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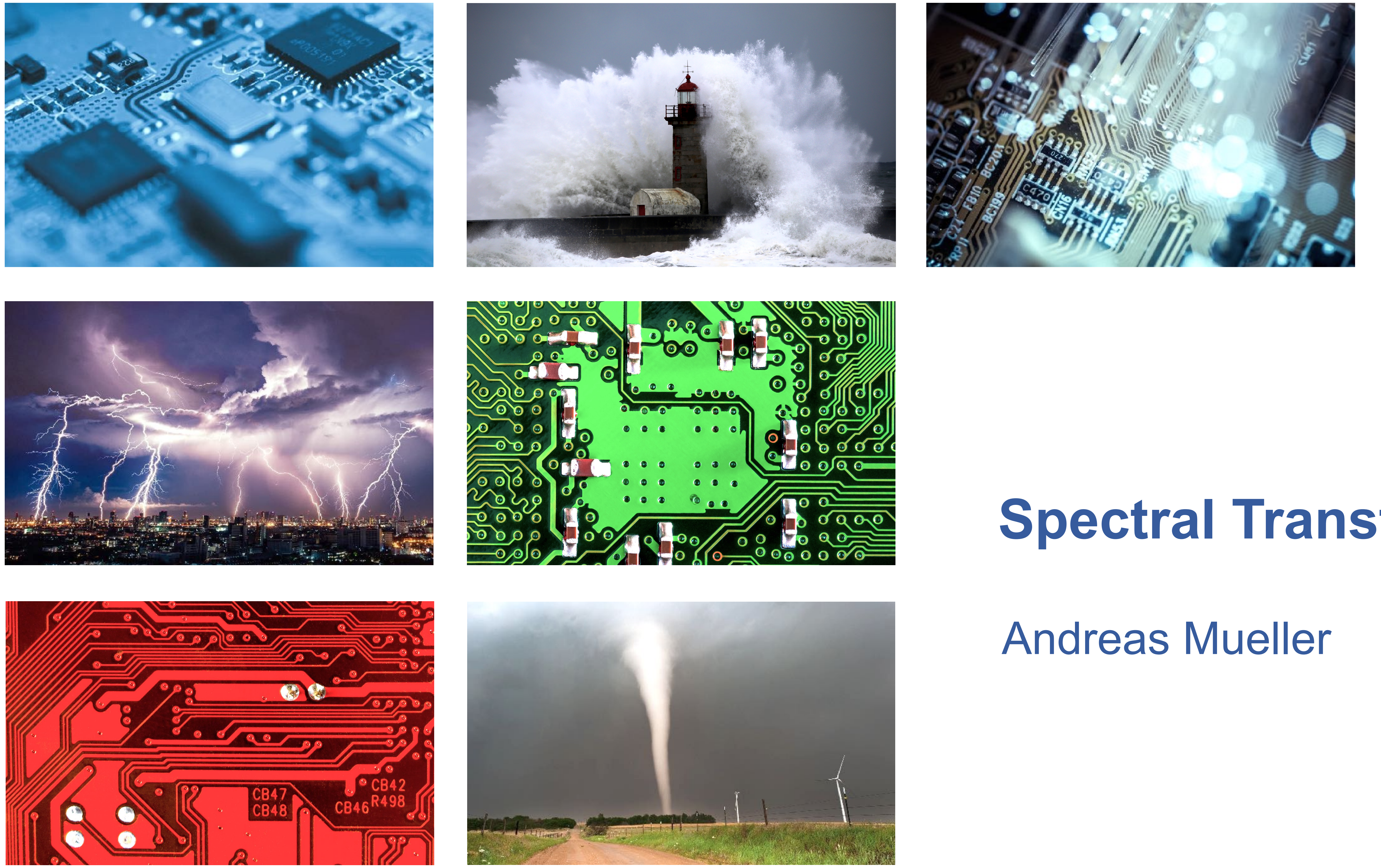

ESCAPE 2

Spectral Transform

Andreas Mueller

The ESCAPE-2 project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 800897

ESCAPE: Energy-efficient Scalable Algorithms for Weather Prediction at Exascale

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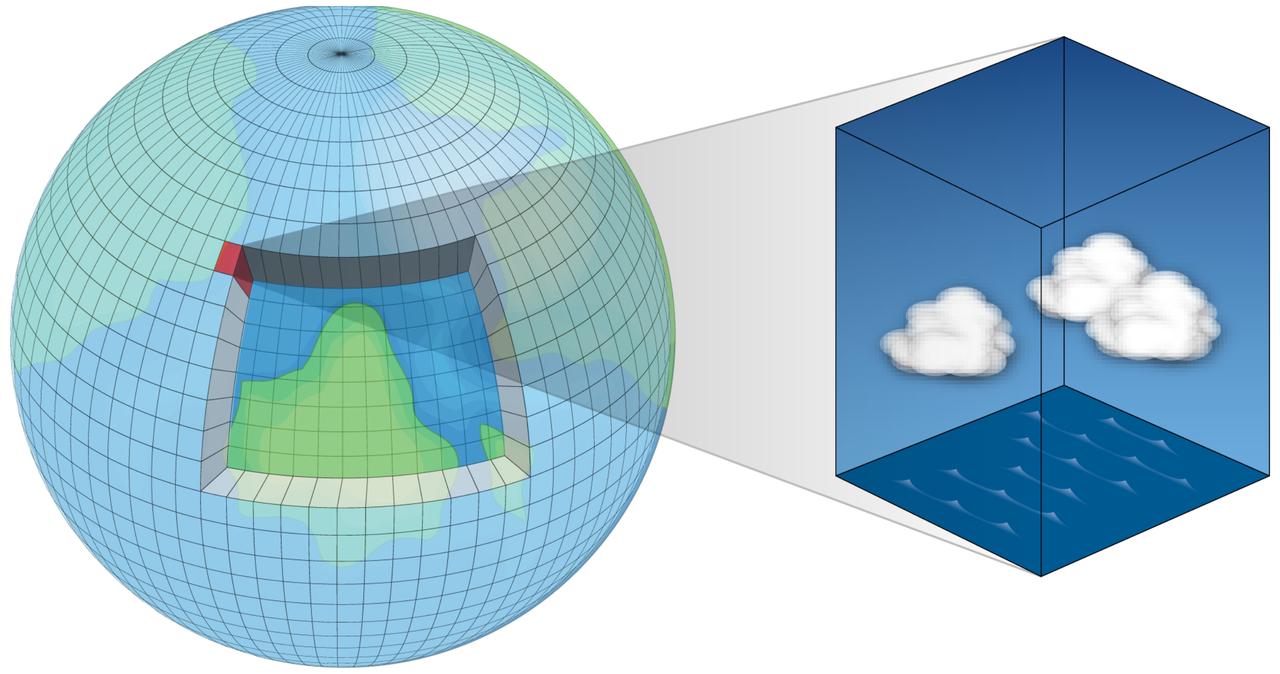
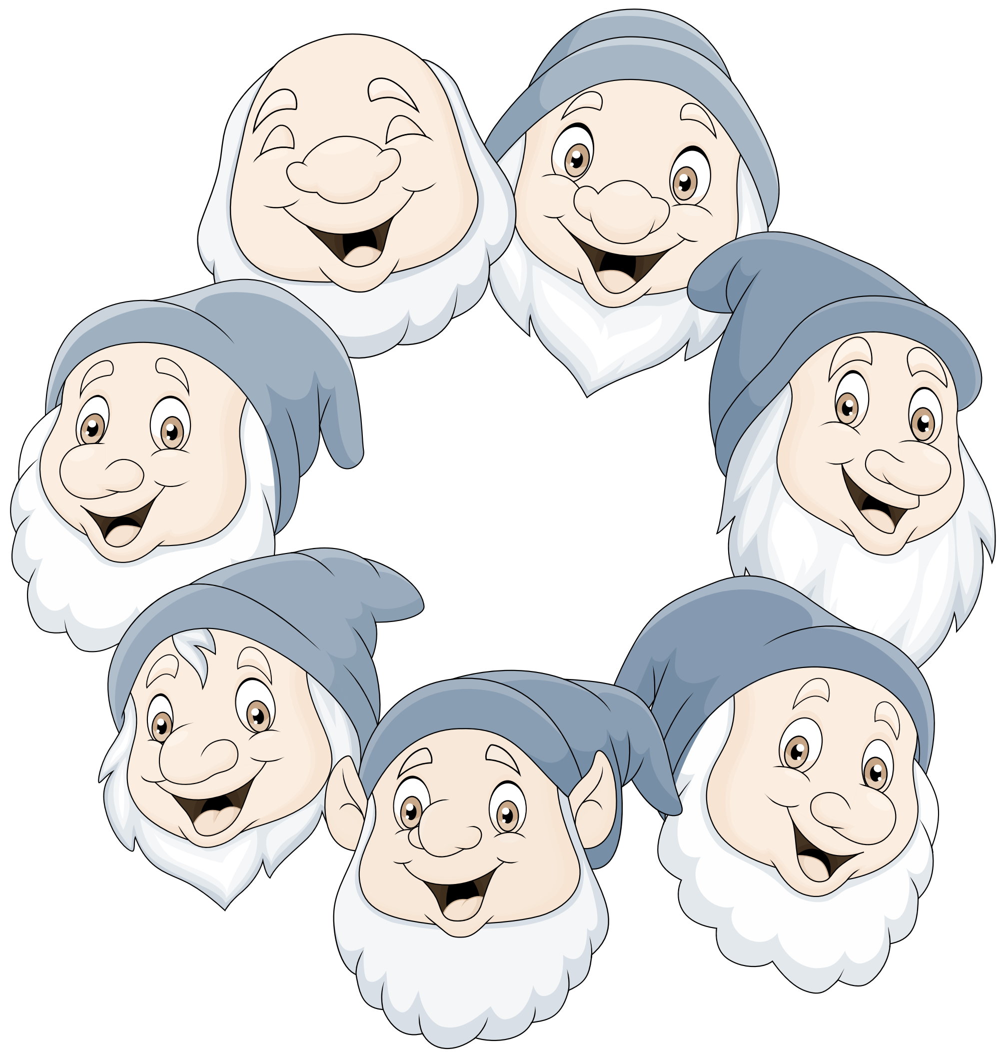


Extract model dwarfs…



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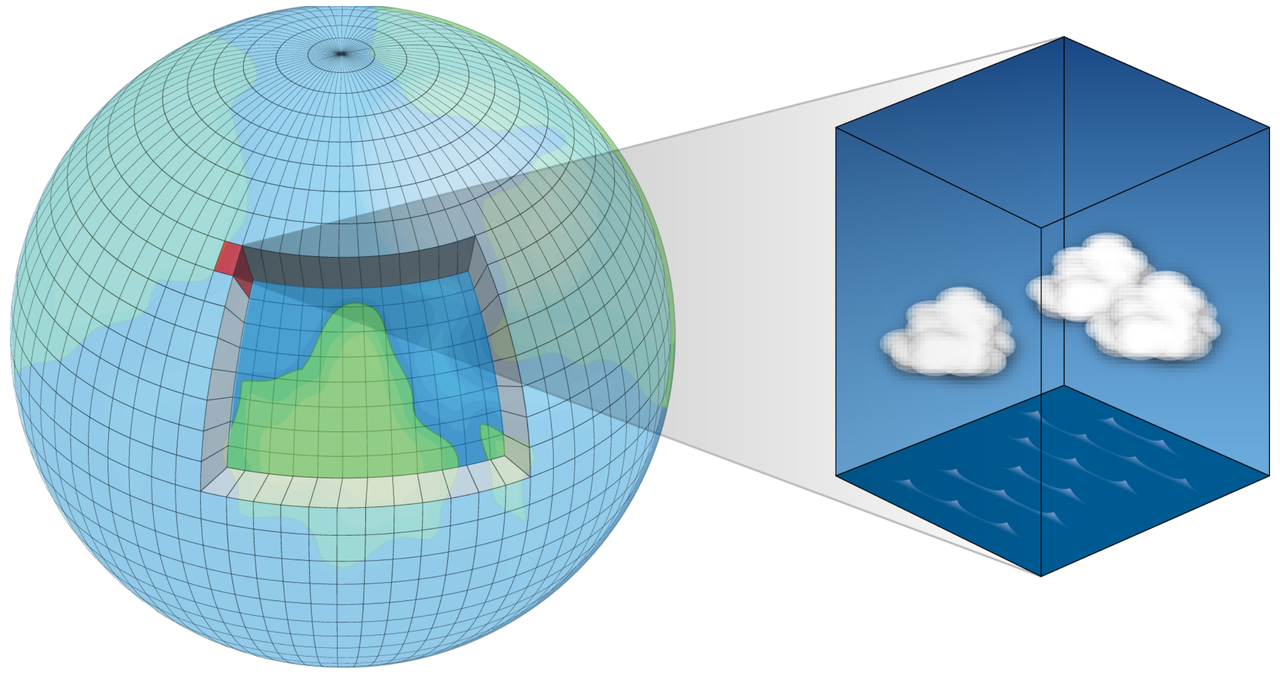
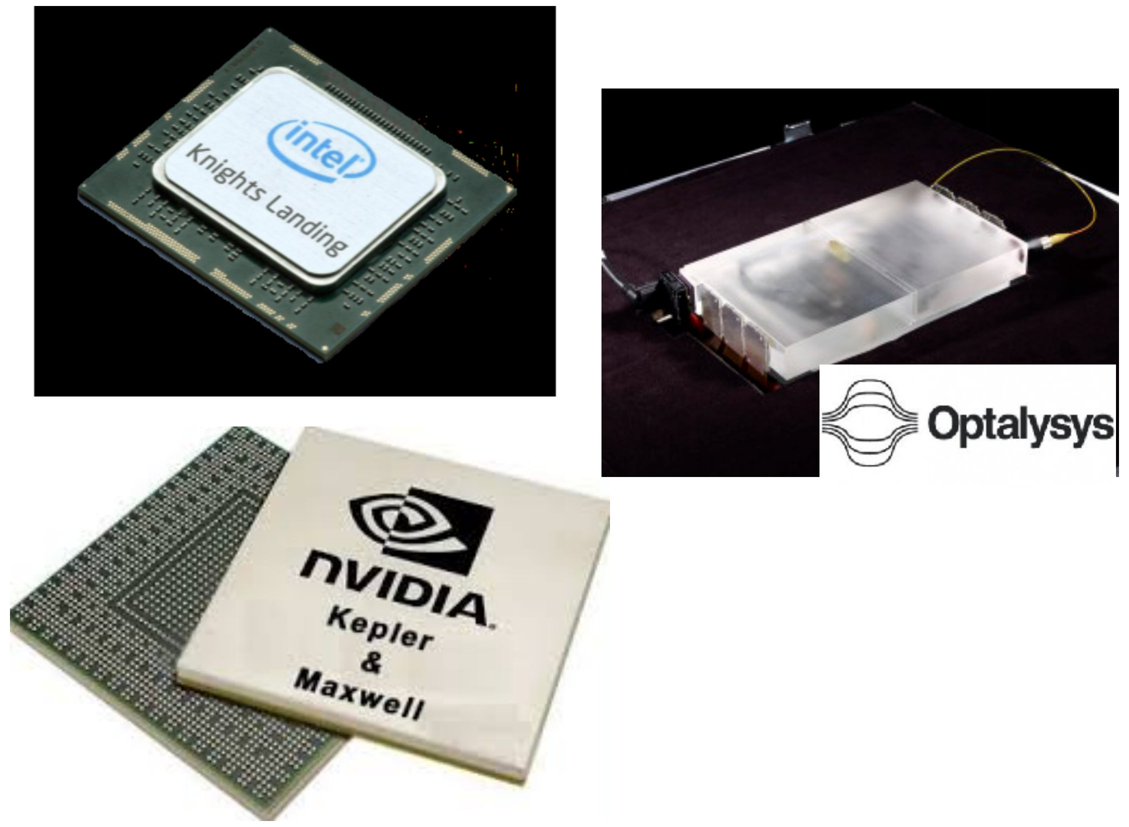


… hardware adaptation …



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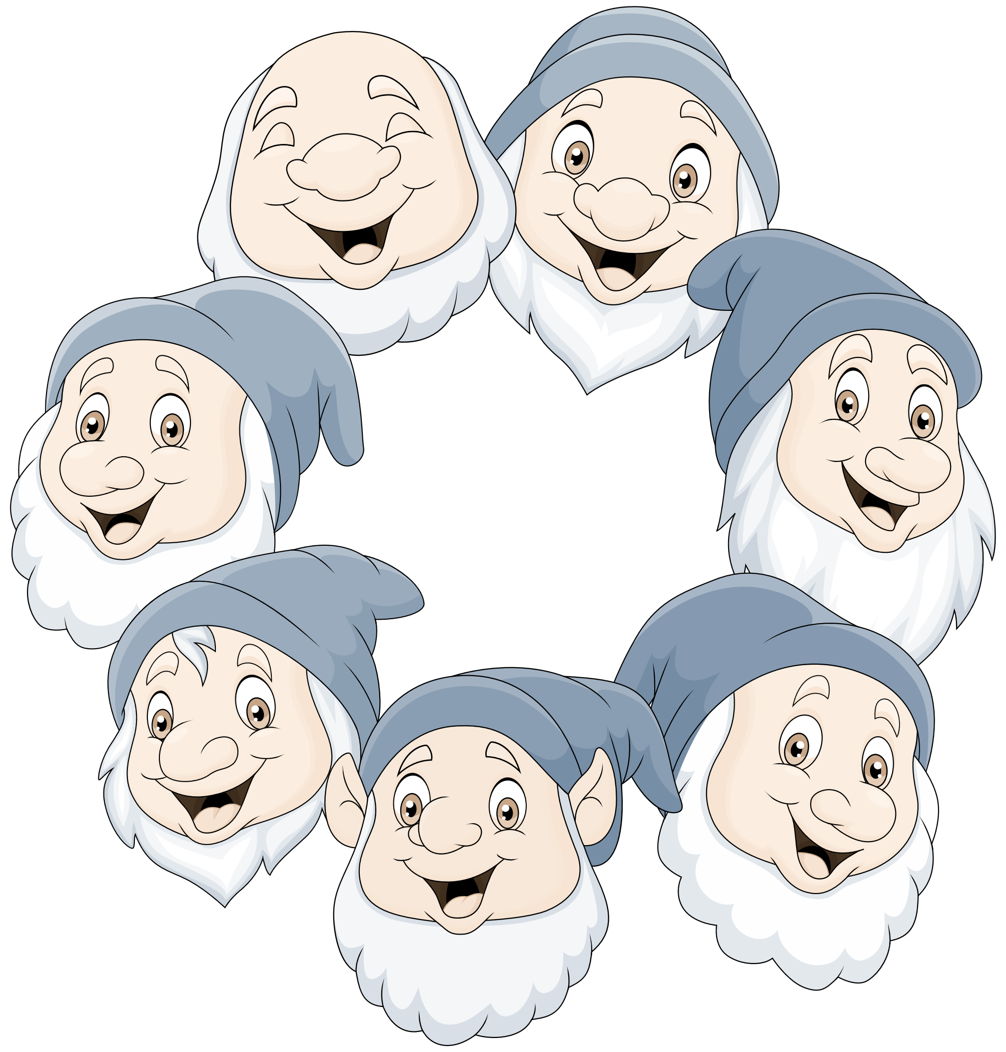

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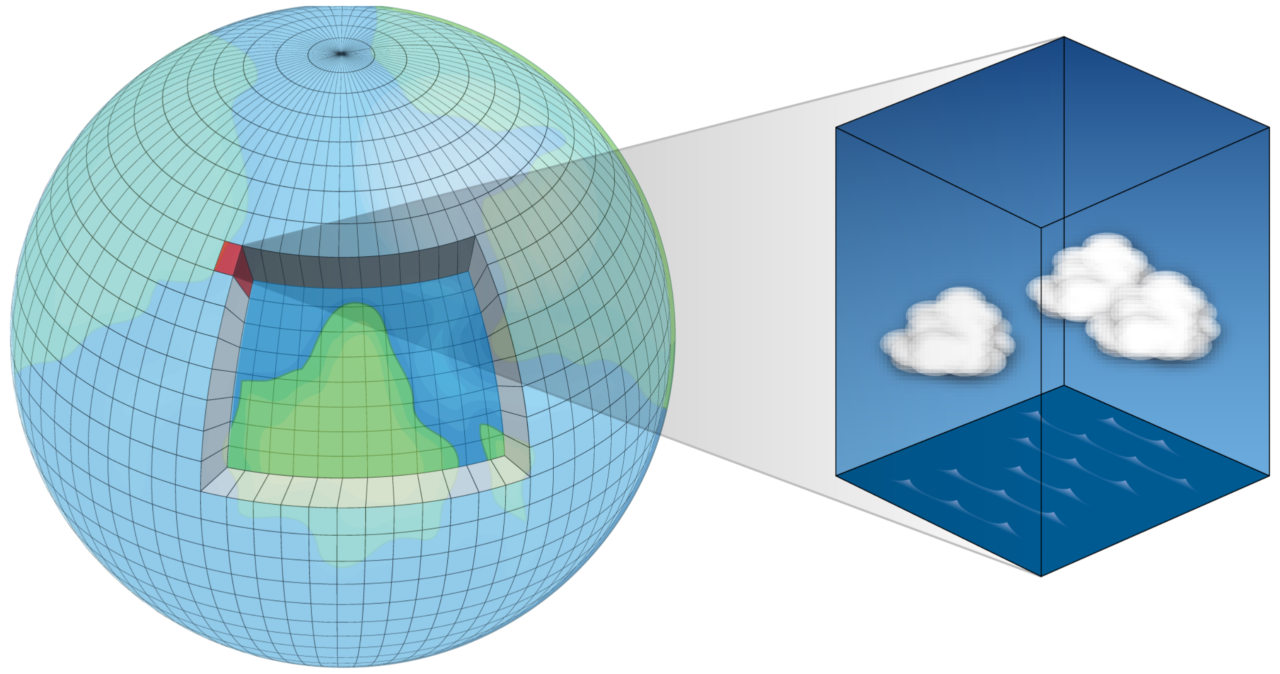

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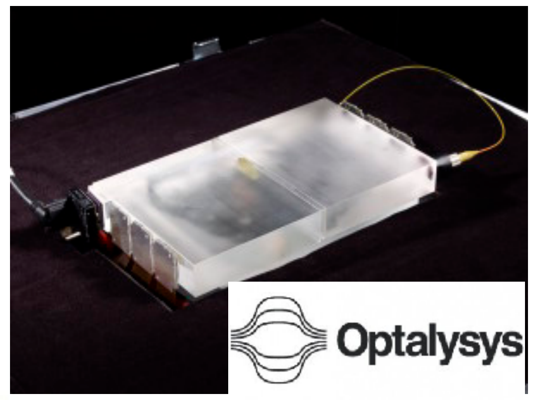

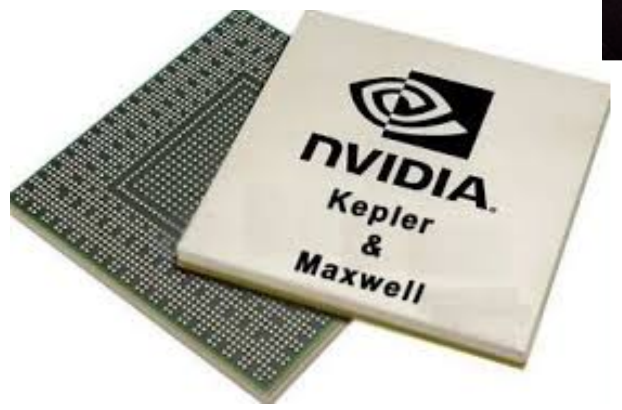

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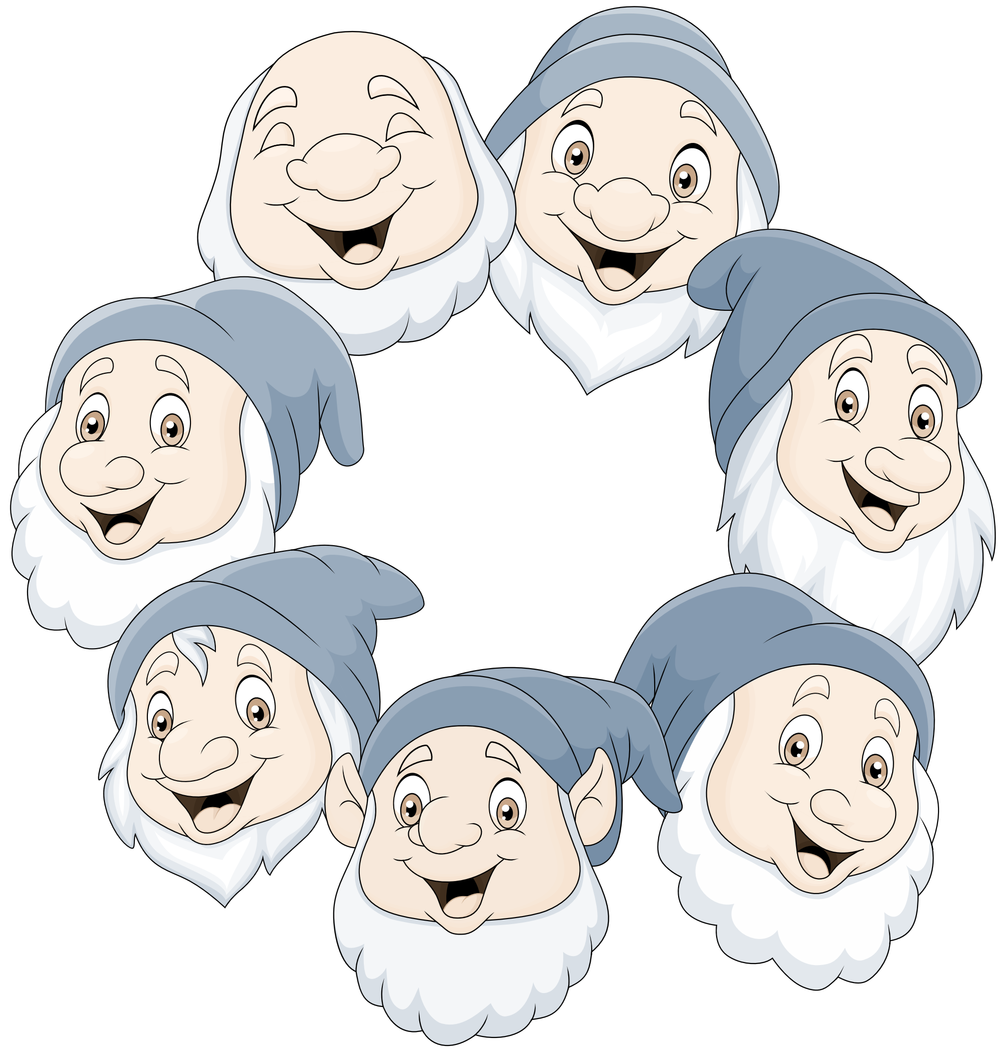
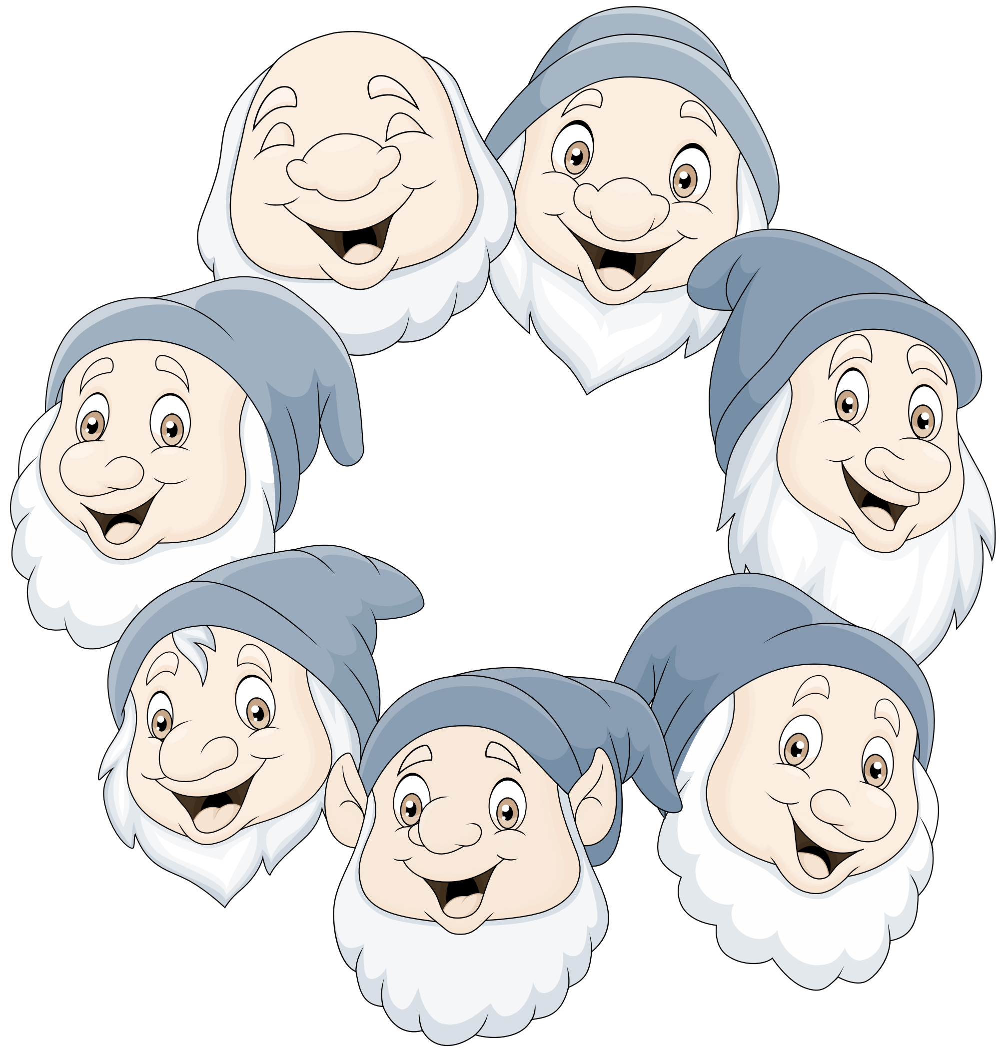


… explore alternative numerical algorithms …



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Overview

10 minutes

- Fourier transform
- Spectral transform

40 minutes

hands-on exercises:

- interactive web-app
- python notebook

IFS (Integrated Forecast System)

Funded by the European Union

technology applied at ECMWF

for the last 30 years

- spectral transform
- semi-Lagrangian
- semi-implicit

IFS (Integrated Forecast System)

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- spectral transform
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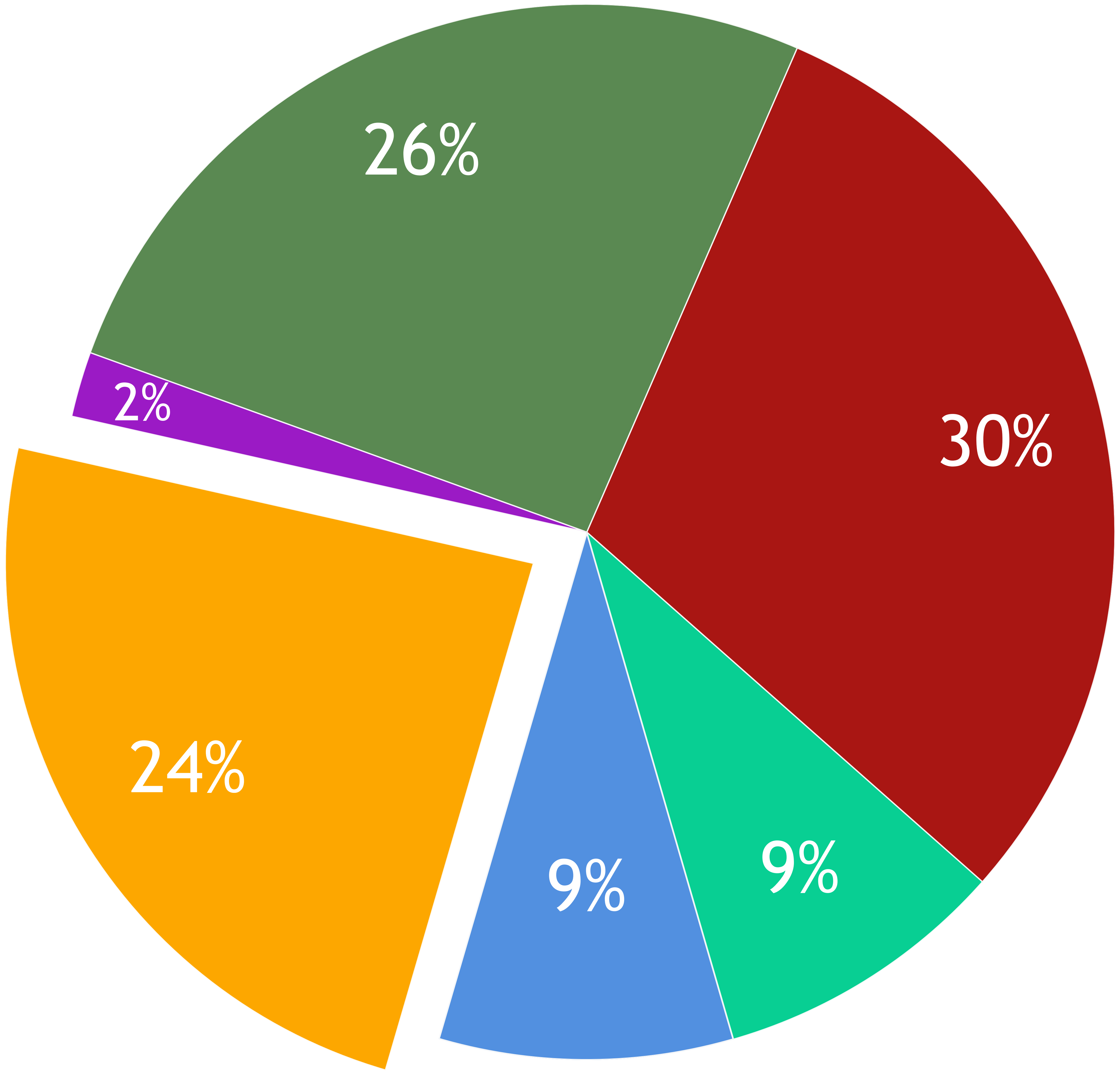
- semi-implicit

pie chart: % of runtime in 9km operational forecast

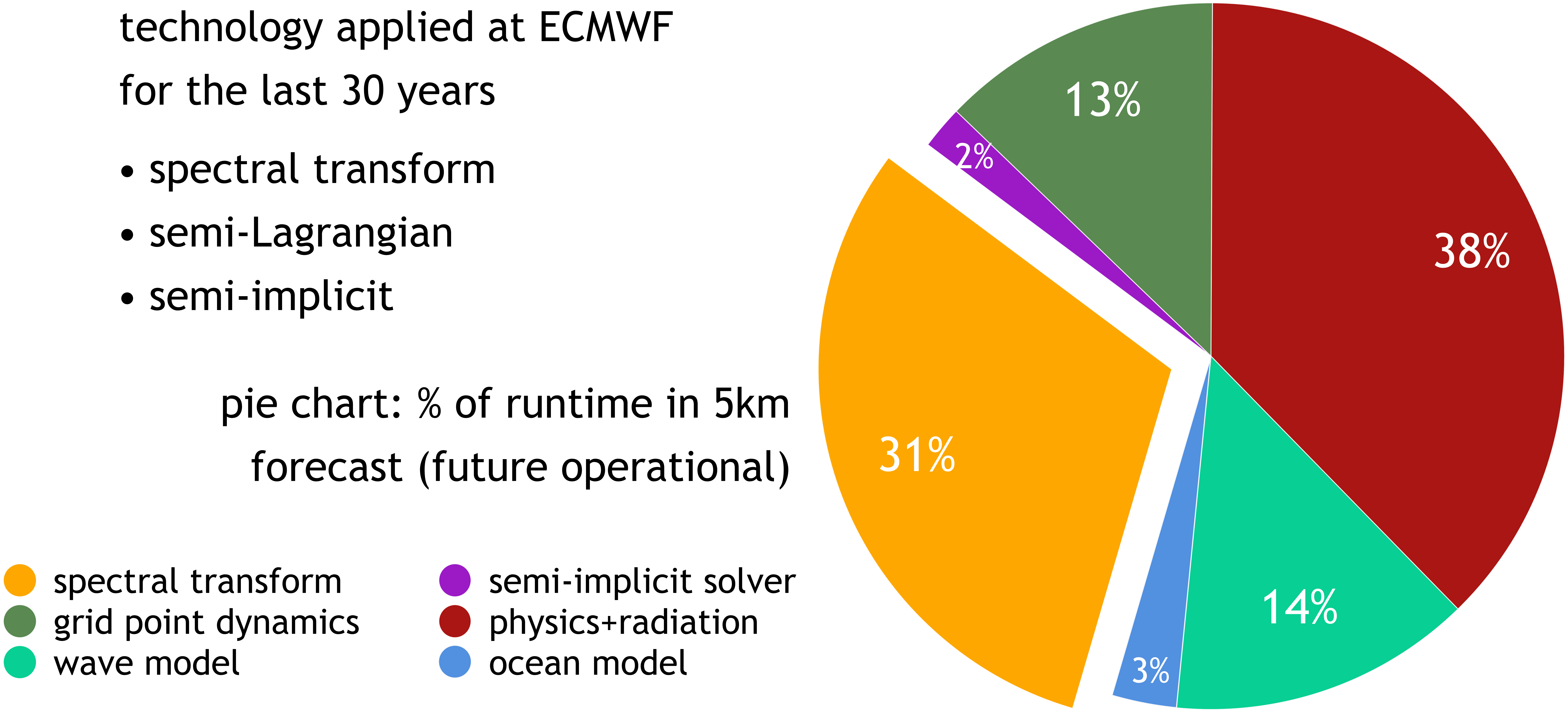


IFS (Integrated Forecast System)

technology applied at ECMWF
for the last 30 years

- spectral transform
- semi-Lagrangian
- semi-implicit

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



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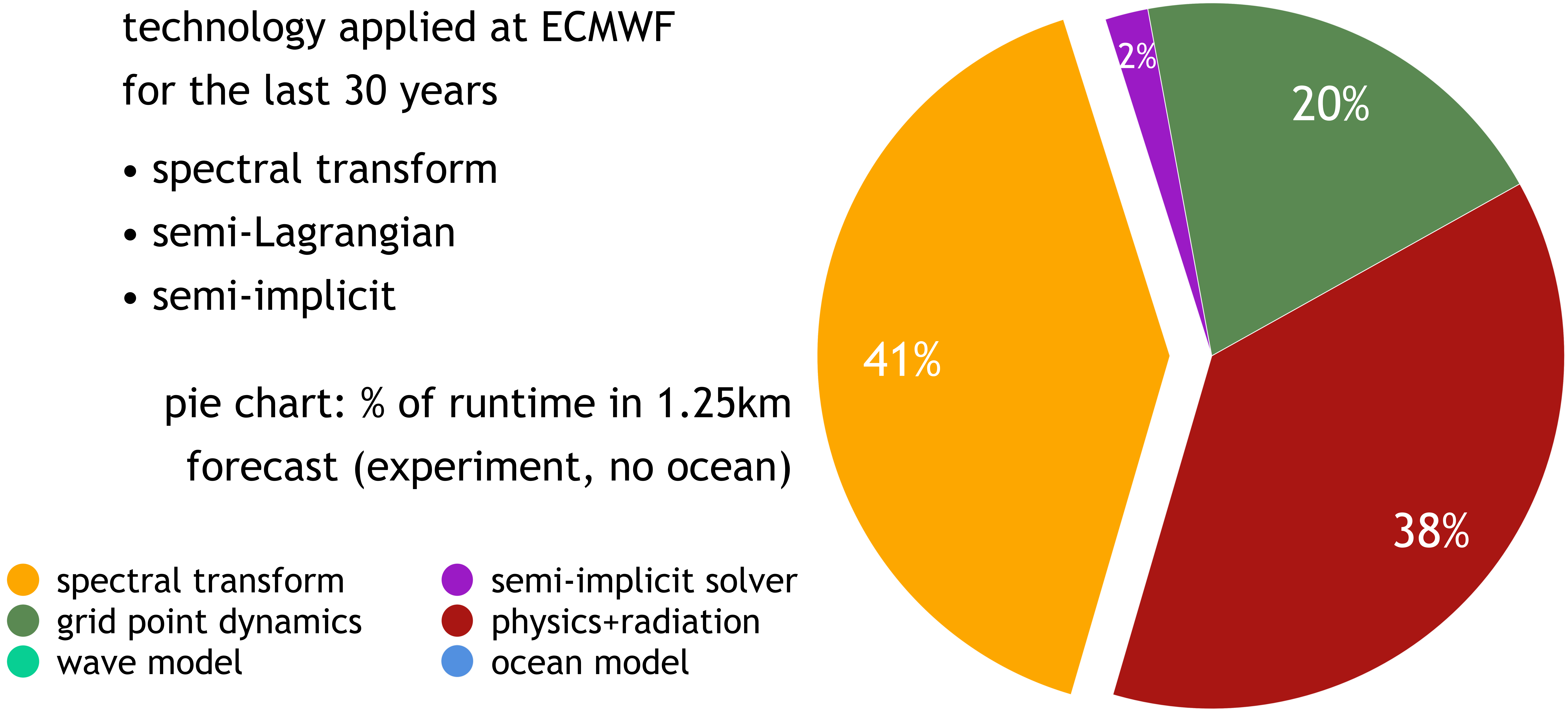
IFS (Integrated Forecast System)

technology applied at ECMWF for the last 30 years

- spectral transform
- semi-Lagrangian
- semi-implicit

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



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Fourier transform

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Fourier transform = Spectral transform in 1D

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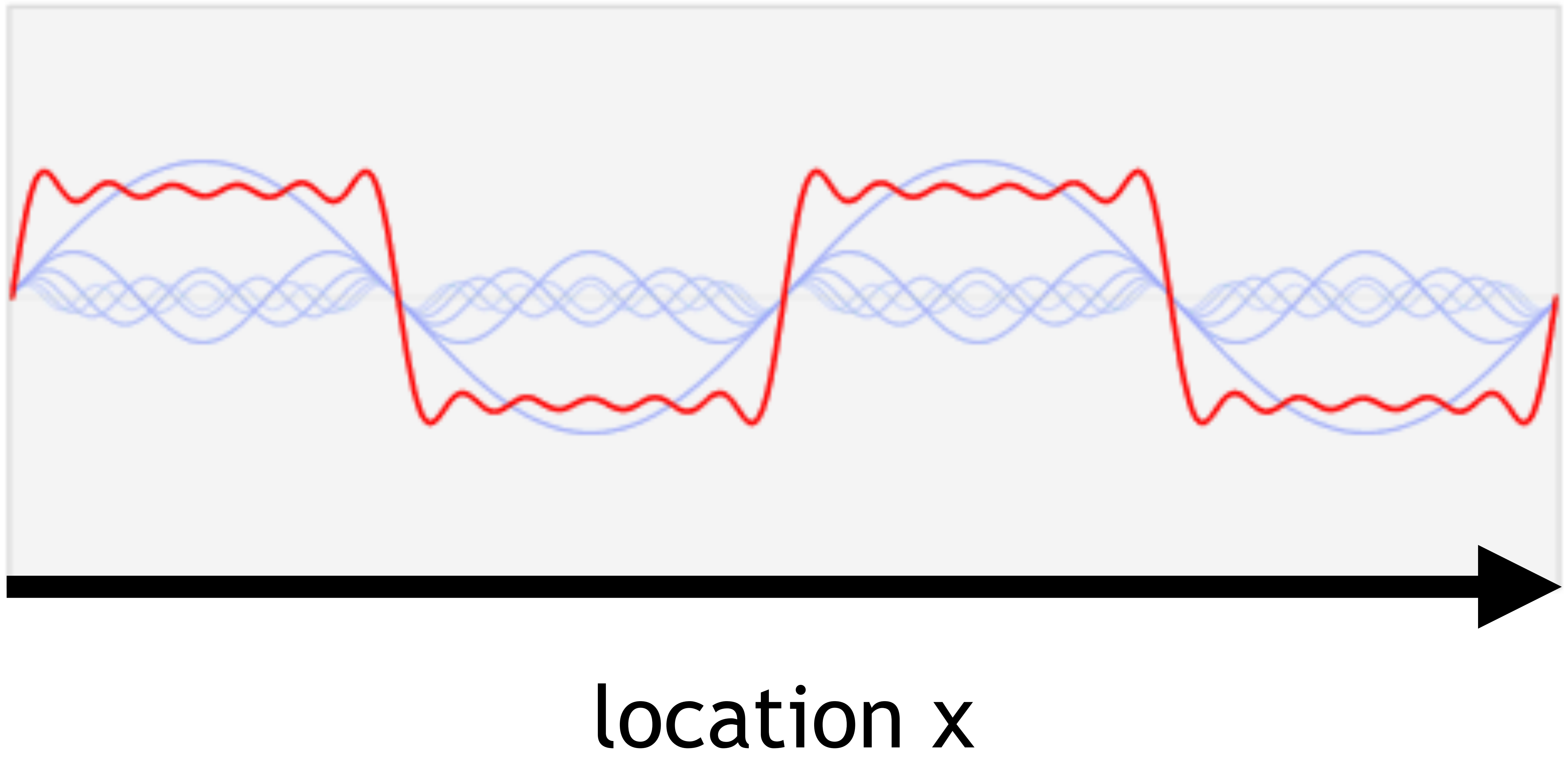
Fourier transform

Fourier transform = Spectral transform in 1D



Fourier transform

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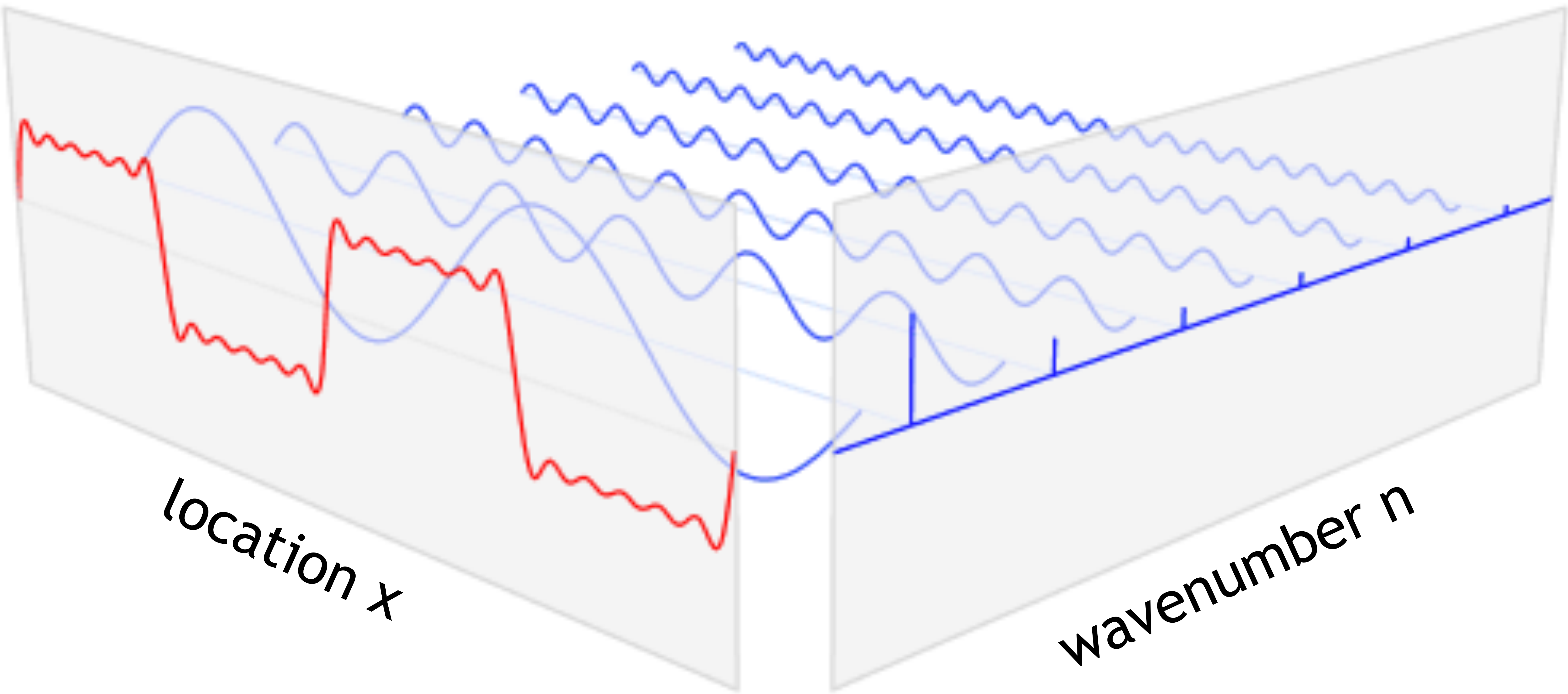
Fourier transform = Spectral transform in 1D



grid point space **Fourier space**

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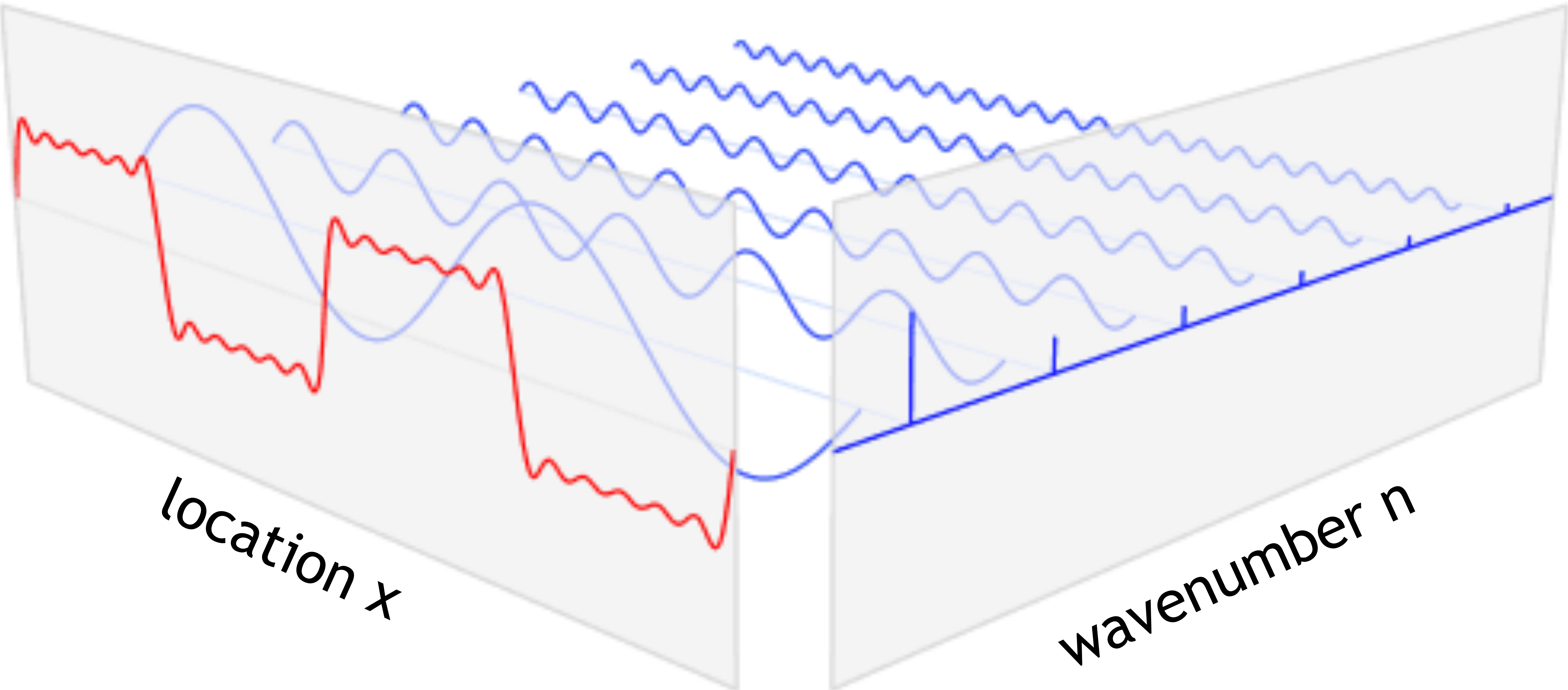
Fourier transform



function in grid point space

Fourier coefficients

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

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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

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

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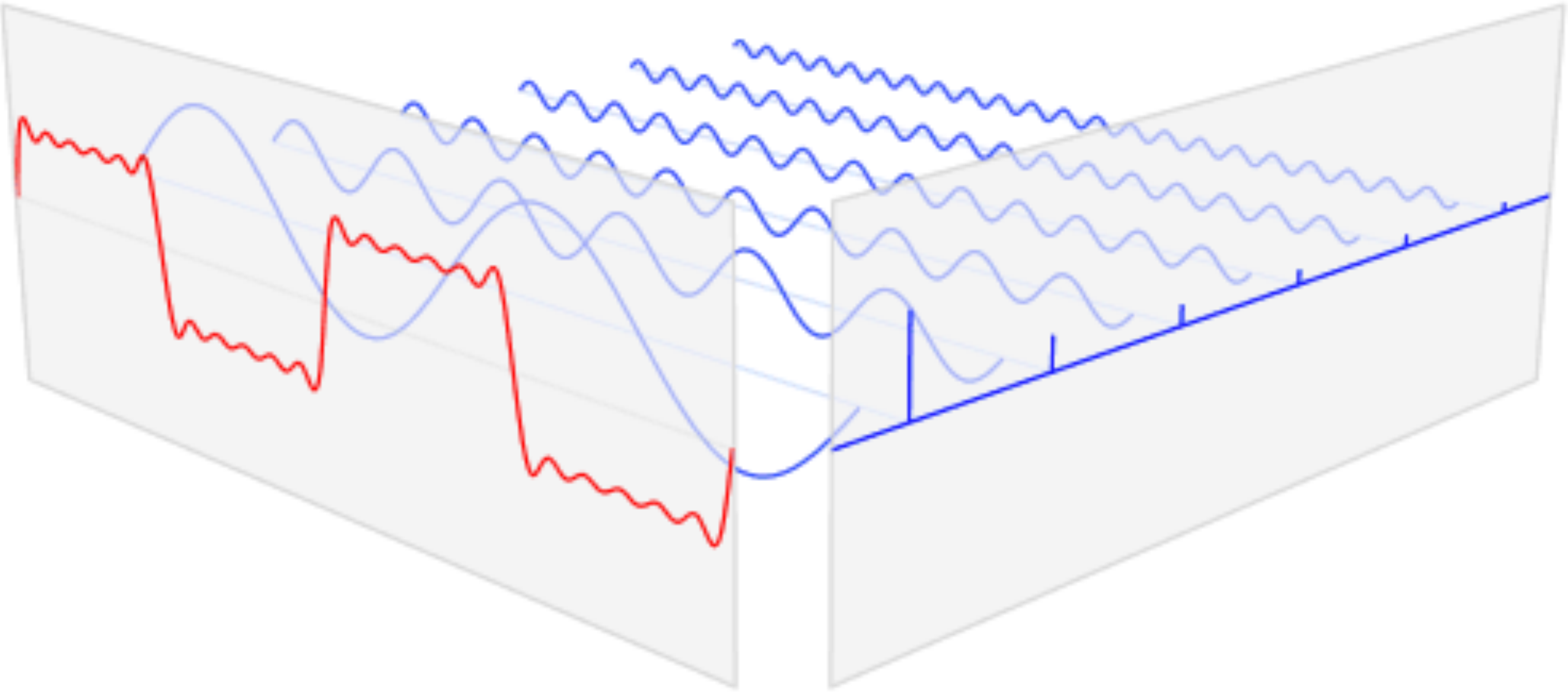
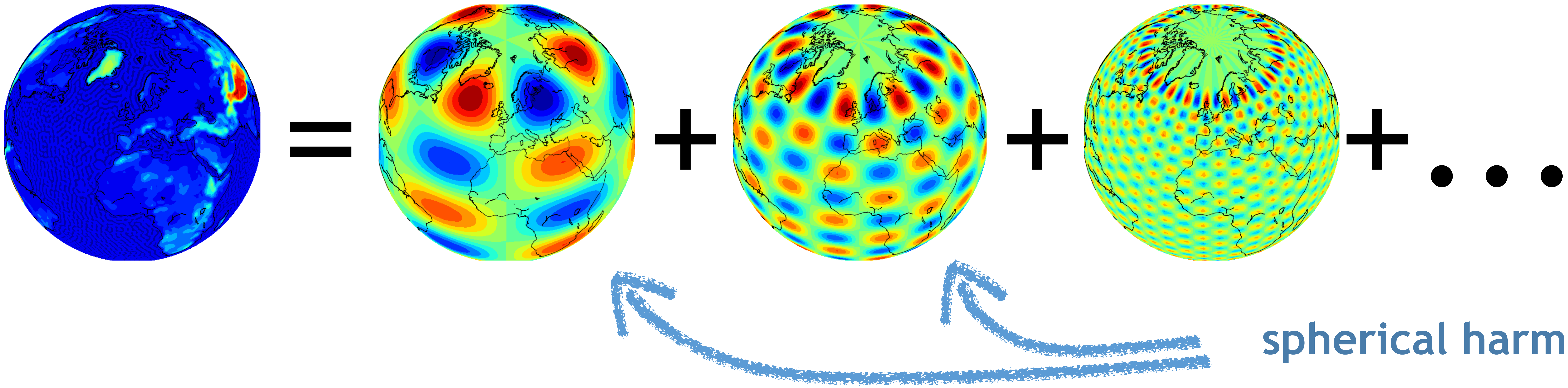
on the sphere: spectral transform



grid point space

spectral space



spherical harmonics

on the sphere: spectral transform

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Spectral coefficients

Latitude

Longitude

Spherical harmonics

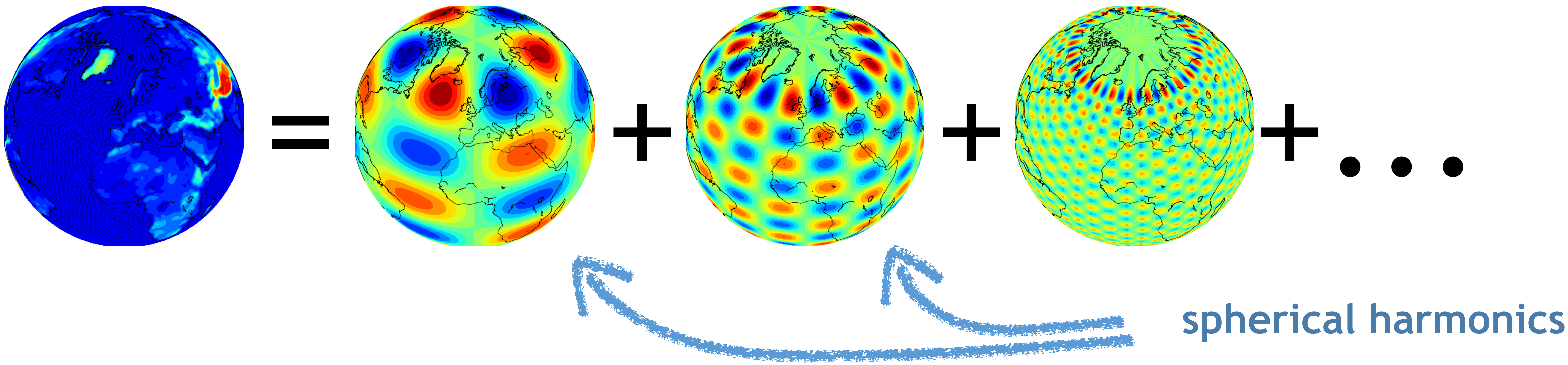
Grid point variable

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

m: zonal wavenumber
n: total wavenumber
M: truncation

grid point space

spectral space



on the sphere: spectral transform

Funded by the European Union

Spectral coefficients

Latitude

Longitude

Spherical harmonics

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

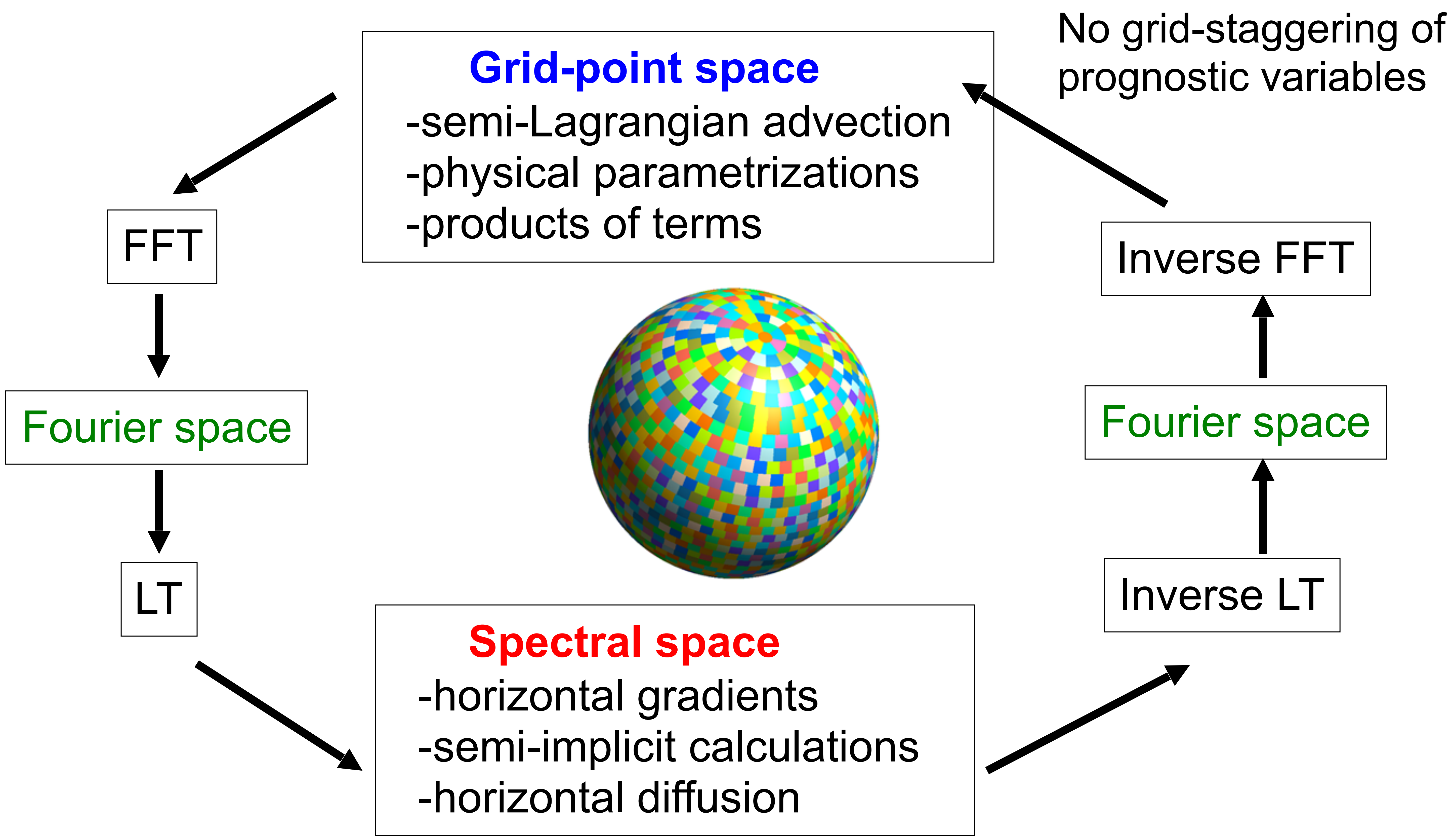
$$f(\phi, \lambda) = \Re\left(\sum_{m=0}^{M} \mathrm{e}^{im\lambda} \sum_{n=m}^{M} f_{m,n} P_n^m(\phi)\right)$$

Legendre transform

Fourier transform

Funded by the European Union

time step in IFS



FFT: Fast Fourier Transform, LT: Legendre Transform

hands-on session

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for everyone: interactive web-app about spectral transform

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

optional: step 2: Python course

in the classroom:
/home/users/swx18100/Monday_training/spectral/install.sh

in the cloud:
https://notebooks.azure.com/anmrde/libraries/tcnm2019
click on clone

files:

exercises.ipynb, TCNM2019.ipynb: Python notebook with exercises
solution.ipynb, TCNM2019solution.ipynb: notebook including sample solutions

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aliasing

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

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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

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aliasing

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

aliasing

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

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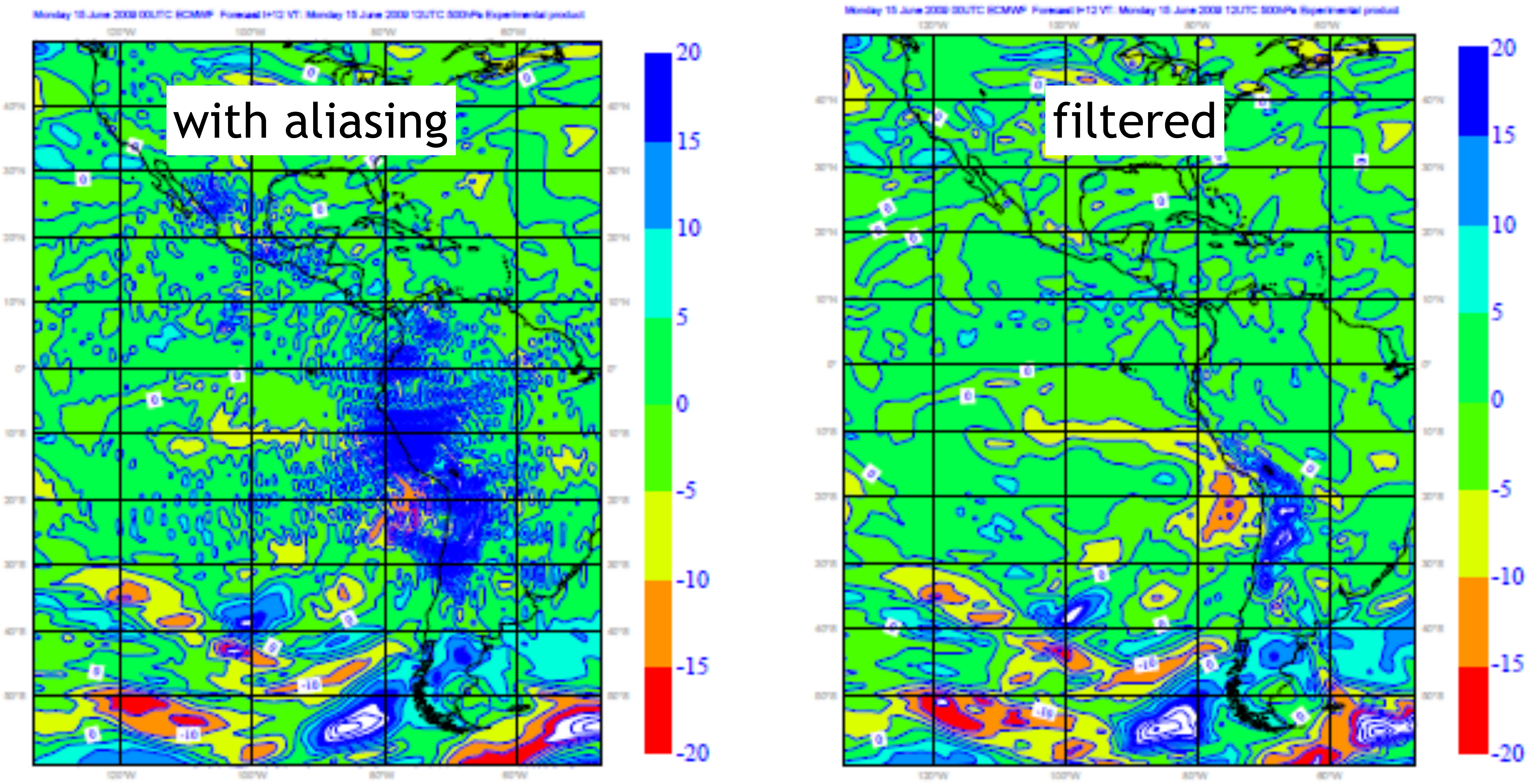
aliasing example

500hPa adiabatic zonal wind tendencies (T159)



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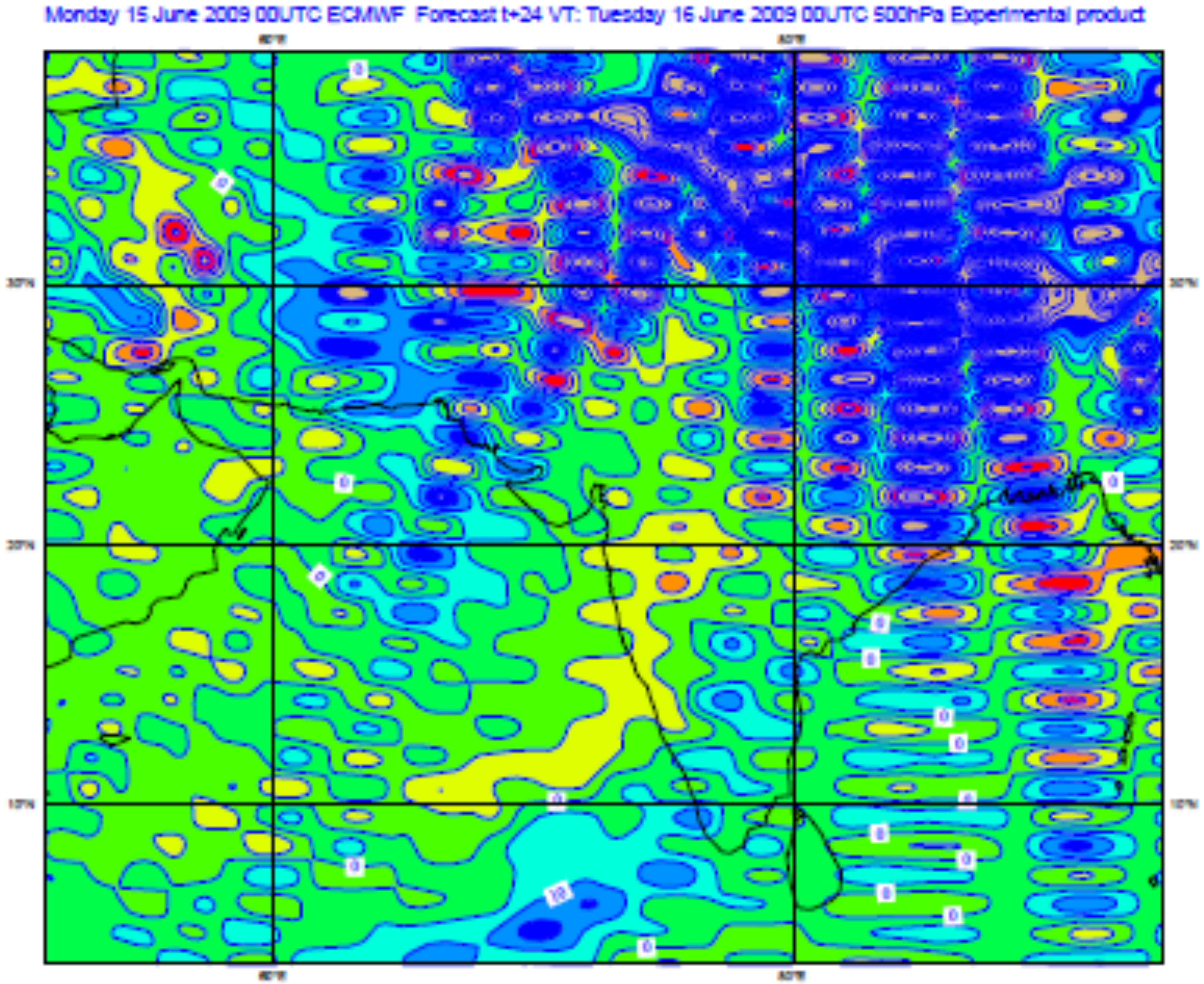
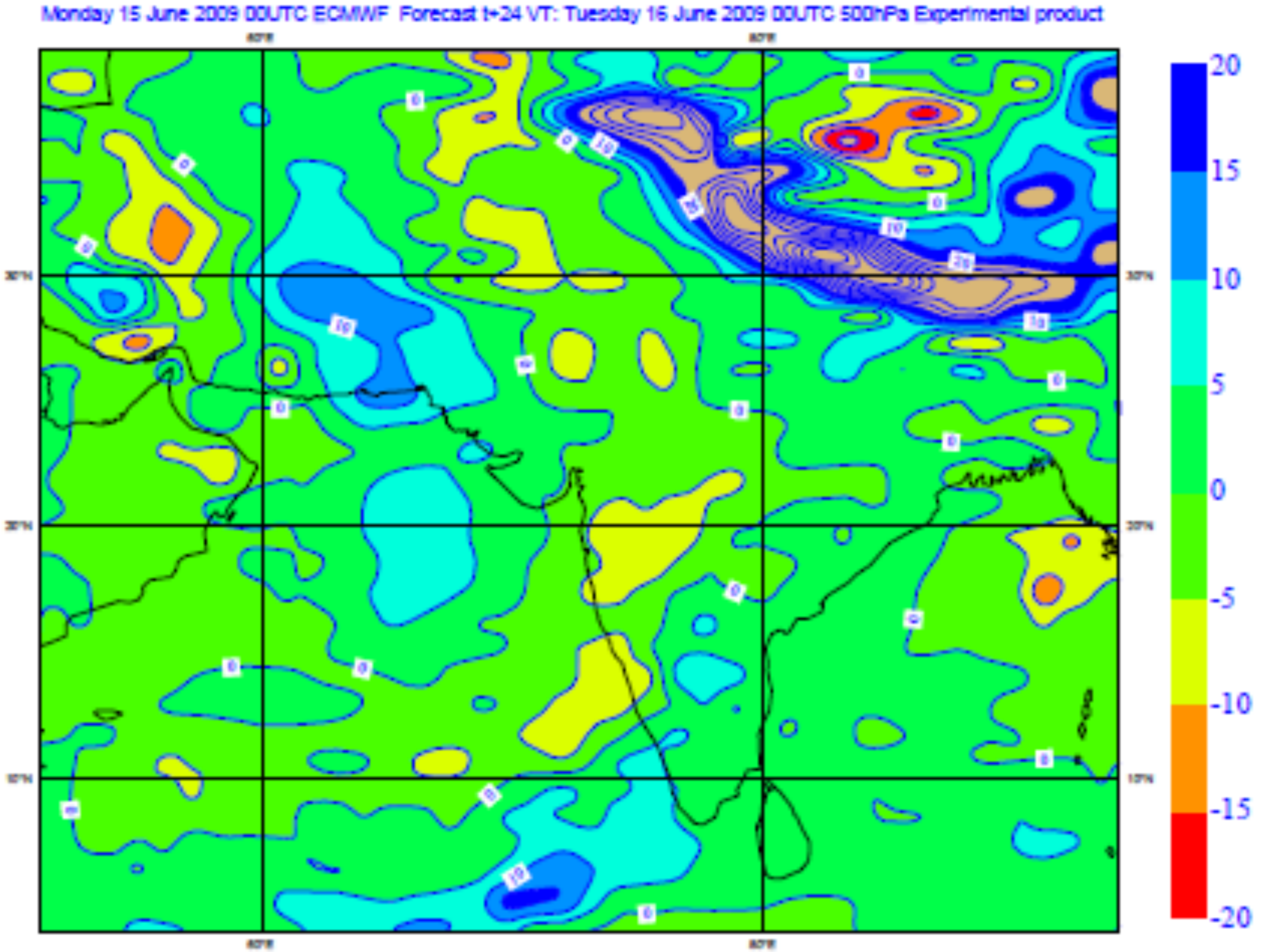
aliasing example

500hPa adiabatic meridional wind tendencies (T159)

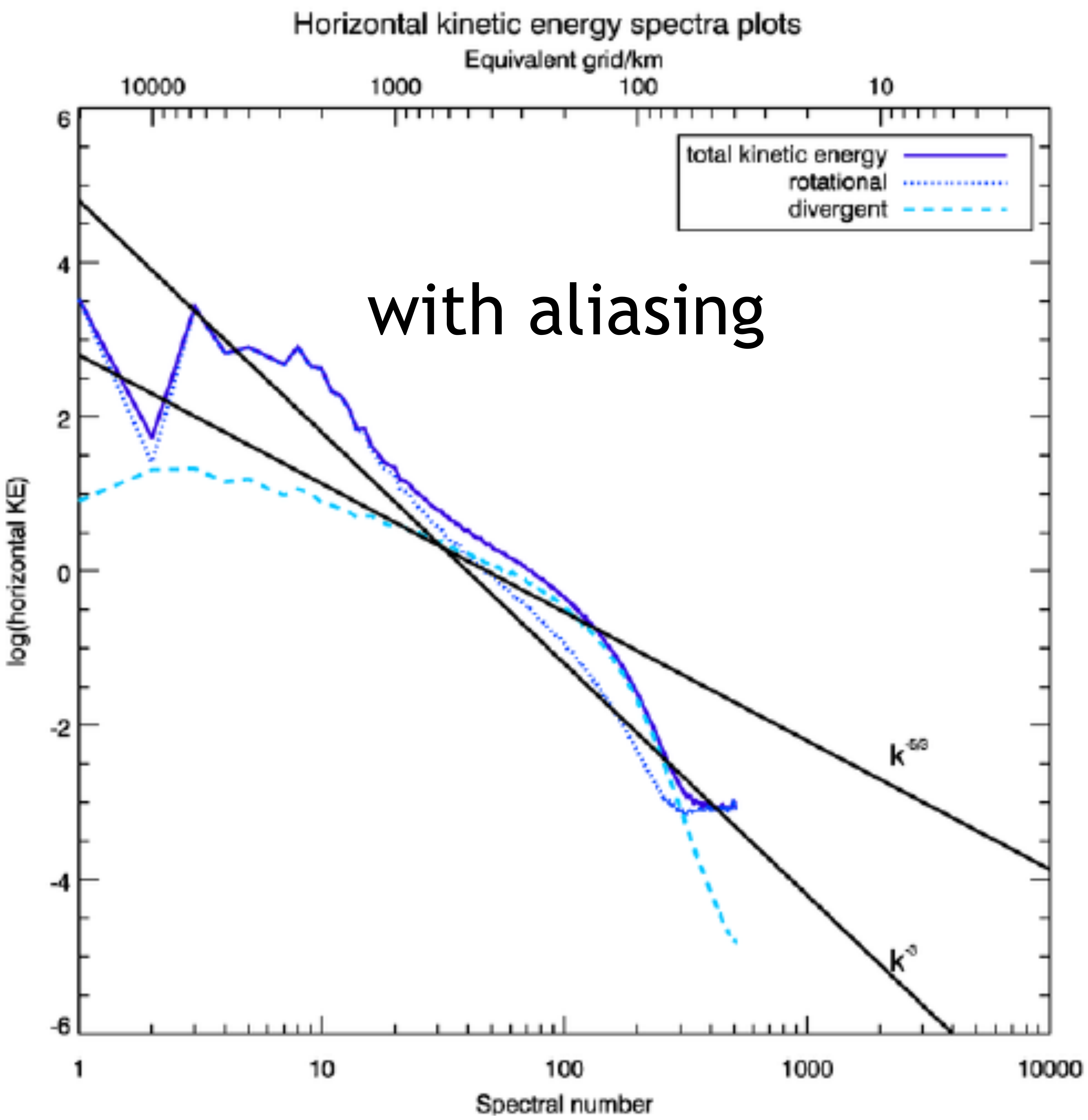
with aliasing

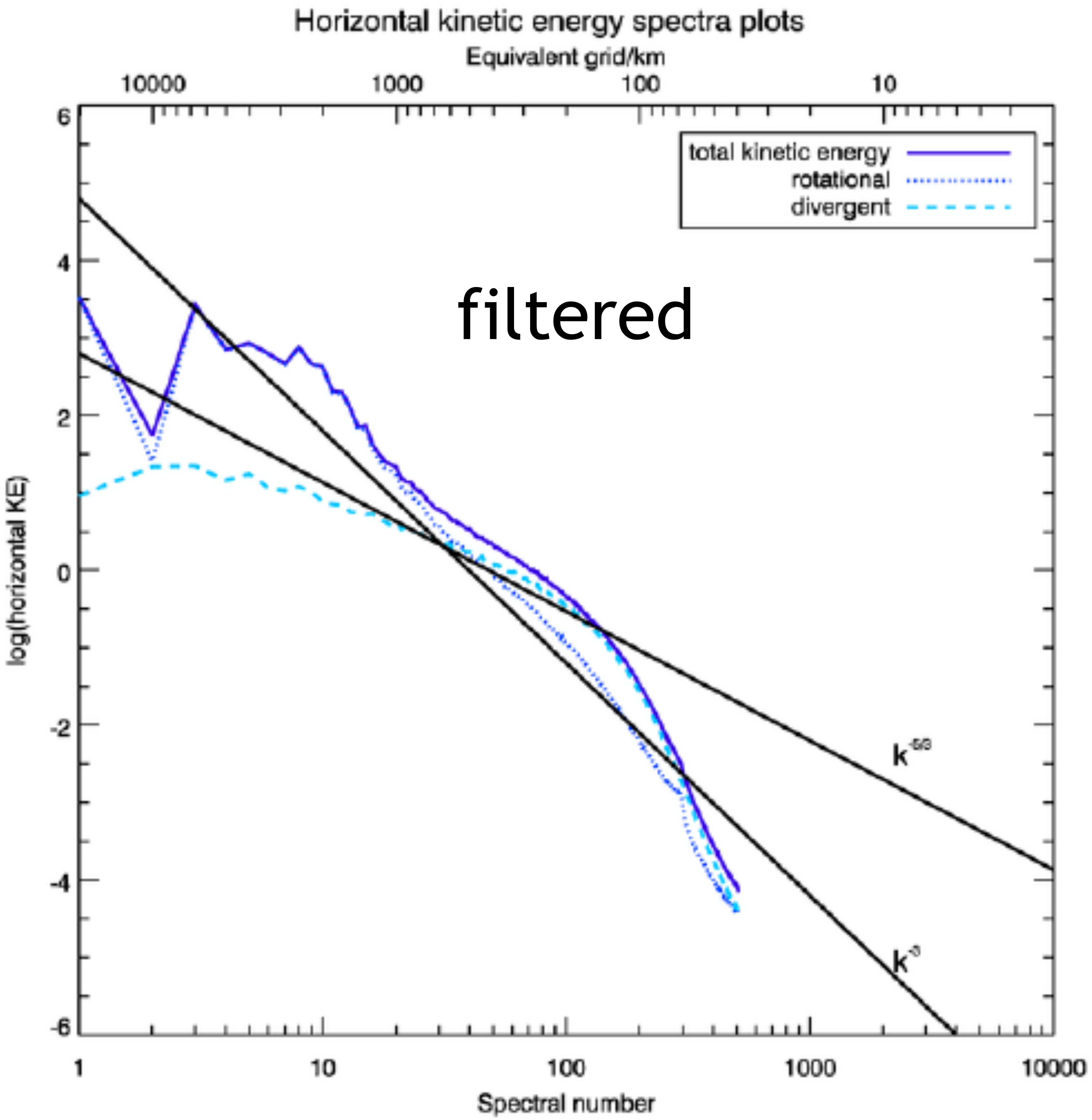


filtered



aliasing example
kinetic energy spectra, 100 hPa





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alternatives to using a filter

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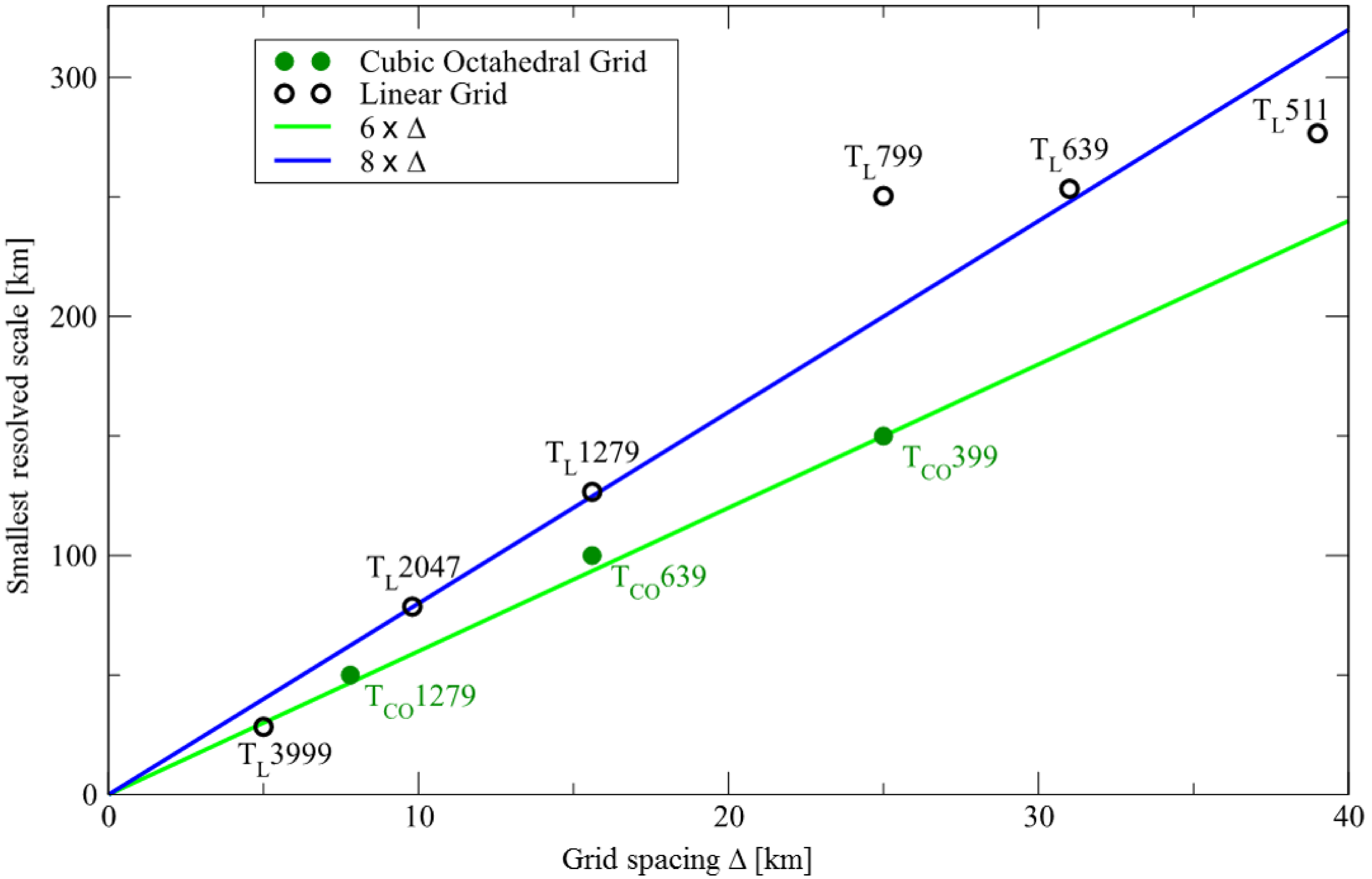
Idea: use more grid points than spectral coefficients

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 *(Wedi, 2014)*
	Spatial filter range

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:

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

matrix multiplications

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inverse spectral transform

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matrix multiplications

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

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

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inverse spectral transform

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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

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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

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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

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

inverse Fourier transform

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

grid point space

inverse spectral transform

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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

ESCAPE 2

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

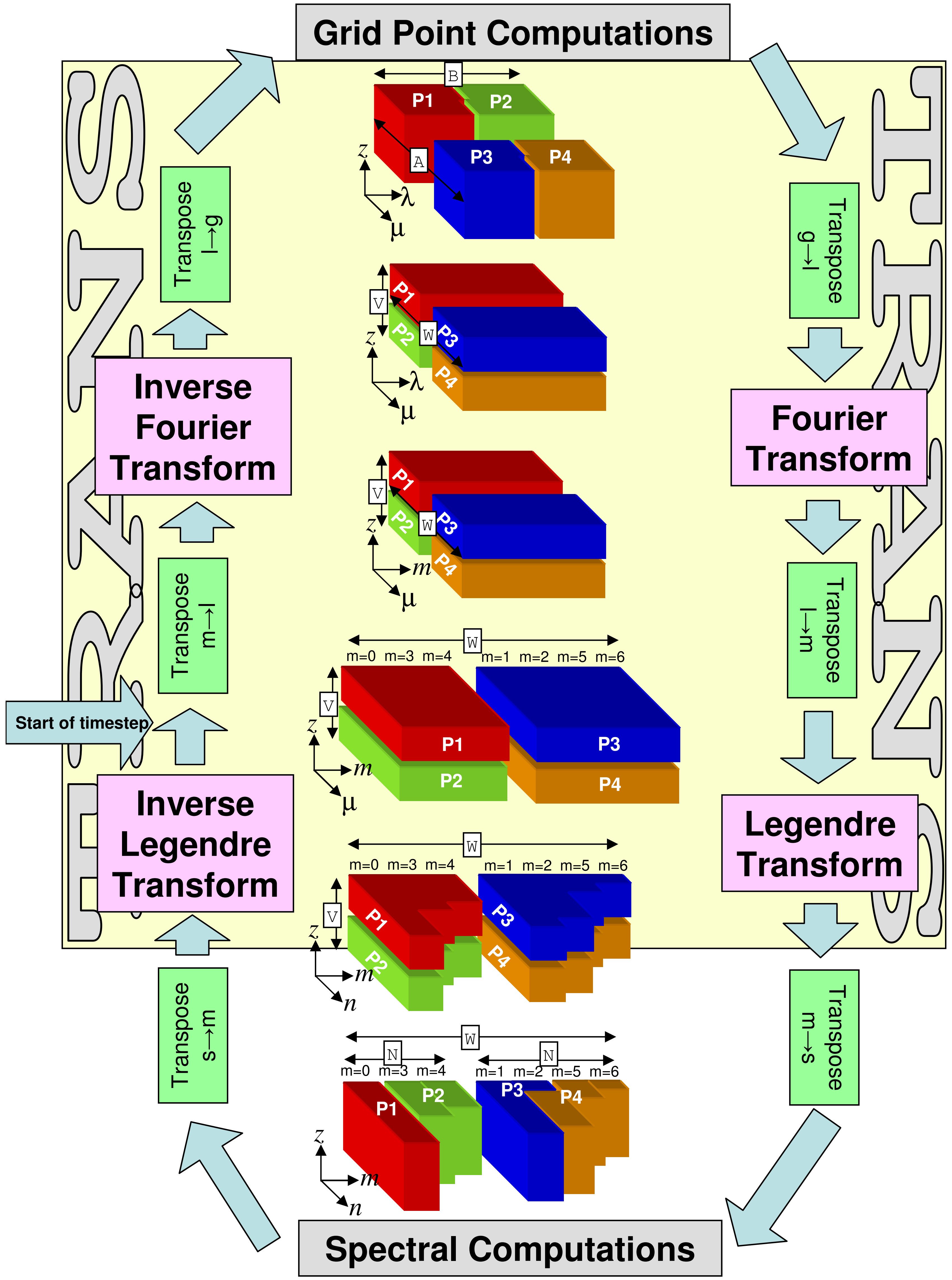
spectral space	m,n
inverse Legendre transform	m,f
inverse Fourier transform	ϕ,f
grid point space	ϕ,λ

parallelisation over these indices

lots of MPI communication

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

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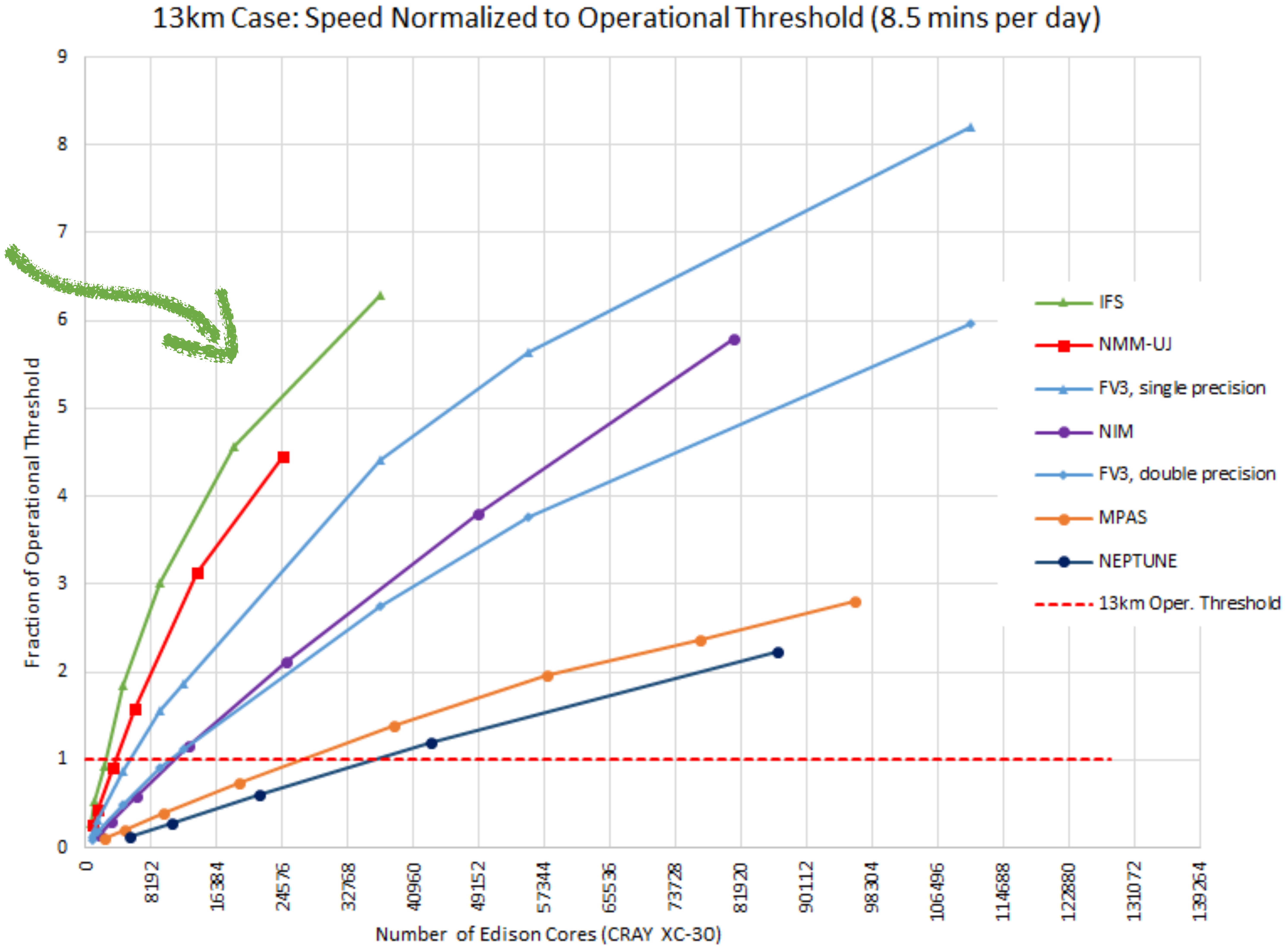
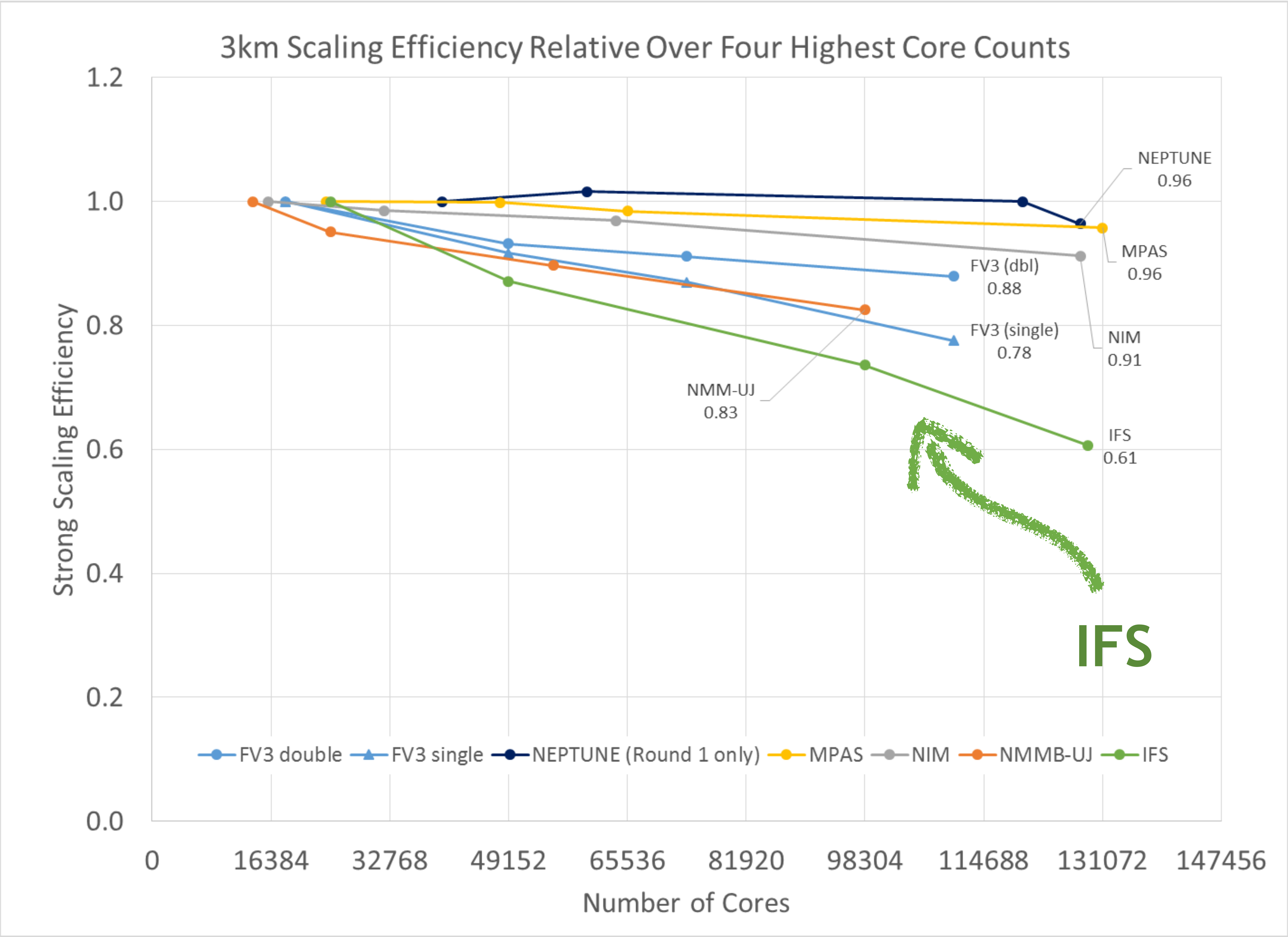
IFS



(Michalakes et al, NGGPS AVEC report, 2015)

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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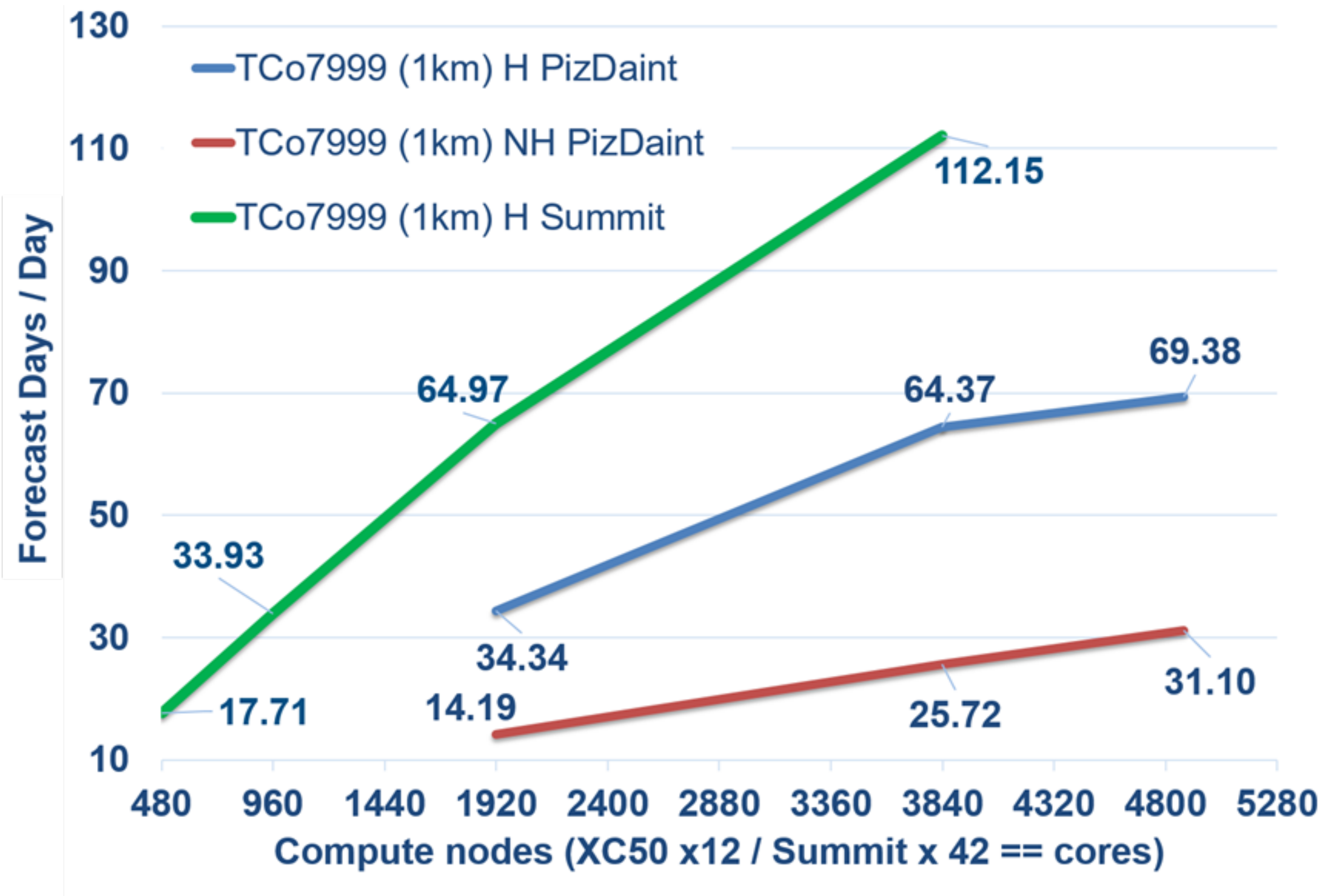


ESCAPE 2

spectral transform vs discontinuous Galerkin

projected for 5km 2-day forecast

Funded by the European Union

	DG, horizontally explicit => 4s time-step, almost no communication
communication volume:	**34 TB on 2880 MPI procs**
time to solution:	**4 hours**

ESCAPE 2

Funded by the European Union

spectral transform vs discontinuous Galerkir

projected for 5km 2-day forecast

	DG, horizontally explicit => 4s time-step, almost no communication	IFS (spectral transform): 240s time-step, lots of communication
communication volume:	**34 TB on 2880 MPI procs**	**427 TB on 2880 MPI procs**
time to solution:	**4 hours**	

spectral transform vs discontinuous Galerkin

projected for 5km 2-day forecast

Funded by the European Union

	DG, horizontally explicit => 4s time-step, almost no communication	IFS (spectral transform): 240s time-step, lots of communication
communication volume:	**34 TB on 2880 MPI procs**	**427 TB on 2880 MPI procs**
time to solution:	**4 hours**	**12 minutes**

spectral transform vs discontinuous Galerkir

projected for 5km 2-day forecast

Funded by the European Union

	DG, horizontally explicit => 4s time-step, almost no communication	IFS (spectral transform): 240s time-step, lots of communication	DG (like on the left)
communication volume:	**34 TB on 2880 MPI procs**	**427 TB on 2880 MPI procs**	**689 TB on 57600 MPI procs**
time to solution:	**4 hours**	**12 minutes**	**12 minutes**

optimisations by NVIDIA in ESCAPE

Funded by the European Union

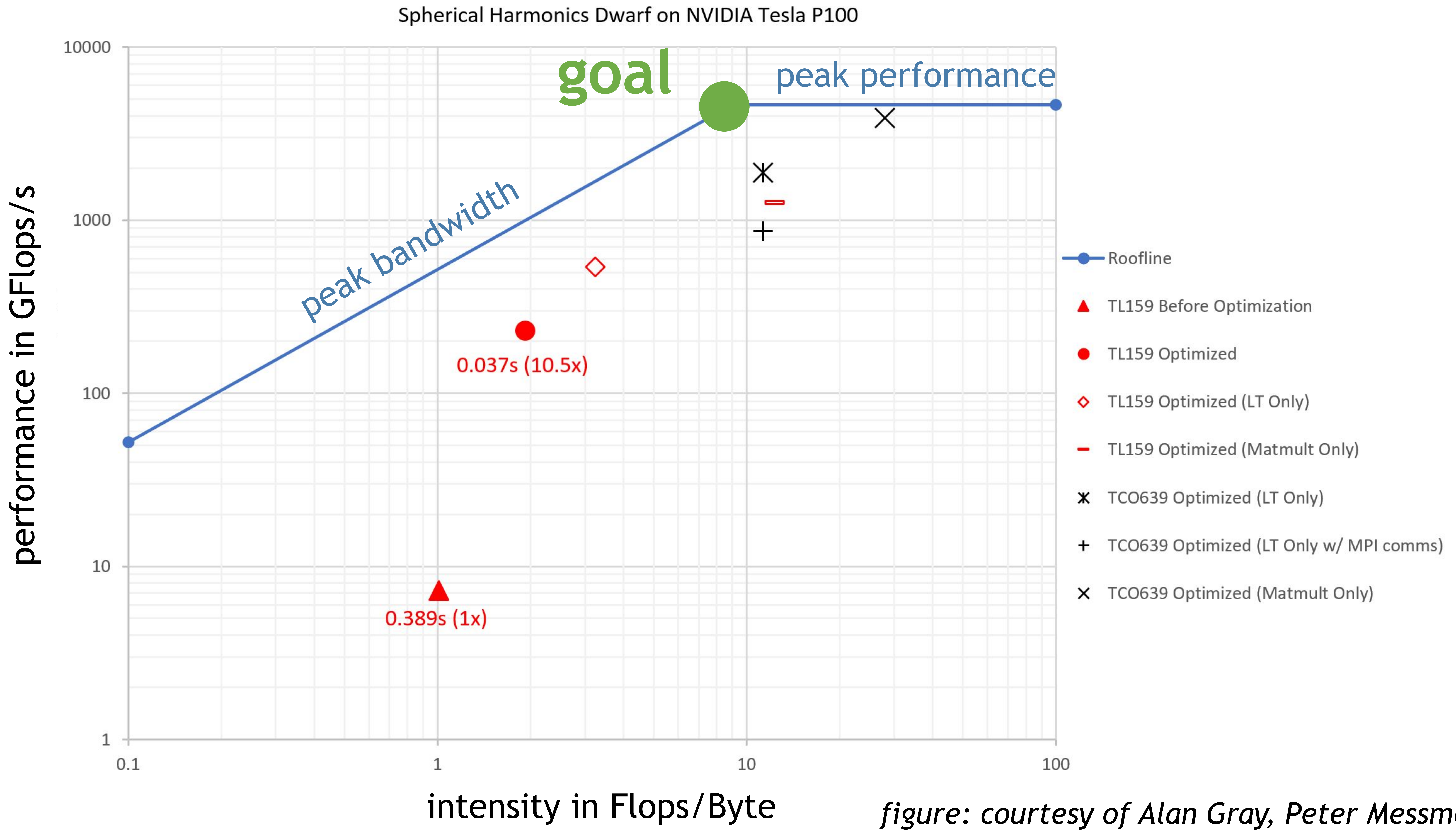


figure: courtesy of Alan Gray, Peter Messmer (NVIDIA)

optimisations by NVIDIA in ESCAPE

Funded by the European Union

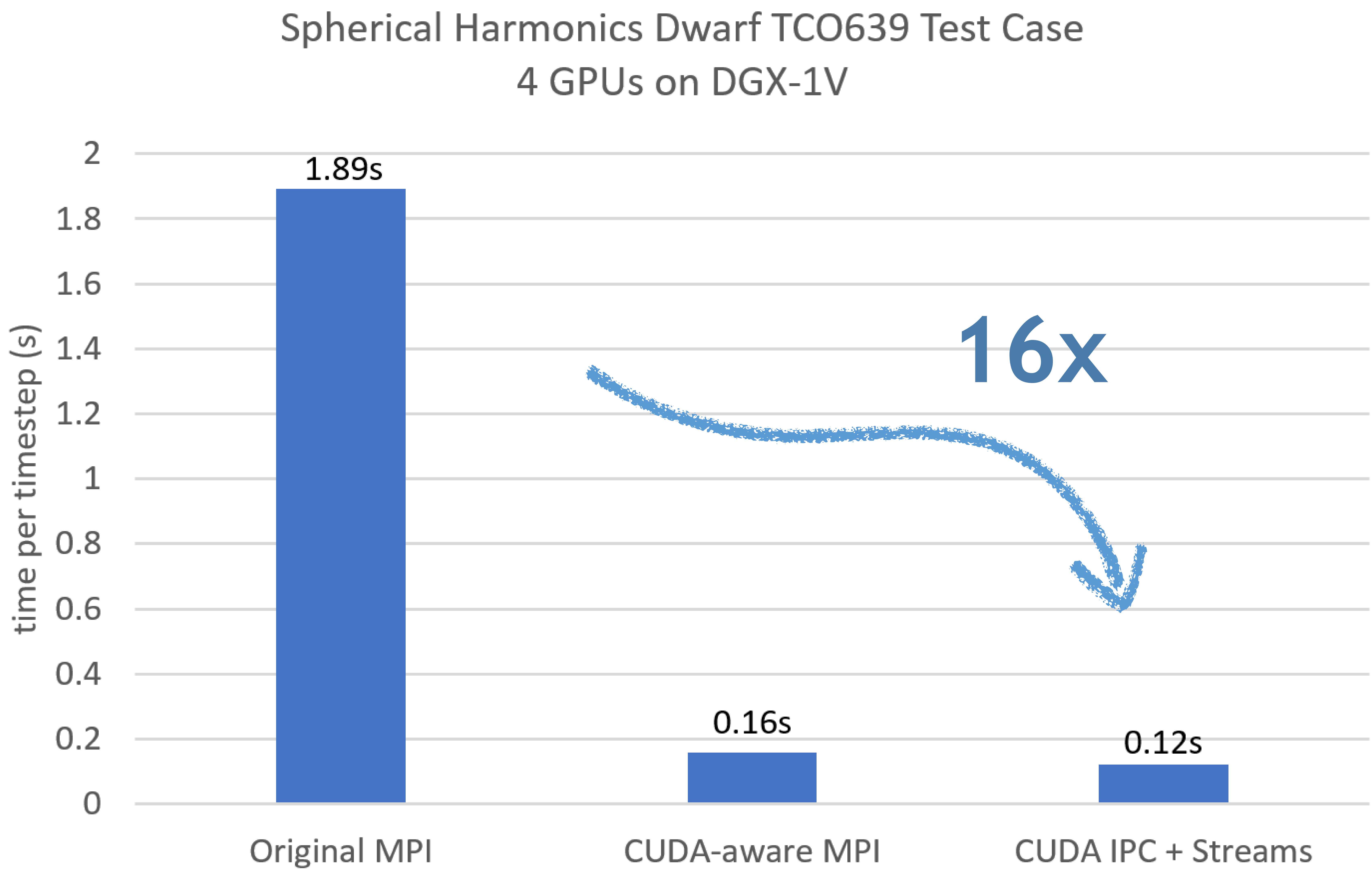
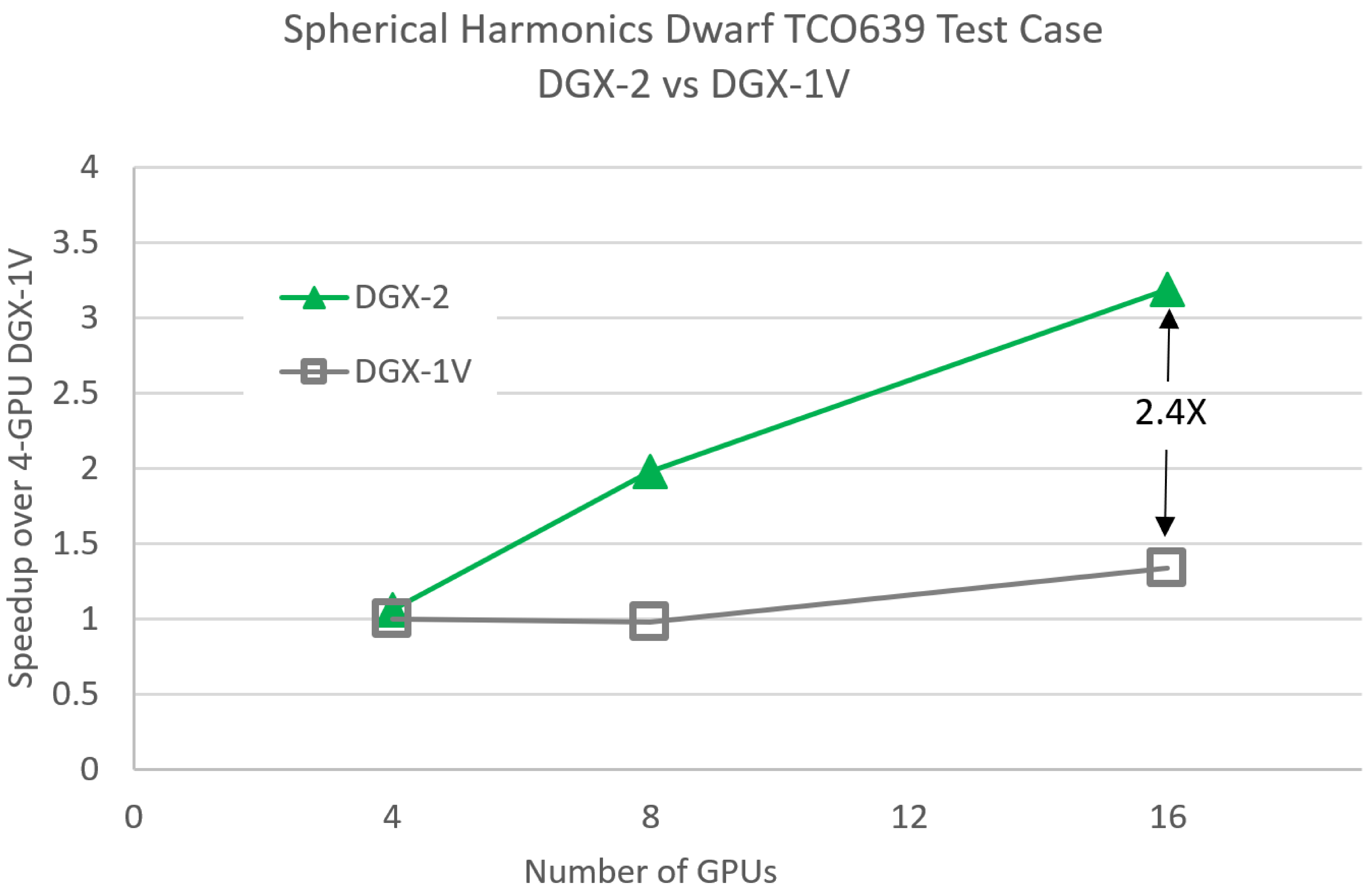


figure: courtesy of Alan Gray, Peter Messmer (NVIDIA)

optimisations by NVIDIA in ESCAPE

Funded by the European Union

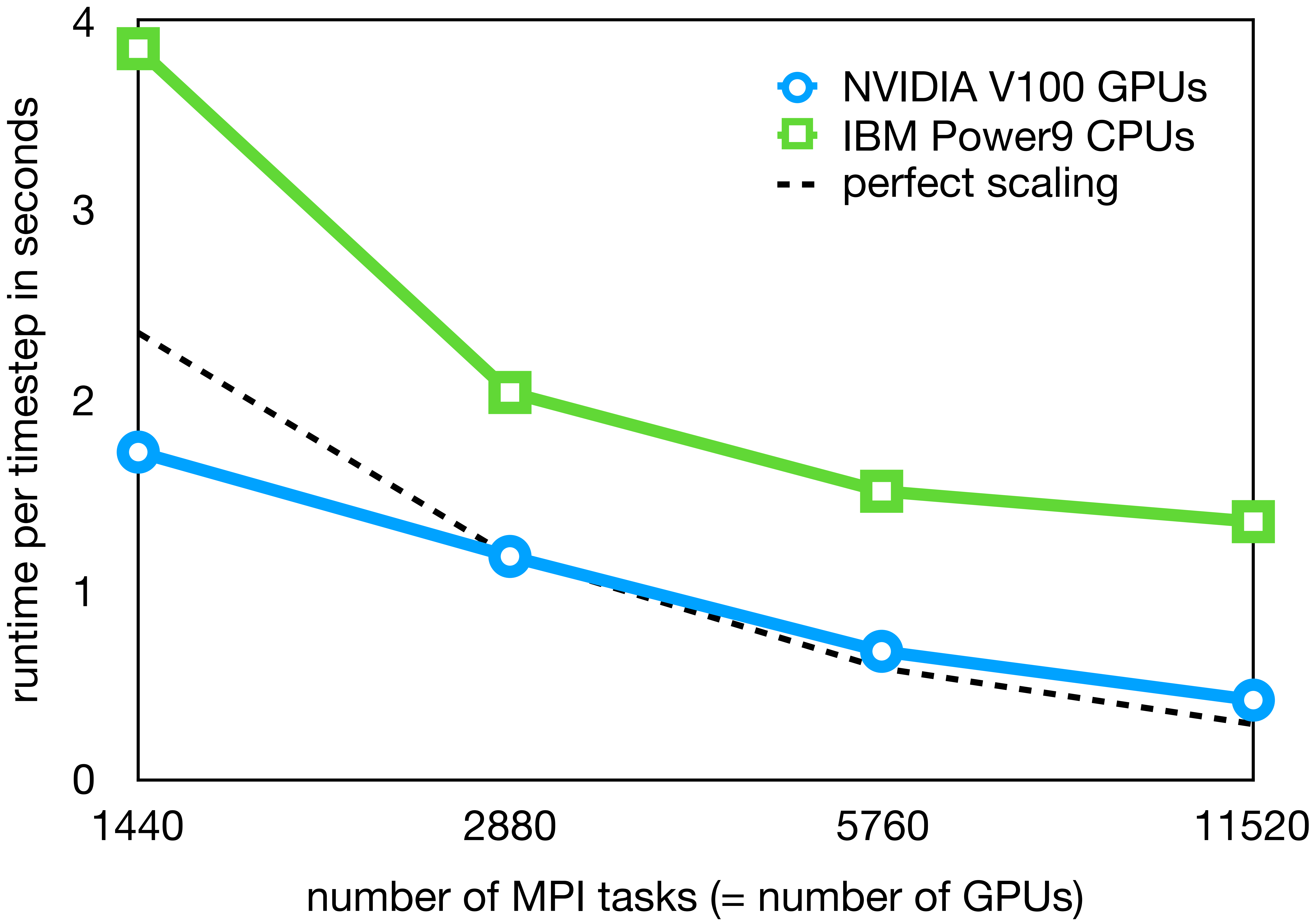


DGX-1V uses MPI for >=8 GPUs (due to lack of AlltoAll links), all others use CUDA IPC.
DGX-2 results use pre-production hardware.

figure: courtesy of Alan Gray, Peter Messmer (NVIDIA)

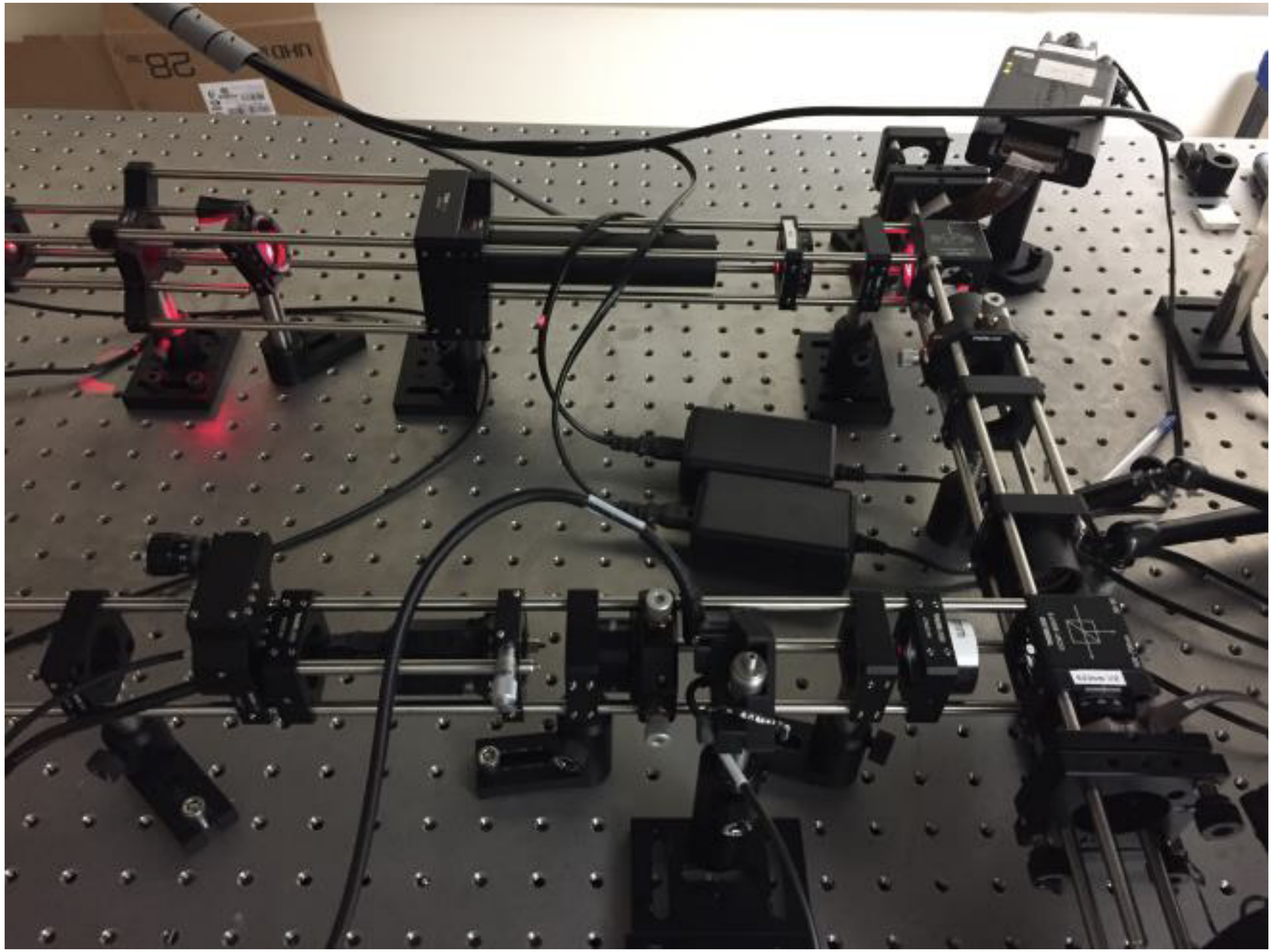
GPUs vs CPUs on Summit

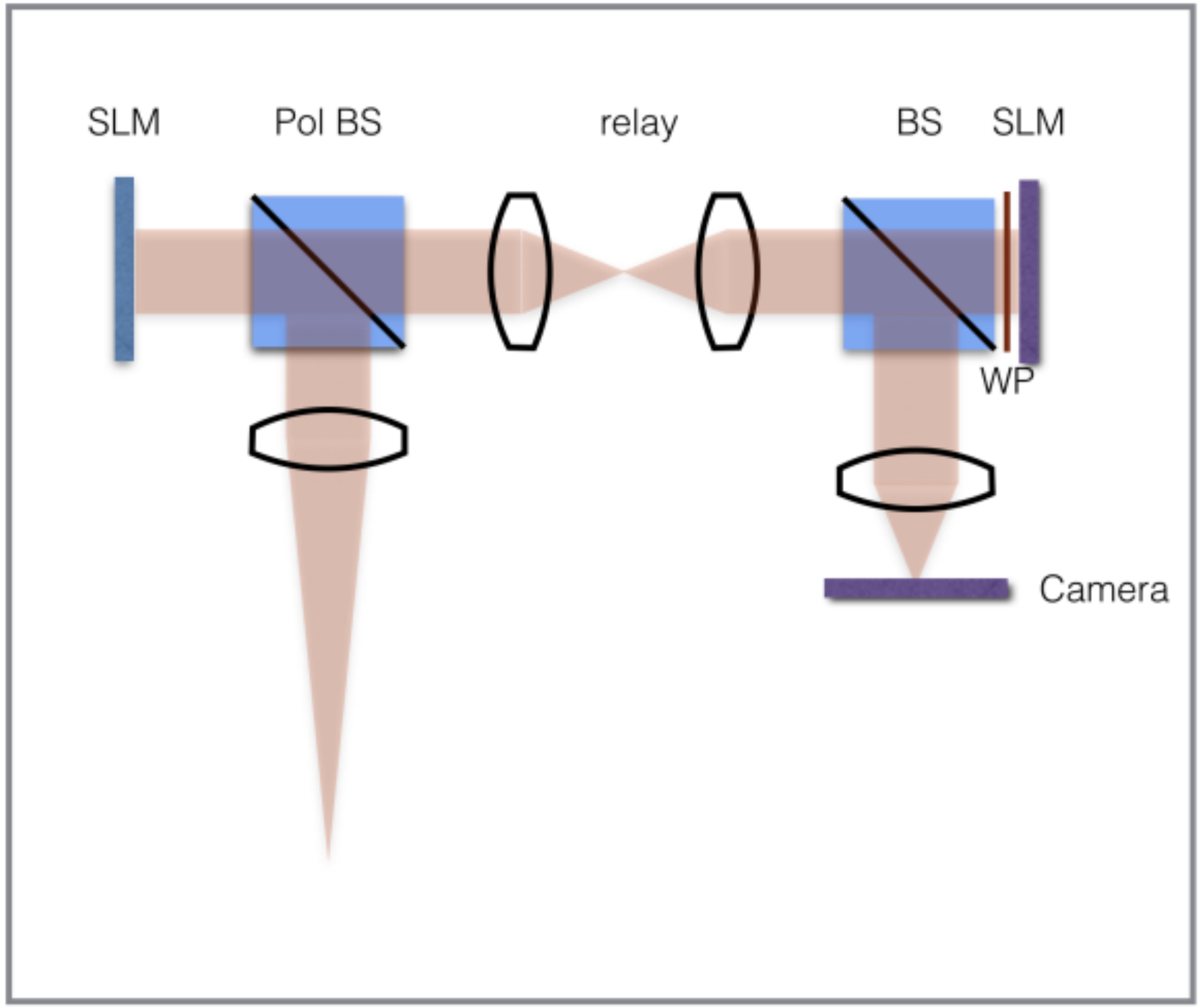
Funded by the European Union



Optalysys: optical processor for spectral transform

Funded by the European Union





Figures used with permission from Optalysys, 2017

Fast Legendre Transform

Funded by the European Union

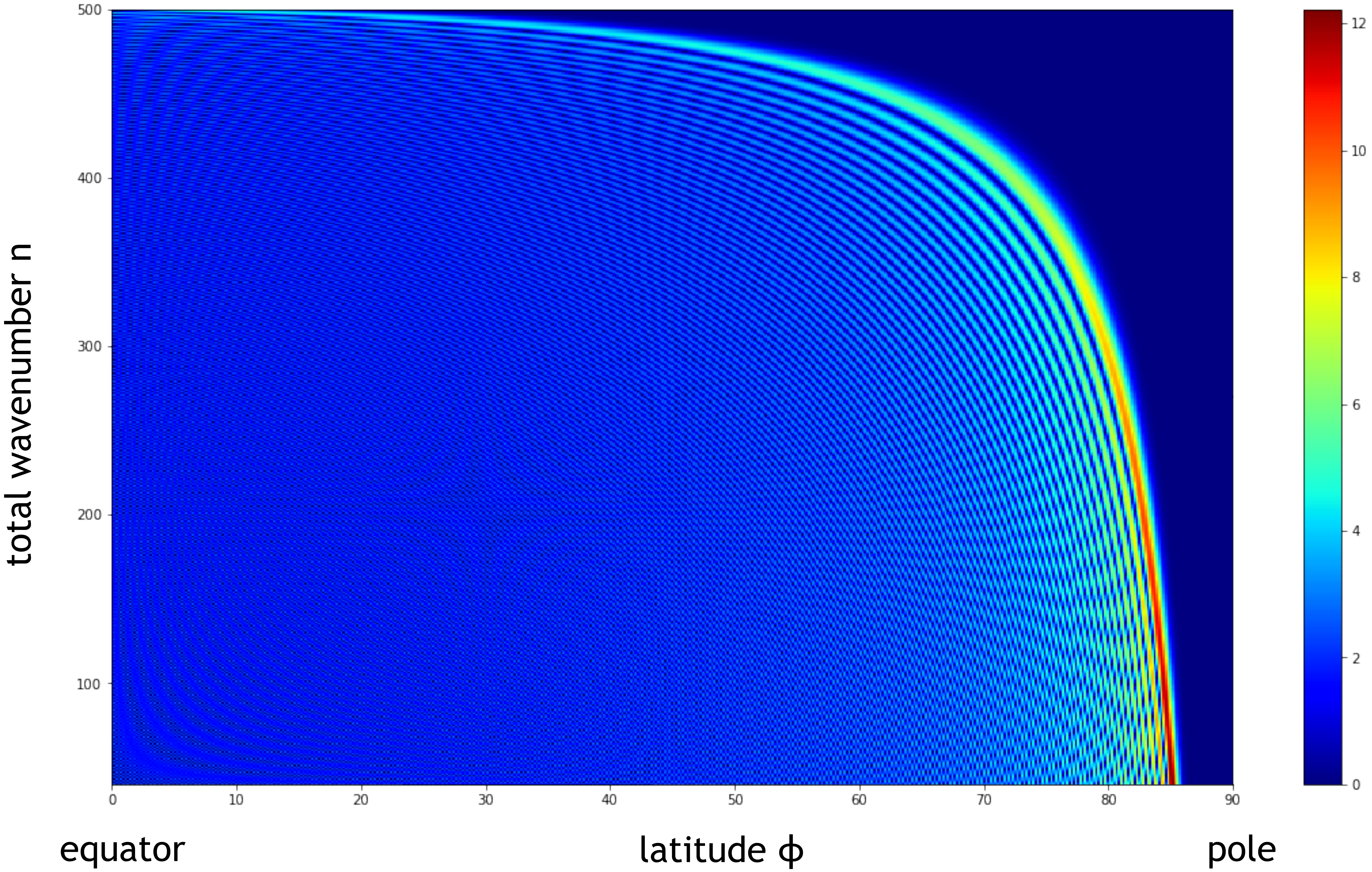
matrix of
Legendre polynomials

truncation N=500,
zonal wavenumber
m=40

FLT:

step 1: split matrix into two rows

step 2: use interpolation to empty half of the columns



Fast Legendre Transform

Funded by the European Union

matrix of Legendre polynomials

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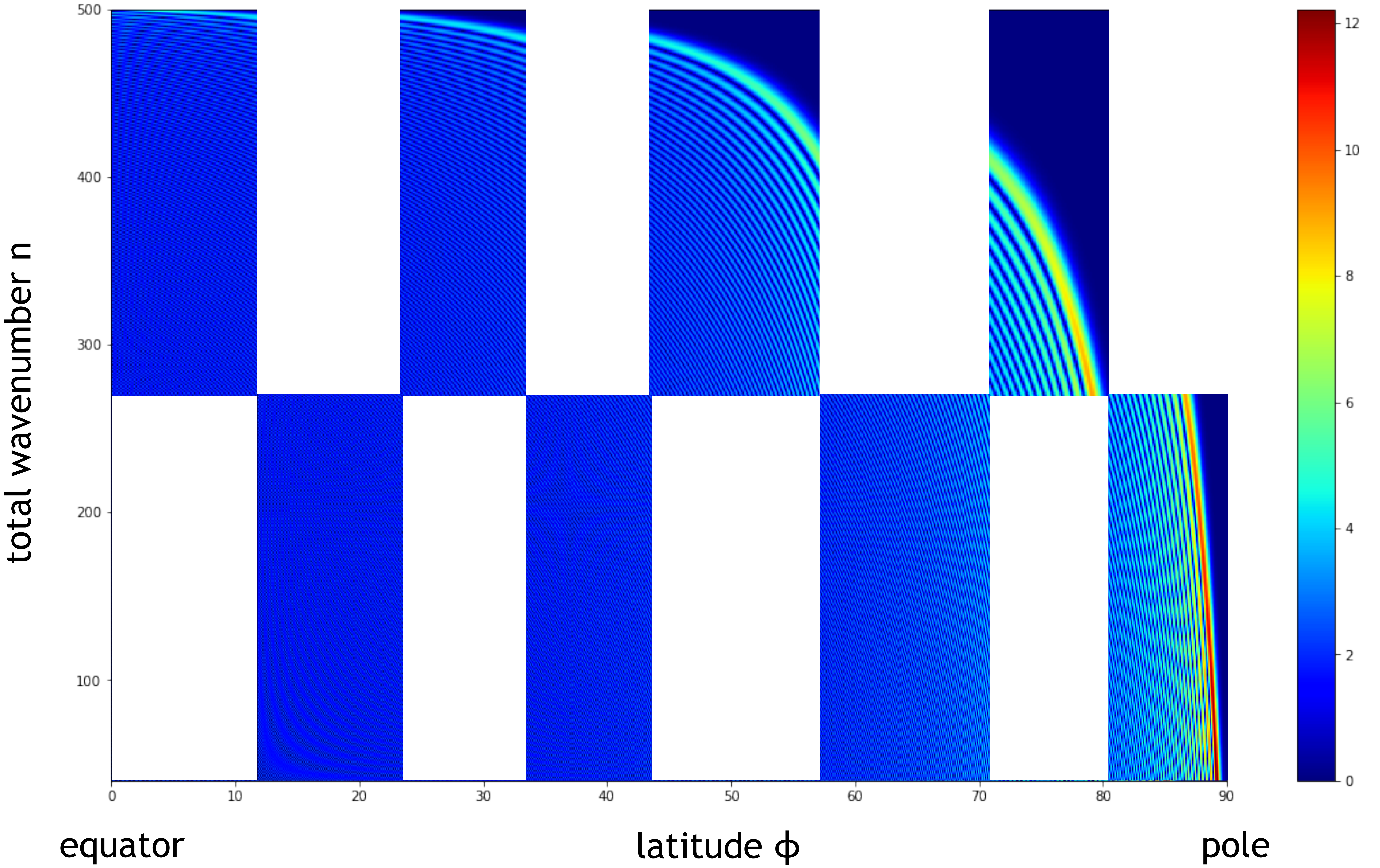
step 3: reorder columns



Fast Legendre Transform

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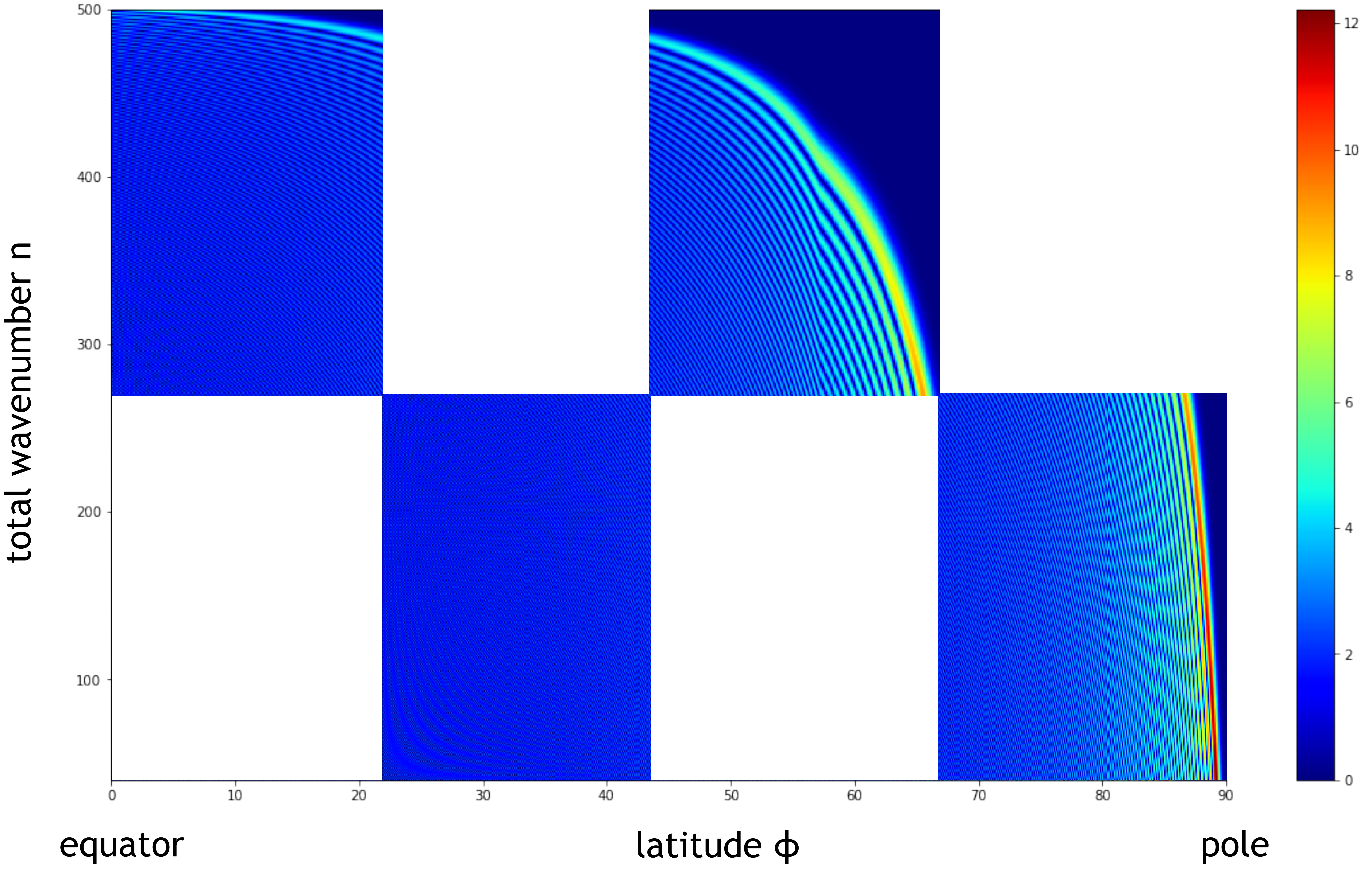
step 4: apply to each block recursively



Funded by the European Union

Fast Legendre Transform

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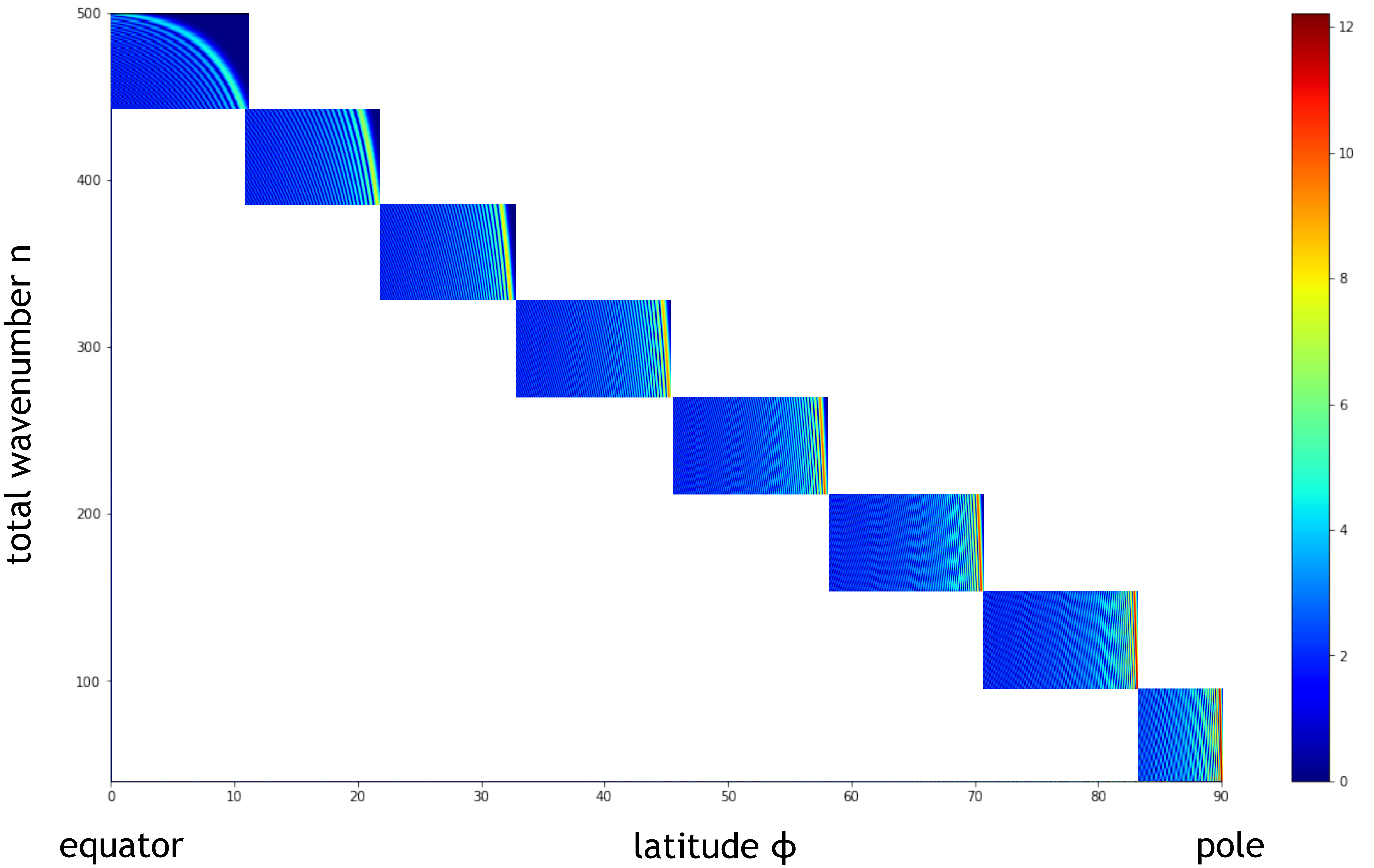


Fast Legendre Transform

Funded by the European Union

matrix of
Legendre polynomials

truncation N=500,
zonal wavenumber
m=40

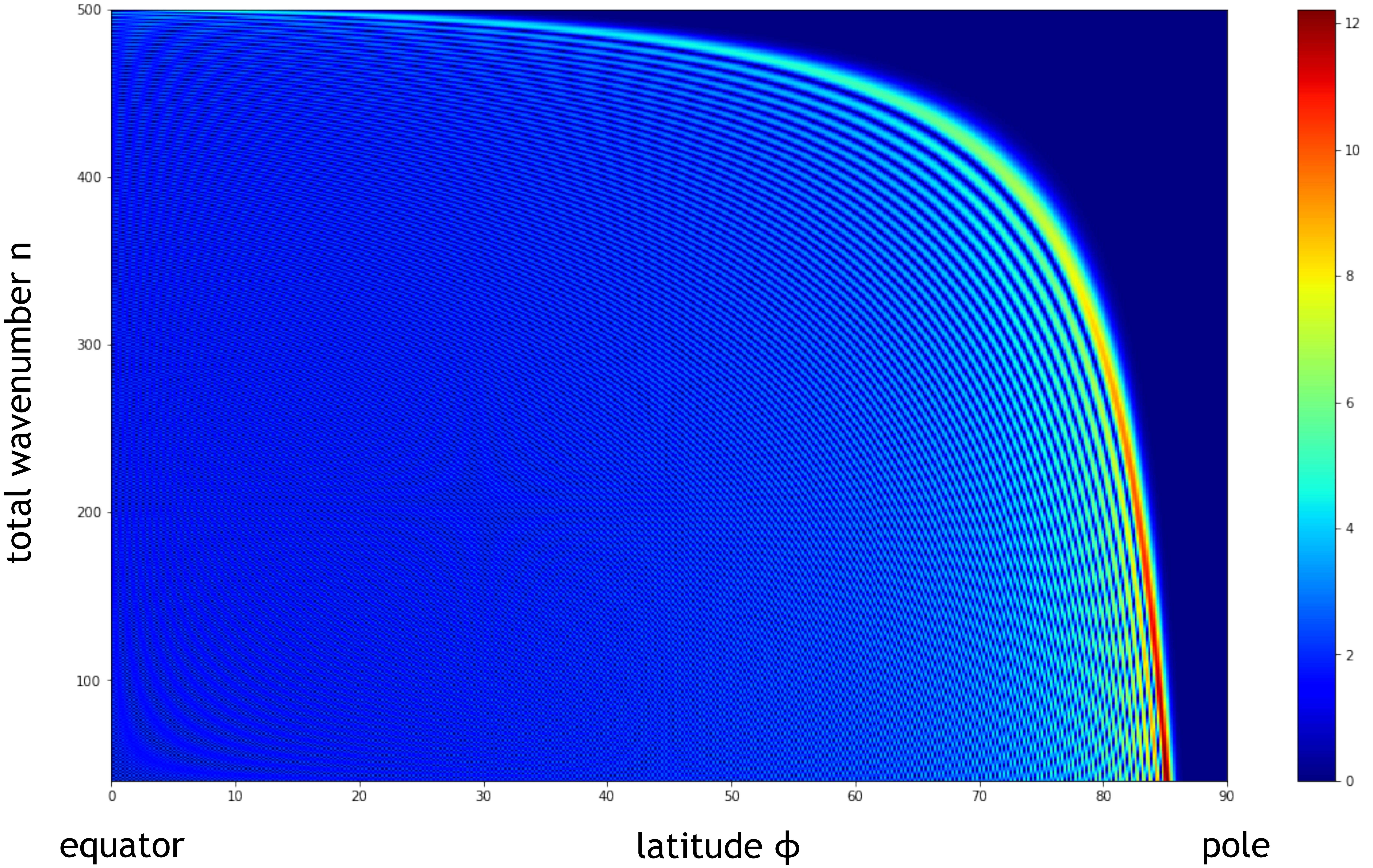
FLT:

step 1: split matrix into two rows

step 2: use interpolation to empty half of the columns

step 3: reorder columns

step 4: apply to each block recursively



Fast Legendre Transform

Funded by the European Union

matrix of
Legendre polynomials

truncation N=500,
zonal wavenumber
m=100

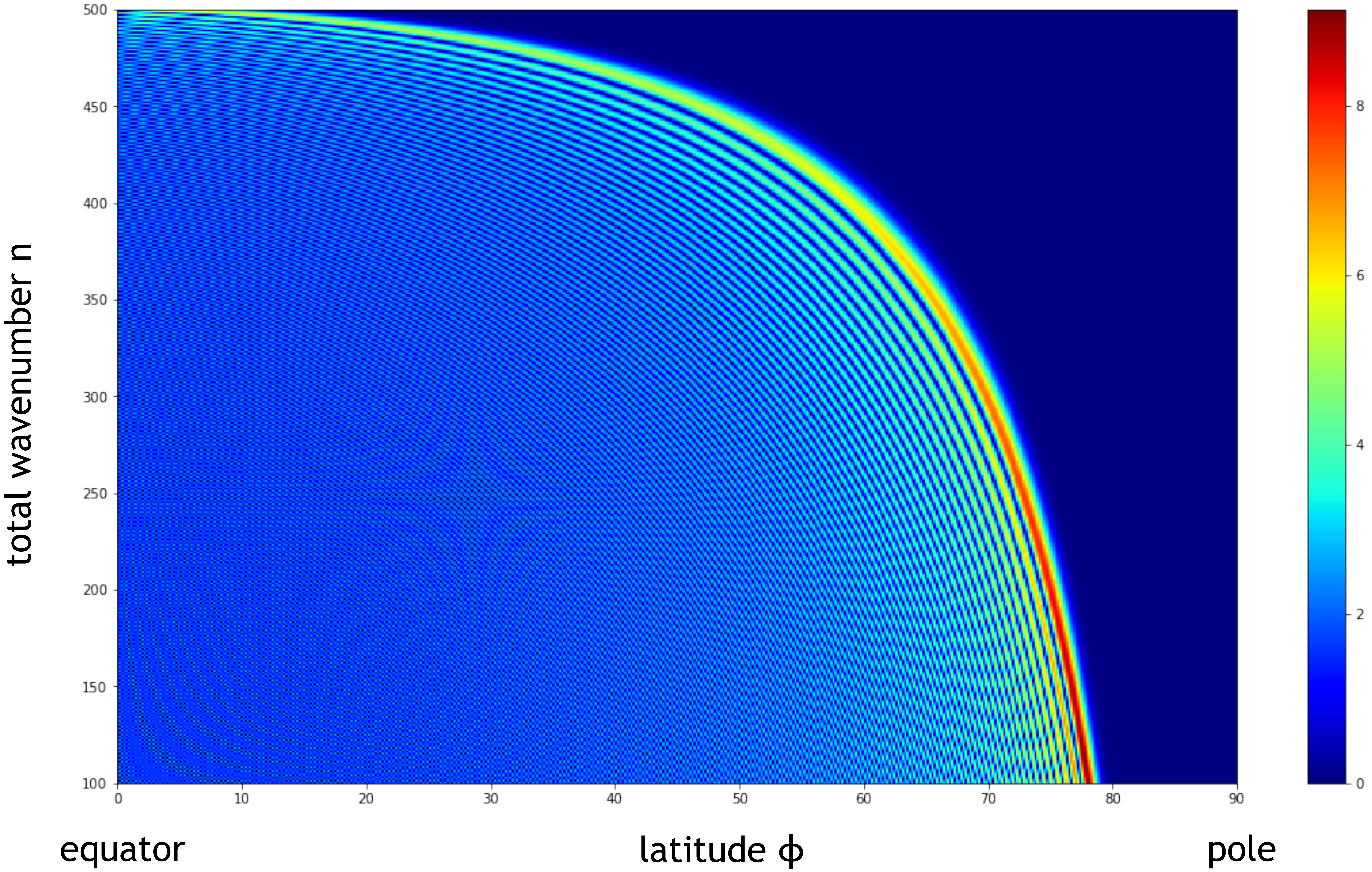
FLT:

step 1: split matrix into two rows

step 2: use interpolation to empty half of the columns

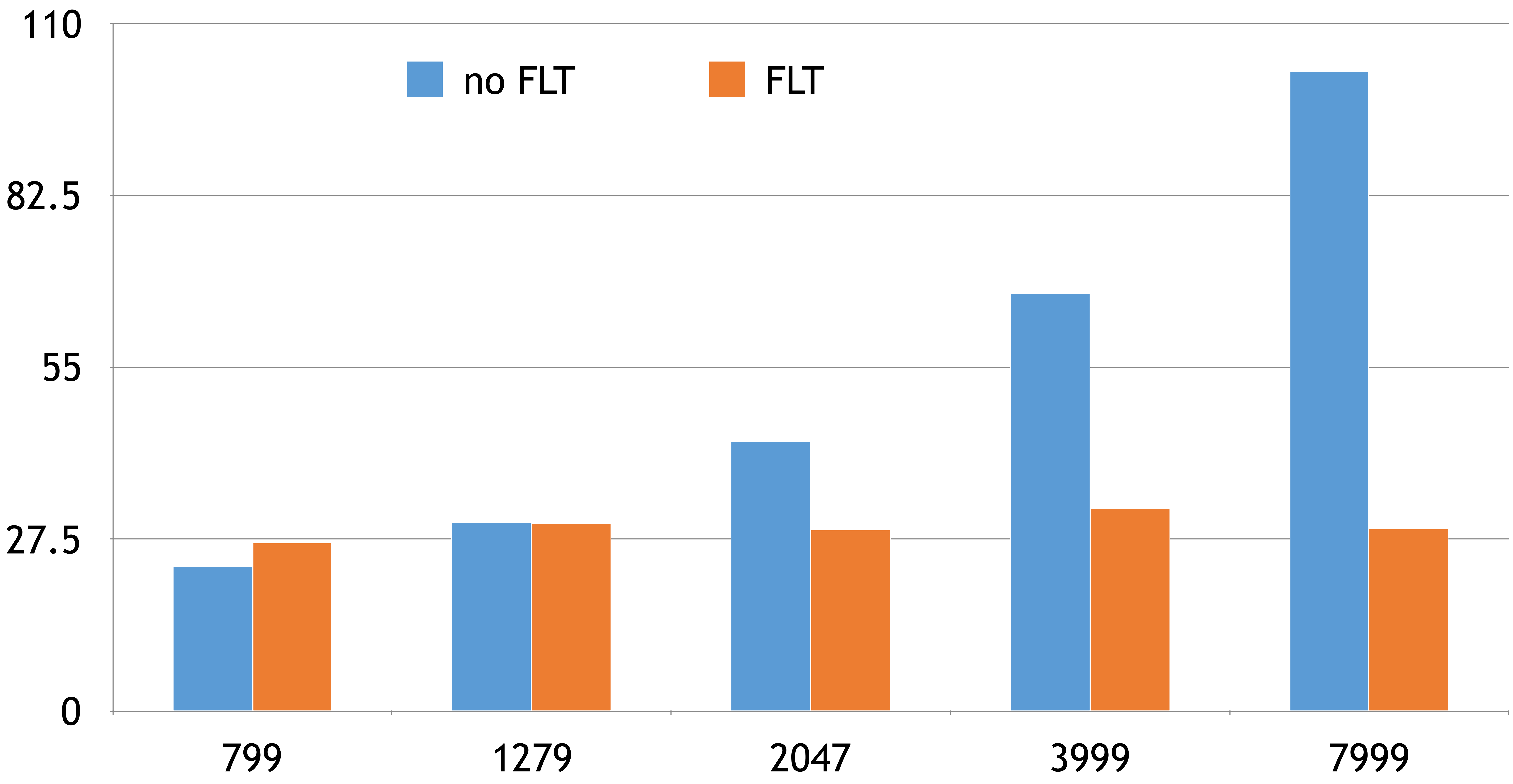
step 3: reorder columns

step 4: apply to each block recursively



Fast Legendre Transform
floating point operations

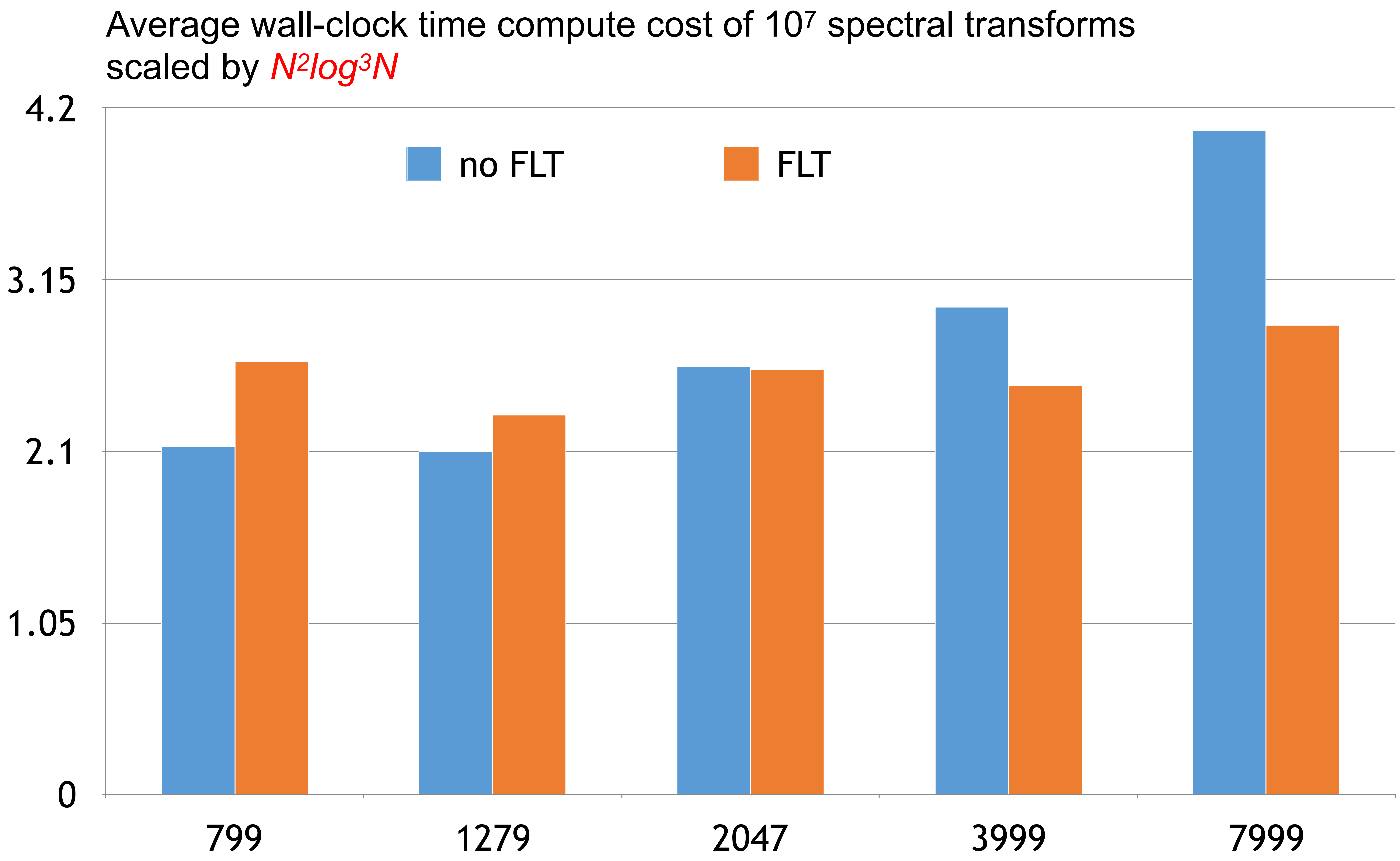
Number of floating point operations for direct or inverse spectral transforms of a single field, scaled by $N^2 log^3 N$



Fast Legendre Transform

wallclock time

Funded by the European Union



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