On Fully Discrete Finite Element Schemes for the Fermi and Fokker-Planck Pencil-beam Equations

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Overview

Introduction

A model for the calculation of the dose (energy deposited per unit mass):

$$\begin{cases} W_x + zW_y = \epsilon W_{zz}, & (x, y, z) \in \Omega = I_x \times I_\perp, \\ W_z(x, y, \pm z_0) = 0 & \text{for } (x, y) \in I_x \times I_y, \\ W(0, x_\perp) = f(x_\perp), & \text{for } x_\perp \equiv (y, z) \in I_\perp \\ W(x, x_\perp) = 0 & \text{on } \Gamma_\beta^-(0, x_\perp). \end{cases} \tag{1}$$

The problem is formulated for the flux W and measure of interest for nuclear engineers.

Motivation

- Many people get some kinds of cancer in their lives.
- One person in 5 will die from that cancer.
- Cancer is one of the biggest causes of death.
- Almost half of the cancer patients receive radiation therapy.
- Any kind of improvement in Radiotherapy will benefit a large number of people.

Radiation cancer therapy

- Internal Radiotherapy
  The patients will take liquid source of radiation in their body.
  Through mouth or by injection into a vein.
- External Radiotherapy
  The machine gives high energy radiation such as x-rays to the cancer part of body and a small area of normal tissue surrounding it.
- Mathematical view of radiotherapy
  In mathematical modeling , one important aspect should be discussed which is calculation of radiation dose which gives information about energy absorbed per unit mass in tissue layers and after this calculation the result is **dose** function which helps doctors to know amount of radiation to give to tumor in patient.

Aim

- To remove the oscillatory behavior and formation of layers in a solution with hyperbolic and maxwellian initial conditions
- Issues
  These oscillations can come from several issues, such as mesh density and time stepping, but also from numerical issues such as underflow and overflow, as well as the scaling of the variables.

The monoenergetic transport equation

let $X \in \tilde{Q} := [0, L] \times R \times R$ a homogeneous slab, and $\omega \in S^2$, consider the equation

$$\omega \cdot \nabla_X \psi(X, \omega) + \sigma_t(X)\psi(X, \omega) = \int_{S^2} \sigma_s(X, \omega.\omega')\psi(X, \omega)d\omega' \tag{2}$$

With in- and out-flow boundary conditions

$$\begin{cases} \psi(L, y, z, \omega) = 0 & \text{if } \xi < 0 \\ \psi(0, y, z, \omega) = \frac{1}{2\pi}\delta(1 - \xi)\delta(y)\delta(z) & \text{if } \xi > 0, \end{cases} \tag{3}$$

The monoenergetic transport equation

With $X = (x, y, z) \in \tilde{Q}, \omega = (1, \eta, \zeta) \in S^2$ describing the spreading of a pencil beam of particles normally incident at the boundary (0, y, z) of the slab $\tilde{Q}$. ψ is the density of the particles at the point X moving in the direction of ω. σ_t is the total cross section and σ_s is the scattering cross section.

The Fermi-pencil beam equation

The Fermi equation is derived from the Fokker-Planck equation.

$$\begin{cases} \omega_0 \cdot \nabla_X \psi^F = \sigma \Delta_{\eta,\zeta} \psi^F, & \\ \psi^F(L, y, z, \eta, \zeta) = 0 & \text{if } \xi < 0 \\ \psi^F(0, y, z, \eta, \zeta) = \delta(y)\delta(z)\delta(\eta)\delta(\zeta) & \text{if } \xi > 0, \end{cases} \tag{4}$$

where $\omega_0 = (1, \eta, \zeta)$, $(\eta, \zeta) \in R \times R$ and $\Delta_{\eta,\zeta} = \partial^2/\partial\eta^2 + \partial^2/\partial\zeta^2$.

A Model problem

$$\begin{cases} W_x + zW_y = \epsilon W_{zz}, & (x, y, z) \in \Omega = I_x \times I_\perp \\ W_z(x, y, \pm z_0) = 0 & \text{for } (x, y) \in I_x \times I_y, \\ W(0, x_\perp) = f(x_\perp), & \text{for } x_\perp \in I_\perp \\ W(x, x_\perp) = 0 & \text{on } \Gamma_\beta^-(0, x_\perp). \end{cases} \tag{5}$$

Where $\Gamma_\beta^- := \{(x, x_\perp) \in \partial\Omega : \beta.\ \mathbf{n} < 0\ \}, \beta = (1, z, 0)$, and $x_\perp \equiv (y, z)$ is the transversal variable. Also $\mathbf{n} := n(x, x_\perp)$ is the outward unit normal to Γ at $(x, x_\perp) \in \Gamma$.
Our model problem is Fermi equation which is a forward-backward (z changes the sign), convection dominated (ϵ is small),convection-diffusion equation of degenerate type (convection is in (x, y) and diffusion in z).

We define the discrete trial function space $V_{h,\beta}$ as
$V_{h,\beta} \subset H^1_\beta(D_\perp)$ such that

$$H^1_\beta(D_\perp) = \left\{ v \in H^1(D_\perp) : v = 0 \text{ on } \Gamma^-_\beta \{(0, x_\perp)\} \right\}. \tag{6}$$

FEM formulation for (5) is
find a solution $u_h \in V_{h,\beta}$ of (5) such that,

$$\begin{cases} A(u_h, \chi)_\perp + (\epsilon u_{h,z}, \chi_z)_\perp = 0 \quad \forall \chi \in V_{h,\beta}, \\ u_h(0, \chi_\perp) = f_h(x_\perp). \end{cases} \tag{7}$$

where $A(\cdot, \cdot)$ is defined as,

$$A(u, v) = (u_x, v)_\perp + (z u_y, v)_\perp, \ \ \forall\ u, v \in V_{h,\beta} \tag{8}$$

Where f_h is a finite element approximation of f. Further the mesh size h should be chosen such that

$$h^2 \leq \epsilon \leq h. \tag{9}$$

The standard finite element discretization

One approach that corresponds to add of extra diffusion is the SSD scheme:
Let

$$a(w,v) = (w_\beta, v)_\perp + \delta(w_\beta, v_\beta)_\perp + (\epsilon w_z, v_z)_\perp + \delta(\epsilon w_z, (v_\beta)_z)_\perp \tag{10}$$

$$b(w,v) = \delta(w, v_\beta)_\perp + (w,v)_\perp, \tag{11}$$

Then we write the problem as,

$$(SSD) \begin{cases} \text{Find a solution } w \in H^1_\beta(I_\perp) \text{ such that}, \\ b(w_x, v) + a(w,v) = 0, \quad \forall\ v \in H^1_\beta(I_\perp). \end{cases} \tag{12}$$

The standard finite element discretization

Let $w_h \in V_{h,\beta}$ be the discrete solution. We represent w_h by separation of variables

$$w_h(x, y, z) = \sum_{i=1}^{M} \xi_i(x)\phi_i(y, z), \tag{13}$$

where $M \sim 1/h$. Letting $v = \phi_j$ for $j = 1, 2, \ldots, M$ and inserting (13) in (12) we get the discretization method,

$$\sum_{i=1}^{M} \xi_i'(x) b(\phi_i, \phi_j) + \sum_{i=1}^{M} \xi_i(x) a(\phi_i, \phi_j) = 0 \qquad j = 1, 2, \ldots, M \tag{14}$$

In matrix form this can be written as

$$B\xi'(x) + A\xi(x) = 0 \tag{15}$$

The standard finite element discretization

We discretize in x direction and use backward Euler method get the fully discrete scheme.

$$B(\xi^n - \xi^{n-1}) + k_n A \cdot \xi^n = 0. \tag{16}$$

backward Euler can be recognized by

$$[B + k_n A]\xi^n = B \cdot \xi^{n-1} \tag{17}$$

Here $B = (b_{ij})$ with matrix entries $b_{ij} = b(\phi_i, \phi_j)$ and $A = (a_{ij})$ with matrix elements $a_{ij} = a(\phi_i, \phi_j)$.
Other fully discrete schemes can be obtained depending on the choice of the discretization method in the direction of x.

The energy equation in COMSOL

Consider the convection diffusion equation as

$$d_a \frac{\partial u}{\partial t} + \beta.\nabla u = \nabla.(c\nabla u) + F, \tag{18}$$

and our Fermi pencil-beam equation is.

$$W_x + zW_y = \epsilon W_{zz}, \tag{19}$$

The parameters β and c refer to the convective velocity and the diffusion coefficient respectively. In our case we took F(source term) =0. This equation could represent the energy equation, that means the heat transfer equation, mass transfer equations used for the transfer of chemical spices, Navier-Stokes equations for the transport of momentum in fluids, in our case Fermi equation for the transport of electrons and protons.

Numerical results

- Exact solution
  The closed form exact solution of our model problem (5) is given by

$$W(x,y,z) = (\sqrt{3}/(\pi\varepsilon x^2))\exp^{-2(3(y/x)^2-3(y/2)z+z^2)/(\varepsilon x)} \tag{20}$$

$(y,z) \in [-1,1]\times[-1,1]$

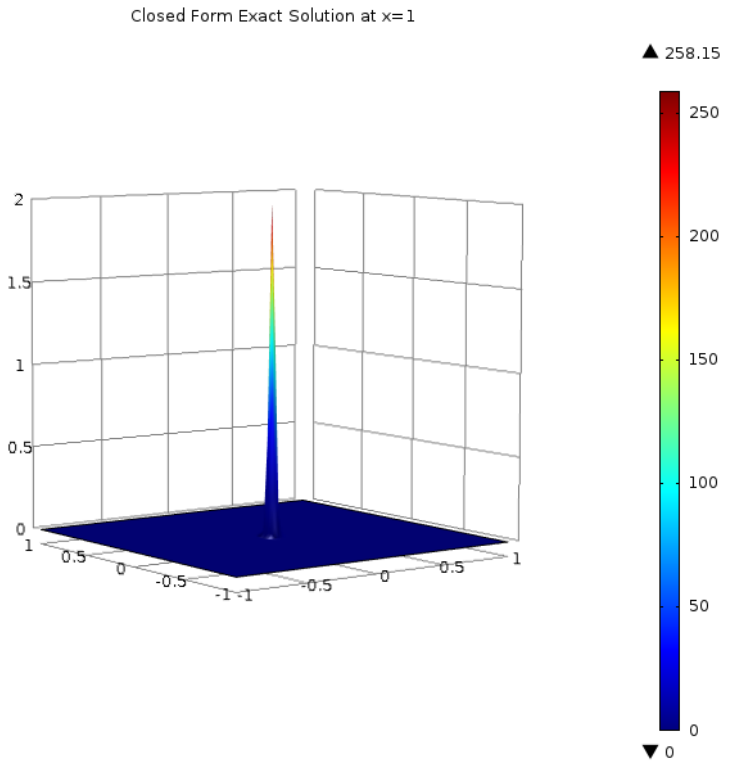


Figure: This is the exact solution of Fermi pencil beam obtained at x =1

Numerical results

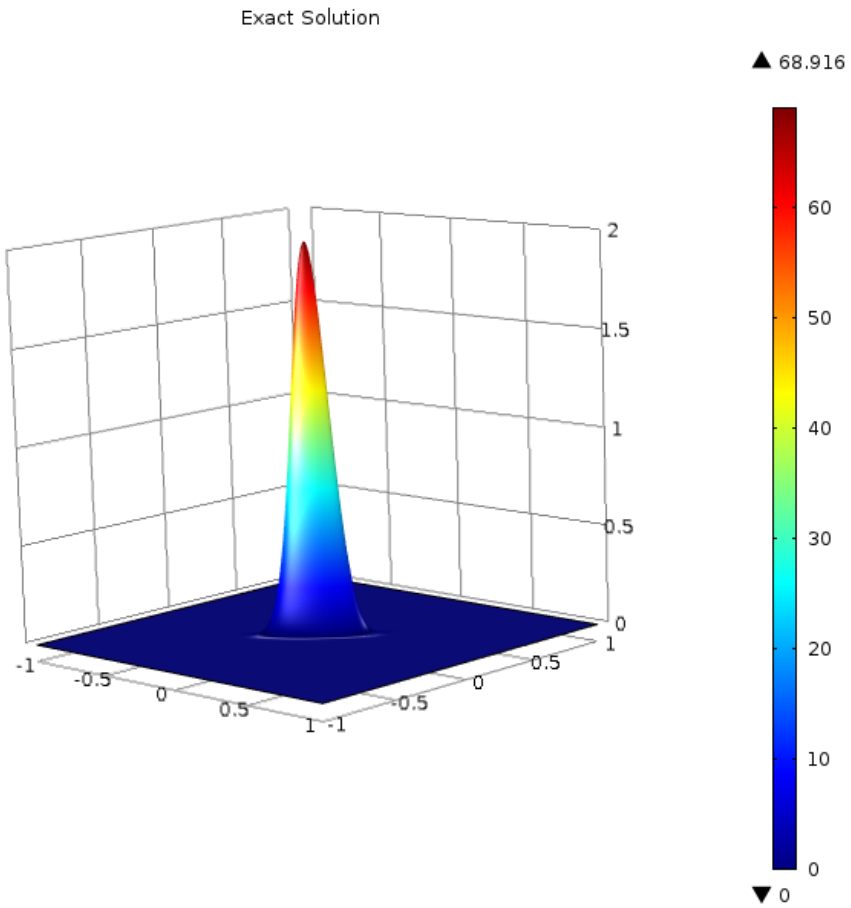


Figure: Exact solution of Fermi pencil beam at x =2

The closed form exact solution when $x = 1$ gives us thin electron beam, so it will cover less area. while when $x = 2$ this gives us thicker beam which means that more area can be covered.

Numerical results

- Geometry

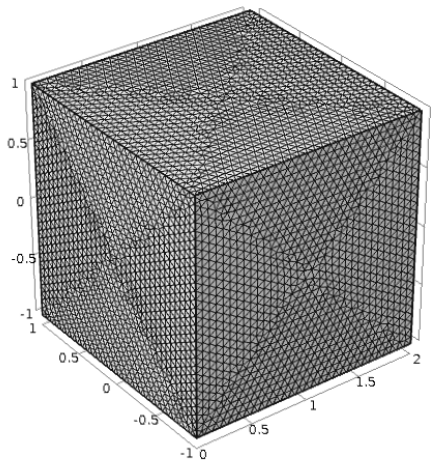


Figure: Example of a three dimensional geometry which we used for getting our numerical results in 3d.

Above example is a cube represented in three dimension and we take it as our domain which we work on it to get the numerical results represented in 3d. The position of cube is $[1, 0, 0]$. So our total number of boundaries in this case is 6 and domain is 1. Number of edges are 12 and the number of vertices 8. The length units are meter and the angular units are degree. Size of the cube is $[2, 2, 2]$ and axis type is x-axis.

Meshing

Whenever use the finite element method, it is important to remember that the accuracy of solution is linked to the mesh size. As mesh size decreases towards zero (leading to a model of infinite size), we move toward the exact solution for the equations we are solving. However, since we are limited by finite computational resources and time, we will have to rely on an approximation of the real solution. The goal of simulation, therefore, is to minimize the difference (error) between the exact and the approximated solution, and to ensure that the error is below some accepted tolerance level

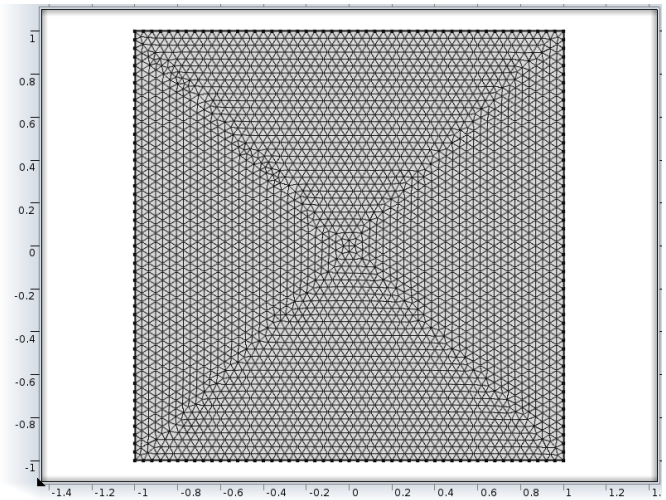


Figure: Mesh in two dimensional figure

Property	Value
Minimum element quality	0.3414
Average element quality	0.9185
Triangular elements	26440
Edge elements	108
Vertex elements	4

Table: Mesh statistics

Element quality

By default, poor quality elements are those having one or more of the following:

- Ratio of maximum side length to minimum side length is larger than 10.
- Minimum interior angle is smaller than 20 degree.
- Maximum interior angle is larger than 120 degree.

Element quality

The element quality q for triangle is obtained by

$$q = \frac{4\sqrt{3}A}{h_1^2 + h_2^2 + h_3^2} \tag{21}$$

where A denote the area and h_1, h_2, h_3 the side-lengths.
For a tetrahedron the quality measures is evaluated using the formula

$$q = \frac{72\sqrt{3}V}{(h_1^2 + h_2^2 + h_3^2 + h_4^2 + h_5^2 + h_6^2)^{\frac{3}{2}}} \tag{22}$$

where V denotes the volume, and the h:s are the edge lengths.

Meshing

- refinement

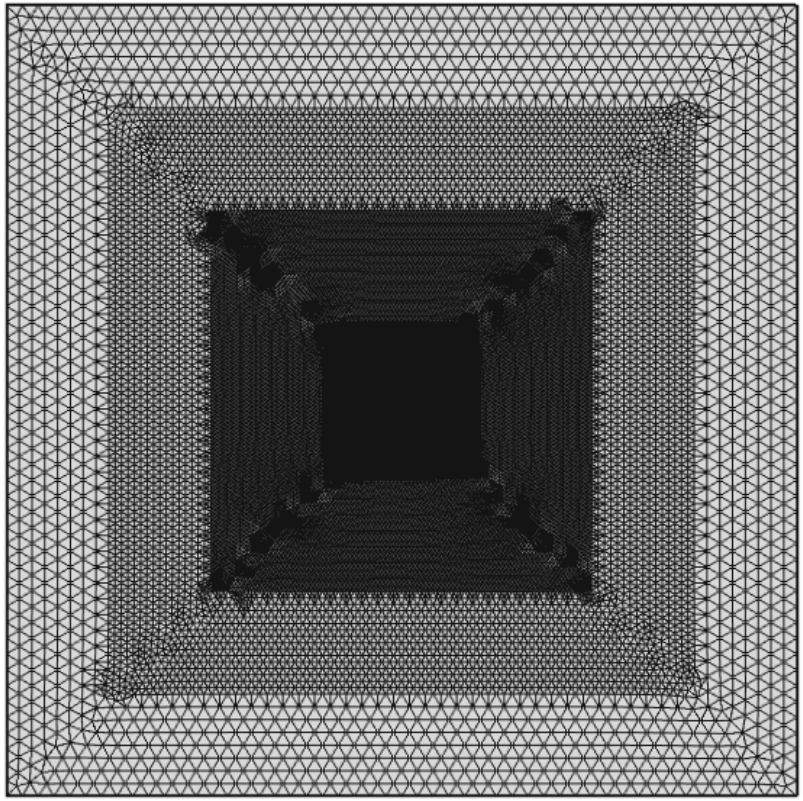


Figure: We used "fine" mesh size with one refinement in -0.25 to 0.25 and then another refinement from -0.5 to 0.5, finally a refinement from -0.75 to 0.75.

Most numerical simulation methods(finite element, finite difference, finite volume) require stabilization methods when modeling transport applications driven mainly by convection rather than diffusion. With FEM stabilization means adding small amount of artificial diffusion.

Numerical results

- Justification of our implementation done in COMSOL Multiphysics and LIVE LINK MATLAB.
- Goal : To decrease formation of layers behavior of the Maxwellian initial data
- Layers associated with large steps in x.

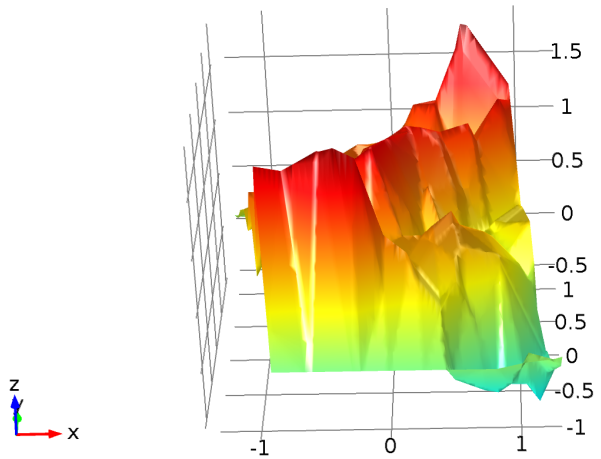


Figure: Formation of layers in a computed solution with maxwillian initial condition

Numerical results

- Solution with maxwillian initial condition using two dimensional model.

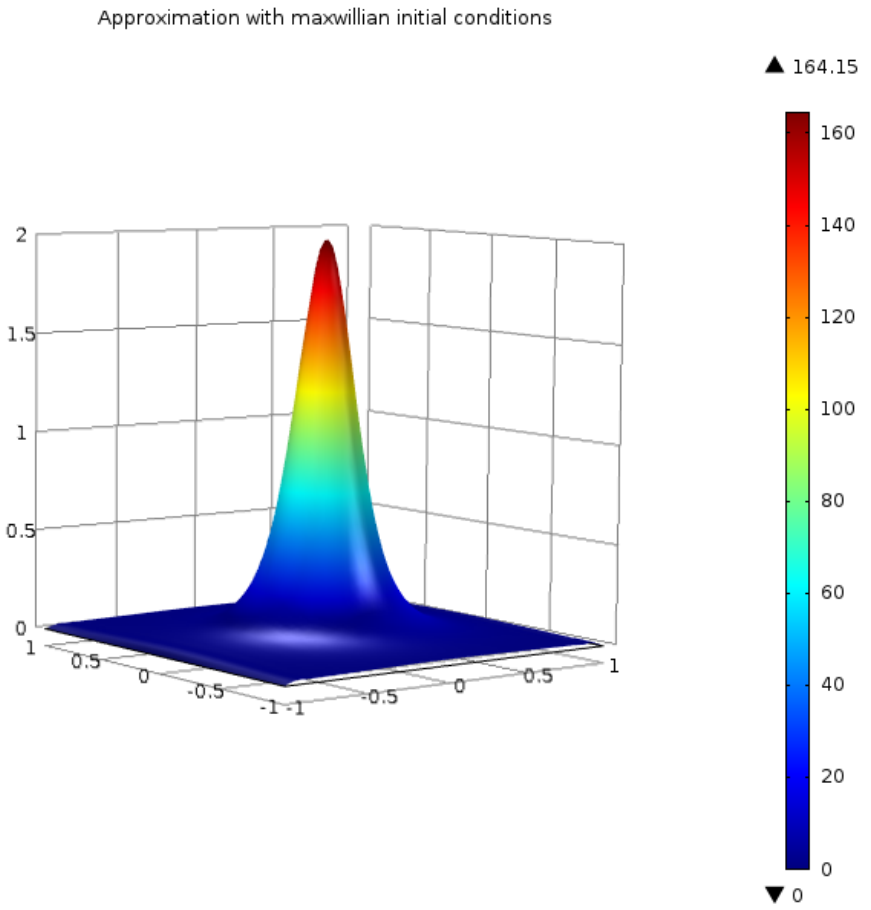


Figure: Computed solution of our model problem with Maxwellian initial conditions

Numerical results

- The exact solution of (20) of fermi pencil-beam obtained in same model in which we calculated the computed solution.

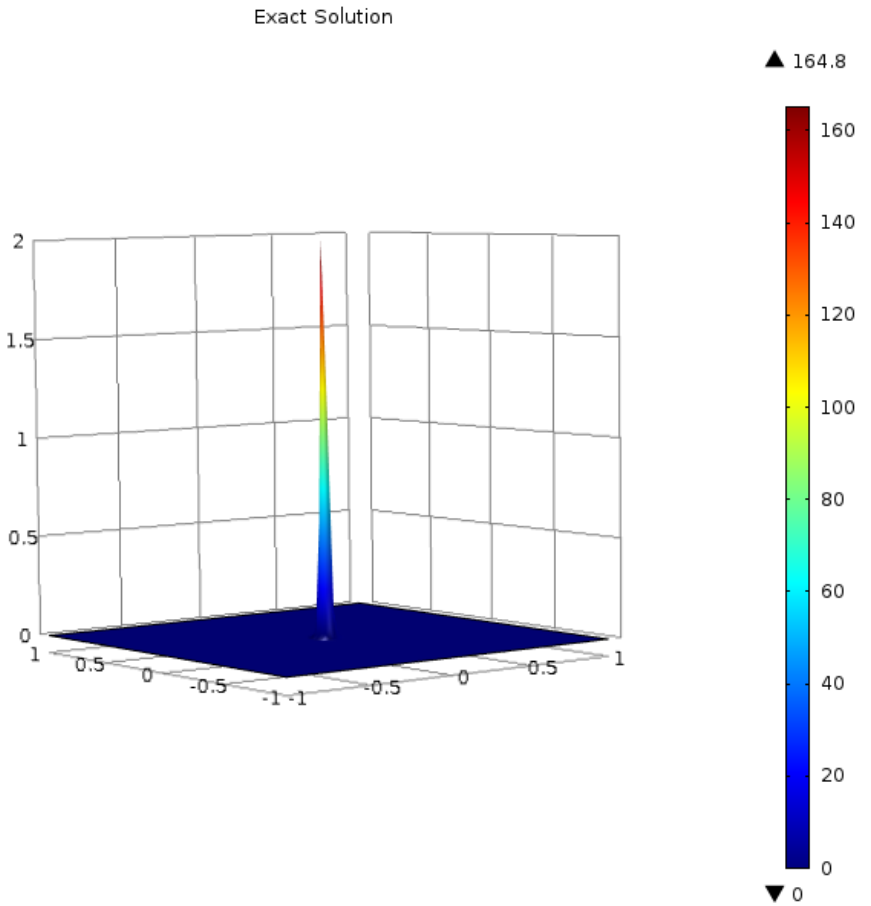


Figure: The exact solution of (20)

Numerical results

- Computed solution in three dimensional model.

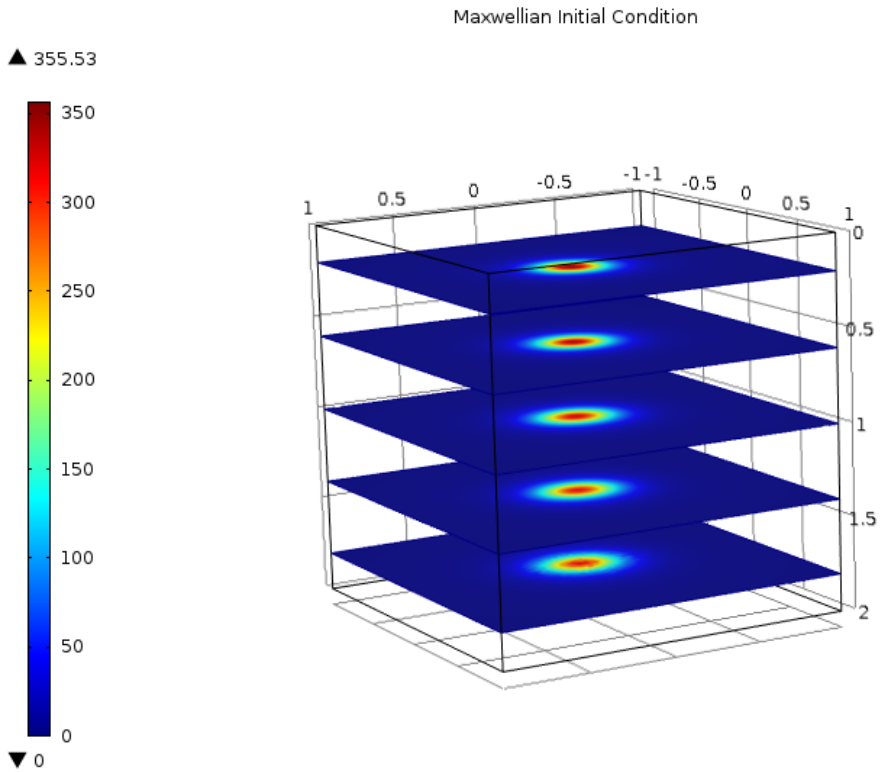


Figure: Computed solution for model problem with Maxwellian initial condition.

Here we use $f = \exp(-(y^2 + z^2) + \alpha)$ with $\alpha = 0.16$ in order to avoid oscillations when both y and z are equal to 0.

Numerical results

- The exact solution of (20) for the three dimensional model.

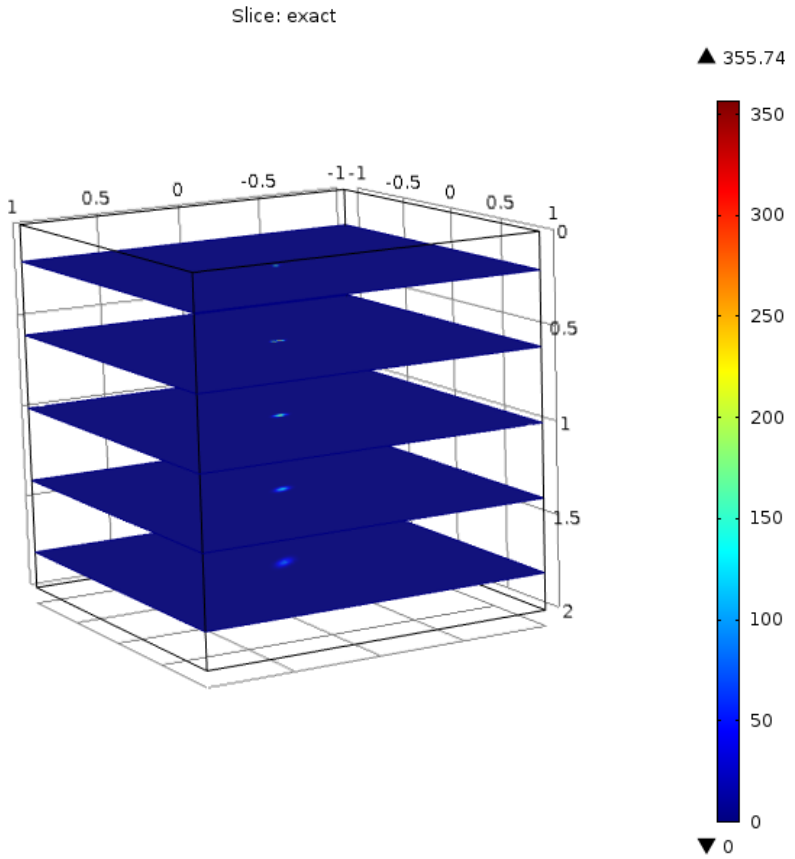
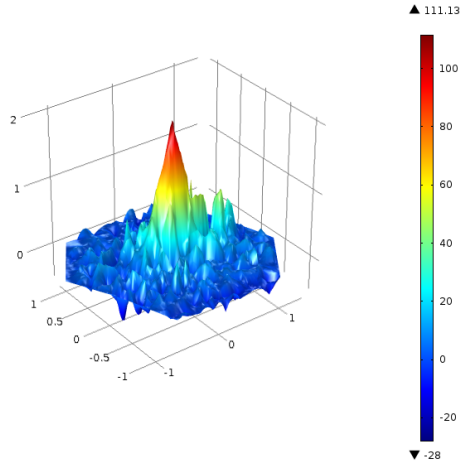


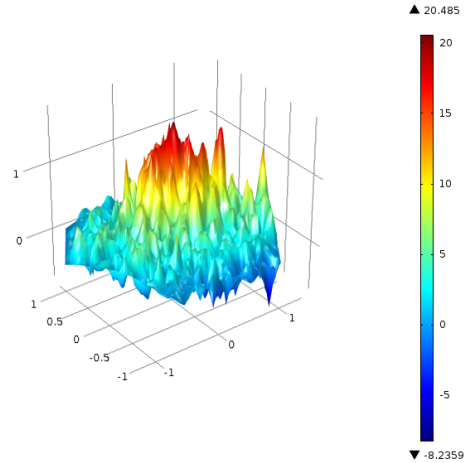
Figure: Computed solution for model problem with Maxwellian initial condition.

Here we use $f = \exp(-(y^2 + z^2) + \alpha)$ with $\alpha = 0.16$ in order to avoid oscillations when both y and z are equal to 0.

Hyperbolic initial condition.



(a) Oscillatory behavior of the computed solution with hyperbolic initial condition



(b) Oscillatory behavior of the computed solution with hyperbolic initial condition

Hyperbolic initial condition.

- Computed solution in two dimensional model with hyperbolic initial condition.

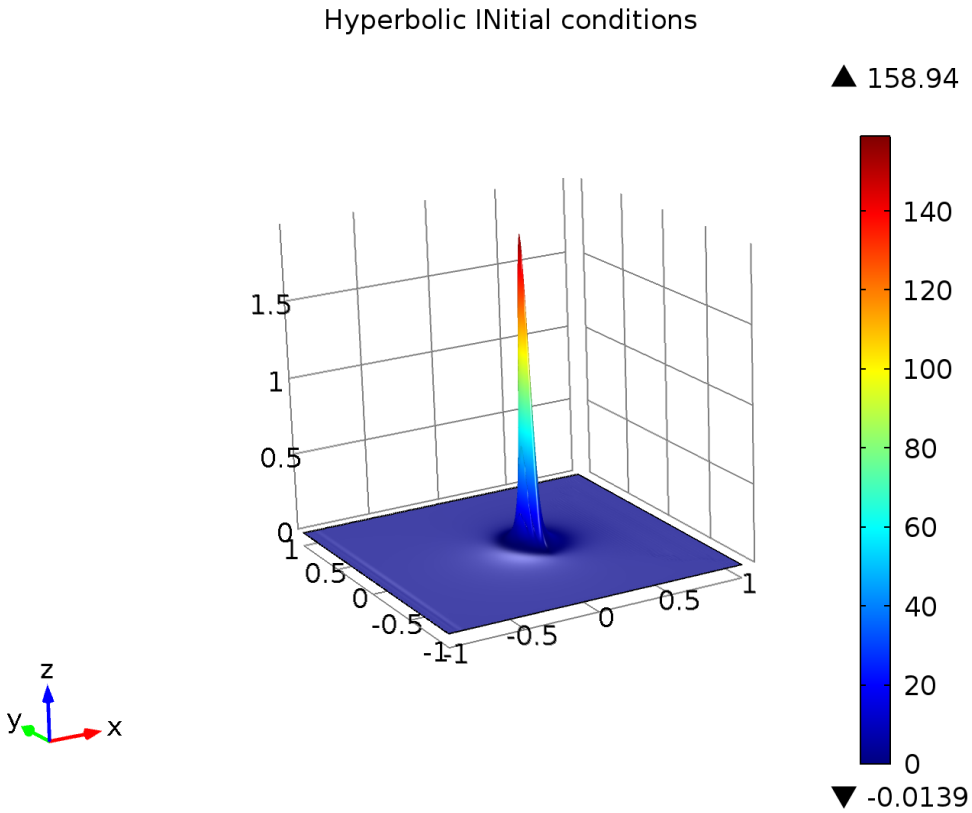


Figure: Computed solution for model problem with hyperbolic initial condition.

In hyperbolic initial condition, the function $f = \frac{1}{\sqrt{x^2+y^2+\alpha}}$ is used and α is 0.19 to avoid having the value of denominator of f equal to 0.

Dirac-I initial condition.

- Computed solution in two dimensional model.

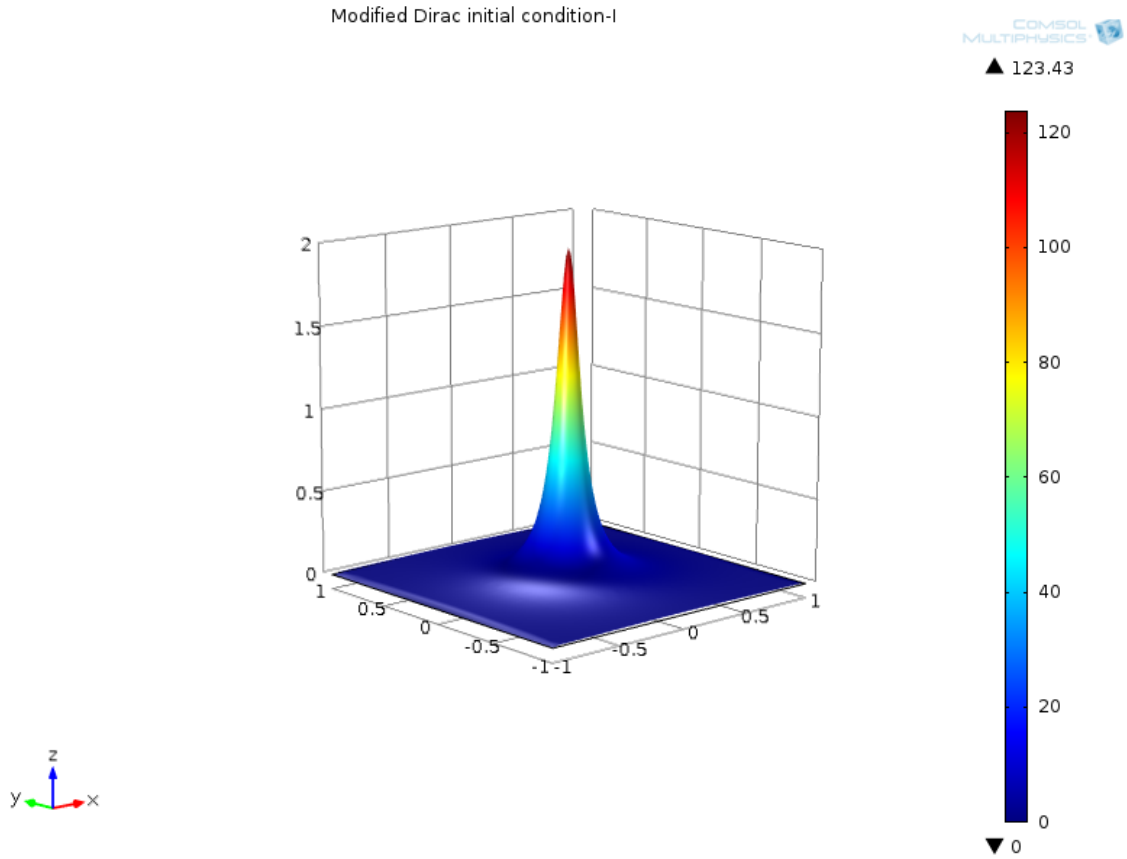


Figure: Computed solution with hyperbolic initial condition.

Computed solution at t = 1.5 of model problem (5) with the Dirac-I initial condition, function $f = 1/(x^2 + y^2 + \alpha)$ and the α is used to avoid undefined value of f at $(x, y) = (0, 0)$.

Discretization

Linear Lagrange shape function representation is to control the material density in our model, the solution contains the sensitivity of the objective function with respect to the discrete density value at each node point in the mesh. Because each node influences the density in a small surrounding region, the size of which varies from node to node, the individual sensitivities are not directly comparable to each other.

Dirac-I initial condition.

- Computed solution in three dimensional model viewed in slab form (Level sets).

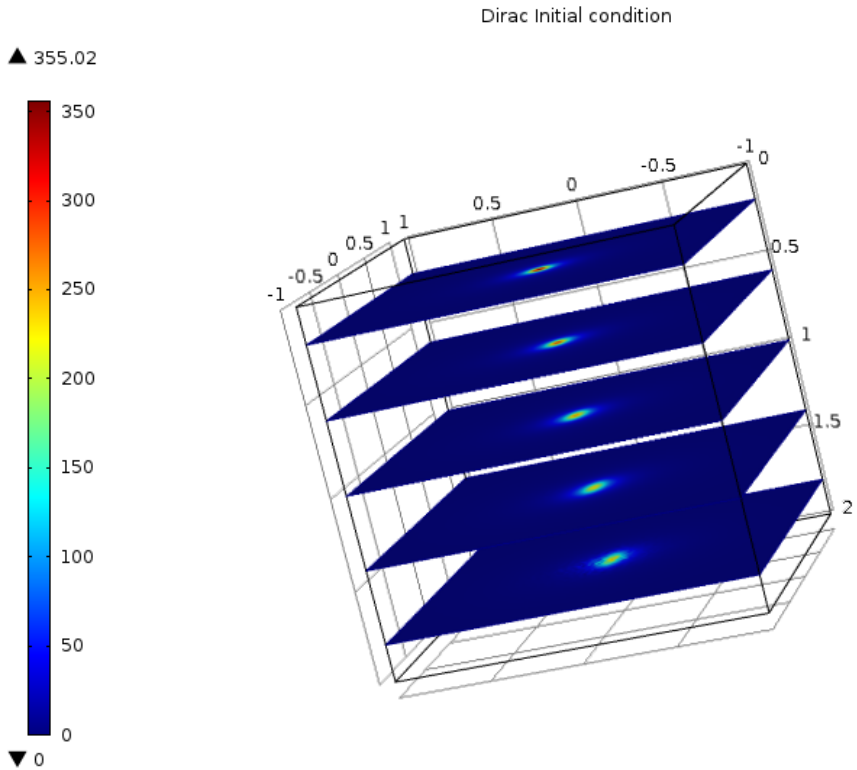


Figure: Computed solution for model problem with $Dirac - I$ initial condition.

In Dirac initial condition, the function $f = 1/(y^2 + z^2 + \alpha)$ is used,where $\alpha = 0.2$ is added in order to avoid having the value of denominator of f equal to 0.

Dirac-I initial condition.

- Computed solution in three dimensional model in height form.

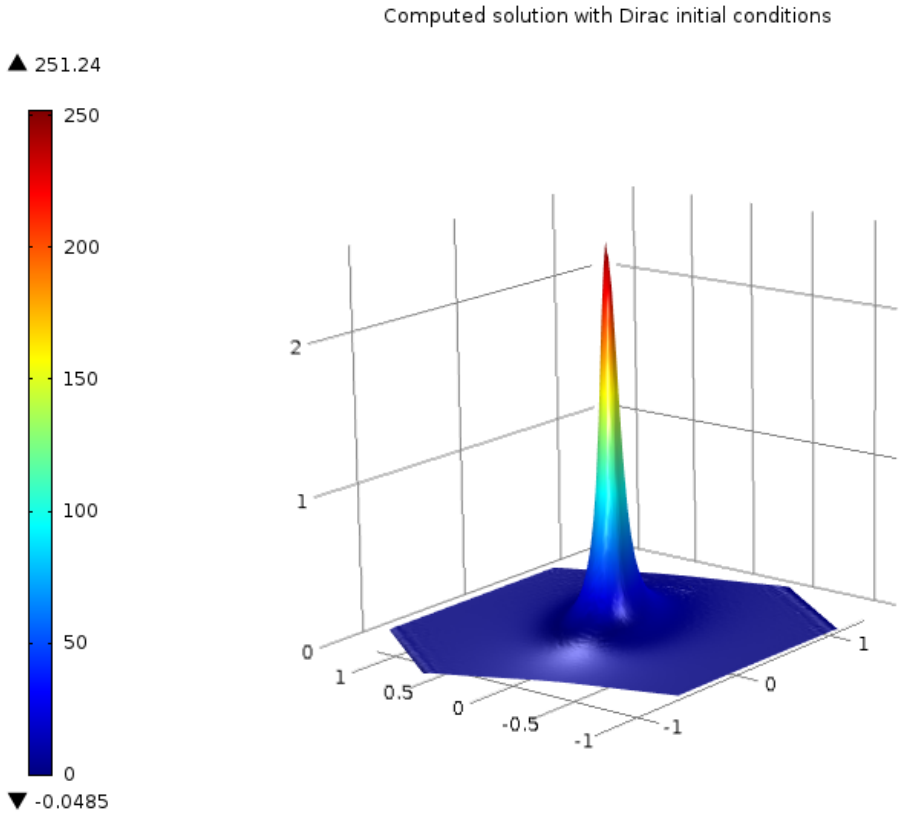


Figure: Computed solution for model problem with $Dirac - I$ initial condition.

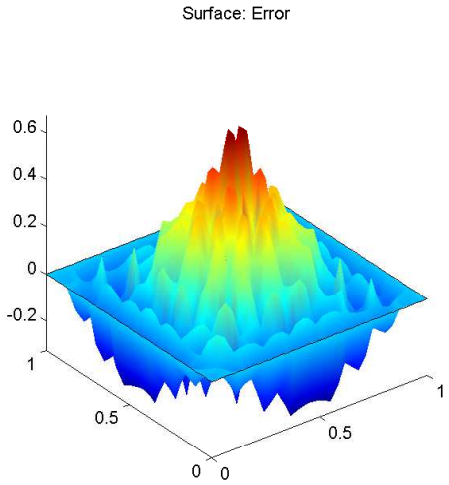
In Dirac initial condition, the function $f = 1/(y^2 + z^2 + \alpha)$ is used, where $\alpha = 0.2$ is added in order to avoid having the value of denominator of f equal to 0.

Convergence study.

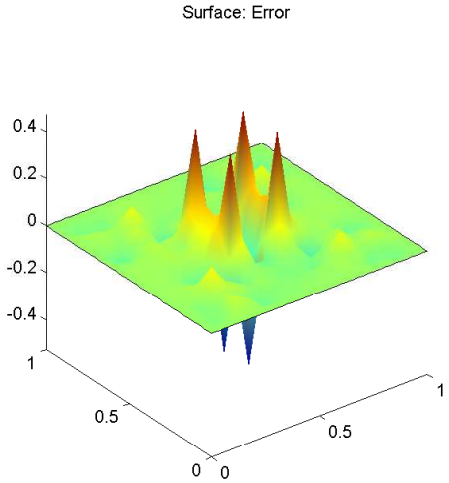
Number of refinement	Element	Vertices	DOF	Error	Sq.Error	ratio of error
0	272	157	157	8.278e-03	6.853e-05	0.00
1	1088	585	585	2.105e-03	4.431e-06	3.93
2	4352	2257	2257	5.290e-04	2.799e-07	3.98
3	17408	8865	8865	1.325e-04	1.754e-08	3.99
4	69632	35137	35137	3.313e-05	1.097e-09	4.00

Table: Table for Lagrange elements with p=1

Convergence study.

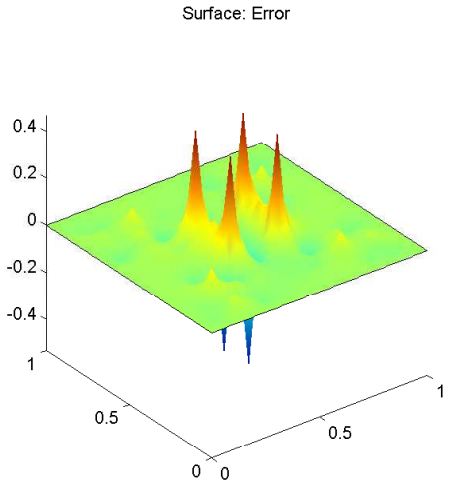


(a) Error view with no refinements

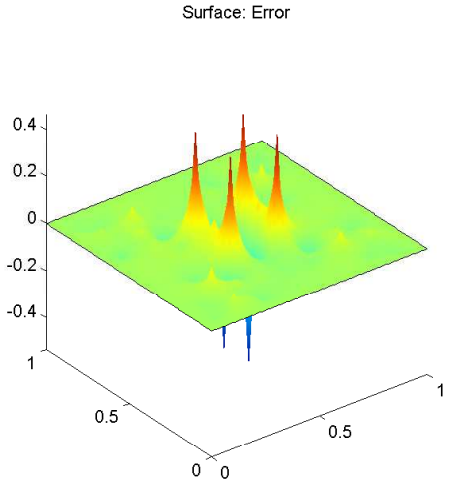


(b) error view with 1 refinements

Convergence study.



(a) Error view with 2 refinements



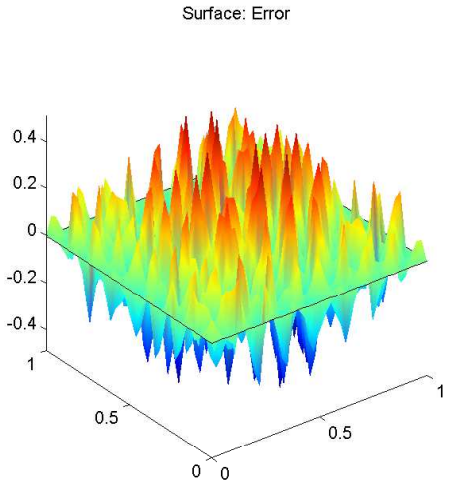
(b) error view with 3 refinements

Convergence study.

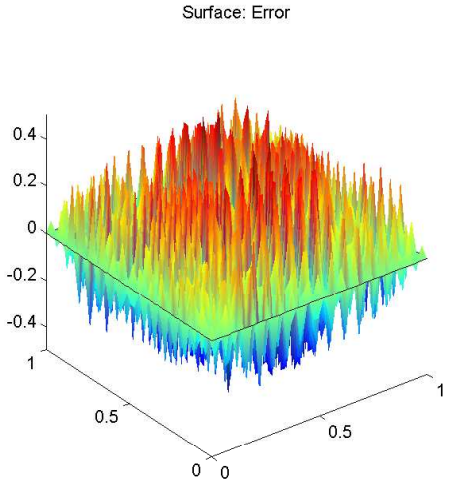
Number of refinement	Element	Vertices	DOF	Error	Sq.Error	ratio of error
0	272	157	585	2.706e-04	7.322e-08	0.00
1	1088	585	2257	3.427e-05	1.175e-09	7.90
2	4352	2257	8865	4.307e-06	1.855e-11	7.96
3	17408	8865	35137	5.398e-07	2.913e-13	7.98
4	69632	35137	139905	6.755e-08	4.564e-15	7.99

Table: Table for Lagrange elements with p=2

Convergence study.

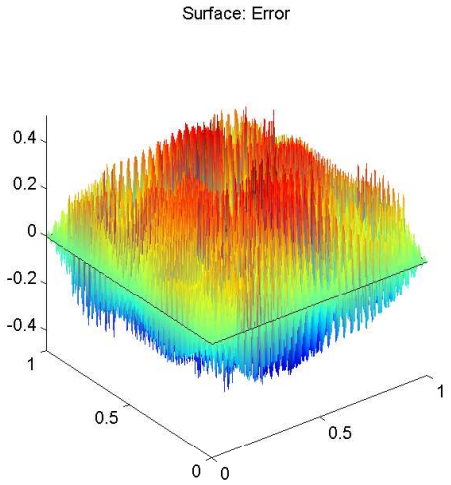


(a) Error view with no refinements

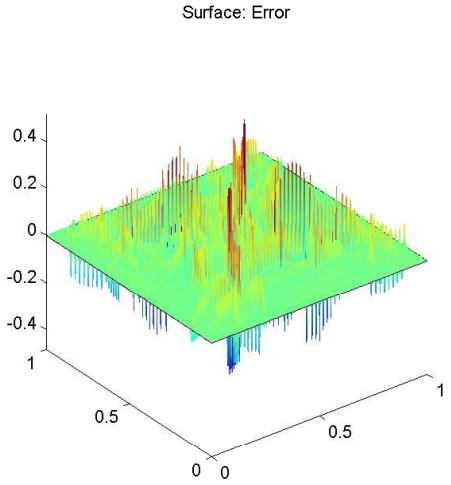


(b) error view with 1 refinements

Convergence study.



(a) Error view with 2 refinements



(b) error view with 3 refinements

Error norms

L_2	Maxwellian	Hyperbolic	Dirac-I	Dirac-II
SSD	0.24	0.18	0.19	18
CSD	0.21	0.10	0.11	9.6
CG	0.19	0.22	0.21	14

Table: Errors: differences from the initial conditions used for FEM, we calculated the error in L_2.

Convergence study.

- Convergence study with respect to element order

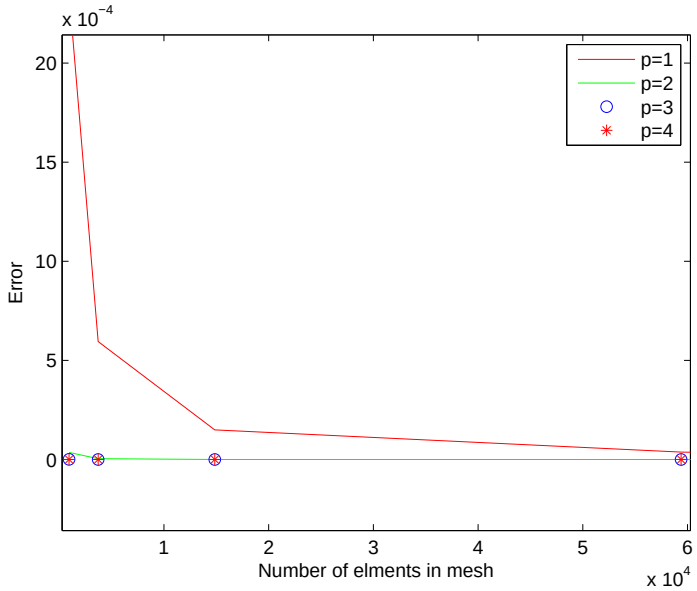


Figure: Convergence study plot.

Convergence study for the Fermi equation, In the figure above we have number of nodes(elements) on the X-axis and the error on Y-axis. From the figure we can see by increasing the spectral order (p) gives faster convergence.

Thank you for your attention