多倍長計算手法

平成24年度第2四半期

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今回から一般の精度問題に関する事柄に関しては,単精度を,倍精度演算も多倍長計算手法に含める様にしました.

1. ルジャンドル陪関数計算

正規化ルジャンドル陪関数

$$\bar{P}_{m-1}{}^{m}(x)=0 \quad \bar{P}_{m}{}^{m}(x)=\sqrt{\frac{1}{2}\frac{2m+1}{(2m)!}}(1-x^2)^{\frac{m}{2}}$$

$$\int_{-1}^{1} P_m{}^m(x)^2 dx=[(2m-1)!!]^2\int_{-1}^{1}(1-x^2)^m dx=\frac{2(2m-1)!!(2m)!!}{2m+1}=\frac{2(2m)!}{2m+1}$$

$$I_n=\int_{-1}^{1}(1-x^2)^n dx=\int_0^{\pi}\sin^{2n+1}\theta d\theta \qquad x=\cos\theta$$

$$I_n=\frac{2n}{2n+1}I_{n-1}=\ldots=\frac{2^n n!}{(2n+1)!!}I_0=\frac{2^{2n+1}n!}{(2n+1)!!}=\frac{2^{n+1}n!2^n n!}{(2n+1)!}=\frac{2^{2n+1}(n!)^2}{(2n+1)!}$$

$$\bar{P}_n{}^m(x)=\sqrt{\frac{2n+1}{2}\frac{(n-m)!}{(n+m)!}}P_n{}^m(x) \quad \bar{P}_m{}^{-m}(x)=(-1)^m\bar{P}_m{}^m(x)$$

$$\bar{P}_n{}^m(x)=\sqrt{\frac{(2n-1)}{(n+m)}\frac{(2n+1)}{(n-m)}}x\bar{P}_{n-1}{}^m(x)-\sqrt{\frac{(2n+1)}{(2n-3)}\frac{(n+m-1)(n-m-1)}{(n+m)(n-m)}}\bar{P}_{n-2}{}^m(x)$$

計算手順

xとして、ルジャンドル多項式の０点をとる。

$$P_0^{\ 0}(x)=1, P_1^{\ 0}(x)=\sqrt{3}x$$

$$P_{n+1}^{\ \ 0}(x)=\frac{\sqrt{(2n+1)(2n+3)}}{n+1}(xP_n^{\ 0}(x)-\frac{nP_{n-1}^{\ \ 0}(x)}{\sqrt{(2n+1)(2n-1)}})$$

$$(1\le n\le nn-1)$$

$m>0$の場合$, m>n$なら$P_n^{\ m}(x)=0.$このため$, P_{n+m}^{\ \ m}(x)$を$P_n^{\ m}(x)$

とする.

$$P_0^{\ m}(x)=\sqrt{2m+1}\sqrt{\frac{(2m-1)!!}{(2m)!!}}(1-x^2)^{\frac{m}{2}}$$

$$P_1^{\ m}(x)=\sqrt{2m+3}xP_0^{\ m}(x)$$

$$P_{n+1}^{\ \ m}(x)=\sqrt{\frac{(2n+2m+3)(2n+2m+1)}{(n+1)(n+2m+1)}}(xP_n^{\ m}(x)-\sqrt{\frac{n(n+2m)}{(2n+2m+1)(2n+2m-1)}}P_{n-1}^{\ \ m}(x))$$

$$(1\le m\le mm, 1\le n\le nn-1)$$

$DP_n^{\ m}(x)=\dfrac{dP_n^{\ m}(x)}{dx}$で表す.

$$DP_0^{\ m}(x)=-\frac{mxP_0^{\ m}(x)}{1-x^2}$$

$$DP_1^{\ m}(x)=\sqrt{2m+3}(P_0^{\ m}(x)+xDP_0^{\ m}(x))$$

$$DP_{n+1}^{\ \ m}(x)=\sqrt{\frac{(2n+2m+3)(2n+2m+1)}{(n+1)(n+2m+1)}}\times$$

$$(P_n^{\ m}(x)+xDP_n^{\ m}(x)-\sqrt{\frac{n(n+2m)}{(2n+2m+1)(2n+2m-1)}}DP_{n-1}^{\ \ m}(x))$$

$$(1\le m\le mm, 1\le n\le nn-1)$$

チェック方法

$$\int_{-1}^{1}(P_n^{\ m}(x))^2dx=2$$

計算例

nn=mm,Gauss-Legendre 積分の分点数を3*mmとする.倍精度演算では,mmが小さい場合特に精度上問題はないが,mm≥960で問題が発生.（次ページのグラフ)

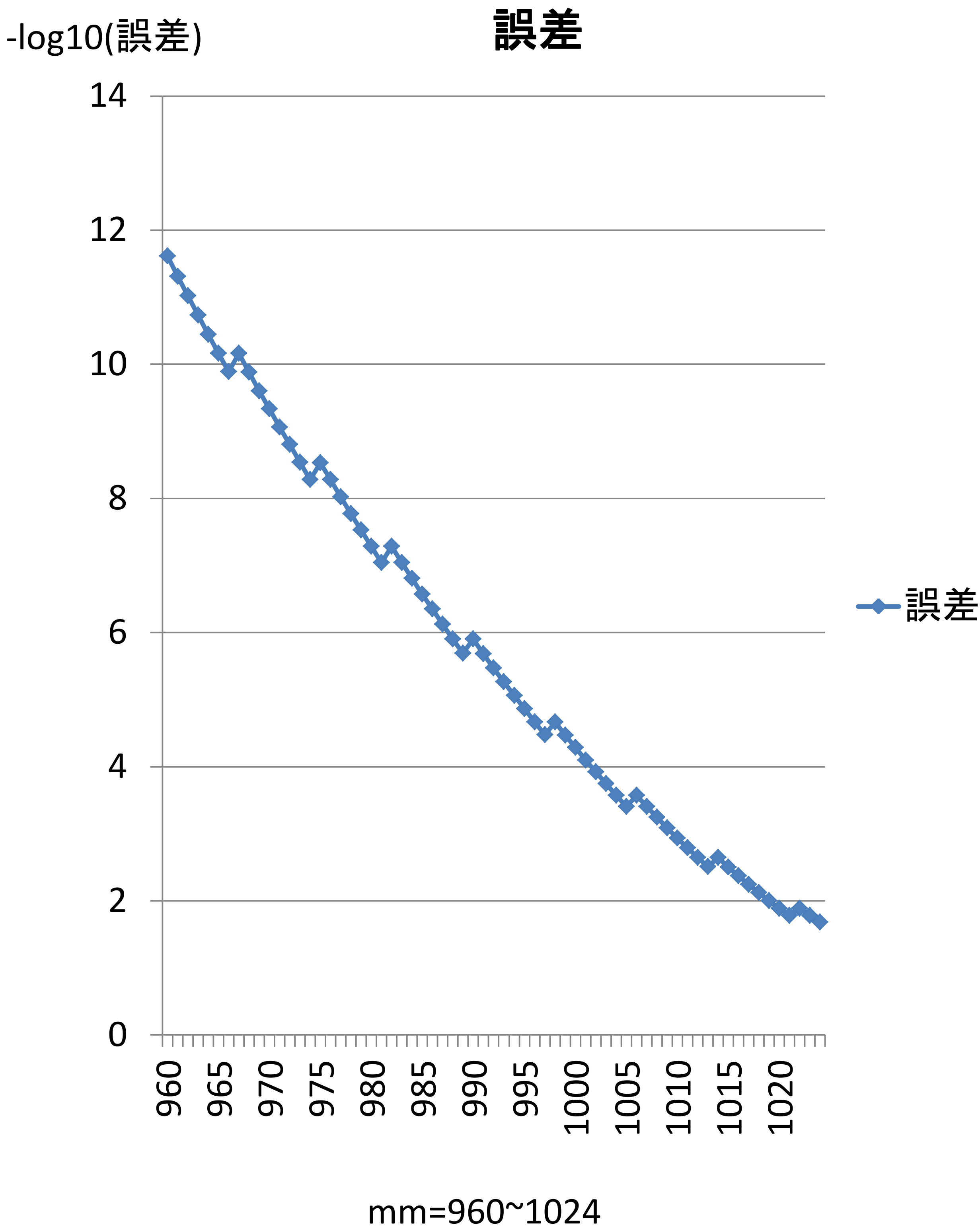
原因はmが大きくなると,$P_0^m(x)$がアンダーフローにより0となり積分値に寄与する$P_n^m(x)$の値が0になる事によります.これは,$m=1024$, $IEEE754-2008$の4倍精度で演算を行い結果を倍精度で格納した値で積分値を計算すると誤差は10^{-15}以下となる事で確認しました.

double = 0.88817841970012523D-15

quad = 0.42178096893673792D-26

倍精度　ルジャンドル陪関数の誤差

サイズ　(mm,mm,3*mm)



2. 4次元積分S221の計算

・一般式

$$S^{221}(s;m_1{}^2,m_2{}^2,m_3{}^2,m_4{}^2,m_5{}^2)=\int_0^1\int_0^{1-x}\int_0^{1-x-y}\int_0^{1-x-y-z}\frac{1}{DC}dudzdydx$$

$$C=(x+y+z+u)(1-x-y-z-u)+(x+y)(z+u)$$
$$E=(1-x-y-z-u)(x+z)(y+u)+(x+y)zu+(z+u)xy$$
$$M^2=xm_1{}^2+ym_2{}^2+zm_3{}^2+um_4{}^2+(1-x-y-z-u)m_5{}^2$$
$$D=-sE+M^2C$$

$$\frac{D}{-s}=E-\frac{M^2}{s}C,\frac{-s}{D}=\frac{1}{E-\frac{M^2}{s}C}.\frac{-s}{DC}=\frac{1}{C(E-\frac{M^2}{s}C)}=\frac{1}{CE}+\frac{M^2}{E(sE-M^2C)}$$

.積分領域をΩで表すと, $\int_\Omega\frac{1}{CE}d\Omega=6\varsigma(3)$ で, $\int_\Omega\frac{M^2}{E(sE-M^2C)}d\Omega$ を求めれば良い

解析解

$$case1 \quad S^{221}(1;0,0,0,0,0) = -6\varsigma(3) = -7.21234141895756568$$

$$case2 \quad S^{221}(-1;0,0,0,0,0) = 6\varsigma(3) = 7.21234141895756568$$

$$case3 \quad S^{221}(0;1,1,1,1,0) = 1$$

$$case4 \quad S^{221}(0;0,1,1,1,0) = \varsigma(2) = \frac{\pi^2}{6} = 1.64493406684822643647 2$$

$$case5 \quad S^{221}(0;1,1,1,1,1) = -\int_0^1 \frac{x(\frac{\ln x(1-x)}{1-x+x^2}+1)}{1-x+x^2} = 0.78130241289648$$

基本的なケースは良く一致する.

実測値

case1 result= -7.21234141895747793

case2 result= 7.21234141895747793

case3 result= 0.99999999999997335

case4 result= 1.64493406684822352

case5 result= 0.78130241289648405 5

$$S^{221}(s;m^2,0,0,0,0) \qquad s=\pm 1, m^2=1$$

$$\text{解析解}\ \mp 3\varsigma(3) = \mp 3.6061707947878284$$

複素平面での実軸への接近の仕方で結果が異なる。

$$s=1, m^2=1$$

計算解（ε-算法なし）=3.60617070947862928
計算解(y=-s/m^2)= 0.107304279342169218+162
計算解(x=-m^2/s)= 0.360617069930836021D+01

$$s=-1, m^2=1$$

計算解（ε-算法なし）＝+****************************
計算解(y=-s/m^2)= -0.200213566025878417D+162
計算解(x=-m^2/s)= -0.360611840086198487D+01

$$S^{221}(s;m^2,0,0,0,0)=\int_0^1\int_0^{1-x}\int_0^{1-x-y}\int_0^{1-x-y-z}\frac{1}{CD}dudzdydx=\int_\Omega\frac{1}{CD}d\Omega$$

$$D=-sE+xm^2C \qquad s=-1,m^2=1 \qquad => D=E+xC$$

$$\frac{1}{CD}=\frac{1}{CE}-\frac{x}{E(E+xC)}$$

$\int_\Omega\frac{1}{CE}d\Omega=6\varsigma(3)$ => 実測結果 result= 7.21234141895747793

$\int_\Omega\frac{x}{E(E+xC)}d\Omega=3\varsigma(3)$ => 実測結果 result= 3.60617070947877494

$\int_\Omega\frac{1}{C^2}d\Omega=S^{221}(0;1,1,1,1,1)$ => 実測結果 result= 0.781302412896484055

$\int_\Omega\frac{1}{C}d\Omega=\frac{1}{6}$ => 実測結果 result= 0.166666666666665747

$\int_\Omega\frac{1}{E}d\Omega=\frac{11}{9}\varsigma(3)$ => 実測結果 result= 1.46918065941728160

$$\int_\Omega\frac{1}{xC^2}d\Omega=-\int_0^1\frac{\ln(1-x)}{1-x}\quad dx$$

$$S^{221}(0;0,1,1,1,0)=\int_0^1\int_0^1\frac{1}{1-xy}dydx=-\int_0^1\frac{\ln(1-x)}{x}dx=\frac{\pi^2}{6}$$

$$S^{221}(0;1,0,1,1,0)=\int_0^1\int_0^1\frac{x}{(1-x+xy)(1-xy)}dydx=-2\int_0^1\frac{\ln(1-x)}{2-x}dx=-2\int_0^1\frac{\ln x}{x+1}=\frac{\pi^2}{6}$$

$$S^{221}(0;1,1,1,0,0)=S^{221}(0;1,1,0,1,0)=\frac{1}{2}\int_0^1\frac{(\ln(1-x))^2}{x^2}dx=\frac{\pi^2}{6}$$

$S^{221}(-1;1,1,1,1,1)$ result = 0.680876150423024185

$S^{221}(1;1,1,1,1,1)$ result = 0.923631826519863641

解析解の数学的根拠

$$\int_0^1 \frac{(\ln(1-x))^2}{x^2}dx = \int_0^1 \frac{(\ln x)^2}{(1-x)^2}dx = [\ln x(\frac{\ln x}{1-x} + \ln\frac{1-x}{x})]_{x=0}^{x=1} - \int_0^1 \frac{\ln x}{1-x}dx - \int_0^1 \frac{\ln(1-x)}{x}dx$$

$$= -2\int_0^1 \frac{\ln(1-x)}{x} = 2SP(1) = 2\varsigma(2) = \frac{\pi^2}{3}$$

$$\int_\Omega \frac{1}{C^2}d\Omega = \int_0^1\int_0^{1-x}\int_0^{1-x-y}\int_0^{1-x-y-z} \frac{1}{C^2}dudzdydx, \int_\Omega \frac{1}{C}d\Omega = \int_0^1\int_0^{1-x}\int_0^{1-x-y}\int_0^{1-x-y-z} \frac{1}{C}dudzdydx$$

これらの場合の変数変換は,

$$x + y = p$$
$$y = pq$$
$$z + u = (1-p)r$$
$$u = (1-p)rs$$

で行う.

$$\int_\Omega \frac{1}{C^2}d\Omega = \int_0^1\int_0^1 \frac{xy}{[x+(1-x)y(1-y)]^2}dydx = -\int_0^1 \frac{x(\frac{\ln x(1-x)}{1-x+x^2}+1)}{1-x+x^2} = 0.78130241289648$$

$$\int_\Omega \frac{1}{C}d\Omega = \int_0^1\int_0^1 \frac{x(1-x)y}{x+(1-x)y(1-y)}dydx = \frac{1}{2}\int_0^1\int_0^1 \frac{x(1-x)}{Ax-(A-1)}dxdy$$

$$A = y^2 - y + 1, \frac{-x^2+x}{Ax-(A-1)} = -\frac{1}{A}x + \frac{1}{A^2} + \frac{1}{Ax-(A-1)}\frac{A-1}{A^2}$$

$$\int_\Omega \frac{1}{C}d\Omega = -\frac{1}{4}\int_0^1 \frac{1}{y^2-y+1}dy + \frac{1}{2}\int_0^1 \frac{1}{(y^2-y+1)^2}dy + \frac{1}{2}\int_0^1 \frac{(y-y^2)\ln y(1-y)}{(y^2-y+1)^3}dy$$

$$a = \int_0^1 \frac{1}{y^2-y+1}dy, b = \int_0^1 \frac{1}{(y^2-y+1)^2}dy, u = \frac{2y-1}{6(y^2-y+1)^2}, v = \ln y(1-y)$$

$$\int_0^1 \frac{(y-y^2)\ln y(1-y)}{(y^2-y+1)^3}dy = \int_0^1 \frac{(2y-1)^2}{6(y^2-y+1)^2(y-y^2)}dy$$

$$= -\frac{1}{2}\int_0^1 \frac{1}{(y^2-y+1)^2(y-y^2)}dy + \frac{2}{3}\int_0^1 \frac{1}{(y^2-y+1)(y-y^2)}dy$$

$$= -\frac{1}{2}\int_0^1 \frac{1}{(y^2-y+1)(y-y^2)}dy - \frac{1}{2}b + \frac{2}{3}a = -\frac{1}{2}a - \frac{1}{2}b + \frac{2}{3}a = \frac{1}{6}a - \frac{1}{2}b$$

$$\int_0^1 \frac{(\ln(1-x))^2}{x^2}dx = \int_0^1 \frac{(\ln x)^2}{(1-x)^2}dx = [\ln x(\frac{\ln x}{1-x} + \ln\frac{1-x}{x})]_{x=0}^{x=1} - \int_0^1 \frac{\ln x}{1-x}dx - \int_0^1 \frac{\ln(1-x)}{x}dx$$

$$= -2\int_0^1 \frac{\ln(1-x)}{x} = 2SP(1) = 2\varsigma(2) = \frac{\pi^2}{3}$$

$$\int_\Omega \frac{1}{C}d\Omega = -\frac{1}{4}a + \frac{1}{2}b + \frac{1}{12}a - \frac{1}{4}b = -\frac{1}{6}a + \frac{1}{4}b = -\frac{1}{6}a + \frac{1}{4}(\frac{2}{3} + \frac{2}{3}a) = \frac{1}{6}$$

$$b = \int_0^1 \frac{1}{(y^2-y+1)^2}dy = \frac{2y-1}{3(y^2-y+1)}\,|_{y=0}^{y=1} + \frac{2}{3}\int_0^1 \frac{1}{y^2-y+1}dy = \frac{2}{3} + \frac{2}{3}a$$

$$E = (1-x-y-z-u)(x+z)(y+u) + (x+y)zu + (z+u)xy$$

$$x+z = p, z = pq, y+u = (1-p)r, u = (1-p)rs$$

$$\int_\Omega \frac{1}{E}d\Omega = \int_0^1 \frac{4(x-x^2)}{(2x-1)(x-x^2-1)}(\ln^2(1-x) - \ln^2(x))dx \quad (q\text{をxに付け直した.})$$

$$= -\frac{4}{3}\int_0^1 \frac{\ln^2(1-x)-\ln^2(x)}{2x-1}dx + \frac{4}{3}\int_0^1 \frac{1-2x}{x-x^2-1}(\ln^2(1-x)-\ln^2(x))dx$$

$$I_1 = \int_0^1 \frac{\ln^2(1-x)-\ln^2(x)}{2x-1}dx = \frac{1}{2}\int_{-1}^1 \frac{\ln^2(\frac{1-x}{2}) - \ln^2(\frac{1+x}{2})}{x}dx$$

$$= \int_0^1 \frac{\ln^2(1-x)-\ln^2(1+x)}{x}dx - \ln(2)\int_{-1}^1 \frac{|\ln(\frac{1-x}{1+x})|}{x}dx$$

$$= \frac{7}{4}\varsigma(3)$$

$$I_2 = \int_0^1 \frac{1-2x}{x-x^2-1}(\ln^2(1-x)-\ln^2(x))dx = 4\int_0^1 \frac{\ln(x^2-x+1)\ln(x)}{x}dx$$

$$= 4(\sum_{n=1}^\infty \frac{(-1)^{n-1}}{n^3} - \frac{1}{9}\sum_{n=1}^\infty \frac{(-1)^{n-1}}{n^3}) = 4\times\frac{3}{4}\times\frac{8}{9}\varsigma(3) = \frac{8}{3}\varsigma(3)$$

$$\int_\Omega \frac{1}{E}d\Omega = (\frac{8}{3}\times\frac{4}{3} - \frac{4}{3}\times\frac{7}{4})\varsigma(3) = \frac{11}{9}\varsigma(3) = 1.469180659...............$$

3 FFTの計算

一次元複素フーリエ変換

$$C_l <-> \quad y_k \quad (l, k = 0,1,\dots, L-1)$$

$$e(x) = e^{2\pi i x} = \cos(2\pi x) + i * \sin(2\pi x)$$

$$C_l = \frac{1}{\sqrt{L}} \sum_{k=0}^{L-1} y_k e(-\frac{lk}{L}) \qquad y_k = \frac{1}{\sqrt{L}} \sum_{l=0}^{L-1} C_l e(\frac{lk}{L})$$

これを以下の様にして演算量を削減します.(FFT)

$$L = MN$$

$$k = p + Mq \qquad p = 0,1,\dots, M-1 \quad q = 0,1,\dots, N-1$$

$$l = Nm + n \qquad m = 0,1,\dots, M-1 \quad n = 0,1,\dots, N-1$$

$$C_l = C_{Nm+n} = \frac{1}{\sqrt{M}} \sum_{p=0}^{M-1} e(-\frac{pm}{M}) e(-\frac{pn}{MN}) [\frac{1}{\sqrt{N}} \sum_{q=0}^{N-1} e(-\frac{qn}{N}) y_{p+Mq}]$$

演算量:フーリエ変換 $L^2 = (MN)^2$

$FFT \qquad MN(M+N+1) \fallingdotseq MN(M+N)$

MとN互いに素 $\qquad MN(M+N)$

$$L = N_1 * N_2 * \dots\dots * N_m$$

$$FFT\text{演算量} \fallingdotseq L(N_1 + N_2 + \dots\dots + N_m)$$

$$FFT\text{の効果} \fallingdotseq \frac{L}{(N_1 + N_2 + \dots\dots + N_m)}$$

例

$$L = 2*3*4*5*6*7*8*9 = 362880$$

$$362880/(2+3+4+5+6+7+8+9) = 8247$$

精度改善例

FFTは性能のみならず精度面でも向上します.

各種コンパイラによる一次元
フーリエ変換とＦＦＴ計算の誤差

cpu	x5570	sr16000	bg/q
フーリエ変換	2.120*10^{-11}	6.233*10^{-10}	6.233*10^{-10}
FFT	4.089*10^{-15}	4.031*10^{-15}	3.960*10^{-15}

サイズは$N = 2^{20}$であるが、
FFTでは精度は倍精度演算
の限界まで出ている.