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Acceleration of diffraction calculations in cylindrically symmetrical optics

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Abstract

We have significantly accelerated diffraction calculations using three independent acceleration devices. These innovations are restricted to cylindrically symmetrical systems. In the first case, we consider Wolf's formula for integrated flux in a circular region following diffraction of light from a point source by a circular aperture or a circular lens. Although the formula involves a double sum, we evaluate it with the effort of a single sum by use of fast Fourier transforms (FFTs) to perform convolutions. In the second case, we exploit properties of the Fresnel-Kirchhoff propagator in the Gaussian, paraxial optics approximation to achieve the propagation of a partial wave from one optical element to the next. Ordinarily, this would involve a double loop over the radial variables on each element, but we have reduced the computational cost by a factor approximately equal to the smaller number of radius values. In the third case, we reduce the number of partial waves, for which the propagation needs to be calculated, in order to determine the throughput of an optical system of interest in radiometry when at least one element is very small, such as a pinhole aperture. As a demonstration of the benefits of the second case, we analyze intricate diffraction effects that occur in a satellite-based solar radiometry instrument.

1. INTRODUCTION

Since the early work by Rayleigh [1], diffraction effects on power received by the detector in a given optics system have been of practical interest and have received considerable attention in the field of optical radiometry. Lommel considered Fresnel diffraction for the case of a point source [2], and Wolf integrated Lommel's irradiance distribution to obtain the integrated flux on the entire area of a detector [3]. Considerable attention to diffraction errors (and their correction) has been brought to bear in standards laboratories such as work by Blevin [4], Sanders and Jones [5], Ooba [6], Steel, De and Bell [7], and Boivin [8]. More recently, one of the authors analyzed the same formula and its asymptotic behavior and demonstrated how one can treat an extended source [9, 10]. Edwards and McCall also studied the same problem [11].

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The authors maintain several computer programs that evaluate Wolf's formula and simulate propagation of radiation through multistage optical systems pertinent to various radiometric applications. Here we show how one can accelerate the evaluation of Wolf's formula and simulated propagation of radiation using fast Fourier transforms (FFTs), and we use properties of traces of products of matrices to reduce the number of waves whose propagation must be computed for an optical system. This constitutes three independent innovations that are respectively discussed in Sections 2-4. We then demonstrate good scaling of computation time with wavelength in a multi-stage system that the authors could not treat as thoroughly for optical wavelengths of interest, i.e., in the visible and near-infrared region, with modest computational resources.

2. STREAMLINED EVALUATION OF WOLF'S FORMULA FOR INTEGRATED FLUX

Consider the problem of light from a point source incident on a circular aperture or lens (with focal length f) with radius R_a . The point source is located on the principle optic axis at distance d_s from the optical element. The fraction of the flux incident on the aperture or lens that falls within a central circular region with radius R_d and distance d_d further downstream was derived by Wolf, and a schematic drawing of the complete geometry is illustrated in Fig. 1. To express this, we introduce the parameters

$$u = \left(\frac{2\pi R_a^2}{\lambda} \right) \left| \frac{1}{d_s} + \frac{1}{d_d} - \frac{1}{f} \right|, \quad (1)$$

$$v = \frac{2\pi R_d R_a}{\lambda d_d} \quad (2)$$

and

$$w = \frac{\min(u, v)}{\max(u, v)}. \quad (3)$$

Here λ is wavelength. In the case of $u < v$, the fraction is given by

$$L(u, v) = 1 - L_B(v, w), \quad (4)$$

with

$$L_B(v, w) = \sum_{s=0}^{\infty} (-1)^s w^{2s} Q_{2s}(v) / (2s+1) \quad (5)$$

and

$$Q_{2s}(v) = \sum_{p=0}^{2s} (-1)^p [J_p(v) J_{2s-p}(v) + J_{p+1}(v) J_{2s+1-p}(v)]. \quad (6)$$

Thus $L(u, v)$ is a combination of products of Bessel functions. In the case of, $u > v$, one has

$$L(u, v) = w^2 [1 + L_B(v, w)] - L_x(v, w), \quad (7)$$

with

$$L_x(v, w) = \left(\frac{4w}{v} \right) \left[Y_1\left(\frac{v}{w}, v\right) \cos(gv) + Y_2\left(\frac{v}{w}, v\right) \sin(gv) \right], \quad (8)$$

$g = (w + w^{-1}) / 2$ and

$$Y_n(u, v) = \sum_{s=0}^{\infty} (-1)^s (n+2s) w^{n+2s} J_{n+2s}(v). \quad (9)$$

The above results were derived by Wolf [3] and are also discussed by Born and Wolf [12].

Because each $Q_{2s}(v)$ term in the sum in Eq. (5) is itself a sum, evaluation of $L_B(v, w)$ is formally a double sum. However, we have found the following approach to reduce the computational cost of finding $L_B(v, w)$ to that of a single sum times a factor that is logarithmic in the number of terms included. We first write

$$Q_{2s}(v) = S_s^{(1)}(v) - S_s^{(2)}(v) + S_s^{(3)}(v) - S_s^{(4)}(v), \quad (10)$$

with

$$S_s^{(1)}(v) = \sum_{p=0}^s J_{2p}(v) J_{2s}(v), \quad (11)$$

$$S_s^{(2)}(v) = \sum_{p=0}^{s-1} J_{2p+1}(v) J_{2s-2p-1}(v), \quad (12)$$

$$S_s^{(3)}(v) = \sum_{p=0}^s J_{2p+1}(v) J_{2s+1-2p}(v) \quad (13)$$

and

$$S_s^{(4)}(v) = \sum_{p=0}^{s-1} J_{2p+2}(v) J_{2s-2p}(v). \quad (14)$$

We also have $S_0^{(2)} = S_0^{(4)} = 0$. We next observe

$$\left. \begin{aligned} S_0^{(1)}(v) &= J_0(v) J_0(v), \\ S_1^{(1)}(v) &= J_0(v) J_2(v) + J_2(v) J_0(v), \\ S_2^{(1)}(v) &= J_0(v) J_4(v) + J_2(v) J_2(v) + J_4(v) J_0(v), \\ &\vdots \end{aligned} \right\} \quad (15)$$

and so forth. If we introduce the function

$$F_k^{(1)}(v) = J_{2k}(v), \quad (16)$$

we have

$$S_k^{(1)}(v) = \sum_{l=0}^k F_l^{(1)}(v) F_{k-l}^{(1)}(v), \quad (17)$$

i.e., the convolution of $F_l^{(1)}$ with itself. By similar analysis, for $k > 0$ we can introduce

$$F_k^{(2)}(v) = J_{2k-1}(v), \quad (18)$$

so that we have another convolution:

$$S_k^{(2)}(v) = \sum_{l=1}^k F_l^{(2)}(v) F_{k-l+1}^{(2)}(v). \quad (19)$$

Because the series $\{F_k^{(1)}(v)\}$ and $\{F_k^{(2)}(v)\}$ are real, the above two convolutions can be carried out simultaneously for all k at the computational cost of two complex FFTs [13]. One may also show

$$S_k^{(3)}(v) = S_{k+1}^{(2)}(v) \quad (20)$$

and

$$S_k^{(4)}(v) = S_{k+1}^{(1)}(v) - 2J_0(v)J_{2k+2}(v). \quad (21)$$

Using FFTs has considerably accelerated diffraction calculations relevant to radiometric calibrations that are described elsewhere [10]. Additional acceleration was achieved by using Debye's formula in cases of large order and argument of Bessel functions [14].

3. GAUSSIAN OPTICS CALCULATIONS IN MULTI-STAGE CYLINDRICALLY SYMMETRICAL SYSTEMS ACCELERATED USING FFTS

In an earlier work, one of the authors presented a method by which the propagation of light within the Fresnel-Kirchhoff (Gaussian or paraxial optics approximation) method could be done for multi-stage optics trains [15]. Gaussian optics are discussed in more detail, for instance, by Goodman [16]. The main idea is to iterate Kirchhoff's method at each element in series. For a cylindrically symmetrical system, it is helpful to express the radiation field incident on an element (say, element l) as a sum over partial waves:

$$u(r, \theta, z_l) = \sum_{m=-\infty}^{+\infty} e^{im\theta} u_{m,l}(r). \quad (22)$$

The field on the subsequent element, which is distance d downstream, is given by

$$u(s, \theta, z_{l+1}) = \frac{1}{i\lambda d} \sum_{m=-\infty}^{+\infty} \int_0^{R_l} dr r u_{m,l}(r) \int_0^{2\pi} d\theta' e^{im\theta'} \times \exp\left[\frac{ik}{2d}(r^2 + s^2 - 2rs\cos(\theta - \theta'))\right], \quad (23)$$

with $k = 2\pi/\lambda$. The angular integration can be done using

$$\exp(-iacos\phi) = \sum_{m=-\infty}^{+\infty} (-i)^m e^{-im\phi} J_m(a), \quad (24)$$

and rearrangement gives

$$u(s, \theta, z_{l+1}) = \frac{2\pi e^{iks^2/(2d)}}{i\lambda d} \sum_{m=-\infty}^{+\infty} (-i)^m e^{im\theta} \times \int_0^{R_l} dr r J_m(krs/d) \left[u_{m,l}(r) e^{ikr^2/(2d)} \right] \quad (25)$$

and

$$u_{m,l+1}(s) = \frac{2\pi e^{iks^2/(2d)}}{i^{m+1}\lambda d} \int_0^{R_l} dr r J_m(krs/d) \left[u_{m,l}(r) e^{ikr^2/(2d)} \right]. \quad (26)$$

We note that the partial waves propagate independently.

To evaluate Eq. (26), we tabulate partial waves on discrete radial grids optimized for extended Gauss-Legendre quadrature, i.e., low-order (we use 16 points) quadrature within each of many contiguous radial intervals. This is done with sufficiently dense sampling to ensure that $k(r+s)^2/(2d)$ does not change by more than about $\pi/2$, which proves to be accurate to better than one part in 10^{10} . Indexing values of $r(s)$ with $v(\mu)$ yields

$$u_{m,l+1}(s_\mu) \approx \frac{2\pi \exp[iks_\mu^2/(2d)]}{i^{m+1}\lambda d} \times \sum_{v=1}^{N_r} w_v r_v J_m(kr_v s_\mu/d) \{ u_{m,l}(r_v) \exp[iks_v^2/(2d)] \}. \quad (27)$$

There are $N_r(N_s)$ values of $r_v(s_\mu)$ and w_v is a quadrature weight.

The number of operations required to compute all values of $u_{m,l+1}(s_\mu)$ as shown above is on the order of $N_r N_s$. However, the scaling can be improved with very modest approximation as follows. We shall first introduce a compressed notation, introducing g_μ , from which the desired partial wave is obtained using

$$u_{m,l+1}(s_\mu) = \left(\frac{2\pi \exp[iks_\mu^2/(2d)]}{i^{m+1}\lambda d} \right) g_\mu \quad (28)$$

and

$$f_v = w_v r_v u_{m,l}(r_v) \exp[iks_v^2/(2d)]. \quad (29)$$

Relating f_v or g_μ to the partial waves has operation counts scaling as N_r or N_s , respectively, and from Eq. (27) we have

$$g_\mu = \sum_{v=1}^{N_r} J_m(kr_v s_\mu/d) f_v. \quad (30)$$

Suppose that the first n_r values of r_v and the first n_s values of s_μ are “small,” in the sense that $kr_v s_\mu/d$ is never much larger than unity. We can use Eq. (30) to evaluate the first n_s values of g_μ . For the remaining values, we may write

$$g_\mu = \sum_{v=1}^{n_r} J_m(kr_v s_\mu/d) f_v + \Gamma_\mu, \quad (31)$$

with

$$\Gamma_\mu = \sum_{v=n_r+1}^{N_r} J_m(kr_v s_\mu/d) f_v. \quad (32)$$

The operations count for all but evaluation of Eq. (32) for all $\mu > n_s$ is small, because we have $n_s n_r \sim 1$.

For Eq. (32), one can introduce two logarithmic grids with radius variables $\rho(\sigma)$ on the $r(s)$ grid, such that a grid begins with a value smaller than $r_{n_r+1}(s_{n_s+1})$ and ends with a value larger than $r_{N_r}(s_{N_s})$. The grids have the same ratio for adjacent values of ρ and σ and are sufficiently dense, so that the argument of the Bessel function changes by no more than about 0.75 for neighboring values of $\rho\sigma$ as per Gottlieb and Orszag [17]. We only need to find $J_m(k\rho\sigma/d)$ for $N_\rho + N_\sigma$ values of $\rho\sigma$ (i.e., not $N_r N_s$ values of $r_v s_\mu$) dramatically reducing storage requirements. Lagrange interpolation using N_L (we use $N_L=20$) values of $\rho(\sigma)$ closest to $r_v(s_\mu)$ gives

$$J_m(kr_v s_\mu/d) \cong \sum_{\sigma,\rho} w_r(r_v, \rho) w_s(s_\mu, \sigma) J_m(k\rho\sigma/d). \quad (33)$$

Interpolating at a point near the middle of the N_L points is also stable for larger N_L , but the value chosen indicates convergence with respect to N_L . This is accurate, because successive

derivatives of Bessel functions are comparable in size. Hence, their Taylor series' in a small neighborhood converge rapidly and are well approximated by a low-order polynomial, for which Lagrange interpolation performs well. Summation in Eq. (33) is done only over terms with non-zero products of interpolation weights. Substituting Eq. (33) in Eq. (32) gives

$$\Gamma_{\mu} = \sum_{v=n_r+1}^{N_r} \sum_{\sigma,\rho} w_r(r_v\rho)w_s(s_{\mu},\sigma)J_m(k\rho\sigma/d)f_v. \quad (34)$$

This can be evaluated simultaneously for all $\mu > n_s$ very efficiently as follows. We first evaluate

$$F(\rho) = \sum_{v=n_r+1}^{N_r} w_r(r_v,\rho)f_v, \quad (35)$$

which requires an operation count $\sim N_L N_r$. This gives

$$\Gamma_{\mu} = \sum_{\sigma,\rho} w_s(s_{\mu},\sigma)J_m(k\rho\sigma/d)F(\rho). \quad (36)$$

We next evaluate

$$G(\sigma) = \sum_{\rho} J_m(k\rho\sigma/d)F(\rho) \quad (37)$$

simultaneously for all σ . This exploits the fact that all arguments of functions in Eq. (37) are on equally tempered logarithmic grids with the Bessel function depending on the *product*, $\rho\sigma$. If we introduce $\alpha = \rho^{-1}$, we have

$$G(\sigma) = \sum_{\alpha} J_m((k/d)\sigma\alpha^{-1})F'(\alpha^{-1}), \quad (38)$$

which is a convolution amenable to discrete FFT methods with operation count $\sim [(N_{\rho} + N_{\sigma})\log_2(N_{\rho} + N_{\sigma})]$. Finally, we evaluate

$$\Gamma_{\mu} = \sum_{\sigma} w_s(s_{\mu},\sigma)G(\sigma), \quad (39)$$

which requires $\sim N_L N_s$ operations. In Section 5, we present sample values of N_r , N_s , N_{ρ} , N_{σ} and FFT grid lengths.

4. OPERATIONS-COUNT REDUCTION FOR THROUGHPUT-ONLY CALCULATIONS

Oftentimes, one wants to relate spectral power $\Phi_\lambda(\lambda)$ incident on a detector and radiance $L_\lambda(\lambda)$ of a uniform, Lambertian source, whereas the spatial distribution of the radiation at the detector is of less interest. We again restrict ourselves to cylindrically symmetrical systems and consider spectrally resolved power and radiance, i.e., the power and radiance for one wavelength. Cylindrical symmetry implies that power can be expressed as a sum over partial wave channels:

$$\Phi_\lambda(\lambda) = L_\lambda(\lambda) \left(\Phi_0 + 2 \sum_{m=1}^{\infty} \Phi_m \right). \quad (40)$$

This exploits $m \leftrightarrow -m$ symmetry. With the prefactor

$$P = (2\pi)^{2+2N} / [\lambda^{2N} (d_0 \dots d_{N+1})^2], \quad (41)$$

we have

$$\begin{aligned} \Phi_m = P & \int_0^{R_0} dr_0 r_0 \int_0^{R_{N+1}} dr_{N+1} r_{N+1} \\ & \times \left| \int_0^{R_1} dr_1 r_1 \dots \int_0^{R_N} dr_N r_N e^{i\phi(r_1, \dots, r_N)} J_m \left(\frac{kr_0 r_1}{d_0} \right) \dots J_m \left(\frac{kr_N r_{N+1}}{d_N} \right) \right|^2. \end{aligned} \quad (42)$$

Here R_0 and R_{N+1} are the source and detector radii, $R_1, \dots, R_N$ are radii of intervening apertures or lenses, and $d_0, \dots, d_N$ are distances between successive elements. The phase $\phi(r_1, \dots, r_N)$ accounts for focusing and other effects involving squares of radii.

Squaring as in Eq. (42) and rearrangement give

$$\Phi_m = P \int_0^{R_0} dr_0 \int_0^{R_1} dr_1 \dots \int_0^{R_N} dr_N \int_0^{R_{N+1}} dr_{N+1} \int_0^{R_N} dr_N \dots \int_0^{R_1} dr_1 \times t_{0,1}(r_0, r_1) t_{1,2}(r_1, r_2) \quad (43)$$

$$\dots t_{N,N+1}(r_N, r_{N+1}) \times [t_{N+1,N}(r_{N+1}, r_N) \dots t_{2,1}(r_2, r_1) t_{1,0}(r_1, r_0)]^*,$$

The t -functions shown follow from examination of Eq. (42). If we discretize radial integrations using quadrature, Φ_m / P is the trace of a product of matrices. The first matrix would have rows and columns associated with the radial grid indices for r_0 and r_1 , respectively, and so forth. The product of the first $N+1$ matrices is the adjoint of the product of the last $N+1$ matrices.

We now indicate the adjoint of a matrix with an overbar and write the matrix product and power conveyed within a partial-wave channel as

$$\Phi_m = P \operatorname{Tr} \left\{ \mathbf{T}_{0,1}^{(m)} \cdots \mathbf{T}_{N,N+1}^{(m)} \bar{\mathbf{T}}_{N+1,N}^{(m)} \cdots \mathbf{T}_{1,0}^{(m)} \right\}. \quad (44)$$

This is a scalar quantity, and the trace contains no information about the spatial distribution of radiation on the detector or anywhere along the optics train. For that price, however, a tremendous computational speed-up can be achieved in optical systems where there is one element, herein the A -th, that has the lowest number of radial grid points. The trace in Eq. (44) is unchanged if the leading matrix is moved from the front of the product to the back. One can repeat this step to obtain

$$\Phi_m = P \operatorname{Tr} \left\{ \mathbf{T}_{A,A+1}^{(m)} \cdots \mathbf{T}_{N,N+1}^{(m)} \bar{\mathbf{T}}_{N+1,N}^{(m)} \cdots \mathbf{T}_{1,0}^{(m)} \mathbf{T}_{0,1}^{(m)} \cdots \mathbf{T}_{A-1,A}^{(m)} \right\}. \quad (45)$$

One can calculate diagonal elements of the matrix product by propagating partial waves as described in Section 3. The product involves passing each point along the optics train twice, once in each direction. This “doubling” of effort can be more than offset by reducing the number of partial waves to propagate.

5. SAMPLE APPLICATION

Several factors determine the scaling of computation time with λ . The number of partial wave channels that one should sum over is set by the maximum order m for which a Bessel function is appreciable, which varies as λ^{-1} . The numbers of radial grid points required for accuracy on the source, aperture, and detector areas also vary as λ^{-1} , because extended Gaussian quadrature must resolve all oscillations in the radiation field or its square. Finally, the number of starting conditions for partial waves of a given m that must be propagated through the optics train varies as λ^{-1} , because it is proportional to the number of radial grid points on at least one element. Thus, for an extended, incoherent source, the worst-scaling parts of the computational vary as $\lambda^{-3} |\log \lambda|^2$, because of using logarithmic grids and FFTs. Without the innovation presented in Section 3, we would have scaling of λ^{-4} .

To demonstrate this numerically, we consider the Laboratory for Atmospheric and Solar Physics (LASP) total-irradiance monitor (TIM) instruments [18]. These measure the total irradiance (in W/m²) at the top of the atmosphere (TOA) one astronomical unit (AU) from the center of the sun. The optics include one defining aperture, three non-limiting apertures that barely avoid vignetting of light, and one aperture immediately in front of a black, NiP-coated electrical-substitution radiometer (ESR). Such an ESR determines incident optical

power by comparing it to electrical power required when the instrument shutter is closed to maintain the same heat load. (The radiometer absorbs nearly all incident light.) The five aperture radii are 3.9894 mm, 5.0800 mm, 6.0325 mm, 6.9850 mm, and 7.6200 mm, so they are successively larger going downstream along the optics train. Successive apertures are separated by 25.4 mm. For the distance to the sun and solar radius, we used as 1.5×10^{14} mm and 6.75×10^{11} mm, respectively. Figure 2 shows a schematic drawing of the layout of the LASP TIM instrument.

Theoretical total power is found by integrating spectral power versus λ over the Planck distribution. If one assumes a 5900 K blackbody temperature for the surface of the sun, the average diffraction effect on total power is close to the diffraction effect on spectral power for 902 nm light. This has been analyzed previously [10], but the computational innovations presented here have enabled us to determine the effects of the middle three apertures in more detail.

Figure 3 shows diffraction effects on spectral power, which is mostly due to the first aperture and which does exhibit roughly linear behavior with λ . The additional diffraction effects of the middle three apertures are presented as a function of λ for several wavelengths between 0 μm and 40 μm in Fig. 4. Although relative diffraction effects usually scale as the first or second power of λ , the nearly-vignetting properties of the apertures precludes applicability of asymptotic analysis to deduce such behavior, which indeed is not observed. Meanwhile, the variety of ways in which light can diffract causes interference effects leading to complicated oscillatory patterns in the diffraction effects versus λ .

The computation time is shown vs wavelength in a log-log plot in Fig. 5, along with a line that demonstrates a hypothetical λ^{-3} scaling. The points are not on one line because of the limitations on sizes of optimal FFT grids. (We allowed the grid length to include prime factors of two and three, and allowed for at most one power of three. This struck a balance between having shorter FFT grids and non-optimal factors of the grid lengths. The optimal grid lengths might depend on the FFT software being used.) At longer λ , other parts of the calculation do not fall off as quickly as λ^{-3} . Table 1 shows the throughput for 902 nm light found using geometrical optics and physical optics without and with the FFT acceleration, as well as computation time and approximate memory use (1 GB=1 gigabyte). The results shown in Table 1 indicate at least 10 decimal digits of accuracy are achieved with the FFT used as we implement it. Table 2 shows the grid lengths. We have found that this accuracy is routinely achievable for the radial grid and Lagrange interpolation performed as discussed in Section 3. The relative speed-up achieved, however, depends on the optical layout.

6. CONCLUSIONS

We have demonstrated improvements in the computational cost of diffraction calculations that are relevant in practical radiometry. Improvements in efficiency were achieved without loss of accuracy and are sufficient to make diffraction calculations for multistage optics trains a desktop project. We have used all these innovations in other applications as well, and astronomical studies such as the work by Witteborn *et al.* [19] and Butler *et al.* [20] can also benefit.

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Fig. 1. Schematic layout of Wolf's idealized system, indicating aperture radius R_a , detector radius R_d , source-to-aperture distance d_s , and detector-to-aperture distance d_d .

Fig. 2.
Schematic layout of the LASP TIM instrument.

Fig. 3.
Diffraction effect of A_1 ; e.g., a loss of about 1 % occurs at $\lambda=21 \mu\text{m}$.

Fig. 4.
Diffraction effect of combination of A_2 , A_3 and A_4 ; e.g., a gain of about 0.021 % occurs at $\lambda=10 \mu\text{m}$.

Fig. 5. Computation time versus wavelength (points), shown as a log-log plot; a purely λ^{-3} trend is indicated by a solid line.

Table 1

Demonstration of acceleration

Method	Throughput	Time (s)	Memory (GB)
Geom. optics	1.000000000000	—	—
Without FFT	0.9995796774708	47470	10.0
With FFT	0.9995796774688	629	1.3

Table 2

Radial grid lengths along optics train

Spacing	N_r	N_s	N_ρ	N_σ	N_{FFT}
Sun-A ₁	80	2512	268	278	768
A ₁ -A ₂	2512	6704	38414	38529	98304
A ₂ -A ₃	6704	9536	63183	62941	131072
A ₃ -A ₄	9536	12592	91271	91708	196608
A ₄ -ESR	12592	9296	119554	119246	262144