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BOTTLENECK POINTS AND POSSIBLE OPTIMIZATIONS METHODS

SOME BOTTLENECK POINTS:

Function digam in e_Tceis

```
if(z == c1)  {  psi = -c1*gama;  return;}


if(z.real() < 0)  psi = diser(c1-z) - PI*cos(PI*z)/sin(PI*z);
else              psi = diser(z);
}
```

Function chypser in e_Tceis

```
848                 while(1)
849                     {
850     3.42 min        cfac=((caa*cbb)/ccc)*cfac;
851     1.42 min        cfac=cfac*x/double(n);
852      31.16 s        cf=ctemp+cfac;
853      48.81 s        if(cf == ctemp) break;
854
855                     ctemp=cf;
856   920.00 ms         n=n+1;
857      34.51 s        caa=caa+c1;
858      31.05 s        cbb=cbb+c1;
859      28.84 s        ccc=ccc+c1;
860                     }
```

BOTTLENECK POINTS AFTER PRESSING THE "CONTINUE" BUTTON

```
int f_numPP(int NCO)
{
int numPP=NUM3[NCO+1];
return numPP;
}
```

In e_F4

```
void CalcOlegSum(double *V)
{
static int counter=0;

      for(int i=0; i<8; i++) sumM[i]=0;

      for(int I=1;   I<=63;   I++) sumM[0] += V[I];
      for(int I=64;  I<=66;   I++) sumM[1] += V[I];
      for(int I=67;  I<=73;   I++) sumM[2] += V[I];
      for(int I=74;  I<=84;   I++) sumM[3] += V[I];
      for(int I=85;  I<=293;  I++) sumM[4] += V[I];
      for(int I=294; I<=326;  I++) sumM[5] += V[I];
      for(int I=327; I<=1283; I++) sumM[6] += V[I];

      for(int i=0; i<7; i++)
                  if(i!=4)
                        sumM[7] += (sumM[i]-1.);

counter++;

}
```

In e_ETACHA

POSSIBLE SOLUTIONS:

-First step will be to optimize numerical calculations by reducing redundant calculations(reducing iterations and more efficient methods of calculation, using temporary variables)

-Parallelize the computation of loops in heavy functions.

-Approximations for Large Iterations

Bottleneck Solutions #1

List of B-N	N~ of Bottleneck w/ line number
e_Tceis	5 from lines 850-859
e_Tceis	Function cGamLn lines 1242-1269
e_Tceis	Function diser lines 1027-1033
e_ETACHA	Function CalcOlegSum lines 1317-1331
e_F4	Function f_numPP line 673
	Function f_numP line 636
	Function f_KK line line 534
e_Tceis	Function digam all lines 879-884

```
while(1)
        {
          qDebug()<<n<<cf.real()<<cf.imag()<<ctemp.real()<<ctemp.imag();
        cfac=((caa*cbb)/ccc)*cfac;
        cfac=cfac*x/double(n);
        cf=ctemp+cfac;
        if(cf == ctemp) break;

        ctemp=cf;
        n=n+1;
        caa=caa+c1;
        cbb=cbb+c1;
        ccc=ccc+c1;
        }
}
```

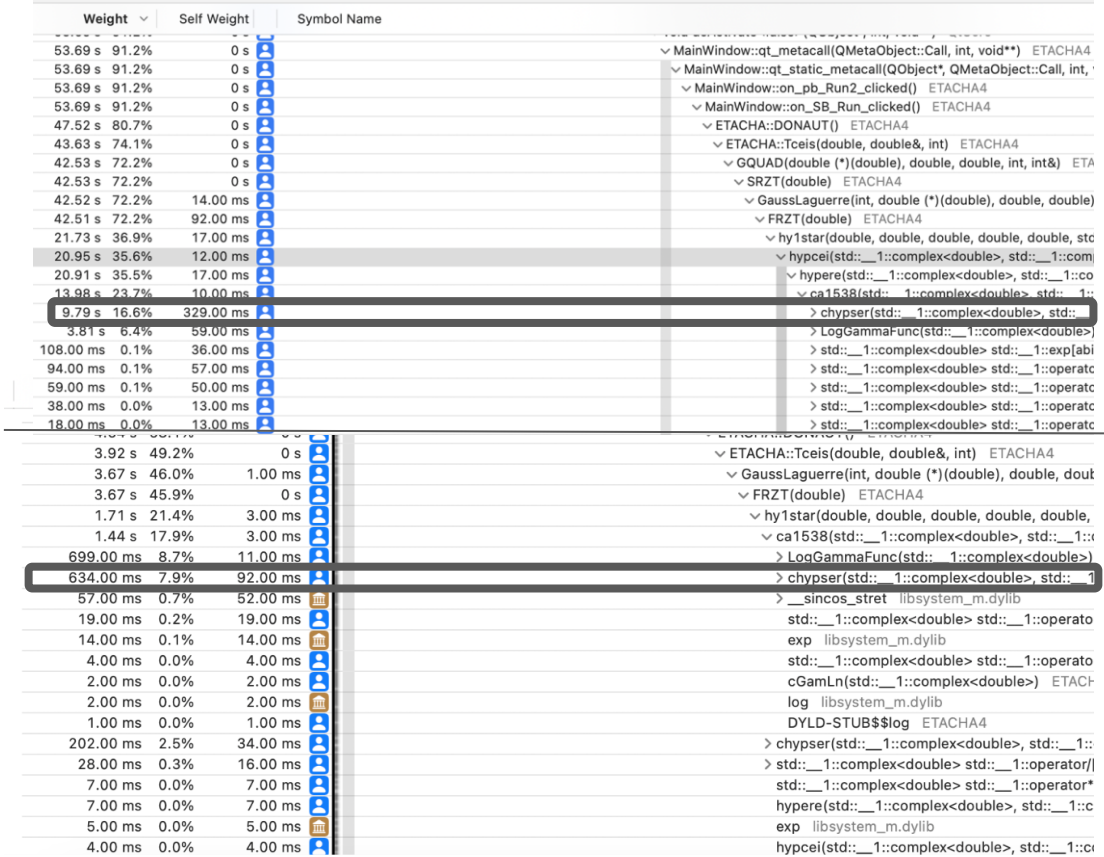
METHODS THAT WE WILL USE TO OPTIMIZE-

-Precompute (caa * cbb / ccc) to avoid redundant calculations.

-Use `abs(cf - ctemp) < EPSILON` instead of direct equality for convergence.

-Parallelize with `#pragma omp parallel` for faster execution.

Result #1



-Made three key improvements to make the function run faster and more reliably:

- Instead of doing the same calculation over and over, it now computes it once and reuses it.
- Instead of looking for an exact match, it checks if the difference is small enough to safely stop.
- Organized the loop better so the function doesn't waste effort.

-Results of optimisation

- Overall function runtime cut by almost 60%
- No longer the heaviest function in e_Tceis

#2

List of B-N	N~ of Bottleneck w/ line number
e_Tceis	5 from lines 850-859
e_Tceis	Function cGamLn lines 1242-1269
e_Tceis	Function diser lines 1027-1033
e_ETACHA	Function CalcOlegSum lines 1317-1331
e_F4	Function f_numPP line 673
	Function f_numP line 636
	Function f_KK line line 534
e_Tceis	Function digam all lines 879-884

```
complex<double>  cGamLn(complex<double> cz)
{
      double rcof[7] = {0,
                        76.18009172947146e0,-86.50532032941677e0,
                        24.01409824083091e0,-1.231739572450155e0,
                        0.1208650973866179e-2,-0.5395239384953e-5};

      double stp=2.5066282746310005;

      if(cz.real() <= 0.) return c0; //// 'real[z] <= 0';

      complex<double> cx(cz);
      complex<double> cy(cx);
      complex<double> ctmp(cx+5.5);
      complex<double> cser(1.000000000190015,0);

      ctmp=(cx+0.5)*log(ctmp)-ctmp;

      for(int j=1; j<=6; j++)
                  {
                  cy   = cy+1.;
                  cser = cser+rcof[j]/cy;
                  }

complex<double> canswer=ctmp+log(stp*cser/cx);

return canswer;
}
```

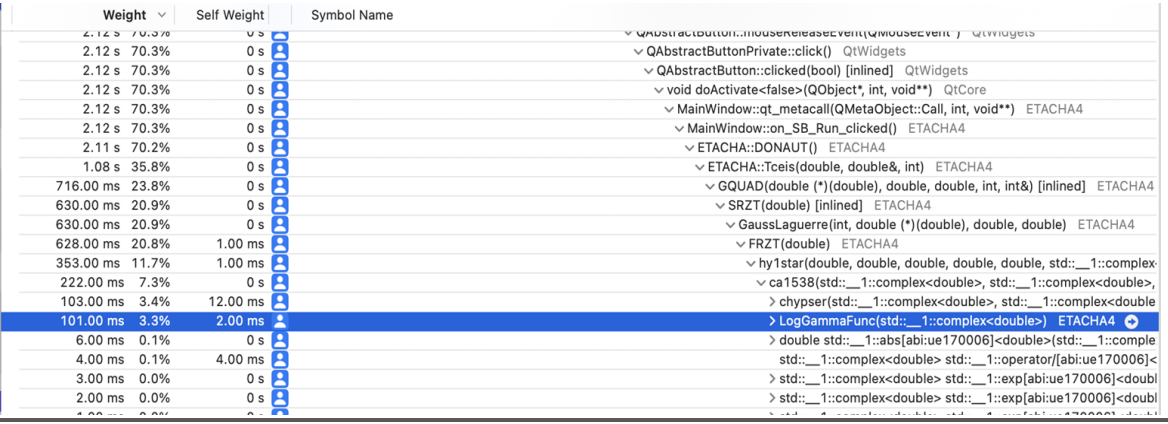
METHODS THAT WE WILL USE TO OPTIMIZE-

-Use of constexpr for Constants

-Avoided unnecessary pre computations in loop

-Use fewer temporary variables in return statement

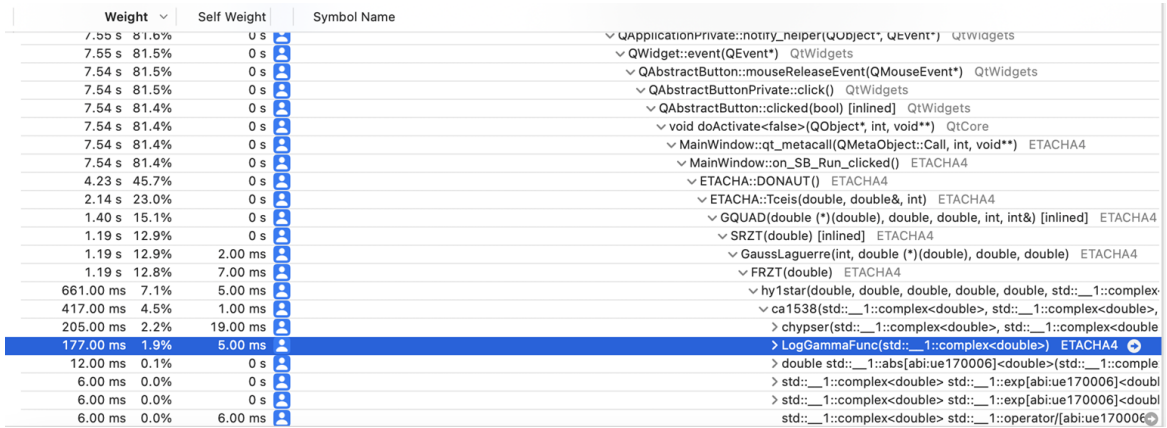
Result #2



Weight	Self Weight	Symbol Name
2.12 s 70.3%	0 s	QAbstractButtonPrivate::click() QtWidgets
2.12 s 70.3%	0 s	QAbstractButton::clicked(bool) [inlined] QtWidgets
2.12 s 70.3%	0 s	void doActivate<false>(QObject*, int, void**) QtCore
2.12 s 70.3%	0 s	MainWindow::qt_metacall(QMetaObject::Call, int, void**) ETACHA4
2.12 s 70.3%	0 s	MainWindow::on_SB_Run_clicked() ETACHA4
2.11 s 70.2%	0 s	ETACHA::DONAUT() ETACHA4
1.08 s 35.8%	0 s	ETACHA::Tceis(double, double&, int) ETACHA4
716.00 ms 23.8%	0 s	GQUAD(double (*)(double), double, double, int, int&) [inlined] ETACHA4
630.00 ms 20.9%	0 s	SRZT(double) [inlined] ETACHA4
630.00 ms 20.9%	0 s	GaussLaguerre(int, double (*)(double), double, double) ETACHA4
628.00 ms 20.8%	1.00 ms	FRZT(double) ETACHA4
353.00 ms 11.7%	1.00 ms	hy1star(double, double, double, double, double, std::__1::complex
222.00 ms 7.3%	0 s	ca1538(std::__1::complex<double>, std::__1::complex<double>,
103.00 ms 3.4%	12.00 ms	chypser(std::__1::complex<double>, std::__1::complex<double
101.00 ms 3.3%	2.00 ms	LogGammaFunc(std::__1::complex<double>) ETACHA4
6.00 ms 0.1%	0 s	double std::__1::abs[abi:ue170006]<double>(std::__1::comple
4.00 ms 0.1%	4.00 ms	std::__1::complex<double> std::__1::operator/[abi:ue170006]<
3.00 ms 0.0%	0 s	std::__1::complex<double> std::__1::exp[abi:ue170006]<doubl
2.00 ms 0.0%	0 s	std::__1::complex<double> std::__1::exp[abi:ue170006]<doubl

-Made three key improvements to make the function run faster and more reliably:

- Use of constexpr for Constants
- Avoided unnecessary pre computations in loop
- Use fewer temporary variables in return statement



Weight	Self Weight	Symbol Name
7.55 s 81.5%	0 s	QWidget::event(QEvent*) QtWidgets
7.54 s 81.5%	0 s	QAbstractButton::mouseReleaseEvent(QMouseEvent*) QtWidgets
7.54 s 81.5%	0 s	QAbstractButtonPrivate::click() QtWidgets
7.54 s 81.4%	0 s	QAbstractButton::clicked(bool) [inlined] QtWidgets
7.54 s 81.4%	0 s	void doActivate<false>(QObject*, int, void**) QtCore
7.54 s 81.4%	0 s	MainWindow::qt_metacall(QMetaObject::Call, int, void**) ETACHA4
7.54 s 81.4%	0 s	MainWindow::on_SB_Run_clicked() ETACHA4
4.23 s 45.7%	0 s	ETACHA::DONAUT() ETACHA4
2.14 s 23.0%	0 s	ETACHA::Tceis(double, double&, int) ETACHA4
1.40 s 15.1%	0 s	GQUAD(double (*)(double), double, double, int, int&) [inlined] ETACHA4
1.19 s 12.9%	0 s	SRZT(double) [inlined] ETACHA4
1.19 s 12.9%	2.00 ms	GaussLaguerre(int, double (*)(double), double, double) ETACHA4
1.19 s 12.8%	7.00 ms	FRZT(double) ETACHA4
661.00 ms 7.1%	5.00 ms	hy1star(double, double, double, double, double, std::__1::complex
417.00 ms 4.5%	1.00 ms	ca1538(std::__1::complex<double>, std::__1::complex<double>,
205.00 ms 2.2%	19.00 ms	chypser(std::__1::complex<double>, std::__1::complex<double
177.00 ms 1.9%	5.00 ms	LogGammaFunc(std::__1::complex<double>) ETACHA4
12.00 ms 0.1%	0 s	double std::__1::abs[abi:ue170006]<double>(std::__1::comple
6.00 ms 0.0%	0 s	std::__1::complex<double> std::__1::exp[abi:ue170006]<doubl
6.00 ms 0.0%	0 s	std::__1::complex<double> std::__1::exp[abi:ue170006]<doubl
6.00 ms 0.0%	6.00 ms	std::__1::complex<double> std::__1::operator/[abi:ue170006

-Results of optimisation

Overall function runtime cut by more than 50%

#3

List of B-N	N~ of Bottleneck w/ line number
e_Tceis	5 from lines 850-859
e_Tceis	Function cGamLn lines 1242-1269
e_Tceis	Function diser lines 1027-1033
e_ETACHA	Function CalcOlegSum lines 1317-1331
e_F4	Function f_numPP line 673
	Function f_numP line 636
	Function f_KK line line 534
e_Tceis	Function digam all lines 879-884

```
nz=xz;
 if(xz != 0.)  divx=nz/xz;
 if(xz == 0. || divx == 1.)
                {
                if(yz == 0.)
                        {
                        cdiser=-gama;
                        for(int k=1; k<=nz-1; k++)
                                cdiser = cdiser+1./k;
                        }
                 else    {
                        digi1(nz,xz,yz,cdiser);
                        }
                }
  else digi2(z,cdiser);
return cdiser;
```

METHODS THAT WE WILL USE TO OPTIMIZE-

-Asymptotic Expansion for Large nz

-Declare xz, yz, and nz as const

-Simplified Conditional Structure

#4

List of B-N	N~ of Bottleneck w/ line number
e_Tceis	5 from lines 850-859
e_Tceis	Function cGamLn lines 1242-1269
e_Tceis	Function diser lines 1027-1033
e_ETACHA	Function CalcOlegSum lines 1317-1331
e_F4	Function f_numPP line 673
	Function f_numP line 636
	Function f_KK line line 534
e_Tceis	Function digam all lines 879-884

```
void CalcOlegSum(double *V)
{
static int counter=0;

    for(int i=0; i<8; i++) sumM[i]=0;

    for(int I=1;   I<=63;   I++) sumM[0] += V[I];
    for(int I=64;  I<=66;   I++) sumM[1] += V[I];
    for(int I=67;  I<=73;   I++) sumM[2] += V[I];
    for(int I=74;  I<=84;   I++) sumM[3] += V[I];
    for(int I=85;  I<=293;  I++) sumM[4] += V[I];
    for(int I=294; I<=326;  I++) sumM[5] += V[I];
    for(int I=327; I<=1283; I++) sumM[6] += V[I];

    for(int i=0; i<7; i++)
                    if(i!=4)
                        sumM[7] += (sumM[i]-1.);
```

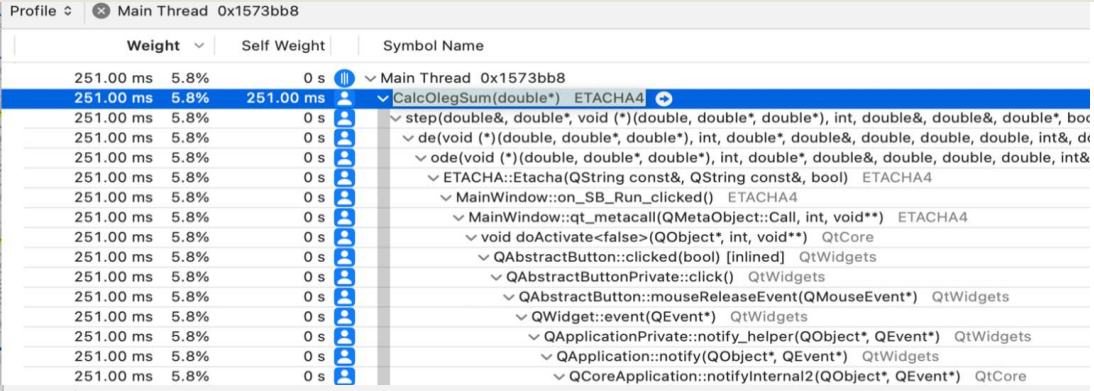
METHODS THAT WE WILL USE TO OPTIMIZE-

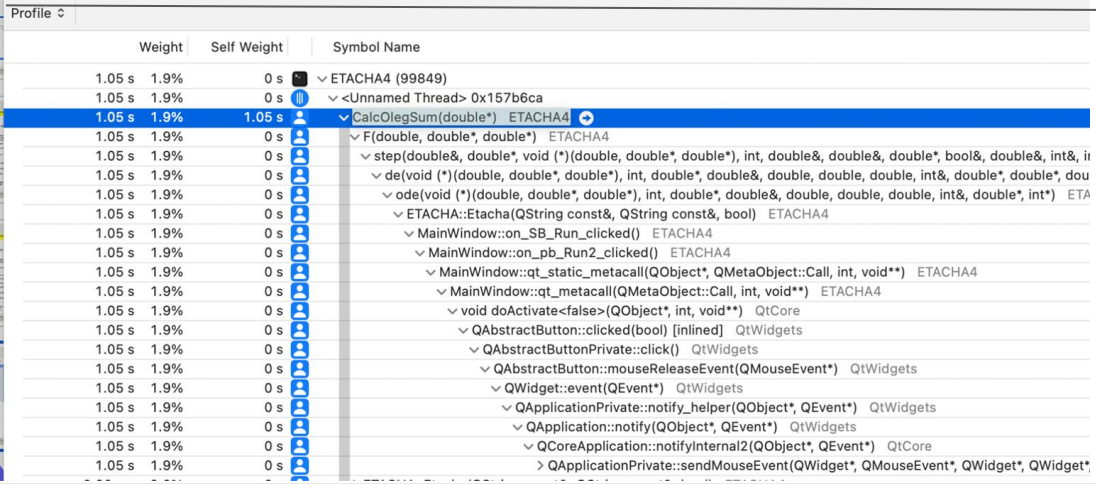
-Reduced Loop Overhead: Instead of looping separately for each sum range, a single loop iterates through V, categorizing values in one pass.

-The categorization is handled via if-else blocks

-Using constexpr for range values

Results #4





Made three key improvements to make the function run faster and more reliably:

- Instead of looping separately for each sum range, a single loop iterates through V, categorizing values in one pass.
- The categorization is handled via if-else blocks

-Results of optimisation

Overall function runtime cut by more than 65%

#5 and #6 and Results

List of B-N	N~ of Bottleneck w/ line number
e_Tceis	5 from lines 850-859
e_Tceis	Function cGamLn lines 1242-1269
e_Tceis	Function diser lines 1027-1033
e_ETACHA	Function CalcOlegSum lines 1317-1331
e_F4	Function f_numPP line 673
	Function f_numP line 636
	Function f_KK line line 534
e_Tceis	Function digam all lines 879-884

```
int f_numPP(int NCO)
{
int numPP=NUM3[NCO+1];
return numPP;
}
```

```
int f_numP(int NCO)
{
int numP=NUM2[NCO+1];
return numP;
}
```

-Results of optimisation

- Removed the unnecessary numPP and numP variable, returned directly
- (f_numPP)-The function runtime has decreased by approximately 29%
- (f_numP)-Function runtime has negligible runtime compared to program runtime(Almost 95% decrease).

#7 and #8 and Results

List of B-N	N~ of Bottleneck w/ line number
e_Tceis	5 from lines 850-859
e_Tceis	Function cGamLn lines 1242-1269
e_Tceis	Function diser lines 1027-1033
e_ETACHA	Function CalcOlegSum lines 1317-1331
e_F4	Function f_numPP line 673
	Function f_numP line 636
	Function f_IKM line 706
	Function f_IN line 700

```
int f_IKM(int N, int num)
{
int f_IKM=IC03[num]-N*100;
return f_IKM;
}
```

```
int f_IN(int num)
{
int f_IN=IC03[num]/100;
return f_IN;
}
```

-Results of optimisation

- Removed the unnecessary f_IKM and f_IN variable, returned directly
- % operator to calculate the remainder instead of subtracting multiples.
- (f_IKM)-The function runtime has decreased by approximately 75%
- (f_IN)-The function runtime has decreased by approximately 75%

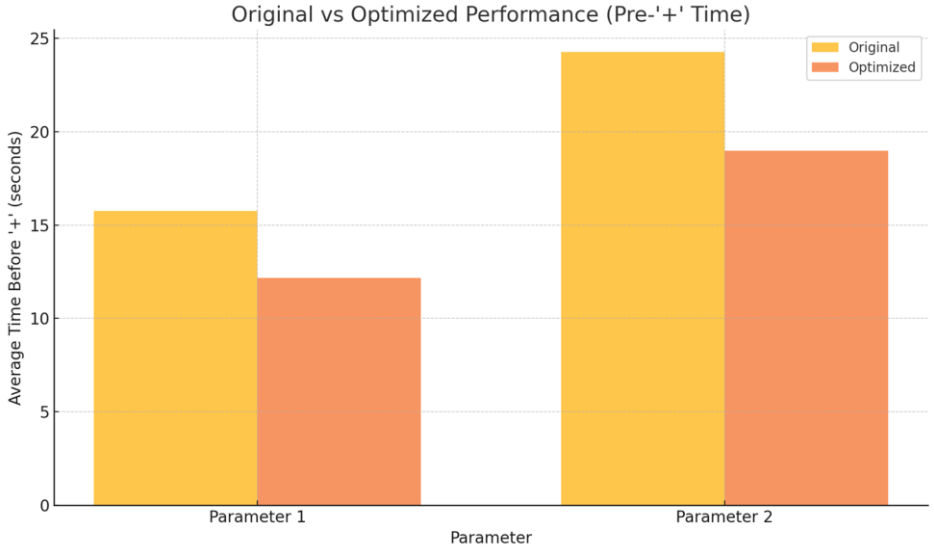
Final Results

Runs

- Each version (optimized & original) was run 3 times with identical parameters(Initial energy, projectile, target etc.) to ensure fairness.

- I averaged the run times and found the time profit between the two versions.

Parameter	Optimized	Original	Time Saved
Parameter 1	13.601666666666700	17.171333333333300	3.5696666666666700
Parameter 2	41.03966666666670	46.76866666666670	5.729000000000000
Parameter 3	22.16033333333330	22.664666666666700	0.5043333333333350
Parameter 4	1.458	1.492	0.03400000000000000



Results

- Parameters 3 and 4 were run on Ionization and Excitation models being set on PWBA(fast). **We see only around a 2.2% time profit.**

- Parameters 1 and 2 were not run on Ionization and Excitation models set on PWBA(fast). Versions v.3 and v.4 were used and both were tested with both integration models. **We saw a huge time profit in this case(around 23%).** The profit was mainly due to faster cross-section calculation.

- The time profit percentages were around the same, suggesting that **the optimized code works for all cases.**