0,…,N; n=0,…,N-m

even n

odd n

P: precomputed Legendre polynomials

for each m:

$$\mathbf{S}_m(f, \mathrm{i}, \phi) = \sum_n \mathbf{D}_{e,m}(f, \mathrm{i}, n) \cdot \mathbf{P}_{e,m}(n, \phi), \quad \mathbf{A}_m(f, \mathrm{i}, \phi) = \sum_n \mathbf{D}_{o,m}(f, \mathrm{i}, n) \cdot \mathbf{P}_{o,m}(n, \phi)$$

matrix multiplications

ECMWF

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matrix multiplications

$$\phi > 0: \quad \mathbf{F}(\mathrm{i}, m, \phi, f) = \mathbf{S}_m(f, \mathrm{i}, \phi) + \mathbf{A}_m(f, \mathrm{i}, \phi)$$

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for each ϕ,f:

$$\mathbf{G}_{\phi,f}(\lambda) = \mathrm{FFT}(\mathbf{F}_{\phi,f}(\mathrm{i}, m))$$

FFT: Fast Fourier Transform

inverse spectral transform

spectral data: $\mathbf{D}(f, \mathrm{i}, n, m)$

m=0,…,N; n=0,…,N-m

P: precomputed Legendre polynomials

even n

odd n

for each m:

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matrix multiplications

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for each ϕ,f: $\mathbf{G}_{\phi,f}(\lambda) = \mathrm{FFT}(\mathbf{F}_{\phi,f}(\mathrm{i},m))$

FFT: Fast Fourier Transform

grid point data: $\mathbf{G}(f,\lambda,\phi)$

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inverse spectral transform

spectral data: $\mathbf{D}(f, \mathrm{i}, n, m)$

spectral space

even n

odd n

for each m:

$$\mathbf{S}_m(f, \mathrm{i}, \phi) = \sum_n \mathbf{D}_{e,m}(f, \mathrm{i}, n) \cdot \mathbf{P}_{e,m}(n, \phi),$$

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inverse Legendre transform

inverse Fourier transform

for each ϕ,f: $\mathbf{G}_{\phi,f}(\lambda) = \mathrm{FFT}(\mathbf{F}_{\phi,f}(\mathrm{i}, m))$

grid point data: $\mathbf{G}(f, \lambda, \phi)$

grid point space

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inverse spectral transform

spectral data: $\mathbf{D}(f, \mathrm{i}, n, m)$ — spectral space — m,n

even n — odd n

parallelisation over these indices

for each m:

$$\mathbf{S}_m(f,\mathrm{i},\phi) = \sum_n \mathbf{D}_{e,m}(f,\mathrm{i},n) \cdot \mathbf{P}_{e,m}(n,\phi),$$
$$\mathbf{A}_m(f,\mathrm{i},\phi) = \sum_n \mathbf{D}_{o,m}(f,\mathrm{i},n) \cdot \mathbf{P}_{o,m}(n,\phi)$$

$$\phi > 0: \ \mathbf{F}(\mathrm{i},m,\phi,f) = \mathbf{S}_m(f,\mathrm{i},\phi) + \mathbf{A}_m(f,\mathrm{i},\phi)$$
$$\phi < 0: \ \mathbf{F}(\mathrm{i},m,\phi,f) = \mathbf{S}_m(f,\mathrm{i},-\phi) - \mathbf{A}_m(f,\mathrm{i},-\phi)$$

inverse Legendre transform — m,f

for each ϕ,f: $\mathbf{G}_{\phi,f}(\lambda) = \mathrm{FFT}(\mathbf{F}_{\phi,f}(\mathrm{i},m))$ — inverse Fourier transform — ϕ,f

grid point data: $\mathbf{G}(f,\lambda,\phi)$ — grid point space — ϕ,λ

inverse spectral transform

spectral data: $\mathbf{D}(f, \mathrm{i}, n, m)$

even n — odd n

for each m:

$$\mathbf{S}_m(f, \mathrm{i}, \phi) = \sum_n \mathbf{D}_{e,m}(f, \mathrm{i}, n) \cdot \mathbf{P}_{e,m}(n, \phi),$$

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for each ϕ,f: $\mathbf{G}_{\phi,f}(\lambda) = \mathrm{FFT}(\mathbf{F}_{\phi,f}(\mathrm{i}, m))$

grid point data: $\mathbf{G}(f, \lambda, \phi)$

spectral space	m,n
inverse Legendre transform	m,f
inverse Fourier transform	ϕ,f
grid point space	ϕ,λ

parallelisation over these indices

lots of MPI communication

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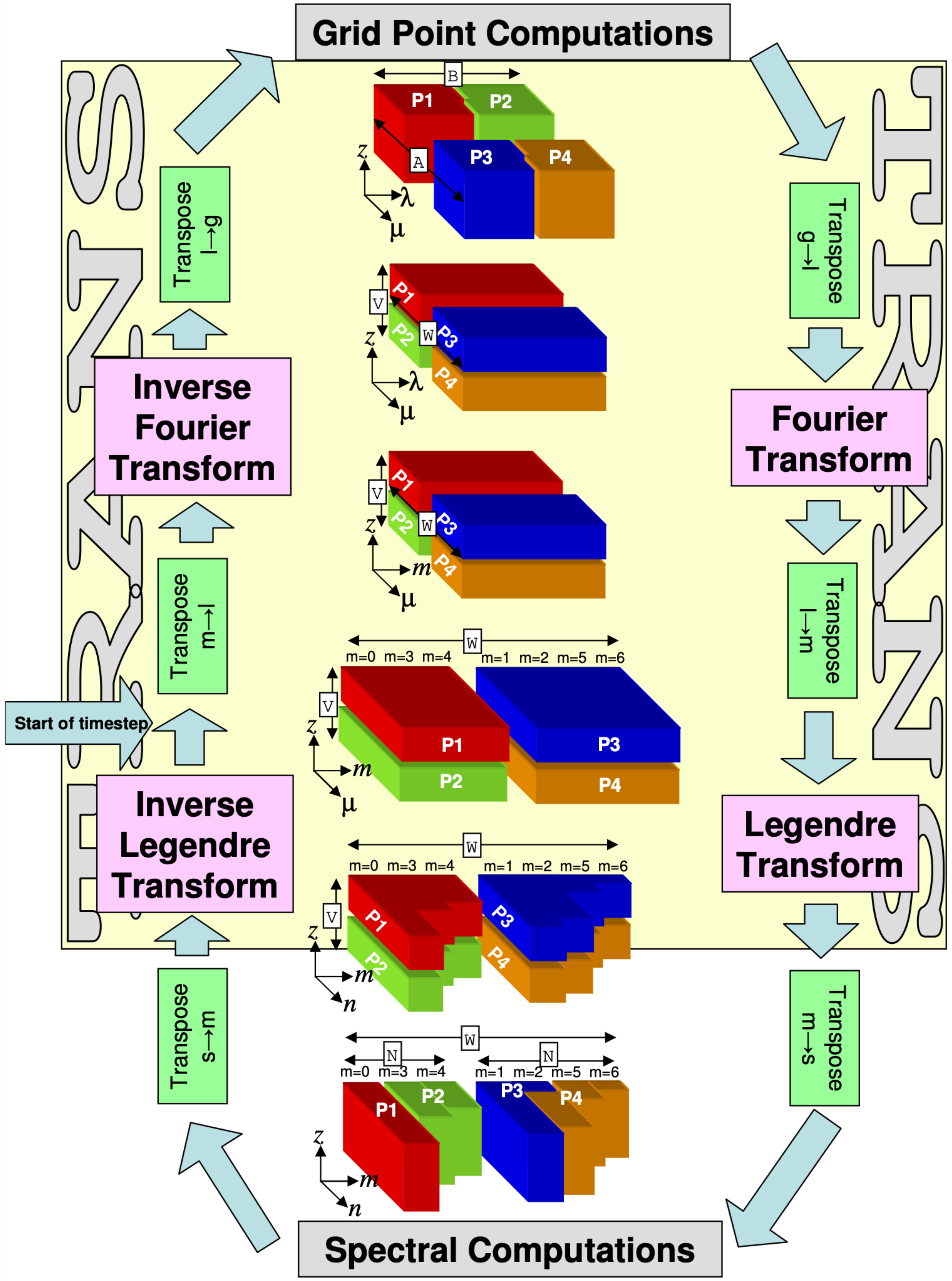
direct spectral transform

- same like inverse spectral transform
- reverse order
- multiply data with Gaussian quadrature weights before Legendre transform



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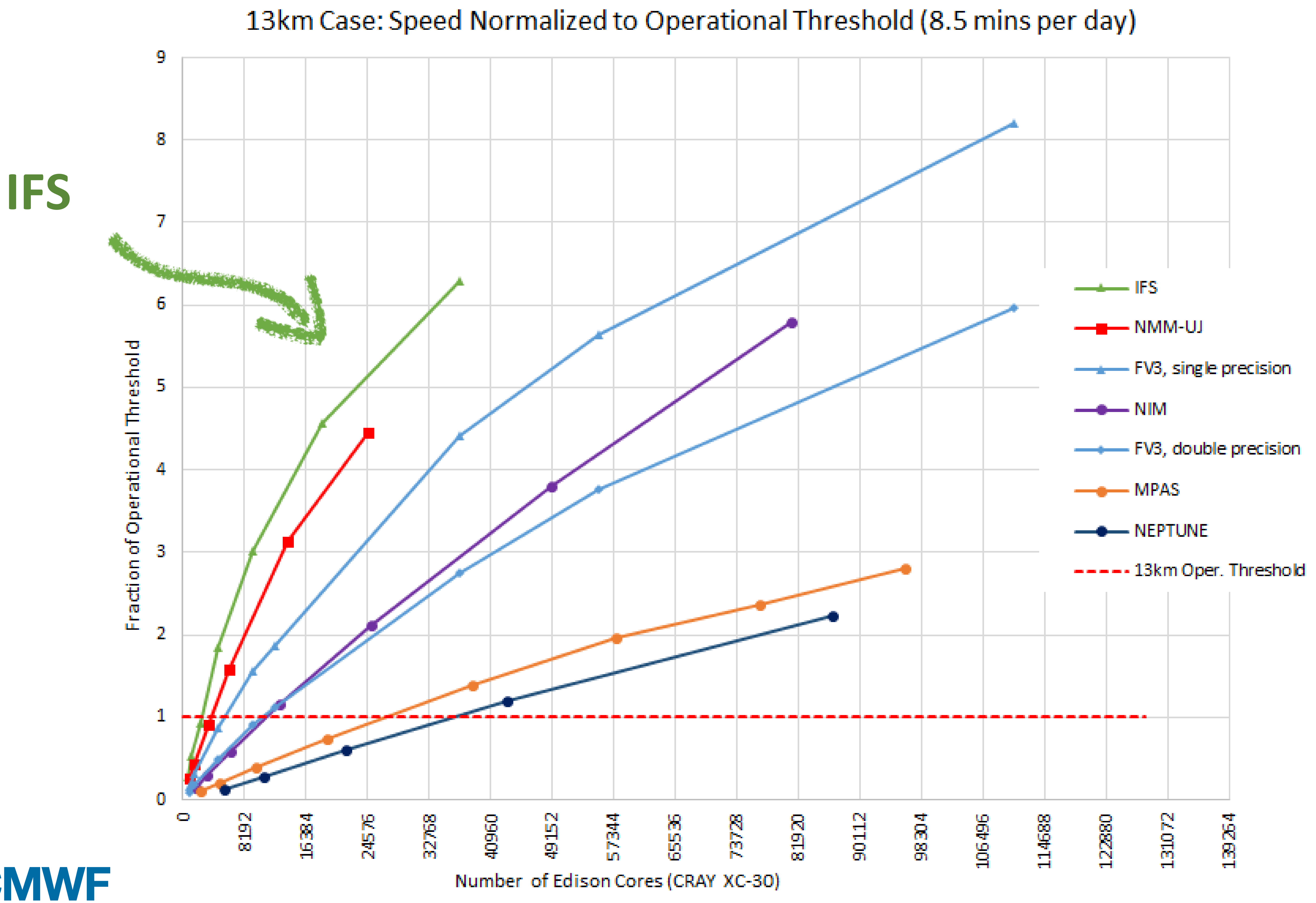
performance comparison of IFS with other models



(Michalakes et al, NGGPS AVEC report, 2015)

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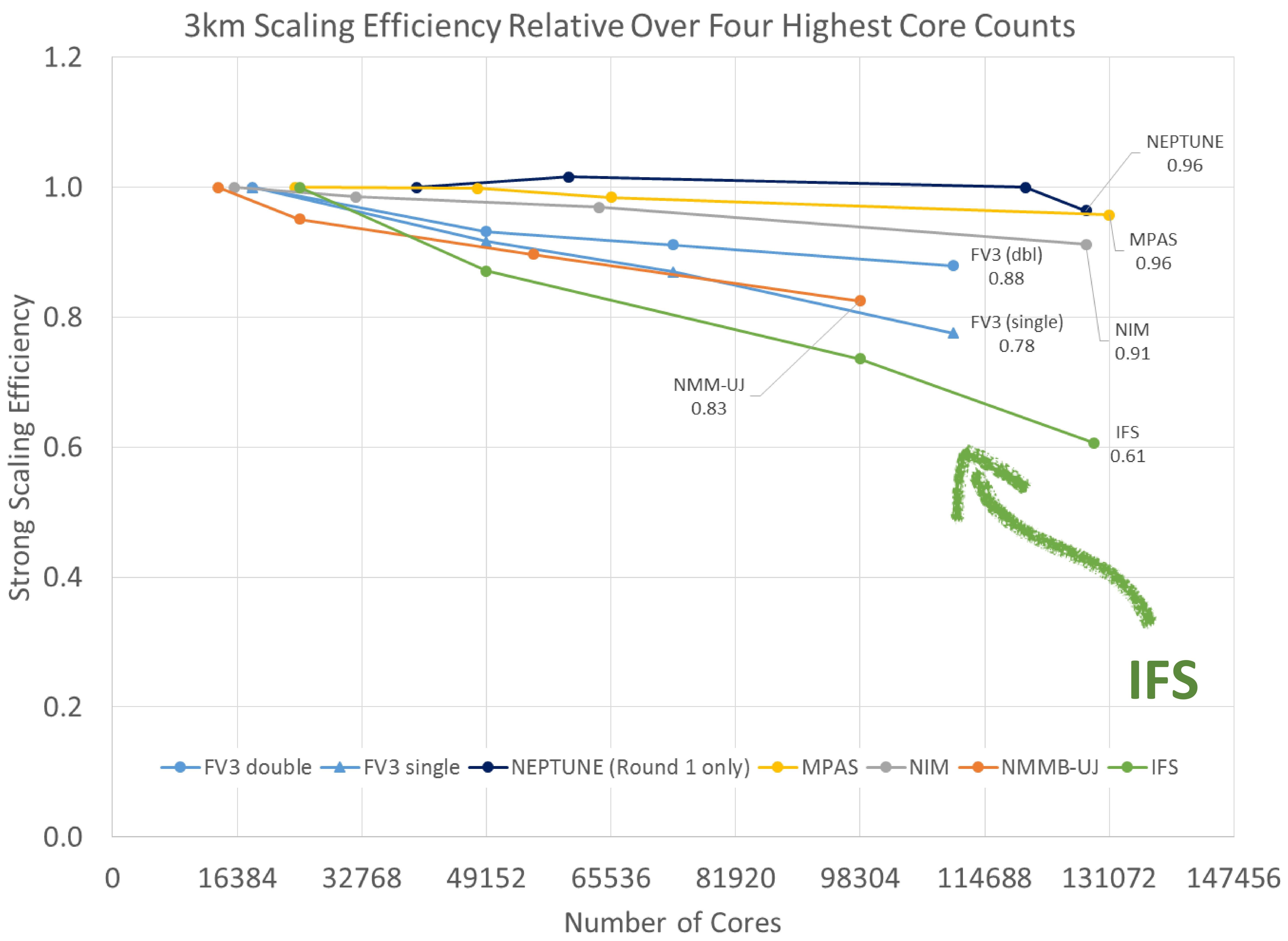
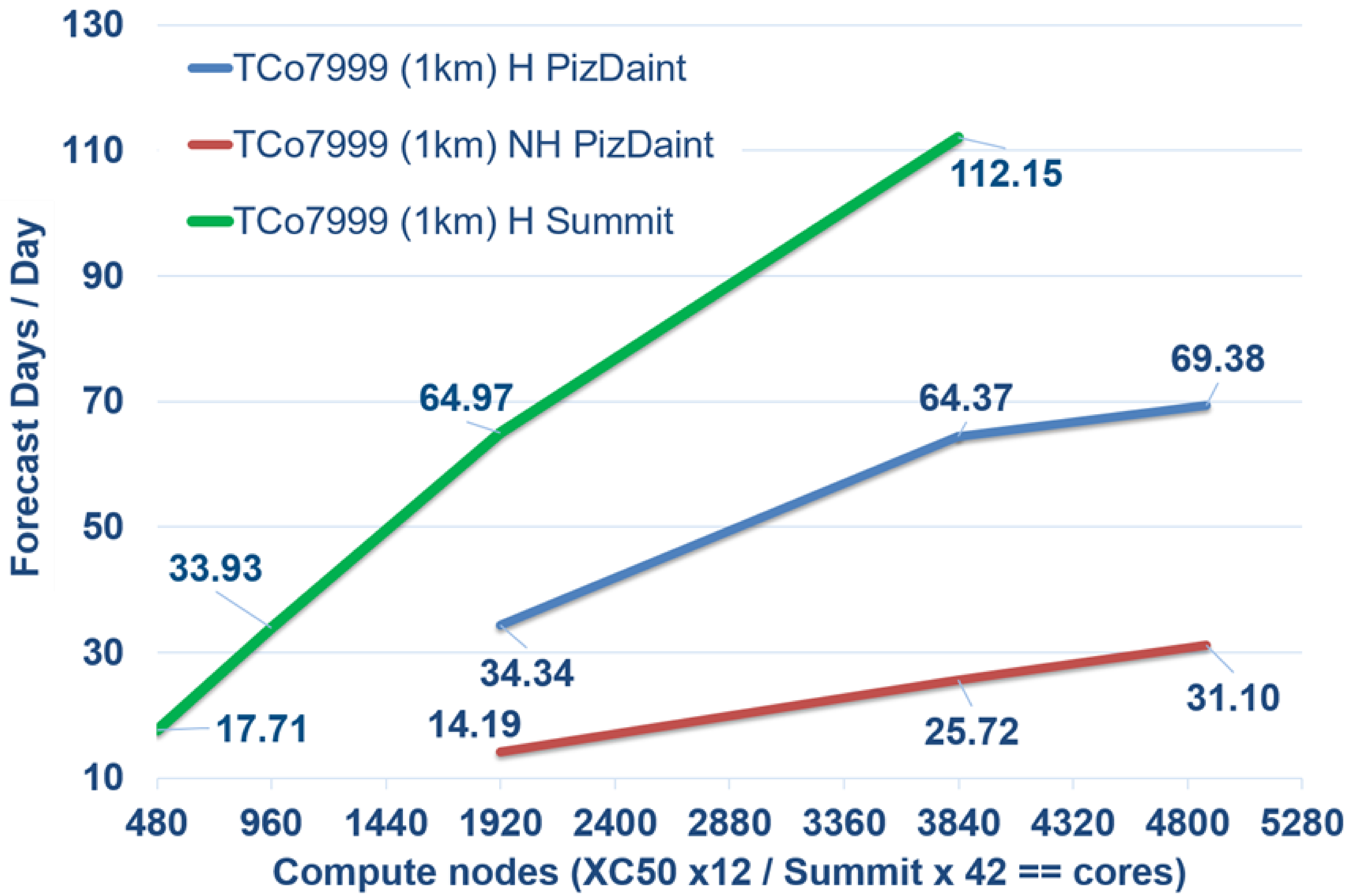
scalability comparison of IFS with other models



(Michalakes et al, NGGPS AVEC report, 2015)

IFS scaling on Summit and PizDaint (CPU only)



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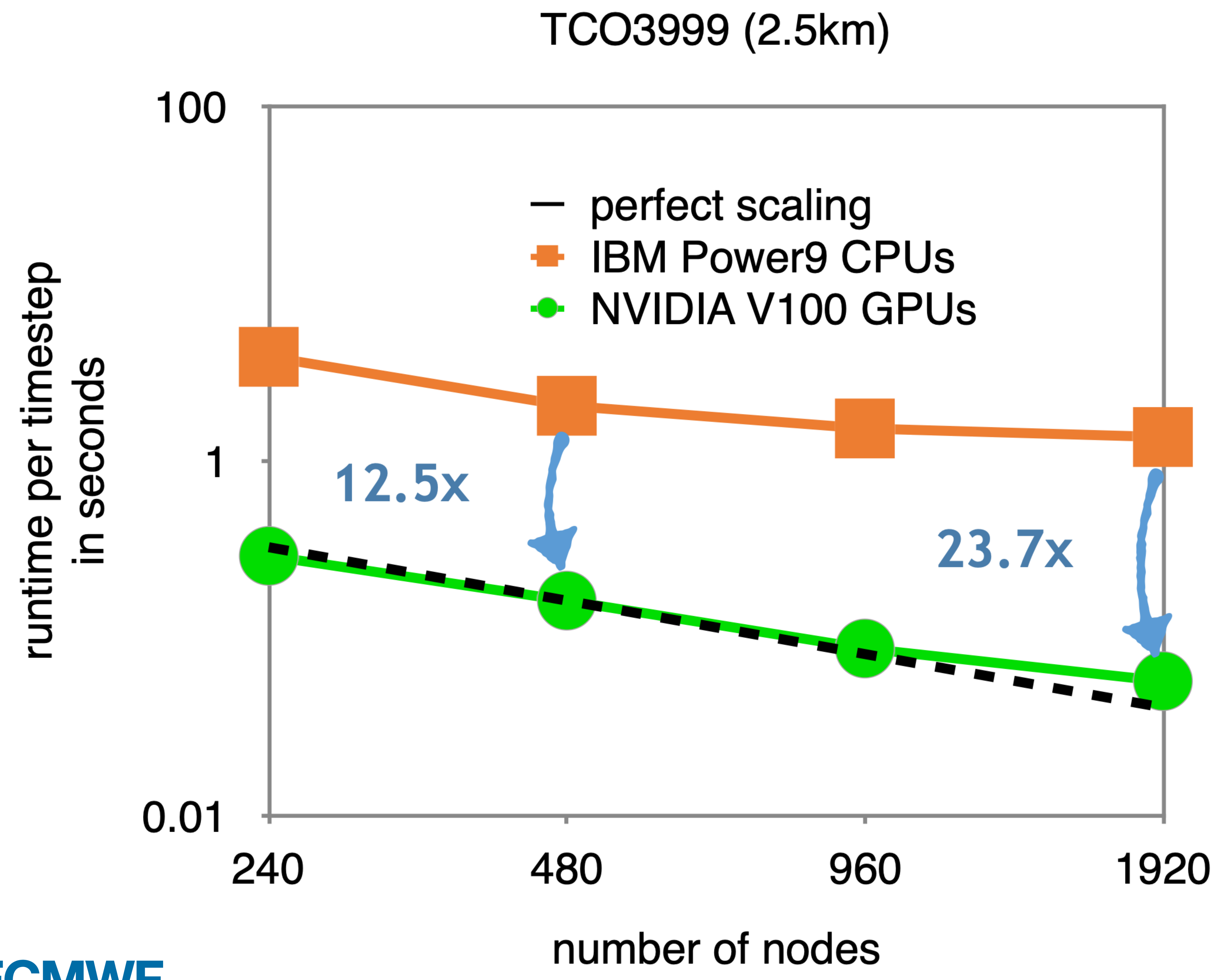
GPUs vs CPUs on Summit

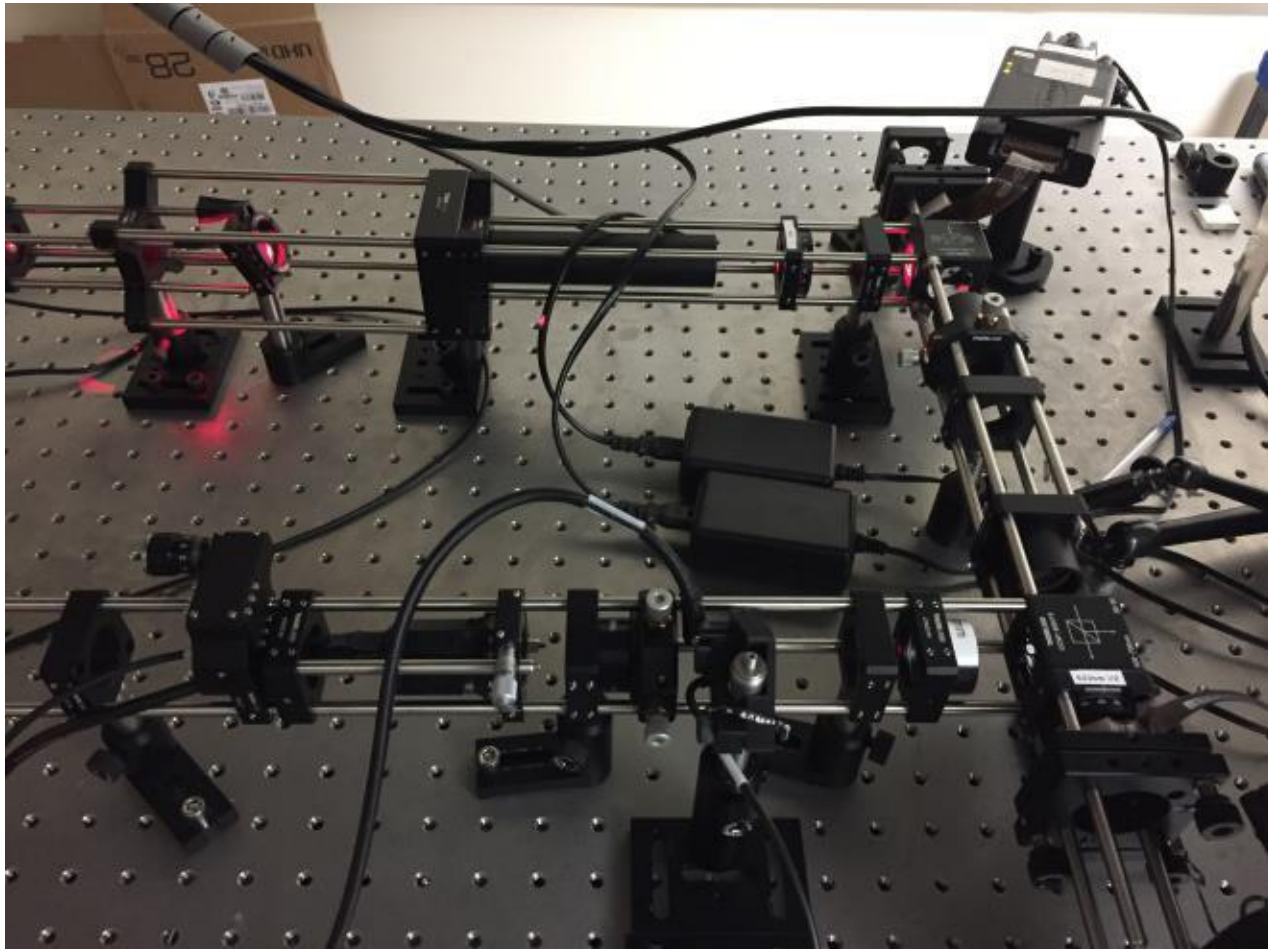
spectral transform only

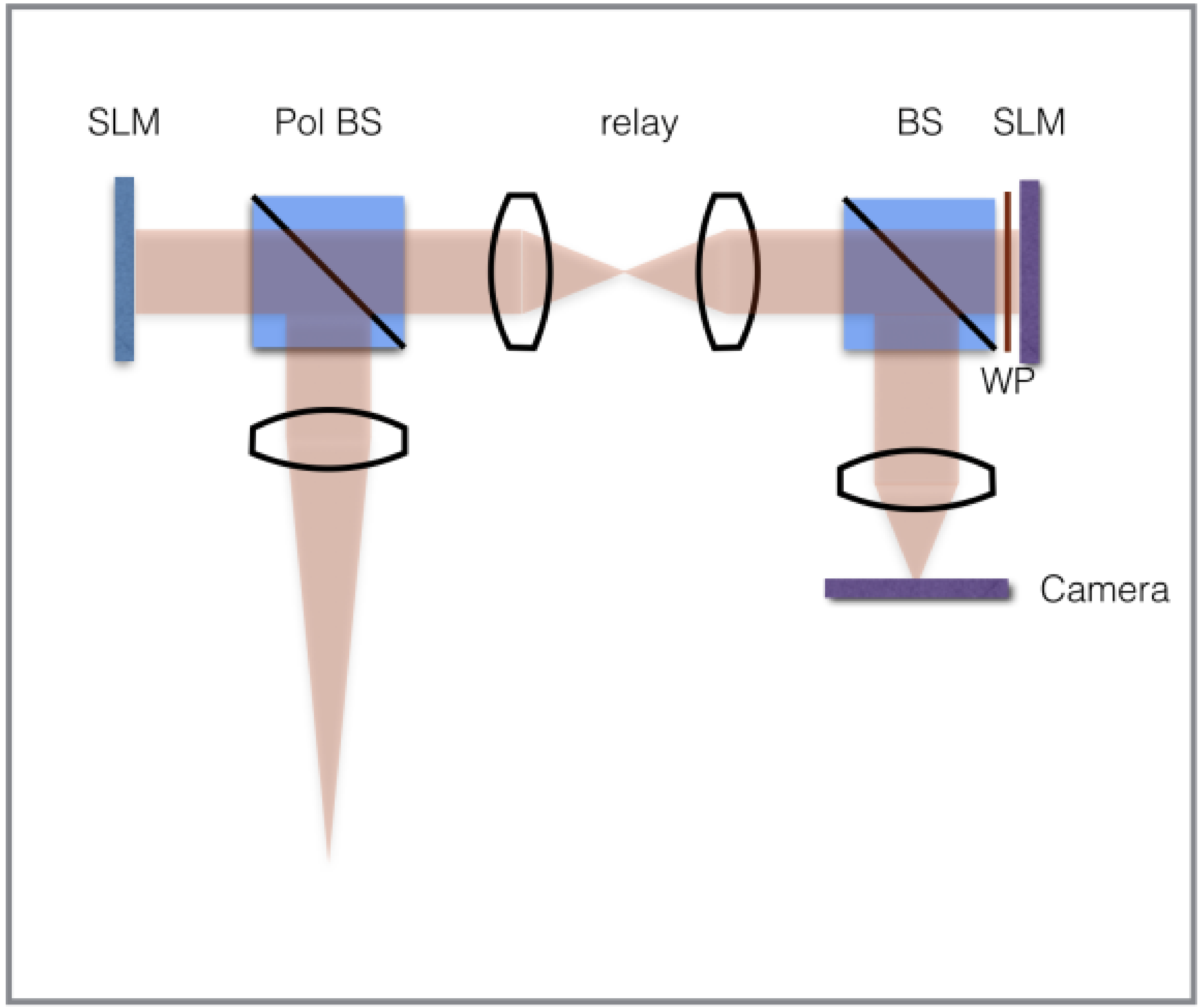


At 2.5km resolution, less than 1s per time-step fits operational needs.

This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE office of Science User Facility supported under contract DE-AC05-00OR22725.

Optalysys: optical processor for spectral transform





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Questions?