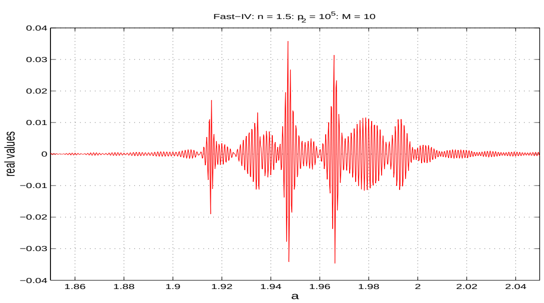
An exploration of exponentially transformed splitting methods for highly oscillatory wave equations

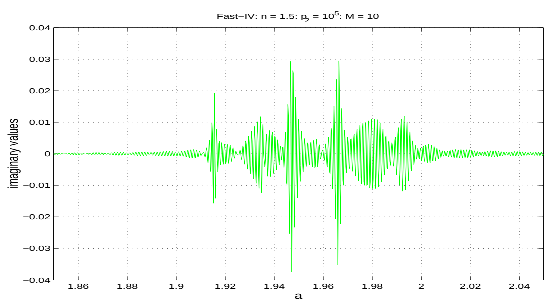
Qin Sheng[1], **Shekhar Guha**[2] **and Leonel Gonzalez**[2]

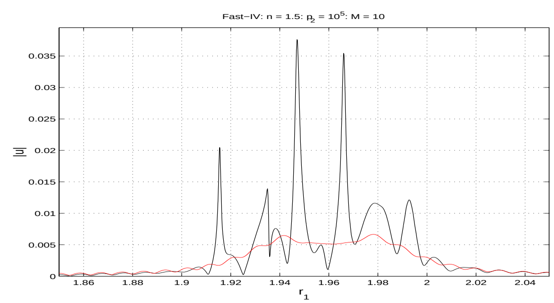
[1]**Baylor University**

[2]**Air Force Research Laboratory**

http://bearspace.baylor.edu/Qin_Sheng/www/







1. Highly oscillatory wave problem

Highly oscillatory optical wave equations, such as the multidimensional paraxial Helmholtz equation, have been used extensively in modeling propagation of the light from lens to the focal region in applications. Numerical approximations of solutions of such equations contain crucial light information in focal regions even when the f-number is small. However, it has been difficult to compute highly oscillatory numerical solutions efficiently. This paper proposes two correlated splitting strategies for fast computations of oscillatory wave solutions. Reinforced by an exponential transformation, the splitting schemes offer straightforward and novel oscillation-free ways for solving underlying differential equations with accuracy and stability.

For a slowly varying envelope approximation of the light beam propagation, consider the paraxial Helmholtz equation,

$$2i\kappa\frac{\partial E}{\partial z} = \frac{\partial^2 E}{\partial x^2} + \frac{\partial^2 E}{\partial y^2},\ 0 \le x,y \le \ell,\ z \ge z_0, \tag{1}$$

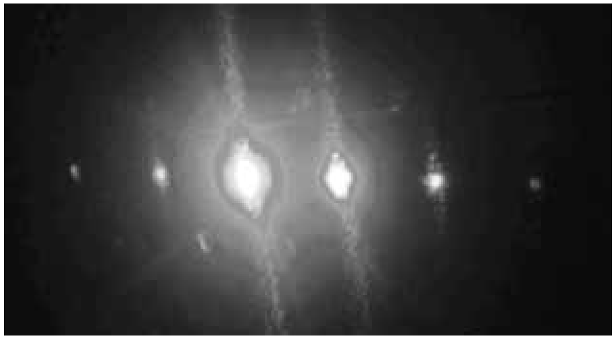
where $i = \sqrt{-1}$, $\kappa = 2\pi/\lambda$ is the wave number, λ is the wavelength, z is the beam propagation direction, z_0 is the initial beam location, x,y are dimensional directions perpendicular to the light, ℓ is a realistic boundary location indicator and E is the complex envelope of the wave function investigated. Values of $\kappa \approx 10^6$.

Since values of κ can be extremely large in optical applications, the complex function u is highly oscillatory. Consequently, the effectively of the numerical solution via conventional finite difference schemes has been extremely difficult to achieve since mesh step sizes cannot be unrealistically small.

Certain spectrum or boundary element methods may possess certain merits, the main challenge pertains in balancing the algorithmic simplicity and accuracy.

Our new approach is based on

– Eikonal Equation - Fermat Principle - Hamilton-Jacobi Equations –



Consider the wave disturbance function in geometrical optics,

$$E(x,y,z) = u(x,y,z)e^{i\omega(x,y,z)}.$$

Set $\omega(x,y,z) = \kappa v(x,y,z)$ and this leads to

$$E(x,y,z) = u(x,y,z)e^{i\kappa v(x,y,z)}. \tag{2}$$

Assume that $u \neq 0$ and substitute (2) into (1) to yield ray equations

$$\frac{\partial u}{\partial z} = a\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) + f_1, \tag{3}$$

$$\frac{\partial v}{\partial z} = b\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + f_2, \tag{4}$$

where

$$a = \frac{u}{2},\ b = -\frac{1}{2\kappa^2 u},\ f_1 = \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial y},\ f_2 = \frac{1}{2}\left(\frac{\partial v}{\partial x}\right)^2 + \frac{1}{2}\left(\frac{\partial v}{\partial y}\right)^2.$$

Note that solutions of (3), (4) are oscillation-free for large κ.

Denote

$$w = \begin{pmatrix} u \\ v \end{pmatrix}, \ f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \ M = \begin{pmatrix} 0 & a \\ b & 0 \end{pmatrix},$$

then (3), (4) can be written as

$$w_z = M w_{xx} + M w_{yy} + f. \tag{5}$$

Lemma 1 *For fixed (x, y, z), M is similar to a skew symmetric matrix and thus its eigenvalues are pure imaginary. Further, the spectral radius $\rho(M) = 1/(2\kappa)$ and the condition number $\mathrm{cond}_2(M) = 1$.*

Initial condition:

$$w(x, y, z_0) = g_0(x, y). \tag{6}$$

$$w(0, y, z) = w(\ell, y, z) = 0, \ w(x, 0, z) = w(x, \ell, z) = 0. \tag{7}$$

or

$$w_x(0, y, z) = w_x(\ell, y, z) = 0, \ w_y(x, 0, z) = w_y(x, \ell, z) = 0, \tag{8}$$

2. Exponential transformation based splitting methods (ETBSM)

Exponential transformation (2) based ADI semi-discretization

$$\begin{aligned} w^{r+1/2} - w^r &= \frac{h_z}{2}\left(Mw_{xx}^{r+1/2} + Mw_{yy}^r\right) + \frac{h_z}{2} f^r, &(9)\\ w^{r+1} - w^{r+1/2} &= \frac{h_z}{2}\left(Mw_{xx}^{r+1/2} + Mw_{yy}^{r+1}\right) + \frac{h_z}{2} f^{r+1/2}. &(10)\end{aligned}$$

Similarly, we may consider the exponential transformation (2) based LOD semi-discretization

$$\begin{aligned} w^{r+1/2} - w^r &= \frac{h_z}{2}\left(Mw_{xx}^{r+1/2} + Mw_{xx}^r\right) + \frac{h_z}{2} f^r, &(11)\\ w^{r+1} - w^{r+1/2} &= \frac{h_z}{2}\left(Mw_{yy}^{r+1/2} + Mw_{yy}^{r+1}\right) + \frac{h_z}{2} f^{r+1/2}. &(12)\end{aligned}$$

Let

$$h_x^2\delta_x^2\omega_{s,t}^{\sigma}=\omega_{s+1,t}^{\sigma}-2\omega_{s,t}^{\sigma}+\omega_{s-1,t}^{\sigma},\ h_y^2\delta_y^2\omega_{s,t}^{\sigma}=\omega_{s,t+1}^{\sigma}-2\omega_{s,t}^{\sigma}+\omega_{s,t-1}^{\sigma}.$$

We acquire

I. Exponential Transformation Based ADI (ETBADI) Scheme:

$$\begin{aligned}
w_{s,t}^{r+1/2}-w_{s,t}^{r} &= \frac{h_z}{2}M_{s,t}^{r}\left(\delta_x^2 w_{s,t}^{r+1/2}+\delta_y^2 w_{s,t}^{r}\right)+\frac{h_z}{2}f_{s,t}^{r},\\
w_{s,t}^{r+1}-w_{s,t}^{r+1/2} &= \frac{h_z}{2}M_{s,t}^{r+1/2}\left(\delta_x^2 w_{s,t}^{r+1/2}+\delta_y^2 w_{s,t}^{r+1}\right)+\frac{h_z}{2}f_{s,t}^{r+1/2},\\
& s=1,2,\ldots,m;\ t=1,2,\ldots,n;\ r=0,1,\ldots
\end{aligned}$$

II. Exponential Transformation Based LOD (ETBLOD) Scheme:

$$\begin{aligned}
w_{s,t}^{r+1/2}-w_{s,t}^{r} &= \frac{h_z}{2}M_{s,t}^{r}\left(\delta_x^2 w_{s,t}^{r+1/2}+\delta_x^2 w_{s,t}^{r}\right)+\frac{h_z}{2}f_{s,t}^{r},\\
w_{s,t}^{r+1}-w_{s,t}^{r+1/2} &= \frac{h_z}{2}M_{s,t}^{r+1/2}\left(\delta_y^2 w_{s,t}^{r+1/2}+\delta_y^2 w_{s,t}^{r+1}\right)+\frac{h_z}{2}f_{s,t}^{r+1/2},\\
& s=1,2,\ldots,m;\ t=1,2,\ldots,n;\ r=0,1,\ldots
\end{aligned}$$

As an illustration, let us consider the homogeneous Dirichlet boundary condition (7). Hence, we can reformulate our schemes into matrix form:

III. ETBADI SCHEME:

$$\begin{aligned} (I-\mu M^r)\, w^{r+1/2} &= (I+\eta N^r)\, w^r + \frac{h_z}{2} f^r, && (13) \\ \left(I-\eta N^{r+1/2}\right) w^{r+1} &= \left(I+\mu M^{r+1/2}\right) w^{r+1/2} + \frac{h_z}{2} f^{r+1/2}, && (14) \\ & r = 0,1,\ldots \end{aligned}$$

IV. ETBLOD SCHEME:

$$\begin{aligned} (I-\mu M^r)\, w^{r+1/2} &= (I+\mu M^r)\, w^r + \frac{h_z}{2} f^r, && (15) \\ \left(I-\eta N^{r+1/2}\right) w^{r+1} &= \left(I+\eta N^{r+1/2}\right) w^{r+1/2} + \frac{h_z}{2} f^{r+1/2}, && (16) \\ & r = 0,1,\ldots, \end{aligned}$$

and μ, η are dimensional Courant numbers.

Here $I \in 2n^2 \times 2n^2$ is an identity matrix and

$$
\begin{aligned}
M^\sigma &= \text{diag}\left(M_1^\sigma, M_2^\sigma, \ldots, M_n^\sigma\right), \\
M_j^\sigma &= \begin{pmatrix}
-2M_{1,j}^\sigma & M_{1,j}^\sigma & & & & & \\
M_{2,j}^\sigma & -2M_{2,j}^\sigma & M_{2,j}^\sigma & & & & \\
& M_{3,j}^\sigma & -2M_{3,j}^\sigma & M_{3,j}^\sigma & & & \\
& & \cdots & \cdots & \cdots & & \\
& & & & M_{n-1,j}^\sigma & -2M_{n-1,j}^\sigma & M_{n-1,j}^\sigma \\
& & & & & M_{n,j}^\sigma & -2M_{n,j}^\sigma
\end{pmatrix}, \\
& \quad j = 1, 2, \ldots, n,
\end{aligned}
$$

and

$$
\begin{aligned}
N^{\sigma} &= \begin{pmatrix}
-2N_1^{\sigma} & N_1^{\sigma} & & & & & \\
N_2^{\sigma} & -2N_2^{\sigma} & N_2^{\sigma} & & & & \\
& N_3^{\sigma} & -2N_3^{\sigma} & N_3^{\sigma} & & & \\
& & \cdots & \cdots & \cdots & & \\
& & & & N_{n-1}^{\sigma} & -2N_{n-1}^{\sigma} & N_{n-1}^{\sigma} \\
& & & & & N_n^{\sigma} & -2N_n^{\sigma}
\end{pmatrix}, \\
N_j^{\sigma} &= \text{diag}\left(M_{1,j}^{\sigma}, M_{2,j}^{\sigma}, \ldots, M_{n,j}^{\sigma}\right) \\
& \quad j = 1, 2, \ldots, n.
\end{aligned}
$$

For the simplicity in discussions, we only consider the ETBADI scheme in following discussions. The discussion of ETBLOD scheme is similar.

Lemma 2 *Matrices M^σ and N^σ are similar.*

Lemma 3 *Eigenvalues of matrices M^σ and N^σ are pure imaginary.*

Further, Let e_j denote the jth column of the identity matrix. Then

$$P = [e_1, e_3, \ldots, e_{2n^2-1}, e_2, e_4, \ldots, e_{2n^2}]$$

is a $2n^2 \times 2n^2$ permutation matrix. Furthermore, we have

$$P^T S^\sigma P = \begin{bmatrix} 0 & \Lambda_\alpha \\ \Lambda_\beta & 0 \end{bmatrix},$$

where

$$\Lambda_\alpha = \mathrm{diag}(\alpha^\sigma_{1,1}, \alpha^\sigma_{2,1}, \ldots, \alpha^\sigma_{n,1}, \alpha^\sigma_{1,2}, \ldots, \alpha^\sigma_{n,n}),\ \Lambda_\beta = \mathrm{diag}(\beta^\sigma_{1,1}, \beta^\sigma_{2,1}, \ldots, \beta^\sigma_{n,1}, \beta^\sigma_{1,2}, \ldots, \beta^\sigma_{n,n}).$$

Moreover, we observe that

$$P^T T_2 P = \begin{bmatrix} L \otimes I_n & 0 \\ 0 & L \otimes I_n \end{bmatrix}, \; P^T T_1 P = \begin{bmatrix} I_n \otimes L & 0 \\ 0 & I_n \otimes L \end{bmatrix},$$

where $L = \mathrm{tridiag}(1, -2, 1) \in \mathbb{R}^{n \times n}$.

Remark:

$$A \otimes B_{n \times m} = \begin{bmatrix} Ab_{11} & Ab_{12} & \cdots & Ab_{1m} \\ Ab_{21} & Ab_{22} & \cdots & Ab_{2m} \\ \cdots & \cdots & \cdots & \cdots \\ Ab_{n1} & Ab_{n2} & \cdots & Ab_{nm} \end{bmatrix}.$$

Therefore, we have

$$P^T M^\sigma P = P^T S^\sigma T_1 P = \begin{bmatrix} 0 & \Lambda_\alpha (I_n \otimes L) \\ \Lambda_\beta (I_n \otimes L) & 0 \end{bmatrix} \equiv \widehat{M},$$

$$P^T N^\sigma P = P^T S^\sigma T_2 P = \begin{bmatrix} 0 & \Lambda_\alpha (L \otimes I_n) \\ \Lambda_\beta (L \otimes I_n) & 0 \end{bmatrix} \equiv \widehat{N}.$$

Part of the following discussions is contributed by W. Sun, University of Macau:

Lemma 4 *We have*

$$\|\Lambda_\alpha\|_2 = \frac{\max\phi}{2} = O(1),\ \|L\|_2 < 4 = O(1),\ \|\Lambda_\beta\|_2 = \frac{1}{2\kappa^2\min\phi} = O\left(\frac{1}{\kappa^2}\right).$$

Lemma 5 *The spectral radius of matrices M^σ and N^σ satisfy the following relations*

$$\rho\left(M^\sigma\right),\ \rho\left(N^\sigma\right) = O\left(\frac{1}{\kappa}\right).$$

Lemma 6 *We have*

$$\|\widehat{M}^2\|_2,\ \|\widehat{N}^2\|_2 = O\left(\frac{1}{\kappa^2}\right).$$

The result is obviously much stronger than that in Lemma 5.

Let

$$A^{\sigma} = \left(I_{2n^2} - \mu M^{\sigma}\right)^{-1}\left(I_{2n^2} + \eta N^{\sigma}\right) \equiv I_{2n^2} + B, \tag{17}$$

where $\mu,\ \eta$ are reasonably small, and

$$B^{\sigma} = \left(I_{2n^2} - \mu M^{\sigma}\right)^{-1}\left(\eta N^{\sigma} + \mu M^{\sigma}\right). \tag{18}$$

Then we can prove

Theorem 7 *Further, the ETBADI scheme is oscillation-free and unconditionally asymptotically stable, that is,*

$$\|A^2\|_2,\ \|B^2\|_2 = O\left(\frac{\mu^2 + \eta^2}{\kappa^2}\right),$$

unconditionally.

3. Optimized computational procedures

For ETBADI Scheme:

$$\begin{aligned} A_r v^{r+1/2} &= \mu D_{b^r} S \phi_1^r + \phi_2^r, & (19)\\ u^{r+1/2} &= \mu D_{a^r} S v^{r+1/2} + \phi_1^r, & (20)\\ B_{r+1/2} v^{r+1} &= \eta D_{b^{r+1/2}} T \phi_3^{r+1/2} + \phi_4^{r+1/2}, & (21)\\ u^{r+1} &= \eta D_{a^{r+1/2}} T v^{r+1} + \phi_3^{r+1/2}, & (22)\\ & r = 0, 1, 2, \ldots, \end{aligned}$$

where

$$\begin{aligned} A_r &= I - \mu^2 D_{b^r} S D_{a^r} S,\\ B_{r+1/2} &= I - \eta^2 D_{b^{r+1/2}} T D_{a^{r+1/2}} T \end{aligned}$$

and $u_0,\ v_0$ are initial values given by (6).

For ETBLOD Scheme:

$$
\begin{aligned}
A_r v^{r+1/2} &= \mu D_{b^r} S \psi_1^r + \psi_2^r, & (23)\\
u^{r+1/2} &= \mu D_{a^r} S v^{r+1/2} + \psi_1^r, & (24)\\
B_{r+1/2} v^{r+1} &= \eta D_{b^{r+1/2}} T \psi_3^{r+1/2} + \psi_4^{r+1/2}, & (25)\\
u^{r+1} &= \eta D_{a^{r+1/2}} T v^{r+1} + \psi_3^{r+1/2}, & (26)\\
& r = 0, 1, 2, \ldots,
\end{aligned}
$$

where

$$
\psi_1^\sigma = u^\sigma + \eta D_{a^\sigma} S v^\sigma + \frac{h_z}{2} f_1^\sigma, \qquad \psi_2^\sigma = v^\sigma + \eta D_{b^\sigma} S u^\sigma + \frac{h_z}{2} f_2^\sigma,
$$

$$
\psi_3^\sigma = u^\sigma + \mu D_{a^\sigma} T v^\sigma + \frac{h_z}{2} f_1^\sigma, \qquad \psi_4^\sigma = v^\sigma + \mu D_{b^\sigma} T u^\sigma + \frac{h_z}{2} f_2^\sigma.
$$

4. Simulation experiments

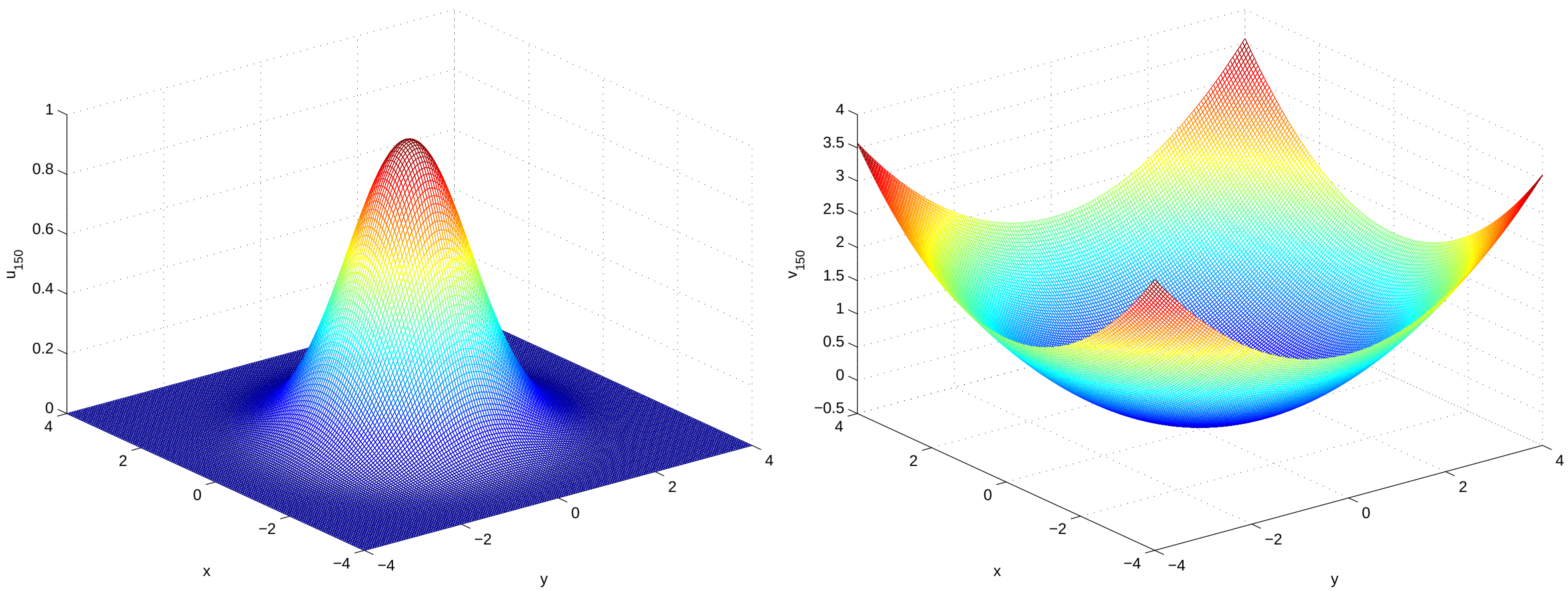


Figure 1: Simulated numerical solutions $u(x, y, z_{150})$ and $v(x, y, z_{150})$.

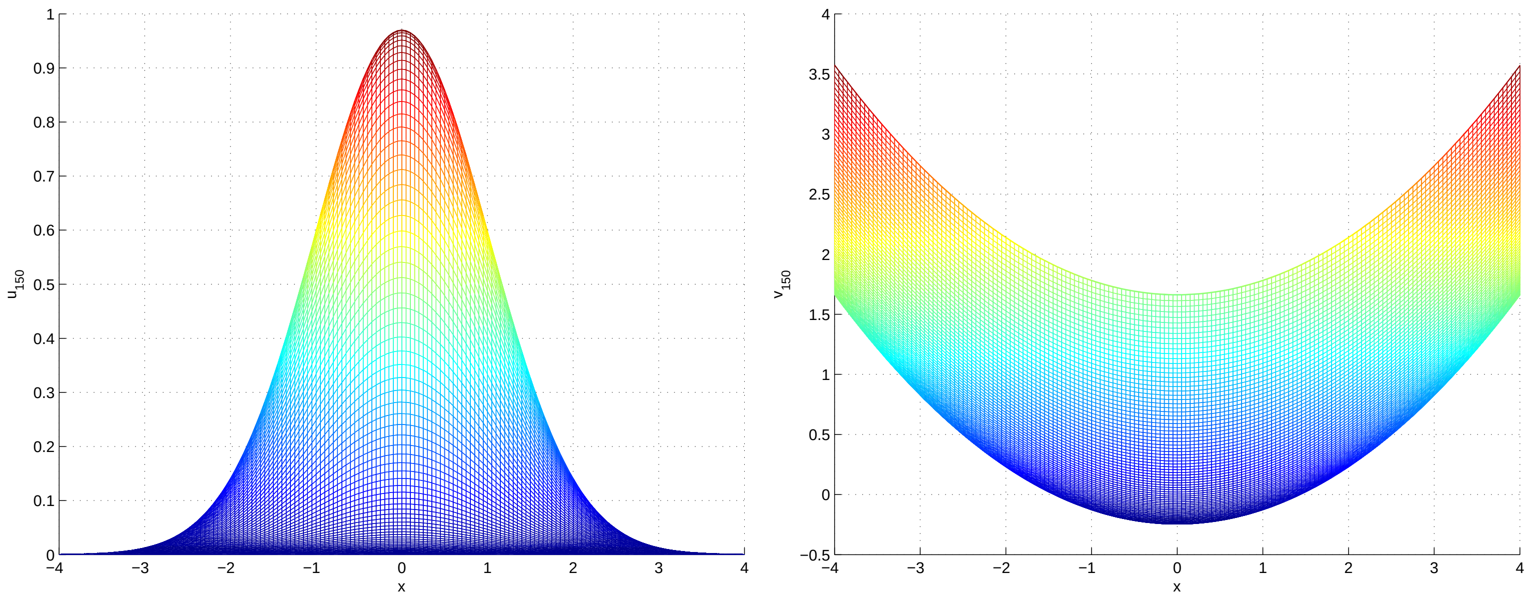


Figure 2: Side projections of simulated numerical solutions $u(x, y, z_{150})$ and $v(x, y, z_{150})$.

We may convert u and v to E which is complex.

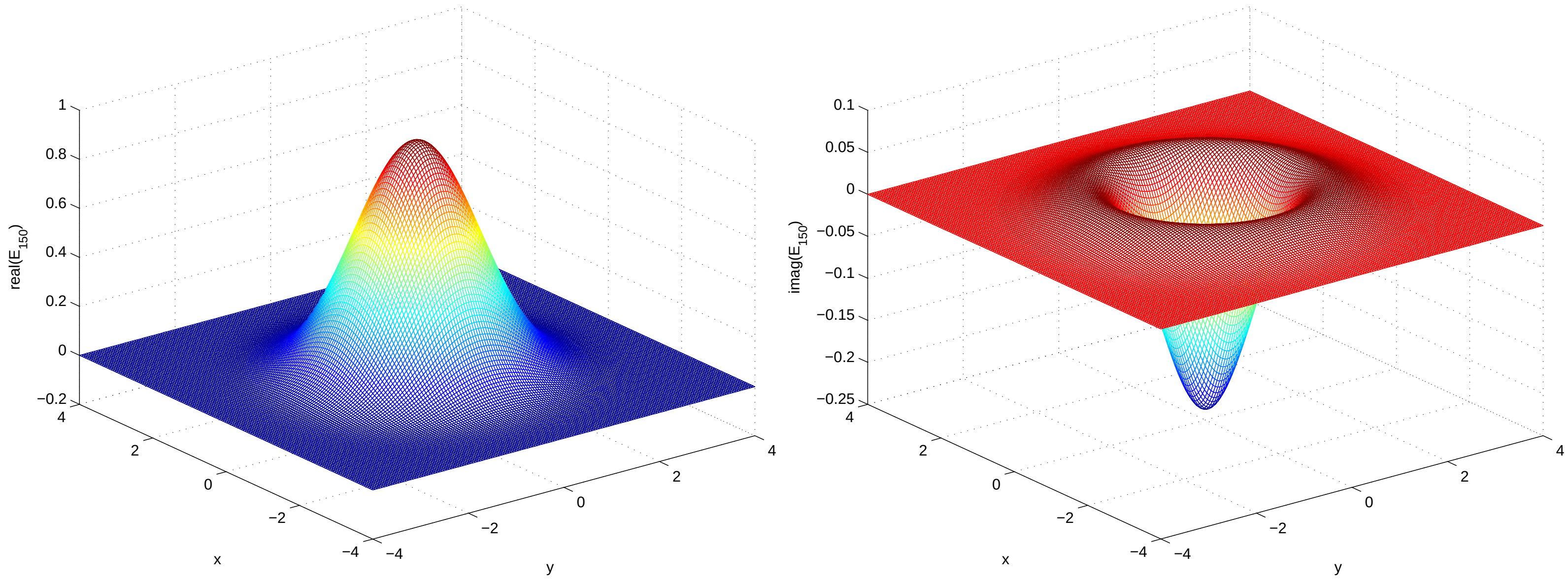


Figure 3: Simulated real and imaginary parts of the solution $E(x, y, z_{150})$.

Further,

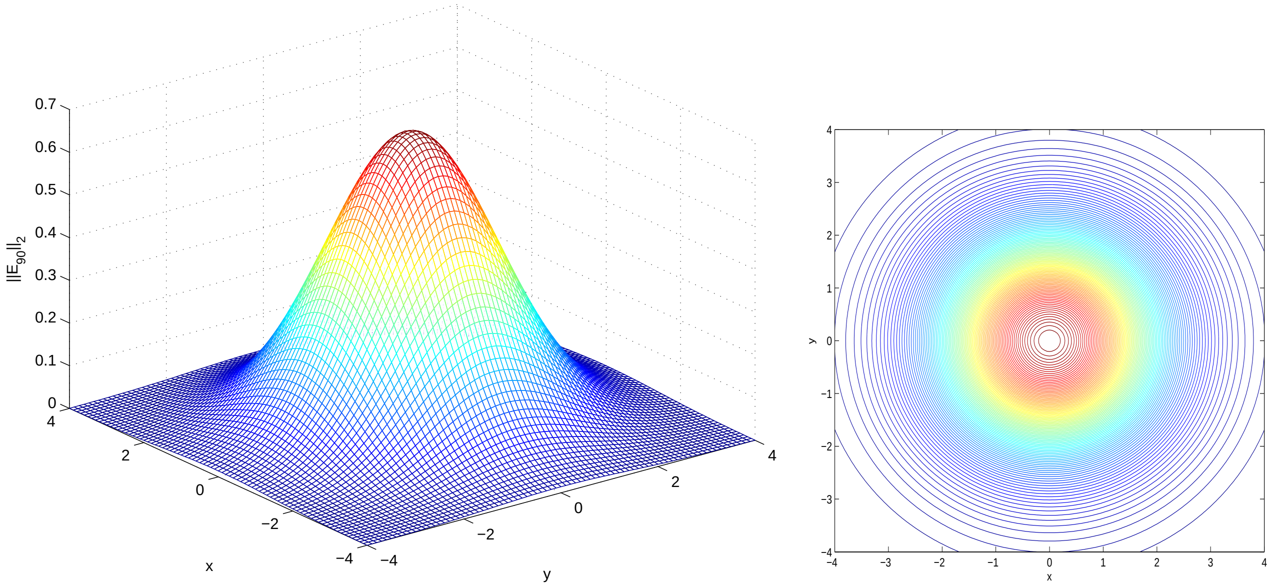


Figure 4: Modules and its contour map of the solution $E(x, y, z_{90})$.

References:

[1] Q. Sheng, S. Guha and L. Gonzalez, An exponential transformation based splitting method for fast computations of highly oscillatory solutions, submitted, 2010.

[2] Q. Sheng, S. Guha and L. Gonzalez, On exponentially transformed decomposition methods for highly oscillatory wave simulations, submitted, 2010.

[3] Q. Sheng and W. Sun, On the stability of an oscillation-free ADI method for highly oscillatory wave equations, submitted, 2010.

Thank you and have a wonderful Symposium on Splitting Methods!