3D Finite Element Approximation of the Resonator Equation in Laser Simulation [1]

Konrad Altmann
LAS-CAD GmbH,
Christoph Pflaum, David Seider
Institut für Angewandte Mathematik und Statistik,
Universität Würzburg
e-mail: Dr.Altmann@las-cad.com
pflaum@mathematik.uni-wuerzburg.de
seider@mathematik.uni-wuerzburg.de

Abstract

The resonator wave in a laser cavity can be described by a complex Helmholtz eigenvalue problem in 3D. This eigenvalue problem has to be approximated by a numerical method, since in general it cannot be solved analytically. A common approach to do this is to apply the method of Fox-Li.

In this paper, we present a new numerical method for approximating the laser resonator eigenvalue problem. First, this method approximates the solution of the resonator eigenvalue problem by two waves between the mirrows of the laser cavity. This leads to an eigenvalue problem of a coupled equation system. The equations of this system, are partial differential equations of second order with a large term of first order. To obtain a stable discretization of this equation, we apply a streamline-diffusion finite element approximation of these partial differential equations. Numerical results are presented.

1 Introduction

Nowadays, different kinds of lasers are needed in several engineering applications. Therefore, new kind of lasers have to be designed. One problem in designing lasers is that the laser beam is very sensitive with respect to physical parameters of the laser. One of them is the deformation of the laser medium caused by heating. Therefore, numerical simulation of lasers plays an important role in designing new lasers (see [?] and [?]). One part of such a simulation is the simulation of the laser beam. This simulation has necessarily to take into account the wave character of light.

[1] **Acknowledgment.** We would like to thank the Bavarian Research Foundation for the financial support of this work.

The Maxwell equations describe the behavior of electro-magnetic waves. By suitable assumptions and simplifications, these equations can be transformed to the scalar wave equation

$$\mu\varepsilon \frac{\partial^2 E}{\partial t^2} = \Delta E, \tag{1}$$

where $E(x, y, z; t)$ is the electric field. Assuming a time harmonic wave E with wavenumber $k \in \mathbb{R}^+$, i.e. $E(x, y, z; t) = \tilde{E}(x, y, z) \cdot e^{jkt}$, equation (1) leads to the Helmholtz equation

$$-\Delta\tilde{E} - n^2k^2\tilde{E} = 0. \tag{2}$$

with refractive index $n = \sqrt{\mu\varepsilon}$. To analyze the behavior of the solution of the scalar wave equation, one has to calculate the eigenmodes $\tilde{E}$ of the laser resonator. The standard approach for solving (2) is to apply the paraxial approximation. This approach uses the ansatz $\tilde{E} = U(x, y, z) \cdot e^{j\omega z}$ where $\omega^2 = n^2k^2$. The second-order derivation U_{zz} is neglected. For constant index n, this leads to the following equation:

$$-\Delta_{x,y}U = 2j\omega \frac{\partial U}{\partial z} \tag{3}$$

For certain boundary conditions, the so–called Gauß–Modes are analytical solutions of (3), see e.g. [?] or [?]. These modes are used to analyze the laser cavity (complex ABCD-matrices).

In general however, the parameter n depends on the spatial coordinates. In this case, analytical solutions of (2) do not exist and the above ansatz is not appropriate. Then, an approximation by Gauß–Modes often is not accurate enough. An improvement can be obtained by the so-called Fox–Li approach, see [?] or [?]. This method utilizes Beam-Propagation-Methods to numerically compute eigenmodes (see [?], [?], [?] or [?]). The idea of the Fox–Li approach is to calculate the profile of a front of a laser beam, which is reflected several times forth and back by the mirrors of the laser cavity. The convergence of this method depends on the eigenvalues of the eigenmodes of the propagation operator. Therefore, this method cannot converge in general, see e.g. [?]. Another disadvantage of the Fox–Li approach is that it neglects the global character of the Helmholtz equation by the paraxial approximation. Therefore, a global approximation of the Helmholtz equation is needed.

The Finite Element method is a successful approach for the numerical solution of partial differential equations. Therefore, we applied the Finite Element method to calculate (what we call) eigenmodes of the resonator equation. To apply the Finite Element method directly to the Helmholtz equation is very difficult in case of high wave numbers k. On one hand a very fine discretization has to be used to resolve the high–oscillatory waves. On the other hand the arising complex symmetric linear systems of equations are hard to solve.

In this report, we present a new 3D–approach for computing eigenmodes of a laser cavity. The considered Helmholtz eigenvalue problem is described in the next section. In Section 3, a two–wave representation of an eigenmode is introduced. By this

representation the Helmholtz equation transforms to an elliptic system of equations with a large first order term. To obtain a stable discretization, streamline–diffusion is applied (see Section 4). Finally, in Section 5 numerical results are presented.
At least, let us remark that the integration variables are not written explicitly, so that the presentation of the formulas becomes clearer. Furthermore, all function spaces in this paper as $H^{1,2}(\Omega)$, consist of complex-valued functions.

2 The Helmholtz Eigenvalue Problem

From Maxwell's equations a scalar wave equation for the electric field E can be derived:

$$\mu\varepsilon \frac{\partial^2 E}{\partial t^2} = \Delta E, \tag{4}$$

where ε is the dielectric constant and μ is the magnetic permeability. The refractive index n is defined by

$$n^2 = \mu\varepsilon.$$

Suitable boundary conditions are introduced below in this section.
For solving (4) let us assume that there exists a basis of eigenfunctions u_i of the generalized eigenvalue problem

$$-\Delta u_i - n^2 k^2 u_i = \lambda_i \, n^2 u_i. \tag{5}$$

with corresponding eigenvalues $\lambda_i \in \mathbb{C}$. Now, consider the sum

$$E = \sum_{i=1}^{\infty} \gamma_i \, u_i(x, y, z) e^{jkt} e^{jk_i t} \tag{6}$$

with $k = \frac{2\pi}{\nu}$ and a small fixed wavelength ν. It converges, if the coefficients γ_i are chosen properly. Furthermore, the sum (6) fulfills equation (4) for suitable parameters k_i, e.g. if the k_i are such that $\lambda_i = (2kk_i + k_i^2)$.
Since we want to find the eigenmodes with wavelengths near to ν, we search for eigenfunctions u_i with eigenvalues of smallest modulus. We call these u_i the eigenmodes of the laser.
Usually, the square of the refractive index n^2 is real. By adding an imaginary part, amplification or damping of a wave can be modeled.
Here, we consider a laser cavity of the form of a cuboid with mirrors at the abbuting faces and open sides, see Figure 1. We assume that we have perfectly reflecting mirrors and that the waves can leave the cavity at the open boundary. So, we define the domain

$$\Omega := [0; 1] \times [0; 1] \times [0; L],$$

and the boundaries

$$\Gamma_0 := [0; 1] \times [0; 1] \times \{0\}, \Gamma_L := [0; 1] \times [0; 1] \times \{L\} \text{ and } \Gamma_r := \partial\Omega \setminus (\Gamma_0 \cup \Gamma_L).$$

The reflection of the mirrors is modeled by enforcing the solutions to vanish at the corresponding boundaries Γ_0, Γ_L (see [?]). Robin–boundary conditions are applied at the open boundary Γ_r.
Combining all requirements, we obtain the eigenvalue problem:
Find u and λ such that

$$\begin{aligned} -\triangle u - n^2 k^2 u &= \lambda \cdot n^2 \cdot u && \text{in } \Omega \\ u &= 0 && \text{on } \Gamma_0 \cup \Gamma_L \\ \partial_n u_r &= jku_r && \text{on } \Gamma_r \end{aligned}$$

Let us describe this problem by a weak formulation. To this end, let

$$H := \{v \in H^{1,2}(\Omega) \mid v|_{\Gamma_0 \cup \Gamma_L} = 0\}$$

and define the sesquilinear forms

$$a(u,v) := \int_\Omega (\nabla u \nabla \overline{v} - n^2 k^2 u \overline{v}) - \int_{\Gamma_r} jku\overline{v}$$

and

$$(u,v)_0 := \int_\Omega n^2 \; u\overline{v}.$$

So, the weak formulation reads as follows:
Find $u \in H$ and $\lambda \in \mathbb{C}$ such that

$$a(u,v) = \lambda (u,v)_0 \qquad \forall v \in H. \tag{7}$$

For a numerical calculation of the eigenvalue and eigenvector with smallest modulus, one has to invert the operator corresponding to the sesquilinear form $a(\cdot,\cdot)$, i.e. one has to solve the equation

$$a(u,v) = (f,v)_0 \qquad \forall v \in H \tag{8}$$

for appropriate right hand sides f.

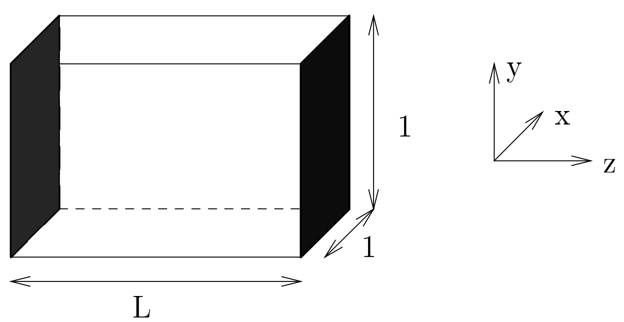

Figure 1: Geometry

It can easily be shown, that $a(\cdot,\cdot)$ fulfills the Gårding inequality. So, the Fredholm alternative applies to equation (8), cf. [**?**]. Existence and uniqueness of the solution follows, if we can show that for right-hand side $f = 0$, only the trivial solution $u = 0$ exists.
For constant and real n^2k^2 this is the case if following condition holds:

$$\rho - n^2k^2 \neq 0 \tag{9}$$

for all eigenvalues $\rho \in \mathbb{R}_0^+$ of the generalized eigenvalue problem:
Find u in H such that

$$\int_\Omega \nabla u \nabla \overline{v} = \rho \int_\Omega u \overline{v} \qquad \forall v \in H.$$

A rigor analysis for more general parameters will be presented in a subsequent paper.
Solving (8) numerically is quite hard when n^2k^2 has a large positive real part and a small or vanishing imaginary part, see [**?**]. The reasons are that a very fine discretization has to be used and that the resulting system of linear equations is ill–conditioned in general.
So other ways have to be found.

3 Two–Wave Representation

The physics of the laser elucidates some important properties of the laser beam which motivate a two–wave approach for approximating equation (7). First, the beam mainly propagates in the direction of the axis formed by the two mirrors and is reflected forth and back. Furthermore, it has a high longitudinal frequency which nearly corresponds to the oscillation in time.
Therefore, let us represent the solution of the eigenvalue problem (7) by a sum of two waves traveling in opposite z-directions:

$$u(x,y,z) = u_r(x,y,z)\, e^{-j\omega z} + u_l(x,y,z)\, e^{j\omega z} \tag{10}$$

where u_r and u_l have to fulfill the boundary conditions

$$u_r(x,y,0) + u_l(x,y,0) = 0 \text{ and } u_r(x,y,L)\, e^{-j\omega L} + u_l(x,y,0)\, e^{j\omega L} = 0$$

with appropriately chosen ω. If n is non-constant, e.g. $n(x,y,z) = n_0 + \tilde{n}(x,y,z)$ with small $\tilde{n}$, the choice $\omega = n_0 k$ would be suitable. So the main idea is, that a standing wave is described by two waves consisting of a part with high oscillation in z-direction ($e^{\mp j\omega z}$) and a part that smoothly varies in z-direction (u_r, u_l). Let us define the space

$$H_\omega := \{u = u_r\, e^{-j\omega z} + u_l\, e^{j\omega z} \mid u_l, u_r \in H^{1,2}(\Omega), u_r + u_l|_{\Gamma_0} = 0, u_r\, e^{-j\omega L} + u_l\, e^{j\omega L}|_{\Gamma_L} = 0\}.$$

It can easily be seen, that $H_\omega = H$. Thus, every function u in H can be represented in the form (10). Of course, this representation is not unique.
Substituting (10) into (7) and integrating by parts, we obtain the variational equation for $u = u_r\, e^{-j\omega z} + u_l\, e^{j\omega z}$

$$
\begin{aligned}
& a(u,v) = \\
& \int_\Omega \left(\nabla u_r \nabla \bar{v}_r + (\omega^2 - n^2k^2) u_r \bar{v}_r + 2j\omega \frac{\partial}{\partial z} u_r \bar{v}_r \right) - jk \int_{\Gamma_r} u_r \bar{v}_r \\
& + \int_\Omega \left(\nabla u_l \nabla \bar{v}_l + (\omega^2 - n^2k^2) u_l \bar{v}_l - 2j\omega \frac{\partial}{\partial z} u_l \bar{v}_l \right) - jk \int_{\Gamma_r} u_l \bar{v}_l \\
& + \int_\Omega e^{-j2\omega z} \left(\nabla u_r \nabla \bar{v}_l - (\omega^2 + n^2k^2) u_r \bar{v}_l - j\omega u_r \frac{\partial}{\partial z} \bar{v}_l - j\omega \frac{\partial}{\partial z} u_r \bar{v}_l \right) \\
& + \int_\Omega e^{j2\omega z} \left(\nabla u_l \nabla \bar{v}_r - (\omega^2 + n^2k^2) u_l \bar{v}_r + j\omega u_l \frac{\partial}{\partial z} \bar{v}_r + j\omega \frac{\partial}{\partial z} u_l \bar{v}_r \right) \qquad (11) \\
& -jk \int_{\Gamma_r} e^{-j2\omega z} u_r \bar{v}_l - jk \int_{\Gamma_r} e^{j2\omega z} u_l \bar{v}_r \\
& \quad = \lambda \left(\int_\Omega n^2\ u_r \bar{v}_r + \int_\Omega n^2\ u_l \bar{v}_l + \int_\Omega e^{-j2\omega z} n^2\ u_r \bar{v}_l + \int_\Omega e^{j2\omega z} n^2\ u_l \bar{v}_r \right) \\
& \quad = \lambda (u,v)_0
\end{aligned}
$$

which has to be fulfilled for every $v = v_r\, e^{-j\omega z} + v_l\, e^{j\omega z} \in H_\omega$.
Under certain conditions, the eigenvalue problem (11) is equivalent to a system eigenvalue problem, namely:
Find $\lambda \in \mathbb{C}$ and $u_r, u_l \in H^{1,2}$ with $u_r + u_l|_{\Gamma_0} = 0$, $u_r\, e^{-j\omega L} + u_l\, e^{j\omega L}|_{\Gamma_L} = 0$ such that

$$
\begin{aligned}
\int_\Omega \left(\nabla u_r \nabla \bar{v}_r + (\omega^2 - n^2k^2) u_r \bar{v}_r + 2j\omega \frac{\partial}{\partial z} u_r \bar{v}_r \right) - jk \int_{\Gamma_r} u_r \bar{v}_r &= \lambda (u_r, v_r)_0 \qquad (12) \\
\int_\Omega \left(\nabla u_l \nabla \bar{v}_l + (\omega^2 - n^2k^2) u_l \bar{v}_l - 2j\omega \frac{\partial}{\partial z} u_l \bar{v}_l \right) - jk \int_{\Gamma_r} u_l \bar{v}_l &= \lambda (u_l, v_l)_0
\end{aligned}
$$

for all $v_r, v_l \in H^{1,2}$ with $v_r + v_l|_{\Gamma_0} = 0$, $v_r\, e^{-j\omega L} + v_l\, e^{j\omega L}|_{\Gamma_L} = 0$.
If (u_r, u_l) is an eigensolution of (12) with eigenvalue λ, then $u := u_r\, e^{-j\omega z} + u_l\, e^{j\omega z}$ is an element of H_ω and $a(u,v) = \lambda(u,v)_0$ for all $v \in H_\omega$. For the converse implication, it has to be shown that every eigensolution u of (11) can be represented as $u = u_r\, e^{-j\omega z} + u_l\, e^{j\omega z}$, where (u_r, u_l) fulfill (12). This will also be done in a subsequent paper.

4 Solving the Two–Wave System

In this section, we briefly explain how we approximate the space H_ω and how we obtain a stable finite element discretization. First, let $V_h \subset H^{1,2}(\Omega)$ be the finite

element space of continuous piecewise linear elements on a structured mesh Ω_h of size h. Observe, that here a function $v_h \subset V_h$ is a complex-valued function, since $H^{1,2}(\Omega)$ is a complex valued function space.
Now, let us define the space

$$H_h = \left\{ u_h = (u_{l,h}, u_{r,h}) \in V_h \times V_h \;\middle|\; u_{r,h} + u_{l,h}|_{\Gamma_0} = 0, u_{r,h}\, e^{-j\omega L} + u_{l,h}\, e^{j\omega L}|_{\Gamma_L} = 0 \right\}.$$

Restricting (12) to the space H_h, we obtain the discrete variational problem:
Find $(u_{r,h}, u_{l,h}) \in H_h$ and $\lambda \in \mathbb{C}$ such that

$$\begin{aligned} b_+(u_{r,h}, v_{r,h}) &= \lambda(u_{r,h}, v_{r,h})_0 \\ b_-(u_{l,h}, v_{l,h}) &= \lambda(u_{l,h}, v_{l,h})_0 \end{aligned} \tag{13}$$

for all $(v_{r,h}, v_{l,h}) \in H_h$, where the sesquilinear forms $b_\pm(u, v)$ are defined by

$$b_\pm(u, v) := \int_\Omega \left(\nabla u \nabla \bar{v} + (\omega^2 - n^2 k^2) u \bar{v} \pm 2 j \omega \frac{\partial}{\partial z} u \bar{v} \right) - jk \int_{\Gamma_r} u \bar{v}.$$

To obtain a stable discretization of the large first order terms in the forms $b_\pm(u, v)$, we choose the stream–line diffusion discretization (see e.g. in [?] or [?]). This discretization perturbs $b_\pm(\cdot, \cdot)$ by

$$b_s(u, v) = \alpha \int_\Omega \omega \frac{\partial d}{dz} u\, \omega \frac{\partial d}{dz} \bar{v}$$

where $\alpha := j \frac{\omega}{|\omega|} \max(0, \frac{2|\omega| h - 1}{4|\omega|^2})$. We see, that $|b_s(u, v)|$ tends to 0 as the meshsize h tends to 0.
Thus, we arrive at a non-conform finite element discretization of (13), see e.g. [?],

$$\begin{aligned} b_+(u_{r,h}, v_{r,h}) + b_s(u_{r,h}, v_{r,h}) &= \lambda(u_{r,h}, v_{r,h})_0 \\ b_-(u_{l,h}, v_{l,h}) + b_s(u_{l,h}, v_{l,h}) &= \lambda(u_{l,h}, v_{l,h})_0. \end{aligned}$$

Provisionally, we use the inverse iteration method to compute the eigenvalue of smallest modulus and the corresponding eigenmode. Let $(u_{r,h}^{(i)}, u_{l,h}^{(i)}) \in H_h$ be a normed approximation of the eigenmode. Then, the next approximation is obtained by solving the system

$$\begin{aligned} b_+(u_{r,h}^{(i+1)}, v_{r,h}) + b_s(u_{r,h}^{(i+1)}, v_{r,h}) &= (u_{r,h}^{(i)}, v_{r,h})_0 \\ b_-(u_{l,h}^{(i+1)}, v_{l,h}) + b_s(u_{l,h}^{(i+1)}, v_{l,h}) &= (u_{l,h}^{(i)}, v_{l,h})_0 \end{aligned} \tag{14}$$

for all $(v_{r,h}, v_{l,h}) \in H_h$.
Solving (14) is the crucial part in numerically determining the smallest eigenmode. This is done by preconditioned GMRES (see [?]). The preconditioner consists of a few number of relaxation steps in the direction of the propagation of the waves.

In future, we would like to apply a preconditioner based on multigrid with semi-coarsening in x- and y- direction and line relaxation. In [?], it is proved that such a multigrid algorithm is a robust multigrid algorithm for a convection in pure z-direction. Furthermore, more sophisticated methods for simultaneously determining several eigenvalues will be applied (see e.g. [?]).

5 Numerical Results

In this section we present results for two test problems. The tests will be performed on a cube, i.e. with $L = 1$. But we emphasize, that our method is also applicable to more general domains.
For the first test problem we choose a real parabolic profile for n^2, which is constant in z-direction:

$$n^2 = 1 - c\left((x-0.5)^2 + (y-0.5)^2\right) \tag{15}$$

where $0 \leq c \ll 1$ determines the curvature of the index n^2. Furthermore, we have $k^2 = 98715.789 \approx (100^2 + 2)\pi^2$. Due to lensing effects, we expect that the beam will be narrower for larger c. Figures 2 to 4 show $|u_r|^2$ for different choices of c. The predicted behavior of focusing can easily be observed.
In the second test problem, the curvature declines in z-direction:

$$n^2 = 1 - c(1-0.5z)\left((x-0.5)^2 + (y-0.5)^2\right). \tag{16}$$

Here, we use the parameters $c = 0.1$ and $k^2 = 987.15789$. Figure 5 depicts two orthogonal slices and Figure 6 an isosurface of $|u_r|^2$.
These tests show, that the two–wave approach yields sensible results. Generalizing this ansatz, e.g. for discontinuous indices n^2, will hopefully enable us to simulate lasers more generally than it could not be done until now.

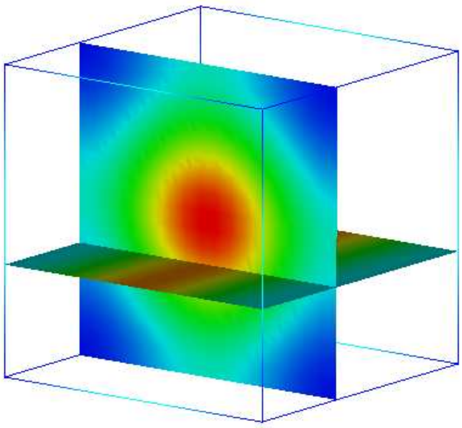

Figure 2: Eigenmode for $c = 0.001$.

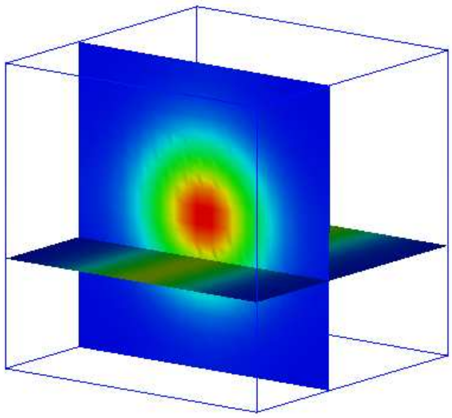

Figure 3: Eigenmode for $c = 0.005$.

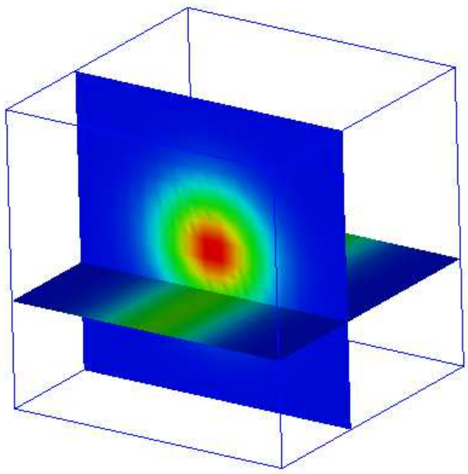

Figure 4: Eigenmode for $c = 0.01$.

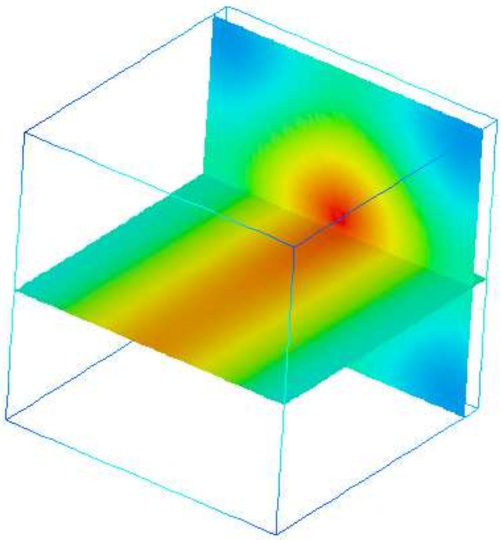

Figure 5: Result for Second Test Problem

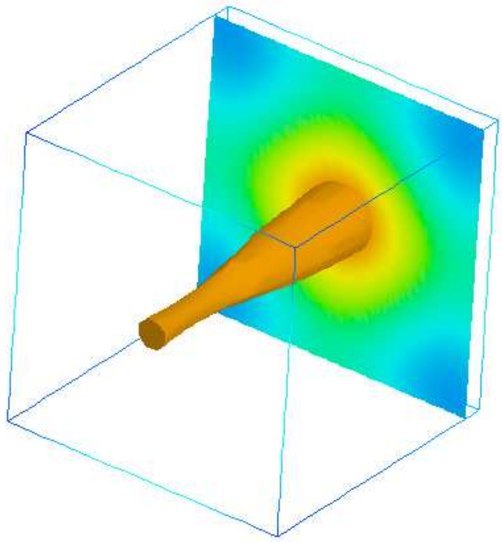

Figure 6: Isosurface for Second Test Problem