Discrete Spherical Harmonic Transforms: Numerical Preconditioning & Optimization

J. A. Rod Blais
Department of Geomatics Engineering
Pacific Institute for the Mathematical Sciences
University of Calgary, Calgary, Alberta T2N 1N4
blais@ucalgary.ca   www.ucalgary.ca/~blais

Introduction

- **Global environmental and other datasets abound!**
- **Discrete spherical harmonics transforms are needed**
- **Quadratures and least squares offer different solutions**
- **Computational efforts are nearly $O(N^3)$ and $O(N^4)$ for degree N**
- **Numerical underflows are really challenging for very large N**
- **Biasing the exponents allow to reach very high degrees & orders**
- **Spherical Harmonic Transforms (SHTs) provide:**

  (a) Harmonic Analysis and Synthesis on the sphere or ellipsoid

  (b) Convolution tools for filtering, BVPs with Green's kernel, etc.

  (c) Multiresolution Analysis of Geopotential Models (GMs), etc.
- **Concluding Remarks**

Spherical Harmonics

Mathematical Formulation:

$$f(\theta,\lambda) = \sum_{n=0}^{\infty} \sum_{|m| \le n} f_{n,m} Y_n^m(\theta,\lambda)$$

with $Y_n^m(\theta,\lambda)$ **denoting the spherical harmonics and**

$$f_{n,m} = \int_{S^2} f(\theta,\lambda) \bar{Y}_n^m(\theta,\lambda) d\sigma$$

$$= \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} \int_{S^2} f(\theta,\lambda) P_n^m(\cos\theta) e^{im\lambda} d\sigma$$

for colatitude θ **and longitude** λ**, where**

$$P_n^m(\cos\theta) = (-1)^m P_{nm}(\cos\theta).$$

Practical Situation

Geodetic Formulation:

$$f(\theta,\lambda) = \sum_{n=0}^{\infty}\sum_{m=0}^{n}[\tilde{c}_{nm}\cos m\lambda + \tilde{s}_{nm}\sin m\lambda]\,\tilde{P}_{nm}(\cos\theta)$$

with

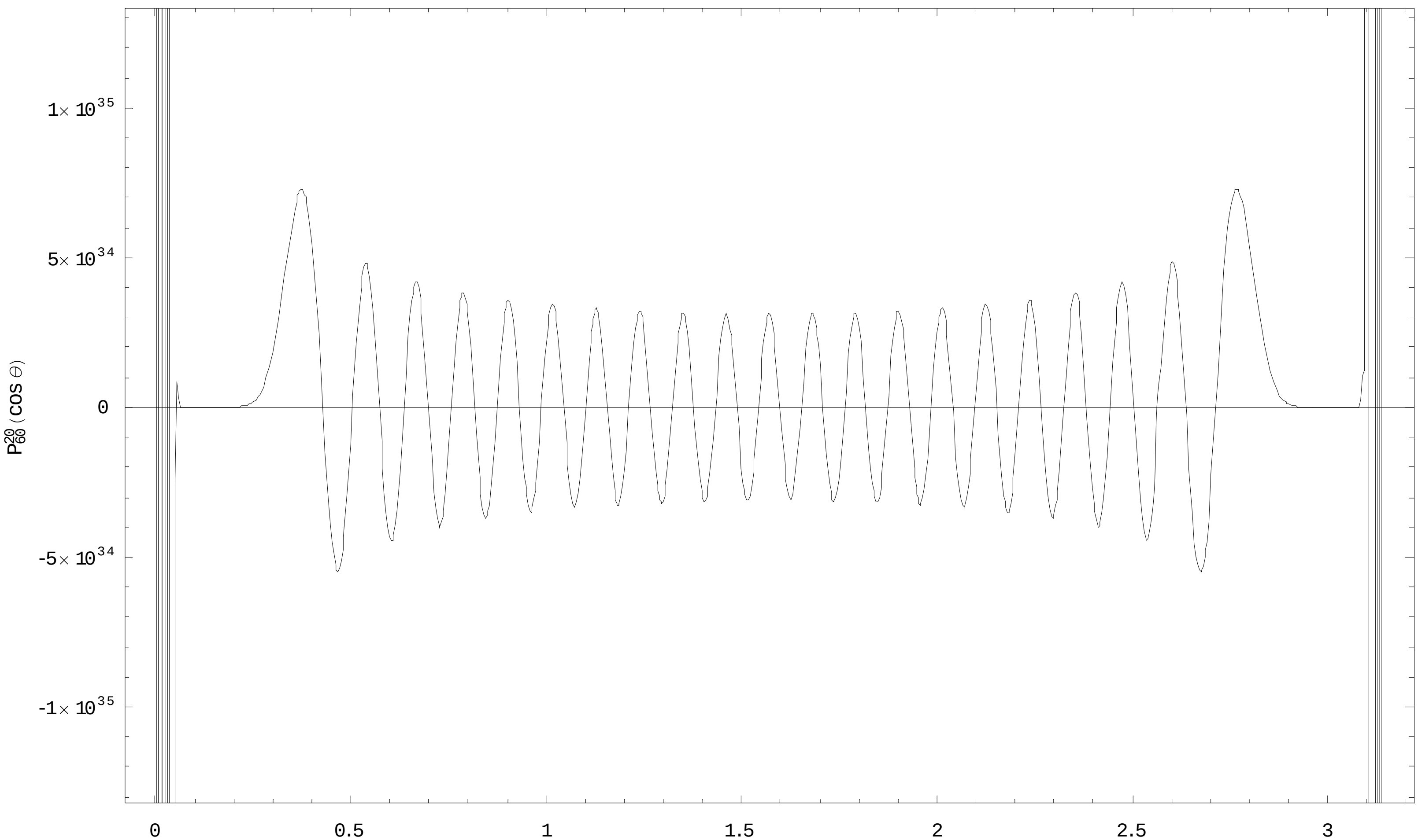
$$\begin{Bmatrix}\tilde{c}_{nm}\\ \tilde{s}_{nm}\end{Bmatrix} = \frac{1}{4\pi}\int_{S^2} f(\theta,\lambda)\begin{Bmatrix}\cos m\lambda\\ \sin m\lambda\end{Bmatrix}\tilde{P}_{nm}(\cos\theta)d\sigma$$

where

$$\tilde{P}_{nm}(\cos\theta) = \sqrt{\frac{2(2n+1)(n-m)!}{(n+m)!}}\,P_{nm}(\cos\theta)$$

$$\tilde{P}_{n}(\cos\theta) = \sqrt{2n+1}\,P_{n}(\cos\theta) \qquad \text{when } m = 0.$$

Example of Legendre Function $P_{60}^{20}(\cos\theta)$

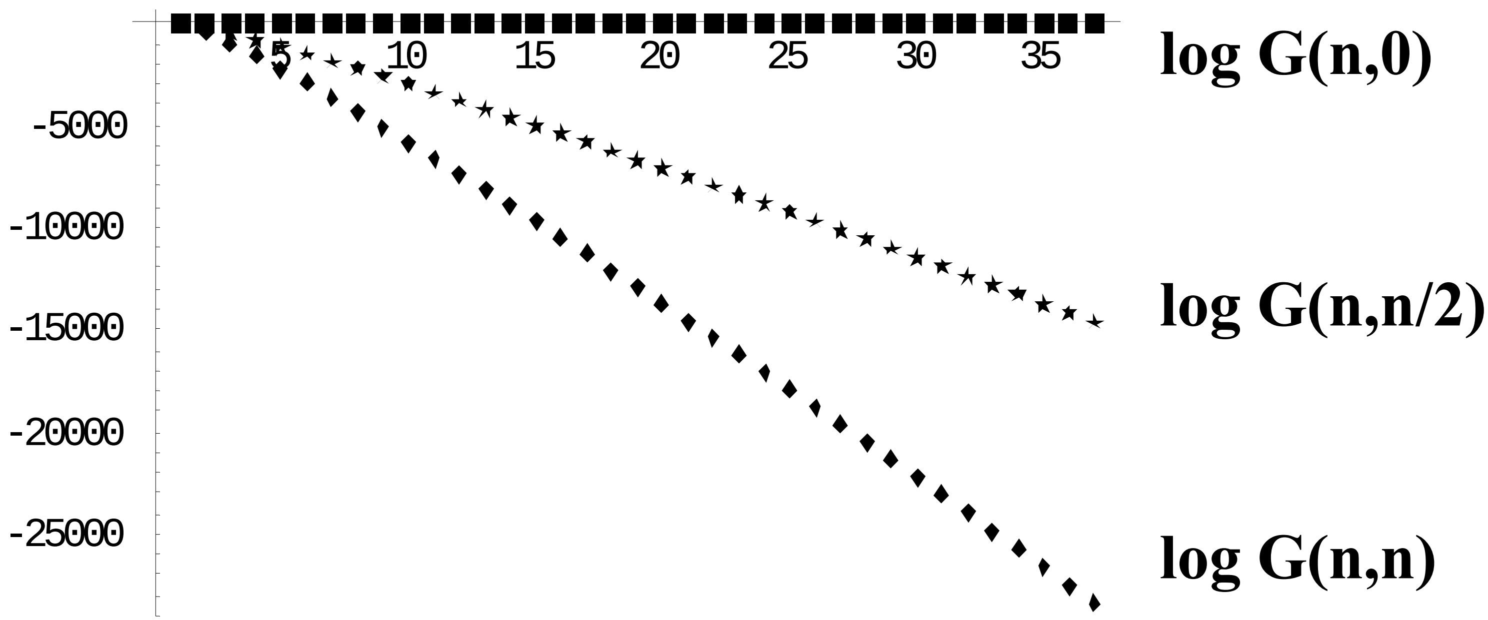


Computational Challenges

Geodetic Normalization:

$$G(n,m) = \sqrt{2(2n+1)(n-m)!/(1+\delta_{nm})(n+m)!}$$

Plots of G(n,0), G(n,n/2), G(n,n) for n = 0,100,…, 3600



Discrete SHTs

SHT: $$\begin{pmatrix} z_{11} & z_{12} & \cdots & z_{1K} \\ z_{21} & z_{22} & \cdots & z_{2K} \\ \cdots & \cdots & \cdots & \cdots \\ z_{J1} & z_{J2} & \cdots & z_{JK} \end{pmatrix} \rightarrow \begin{pmatrix} c_{00} & s_{11} & \cdots & s_{\nu 1} \\ c_{10} & c_{11} & \cdots & s_{\nu 2} \\ \cdots & \cdots & \cdots & \cdots \\ c_{\nu 0} & c_{\nu 1} & \cdots & c_{\nu\nu} \end{pmatrix}$$

with equal data spacing in latitude, $\Delta\theta$,

$$\begin{Bmatrix} c_{nm} \\ s_{nm} \end{Bmatrix} = \sum_{j=1}^{J} \sum_{k=1}^{K} q_j \, z_{jk} \begin{Bmatrix} \cos m\lambda_k \\ \sin m\lambda_k \end{Bmatrix} \tilde{P}_{nm}(\cos\theta_j)$$

and with equal data spacing in longitude, $\Delta\lambda$,

$$c_{nm} + i\, s_{nm} = \text{'const.'} \cdot \sum_{j=1}^{J} q_j \tilde{P}_{nm}(\cos\theta_j) \underset{k=1,K}{\mathrm{DFT}} [z_{jk}]$$

in which q_j denote the Chebychev quadrature weights.

Inverse Discrete SHTs

ISHT: $$\begin{pmatrix} c_{00} & s_{11} & \cdots & s_{\nu 1} \\ c_{10} & c_{11} & \cdots & s_{\nu 2} \\ \cdots & \cdots & \cdots & \cdots \\ c_{\nu 0} & c_{\nu 1} & \cdots & c_{\nu\nu} \end{pmatrix} \rightarrow \begin{pmatrix} z_{11} & z_{12} & \cdots & z_{1K} \\ z_{21} & z_{22} & \cdots & z_{2K} \\ \cdots & \cdots & \cdots & \cdots \\ z_{J1} & z_{J2} & \cdots & z_{JK} \end{pmatrix}$$

with

$$z_{jk} = \sum_{n=0}^{\nu} \sum_{m=0}^{n} (c_{nm} \cos m\lambda_k + s_{nm} \sin m\lambda_k)\, \tilde{P}_{nm}(\cos\theta_j)$$

and assuming equal data spacing in longitude, Δλ,

$$z_{jk} = \text{'const.'} \cdot \underset{m=1,\nu}{\text{IDFT}} \left\{ \sum_{n=m}^{\nu} (c_{nm} + i\, s_{nm}) \tilde{P}_{nm}(\cos\theta_j) \right\}$$

Least-Squares Analysis

From the previous synthesis formulation, one has for discrete colatitudes θ_j

$$\underset{k=1,K}{\mathrm{DFT}}[z_{jk}] = \text{'const.'}\cdot\left\{\sum_{n=m}^{\nu}(c_{nm} + i\,s_{nm})\tilde{P}_{nm}(\cos\theta_j)\right\}$$

which leads to a least-squares estimation problem per order m, for the unknowns $c_{nm} + is_{nm}$, given spatial data at

$\theta_j = j\,\Delta\theta$, **with** $\Delta\theta = \pi/N$, $j = 0, 1, \ldots, N-1$

$\lambda_k = k\,\Delta\lambda$, **with** $\Delta\lambda = \pi/N$, $k = 0, 1, \ldots, 2N-1$

for c_{nm} and s_{nm} with $m \leq n$, $n = 0, 1, \ldots, N-1$.

Note that $\Delta\theta$ need not be constant and $\Delta\lambda$ could be smaller than π/N, i.e., $2\pi/sN$ with $s \geq 2$.

SHT Computations for Degree N

For gridded data with at least 2N equispaced isolatitude data

$$\left\{\mathbf{z}_{jk}\right\} \xrightarrow[\text{per row}]{\text{DFT}} \left\{\mathbf{u}_{jh} + i\mathbf{v}_{jh}\right\} \xrightarrow[\text{per row}]{\text{IDFT}} \left\{\hat{\mathbf{z}}_{jk}\right\}$$

For gridded data with 2N data per column with constant $\Delta\theta$

$$\left\{\mathbf{c}_{nm} + i\mathbf{s}_{nm}\right\} \xrightarrow{\Sigma} \left\{\mathbf{u}_{jh} + i\mathbf{v}_{jh}\right\} \xrightarrow[\text{Quadrature}]{\text{Chebychev}} \left\{\hat{\mathbf{c}}_{nm} + i\hat{\mathbf{s}}_{nm}\right\}$$

For gridded data with N data per column with variable $\Delta\theta$

$$\left\{\mathbf{c}_{nm} + i\mathbf{s}_{nm}\right\} \xrightarrow{\Sigma} \left\{\mathbf{u}_{jh} + i\mathbf{v}_{jh}\right\} \xrightarrow[\text{Squares}]{\text{Least}} \left\{\hat{\mathbf{c}}_{nm} + i\hat{\mathbf{s}}_{nm}\right\}$$

Note that only DFTs are generally invertible above.

Numerical Computations

Full Tests with Unit and 1/deg^2 Spectral Coefficients:

$$\left\{\mathbf{c}_{nm} + i\mathbf{s}_{nm}\right\} \xrightarrow[\text{(CQ \& LS)}]{\text{SHT}^{-1}} \left\{\hat{\mathbf{z}}_{jk}\right\} \xrightarrow[\text{(CQ \& LS)}]{\text{SHT}} \left\{\hat{\mathbf{c}}_{nm} + i\hat{\mathbf{s}}_{nm}\right\}$$

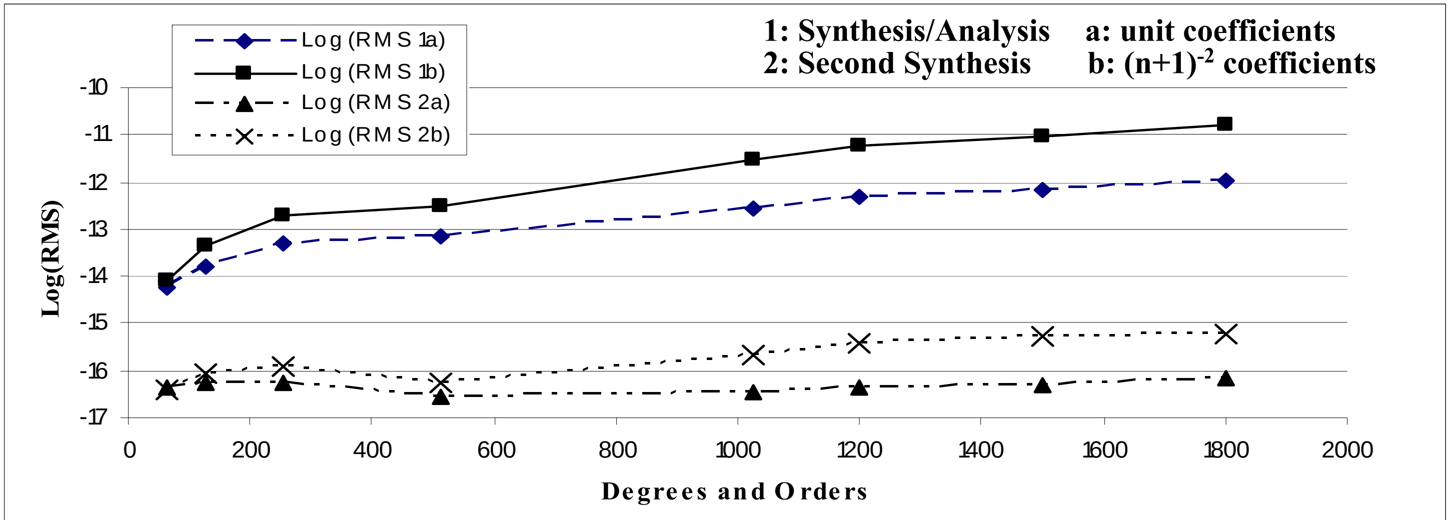
$$\left\{\hat{\mathbf{c}}_{nm} + i\hat{\mathbf{s}}_{nm}\right\} \xrightarrow[\text{(CQ \& LS)}]{\text{SHT}^{-1}} \left\{\hat{\hat{\mathbf{z}}}_{jk}\right\}$$

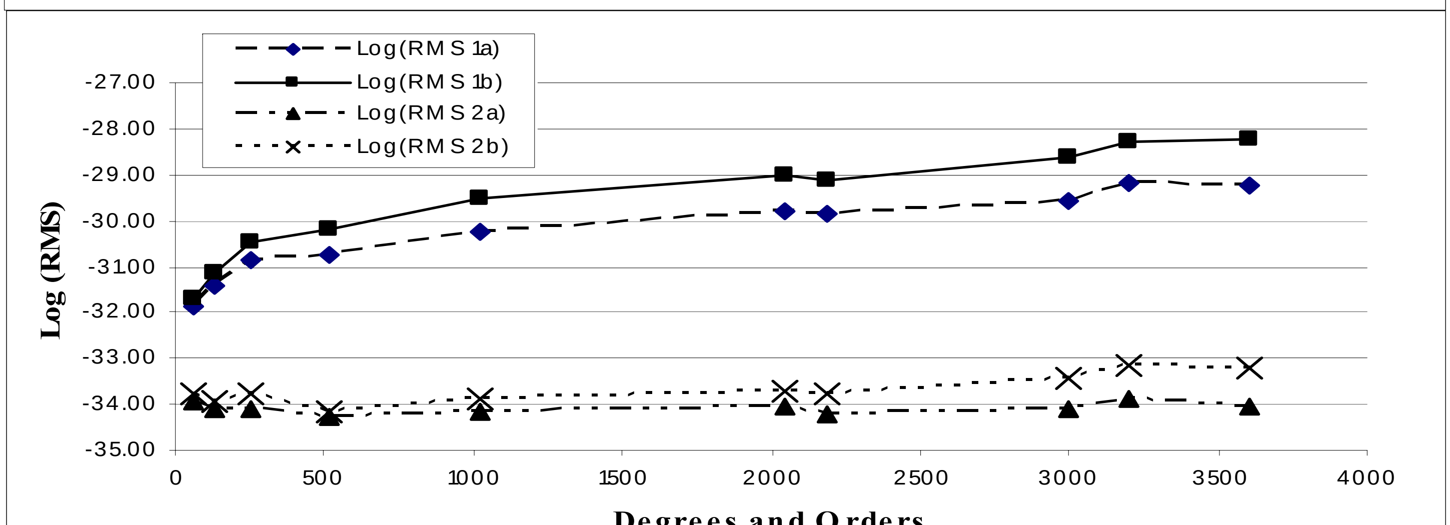
Partial Tests with Unit and 1/deg^2 Spectral Coefficients:

$$\left\{\mathbf{c}_{nm} + i\mathbf{s}_{nm}\right\} \xrightarrow{\Sigma} \left\{\hat{\mathbf{u}}_{jh} + i\hat{\mathbf{v}}_{jh}\right\} \xrightarrow[\text{Quadrature}]{\text{Chebychev}} \left\{\hat{\mathbf{c}}_{nm} + i\hat{\mathbf{s}}_{nm}\right\}$$

$$\left\{\mathbf{c}_{nm} + i\mathbf{s}_{nm}\right\} \xrightarrow{\Sigma} \left\{\hat{\hat{\mathbf{u}}}_{jh} + i\hat{\hat{\mathbf{v}}}_{jh}\right\} \xrightarrow[\text{Squares}]{\text{Least}} \left\{\hat{\hat{\mathbf{c}}}_{nm} + i\hat{\hat{\mathbf{s}}}_{nm}\right\}$$

CHEBYCHEV & LEAST SQUARES IN DP & QP





[Blais et al. 2006]

EXPONENT Limits on PCs and Similar Computers

Variable Type	Minimum EXPONENT	Maximum EXPONENT
REAL*4 or SP	-125	128
REAL*8 or DP	-1021	1024
REAL*16 or QP	-16381	16384

To avoid underflows in REAL*8 or DP , the EXPONENT can simply be biased by ~1000 for numerical stability.

Experimental Results

Degrees N	CQ RMS (data grid: 2Nx2N)	LS RMS (data grid: Nx2N)
1000	1.24557E-12	5.53768E-14
2000	3.16427E-12	1.13533E-13
3000	6.72616E-12	1.67988E-13
3200	2.59890E-12	1.66504E-13
3400	3.86647E-12	1.65382E-13
3600	3.54980E-12	1.64626E-13
3800	5.63723E-11	2.08633E-13
3900	3.96248E-04	2.16095E-13
4000	---	3.09623E-09

On-Going Optimization

Christoffel-Darboux Formula:

- Closed form for $M_{jh}^{m} = \sum_{k=m}^{N-1} \tilde{P}_{km}(\cos\theta_j)\, \tilde{P}_{km}(\cos\theta_h)$

  in terms of $\tilde{P}_{N-1,m}(\cos\theta_i)$ and $\tilde{P}_{Nm}(\cos\theta_i)$, for $i = j \neq h$,

  and their first derivatives when $j = h$.

- Implying major simplifications in constructing the normal equations in the least-squares formulation.

Parallel Computations:

- Colatitudes θ can be distributed over the available processors
- Calls to $P_{nm}(\cos\theta)$ significantly decreased in Synthesis & Analysis
- Both OpenMP & MPI were experimented with [Soofi & Blais, 2005]

Geopotential Models

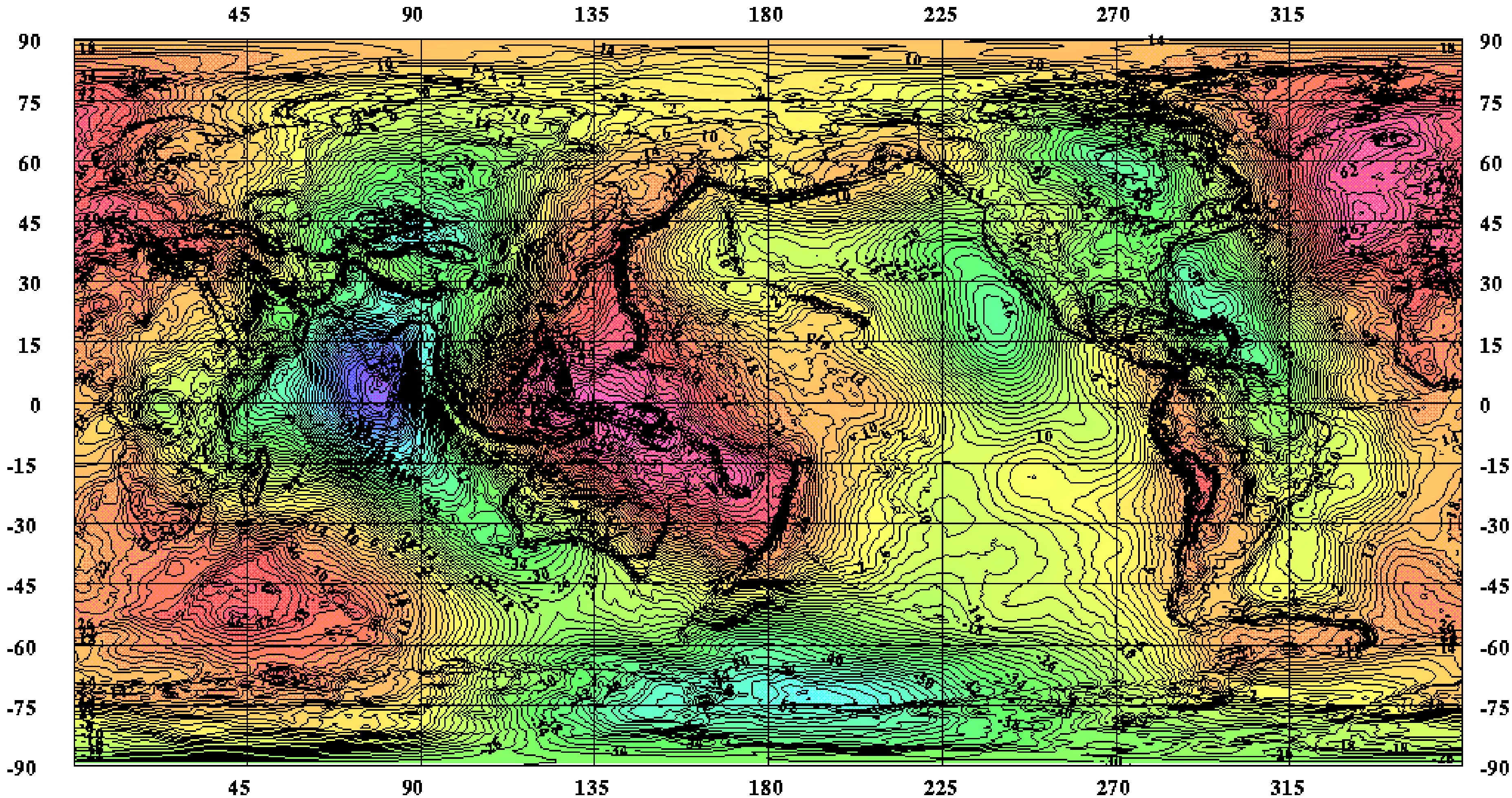
EGM96 MODEL:

- Standard reference geopotential model from GSFC, NIMA & OSU
- Spatial resolution of 30'x30' implied by max. degree and order 360
- Based on some satellite, surface gravity, elevation and altimetry data
- Available thru http://cddis.nasa.gov/926/egm96/

EGM08 MODEL:

- High resolution geopotential model developed by the US NGA
- Spatial resolution of 5'x5' implied by max. degree and order 2160
- Based on satellite, surface gravity, elevation and altimetry data
- Low-order harmonics computed using CHAMP and GRACE data
- Available thru http://earth-info.nga.mil/GandG/

EGM96 Shaded Contour Map



EGM96 15 MINUTE GEOID CI = 2 Meters

Concluding Remarks

- Discrete SHTs are computationally challenging!
- SHTs and SHT^{-1} using quadratures & least squares
- Computations are $\sim O(N^3)$ and $\sim O(N^4)$, respectively
- Without preconditioning, max deg. ~ 2700 in DP
- With EXP. bias, SHT & SHT^{-1} stable over 3800 in DP
- LS optimizable using Christoffel-Darboux' formula
- Parallel and grid computations under experimentation
- Space data can be processed globally to ~5 km resolution