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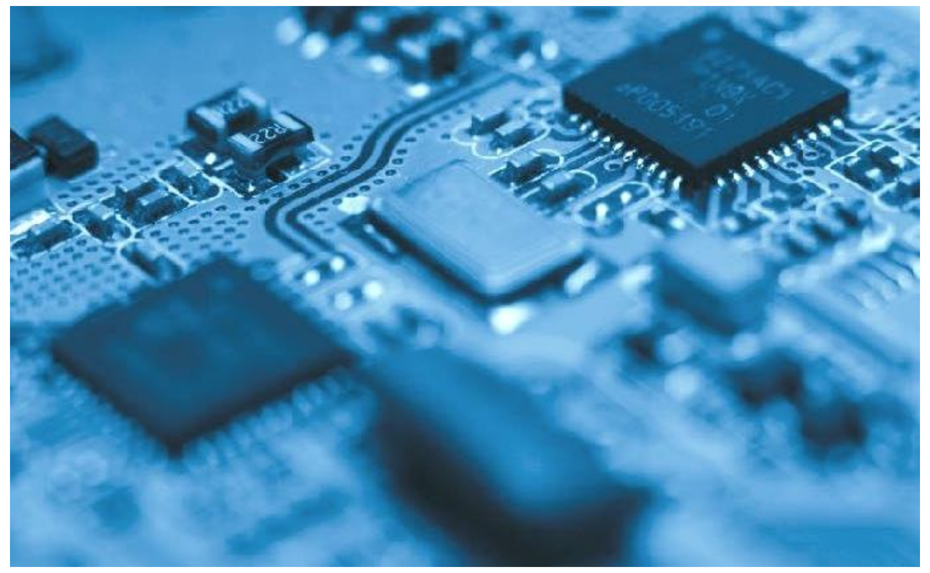
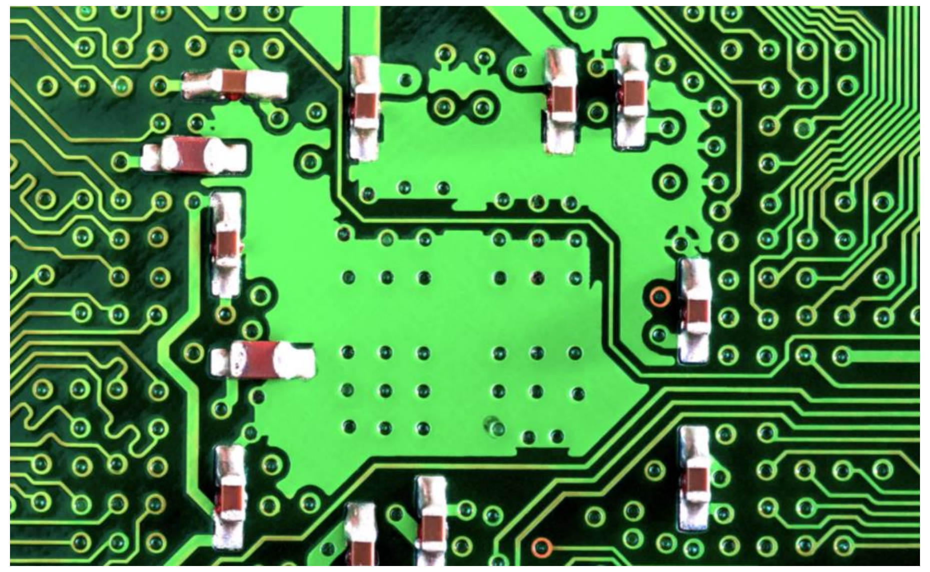
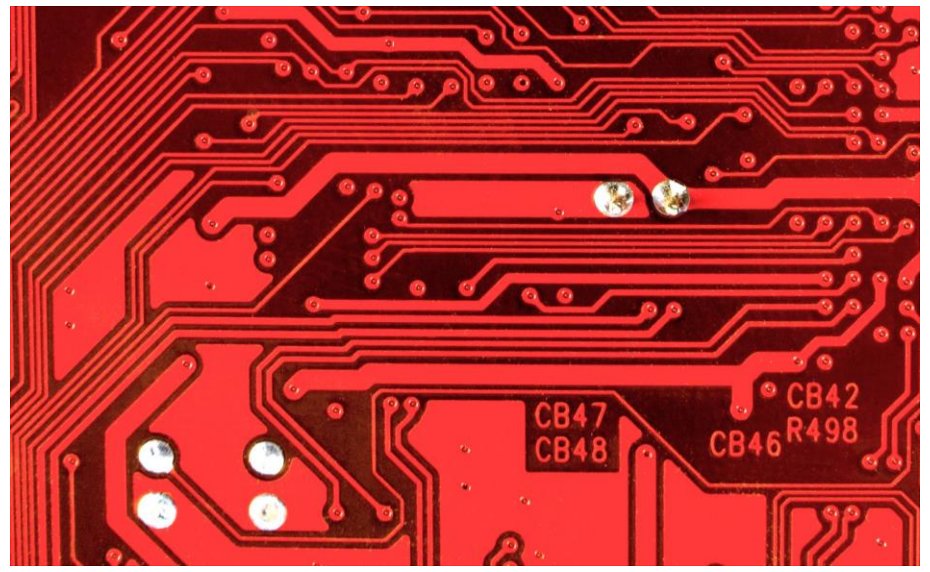


ESCAPE 2

# Spectral Transform

***Michail Diamantakis***

based on the lecture slides by **Andreas Mueller**

ECMWF DKRZ Max-Planck-Institut für Meteorologie MeteoSwiss Barcelona Supercomputing Center cea Loughborough University RMI Politecnico Milano MOX DMI cmcc Bull atos technologies

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# IFS (Integrated Forecast System)

ESCAPE 2

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technology applied at ECMWF for
the last 30 years

- spectral transform
- semi-Lagrangian
- semi-implicit

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

https://www.ecmwf.int/escape

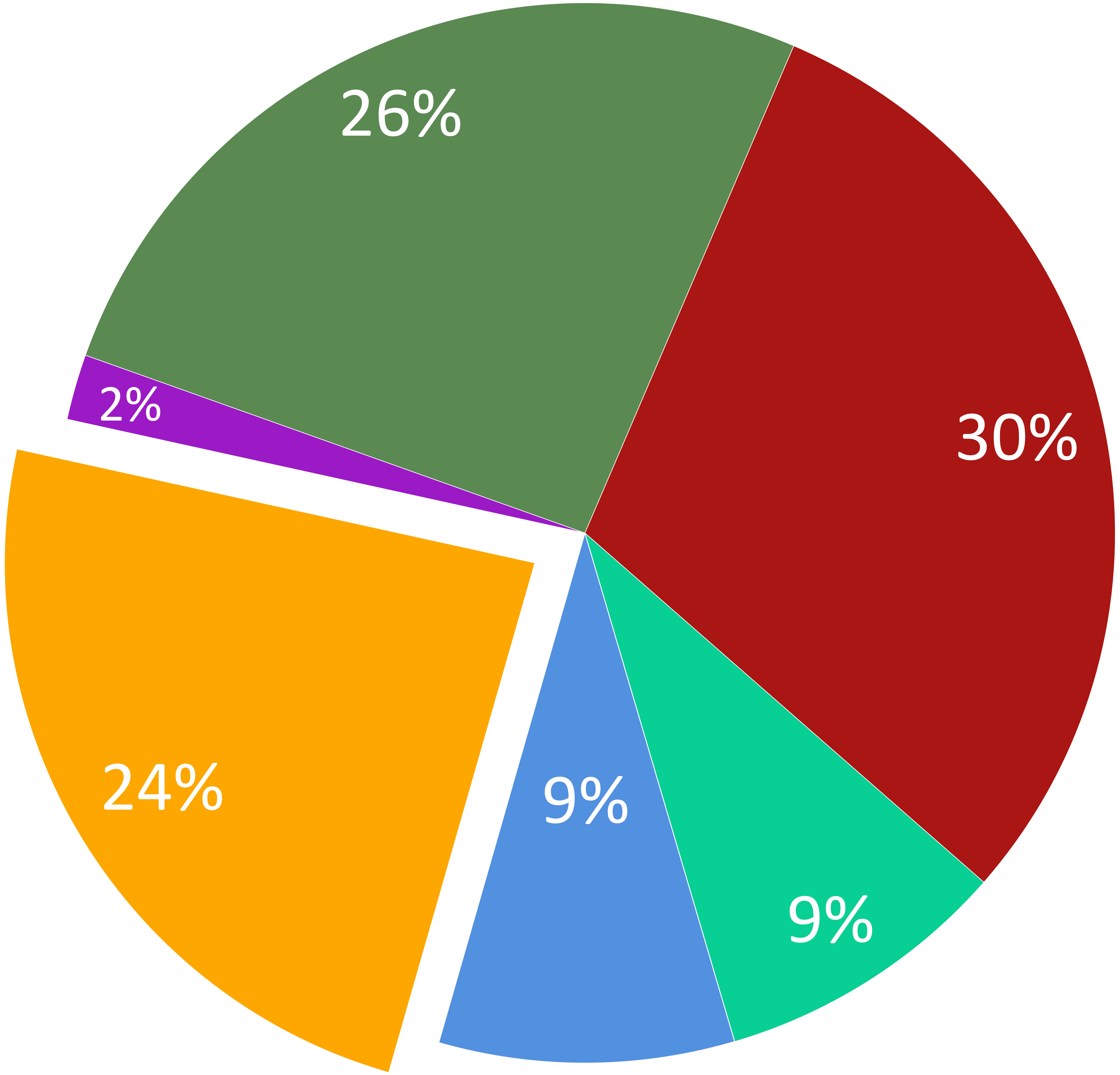
*"ESCAPE aimed to develop world-class, extreme-scale computing capabilities for European operational numerical weather prediction (NWP) and future climate models."*

# IFS (Integrated Forecast System)

technology applied at ECMWF for the last 30 years

- spectral transform
- semi-Lagrangian
- semi-implicit

pie chart: % of runtime in 9km operational forecast




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

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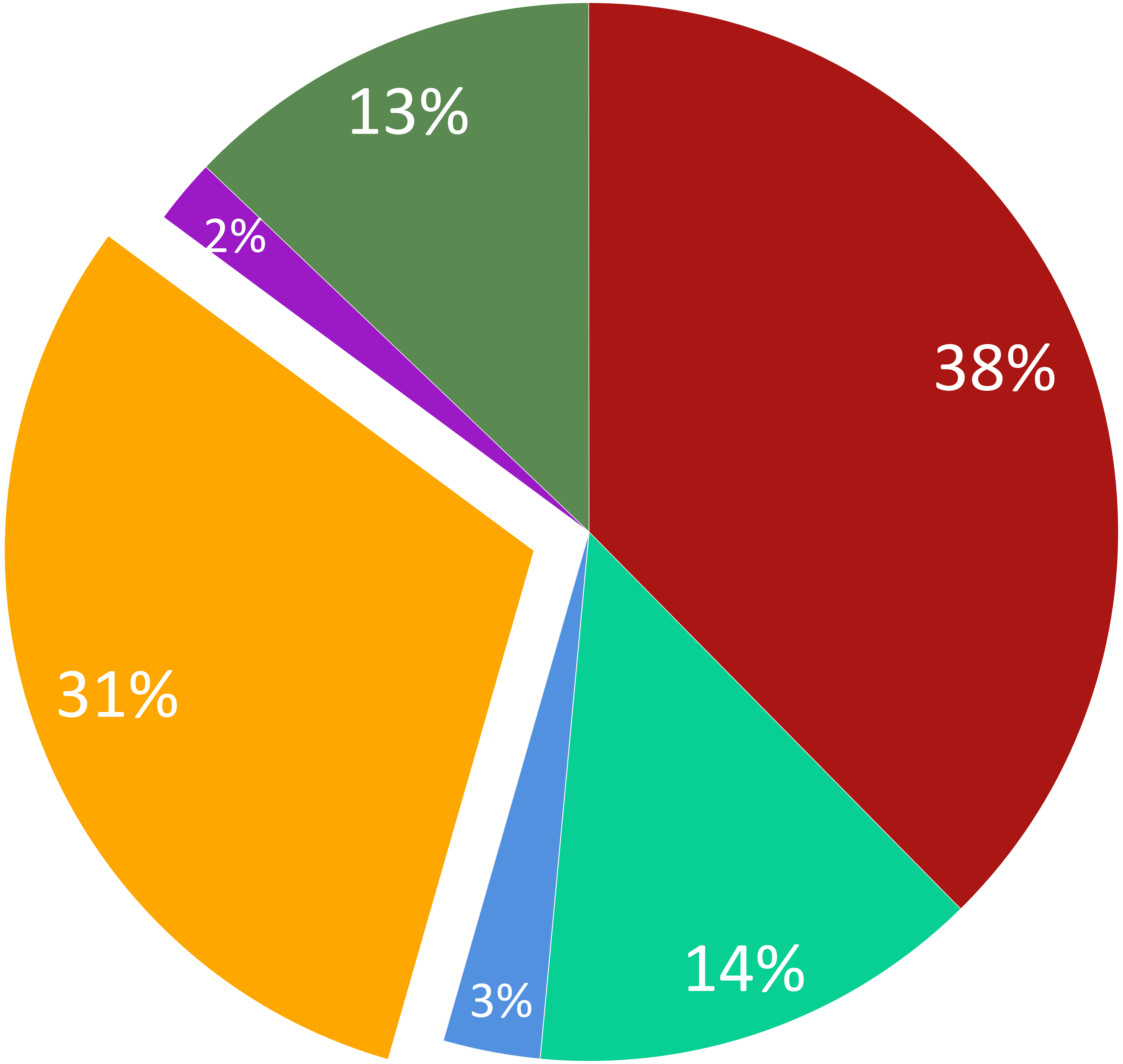
# IFS (Integrated Forecast System)

technology applied at ECMWF for the last 30 years

- spectral transform
- semi-Lagrangian
- semi-implicit

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

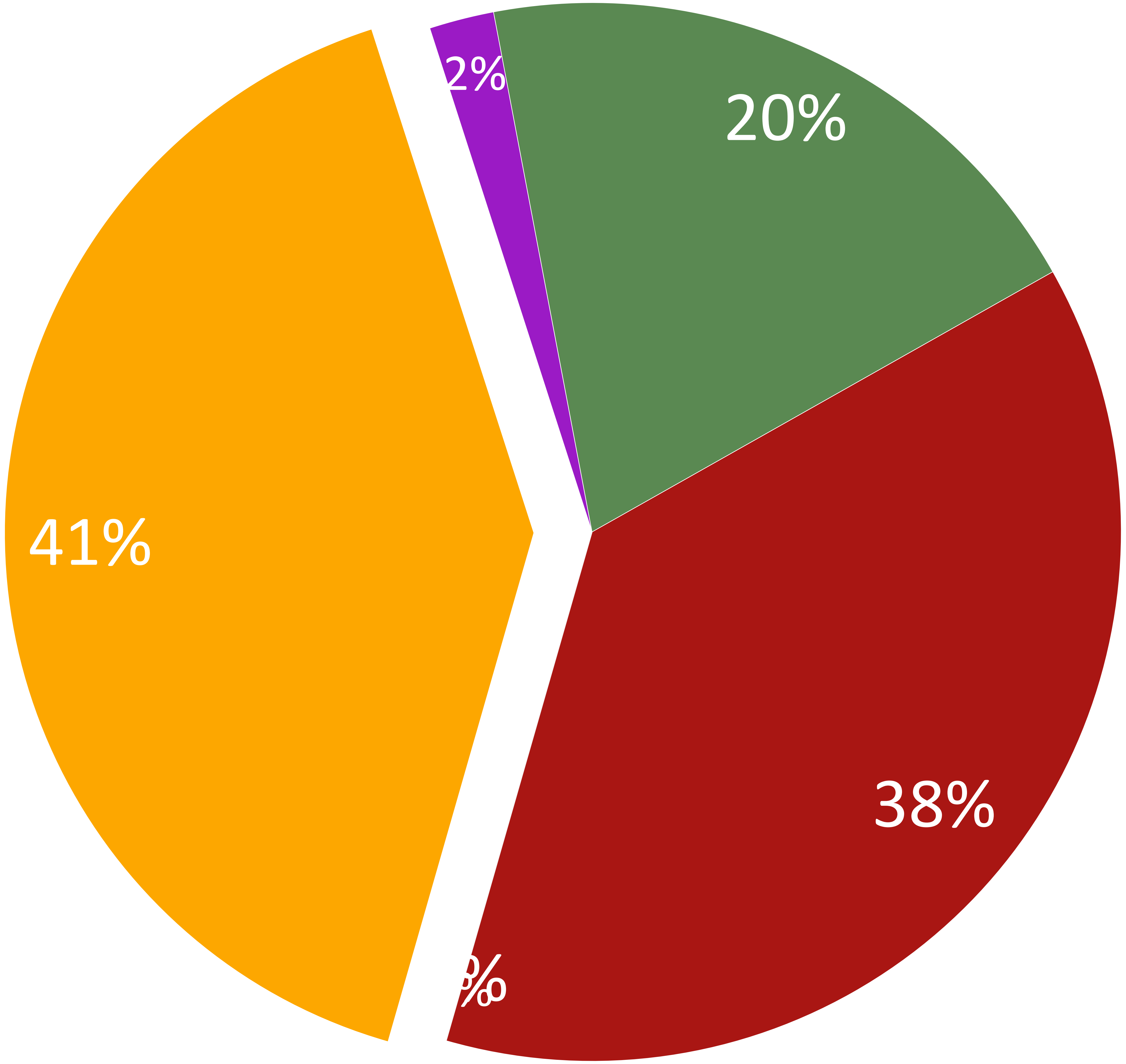


# IFS (Integrated Forecast System)

technology applied at ECMWF for the last 30 years

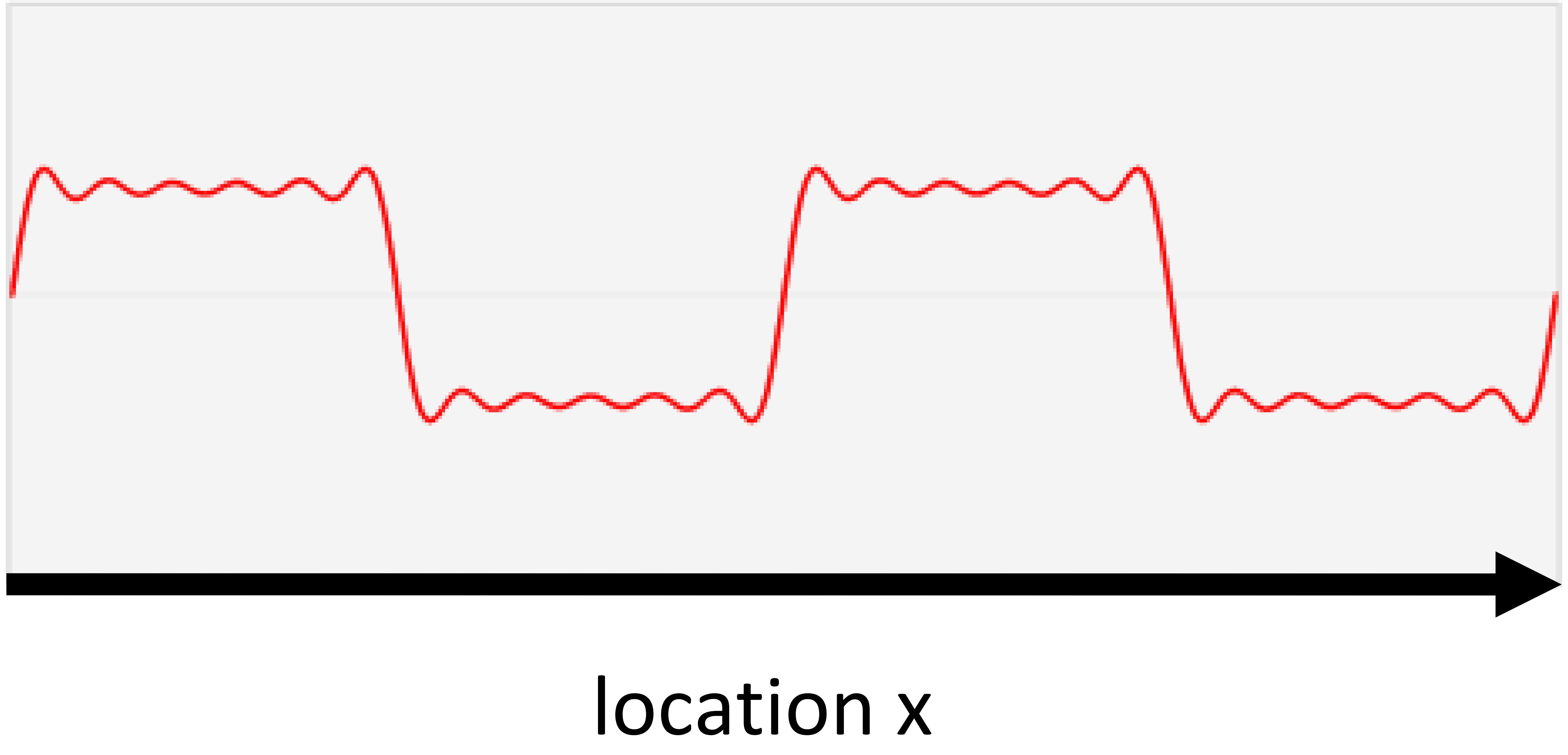
- spectral transform
- semi-Lagrangian
- semi-implicit

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



# Fourier transform

Fourier transform = Spectral transform in 1D



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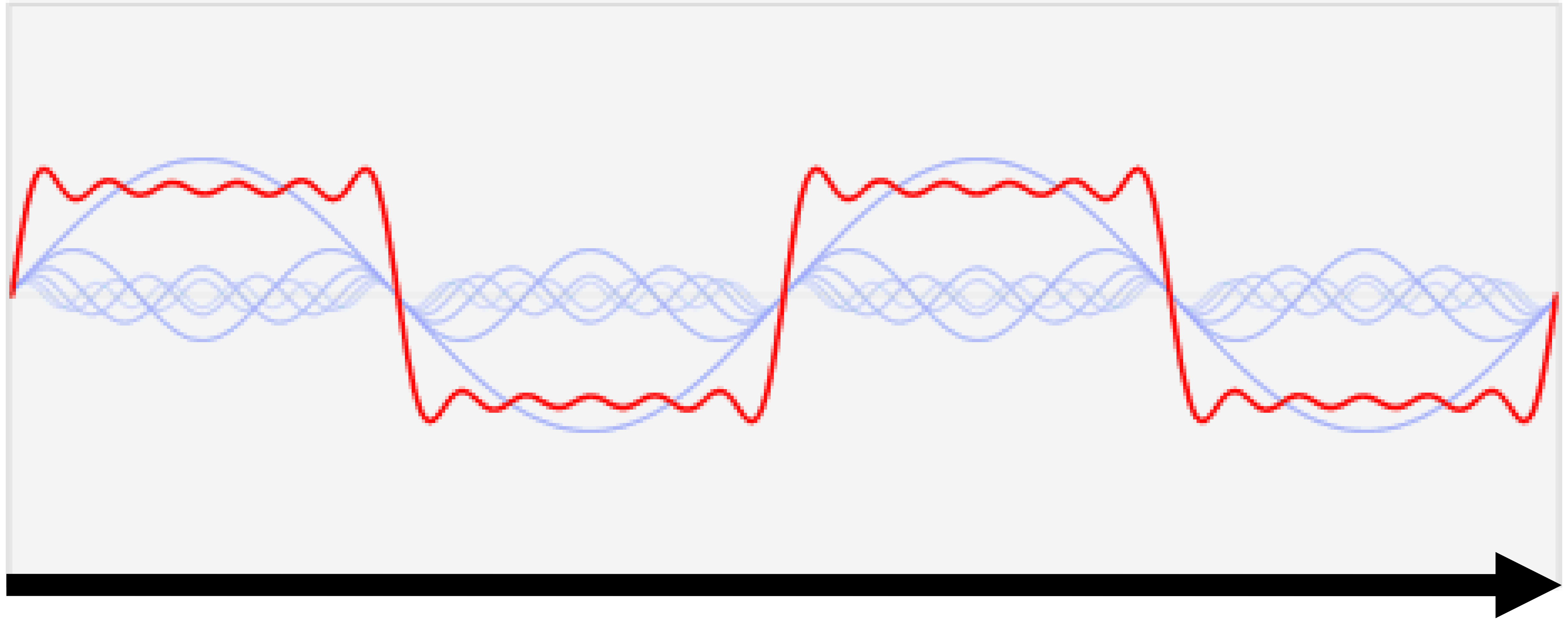
# Fourier transform

Fourier transform = Spectral transform in 1D



location x

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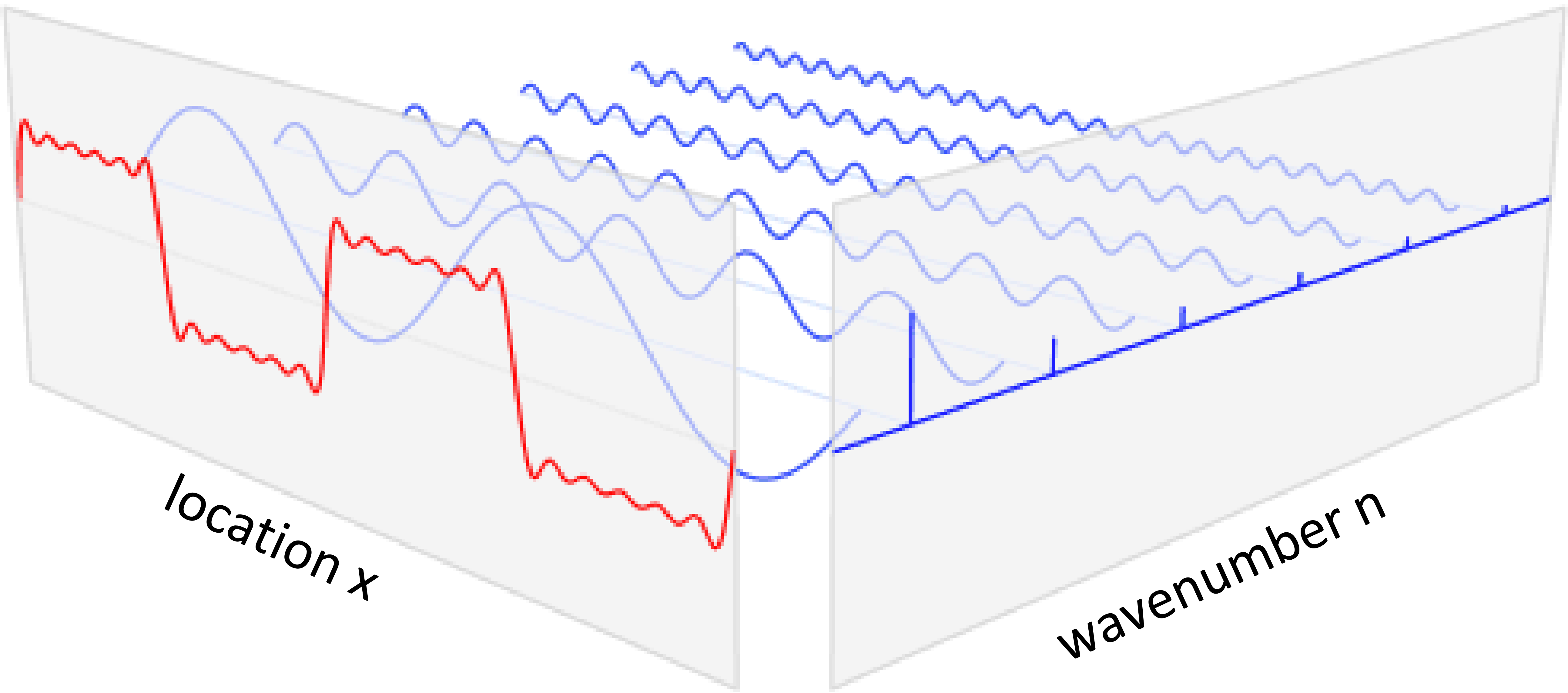
# Fourier transform

Fourier transform = Spectral transform in 1D




**grid point space** **Fourier space**

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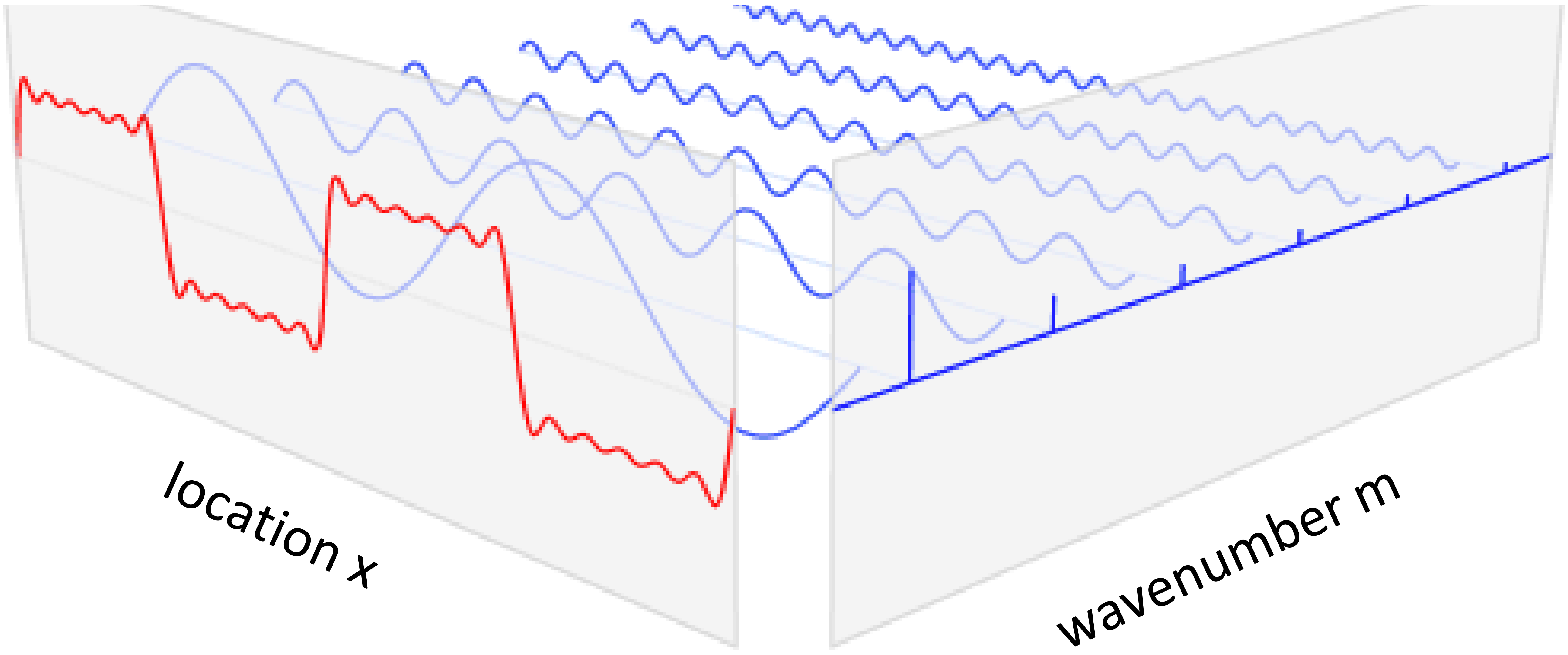
# Fourier transform and its inverse




function of a real variable x

Fourier coefficients

$$f(x)=\sum_{m=-\infty}^{\infty} f_m e^{imx}, \quad x\in[0,2\pi]$$

Inverse Fourier transform

where,

$$f_m=\frac{1}{2\pi}\int_0^{2\pi} f(x)e^{-imx}dx$$

Fourier transform

In practice these transforms are discrete in nature transforming grid-point functions (fields) to a finite number of discrete Fourier coefficients and vice versa.

The Fast Fourier Transform (FFT) is the standard way of performing this operation.

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# Spatial derivatives and Fourier representation

function of x

Fourier coefficients

$$f(x) = \sum_{m=-\infty}^{\infty} f_m e^{imx}, \quad x \in [0, 2\pi]$$

simple multiplication

derivative

$$\frac{df(x)}{dx} = \sum_{m=-\infty}^{\infty} i m f_m e^{imx}$$

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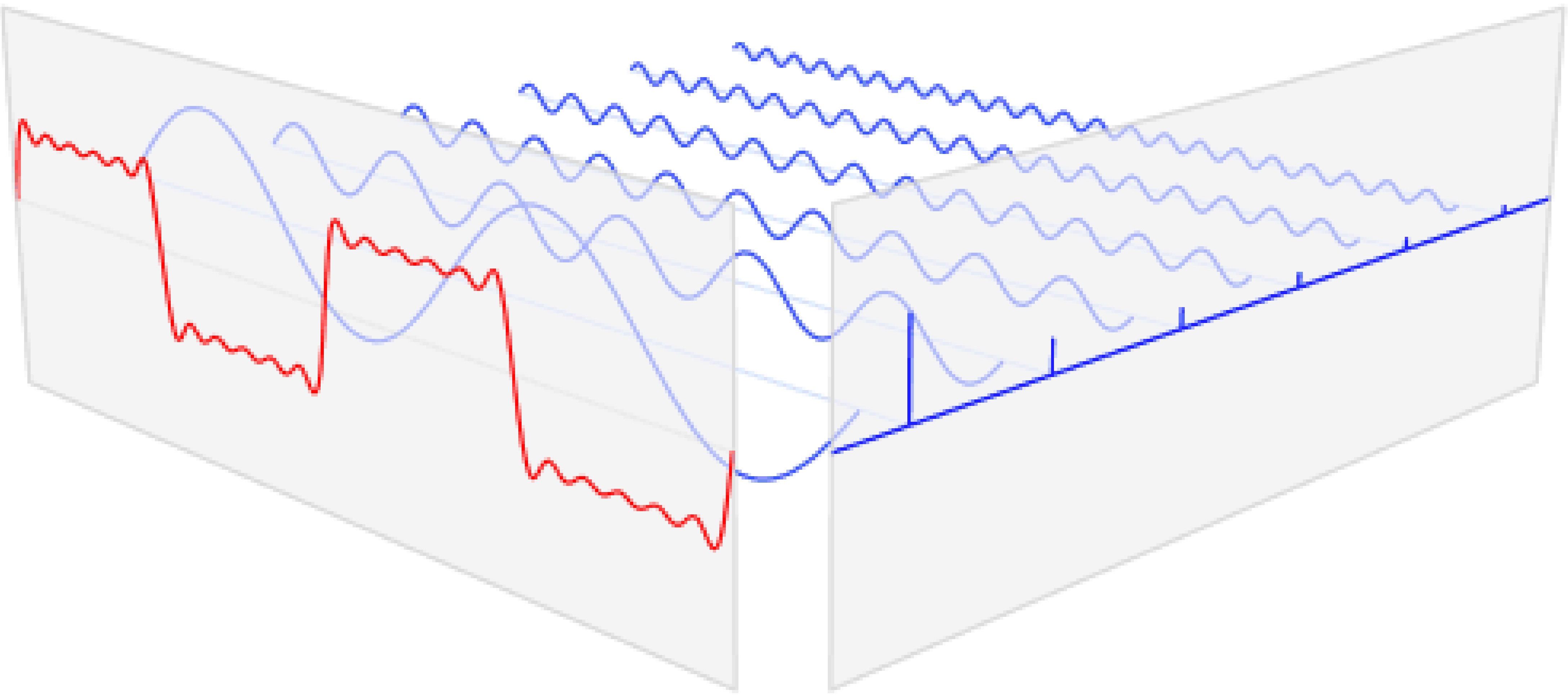
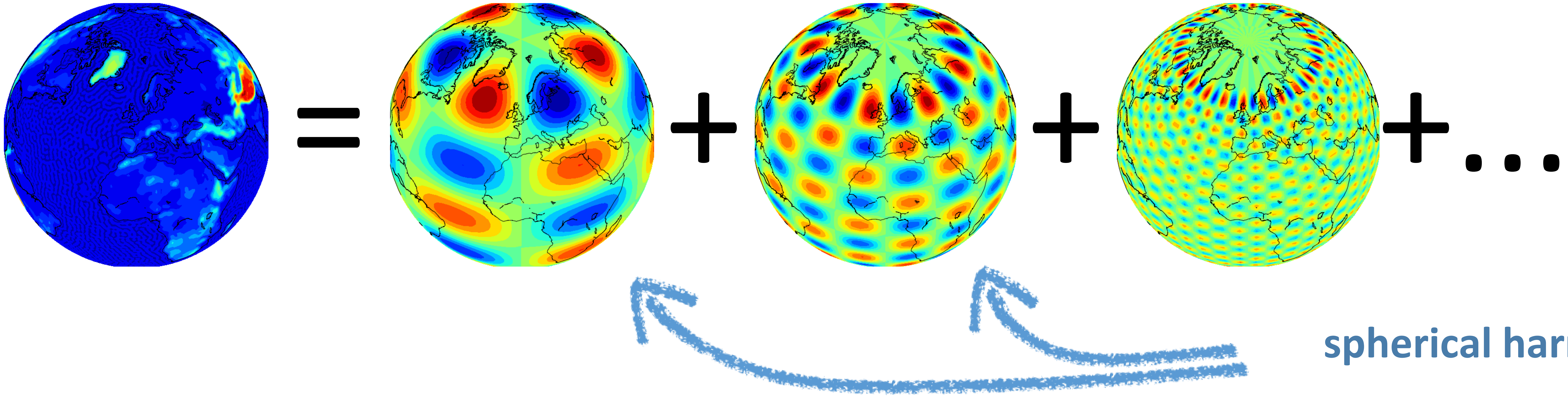
# on the sphere: spectral transform



grid point space

spectral space



spherical harmonics

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# Truncated spectral transform series

Spectral coefficient — longitude — latitude — Spherical harmonics

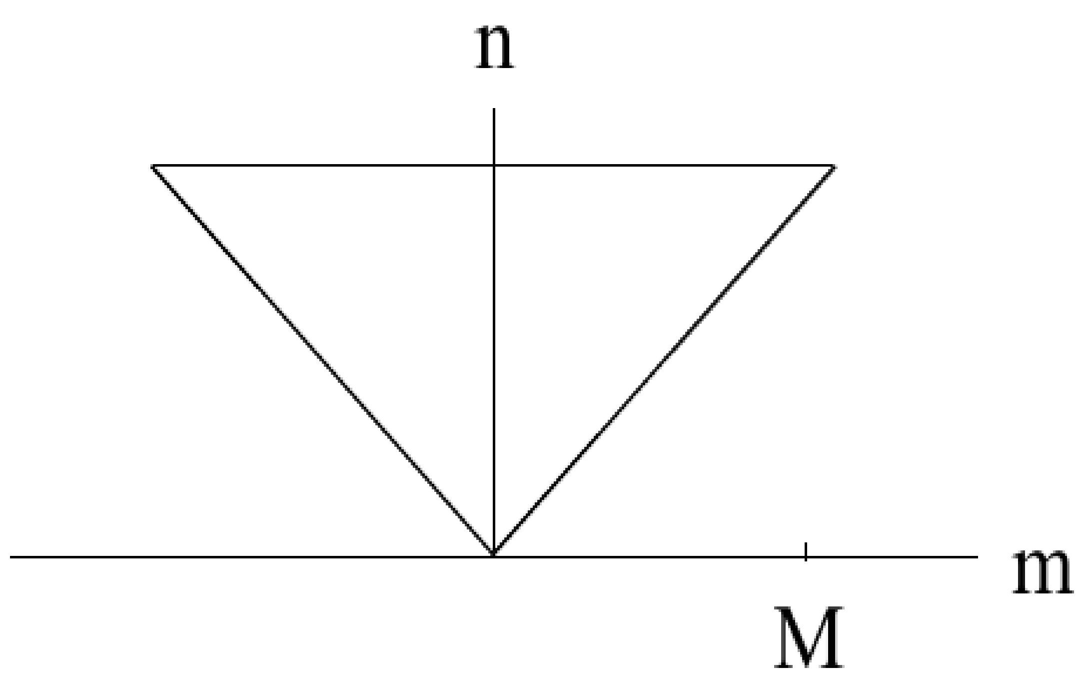
$$f(\lambda,\phi)=\sum_{m=-\infty}^{\infty}\sum_{n=|m|}^{\infty} f_n^m Y_n^m(\lambda,\phi),\quad Y_n^m(\lambda,\phi)=P_n^m(\sin\phi)\,e^{im\lambda}$$

m: zonal wavenumber
n: total wavenumber

Associated Legendre Polynomials (normalised)

Truncated series:

$$f(\lambda,\phi)=\sum_{m=-M}^{M}\sum_{n=|m|}^{M} f_n^m Y_n^m(\lambda,\phi),\quad Y_n^m(\lambda,\phi)=P_n^m(\mu)\,e^{im\lambda},\quad \mu=\sin\phi$$




Triangular truncation: (n,m) indices lie within a triangle.

Uniform resolution over entire surface of the sphere

# Spherical harmonics: where do they come from?

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Consider Laplace's equation on the sphere, assuming a solution (separation of variables, see book by Krishnamurti et al) of the form:

$$Y(\lambda, \mu) = L(\lambda)P(\mu), \quad \lambda: \text{ longitude}, \mu = \sin\phi$$

then, we obtain two ODEs:

$$\frac{d^2 L}{d\lambda^2} + m^2 L = 0, \qquad \frac{1-\mu^2}{P}\frac{d}{d\mu}\left(\left(1-\mu^2\right)\frac{dP}{d\mu}\right) + n(n+1)\left(1-\mu^2\right) = m^2$$

Solving for L, P the above we find that the solution is the *spherical harmonics function*:

$$Y_n^m(\lambda, \mu) = \underbrace{e^{im\lambda}}_{L(\lambda):\text{ Fourier mode}} \cdot \underbrace{P_n^m(\mu)}_{P(\mu):\text{ associated Legendre poly}}$$

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# Properties of spherical harmonics

- Derivatives can be accurately, cheaply and trivially computed:

$$\frac{\partial Y_n^m}{\partial \lambda} = imY_n^m$$

$$\left(1-\mu^2\right)\frac{\partial Y_n^m}{\partial \mu} = -n\varepsilon_{n+1}^m Y_{n+1}^m + (n+1)\varepsilon_n^m Y_{n-1}^m, \quad \varepsilon_n^m = \sqrt{\frac{n^2-m^2}{4n^2-1}}$$

- Spherical harmonics are the Eigenfunctions of the horizontal Laplace operator and they are orthogonal (due to orthogonality of Legendre polynomials)

$$\nabla^2 Y_n^m = \frac{-n(n+1)}{a^2} Y_n^m, \quad a: \text{ Earth radius}$$

- Thus, elliptic equations are easy and cheap to solve ⇨ important for semi-implicit time-stepping

- Spectral transform methods do not suffer from pole singularities and have uniform spatial resolution over entire sphere with triangular truncation for m, n (used in these notes)

# Continuous transforms in space-time

$$f(\lambda,\mu,z,t) = \sum_{m=-\infty}^{\infty} \sum_{n=|m|}^{\infty} f_n^m(z,t) Y_n^m(\lambda,\mu)$$

$$f_m(\mu,z,t) = \frac{1}{2\pi} \int_0^{2\pi} f(\lambda,\mu,z,t) e^{-im\lambda} d\lambda$$

$$f_n^m(z,t) = \frac{1}{2} \int_{-1}^{1} f_m(\mu,z,t) P_n^m(\mu) d\mu$$

**Continuous spectral transform for a 4-dimensional equation model (space-time)**

**Continuous Fourier transform in longitude**

**Continuous Legendre transform in latitude**

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# Discrete transforms in space-time

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$$f_m(\mu_k, z, t) = \frac{1}{L}\sum_{j=1}^{L} f(\lambda_j, \mu_k, z, t) e^{-im\lambda_j}$$

Fourier transform at latitude $\phi_k$: computed using a FFT

$$f_n^m(z,t) = \frac{1}{2}\sum_{k=1}^{K} w_k \; f_m(\mu_k, z, t) P_n^m(\mu_k)$$

Legendre transform: a Gaussian quadrature exact for all polynomials of degree 2K-1

$$\left.\begin{array}{l} w_k : \text{Gaussian weights} \\ \mu_k : \text{Gaussian quadrature points} \end{array}\right\}, \quad k = 1, 2, \ldots, K$$

$$f_m(\mu_k, z, t) = \sum_{n=|m|}^{M} f_n^m(z,t) P_n^m(\mu_k)$$

Inverse Legendre transform

$$f(\lambda_j, \mu_k, z, t) = \sum_{m=-M}^{M} f_m(\mu_k, z, t) e^{im\lambda_j}$$

Inverse Fourier transform

**For accurate LTs a Gaussian grid must be used: grid-point latitudes coincide with the latitude of Gaussian quadrature points (roots of Legendre polynomials)**

# aliasing

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

# aliasing

wave generated in spectral space

**Issue**: multiplication of two waveform variables produces a new variable with shorter wavelength than the one the grid can handle

# aliasing


**Issue**: multiplication of two waveform variables produces a new variable with shorter wavelength than the one the grid can handle

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# aliasing

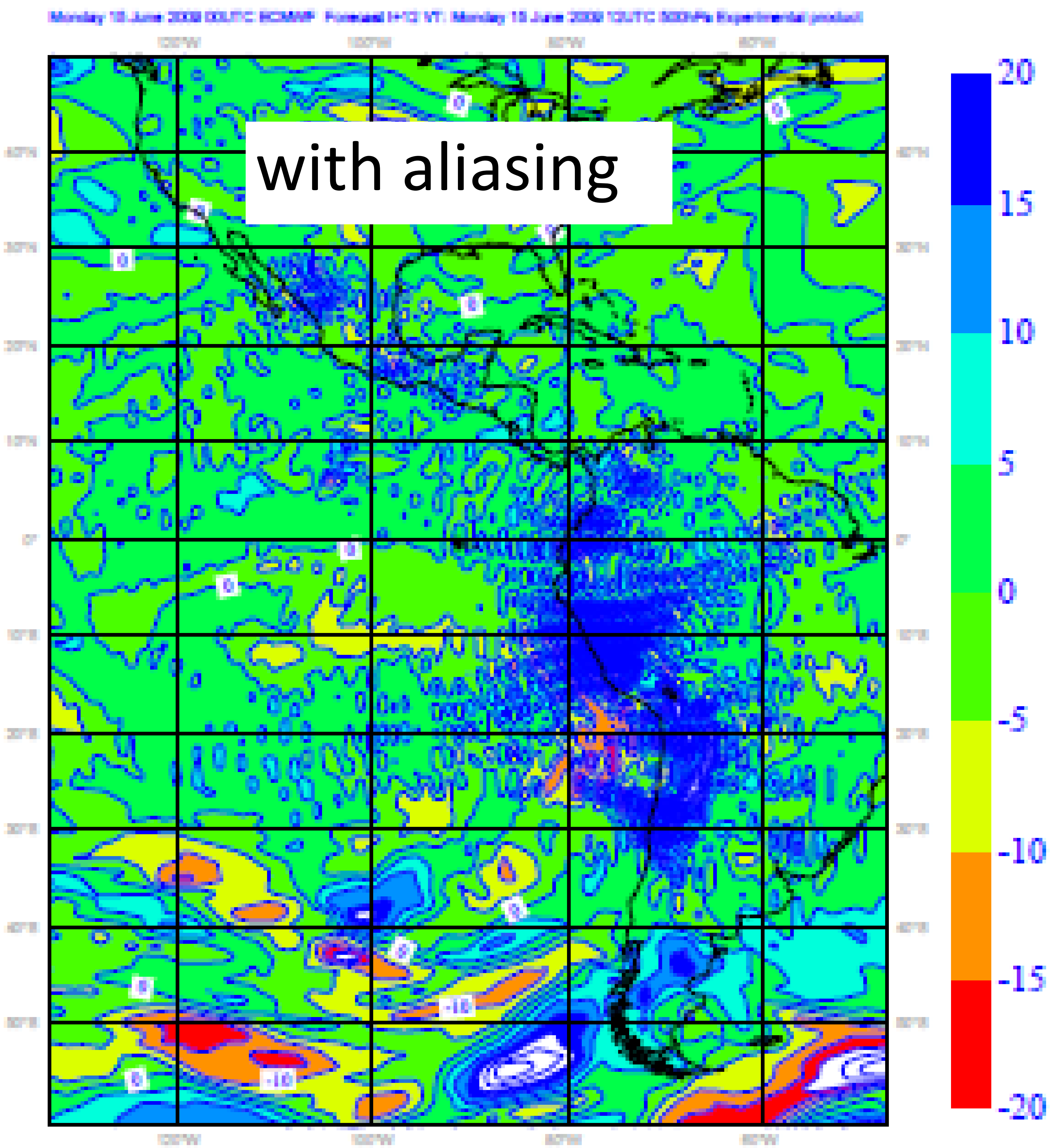

**Issue**: multiplication of two waveform variables produces a new variable with shorter wavelength than the one the grid can handle

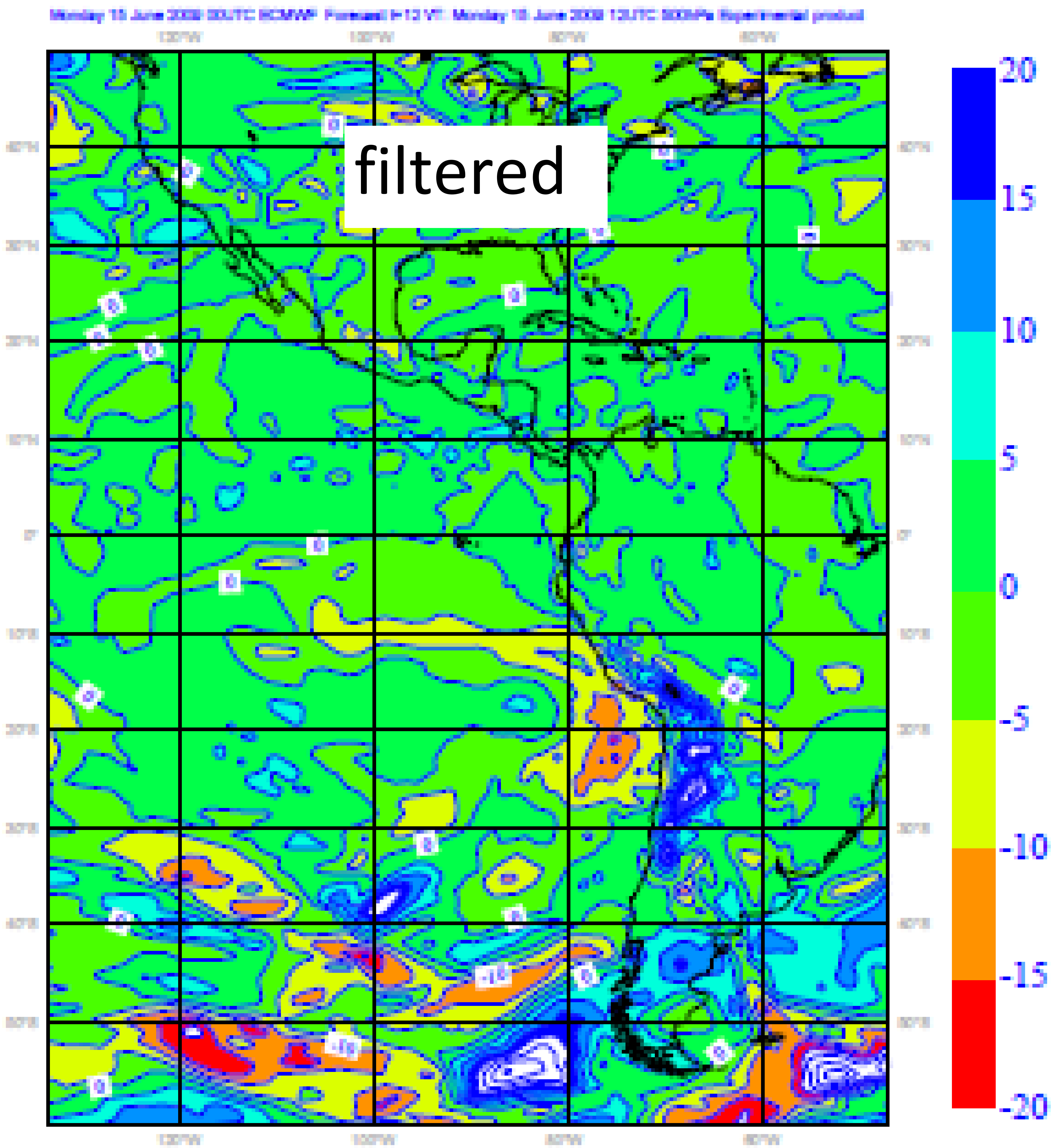
# aliasing


**Issue**: multiplication of two waveform variables produces a new variable with shorter wavelength than the one the grid can handle

# aliasing example

## 500hPa adiabatic zonal wind tendencies (T159)

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# aliasing example

## 500hPa adiabatic meridional wind tendencies (T159)

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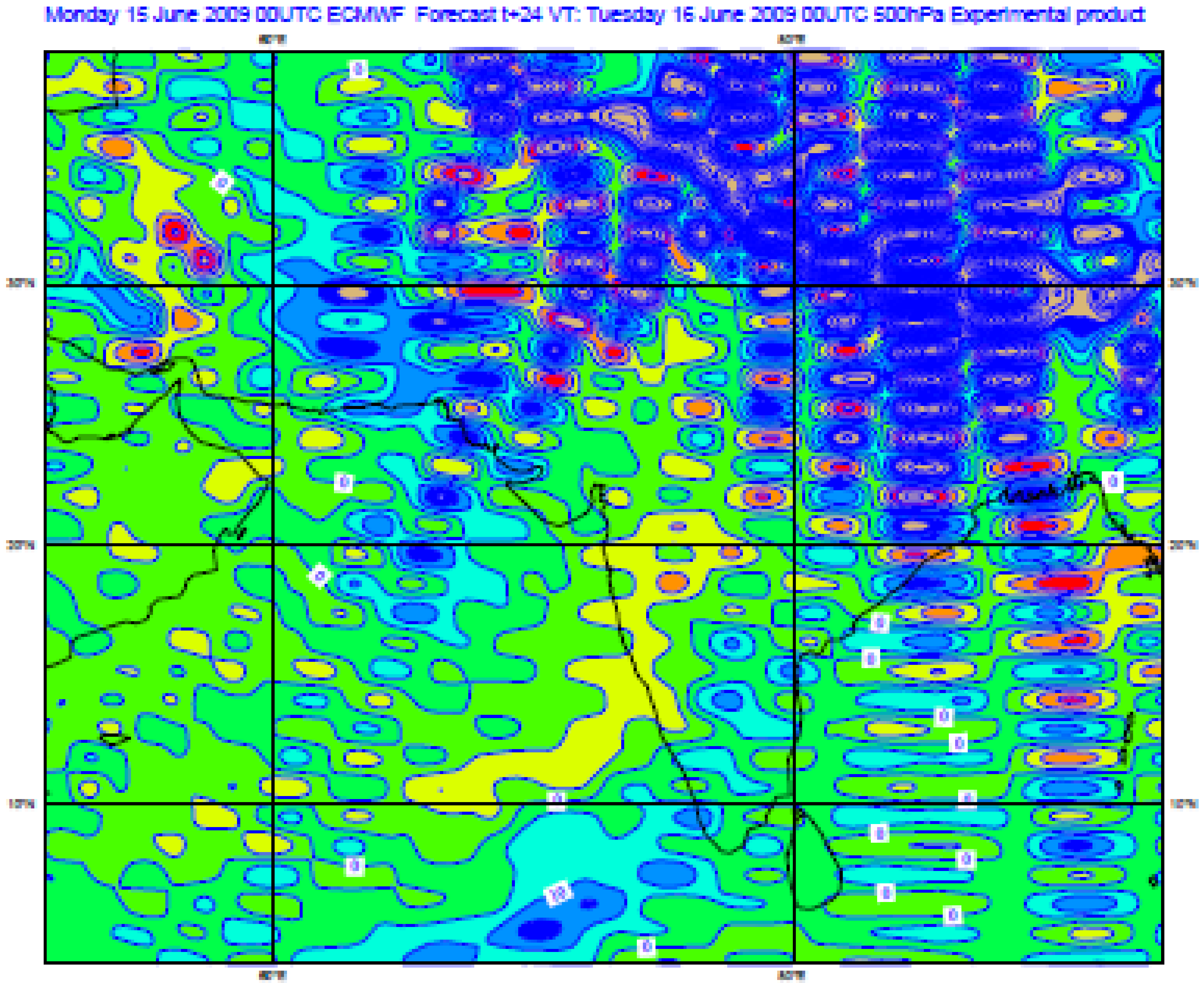
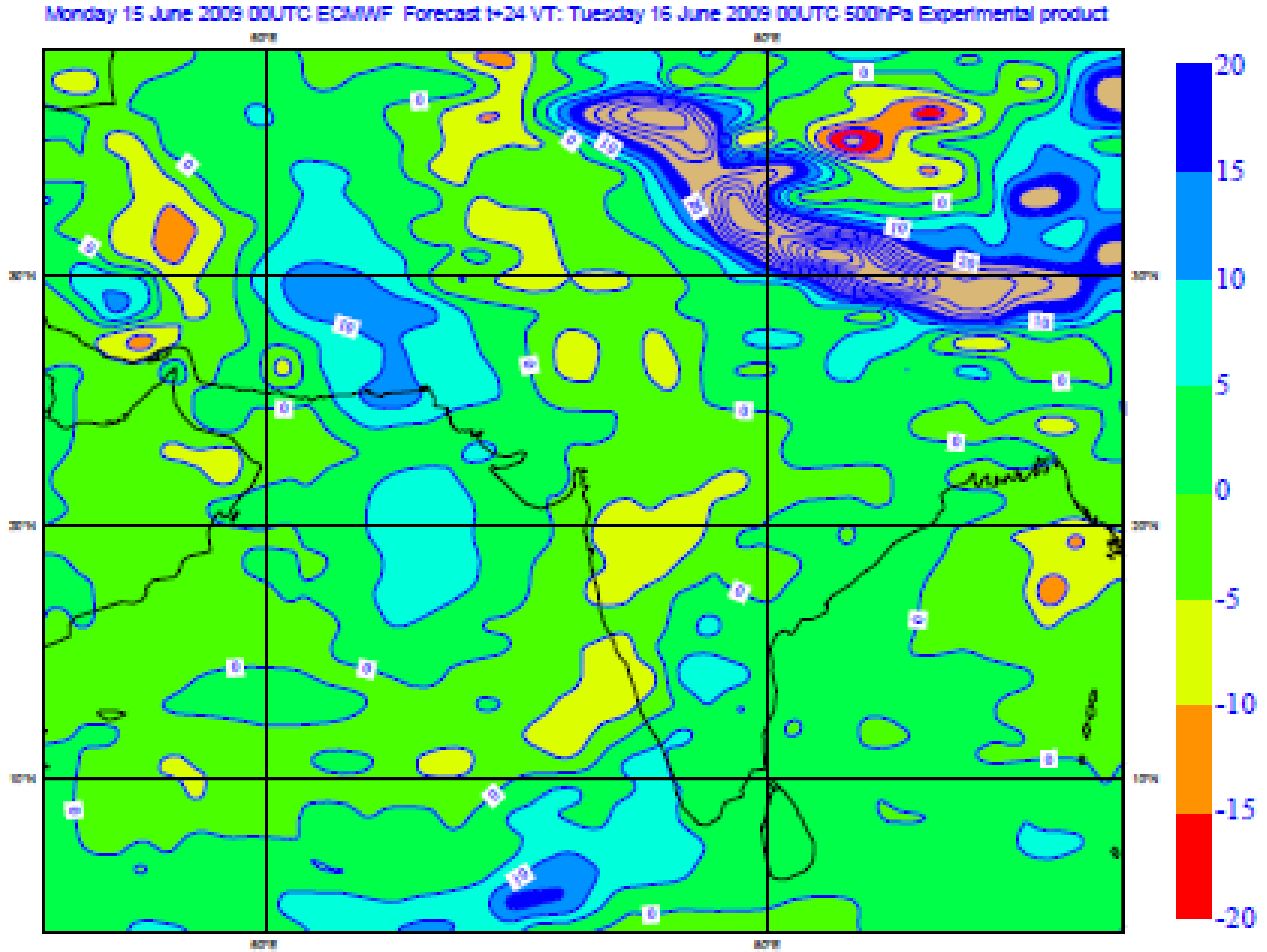
### with aliasing




### filtered



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# alternatives to using a filter

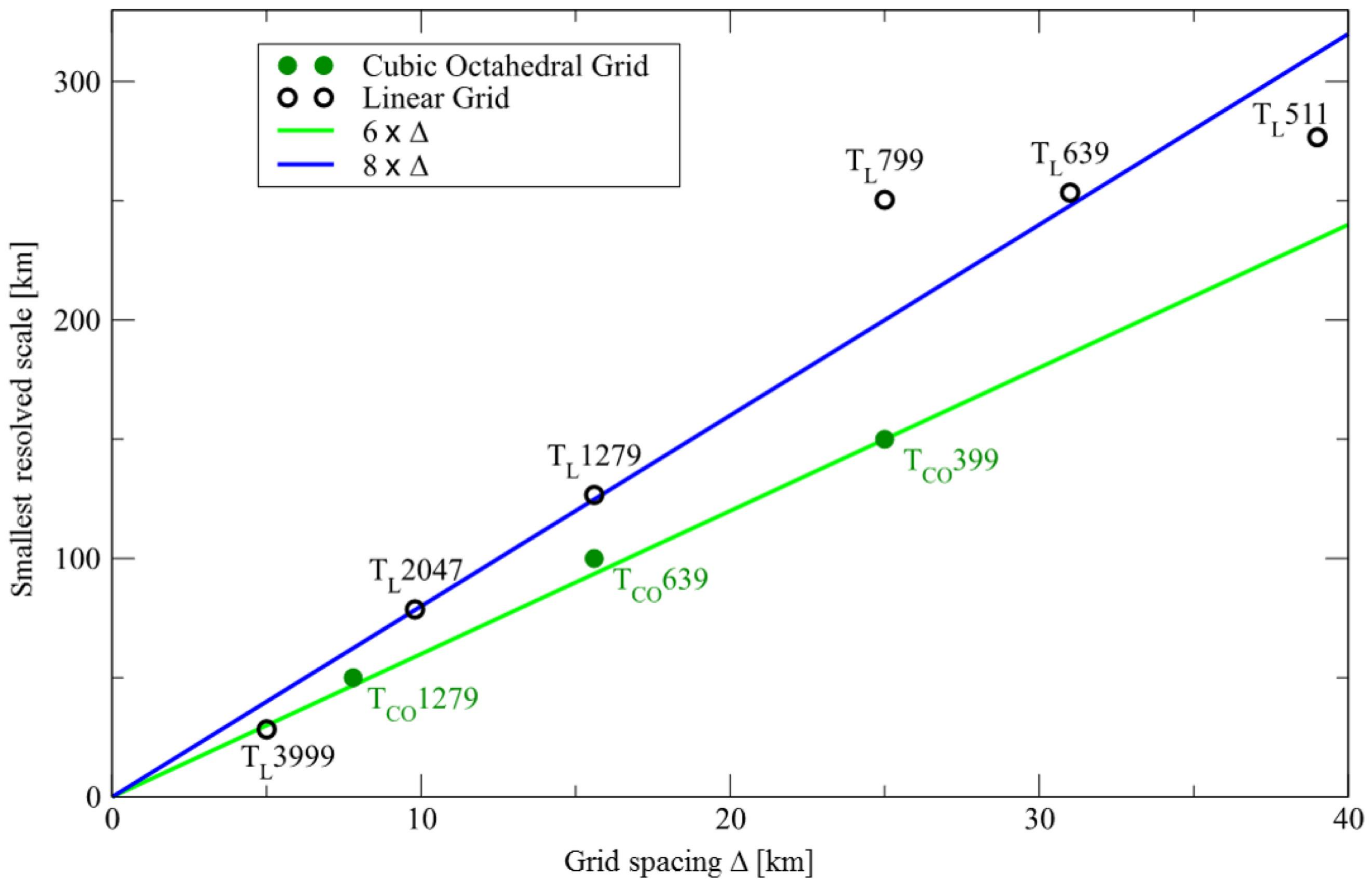
**Idea**: use more grid points than spectral coefficients

| Orszag, 1971: | Spatial filter range<br>Δ : grid-length<br>*(Wedi, 2014)* | Equation terms accurately represented without aliasing |
|---|---|---|
| 2N+1 gridpoints to N waves : linear grid | ~ 1-2 Δ | Linear |
| 3N+1 gridpoints to N waves : quadratic grid | ~ 2-3 Δ | Quadratic |
| 4N+1 gridpoints to N waves : cubic grid | ~ 3-4 Δ | Cubic |

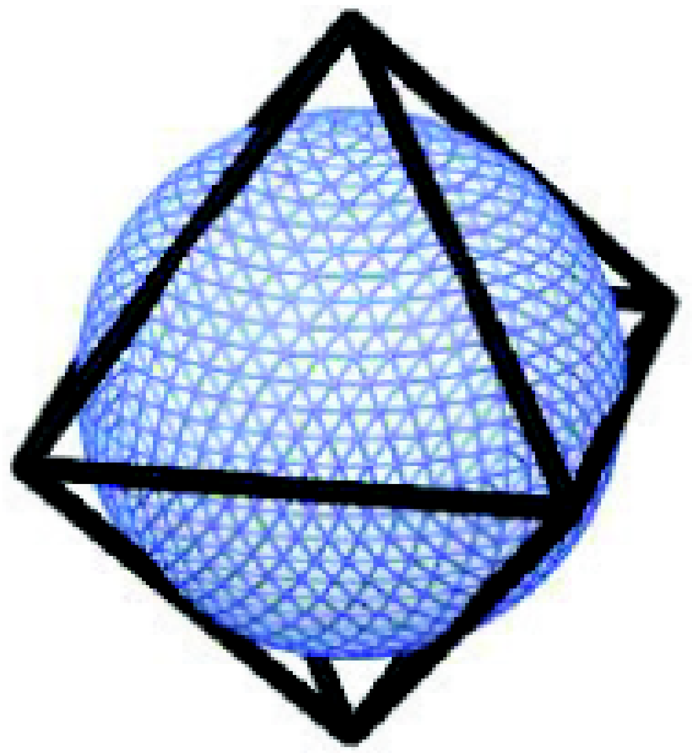
- Cubic grid filters 3-4 grid-length oscillations therefore no need to apply an extra de-aliasing filter as in the linear grid
- The smallest wavelength 2πα/N is resolved by 2,3,4 points by the linear, quadratic, cubic grids

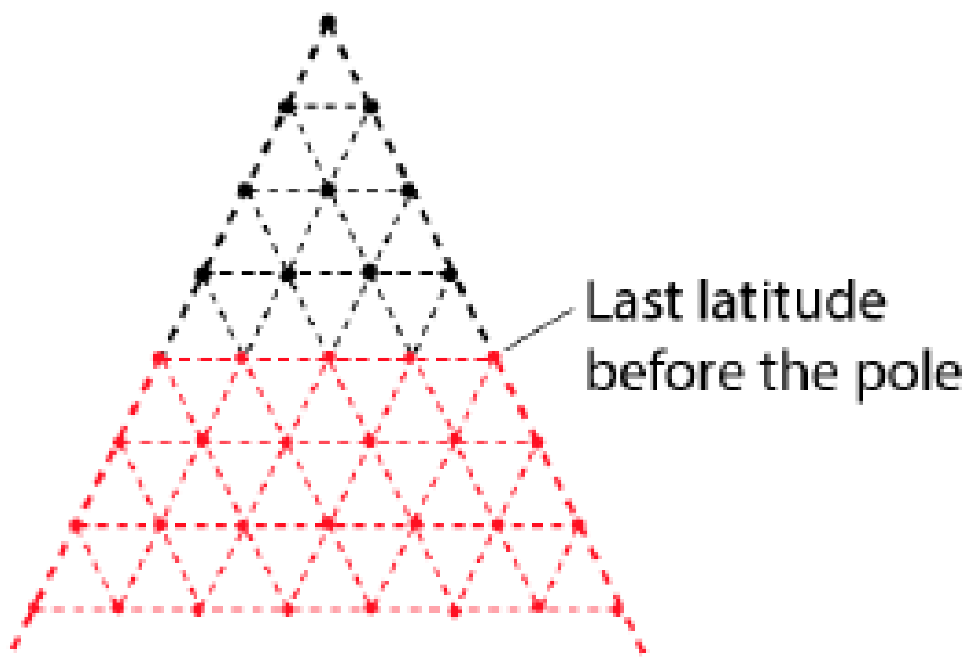
# effective resolution

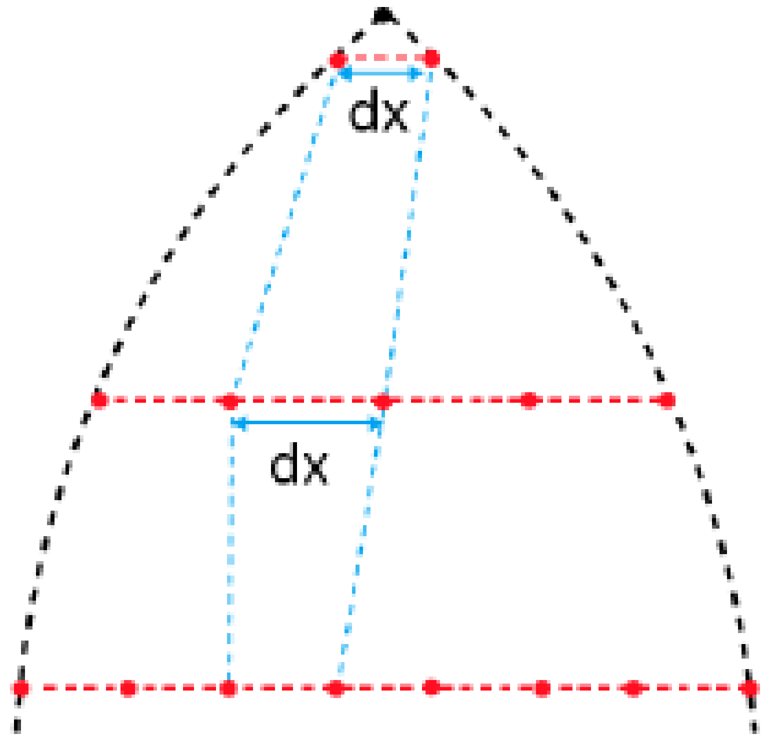
of linear and cubic grids (Abdalla et al. 2013)



# Cubic octahedral (Gaussian) grid of IFS

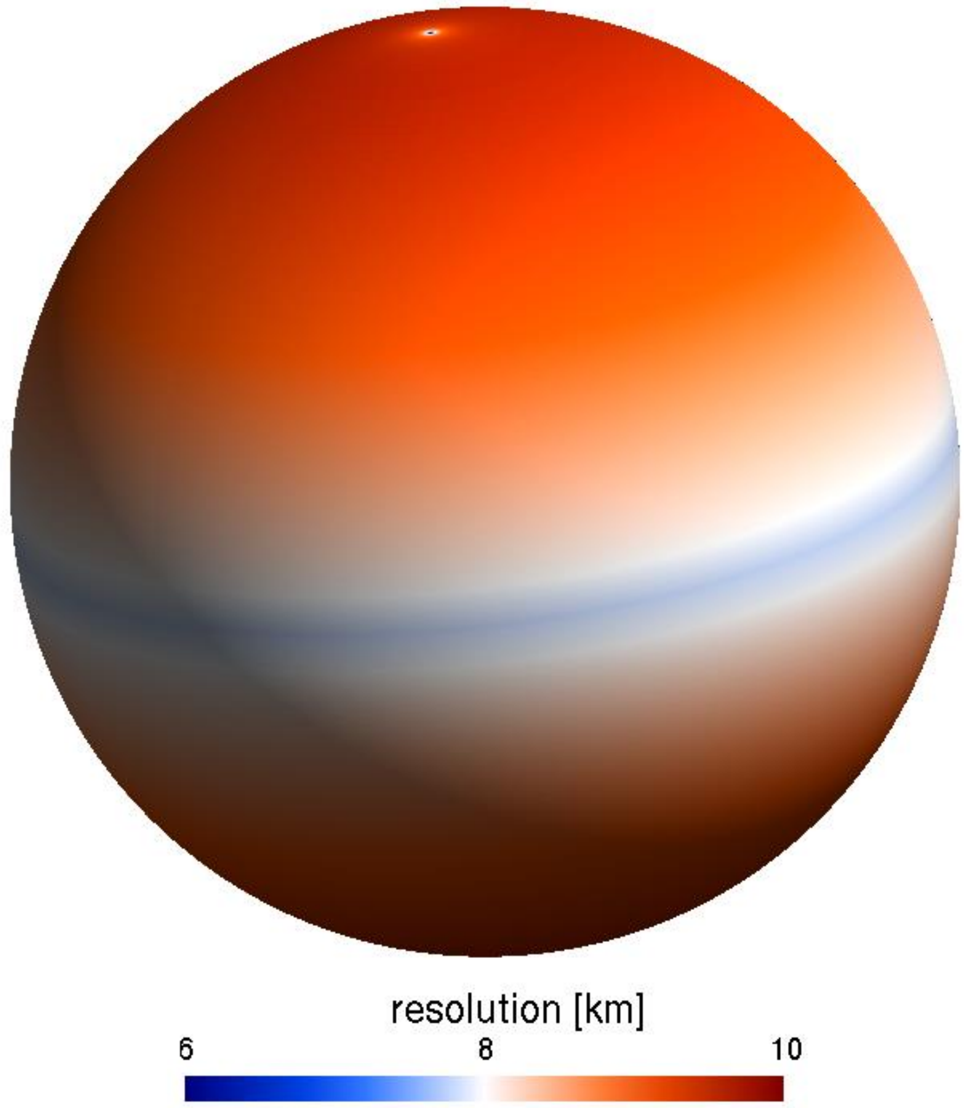





- No aliasing in nonlinear products
- Improved accuracy and mass conservation compared with linear grid
- Efficiency and scalability for large size problems: high grid-point resolution for a given spectral truncation i.e. expensive transforms become a smaller fraction of total computations

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



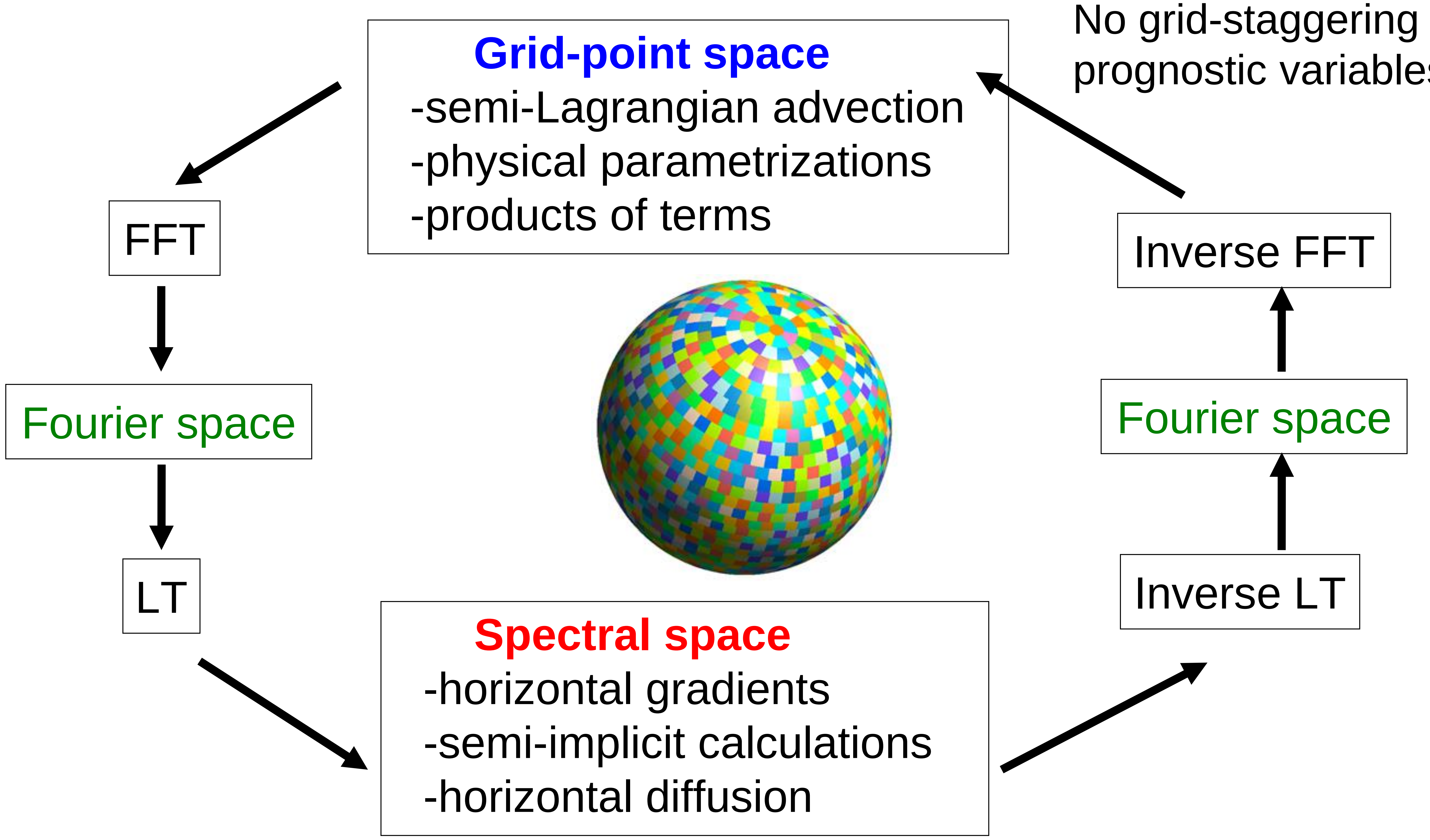

Variation of grid-point resolution with latitude

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

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

# time step in IFS

No grid-staggering of prognostic variables




FFT: Fast Fourier Transform, LT: Legendre Transform

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# Inverse transforms: use of symmetry properties of Legendre polynomials in computation

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

spectral space

**even n** | **odd n**

for each m:

Normalised associated Legendre polynomial

**parallelisation over m, n indices**

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

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

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

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

**lots of MPI communication**

inverse Legendre transform

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

inverse Fourier transform

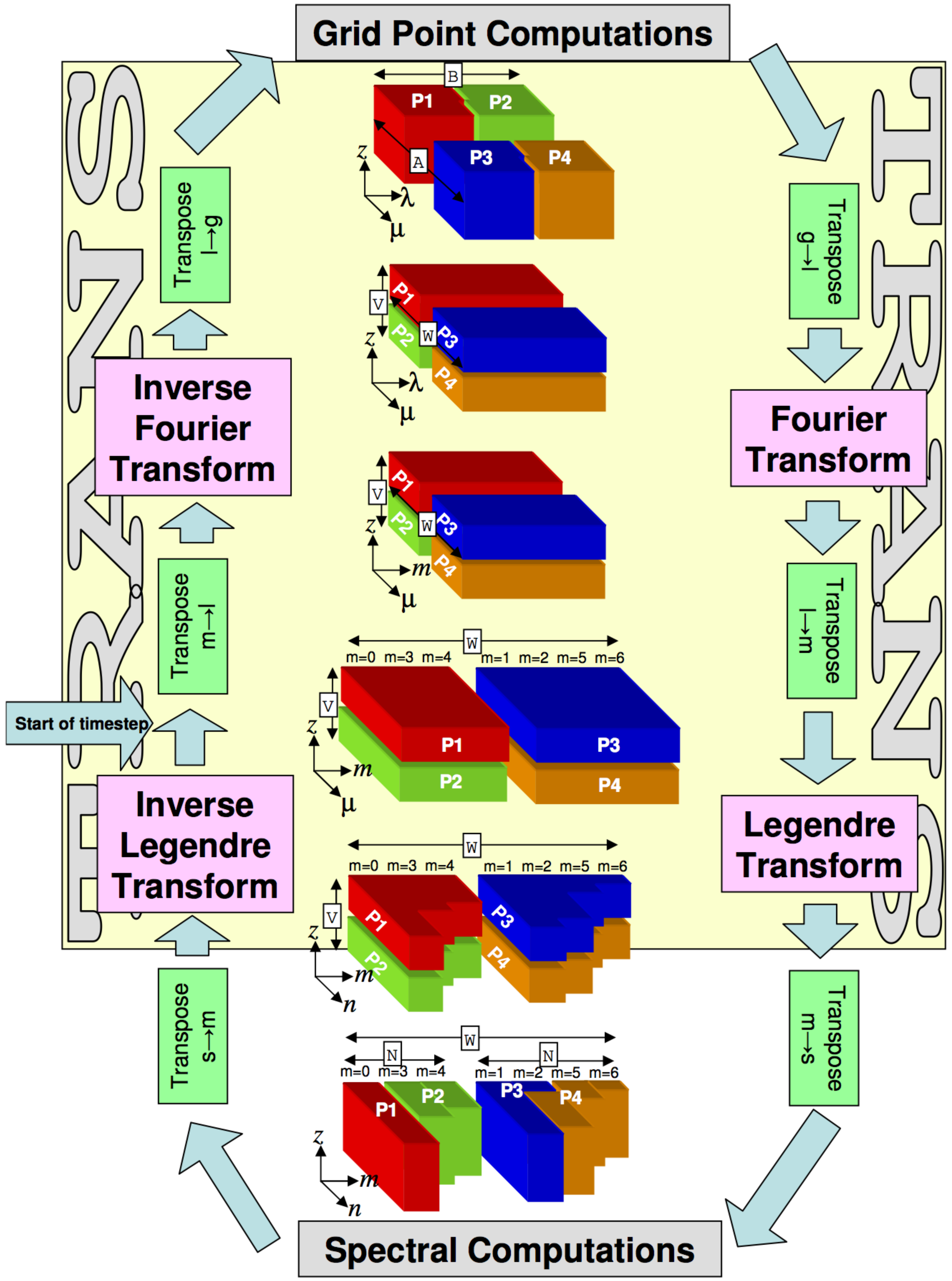
grid point data: $\mathbf{G}(f, \lambda, \phi)$

grid point space

# Domain decomposition in spectral transform semi-implicit solver

Direct Legendre transform:

- multiply data with Gaussian quadrature weights
- Same as an inverse transform but in reverse order
- The data transpositions needed by spectral transforms imply heavy communication load





**References**:
*Foster et al, Parallel Algorithms for the Spectral Transform Method, SIAM J Sci Com, 1997*
*Baros et al, The IFS model: A parallel production weather code, Parallel computing 21*

# Matrix-matrix multiply in a LT

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Legendre and inverse Legendre transforms are expressed as a matrix-matrix multiply for each wavenumber m (Wedi et al, MWR 2013)

$$f_n^m(z,t) = \frac{1}{2}\sum_{k=1}^{K} w_k \; f_m(\mu_k, z, t) P_n^m(\mu_k)$$

$$f_m(\mu_k, z, t) = \sum_{n=|m|}^{M} f_n^m(z,t) P_n^m(\mu_k)$$

**Left: LT**
**Right: Inverse LT**

$$\left[\; f^m(\mu_k)_l \;\right] = \left[\; P_n^m(\mu_k)_l \;\right]\left[\; f_{n,l}^m \;\right]$$

A matrix-matrix multiply for each zonal wavenumber m across all Gaussian Latitudes and vertical levels

Gaussian latitude

Vertical level

Fast LT: apply "butterfly" compression (Tygart 2010)

Spectral coefficient at vertical level l

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# Interpolative decomposition ("butterfly compression")

The ***left hand-side matrix*** in a LT transform (matrix-matrix multiply) ***remains the same*** *regardless the timestep*. It can be compressed and approximated in a form that accelerates computation

$$A_{m\times n} \approx R_{m\times k} S_{k\times n}$$

- A: rank deficient matrix
- R: contains blocks with full rank
- S: "interpolation matrix". A subset of its columns makes up the identity matrix -cannot be further compressed so must be saved
- The approximation is valid within a tolerance selected so that it doesn't change significant the results

$$A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} R_1 \cdot S_1 \\ R_2 \cdot S_2 \end{bmatrix}$$

Split matrix in two halves applying decomposition

$$\begin{bmatrix} R_1 \cdot S_1 & 0 \\ 0 & R_2 \cdot S_2 \end{bmatrix} = \begin{bmatrix} R_1 & 0 \\ 0 & R_2 \end{bmatrix} \begin{bmatrix} S_1 & 0 \\ 0 & S_2 \end{bmatrix}$$

Rewrite matrix as the product of two block matrices emptying half of each column

The above algorithm can be repeated until the residual block matrix contains a single diagonal of full-rank blocks

# Fast Legendre Transform

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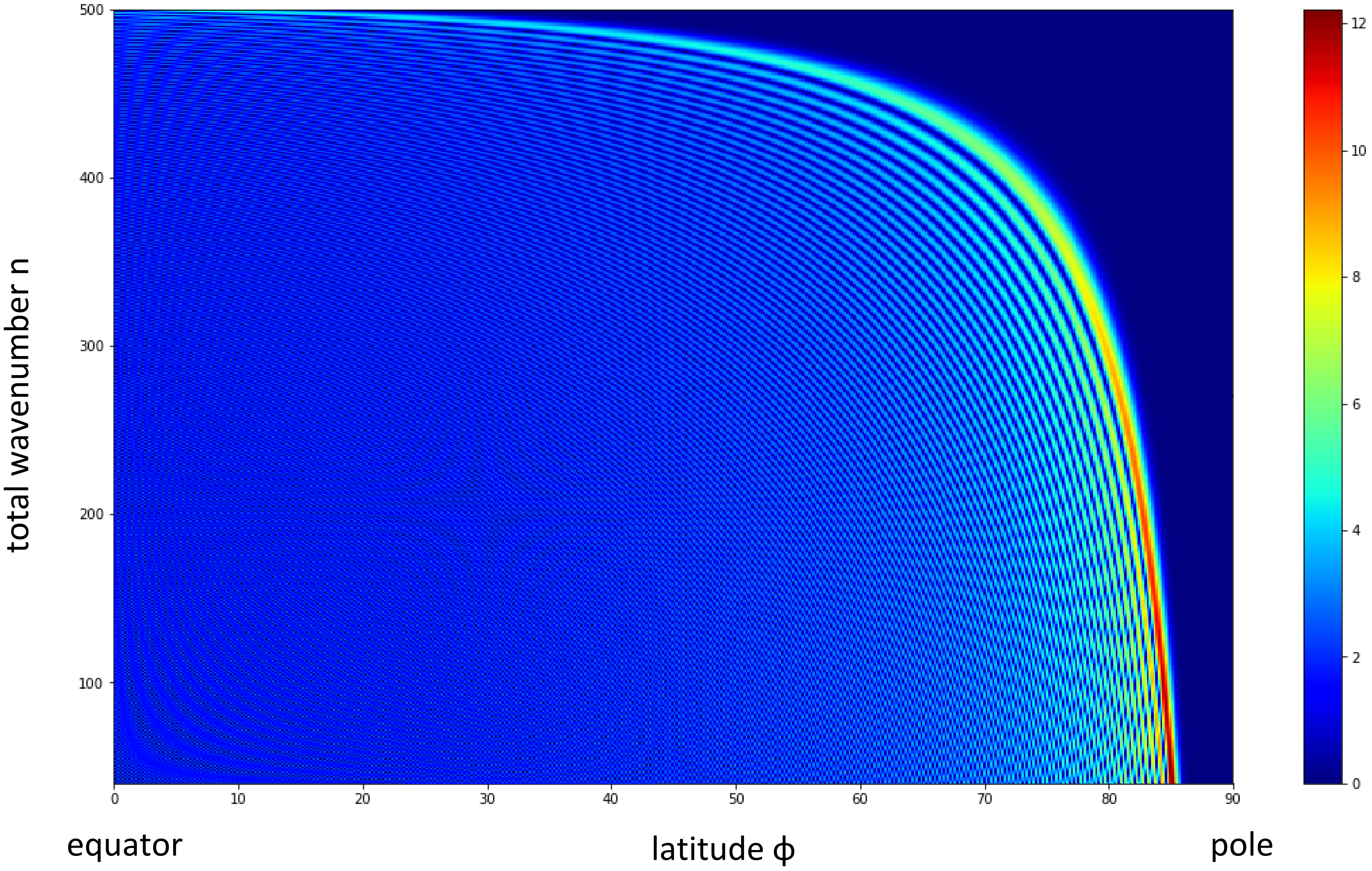
Matrix of
Legendre polynomials

truncation N=500,
zonal wavenumber
m=40

**FLT:**

**step 1**: split matrix into two halves

**step 2**: empty half of each column and apply "interpolative decomposition”



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Funded by the European Union

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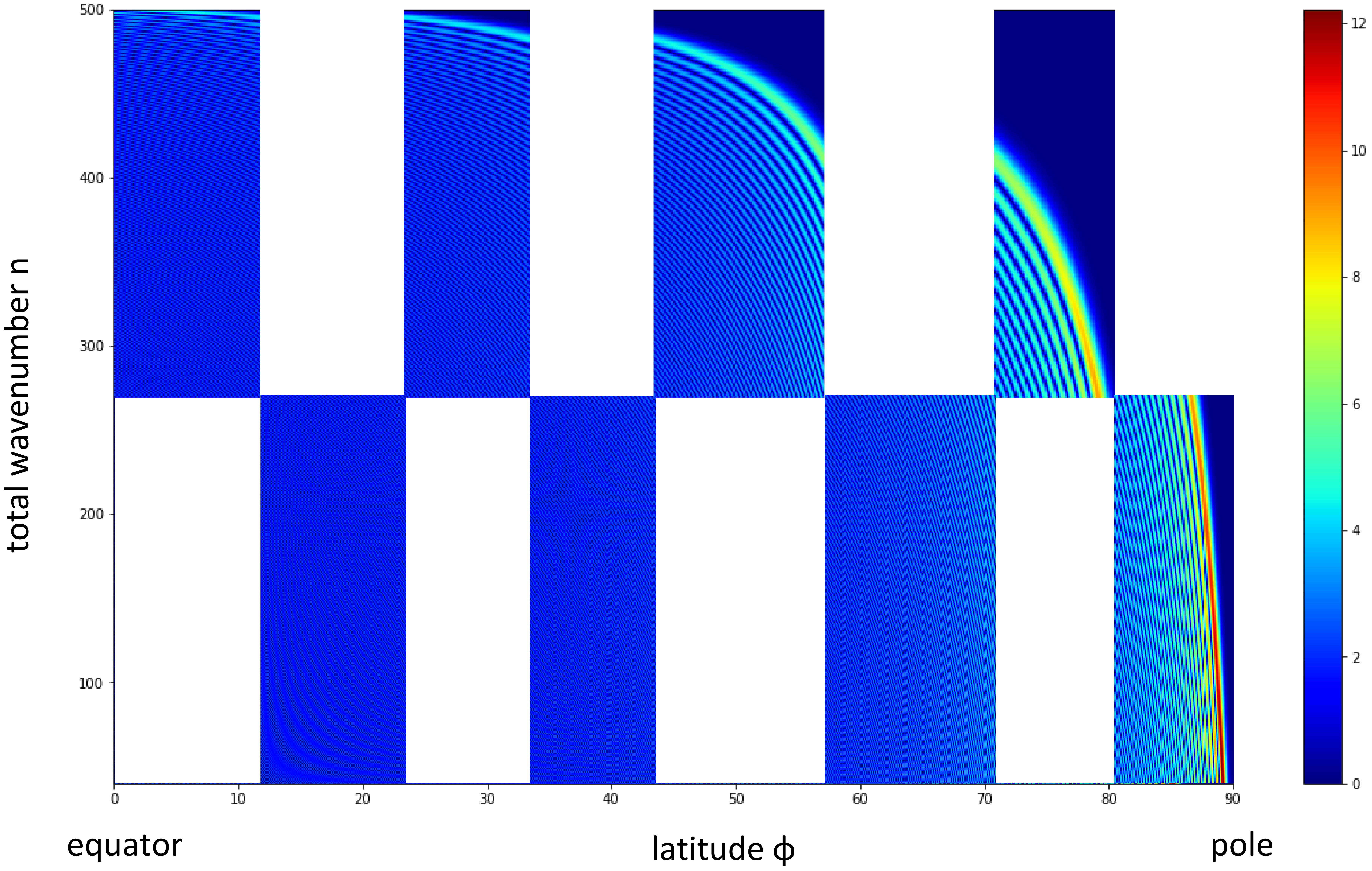
**step 3**: reorder columns



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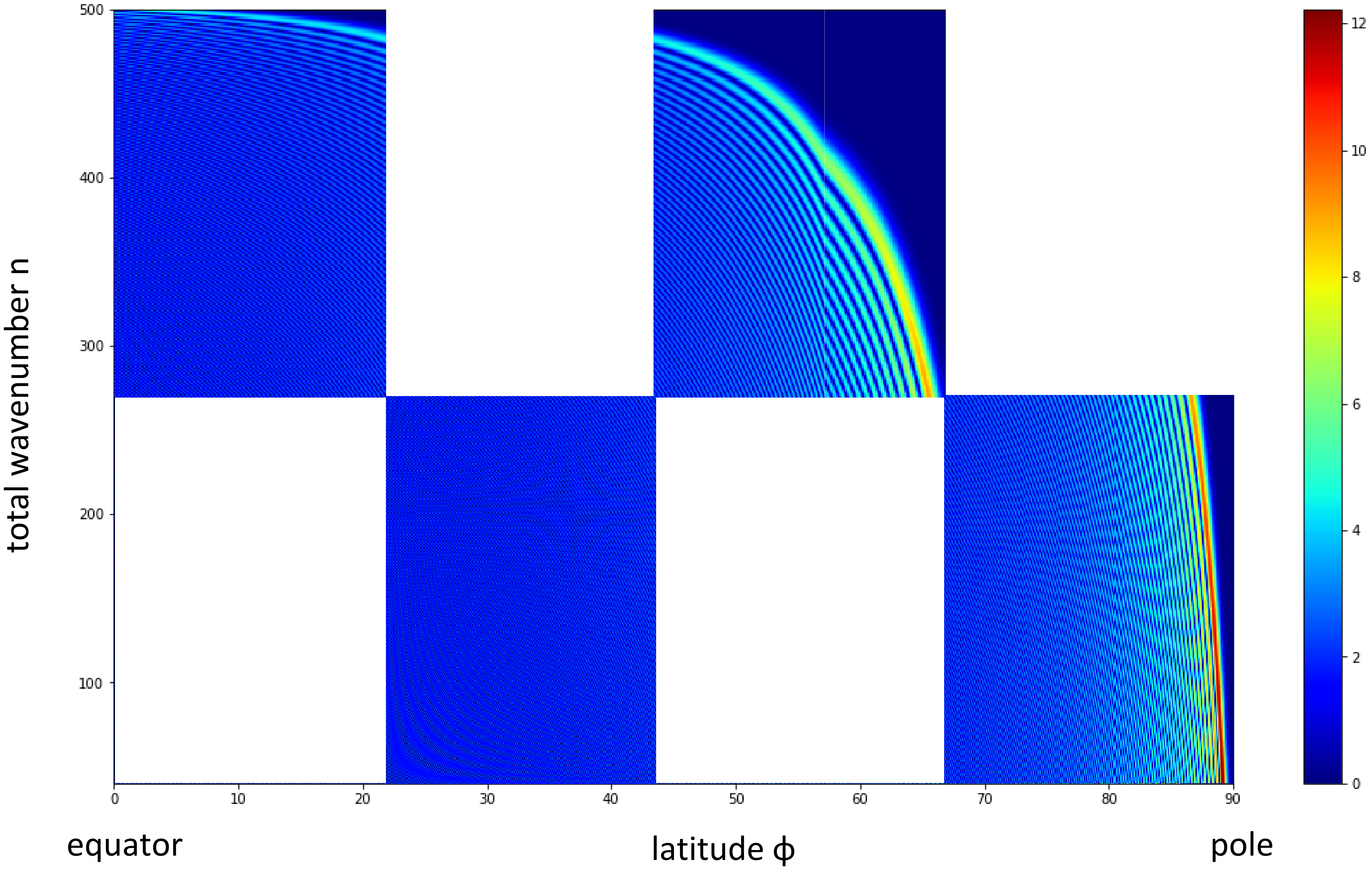
**step 3**: reorder columns

**step 4**: apply to each block recursively



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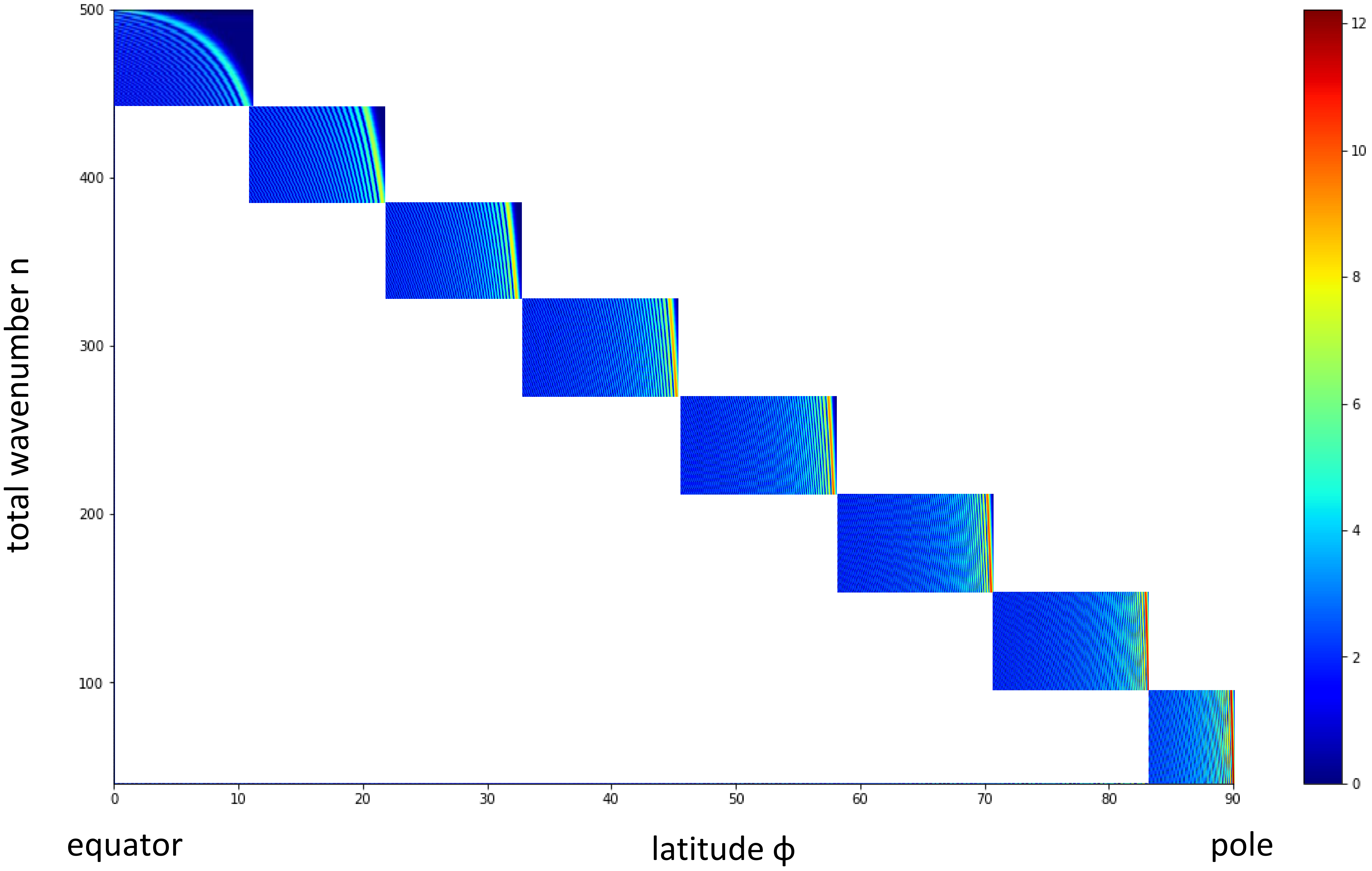

# Fast Legendre Transform

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Matrix of
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truncation N=500,
zonal wavenumber
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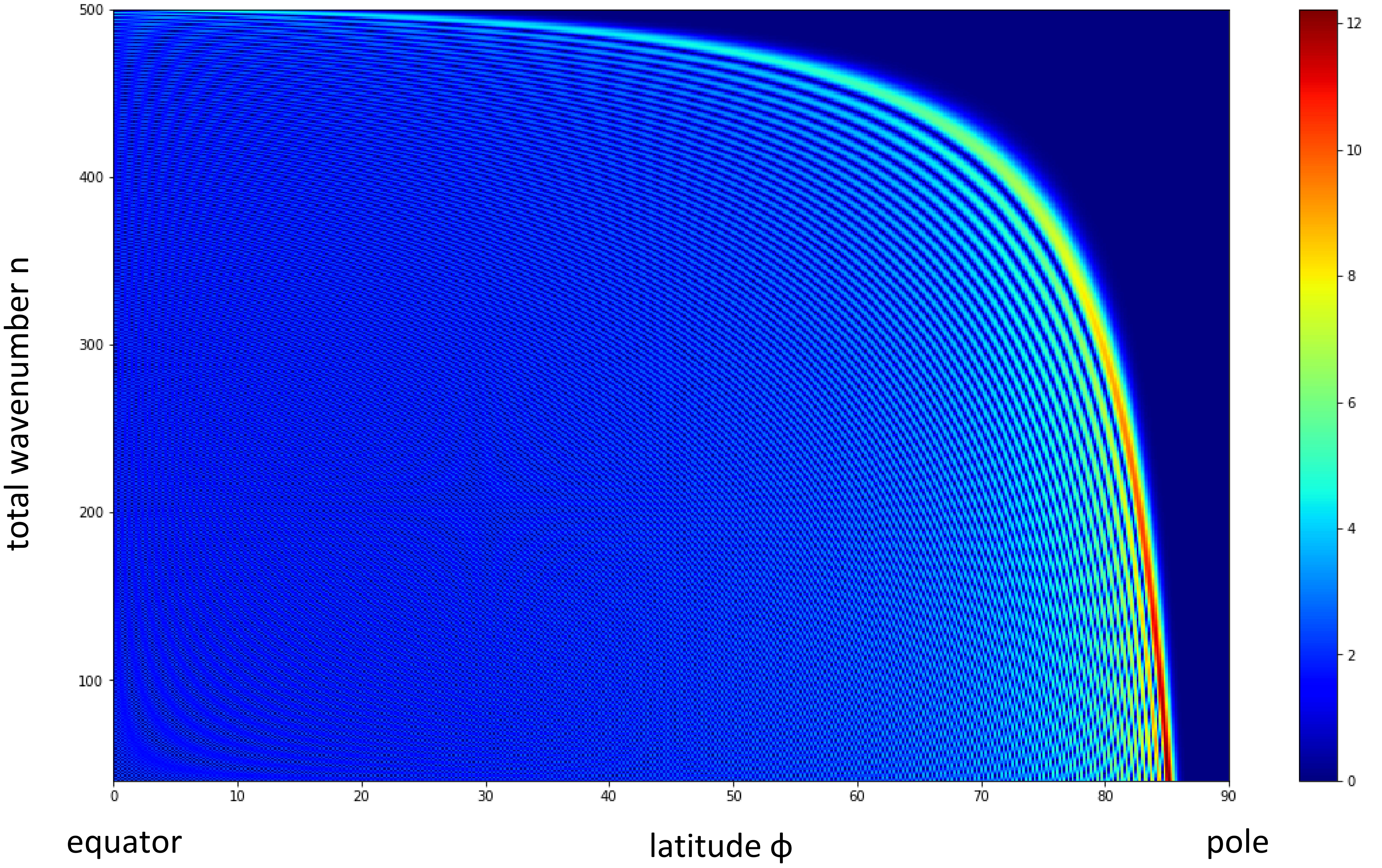

# Fast Legendre Transform

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Matrix of
Legendre polynomials

truncation N=500,
zonal wavenumber
m=100

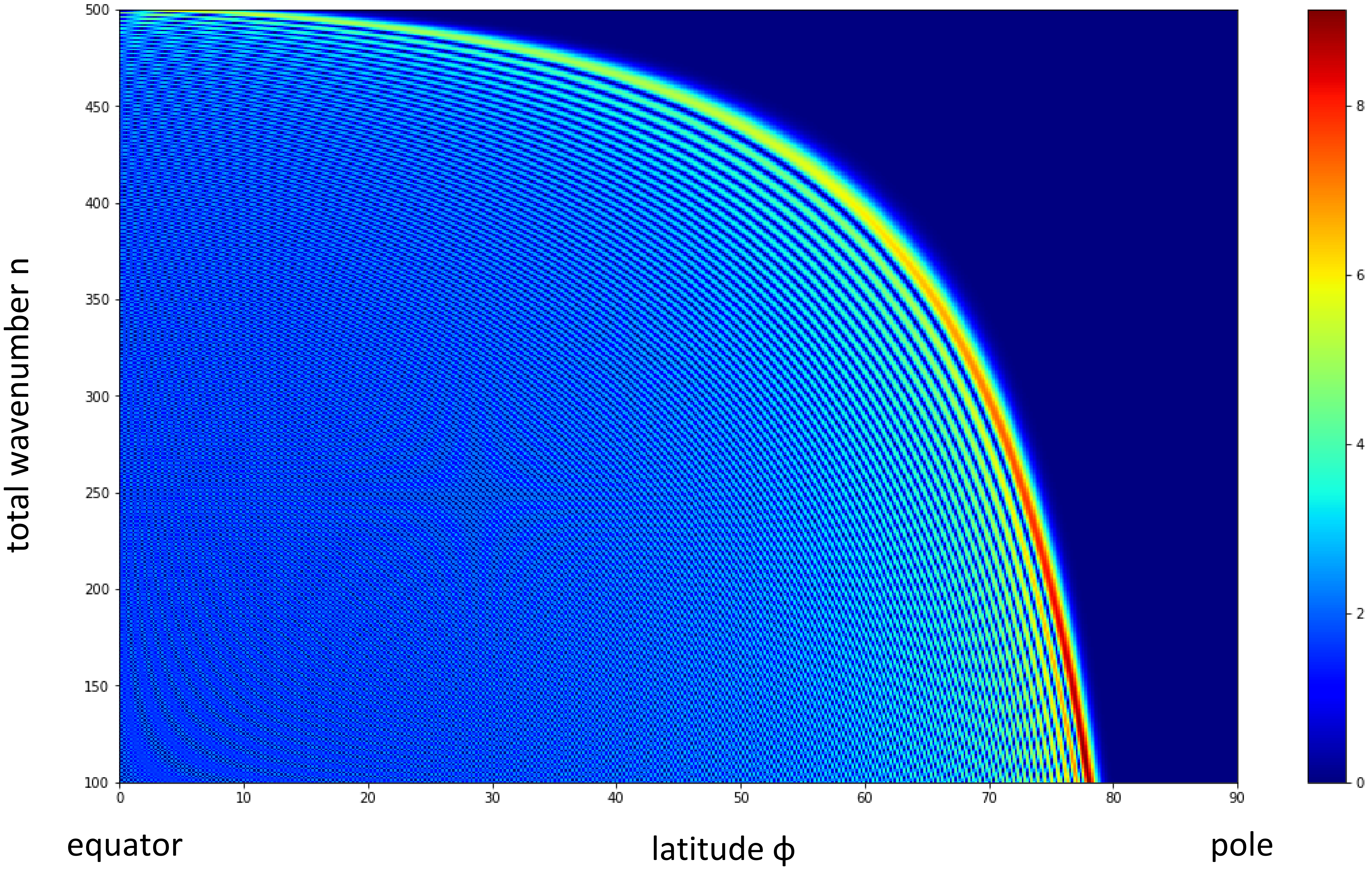
**FLT:**

**step 1**: split matrix into two halves

**step 2**: empty half of each column and apply "interpolative decomposition”

**step 3**: reorder columns

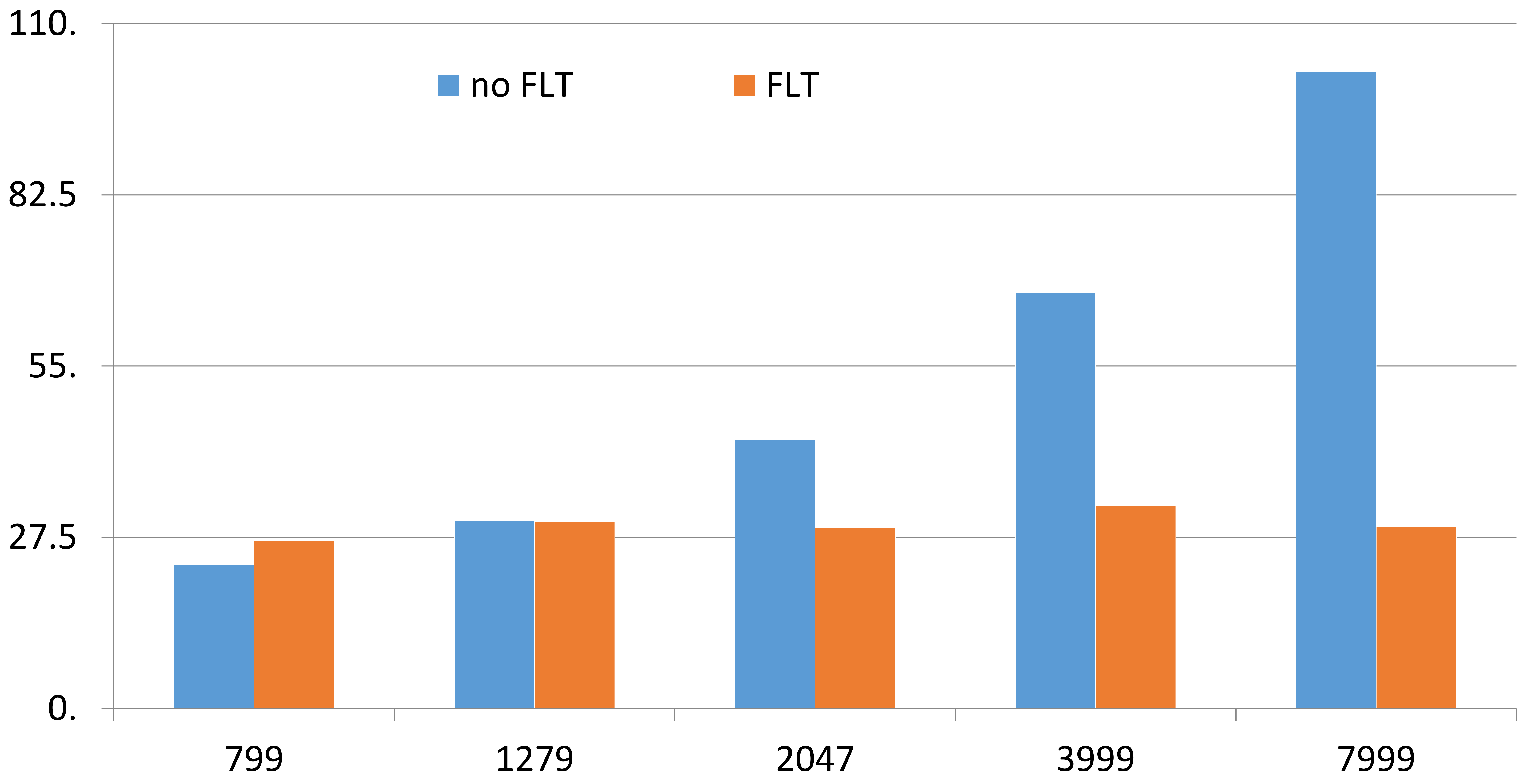
**step 4**: apply to each block recursively



# Fast Legendre Transform

## floating point operations

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

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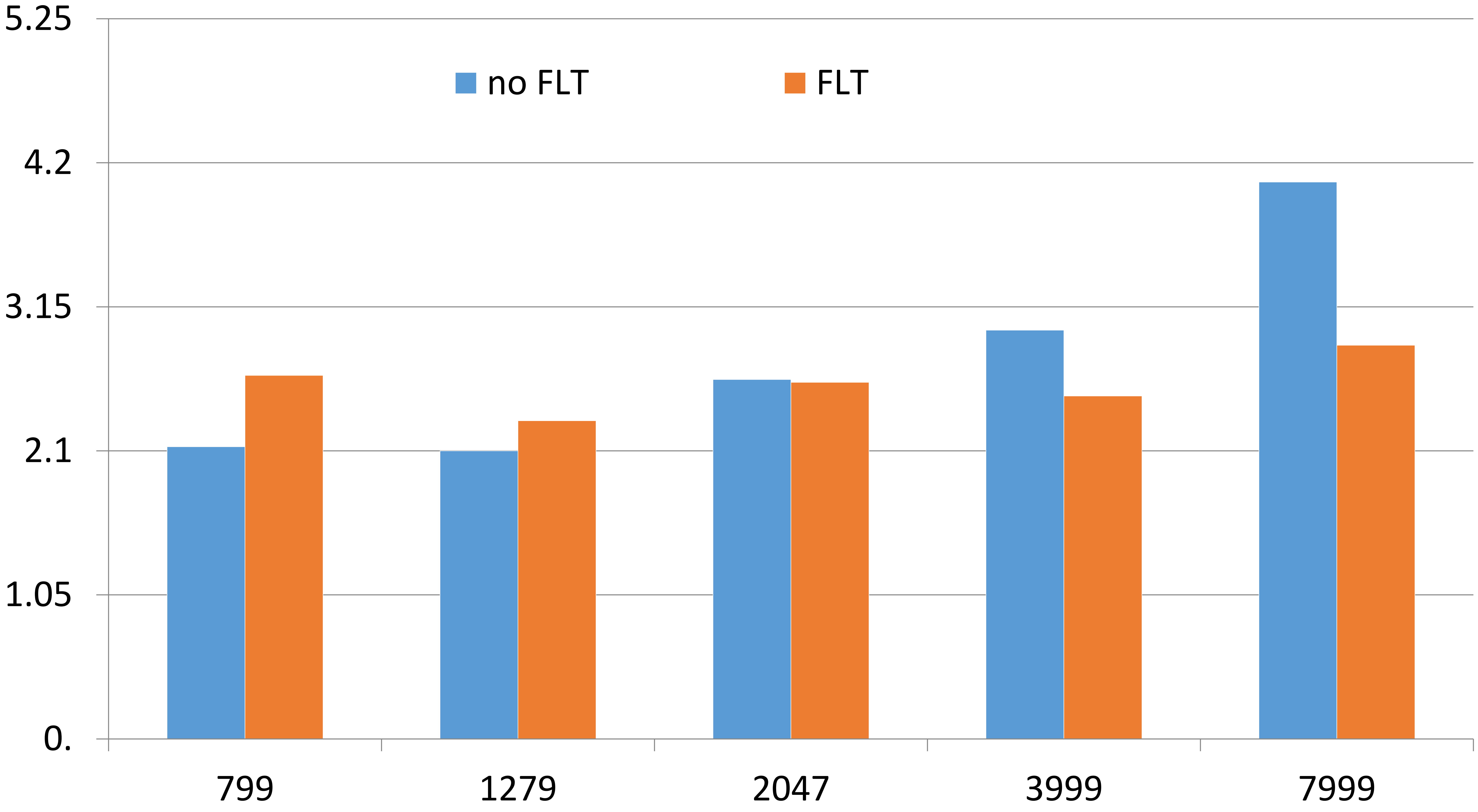
# Fast Legendre Transform

wallclock time

Average wall-clock time compute cost of $10^7$ spectral transforms scaled by $N^2 \log^3 N$

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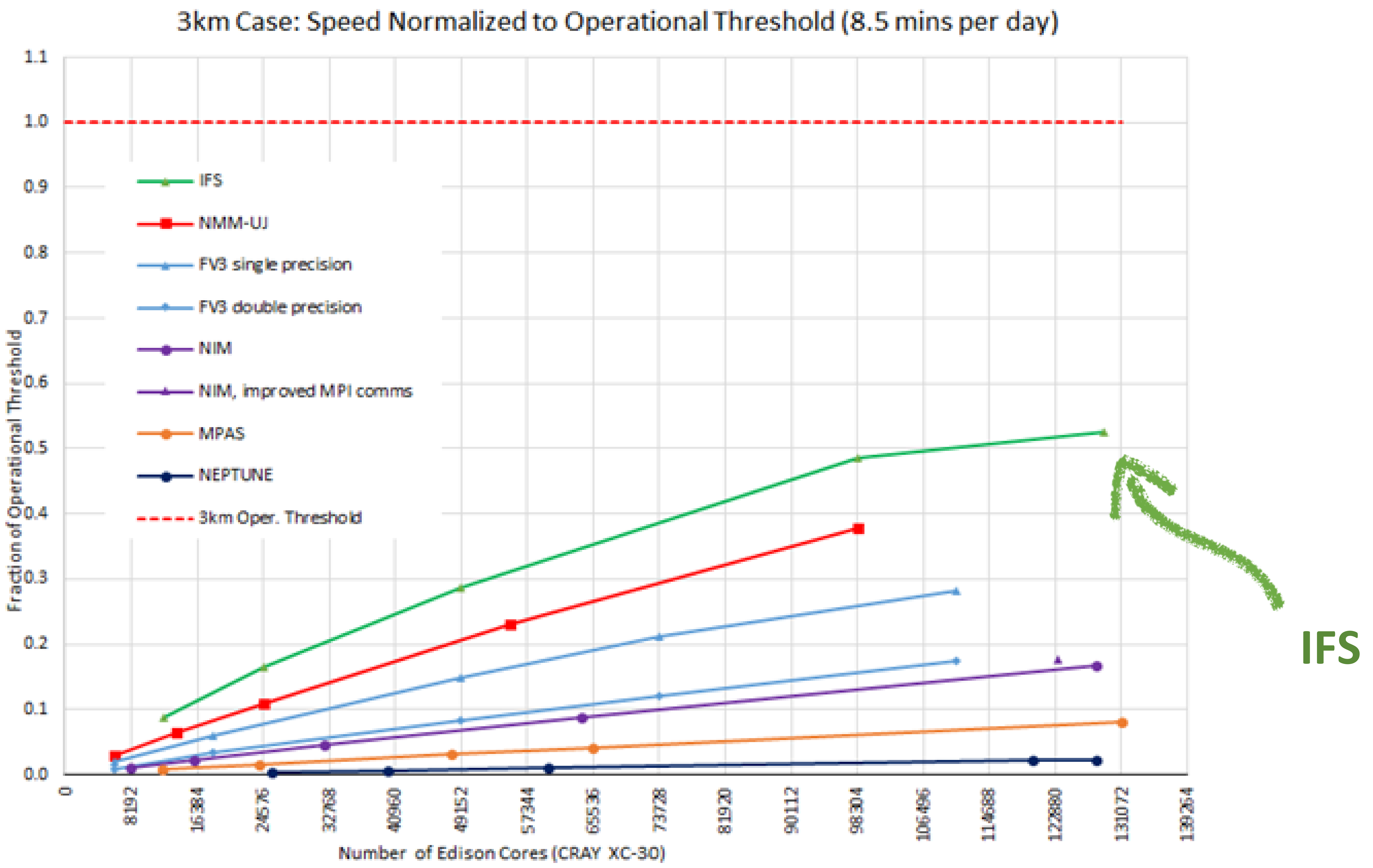
# performance comparison

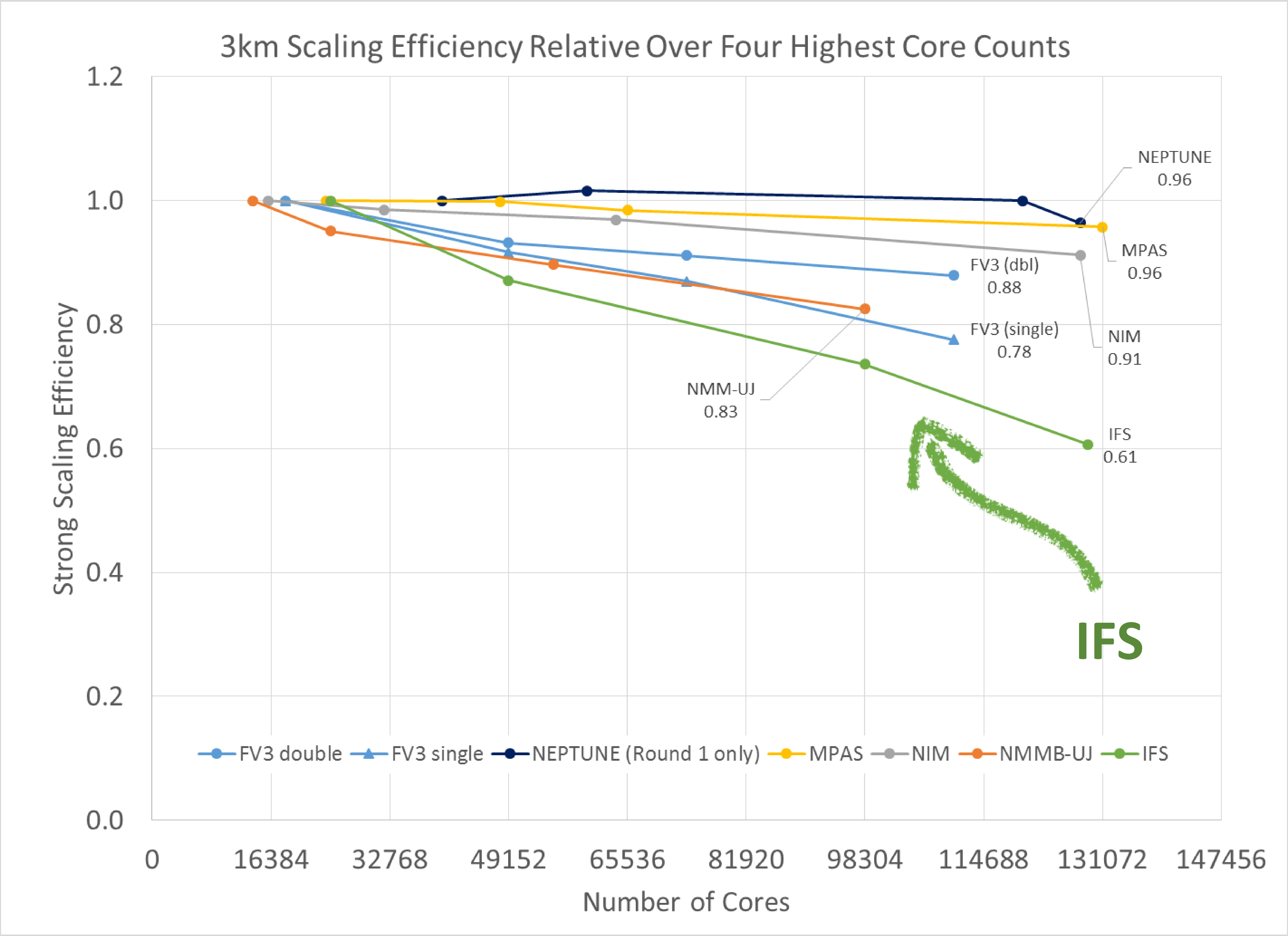
## of IFS with other models




*(Michalakes et al, NGGPS AVEC report, 2015)*

# scalability comparison

## of IFS with other models




*(Michalakes et al, NGGPS AVEC report, 2015)*

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ESCAPE 2

# IFS scaling on Summit and PizDaint (CPU only)

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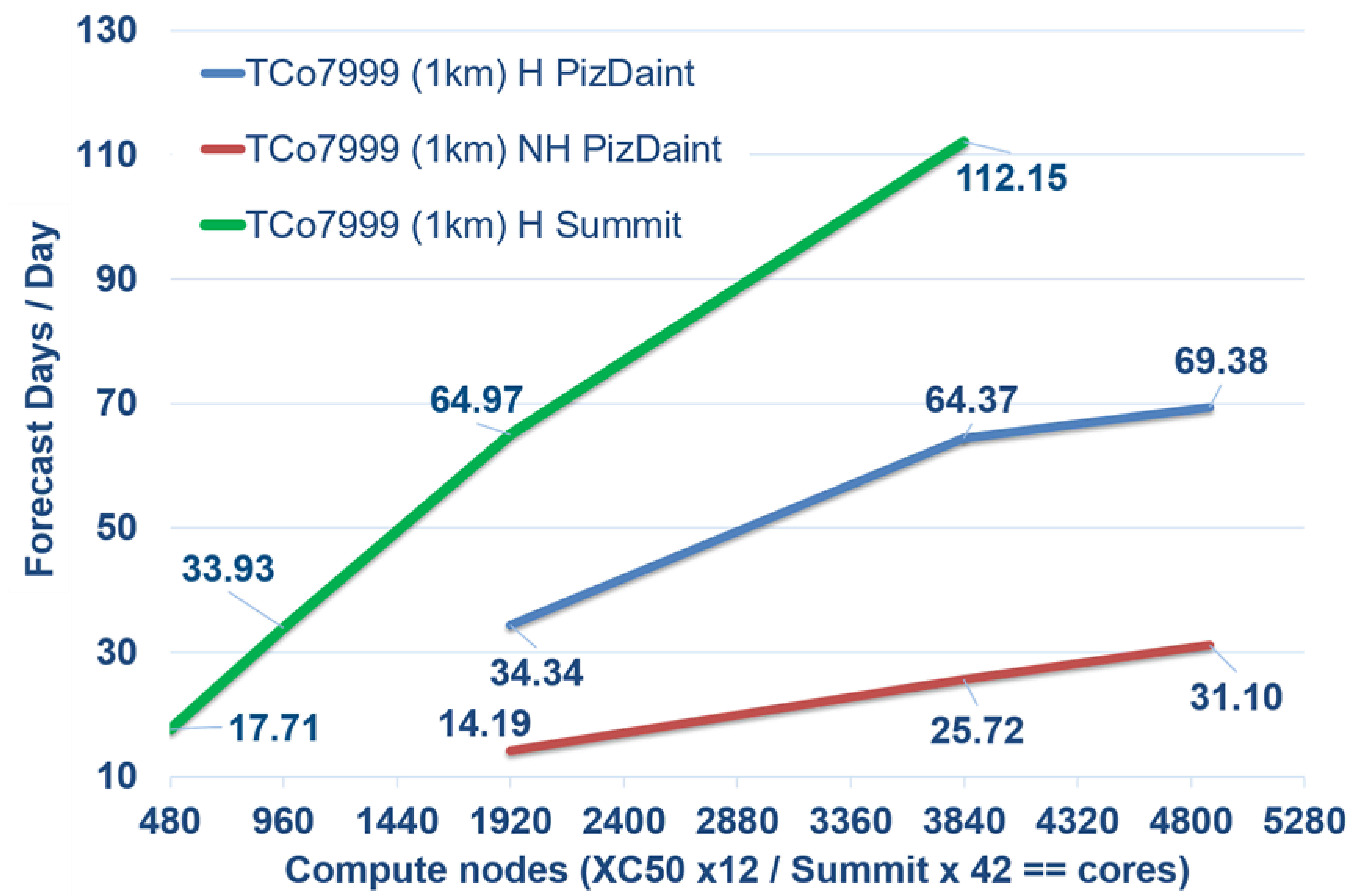

# optimisations by NVIDIA in ESCAPE

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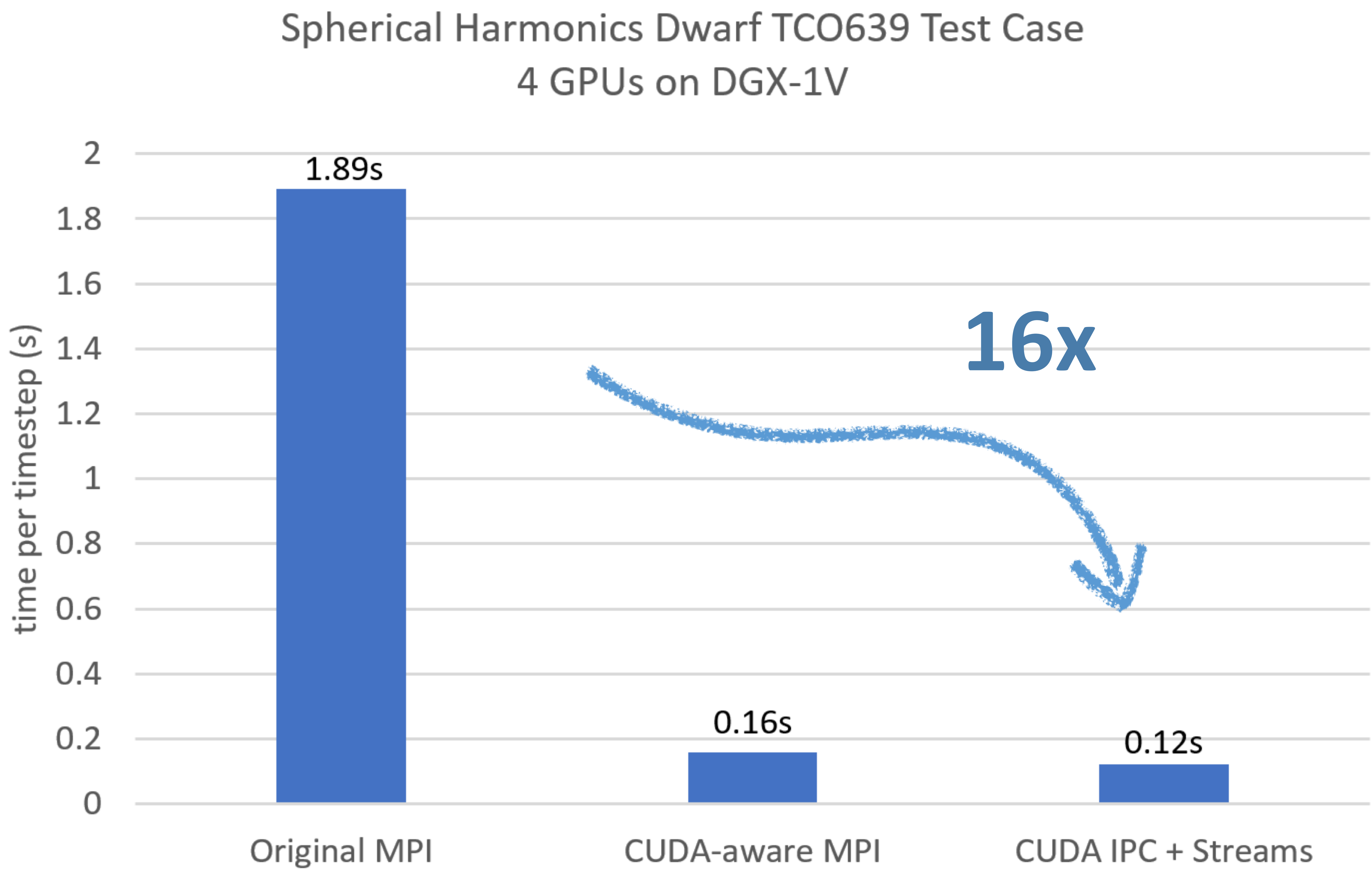


*figure: courtesy of Alan Gray, Peter Messmer (NVIDIA)*

# GPUs vs CPUs on Summit

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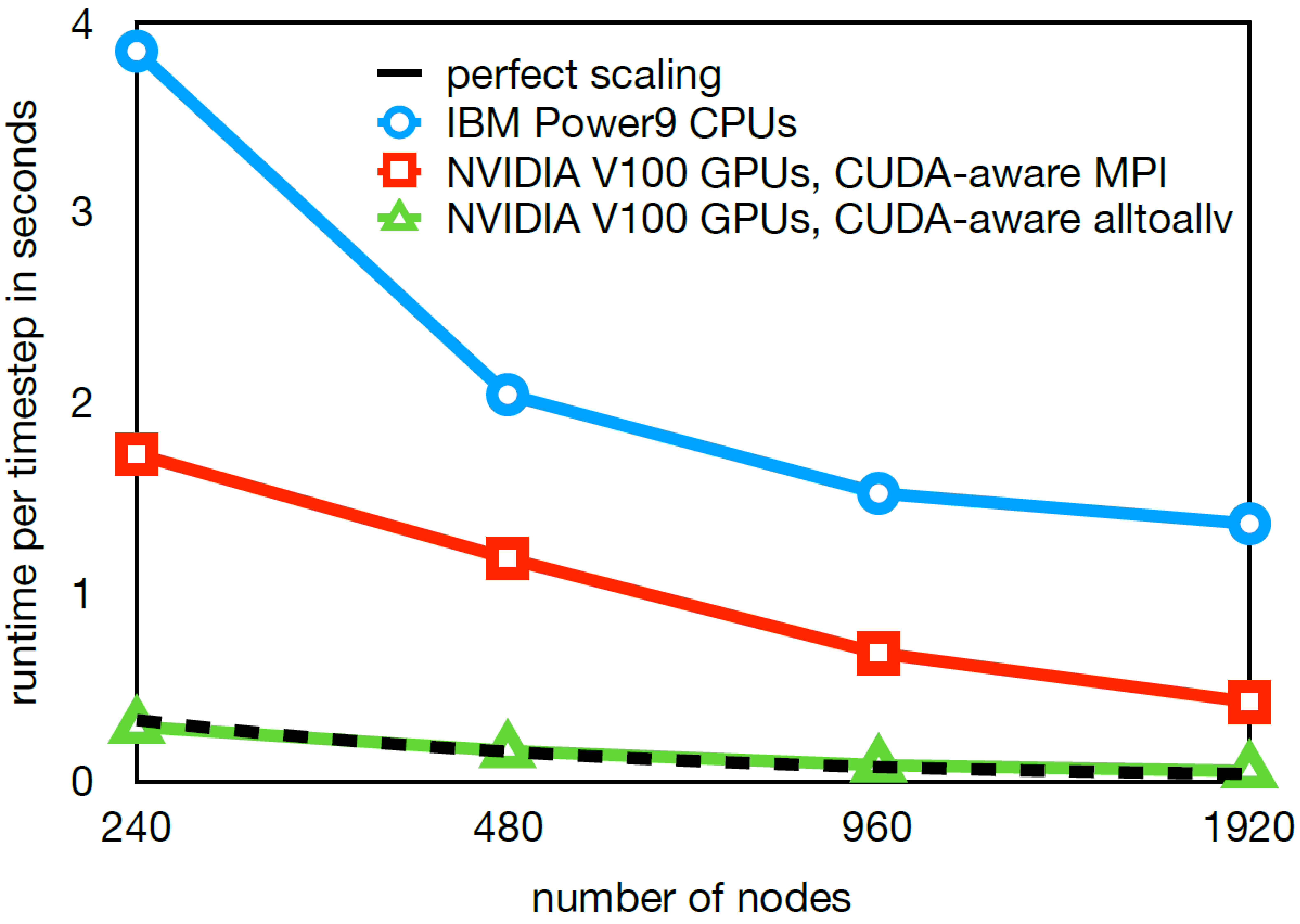

# References & Acknowledgements

*Seljebotn 2012, WAVEMOST-fast spherical transforms by butterfly matrix compression (Astrophysical Journal Supplement, vol 199)*

*Tygert 2010, Fast algorithms for spherical harmonic expansions III (JCP vol 229)*

*Wedi et al 2013, A fast spherical harmonics transform for global NWP and climate models (MWR vol 141)*

*Krishnamurti, T.N., Bedi, H.S., Hardiker, V., Watson-Ramaswamy, L., An Introduction to Global Spectral Modeling, 2006*

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# Some practice …

**interactive web-app by Andreas Müller about spectral transform**

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

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