MATHEMATICAL ALGORITHMS OF SOFTWARE FOR NUMERICAL SIMULATION OF ABERRATED LASER BEAM PROPAGATION

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1. Introduction.

The method of computational experiment requires finding numerical approximation of the solution of given problem. Similar to physical experiments it not sufficient to find only particular value of this solution. We must give boundaries of the error of obtained discrete solution. The key ingredient of such methodology is a reliable method of assessing the accuracy of computed approximation. Such aposteriori error estimation must be computed using the data for the given problem and discrete approximation itself.

Computational efficiency is the second requirement for numerical methods used in computational experiments. Realisation of the basic numerical method must be economical and the costs of obtaining the error estimation must be small compared with the computation of numerical solution.

The development of such methods for numerical simulation of aberrated laser beam propagation is considered in this article. Algorithms and their computational performance are given.

2. Problem formulation.

Modelling of diffraction and propagation of laser beams is one of the most difficult computational problem of non–linear optics [1–3]. Such phenomena is very important for many laser applications (see [4–6]) and laser technology [7,8]. High quality laser beams must be generated for industrial applications and computational experiments are widely used to investigate this process.

The propagation properties of a light beam after it has passed through a focussing lens are assumed to be governed by the equation

$$2ik\frac{\partial u}{\partial z}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)=0 \tag{1}$$

together with the initial and boundary conditions

$$u(0,r)=u_0(r), \tag{2}$$

$$r\frac{\partial u}{\partial r}(z,0)=0, \qquad u(z,R)=0. \tag{3}$$

We want to evaluate the field at a typical plane $z=Z\neq 0$, when a prescribed field at $z=0$ is given.

The direct application of numerical methods for evaluation of diffraction integrals is not efficient approach [9,10]. Here we must use special numerical algorithms for accurate integration of the rapidly oscillating diffraction integrands. Many modifications of such methodology are proposed. They are based on methods in which the integrand of the diffraction formula is replaced locally by expressions that can by integrated analytically or calculated by finite–element methods. The other approach is based on the Hermite–Gaussian and Laguarre–Gaussian wave expansion [11–13]. We have used this method for simulation of non–linear laser beam propagation and interaction [14,15]. Only sufficiently smooth field and phase radial distributions were considered in these cases. Hence we had no problems with the selection of basis functions. The situation becomes much more difficult in the case of numerical simulation of aberrated laser beam propagation.

The primary objective of this paper is to optimise the selection of basis functions in wave expansions and to give aposteriori error estimations of the obtained numerical solution. These results were used in software package for the numerical analysis of laser beam quality [16].

3. Laguerre-Gauss expansion.

We find the solution of problem (1)–(3) as a series expansion

$$U(z,r)=\sum_{p=0}^{P} c_p W_p(z,r), \tag{4}$$

where $W_p(z,r)$ is given by

$$W_p(z,r)=\frac{2}{w(\tilde{z})}L_p\left(\frac{2r^2}{w^2(\tilde{z})}\right)\exp\left(-\frac{r^2}{w^2(\tilde{z})}\left(1+i\frac{\tilde{z}}{z_0}\right)\right)\exp(i(2p+1)\operatorname{atan}\frac{\tilde{z}}{z_0}),$$

$$w^2(\tilde{z})=2z_0\left(1+\left(\frac{\tilde{z}}{z_0}\right)^2\right)/k,\quad z_0=\frac{z_R f^2}{f^2+z_R^2},\quad z_R=kw_0^2/2,\quad \tilde{z}=z-\frac{fz_R^2}{f^2+z_R^2},$$

and L_p denotes the p th Laguerre polynomial. We have two free parameters, i.e., w_0 and f, in the definition of basis functions. The selection of these parameters enables us to minimize the costs of calculation of needed approximation. Functions W_p obey the orthonormality condition

$$(W_p,W_k)=\delta_{pk}, \tag{5}$$

where δ_{nm} is the Kronecker symbol and (U,V) denotes the scalar product

$$(U,V)=\int_0^\infty rU(r)V^*(r)dr.$$

Once the coefficients c_p are known the solution (4) can by calculated at any typical plane $z=Z$. Functions L_p are generated by the well-known recurrence relation.

Now we will estimate the costs of calculation at the solution evaluation stage. Usually we need to find an approximation of $u(z,r)$ at some space mesh of N distinct points r_i, $i=1,...,N$. There is no fast algorithm for the calculation of Laguerre's series expansion like the Fast Fourier Transform. Hence realization costs of the algorithm are estimated by $O(NP)$ floating point operations. This makes the Laguerre expansion method not efficient in the case of non-linear laser beam propagation when we need to calculate sums (4) at N_2 distinct planes $z=Z_k$, $k=1,...,N_2$.

By using basis orthonormality condition (5) we find that c_p is defined by

$$c_p=(u_0(r),W_p(0,r)). \tag{6}$$

Numerical approximation of c_p is obtained by using some method of numerical integration, e.g.,the Simpson method

$$C_p=\sum_{j=1}^{N}\left(g(r_j)+4g(r_{j-0.5})+g(r_{j-1})\right)(r_j-r_{j-1})/6,$$

where $g(r)=ru_0(r)W_p^*(r)$, and r_j are integration knots

$$\Delta=\left\{r_j: r_j<r_{j+1},\ r_{j-0.5}=0.5(r_j+r_{j-1}),\ r_0,\ r_N=R\right\}.$$

The *apriori* error estimate is well-known for the Simpson method

$$|c_p-C_p|\le M_4\max_{1\le j\le N}(r_j-r_{j-1})^4.$$

The value of constant M_4 is not known in most cases, hence we can't estimate the numerical integration error by this inequality. We are interested in obtaining an *aposteriori* error estimate. Two well-known methods were used in our experiments.

The first aposteriori error estimate is given by the *Runge rule*

$$|c_p-C_p|=\frac{|\tilde{C}_p-C_p|}{15}+O\left(\max_{1\le j\le N}(r_j-r_{j-1})^5\right),$$

where $\tilde{C}_p$ is the numerical value of c_p obtained by the same Simpson's integration method with the number of knots $N/2$:

$$\tilde{C}_p = \sum_{j=1}^{N/2} \left(g(r_{2j}) + 4g(r_{2j-1}) + g(r_{2j-2}) \right) (r_{2j} - r_{2j-2}) / 6.$$

The calculation of $\tilde{C}_p$ is economical, because we do not need to calculate additional values of the integrand function $g(r)$.

The second aposteriori error estimate is evaluated as follows

$$|c_p - C_p| = |C_p^H - C_p| + O\left(\max_{1 \le j \le N} (r_j - r_{j-1})^l \right),$$

where C_p^H is the approximation of c_p, which is calculated by high order numerical integration method of l th order, $l \ge 5$.

Now lets consider the errors introduced in series expansion (4) when the series is truncated after the P th term. This gives rise to the P th order approximation of $u(r)$

$$\left\| u - U^{(P)} \right\|_A \le M_A P^{-\alpha},$$

where $\|.\|_A$ is some norm, e. g., the L_2 or L_∞ norm, and $\alpha > 0$ is the convergence order which depends on the smoothness of $u(z,r)$. The estimate given above is again apriori and constants α, M_A are usually not known for a given problem. We note that some simple rules of apriori estimation of P are given in [17] for the evaluation of the diffracted field emerging from a circular function.

In order to obtain aposteriori error estimate of the truncated solution $U^{(P)}(z,r)$ we propose to use the fact that the free–space propagation operator (1) is *unitary*, i.e.

$$\left\| u(z) - U^{(P)}(z) \right\| = \left\| u(0) - U^{(P)}(0) \right\|,$$

where $\|.\|$ is the L_2 norm, $\|v\|^2 = (v,v)$.

The intensity distribution of the initial field $u(0,r)$ is given explicitly. Once the requested error level has been fixed, the number of terms P in the truncated series can be obtained by direct numerical procedure, in order to fulfill the estimate

$$\left\| u(0) - U^{(P)}(0) \right\|_A \le \varepsilon.$$

It remains to determine parameters ω_0 and f in the definition of basis functions $V_p(z,t)$. The relation for z_0 is exact only for a pure Gaussian beam but it remains a good approximation for other distributions with small aberrations (see [18], where analysis for low–order super–Gaussian beams is given).

The parameter ω_0 provides an essential degree of flexibility and we can optimize the costs of calculation by selecting appropriate value of ω_0. This problem was studied in detail in [11, 12, 17]. For smooth distributions such as low–order super–Gaussian fields

$$I(r) = I_0 \exp\left(-\left(\frac{r}{a_0} \right)^{2n} \right)$$

the relation $\omega_0 = a_0$ is used. For other beams of width a_0 the scale factor $\omega_0 \sim a_0 / P^{0.5}$ is optimal.

Numerical Laguerre–Gaussian calculations are carried out using numerical values calculated at discrete points of quasiuniform space mesh. An aposteriori error estimation of this discretization error is obtained by testing numerical integration formula for overlapping integrals

$$(V_p,V_j)=\delta_{p,j}, \qquad 0\le p,j\le P.$$

It is sufficient to test a few largest values of p,j as the error is very much less for smaller values of mode numbers.

4. Integral representation.

The solution of laser beam free propagation problem (1)–(3) can be represented by diffractional integral as follows

$$u(z,r)=-\frac{ike^{-ikz}}{z}\int_0^R pu_0(p)e^{0.5ik\left(p^2+r^2\right)/z}J_0\left(\frac{krp}{z}\right)dp, \qquad (7)$$

where J_0 is the Bessel function. The adaptive integration method is used to find numerical approximation of $u(z,r)$. Two adaptivity techniques are tested.

We denote by $U(a,b,\varepsilon_1)$ the approximation of the integral (7) at (z,r) over interval $[a,b]$, which is correct to some error tolerance ε_1. Our goal is find $U(0,R,\varepsilon)$.

Algorithm 1 (*a divide and conquer approach*).

1. Calculate S_1 numerical approximation of $U(a,b,\varepsilon)$ by same quadrature rule, e.g., the Simpson method

$$S_1=\frac{b-a}{6}\left(f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right),$$

where f is the integrand function.

2. Estimate the error of S_1. For example, a composite Simpson method approximation S_2 is used

$$S_2=\frac{b-a}{12}\left(f(a)+4f\left(\frac{3a+b}{4}\right)+2f\left(\frac{a+b}{2}\right)+4f\left(\frac{a+3b}{4}\right)+f(b)\right),$$

$$error=|S_2-S_1|/15.$$

3. If $error\le\varepsilon$ then S_2 (or S_1) is a needed approximation of $U(a,b,\varepsilon)$, which is correct to the specified accuracy tolerance. Otherwise we define two new problems

$$U\left(a,\frac{b+a}{2},\frac{\varepsilon}{2}\right), \qquad U\left(\frac{b+a}{2},b,\frac{\varepsilon}{2}\right).$$

The algorithm is *recursive* and we start with $U(0,R,\varepsilon)$.

The second algorithm requires more memory for storage of a list of subdivisions, but it can give more efficient results in many cases. We note that similar strategy is also used in NAG standard integration routine.

Algorithm 2. Let assume that we have a subdivision of the interval $[0,R]$

$$[0,R]=\bigcup_{j=1}^{N}[a_j,b_j]$$

and numerical approximations of the integrals $U(a_j,b_j,\varepsilon_j)$ are defined.

1. Calculate the total error

$$error=\sum_{j=1}^{N}\varepsilon_j.$$

If *error* $\le\varepsilon$ then the approximation $U(0,R,\varepsilon)$ is given by

$$U(0,R,\varepsilon)=\sum_{j=1}^{N}U(a_j,b_j,\varepsilon_j).$$

2. Otherwise find an interval $[a_j,b_j]$ with the largest error estimate, bisect it, and apply quadrature and aposteriori error estimation rules to both of them.

Numerical calculation of integrals at many discrete points η_k, $k=1,...,M$ demands for large amounts of computing time. Hence parallel adaptive algorithms were also implemented. These algorithms will be reported in separate paper, as well as detailed results of numerical experiments.

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