

UCLA
COMPUTATIONAL AND APPLIED MATHEMATICS

**Finite Difference Methods for Geometrical Optics and
Related Nonlinear PDEs Approximating the High Frequency
Helmholtz Equation**

**E. Fatemi
B. Engquist
S. Osher**

**March 1995
(Revised November 1995)**

CAM Report 95-11

Finite difference methods for geometrical optics and related nonlinear PDEs approximating the high frequency Helmholtz equation

E. Fatemi, B. Engquist, and S. Osher ¹
University of California, Department of Mathematics, 405 Hilgard Avenue
Los Angeles, CA 90024-1555

Subject Classification: 65M06, 78A05, 78-08

Key Words: wave equation, geometrical optics, eikonal equation, difference methods

¹This research was supported by ONR # N00014-91-J-1034, NSF # DMS 94-04942, and ARPA URL-ONR-N00014-92-J-1890

Running Head: Finite difference methods for geometrical optics and related nonlinear PDEs approximating the high frequency Helmholtz equation

Proofs to be sent to:
Stanley Osher
University of California
Department of Mathematics
405 Hilgard Avenue
Los Angeles, CA 90024-1555

Abstract

Finite difference methods are developed to solve the nonlinear PDEs approximating some solutions of the Helmholtz equation in high frequency regime. Numerical methods are developed for solving the geometrical optics approximation, classical asymptotic expansion, and a new perturbed geometrical optics system. We propose a perturbed geometrical optics system to recover diffraction phenomena that are lost in geometrical optics approximations. We discuss some of the techniques that we have developed for recovering multivalued solutions and we present some numerical examples computed using the finite difference approximations of the above systems.

1 Introduction

We have developed finite difference methods for solving the nonlinear partial differential equations that approximate high frequency solutions of the scalar wave equation, starting from the geometrical optics approximation, continuing to the classical asymptotic expansion and then to a new perturbed geometrical optics system. The motivation is to solve numerically very high frequency solutions of the Maxwell's equations on a coarse grid, coarse compared to the wavelength of the solution. Our methods could be interpreted as ray tracing on a fixed grid and potentially will replace ray tracing methods for high frequency calculations in many cases.

Here we concentrate on the scalar linear wave equation in two spatial variables,

$$v_{tt} = c^2 \Delta v = c^2(x, y)(v_{xx} + v_{yy}), \quad (1)$$

to develop the methods. x and y are the spatial variables, t is time, v is the amplitude of the wave and $c(x, y)$ is the speed of the wave in the medium. Time harmonic solutions of the wave equation of the form

$$v(x, y, t) = e^{i\omega t} u(x, y), \quad (2)$$

are of special interest. Here ω is the time frequency of the wave as imposed by the boundary conditions. For time harmonic solutions the wave equation is reduced to the Helmholtz equation

$$\Delta u + \frac{\omega^2}{c^2} u = \Delta u + k^2 n^2 u = 0. \quad (3)$$

$n(x, y)$ is the index of refraction and the non-dimensional quantity, k , represents the relative size of the wavelength of the wave with respect to the physical size of the problem. Direct numerical solution of the Helmholtz equation for large values of parameter k is difficult. The fundamental difficulty is the fact that the necessary mesh size in each coordinate direction is proportional to k^{-1} . To resolve each wavelength one approximately needs ten points. For a three dimensional calculation one needs approximately $O((10k)^3)$ number of points to resolve the solution. Values of $k = 1000$ are common for many applications.

Since direct solutions are not practical, approximate methods are of special interest. The geometrical optics approximation is a qualitatively correct approximation in the limit of infinite frequency [3]. The geometrical optics could be derived formally by considering a solution of the form

$$u(x, y) = A(x, y)e^{ik\phi(x, y)}, \quad (4)$$

for the Helmholtz equation. The amplitude, A , and the phase, ϕ , satisfy the geometrical optics system:

$$\begin{cases} 0 = |\nabla\phi|^2 - n^2 \\ 0 = 2\nabla A \cdot \nabla\phi + A\Delta\phi. \end{cases} \quad (5)$$

This approximation is valid for infinite frequency and it does not include solutions that manifest the wave nature of the solutions of the Helmholtz equation.

A substantial correction to the above approximation could be achieved by expanding solutions of the Helmholtz equation around zero wavelength, in inverse powers of k in the following form

$$u(x, y) = e^{ik\phi(x, y)} \sum_{n=0}^{\infty} A_n(x, y)(ik)^{-n}. \quad (6)$$

By substituting the above expansion in the Helmholtz equation and equating the coefficients of different powers of k , partial differential equations for the coefficients ϕ, A_0, A_1 , etc are derived,

$$\begin{cases} 0 = |\nabla\phi|^2 - n^2 \\ 0 = 2\nabla\phi \cdot \nabla A_0 + A_0\Delta\phi \\ 0 = 2\nabla\phi \cdot \nabla A_{n+1} + A_{n+1}\Delta\phi + \Delta A_n. \end{cases} \quad (7)$$

The asymptotic expansion is based on the phase defined for the geometrical optics limit and it fails where geometrical optics fails, notably on shadow lines. We have developed methods for the above classical asymptotic expansion previously in Fatemi, Engquist, and Osher [2], and this paper is a continuation of the previous work.

We have investigated a new approximation which we shall name perturbed geometrical optics system. This system is the geometrical optics equations including the usually omitted terms of order k^{-2} ,

$$\begin{cases} 0 = |\nabla\phi|^2 - n^2 + k^{-2}(\Delta A/A) \\ 0 = 2\nabla A \cdot \nabla\phi + A\Delta\phi. \end{cases} \quad (8)$$

We can easily show that these equations are equivalent to the Helmholtz equation in a compact simply connected domain as long as the amplitude is bounded away from zero everywhere. Numerical results show us that this system has qualitatively correct solutions near shadow lines.

2 Perturbed Geometrical Optics

We propose a new approach for including the effects of finiteness of frequency. In this approach we augment the geometrical optics equations by including terms of order k^{-2} in the equations. A nonlinear elliptic system for phase and amplitude is obtained. This system is a singular perturbation of the geometrical optics equations. We claim that our system is equivalent to the Helmholtz equation in a simply connected domain if the amplitude of the solution to the Helmholtz equation is bounded away from zero everywhere in the domain.

We assume that $u(x)$ is a complex solution to the Helmholtz equation in a compact simply connected domain Ω contained in R^3 ,

$$\Delta u(x) + k^2 n^2(x)u(x) = 0. \quad (9)$$

On the boundary we specify either Dirichlet boundary conditions or Sommerfeld radiation condition of the form

$$\frac{\partial u}{\partial \mathbf{n}} = ik u, \quad (10)$$

where \mathbf{n} is the unit vector normal to the boundary.

Since we are interested in calculating high frequency solutions of the wave equation we use a transformation of the form

$$u(x) = A(x)e^{ik\phi(x)} = e^{v(x)+ik\phi(x)}, \quad (11)$$

to derive a new set of equations for amplitude and phase, (A, ϕ) or for (v, ϕ) . This transformation is nothing but the inverse of the Cole-Hopf transformation used to transfer the Burgers equation into the linear heat equation.

The important question is whether this transformation is always possible. We make the observation that given any twice differentiable complex function defined on a simply connected compact domain $\Omega \subset R^3$, we can write it as

$$u(x) = A(x)e^{ik\phi(x)} + c,$$

for $A(x) > 0$, $\phi(x)$ a real function, and c a complex constant. Since $|u(x)|$ is a continuous function in a compact domain it is bounded from above and there is a constant c such that $|u - c| \geq \epsilon > 0$. Therefore we let $u(x) = u(x) - c + c = \hat{u}(x) + c$, where we have $|\hat{u}| > 0$. We define the amplitude function simply as

$$A(x) = |\hat{u}(x)|. \quad (12)$$

Then we define a new function $g(x) = \hat{u}(x)/A(x)$. Since $\nabla \times (-i \frac{\nabla g}{g}) = 0$, the phase is defined uniquely by the above equation, as long as the domain Ω is simply connected.

Now given a twice differentiable solution of the Helmholtz equation we write it as $u(x) = A(x)e^{ik\phi} + c = e^{v+ik\phi} + c$. If we substitute the above ansatz in the Helmholtz equation we obtain the following system for the v and ϕ functions

$$\begin{aligned} |\nabla\phi|^2 - n^2 - k^{-2}(\Delta v + |\nabla v|^2) + \text{Real}(ce^{-v-ik\phi}) &= 0 \\ 2\nabla v \cdot \nabla\phi + \Delta\phi - k\text{Imag}(ce^{-v-ik\phi}) &= 0. \end{aligned} \quad (13)$$

If $c \neq 0$ the equations are correct but have little use. The new nonlinear system has terms that are highly oscillatory and solving the resulting system requires a fine mesh equivalent to the mesh necessary for the original Helmholtz equation. If we assume that $c = 0$ and drop terms of order k^{-2} we obtain the equations of geometrical optics

$$\begin{cases} |\nabla\phi|^2 - n^2 = 0 \\ 2\nabla v \cdot \nabla\phi + \Delta\phi = 0. \end{cases} \quad (14)$$

We consider the case where $c = 0$ but we keep the terms of order k^{-2} . We hope that this new system has solutions that are close to the geometrical optics limit, yet it recovers some of the wave phenomena that are lost in the geometrical optics equations.

The perturbed geometrical optics equations are of the form

$$\begin{cases} |\nabla\phi|^2 - n^2 - k^{-2}(\Delta v + |\nabla v|^2) = 0 \\ 2\nabla v \cdot \nabla\phi + \Delta\phi = 0. \end{cases} \quad (15)$$

The above system is equivalent to the following system for (A, ϕ) variables

$$\begin{cases} |\nabla\phi|^2 - n^2 - k^{-2}(\Delta A/A) = 0 \\ 2\nabla A \cdot \nabla\phi + A\Delta\phi = 0. \end{cases} \quad (16)$$

We can choose either set of variables. We have performed computations using both sets and the numerical results are similar. The (v, ϕ) variables seem a little more natural since the equations have constant coefficients for the highest order derivatives.

The above systems are nonlinear elliptic systems and either one could be solved for steady state solutions of the Helmholtz equation by fixed point methods or by Newton's method. We use an artificial time marching method to obtain the steady state solution.

$$\begin{cases} \phi_\tau = |\nabla\phi|^2 - n^2 - k^{-2}(\Delta v + |\nabla v|^2) \\ v_\tau = 2\nabla v \cdot \nabla\phi + \Delta\phi \end{cases} \quad (17)$$

We have observed that this specific time marching is equivalent to solving the Helmholtz equation by writing it as a time dependent Schroedinger equation,

$$iku_\tau = \Delta u + k^2 n^2 u. \quad (18)$$

If we substitute $u = e^{v+ik\omega\phi}$ in the above equation and separate real and imaginary parts we obtain our time marching scheme.

2.1 Linear Analysis of the Perturbed System

To determine the type of the system and design the numerical methods, a linear analysis of the system is useful. We linearize the following system

$$\begin{cases} \phi_\tau = |\nabla\phi|^2 - n^2 - k^{-2}(\Delta v + |\nabla v|^2) \\ v_\tau = 2\nabla v \cdot \nabla\phi + \Delta\phi, \end{cases} \quad (19)$$

around the solution $(\dot{v}, \dot{\phi})$. We let

$$\phi = \dot{\phi} + \tilde{\phi} \quad v = \dot{v} + \tilde{v}. \quad (20)$$

We obtain the following equations for $\tilde{\phi}$ and \tilde{v}

$$\begin{cases} \tilde{\phi}_\tau = 2\nabla\dot{\phi} \cdot \nabla\tilde{\phi} - 2k^{-2}\nabla\dot{v} \cdot \nabla\tilde{v} - k^{-2}\Delta\tilde{v} \\ \tilde{v}_\tau = 2\nabla\dot{v} \cdot \nabla\tilde{\phi} + 2\nabla\dot{\phi} \cdot \nabla\tilde{v} + \Delta\tilde{\phi}. \end{cases} \quad (21)$$

We take the Fourier transform in spatial variables and we obtain

$$\begin{pmatrix} \hat{\phi} \\ \hat{v} \end{pmatrix}_\tau = \begin{pmatrix} 2\nabla\dot{\phi} \cdot i\zeta & -2k^{-2}\nabla\dot{v} \cdot i\zeta \\ 2\nabla\dot{v} \cdot i\zeta & 2\nabla\dot{\phi} \cdot i\zeta \end{pmatrix} \begin{pmatrix} \hat{\phi} \\ \hat{v} \end{pmatrix} + \begin{pmatrix} 0 & k^{-2}|\zeta|^2 \\ -|\zeta|^2 & 0 \end{pmatrix} \begin{pmatrix} \hat{\phi} \\ \hat{v} \end{pmatrix}. \quad (22)$$

The eigenvalues of the matrix are calculated to be

$$\lambda_{1,2} = 2i\zeta \cdot \nabla\dot{\phi} \pm k^{-1}i|\zeta|^2 \pm 2k^{-1}\nabla\dot{v} \cdot \zeta. \quad (23)$$

If k^{-1} is zero the linearized system has two hyperbolic modes and the solution to the system is

$$\begin{pmatrix} \hat{\phi} \\ \hat{v} \end{pmatrix} = \begin{pmatrix} e^{2i\zeta \cdot \nabla\dot{\phi}t} & 0 \\ (2i\zeta \cdot \nabla\dot{v} - |\zeta|^2)te^{i\zeta \cdot \nabla\dot{\phi}t} & e^{2i\zeta \cdot \nabla\dot{\phi}t} \end{pmatrix} \begin{pmatrix} \hat{\phi}(0) \\ \hat{v}(0) \end{pmatrix}. \quad (24)$$

The above solution is only weakly stable although the nonlinear system is stable.

For k^{-1} non-zero we have a system with Schroedinger modes and the eigenvalues become distinct. The system has an exponentially growing mode that in our numerical calculations was not observed. That is due to the stability of the nonlinear problem and our upwind numerical methods. This phenomena is similar to the following Schroedinger equation with a variable coefficient, $p(x) > p_0 > 0$,

$$u_t = i(p(x)u_x)_x = ip(x)u_x + ip_x(x)u_x, \quad (25)$$

which is well-posed, but the frozen coefficient problem is ill-posed [4]. The system written for A and ϕ can be analyzed in a similar fashion. From the system

$$\begin{cases} \phi_\tau = |\nabla\phi|^2 - n^2 - k^{-2}(\Delta A/A) \\ A_\tau = 2\nabla A \cdot \nabla\phi + A\Delta\phi, \end{cases} \quad (26)$$

we obtain the linearized system,

$$\begin{cases} \tilde{\phi}_\tau = 2\nabla\dot{\phi} \cdot \nabla\tilde{\phi} + k^{-2}\frac{\tilde{A}\Delta\dot{A}}{A^2} - k^{-2}\frac{\Delta\dot{A}}{A} \\ \tilde{A}_\tau = 2\nabla\dot{A} \cdot \nabla\tilde{\phi} + 2\nabla\dot{\phi} \cdot \nabla\tilde{A} + \dot{A}\Delta\tilde{\phi} + \tilde{A}\Delta\dot{\phi}. \end{cases} \quad (27)$$

The Fourier transform of the system is calculated to be

$$\begin{pmatrix} \hat{\phi} \\ \hat{A} \end{pmatrix}_\tau = \begin{pmatrix} 2\nabla\dot{\phi} \cdot i\zeta & 0 \\ 2\nabla\dot{A} \cdot i\zeta & 2\nabla\dot{\phi} \cdot i\zeta \end{pmatrix} \begin{pmatrix} \hat{\phi} \\ \hat{A} \end{pmatrix} + \begin{pmatrix} 0 & k^{-2}|\zeta|^2/\dot{A} \\ -|\zeta|^2\dot{A} & 0 \end{pmatrix} \begin{pmatrix} \hat{\phi} \\ \hat{A} \end{pmatrix} + \begin{pmatrix} 0 & -k^{-2}\Delta\dot{A}/\dot{A}^2 \\ \Delta\dot{\phi} & 0 \end{pmatrix} \begin{pmatrix} \hat{\phi} \\ \hat{A} \end{pmatrix}. \quad (28)$$

The eigenvalues of the matrix are calculated to be

$$2i\zeta \cdot \nabla\dot{\phi} \pm$$

$$ik^{-1}\sqrt{|\zeta|^4 - 2i|\zeta|^2\zeta \cdot \nabla\dot{A}/\dot{A} - |\zeta|^2\Delta\dot{\phi}/\dot{A} - |\zeta|^2\Delta\dot{A}/\dot{A} + 2i\nabla\dot{A} \cdot \zeta\Delta\dot{A}/\dot{A}^2 + \Delta\dot{A}\Delta\dot{\phi}/\dot{A}^2}. \quad (29)$$

For large ζ we have

$$\lambda_{1,2} \approx 2i\zeta \cdot \nabla\dot{\phi} \pm ik^{-1}|\zeta|^2 \pm k^{-1}\zeta \cdot \nabla\dot{A}/\dot{A}. \quad (30)$$

Although the linear problems have growing modes, the nonlinear problem is stable.

Our numerical method is stable due to a combination of our upwind methods and the nonlinear stability of the underlying problem. The time marching scheme is compactly written as

$$iku_\tau = \Delta u + k^2 n^2 u. \quad (31)$$

From the above equation one can easily see that our marching scheme satisfies the following conservation law for amplitude of u in the finite domain Ω ,

$$\partial_\tau \int_\Omega \bar{u}u = (2k^{-1}) \int_{\partial\Omega} \text{Imag}(\bar{u}\nabla u \cdot \mathbf{n}). \quad (32)$$

The index of refraction is a positive bounded function, $0 < n^2 < C$ and we can bound the gradient of the solution using the following relation,

$$\begin{aligned} \partial_\tau \left[\int_\Omega \nabla u \cdot \nabla \bar{u} + k^2 \int_\Omega (C - n^2) \bar{u}u \right] = \\ 2 \int_{\partial\Omega} \text{Real}(\bar{u}_\tau \nabla u \cdot \mathbf{n}) + (2Ck) \int_{\partial\Omega} \text{Imag}(\bar{u}\nabla u \cdot \mathbf{n}). \end{aligned} \quad (33)$$

The above identities could be translated in terms of the variables A and ϕ ,

$$\partial_\tau \int_\Omega A^2 = 2 \int_{\partial\Omega} \text{Imag}(A^2 \nabla \phi \cdot \mathbf{n}) \quad (34)$$

$$\begin{aligned} \partial_\tau \left[\int_\Omega (|\nabla A|^2 + k^2 A^2 |\nabla \phi|^2) + k^2 \int_\Omega (C - n^2) A^2 \right] = \\ 2 \int_{\partial\Omega} A_t \nabla A \cdot \mathbf{n} + k^2 A^2 \phi_t \nabla \phi \cdot \mathbf{n} + (2Ck^2) \int_{\partial\Omega} (A^2 \nabla \phi \cdot \mathbf{n}). \end{aligned} \quad (35)$$

3 Numerical Methods

We have developed finite difference methods to solve the nonlinear PDEs that we have discussed. The schemes for the geometrical optics system and the asymptotic expansion system are explained in our previous paper and we do not describe them here. The numerical method for the perturbed geometrical system is an implicit scheme that uses the previous schemes as building blocks. To achieve high order accuracy we also use the ENO, essentially non-oscillatory, method. The ENO method is based on an adaptive stencil to calculate the derivative of a function defined on a grid. Use of this method allows us to calculate solutions of the eikonal equation with discontinuous first derivatives without smoothing the solution.

We use the following notation to denote the discretization. Δx , Δy , and Δt are the mesh sizes. $\phi_{i,j}^n$ is the numerical approximation to the solution of the eikonal equation,

$$\phi_{i,j}^n \approx \phi(x_i, y_j, t^n) = \phi(i\Delta x, j\Delta y, n\Delta t), \quad (36)$$

and $v_{i,j}^n$ is the numerical approximation to $v(x, y, t)$,

$$v_{i,j}^n \approx v(x_i, y_j, t^n) = v(i\Delta x, j\Delta y, n\Delta t). \quad (37)$$

We use standard notation for forward, backward, and centered differences,

$$D_x^+ \phi_{ij} = \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x} \quad D_x^- \phi_{ij} = \frac{\phi_{i,j} - \phi_{i-1,j}}{\Delta x} \quad D_x^0 \phi_{ij} = \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2\Delta x}. \quad (38)$$

A time marching scheme is used to solve the perturbed geometrical optics system. We consider the discretization of the following system for the variables (v, ϕ) . The discretization for variables (A, ϕ) is similar,

$$\begin{cases} \phi_\tau = |\nabla \phi|^2 - n^2 - k^{-2}(\Delta v + |\nabla v|^2) \\ v_\tau = 2\nabla v \cdot \nabla \phi + \Delta \phi \end{cases} \quad (39)$$

Since we are interested only in the steady state case we consider a simple time discretization. We discovered through linearization of the system that it has two complex eigenvalues, therefore a forward Euler time discretization of the system will be unstable. We do a mixed discretization in time of the system. We treat the linear part implicitly and the nonlinear part explicitly. This will enable us to have time steps which are proportional to Δx , since we are treating the nonlinear transport terms explicitly. To see this point we consider the simple linear equation

$$u_t = iu_{xx} + au_x, \quad (40)$$

where $i = \sqrt{-1}$ and a is a real positive number. Then a forward Euler discretization of this equation is

$$u_j^{n+1} = u_j^n + \Delta t i D_x^+ D_x^- u_j^n + \Delta t a D_x^+ u_j^n. \quad (41)$$

We can do a linear stability analysis of the above scheme using a solution of the form $u_j^n = \kappa^n e^{ij\Delta x \omega}$. We substitute the above ansatz in the scheme and solve for κ ,

$$\kappa = 1 + \frac{\Delta t}{\Delta x^2} i (2 \cos(\omega \Delta x) - 2) + \frac{\Delta t}{\Delta x} a (e^{i\Delta x \omega} - 1). \quad (42)$$

If $a = 0$ we can easily show that $\kappa > 1$ for all values of Δt and Δx . If $a \neq 0$ then the upwind discretization sometimes can stabilize the scheme for $\Delta t \propto \Delta x^2$, but that is a very small and restrictive time step.

A mixed discretization of the following form where the first order derivative is discretized explicitly and the second order terms implicitly results in a time step of order Δx ,

$$u_j^{n+1} - \Delta t D_x^+ D_x^- u_j^{n+1} = u_j^n + \Delta t a D_x^+ u_j^n. \quad (43)$$

We calculate κ for the above scheme and we obtain

$$\kappa = \frac{1 + \frac{\Delta t}{\Delta x} a(e^{i\Delta x \omega} - 1)}{1 + \frac{\Delta t}{\Delta x^2} i(2 \cos(\omega \Delta x) - 2)}. \quad (44)$$

We can easily show that $|\kappa| < 1$ for all ω if $a\Delta t/\Delta x < 1$, since the absolute value of the numerator is less than one and the absolute value of the denominator is greater than one.

The numerical scheme for the system is:

$$\begin{aligned} & \phi_{i,j}^{n+1} + k^{-2} \Delta t (D_x^+ D_x^- v_{i,j}^{n+1} + D_y^+ D_y^- v_{i,j}^{n+1}) = \\ & \phi_{j,j}^n + \Delta t \hat{G}(D_x^+ \phi_{i,j}^n, D_x^- \phi_{i,j}^n, D_y^+ \phi_{i,j}^n, D_y^- \phi_{i,j}^n) - k^{-2} \Delta t ((D_x^0 v_{i,j}^n)^2 + (D_y^0 v_{i,j}^n)^2) \end{aligned} \quad (45)$$

$$\begin{aligned} & v_{i,j}^{n+1} - \Delta t (D_x^+ D_x^- \phi_{i,j}^{n+1} + D_y^+ D_y^- \phi_{i,j}^{n+1}) = \\ & 2\Delta t D_x^u v_{i,j}^n \cdot D_x^0 \phi_{i,j}^n + 2\Delta t D_y^u v_{i,j}^n \cdot D_y^0 \phi_{i,j}^n. \end{aligned} \quad (46)$$

The numerical flux, denoted by \hat{G} , is calculated based on the exact or an approximate solution of a Riemann problem for the eikonal equation. We use two different numerical fluxes, one is the Godunov type flux and the second is a Lax-Friedrichs type. In the first method the flux is defined through a third order ENO interpolation and a Godunov type Riemann solver. The values of the derivatives, D^+ and D^- , are replaced by D^{ENO} and are calculated based on third order interpolation with an adaptive stencil [5]. The Godunov flux is defined by

$$\hat{G}(u^+, u^-, v^+, v^-) = \text{ext}_{u \in I(u^-, u^+)} \text{ext}_{v \in I(v^-, v^+)} H(u, v). \quad (47)$$

$H(u, v) = (u^2 + v^2) - n^2$ and $I(a, b) = [\min(a, b), \max(a, b)]$. The function ext is defined by

$$\text{ext}_{u \in I(a, b)} = \max_{u \in I(a, b)} \quad \text{if } a \leq b, \quad (48)$$

$$\text{ext}_{u \in I(a, b)} = \min_{u \in I(a, b)} \quad \text{if } b < a. \quad (49)$$

Note that in general the operations of taking \max and \min do not commute and the Godunov flux is not always uniquely defined. But for many cases, including our $H(u, v)$, the flux is uniquely defined. Use of a third order ENO interpolation and the exact Riemann solver results in the excellent resolution of the discontinuities in the solution of the phase.

The Lax-Friedrich flux is simpler to describe and is defined as

$$\hat{G}(u^+, u^-, v^+, v^-) = H((u^+ + u^-)/2, (v^+ + v^-)/2) - \alpha_x (u^+ - u^-) + \alpha_y (v^+ + v^-). \quad (50)$$

α_x and α_y are local upper bounds for absolute values of the partial derivatives of the Hamiltonian $H(u, v)$

$$\left| \frac{\partial H}{\partial u} \right| < \alpha_x \quad \text{for } u \in (u^-, u^+), \quad (51)$$

$$\left| \frac{\partial H}{\partial v} \right| < \alpha_y \quad \text{for } v \in (v^-, v^+). \quad (52)$$

The terms D_x^u and D_y^u refer to the upwind discretization of the transport terms and for a first order discretization they are defined as the following

$$\begin{aligned} D_x^u v_{i,j} &= D_x^+ v_{i,j} & \text{if } D_x^0 \phi_{i,j} > 0 \\ D_x^u v_{i,j} &= D_x^- v_{i,j} & \text{if } D_x^0 \phi_{i,j} \leq 0. \end{aligned} \quad (53)$$

In our code we have used a second order ENO method to calculate D_x^u to achieve higher order accuracy.

4 Numerical Results

In this section we present some of the computed numerical results. Our methods are appropriate for very high frequency regimes and direct comparison of our solutions with exact solutions of the Helmholtz equation is not possible. Nevertheless we compare our solutions with exact solutions calculated at a lower frequency whenever possible.

Our first computed example corresponds to calculation of the phase and the amplitude around a shadow line using the perturbed geometrical optics system. We set up the problem in the domain $[-1, 1] \times [-1, 1]$. We specify Dirichlet boundary conditions on one side and Neumann type boundary conditions on rest of the domain. Let us recall that the solution u is

$$u = e^{v+ik\phi}. \quad (54)$$

For Dirichlet boundary conditions we specify

$$\begin{aligned} v(-1, y) = 0 & \quad \phi(-1, y) = 0 & \text{if } y > 0 \\ v(-1, y) = -10 & & \text{if } y < 0. \end{aligned} \quad (55)$$

For rest of the boundary we specify $\nabla\phi \cdot \mathbf{n}$. Since the values of the $\nabla\phi \cdot \mathbf{n}$ are not known *a priori*, we extrapolate the values from neighboring points. The solution of the system is graphed in figures 1 and 2, the amplitude is shown in figure 1 and the phase is contoured in figure 2. Note that we have used value $k = 100$ in this calculation and that the amplitude shows the typical oscillatory behavior around the shadow line ([1] p. 434). In figure 3 we graph the intensity of a diffracted plane wave from an edge using the Fresnel approximation ([1] p. 434). Our computed solution has the correct qualitative behavior.

Next we consider reflection of an incident wave off a cylinder. We consider a cylinder of radius one at the origin. The source of the wave is at point $(0, 7)$. We use polar coordinates for calculations. We assume that the solution is of the form

$$u = A_1 e^{ik\phi_1} - A_2 e^{ik\phi_2}. \quad (56)$$

The physical problem is posed in all of R^2 but our computational domain is $[1, 6] \times [-\pi, \pi]$. The boundary conditions for ϕ_1 and A_1 are specified as the following. We specify the Dirichlet boundary conditions for phase and amplitude in the region of the domain where

it is illuminated by the source. Everywhere else the boundary conditions are based on the local direction of the characteristics. If the characteristic line is pointed to the outside of the domain, there is no need for boundary conditions. If the characteristic line is directed to the inside, we use $\hat{G}(0,0,0,0)$ to calculate the numerical flux for the phase. For the transport equations the numerical flux is set to zero. The direction of the characteristic line is simply determined based on the sign of the normal derivative of the phase. In (r, θ) coordinates, the normal derivatives are simply $d\phi/d\theta$ and $d\phi/dr$. The boundary conditions for the reflected wave, ϕ_2 and A_2 , are specified as the following. For $r = 6$, $\theta = \pi$, and $\theta = -\pi$ the boundary conditions are based on the local direction of the characteristic line. The phase and amplitude of the reflected wave at the surface of the cylinder is set equal to the incident wave and therefore at $r = 1$ we specify the boundary condition for ϕ_2 and A_2 according to

$$\phi_2(1, \theta) = \phi_1(1, \theta), \quad A_2(1, \theta) = A_1(1, \theta). \quad (57)$$

The problem is solved numerically in (r, θ) space and the results are interpolated to a Cartesian grid. We use our numerical method to solve the solution for the incident and the reflected wave. We recover the amplitude of the solution by adding the two solutions, assuming a value of $k = 3$. The amplitude and phase are computed for infinite k , but we use them for finite k . In figure 5 we present the exact solution computed from the expansion of the solution in Bessel functions.

The multivalued solutions of the eikonal equation in domains with constant index of refraction outside a convex domain have a simple structure which could be exploited. If one considers a boundary fitted coordinate system where one of the coordinates is radially outward from center of the body and the other coordinate is the local coordinate on the surface of the object, then the incident and reflected solutions of the eikonal equation become unique in this coordinate system. We consider reflection of a plane wave from a cylinder again. We extend the domain for θ from $(-\pi, \pi)$ to the whole real line. The multivalued solutions in this case are numerated by the integers. For computational purposes we have to cut the domain. We show the results for such a calculation in the domain $(-2\pi, 2\pi)$. In figures 6 and 7 we show the multivalued phase of the incident and reflected wave from the cylinder. In figures 8 and 9 we show the calculated amplitude.

5 Conclusion

We have developed finite difference methods for solving the nonlinear PDEs that approximate high frequency solutions of the reduced wave equation. These approximation can be very useful and powerful tools for calculating high frequency solutions since the mesh size for the numerical solution of these equations is essentially independent of k . The geometrical optics approximation consists of the eikonal system and the transport equation. The behavior of this system is well understood and our numerical method solves this system as long as the phase stays single valued. To correct for the effects of finiteness of frequency we also have developed numerical methods for solving the classical asymptotic expansion.

This approximation can be calculated in situations where geometrical optics equations can be solved.

We have also proposed a new system, the perturbed geometrical optics system, to recover the effects of finiteness of frequency. This system has solutions that are more general than those of the geometrical optics system. In particular we have recovered solutions of the Helmholtz equation around a shadow line. This system is equivalent to the Helmholtz equation as long as the phase stays a single valued function and the amplitude is bounded away from zero everywhere. The major obstacle in recovering all high frequency solutions of the Helmholtz equation using the above approximations is the multivalued nature of the phase. We have developed some special procedures to recover some multivalued solutions. One method relies on detecting a discontinuity in the gradient of the phase and using that as a branch surface to generate a new sheet of the multivalued solution. This approach can be applied to problems where the multivalued nature of the solution is not known *a priori*. Another approach for the exterior of convex objects is to use polar coordinates and extending the domain to calculate phase in multiple copies of the original domain. These methods are special and a general method needs to be developed for recovering all multivalued solutions.

6 Acknowledgment

We wish to thank E. Harabetian for many helpful discussions.

References

- [1] M. Born and E. Wolf, Principles of Optics, Pergamon Press, sixth edition, 1989.
- [2] E. Fatemi, B. Engquist, and S. Osher, Numerical solution of the high frequency asymptotic expansion for the scalar wave equation, to appear in *JCP*.
- [3] J. B. Keller, A Geometrical Theory of Diffraction, *Calculus of variations and its Applications*, McGraw-Hill, New York, 1958, p. 27.
- [4] H-O Kreiss and J. Lorenz, Initial-Boundary Value Problems and the Navier-Stokes Equations, *Academic Press, Inc.*, San Diego, 1989.
- [5] S. Osher and C-W Shu, High order essentially non-oscillatory schemes for Hamilton-Jacobi equations, *SIAM J. Numer. Analys.* XXVIII (1991), 907-922.

Amplitude, $k=100$

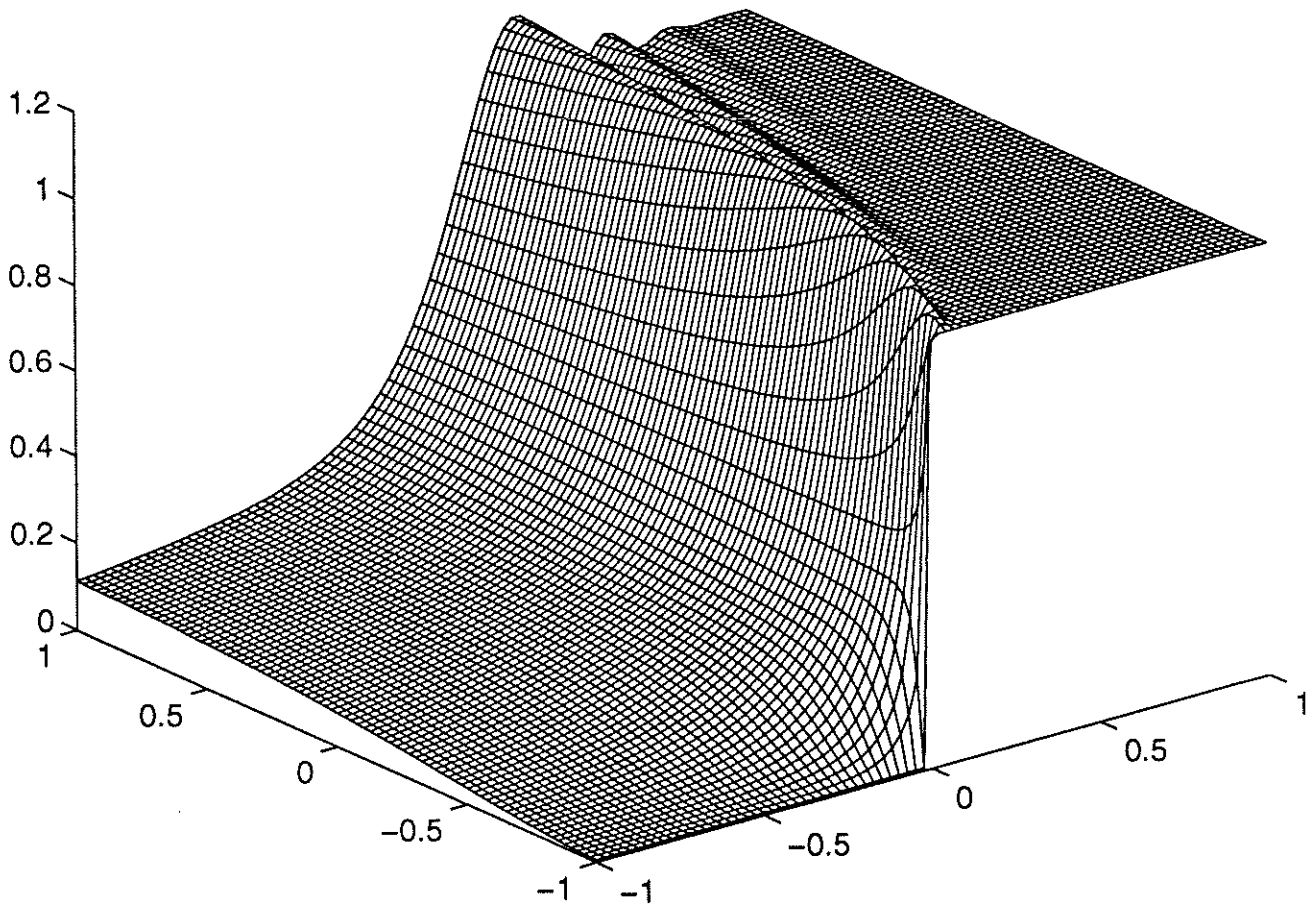


Figure 1: Amplitude of the solution of the perturbed geometrical optics system around a shadow line, $k=100$, $A = e^v$

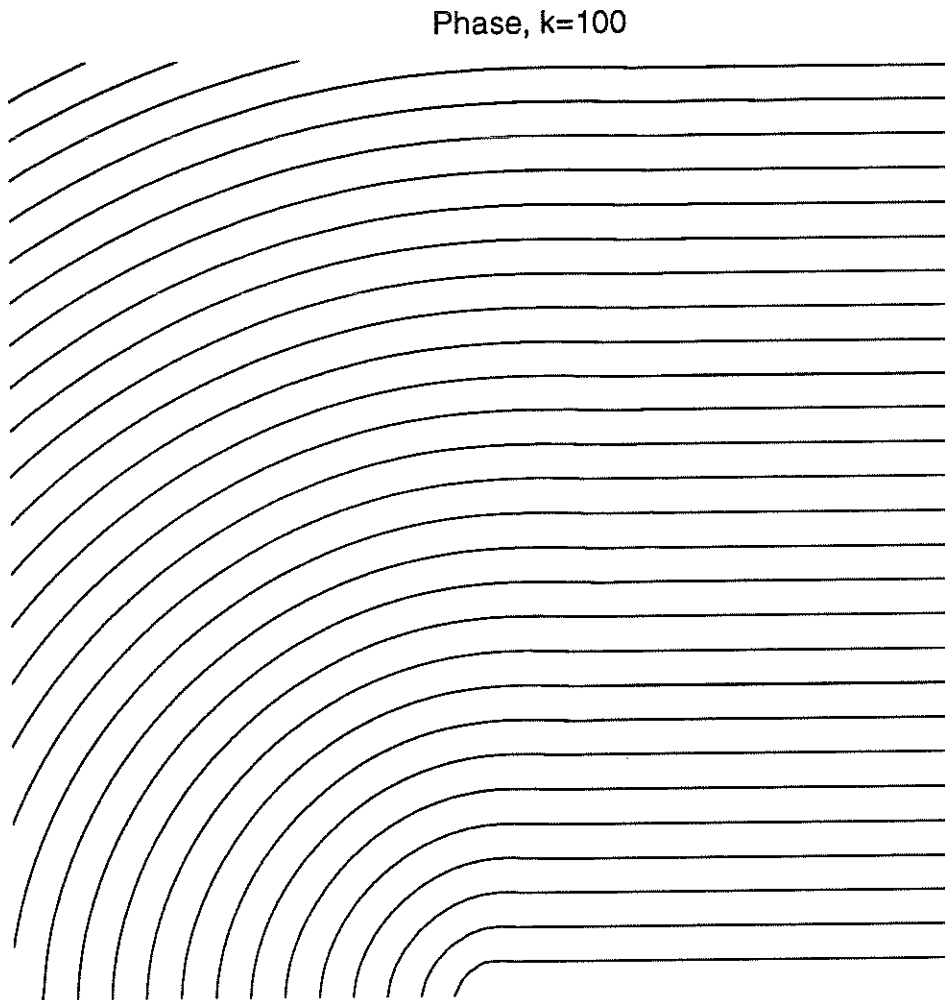


Figure 2: Phase of the solution of the perturbed geometrical optics system around a shadow line, $k=100$

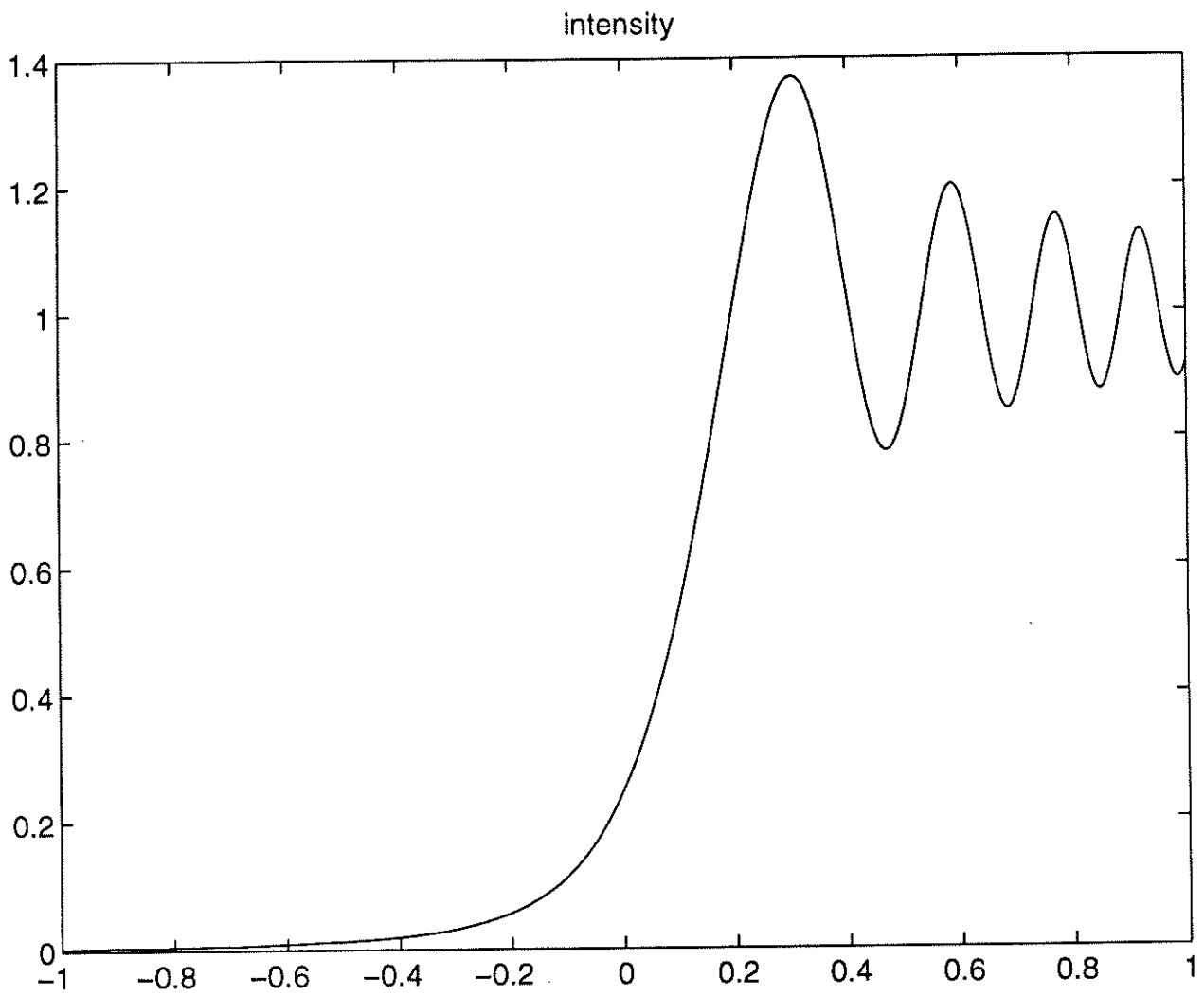


Figure 3: Fresnel diffraction pattern of a straight edge

Amplitude of the solution, computed

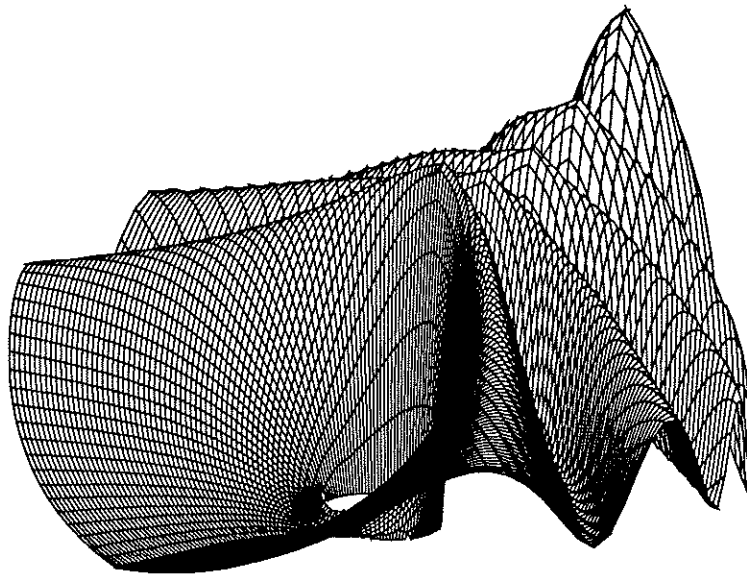


Figure 4: Amplitude of the computed solution outside a cylinder

Amplitude of the solution, exact

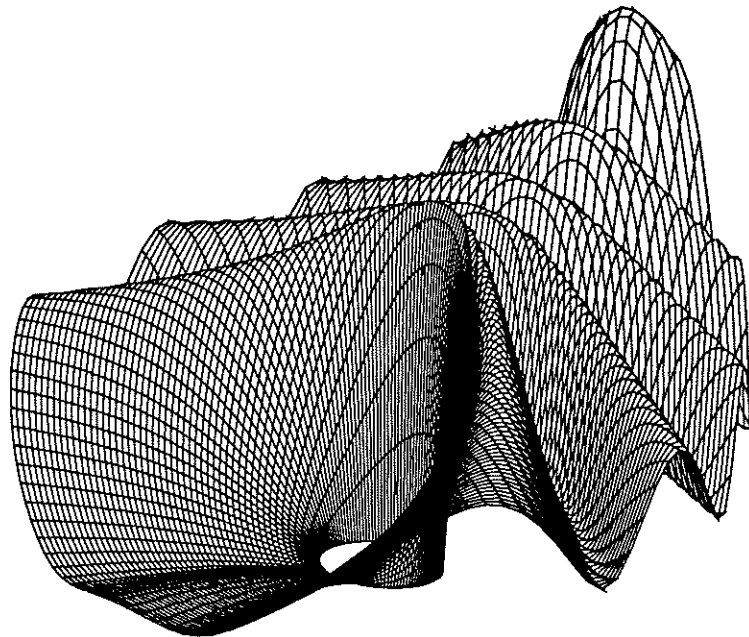


Figure 5: Amplitude of the exact solution outside a cylinder, $k=3$

Phase of the incident wave

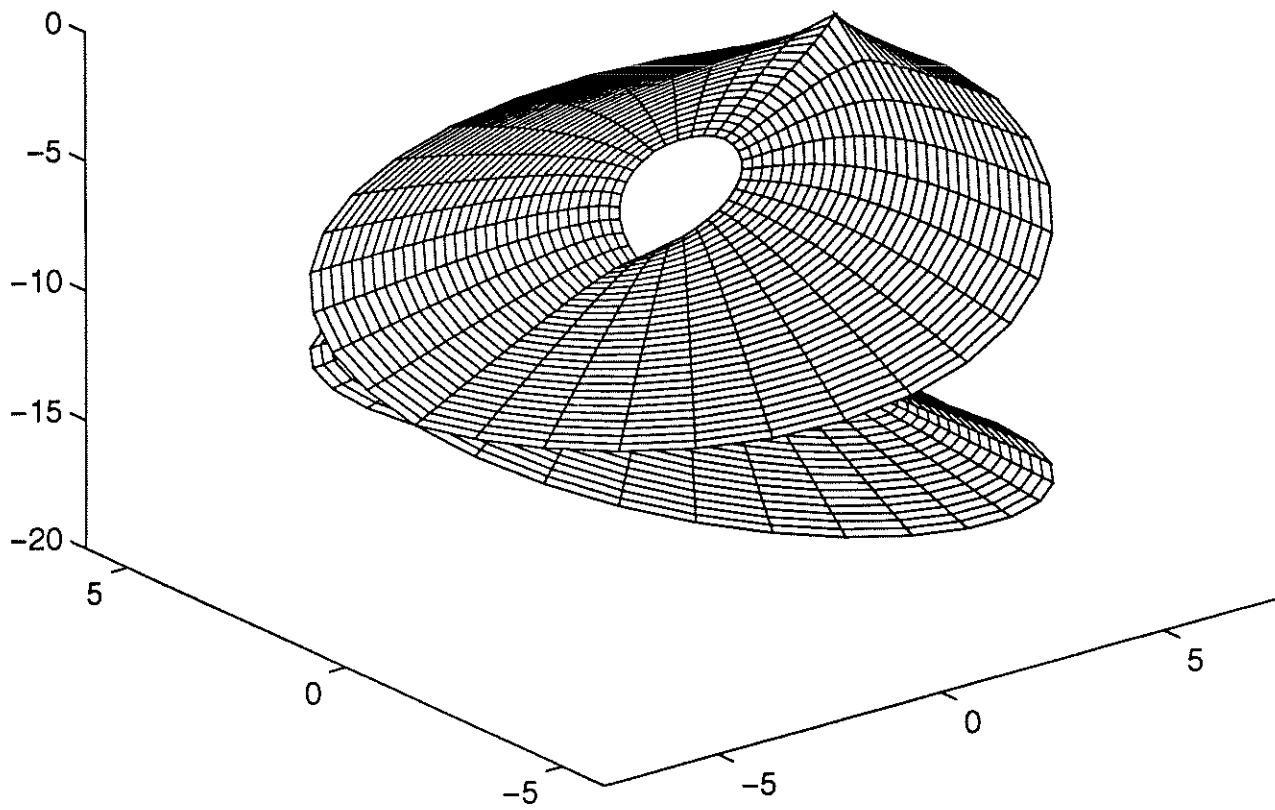


Figure 6: Multivalued phase of the incident wave, ϕ_1

Phase of the reflected wave

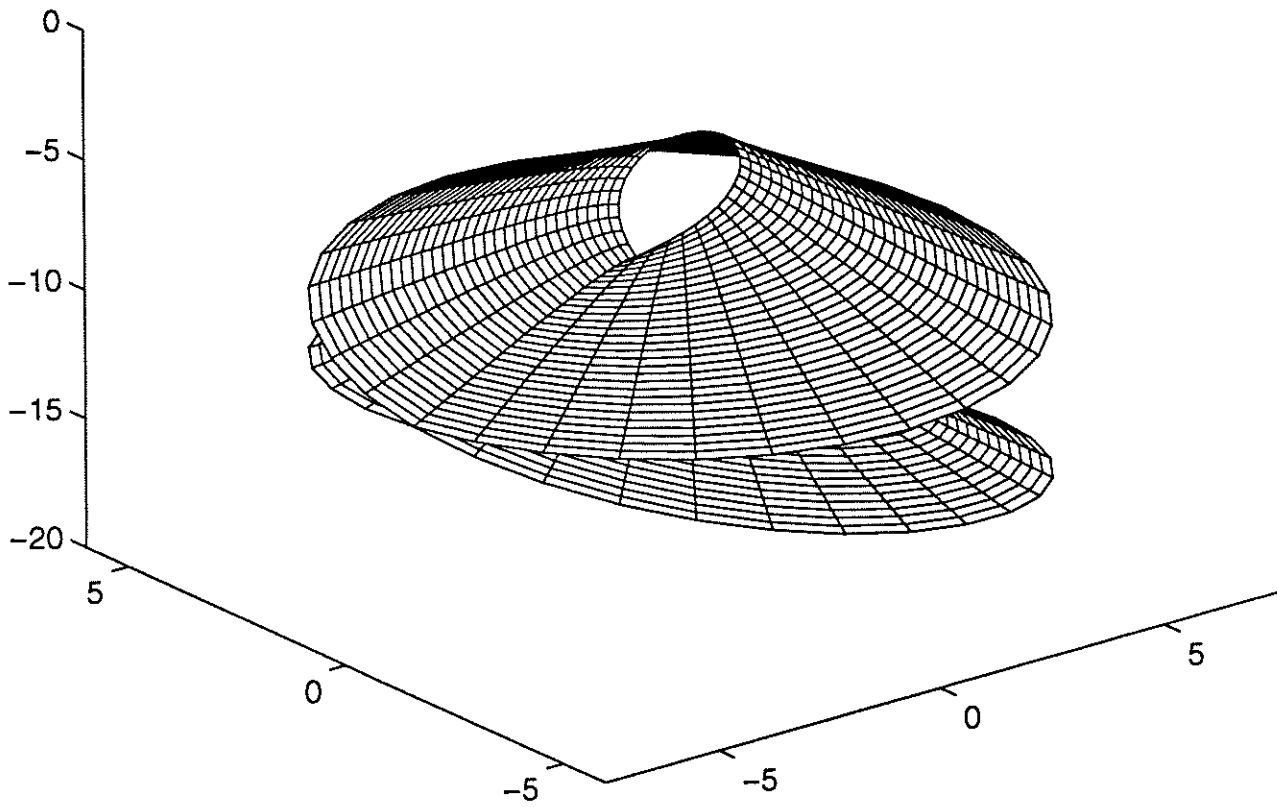


Figure 7: Multivalued phase of the reflected wave, ϕ_2

Amplitude of the incident wave

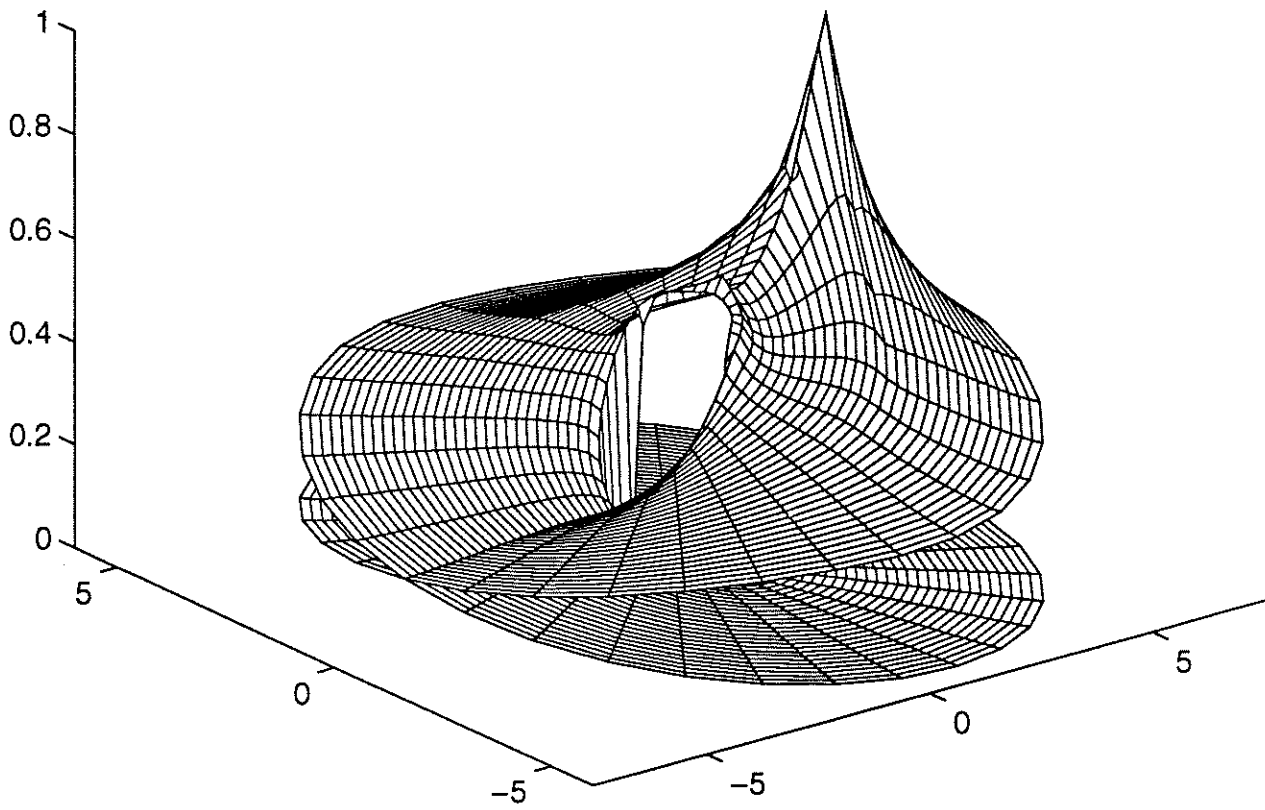


Figure 8: Multivalued amplitude of the incident wave, A_i

Amplitude of the reflected wave

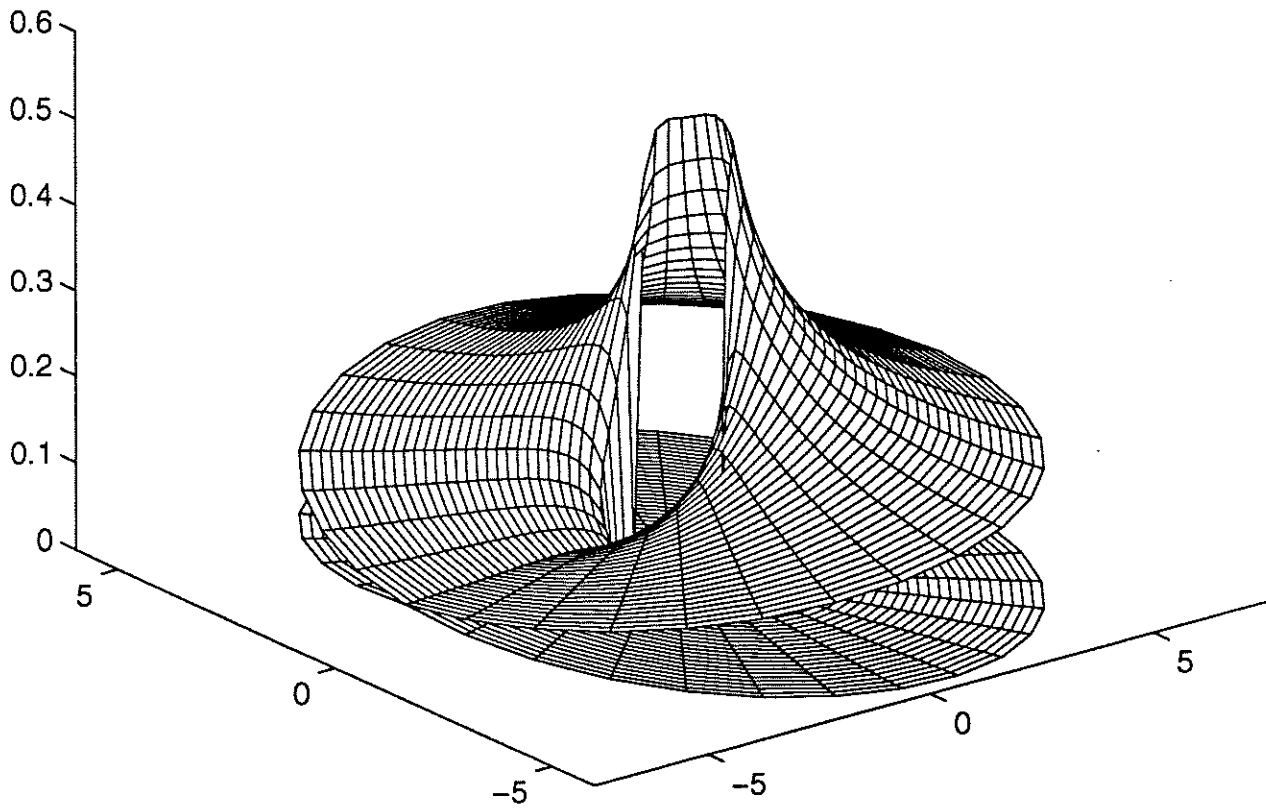


Figure 9: Multivalued amplitude of the reflected wave, A_2