ccSHT: A C Library for Computing a Fast Parallel Spherical Harmonic Transform

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What is the CMB?

Universe began as a hot dense ionized plasma filled with photons.

Universe expanded and cooled to the point where electrons could bind to nuclei.

Suddenly the Universe was transparent to photons about 100,000 years after the Big Bang.

This creates the surface of last scattering which we observe as the Cosmic Microwave Background (CMB).

The expansion of the Universe has stretched the wavelength of the photons to the microwave band.

We observe the CMB with microwave telescopes in dry places on land and in space.

The CMB offers a snap shot of the density of the Universe when it was very young.

The Universe was very homogeneous.

Small anisotropies can tell you about makeup and basic physical properties of our Universe.

The apparent temperature of the anisotropies seen on the sky are theorized to be normally distributed and correlated.

The correlation of the apparent temperature between two points on the sky is theorized to be dependent only on the angle which separates them.

Because of this the CMB should be completely characterized by an angular power spectrum, which we will refer to as C_l. This sufficient statistic is the goal of all CMB data analysis.

Power Spectrum Estimation

Exact calculation is $O(n^3)$ in time and $O(n^2)$ in memory.

This is impossible when $n = 10^7$.

Requires approximate methods in order to break $O(n^3)$ scaling.

These approximate methods require the ability to multiply by the signal covariance matrix, S.

S is n by n, so this would be $O(n^2)$ in both time and memory.

The $O(n^2)$ memory requirement is too much.

Using fast SHT to do S matrix multiplication is $O(n^{3/2})$ in time and $O(n)$ in memory.

What is the Spherical Harmonic Transform?

The spherical harmonics are the eigen functions of the Laplace operator (∇^2 or Δ) on the surface of the unit sphere. The spherical harmonics satisfy the following equation

$$\nabla^2 \psi = -\psi$$

Basis functions of the Fourier transform are a set of orthonormal solutions to the above equation on $\mathcal{R}^n$, Euclidean space.

Basis functions of the spherical harmonic transform are a set of orthonormal solutions to the above equation on $\mathcal{S}^2$, the surface of the unit sphere.

The spherical harmonic transform is just the Fourier transform for the unit sphere.

Pixelization Assumptions

First define our coordinate system (θ, ϕ).

θ is the angle down from the north pole (latitude). This angle is in radians and is 0 at the north pole and π at the south pole.

ϕ is the azimuthal angle (longitude). This angle is in radians and goes from 0 to 2π.

The pixels must lay on rows of constant θ.

Pixels in same row must cover equal area.

The longitudinal separation between pixels must be fixed for each row.

Given these requirements of the pixelization we can use FFT's in the SHT calculation.

$Y_{l,m}$: the Spherical Harmonic Basis

$Y_{l,m}$ are the basis functions for the SHT and are defined as follows for $0 \le l \le \infty$ and $0 \le m \le l$:

$$\begin{aligned} Y_{l,m}(\theta,\phi) &= \sqrt{\frac{2l+1}{4\pi}} Q_{l,m}(cos(\theta))\; e^{\sqrt{-1}m\phi} \\ Y_{l,-m}(\theta,\phi) &= (-1)^m Y^*_{l,m}(\theta,\phi) \end{aligned}$$

$Q_{l,m}(x)$ are the scaled associated Legendre polynomials:

$$Q_{l,m}(x) = \sqrt{\frac{(l-m)!}{(l+m)!}} P_{l,m}(x)$$

$P_{l,m}(x)$ are the associated Legendre polynomials which solve this second order differential equation:

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \left(l(l+1) - \frac{m^2}{1-x^2}\right) y = 0$$

Computing Associated Legendre Polynomials

We use the following recursion for computing the scaled associated Legendre polynomials:

$$
\begin{aligned}
Q_{m,m}(x) &= \sqrt{\prod_{i=1}^{m}\left(1-\frac{1}{2i}\right)}(-1)^m(1-x^2)^{m/2} \\
Q_{m+1,m}(x) &= \sqrt{2m+1}\,xQ_{m,m}(x) \\
Q_{l,m}(x) &= (l^2-m^2)^{-1/2}\,\cdot \\
&\quad [x(2l-1)Q_{l-1,m}(x) - \\
&\quad \sqrt{(l-1)^2-m^2}\,Q_{l-2,m}(x)]
\end{aligned}
$$

The Forward SHT

We would like to calculate

$$a_{l,m} = \int_{\mathcal{S}^2} f(\theta,\phi) Y^*_{l,m}(\theta,\phi)\, dA$$

Approximate with Riemann sum. Assume pixels lie on azimuthal rings and that pixels on the same ring have equal area.

$$a_{l,m} = \sum_{i=0}^{r-1} \sum_{j=0}^{s_i-1} f(\theta_i,\phi_{i,j}) Y^*_{l,m}(\theta_i,\phi_{i,j}) A_i$$

In order to use the FFT's we must assume that rows are evenly spaced in ϕ

$$\phi_{i,j} = \phi_{i,0} + \frac{2\pi}{s_i} j$$

Lets define a phase shift constant:

$$\kappa_{i,m} = e^{\sqrt{-1} m \phi_{i,0}}$$

Now we can write the following expression for $a_{l,m}$:

$$a_{l,m} = \sqrt{\frac{2l+1}{4\pi}} \sum_{i=0}^{r-1} A_i \kappa_{i,m}^* Q_{l,m}(\cos(\theta_i)) \cdot \sum_{j=0}^{s_i-1} f_{i,j} e^{-\sqrt{-1} m j \frac{2\pi}{s_i}}$$

Lets define F which can be calculated with an FFT:

$$F_{i,m} = \sum_{j=0}^{s_i-1} f_{i,j} e^{-\sqrt{-1} m j \frac{2\pi}{s_i}}$$

finally

$$a_{l,m} = \sqrt{\frac{2l+1}{4\pi}} \sum_{i=0}^{r-1} A_i \kappa_{i,m}^* Q_{l,m}(\cos(\theta_i)) F_{i,m}$$

The Backward SHT

We would like to calculate

$$g(\theta, \phi) = \sum_{l=0}^{L} \sum_{m=-l}^{l} a_{l,m} Y_{l,m}(\theta, \phi)$$

Substitute and switch sum order:

$$g_{i,j} = \sum_{m=-L}^{L} \sum_{l=|m|}^{L} \sqrt{\frac{2l+1}{4\pi}} Q_{l,m}(\cos(\theta_i)) \kappa_{i,m} a_{l,m} e^{\sqrt{-1} m j \frac{2\pi}{s_i}}$$

Define α:

$$\alpha_{m,i} = \sum_{l=|m|}^{L} \sqrt{\frac{2l+1}{4\pi}} Q_{l,m}(\cos(\theta_i))\kappa_{i,m} a_{l,m}$$

Sum equivalent modes:

$$\hat{\alpha}_{m,i} = \sum_{k=-\downarrow\frac{L+m}{s_i}\downarrow}^{\downarrow\frac{L-m}{s_i}\downarrow} \alpha_{m+ks_i,i}$$

Where $\hat{\alpha}_{m,i}$ is defined for $m \in \{0, 1, ..., s_i - 1\}$ and $\downarrow x \downarrow$ means the largest integer less than or equal to x Finally we can compute the following expression for g with FFT's.

$$g_{i,j} = \sum_{m=0}^{s_i-1} \hat{\alpha}_{m,i} e^{\sqrt{-1}mj\frac{2\pi}{s_i}}$$

Define Indexing Functions for $a_{l,m}$ and Discrete Functions on the Sphere

Lets introduce some notation which will allow us to write the discrete SHT as a linear operator.

In order to do this we must convert our discrete functions on the sphere and spherical harmonic domain $a_{l,m}$'s as vectors.

Lets use a row major ordering for our vectorization of pixelized functions on the sphere. Given this ordering lets define functions $\theta(j)$ and $\phi(j)$ which map pixel numbers to angles.

The indexing function which orders the $a_{l,m}$'s is unimportant. Lets call this bijective function ζ:

$$\begin{aligned} \zeta : (k) &\rightarrow (l, m) \\ k &\in [0, 1, ..., (L+1)^2) \\ l &\in [0, 1, ..., L] \\ m &\in [-l, -l+1, ..., l] \end{aligned}$$

The inverse of one such function is the following:

$$\zeta^{-1}(l, m) = l^2 + m + l$$

SHT as a Linear Operator

Now that we have an ordering for the $a_{l,m}$'s and the pixels we can construct a matrix $\mathcal{Y}$ which is $(L+1)^2$ by n. Each element of this matrix is defined the following way:

$$\mathcal{Y}_{i,j} = Y_{(\zeta(i))}(\theta(j), \phi(j))$$

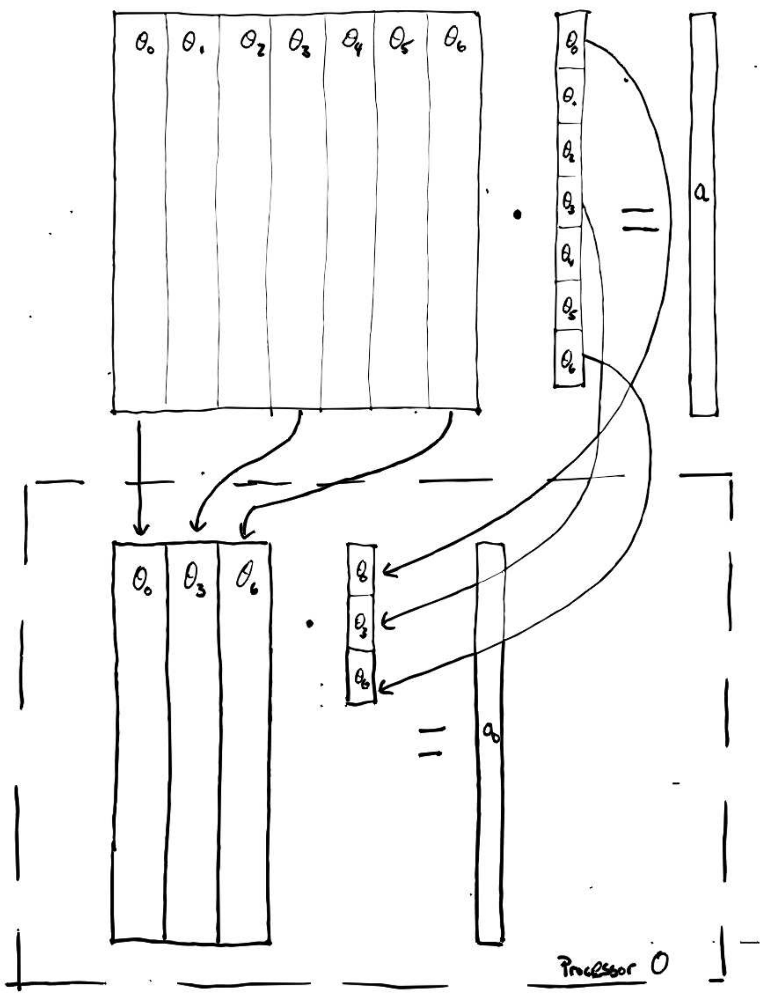
Given this definition of $\mathcal{Y}$ and an area weighted pixel vector p, we can denote the forward transform of p to the vectorized $a_{l,m}$ called a as follows:

$$a = \mathcal{Y}^* p$$

and the backward transform of a vectorized $a_{l,m}$ called a to the pixel vector p can be written as follows:

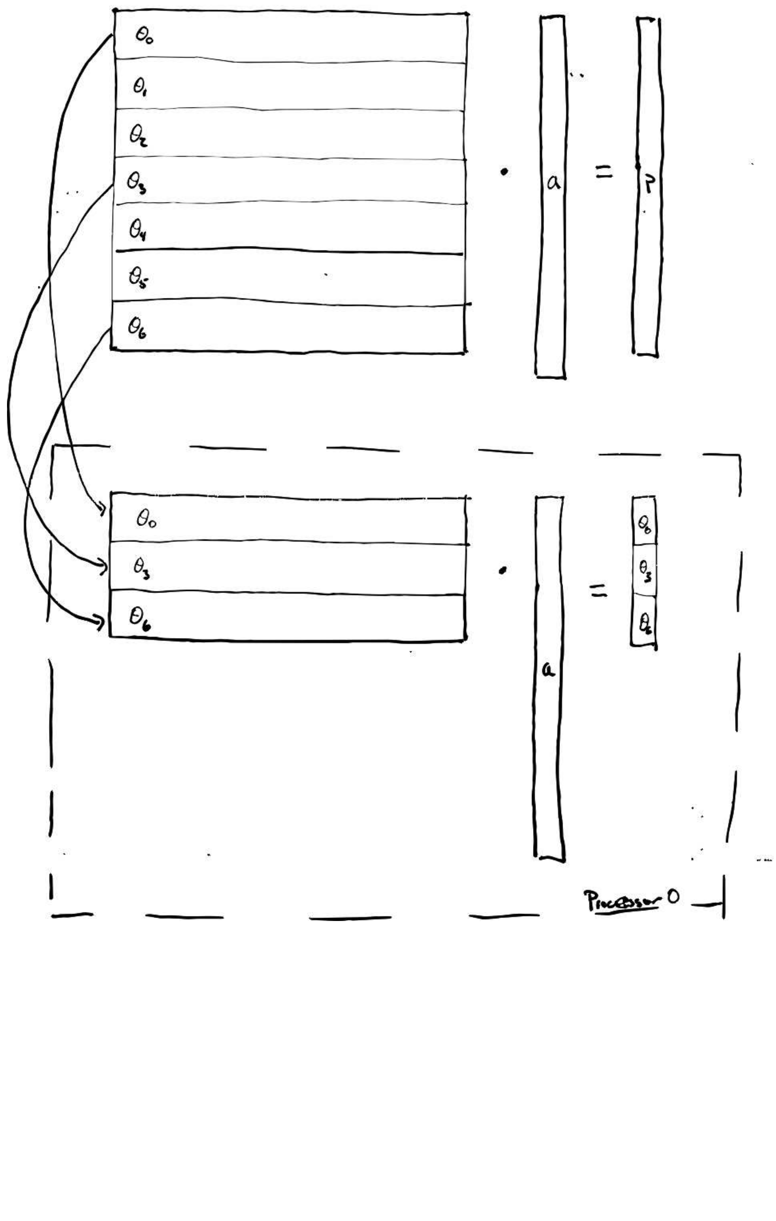
$$p = \mathcal{Y}^T a$$

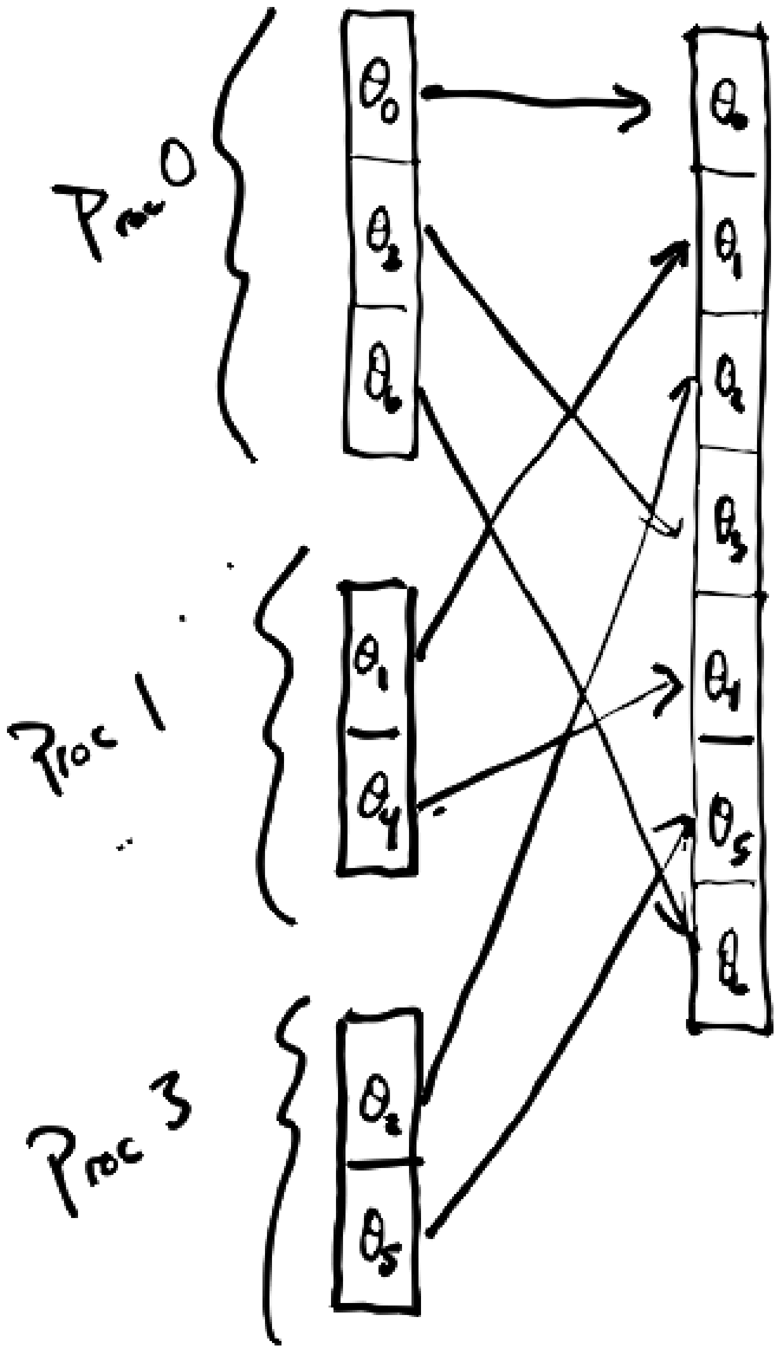
$$Y^*_p = a$$

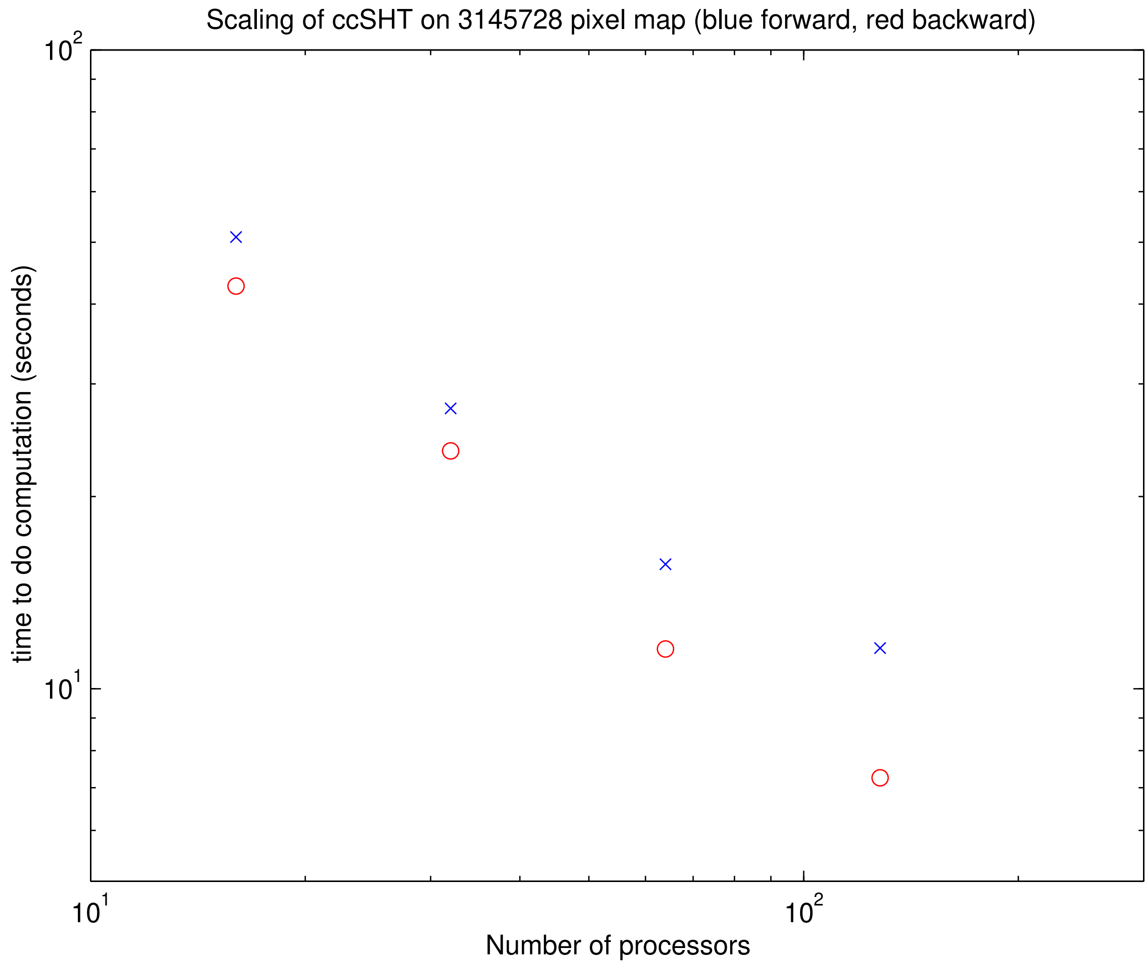


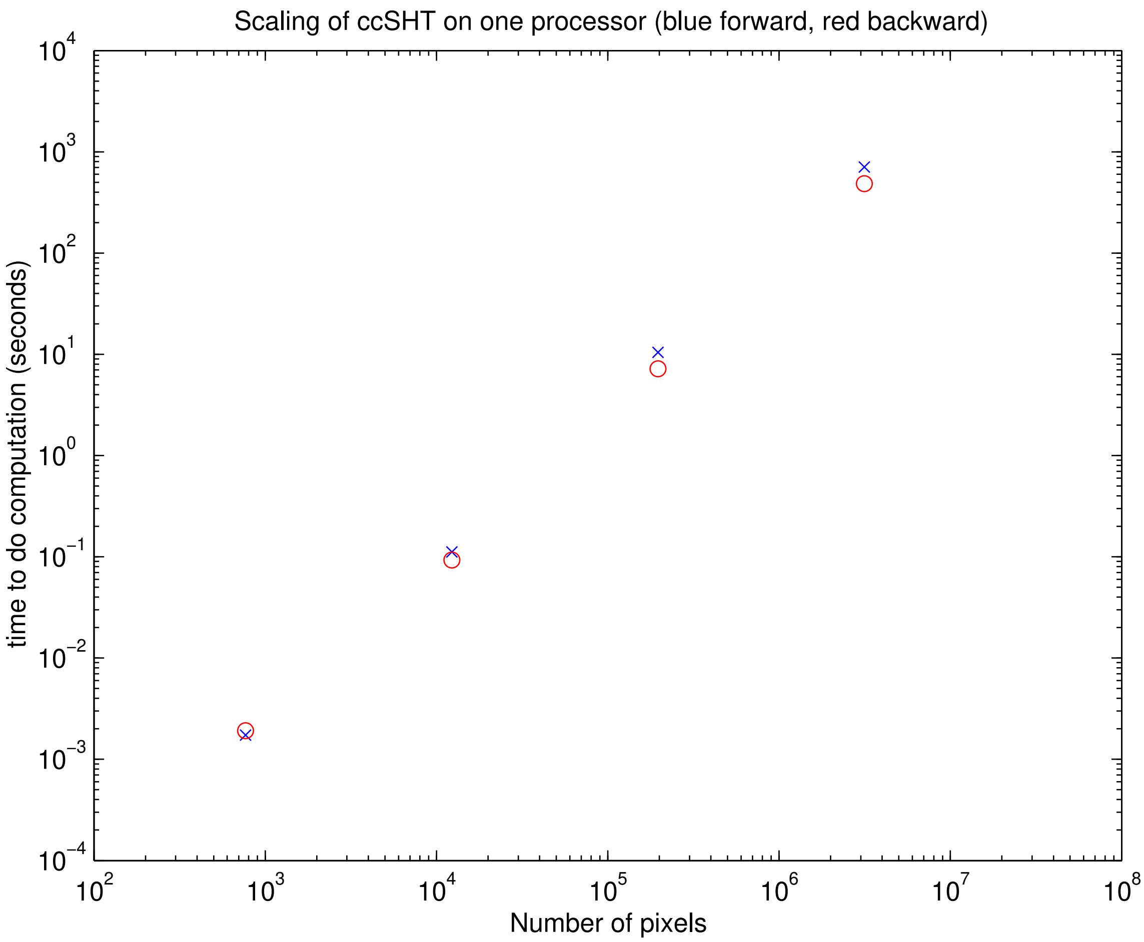
$$a = \sum_{i=0}^{n_p - 1} a_i$$

$Y^T a = p$




Proc 0
Proc 1
Proc 3
θ_0
θ_2
θ_6
θ_1
θ_4
θ_3
θ_5
θ_0
θ_1
θ_2
θ_3
θ_4
θ_5
θ_6


Scaling of ccSHT on 3145728 pixel map (blue forward, red backward)
time to do computation (seconds)
Number of processors
10^2
10^1
10^1
10^2


Scaling of ccSHT on one processor (blue forward, red backward)
time to do computation (seconds)
Number of pixels
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
10^{8}

Relationship Between SHT and CMB Analysis

The pixel-pixel signal correlation matrix, S is used in the MLE of the signal angular power spectrum. The analysis assumes that the signal component of the correlation between two pixels is simply a function of the angular separation between the two pixels. Lets define ξ as follows:

$$\xi_{p,q} = \cos([\theta_p, \phi_p]; [\theta_q, \phi_q])$$

If the multi-pole angular power spectrum is given by C_l then S is defined as follows:

$$S_{p,q} = \sum_{l=0}^{L} \frac{2l+1}{4\pi} C_l P_l(\xi_{p,q})$$

where $P_l(x)$ are the Legendre polynomials.

The following identity relates spherical harmonics to Legendre polynomials:

$$P_l(\xi_{p,q}) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{l,m}(\theta_p, \phi_p) Y^*_{l,m}(\theta_q, \phi_q)$$

When estimating the power spectrum we need to compute $Sx = z$:

$$\begin{aligned} z_p &= \sum_{q=0}^{n-1} x_q S_{p,q} \\ &= \sum_{q=0}^{n-1} x_q \sum_{l=0}^{L} C_l \sum_{m=-l}^{l} Y_{l,m}(\theta_p, \phi_p) Y^*_{l,m}(\theta_q, \phi_q) \\ &= \sum_{l=0}^{L} \sum_{m=-l}^{l} Y_{l,m}(\theta_p, \phi_p) C_l \sum_{q=0}^{n-1} x_q Y^*_{l,m}(\theta_q, \phi_q) \end{aligned}$$

This can be rewritten as follows:

$$z = \mathcal{Y}^T diag(C_l) \mathcal{Y}^* x$$

Conclusions

ccSHT is a great way to do spherical harmonic transforms in parallel.

Applications to CMB analysis have been fruitful.

Many other possible applications exist:

- Heleoseismology
- Geophysics
- Ocean simulations?
- Quantum mechanics?

For more information see

http://www.nersc.gov/ cmc/ccSHTlib/doc

On seaborg: module ccSHT