Analytic Number Theory, Complex Variable and Supercomputers[1]

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Abstract

This paper is the final report of an undergraduate honors thesis project advised by Prof. Dennis Hejhal of the School of Mathematics, University of Minnesota. The main purpose of this project is to examine the analytic properties of certain "quantum-mechanical particles" in Lobachevsky space. The results were obtained on vectorized CRAY serial supercomputers, a CRAY 64-CPU T3D massively parallel system, and a 1K-CPU massively parallel system CM-5 located in University of Minnesota. Using complex arithmetic, we have successfully determined numerous Fourier coefficients for certain types of holomorphic modular forms, including the Ramanujan τ-function. Our experiments involve both arithmetic and non-arithmetic groups. The treatment of the latter is new. Analyzing the output data enables us to experimentally justify a number of properties. Finally, a verification of a Central Limit Theorem for automorphic functions on Hecke Groups was attempted, and very promising results have been obtained.

1 Introduction.

We study the group $G(2\cos\frac{\pi}{N})$ of Möbius transformations with two generators:

$$\begin{cases} T(\tau) = \tau + 2\cos\frac{\pi}{N} \\ S(\tau) = -\frac{1}{\tau} \end{cases} \tag{1}$$

for $N \geq 3$.

It is customary to associate a matrix $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SL(2, \mathcal{R})$ (i.e. $ad - bc = 1$) [4] with the linear fractional mapping

$$A\tau = \frac{a\tau + b}{c\tau + d}. \tag{2}$$

Definition. If G is a subgroup of the group $SL(2, \mathcal{R})$, an open subset R_G of the upper half plane H is called a *fundamental region* for G if it satisfies the following properties:

(a) No two distinct points of R_G are equivalent under the group G.

(b) If $\tau \in H$, there is a point $\tau' \in \overline{R_G}$ such that $\tau' = A\tau$ for $A \in G$. That is, τ' is equivalent to τ under G. ($\overline{K}$ means the closure of K)

It is not hard to prove that the region $\mathcal{F}_N : \{|Re(\tau)| < 2\cos\frac{\pi}{N}, |\tau| > 1\}$ is a fundamental region for the group $G(2\cos\frac{\pi}{N})$. We shall take $G = G(2\cos\frac{\pi}{N})$. For $N = 3$, G reduces to $SL(2, \mathcal{Z})$. For $N \neq 3, 4, 6$, the group G is non-arithmetic in nature[11].

Definition. A *modular form of weight* k is a meromorphic function f on H such that

$$f(A\tau) = f(\tau)(c\tau + d)^k \qquad for\ every\ A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in G. \tag{3}$$

Definition. An *entire modular form of weight* k is an *analytic* function defined on H such that

$$f\left(\frac{a\tau + b}{c\tau + d}\right) = f(\tau)(c\tau + d)^k \quad whenever \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in G \tag{4}$$

and such that f has a Fourier expansion of the form

$$f(\tau) = \sum_{n=0}^{\infty} c_n e^{2\pi i n\tau/L} \quad with \ \ L = 2\cos\frac{\pi}{N} \ \ . \tag{5}$$

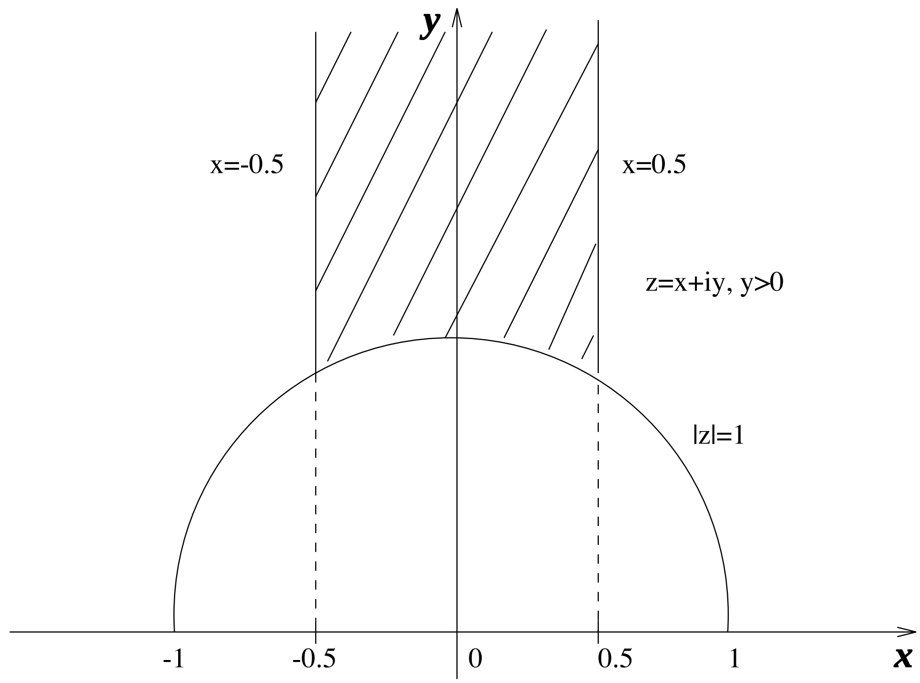

Figure 1: **Fundamental region of the modular group** $G(2cos\frac{\pi}{3})$

The Ramanujan τ-function is the coefficient function τ_n of a special modular form of weight 12 defined for $N=3$ by the generating function [3]

$$\Delta(z) = (2\pi)^{12}\sum_{n=1}^{\infty}\tau_n e^{2\pi inz} = (2\pi)^{12}e^{2\pi iz}\prod_{m=1}^{\infty}(1-e^{2\pi imz})^{24} \quad . \tag{6}$$

When f has $c_0=0$, we call it a *cusp form*. The function $\Delta(z)$ is thus a cusp form.

Deligne proved that $|c_n n^{-\frac{k-1}{2}}| = O(n^{\epsilon})$ for cusp forms with $N=3$ (see [3], section 6.15). For general N, $|c_n n^{-\frac{k-1}{2}}| = O(n^{\frac{1}{2}})$.

We set $c_n = d_n n^{\frac{k-1}{2}}$ ($d_n \equiv 0$ for $n \leq 0$). Let $z = x+iy$, and $G(u) = u^{\frac{k-1}{2}}e^{-2\pi u/L}$. To obtain the relation

$$u(Az) = u(z)\frac{(cz+d)^k}{|cz+d|^k} = u(z)e^{ikArg(cz+d)} \qquad for \quad A \in G, \tag{7}$$

we consider

$$u(z) = y^{\frac{k}{2}}f(z) \quad = \quad \sum_{n=1}^{\infty}c_n y^{\frac{k}{2}}e^{2\pi inz/L}$$

$$= \sum_{n=1}^{\infty} (d_n n^{\frac{k-1}{2}}) y^{\frac{k}{2}} e^{-2\pi ny/L} e^{2\pi inx/L} \tag{8}$$
$$= \sum_{n=1}^{\infty} d_n \sqrt{y} (ny)^{\frac{k-1}{2}} e^{-2\pi ny/L} e^{2\pi inx/L}$$
$$= \sum_{n=1}^{\infty} d_n \sqrt{y} G(ny) e^{2\pi inx/L} \quad .$$

We then find the Fourier coefficients[7] are

$$d_n \sqrt{y} G(ny) = \frac{1}{L} \int_{-L/2}^{L/2} u(z) e^{-2\pi inx/L} dx \quad for \quad n \geq 1, \; y > 0 \quad . \tag{9}$$

There are simple formulas for calculating the dimension of the space of cusp forms of weight k on $G(2\cos\frac{\pi}{N})$ (see [10] pp. 485, 494 in volume 2). In many cases, this dimension is either 0 or 1.

Table 1 shows the dimension of the space of cusp forms in various ranges.

Group	$k=4$	$k=6$	$k=8$	$k=10$	$k=12$	$k=14$	$k=16$
$N=3$	0	0	0	0	1	0	1
$N=4$	0	0	1	0	1	1	2
$N=5$	0	0	1	1	1	1	2
$N=6$	0	0	1	1	2	1	2
$N=7$	0	0	1	1	2	2	2

Table 1: **Dimension of the space of cusp forms for certain groups and weights.**

2 Numerically solving for the Fourier coefficients d_n.

In order to numerically solve for the Fourier coefficients, we imagine that our function u actually satisfies

$$u(z) \equiv \sum_{n=1}^{M} d_n \sqrt{y} G(ny) e^{2\pi inx/L} \tag{10}$$

for some big M, $M = M(y)$ being determined later to ensure sufficient accuracy. By finite Fourier series expansion, we easily convert the above equation into

$$d_n \sqrt{y} G(ny) = \frac{1}{2Q} \sum_{j=1-Q}^{Q} u(z_j) e^{-2\pi inx_j/L} \tag{11}$$

for any $Q \geq M \geq n \geq 1$, where

$$z_j \equiv x_j + iy = \left(j - \frac{1}{2}\right)\frac{L}{2Q} + iy \tag{12}$$

for all $1 - Q \leq j \leq Q$. [In fact, by linearity in (10) and (11), it suffices to treat the case where $d_n = \delta_{k,n}$, $1 \leq k \leq M$. Here $\delta_{k,n}$ is just the Kronecker δ. For this choice of d_n, we have:

$$\begin{aligned}
&\frac{1}{2Q}\sum_{j=1-Q}^{Q} u(z_j)e^{-2\pi i n x_j/L} \\
&= \frac{1}{2Q}\sqrt{y}G(ky)\sum_{j=1-Q}^{Q} e^{2\pi i k x_j/L}e^{-2\pi i n x_j/L} \\
&= \frac{1}{2Q}\sqrt{y}G(ky)\sum_{j=1-Q}^{Q} e^{2\pi i(k-n)(j-\frac{1}{2})/(2Q)} \\
&= \frac{1}{2Q}\sqrt{y}G(ky)e^{\pi i(n-k)/(2Q)}\sum_{j=1-Q}^{Q} e^{2\pi i(k-n)j/(2Q)} \\
&= \frac{1}{2Q}\sqrt{y}G(ky)e^{\pi i(n-k)/(2Q)}\sum_{j=1-Q}^{Q} \zeta^j
\end{aligned} \tag{13}$$

where $\zeta = e^{2\pi i(k-n)/(2Q)}$. The number ζ is a (2Q)-th root of unity. Therefore, automatically,

$$\sum_{j=1-Q}^{Q} \zeta^j = \left\{ \begin{array}{ll} 0, & \zeta \neq 1 \\ 2Q, & \zeta = 1 \end{array} \right\} . \tag{14}$$

For $\zeta = 1$ to hold, we need $n \equiv k \ mod\ 2Q$. Since $Q \geq M$, and n and k both lie in $[1, M]$, this is equivalent to saying $n = k$. In other words:

$$\frac{1}{2Q}\sum_{j=1-Q}^{Q} u(z_j)e^{-2\pi i n x_j/L} = \left\{ \begin{array}{ll} 0, & n \neq k \\ \sqrt{y}G(ky), & n = k \end{array} \right\} \tag{15}$$

exactly as required.]

When $y \geq \sin(\frac{\pi}{N})$, we assume that M can be uniformly replaced by a fixed number M_0. Let z_j^* be the image of z_j in $\mathcal{F}_N$. For $y < \sin(\frac{\pi}{N})$, we then get:

$$d_n\sqrt{y}G(ny) = \frac{1}{2Q}\sum_{j=1-Q}^{Q} u(z_j^*)e^{-ikArg(c_j z_j + d_j)}e^{-2\pi i n x_j/L}$$

$$= \frac{1}{2Q}\sum_{j=1-Q}^{Q}\Big[\sum_{l=1}^{M_0} d_l\sqrt{y_j^*}G(ly_j^*)e^{2\pi i l x_j^*/L}\Big]e^{-ikArg(c_jz_j+d_j)}e^{-2\pi i n x_j/L} \qquad (16)$$

$$= \frac{1}{2Q}\sum_{l=1}^{M_0}\sum_{j=1-Q}^{Q} d_l\sqrt{y_j^*}G(ly_j^*)e^{2\pi i l x_j^*/L}e^{-ikArg(c_jz_j+d_j)}e^{-2\pi i n x_j/L}$$

$$= \sum_{l=1}^{M_0} d_l\Big(\frac{1}{2Q}\sum_{j=1-Q}^{Q}\sqrt{y_j^*}G(ly_j^*)e^{2\pi i l x_j^*/L}e^{-ikArg(c_jz_j+d_j)}e^{-2\pi i n x_j/L}\Big)$$

Let n now go from 1 to M_0. We clearly obtain a linear system of dimension M_0:

$$d_n\sqrt{y}G(ny) = \sum_{l=1}^{M_0} d_l V_{nl} \ , \qquad (17)$$

where

$$V_{nl} = \frac{1}{2Q}\sum_{j=1-Q}^{Q}\sqrt{y_j^*}G(ly_j^*)e^{2\pi i l x_j^*/L}e^{-ikArg(c_jz_j+d_j)}e^{-2\pi i n x_j/L}. \qquad (18)$$

Moving the left hand side of equation(17) to the right hand side, we get a new linear system

$$0 = \sum_{l=1}^{M_0} d_l U_{nl} \ , \qquad 1 \le n \le M_0 \ , \qquad (19)$$

where

$$U_{nl} = \frac{1}{2Q}\sum_{j=1-Q}^{Q}\sqrt{y_j^*}G(ly_j^*)e^{2\pi i l x_j^*/L}e^{-ikArg(c_jz_j+d_j)}e^{-2\pi i n x_j/L} - \delta_{nl}d_n\sqrt{y}G(ny) \qquad (20)$$

If the space of cusp forms of weight k has dimension 1, we can presumably normalize things by setting $d_1 = 1$. In that case:

$$0 = U_{n,1} + \sum_{l=2}^{M_0} d_l U_{nl} \ . \qquad (21)$$

We thus get a $M_0 - 1$ dimensional linear system

$$\sum_{l=2}^{M_0} U_{nl}d_l = -U_{nl} \ , \qquad 2 \le n \le M_0 \ , \qquad (22)$$

i.e.

$$\begin{pmatrix} U_{2,2} & U_{2,3} & \ldots\ldots & U_{2,M_0} \\ U_{3,2} & U_{3,3} & \ldots\ldots & U_{3,M_0} \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ U_{M_0,2} & U_{M_0,3} & \ldots\ldots & U_{M_0,M_0} \end{pmatrix}\begin{pmatrix} d_2 \\ d_3 \\ \ldots \\ d_{M_0} \end{pmatrix} = -\begin{pmatrix} U_{2,1} \\ U_{3,1} \\ \ldots \\ U_{M_0,1} \end{pmatrix} \quad . \qquad (23)$$

The system is solvable numerically using complex Gaussian Elimination. Professor Hejhal has used symmetry in the y-axis to show that the quantities U_{nl} are actually all real. (See Figure 1.)

To be successful in computing d_n, $n \leq M_0$, we should now ensure two concerns:

- good conditioning in (23) for each chosen $y < \sin \frac{\pi}{N}$;
- a solution vector (d_n) which is *stable* when y is varied.

The second condition is essential because the coefficients d_n in (8) must *not* depend on y.

3 Error analysis.

We first need to determine the appropriate value of M_0 in (16) for certain N and k. Our goal is to make the error from neglecting $n > M_0$ terms small. For CRAY single precision computation, we wish the error to be less than 10^{-16}. Since one expects the coefficients d_n to be bounded by $O(\sqrt{n})$ with a *modest* implied constant, we need to study the size of $\sum_{n=M_0+1}^{\infty} \sqrt{ny}G(ny)$ for $y \geq \sin(\frac{\pi}{N})$.

But,

$$lnG(u) = \frac{k-1}{2} lnu - \frac{2\pi}{L}u \tag{24}$$

and

$$\frac{G'(u)}{G(u)} = \frac{k-1}{2u} - \frac{2\pi}{L}. \tag{25}$$

By setting $G'(u) = 0$, we conclude that when $u = \frac{(k-1)L}{4\pi}$ the maximum of $G(u)$ is obtained and

$$max\ G(u) = \left(\frac{(k-1)L}{4\pi}\right)^{\frac{k-1}{2}} e^{-\frac{k-1}{2}} = \left(\frac{(k-1)L}{4\pi e}\right)^{\frac{k-1}{2}}. \tag{26}$$

Now replace $k-1$ by k. To get a steady decay in $\sum_{n=M_0+1}^{\infty} \sqrt{ny}G(ny)$ with respect to n, one should therefore take

$$(M_0 y \geq)\, M_0 \sin\frac{\pi}{N} > \frac{k}{4\pi} L \quad , \tag{27}$$

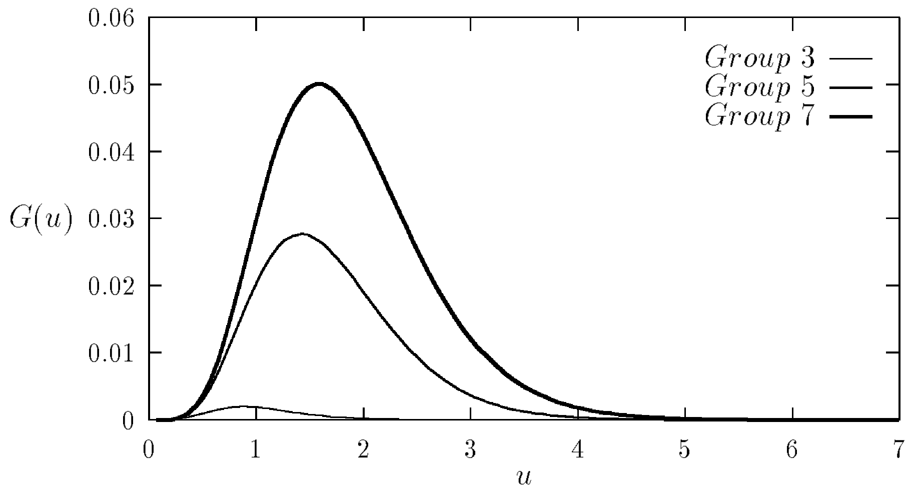

Figure 2: **Plots of $G(u) = u^{\frac{k-1}{2}} e^{-2\pi u/L}$ for k=12 and N=3,5,7**

i.e.

$$M_0 > \frac{\frac{k}{2}}{\pi \tan \frac{\pi}{N}} \quad . \tag{28}$$

In this case, for $y \geq \sin \frac{\pi}{N}$,

$$\sum_{l=M_0+1}^{\infty} \left| d_l \sqrt{y} G(ly) e^{2\pi i l x/L} \right| \tag{29}$$

is majorized by the series

$$\sum_{l=M_0+1}^{\infty} \left(l \sin \frac{\pi}{N} \right)^{\frac{k}{2}} e^{-l\pi \tan \frac{\pi}{N}} \ . \tag{30}$$

For safety in a ratio test of convergence, we can require that

$$\left(\frac{l+1}{l} \right)^{\frac{k}{2}} e^{-\pi \tan \frac{\pi}{N}} < \frac{2}{3} \ , \quad l \geq M_0 + 1 \ . \tag{31}$$

Table 2 then shows us some appropriate M_0 values for certain groups and weights.

The determination of an admissible $M = M(y)$ for $y < \sin \frac{\pi}{N}$ is similar to our treatment of M_0. One needs to ensure that

$$O(1) \sum_{l=M+1}^{\infty} \sqrt{ly} G(ly) < 10^{-16} \ . \tag{32}$$

Group	$4 \leq k \leq 12$	*err. estimation*	$14 \leq k \leq 22$	*err. estimation*
$N=3$	$M_0 = 9$	$O(1)[9.9 * 10^{-19}]$	$M_0 = 12$	$O(1)[6.7 * 10^{-18}]$
$N=4$	$M_0 = 20$	$O(1)[4.1 * 10^{-21}]$	$M_0 = 25$	$O(1)[4.1 * 10^{-21}]$
$N=5$	$M_0 = 25$	$O(1)[1.7 * 10^{-18}]$	$M_0 = 32$	$O(1)[2.0 * 10^{-18}]$
$N=6$	$M_0 = 30$	$O(1)[2.7 * 10^{-17}]$	$M_0 = 40$	$O(1)[6.3 * 10^{-18}]$
$N=7$	$M_0 = 36$	$O(1)[3.2 * 10^{-17}]$	$M_0 = 48$	$O(1)[9.3 * 10^{-18}]$

Table 2: M_0 **values and the estimation of series (30)**

The implied constant in $O(1)$ is the same as in the relation $d_n = O(\sqrt{n})$. We have already *assumed* that this constant is modest.

As a working hypothesis, it is now reasonable to simply require that:

$$\sum_{l=M+1}^{\infty} (ly)^{\frac{k}{2}} e^{-2\pi ly/L} < 10^{-16} \ . \tag{33}$$

Here it is also natural to take

$$My > \frac{kL}{4\pi} \quad , \quad i.e. \quad M > \frac{kL}{4\pi y} \tag{34}$$

since this ensures monotonic decay with respect to l. One can then compare things to an integral. That is, we want:

$$\int_M^{\infty} (ty)^{\frac{k}{2}} e^{-2\pi ty/L} dt < 10^{-16} \ . \tag{35}$$

This reduces to

$$\frac{1}{y}\left(\frac{L}{2\pi}\right)^{\frac{k}{2}+1} \int_{2\pi My/L}^{\infty} u^{\frac{k}{2}} e^{-u} du < 10^{-16} \ . \tag{36}$$

In our work, we shall always keep $k \leq 22$. See Table 2. In this k-range, a trivial calculation shows that

$$\frac{(u+1)^{\frac{k}{2}} e^{-u-1}}{u^{\frac{k}{2}} e^{-u}} = \left(1 + \frac{1}{u}\right)^{\frac{k}{2}} e^{-1} \leq \frac{1}{2} \tag{37}$$

for $u \geq 40$. This ratio suggests that we now take

$$\frac{2\pi My}{L} > 40 \tag{38}$$

in (36). That is,

$$M > \frac{20L}{\pi y} \quad . \tag{39}$$

Notice incidentally that

$$\frac{20L}{\pi y} > \frac{kL}{4\pi y} \quad for \quad k \leq 22 \quad . \tag{40}$$

To ensure (36), we must now take M big enough so that

$$\frac{2}{y}\left(\frac{L}{2\pi}\right)^{\frac{k}{2}+1}\left(\frac{2\pi My}{L}\right)^{\frac{k}{2}} e^{-2\pi My/L} < 10^{-16} \quad , \tag{41}$$

i.e.

$$\frac{L}{\pi y}(My)^{\frac{k}{2}} e^{-2\pi My/L} < 10^{-16} \quad . \tag{42}$$

But $L = 2\cos\frac{\pi}{N} \leq 2$. It is therefore sufficient to go with the *combined restriction*

$$\begin{cases} M > \frac{20L}{\pi y} \\ \frac{1}{y}\ (My)^{\frac{k}{2}} e^{-2\pi My/L} < 10^{-16} \end{cases} \tag{43}$$

in determining the correct value of $M = M(y)$.

4 Deriving the low-index Fourier coefficients.

The idea of Section 2 can now be implemented very easily on the computer.

To obtain optimal accuracy in d_l, it is necessary to use y-values in (17) which are less than $\sin\frac{\pi}{N}$ but *not* too small. One needs to avoid excessively large $Q \geq M(y)$ as well as excessively large errors in V_{nl}.

A rough indicator of the numerical conditioning in (22) is obtained by looking at the ratios

$$\frac{norm\ of\ right\ hand\ side\ of\ (23)}{norm\ of\ l^{th}\ column\ in\ (23)} \tag{44}$$

for $2 \leq l \leq M_0$. A *cruder* indicator would be to simply look at

$$\frac{\max\ G\ as\ in\ (26)}{\sqrt{y}\min[G(2y),\ G(M_0 y)]} \tag{45}$$

When these indicators exceed $O(10^\alpha)$, this is a warning that the computed d_l should be accurate to at most $14-\alpha$ decimal places.

Our code for the implementation of (23) always tested *two* y-values at a time, and always displayed the values of the above indicators. This made it very easy to gauge the accuracy of d_1, d_2, ... , d_{M_0} in the examples we tested.

The trick, of course, is to test many different sets of y-values, always seeking to keep the control ratios as small as possible (or at least below some acceptable limit).

We studied:

N=3	k= 12 (i.e. the Ramanujan τ-function)
N=5	k= 8, 10, 12, 14
N=7	k= 8, 10

(also see Table 1) and obtained excellent results.

For example, with $N = 5$ and $k = 12$, we got the following table.

n	*coefficient* $d(n)$	n	*coefficient* $d(n)$	n	*coefficient* $d(n)$
1	1.000000000000	10	−0.443170826278	19	0.028586186214
2	0.736336215000	11	−0.274712554221	20	1.658396083173
3	0.848487667494	12	−0.656350645623	21	−0.238573742440
4	0.395961414268	13	0.968514715109	22	−0.081802260909
5	−0.965816702987	14	0.652137510007	23	−0.128175671584
6	−0.869840448856	15	−0.248097509310	24	−0.423752374537
7	1.702552411952	16	−0.026120840405	25	−0.483905879531
8	−0.511616761795	17	−0.793461234486		
9	0.363297826112	18	−0.562956805635		

Table 3: **Coefficients d(n) of the modular form with N=5 and k=12**

For the full results, see the Appendix. This is the first time that anyone has ever computed d_l for $N = 5, 7$.

5 Generating the high-index Fourier coefficients.

After the first M_0 Fourier coefficients are successfully stabilized, we may proceed to calculate additional d_n by appropriately using the relation

$$d_n = \frac{1}{\sqrt{y}G(ny)} \sum_{l=1}^{M_0} d_l \left(\frac{1}{2Q} \sum_{j=1-Q}^{Q} \sqrt{y_j^*} G(ly_j^*) e^{2\pi i l x_j^*/L} e^{-ikArg(c_j z_j + d_j)} e^{-2\pi i n x_j / L} \right) \tag{46}$$

for $M_0 < n \leq M(y) \leq Q$. For optimum accuracy, one needs to ensure that the denominator $\sqrt{y}G(ny)$ is not too small. The basic idea is to run through a succession of n-intervals, each having its own appropriately chosen y.

If we denote one of these intervals by $[N_A, N_B]$, then the essential thing will be to try to select y so that on $[yN_A, yN_B]$, the function G(u) does not dip too far *below* max G. Cf Figure 2.

It is this aspect which determines how big the ratio N_B/N_A can be in practice (i.e. how big a "step" we can make).

To gauge the accuracy of the resulting d_n, it is convenient to retain

$$\frac{max\ G}{min_n\ \sqrt{y}G(ny)} \quad and \quad \frac{max\ G}{avg_n\ \sqrt{y}G(ny)} \tag{47}$$

as control values. Here n ranges over $[N_A, N_B]$.

These values are completely analogous to the earlier control values in Section 4.

In setting up the production runs, we typically used a pre-processor to evaluate (47) for many different (N_A, N_B, y) and then sought to optimize things by getting these control ratios down to something like 100 or so. The pre-processor also produced a Q-value consistent with (43). The accuracy of d_n will clearly be affected by

- the size of (47)
- the size of Q
- the intrinsic accuracy of d_1, d_2, ... , d_{M_0}
- the intrinsic accuracy of V_{nl}

Using the available CRAY computer time, the author and his group were able to generate 10,000 Fourier coefficients for a variety of modular forms (with $N = 3, 5$) using the aforementioned iterative scheme. Some results from the production runs can be found in the Appendix.

6 Verification of certain known properties of the Fourier coefficients when N=3, k=12.

For the case $N = 3$, $k = 12$, we found very good agreement with the known formula

$$c(p)c(q) = c(pq) \quad for\ prime\ numbers\ p \neq q \ . \tag{48}$$

We also compared our $c(n)$-values with those produced by the Ramanujan recursion[9] formula from $\tau(n)$.

Definition. Let $\sigma_s(n)$ denote the sum of the s_{th} powers of the divisors of n (including 1 and n). The *Ramanujan recursion formula* then states that:

$$\begin{aligned} \tau(n) &= \frac{24}{1-n}\left\{\sigma_1(1)\tau(n-1) + \sigma_1(2)\tau(n-2) + \ldots + \sigma_1(n-1)\tau(1)\right\} \\ &= \frac{24}{1-n}\sum_{i=1}^{n-1}\left[\sigma_1(i)\tau(n-i)\right] \quad . \end{aligned} \tag{49}$$

As we set $\tau_n = d_n n^{\frac{12-1}{2}} = d_n n^{5.5}$, we may rewrite the recursion formula as

$$d(n) = \frac{24}{1-n}\sum_{i=1}^{n-1}\left[\sigma_1(i)d(n-i)\left(\frac{n-i}{n}\right)^{5.5}\right] \tag{50}$$

in order to prevent over-flow errors. See the Appendix for a complete listing of the first 1500 $d(n)$'s in the case $N = 3$ and $k = 12$.

As a test, we also calculated the first 1000 $d(n)$'s using Section 5. The maximum error between the two methods was found to be $4.18 * 10^{-11}$. This gives a very good verification of the accuracy of our programs.

Finally, we also checked the famous result that

$$|d(p)| \leq 2 \tag{51}$$

holds for *prime* p, at least out to 10000.

Table 4 lists those $d(n)$ with $n \leq 10^4$ whose absolute value exceeds 2.

n	*coefficient* $d(n)$	n	*coefficient* $d(n)$	n	*coefficient* $d(n)$
799	−2.01622560964	1751	2.26352995029	2987	−2.23064957091
3149	−2.39439922307	3713	2.38206562861	4841	−3.27958325463
5321	2.20799919895	6157	2.44448162997	6283	−2.02352350833
6901	2.68808923389	7003	−2.12669409509	7849	2.80504993524
8137	−2.67424283678	8143	−2.24617606452	8777	−2.00360358063
8789	−2.01798559212	9071	2.50040320311	9077	−2.17592546769

Table 4: **Coefficients d(n) that are greater than 2 in absolute value**

7 Other related works in progress.

At the same time this paper is written, we are trying to finish another important experiment using various supercomputers.

In (8), note that we have the identity

$$\frac{1}{\sqrt{Q}}\sum_{j=0}^{Q-1} f\left(\frac{z+jL}{Q}\right) = \sum_{n=1}^{\infty} d_{Qn}\sqrt{y}G(ny)e^{2\pi inx/L} \quad . \tag{52}$$

This means that

$$d_Q\sqrt{y}G(y) = \frac{1}{L}\int_{-L/2}^{L/2}\left[\frac{1}{\sqrt{Q}}\sum_{j=0}^{Q-1} f\left(\frac{z+jL}{Q}\right)\right] e^{-2\pi ix/L}dx \tag{53}$$

for $y > 0$. To analyze the size of d_Q, it is natural to try to study the size of the square bracket as exactly as possible.

This size will depend on where the image (in $\mathcal{F}_N$) of the points $(z+jL)/Q$ are located for $j = 0, 1, 2, ..., Q-1$.

One is especially interested in cases where $y = Q^{-\beta}$ with a small value of β.

Figure 3 shows how the set of image points changes for $Q = 100,000$ as β goes from slightly negative to slightly positive.

Professor Hejhal has conjectured that, for $\beta > 0$, a Central Limit Theorem holds for

$$u_Q(x,y) = \frac{1}{\sqrt{Q}}\sum_{j=0}^{Q-1} f\Big(\frac{x+jL}{Q}, \frac{y}{Q}\Big) \tag{54}$$

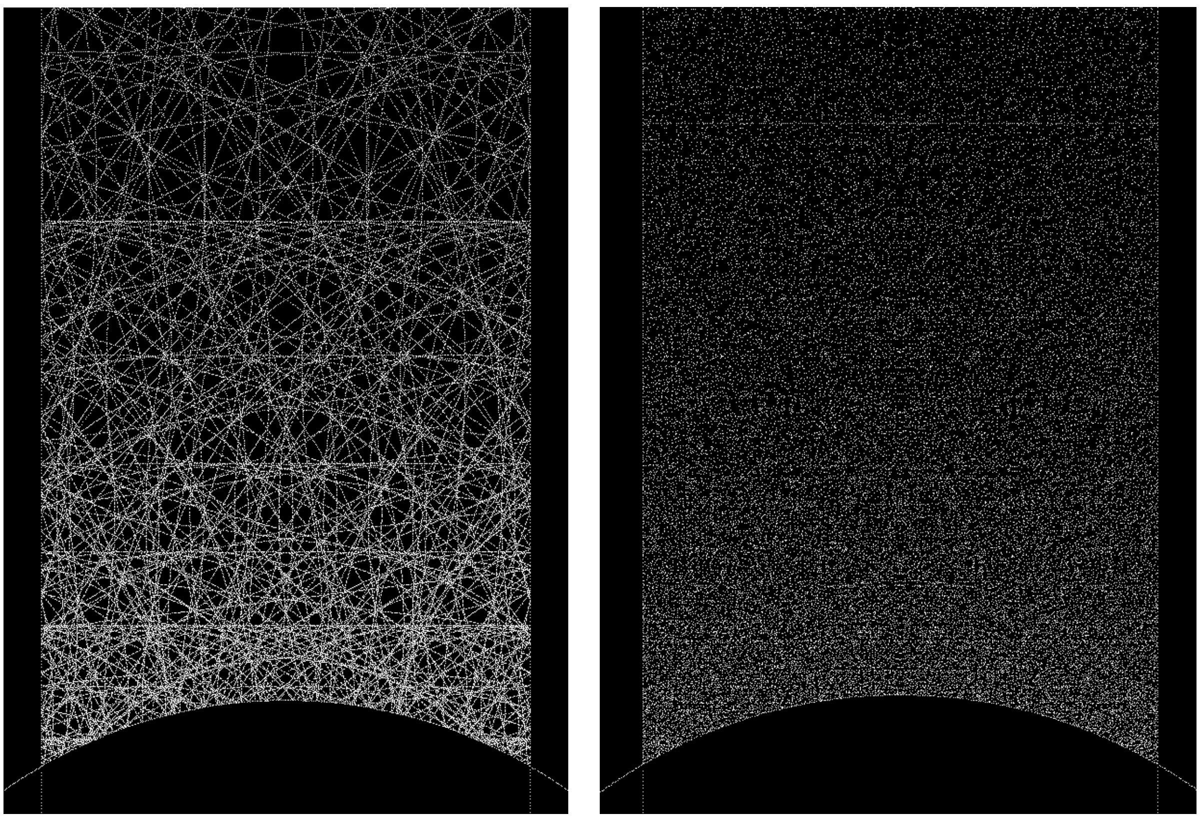

Figure 3: **Mapping of lines parallel to y=0 into the fundamental polygon**

over a large family of functions f so long as the group G is *non*-arithmetic (i.e. $N \neq 3, 4, 6$). The variance σ^2 will be a certain multiple of

$$\iint_{\mathcal{F}_N} |f(x,y)|^2 \frac{dx\,dy}{y^2} \quad . \tag{55}$$

The conjecture is reasonable because in Lobachevsky space (i.e the upper half-plane H), two nearby points have distance $\frac{1}{y}\sqrt{(\Delta x)^2 + (\Delta y)^2}$ instead of $\sqrt{(\Delta x)^2 + (\Delta y)^2}$ as in Euclidean space. The Lobachevsky distance between successive $(z + jL)/Q$ thus tends to infinity whenever $\beta > 0$. A random mixing of the image points in $\mathcal{F}_N$ is therefore likely. See Figure 3 (right).

For arithmetic groups, the Central Limit Theorem should *not* hold (because of hidden symmetries called *Hecke operators*).

The classical version of the Central Limit Theorem is as follows.

Theorem *(Central Limit Theorem)* Let X_1,X_2,... be independent, identically distributed random variables having mean μ and finite nonzero variance σ^2. Set $S_n = X_1 + X_2 + ... + X_n$. Then

$$\lim_{Q\to\infty} P\left(\frac{S_Q - Q\mu}{\sigma\sqrt{Q}} \leq t\right) = \Phi(t) \tag{56}$$

for $-\infty < t < \infty$. Here $\Phi(t)$ is the standard normal distribution function.

The proof of this theorem is in [13].

In Professor Hejhal's conjecture, the functions $f((z + jL)/Q)$ play the role of the x_j.

Testing Hejhal's conjecture using a true modular form of weight k would require an inadmissibly long CPU time — because of the need to find and store many transform matrices $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ like those in (16).

For this reason, we tested (54) using a collection of fairly simple, *real*-valued, functions first. Here $k = 0$.

Actual computation showed that Prof. Hejhal's predictions seem to be correct. The distribution functions of $u_Q(x, y)$ for some f's on Group 3, Group 5 and Group 7 have been included in Figure 4 – 9.

In the non-arithmetic cases, the value of

$$\frac{1}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} u_Q^2(x,y)dx \tag{57}$$

was also computed to 3 to 4 places and was found to be within $1 - 2\%$ of the predicted value (55).

See the Appendix for the *density* functions of $u_Q(x, y)$ on Group 5. The job depicted there requires about 40 hours CPU time on the fastest machines in the world. Jobs with Q closer to 10^6 take on the order of *4* hours; we ran many of these less expensive ones.

Vendor	*System*	*# of CPU used*	*Architecture*	*Performance*
CRAY	*C90*	1	*Vector*	1.000
CRAY	*T3D*	64	*3D torus*	1.098
Connection Machine	$CM-5$	512	*fat tree*	0.914
CRAY	*II*	1	*Vector*	0.278
Silicon Graphics	*Indigo II*	1	*Serial*	0.013

Table 5: **Comparison of machine performance**
(Based on several jobs ranging from 3.0 minutes to 40 hours C90 CPU time)

For this project, we used several computer systems including the newest available ones: CRAY C90, Connection Machine CM-5 and CRAY T3D. The CRAY C90 is the world's best sequential vector supercomputer. Our vectorized version code runs at over 50% of the peak performance of one CRAY C90 processor. Since our algorithm is ideally suited for distributed memory multiple instruction multiple data (MIMD) massively parallel processing (MPP) machines, we have also implemented and tested the problem on the 512-CPU Thinking Machine CM-5 system using CMMD message passing library with both hostless and host-node programming mode. In order to achieve a 12-places accuracy, we used double precision on CM-5. Then we translated our code into Parallel Virtual Machine (PVM) form for the new CRAY T3D system. PVM is a software system that facilitates the inter-process communication in UNIX network programming. Figure 10 illustrated the structure of CRAY-T3D system. On a system having 64 processors like the CRAY T3D, we partitioned the entire x-interval into 64 equal length subintervals and sent them uniformly to 64 processors. Information packages containing the partial computing results, the values of the selected functions and records on number of iterations, are sent to one master (or host) processor via the inter-communication network. In the host-node version of the program, we use the CRAY C90 as the host. It collects the message packages received from the nodal processors, distinguishes them by tags and computes the overall statistical tally. After all

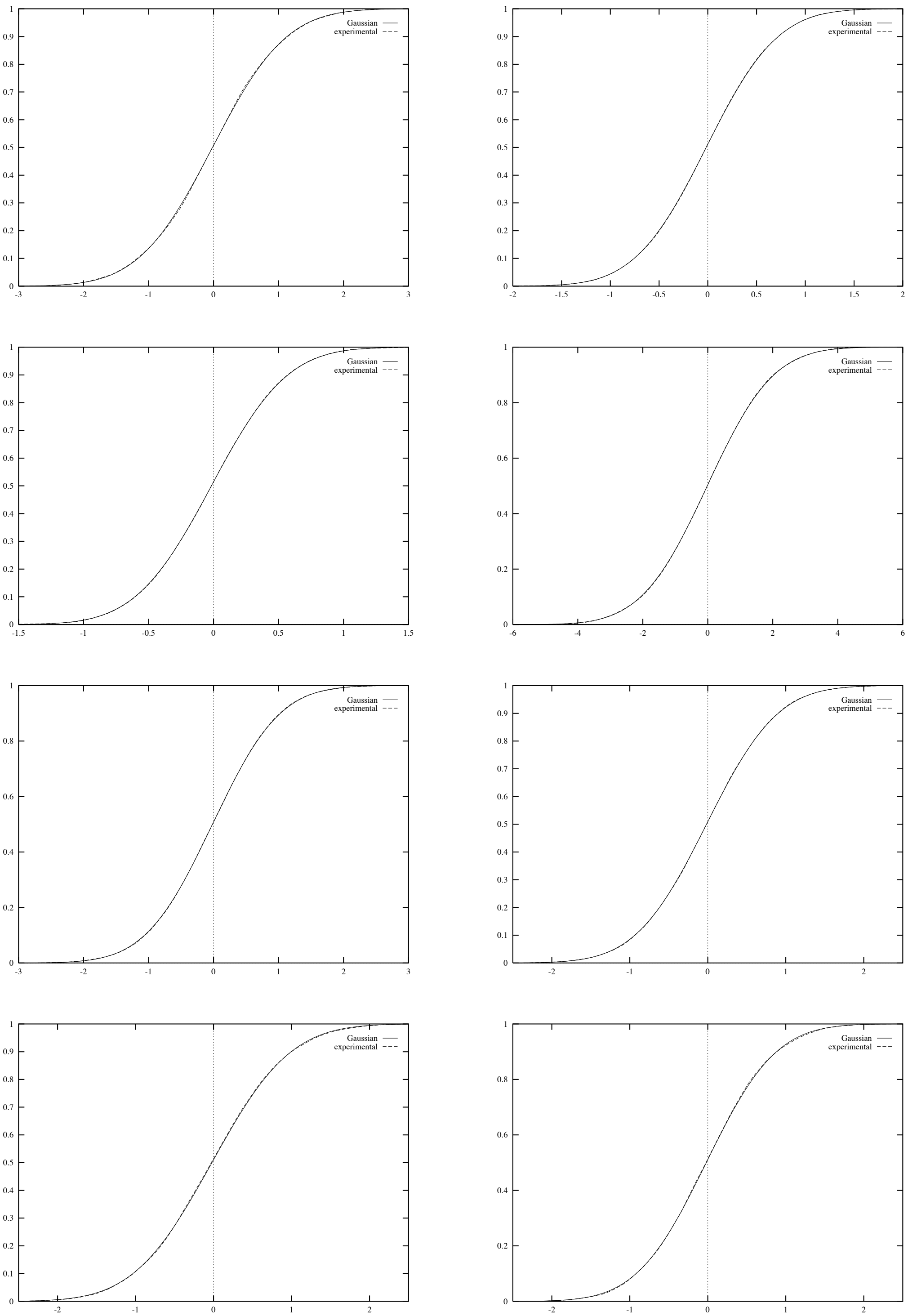

Figure 4: **Probability distribution functions for Group 5, Q=10423507,** $\beta = 0.385$

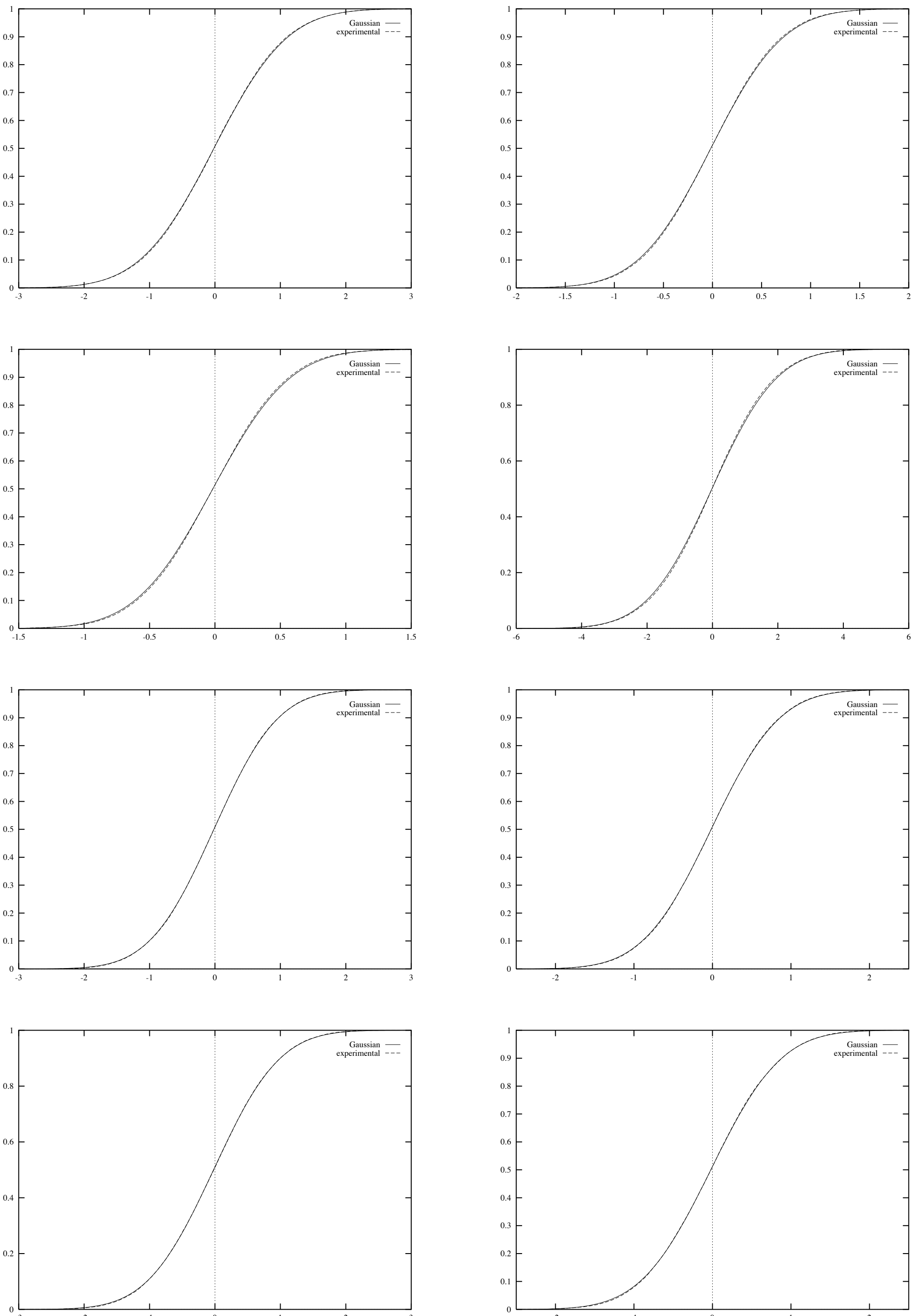

Figure 5: **Probability distribution functions for Group 7, Q=1000193,** $\beta = 0.500$

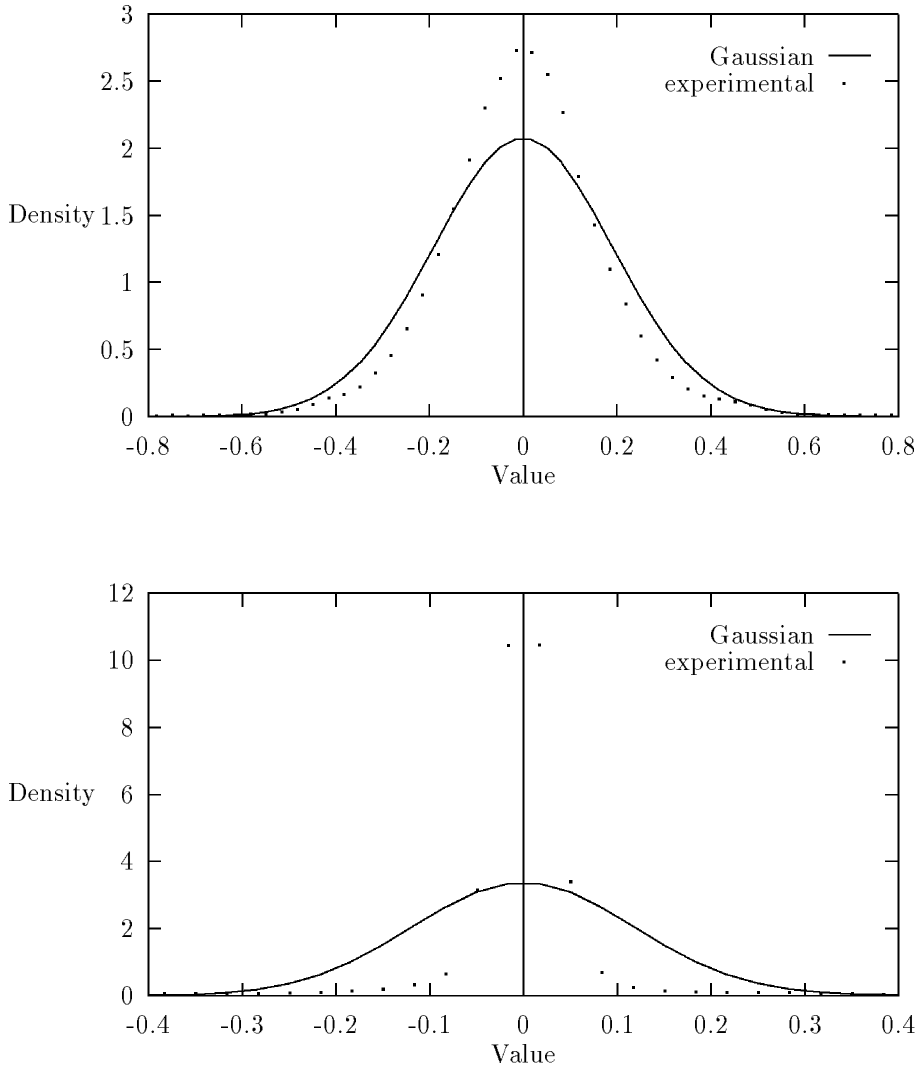

Figure 6: **NON-GAUSSIAN density for Group 3 (Function 1 and 2)** Q=1000619, $\beta = 0.500$

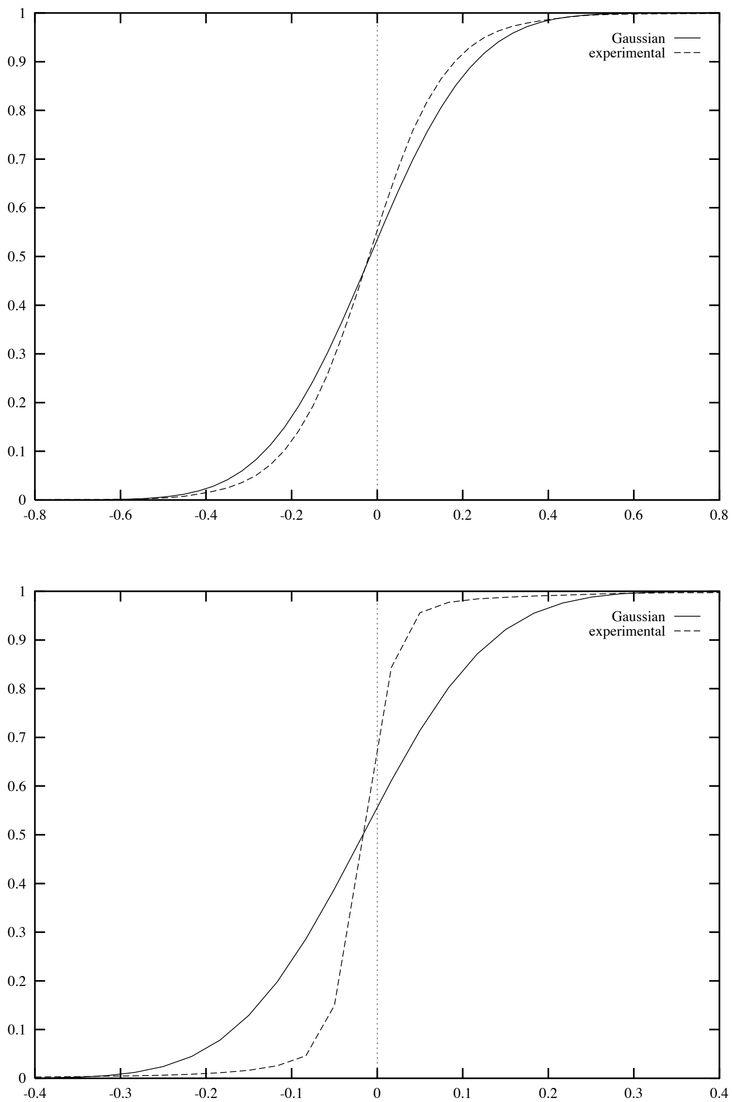

Figure 7: **NON-GAUSSIAN distribution for Group 3 (Function 1 and 2)**
Q=1000619, $\beta = 0.500$

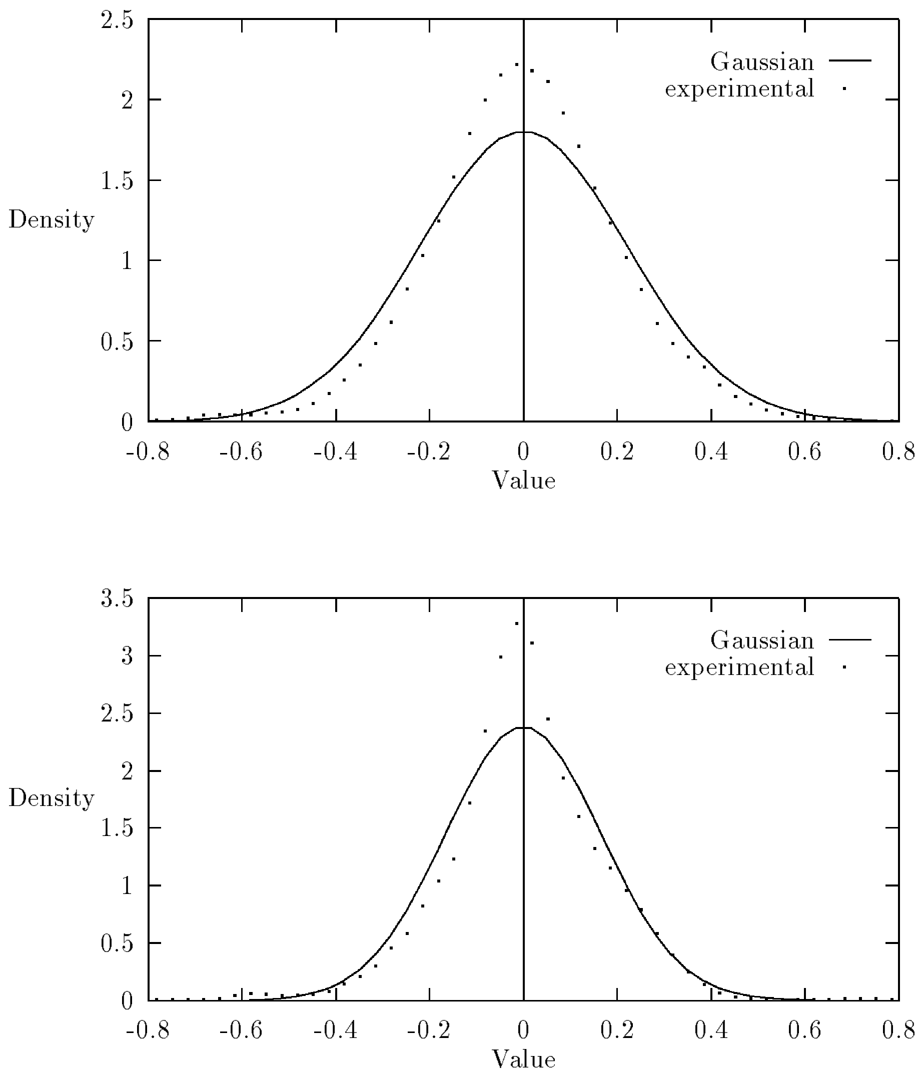

Figure 8: **NON-GAUSSIAN density for Group 3 (Function 3 and 4)**
Q=1000619, $\beta = 0.500$

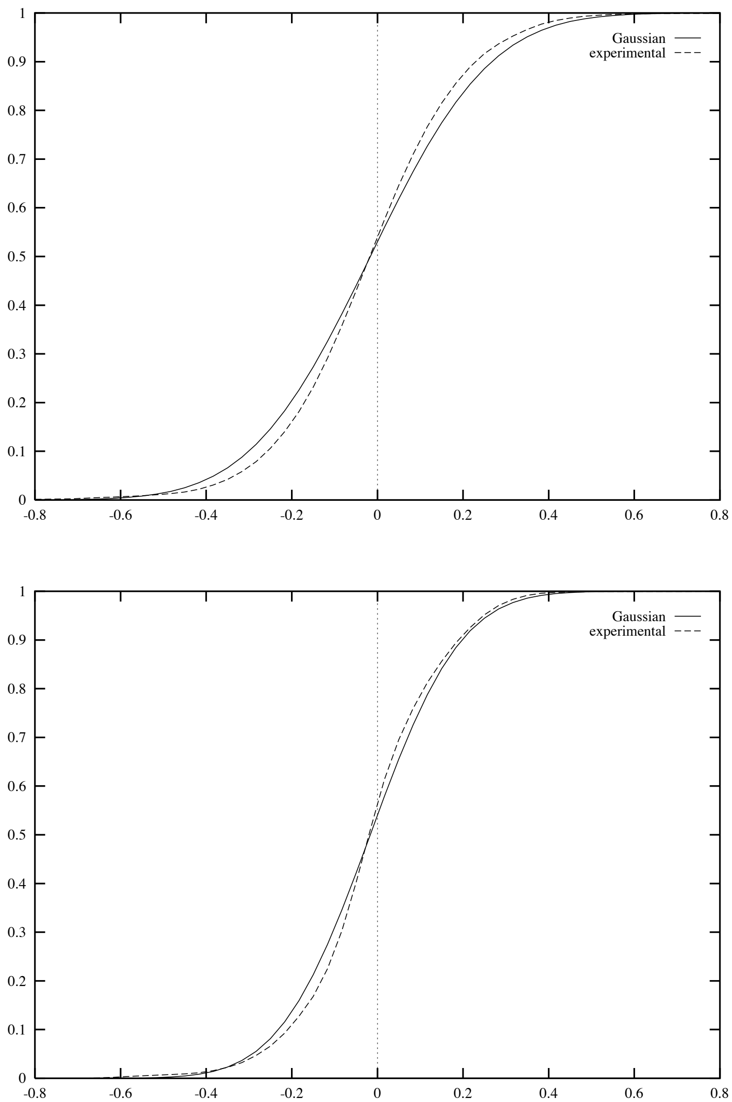

Figure 9: **NON-GAUSSIAN distribution for Group 3 (Function 3 and 4)**
Q=1000619, $\beta = 0.500$

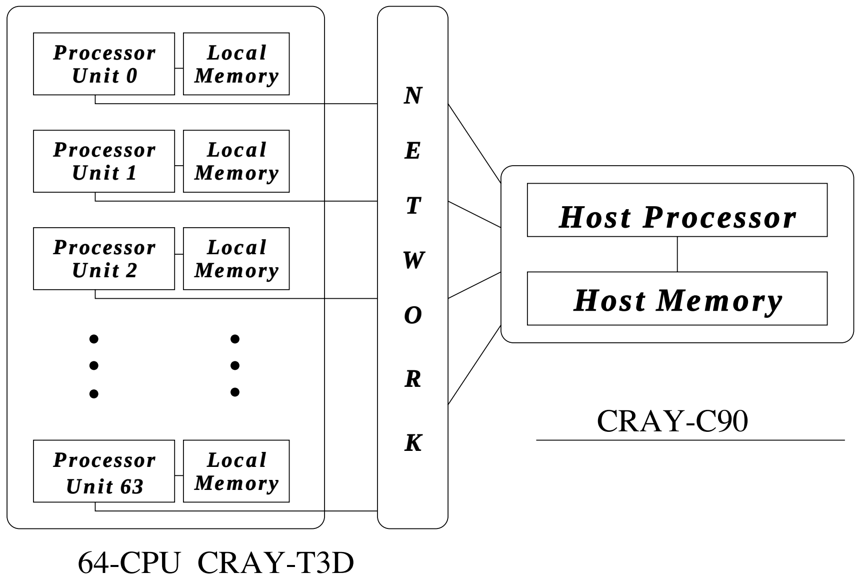

Figure 10: **Massive Parallel Machine CRAY-T3D**

the nodes finish running, the host starts to process the probability density analysis routine. Since the nodal operations are perfectly parallel and scalable, it is expected to have a 64 times speed-up. Though processors on a parallel system are only at the workstation level, real time computations have showed a faster speed than the C90.

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References

[1] Lars V. Ahlfors, *Complex Analysis: An Introduction to the Theory of Analytic Functions of One Complex Variable*, 3rd edition, McGraw-Hill, New York, 1979.

[2] Tom A. Apostol, *Introduction to Analytic Number Theory*, Undergraduate Texts in Mathematics, Springer-Verlag, New York, 1976.

[3] Tom A. Apostol, *Modular Functions and Dirichlet Series in Number Theory*, Graduate Texts in Mathematics, Springer-Verlag, New York, 1976.

[4] Michael Artin, *Algebra*, Prentice Hall, New York, 1991.

[5] Kendall E. Atkinson, *Elementary Numerical Analysis*, Wiley, New York, 1985.

[6] Ruel V. Churchill, *Fourier Series and Boundary Value Problems*, McGraw-Hill, New York, 1987.

[7] Gerald B. Folland, *Fourier Analysis and Its Applications*, Pacific Grove, Calif., 1992.

[8] Gene Golub and James M. Ortega, *Scientific Computing : an introduction with parallel computing*, Academic Press, Boston, 1993.

[9] G.H. Hardy, P.V. Seshu Aiyar and B.M. Wilson, *Collected Papers of Srinivasa Ramanujan* Chelsea Publishing Company, New York, 1927, 1962.

[10] Dennis A. Hejhal *The Selberg trace formula for PSL(2,R)* Vol. 1-2, Lecture Notes in Math. No. 548, 1001, Springer-Verlag, Berlin, New York, 1976-1983.

[11] Dennis A. Hejhal *"Eigenvalues of the Laplacian for Hecke Triangle Groups"*, AMS Memoirs 469, May 1992.

[12] Dennis A. Hejhal and Barry N. Rackner, *On the Topography of Maass Waveforms for $PSL(2, Z)$: Experiments and Heuristics*, Experimental Mathematics, Vol. 1, No. 4, 1992, 275-305.

[13] Paul G. Hoel, Sidney C. Port and Charles J. Stone, *Introduction to Probability Theory*, Houghton Mifflin, Boston, 1971.

[14] Srinivasa Ramanujan, *"On Certain Arithmetical Functions"*, Transactions of the Cambridge Philosophical Society, XXII, No. 9, 1916, 159-184.