

# Software Requirements Specification for SPDFM: Surface Plasmon Dynamics Finite Method (SPDFM)

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## Revision History

Date	Version	Notes
8/10/2020	1.0	First Draft

# 1 Reference Material

This section records information for easy reference.

## 1.1 Table of Units

Throughout this document SI (Système International d'Unités) is employed as the unit system. In addition to the basic units, several derived units are used as described below. For each unit, the symbol is given followed by a description of the unit and the SI name.

symbol	unit	SI
m	length	metre
$\text{m}^{-1}$	reciprocal metre	wave number
s	time	second
$\text{m s}^{-1}$	velocity	metre per second
kg	mass	kilogram
$\text{s}^{-1}$	frequency	hertz
$\text{V m}^{-1}$	electric field strength	volt per meter
$\text{A m}^{-2}$	electric current density	ampere per square metre
$\text{F m}^{-1}$	permittivity	farad per metre
$\text{H m}^{-1}$	permeability	henry per metre

## 1.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units if applicable.

symbol	unit	description
$\mathbf{B}$		Basis of the Cartesian space $\in \mathbb{R}^3$
$\mathbf{u}_x$		Unitary vector of basis $\mathbf{B} \in \mathbb{R}$
$\mathbf{u}_y$		Unitary vector of basis $\mathbf{B} \in \mathbb{R}$
$\mathbf{u}_z$		Unitary vector of basis $\mathbf{B} \in \mathbb{R}$
$\mathbf{E}$		3D electric field vector $\in \mathbb{C}^3$
$\mathbf{E}_x$	$\text{V m}^{-1}$	Electric field strength along $\mathbf{u}_x \in \mathbb{C}$
$\mathbf{E}_y$	$\text{V m}^{-1}$	Electric field strength along $\mathbf{u}_y \in \mathbb{C}$
$\mathbf{E}_z$	$\text{V m}^{-1}$	Electric field strength along $\mathbf{u}_z \in \mathbb{C}$
$\mathbf{E}_i$		3D electric field vector of an incident light $\in \mathbb{C}^3$
$\mathbf{J}_{HD}$		3D hydrodynamic electric current density vector $\in \mathbb{C}^3$

$\mathbf{J}_{HD,x}$	$\text{A m}^{-2}$	Component of hydrodynamic electric current density along $\mathbf{u}_x \in \mathbb{C}$
$\mathbf{J}_{HD,y}$	$\text{A m}^{-2}$	Component of hydrodynamic electric current density along $\mathbf{u}_y \in \mathbb{C}$
$\mathbf{J}_{HD,z}$	$\text{A m}^{-2}$	Component of hydrodynamic electric current density along $\mathbf{u}_z \in \mathbb{C}$
$\varepsilon_0$	$\text{F m}^{-1}$	Permittivity constant $\in \mathbb{R}$
$\varepsilon_{loc}$	$\text{F m}^{-1}$	Permittivity of the local response $\in \mathbb{C}$
$\mu_0$	$\text{H m}^{-1}$	Permeability constant $\in \mathbb{R}$
$\nu_F$	$\text{m s}^{-1}$	Fermi velocity $\in \mathbb{R}$
$\beta$		Fermi velocity proportionality constant $\in \mathbb{R}$
$\omega_p$	$\text{s}^{-1}$	Plasma frequency of the free electron gas $\in \mathbb{R}$
$\omega$	$\text{s}^{-1}$	Angular frequency of the propagating wave $\in \mathbb{R}$
$t$	$\text{s}$	Time variable $\in \mathbb{R}$
$\mathbf{p}$		Polarization vector of the incident light in 3D space $\in \mathbb{R}^3$
$p_x$		Component of polarization vector of the incident light along $\mathbf{u}_x \in \mathbb{R}$
$p_y$		Component of polarization vector of the incident light along $\mathbf{u}_y \in \mathbb{R}$
$p_z$		Component of polarization vector of the incident light along $\mathbf{u}_z \in \mathbb{R}$
$\mathbf{d}$		Unit direction vector of the incident light in 3D space $\in \mathbb{R}^3$
$d_x$		Component of unit direction vector of the incident light along $\mathbf{u}_x \in \mathbb{R}$
$d_y$		Component of unit direction vector of the incident light along $\mathbf{u}_y \in \mathbb{R}$
$d_z$		Component of unit direction vector of the incident light along $\mathbf{u}_z \in \mathbb{R}$
$\lambda$	$\text{m}$	Wavelength of the incident light $\in \mathbb{R}$
$k$	$\text{m}^{-1}$	Wave number of the incident light $\in \mathbb{R}$
$i$		Imaginary unit $\in \mathbb{C}$
$\mathbf{r}$		Displacement vector in 3D space $\in \mathbb{R}$
$\varnothing()$	$\text{m}$	Diameter operator (length of the largest diameter in a geometry) $\in \mathbb{R}$
$e$		Exponential operator
$\nabla$		Gradient operator
$\times$		Cross product operator
$\cdot$		Dot product operator
$\Omega$		Finite 3D meshed volume
$\partial\Omega$		2D meshed boundary
$DtN$		Dirichlet to Neumann operator

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### 1.3 Abbreviations and Acronyms

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symbol	description
A	Assumption
DD	Data Definition
GD	General Definition
GS	Goal Statement
IM	Instance Model
LC	Likely Change
PS	Physical System Description
R	Requirement
SRS	Software Requirements Specification
SPDFM	Surface Plasmon Dynamics Finite Method
T	Theoretical Model

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## 2 Introduction

Surface plasmon activities are known as a bridge between the photonic realm and electronic physics. This material property that exist in some materials has opened new doors into the design of novel systems that work based on photon/electron interactions such as photocatalytic and optoelectronic systems. Therefore, it is a paramount importance to study the impact of surface plasmon activities on the electronic parameters in the material. This document provides the Software Requirements Specification (SRS) for a software designed to calculate the electric field and electric current density generated due to surface plasmon excitation in an arbitrary geometry.

### 2.1 Purpose of Document

The purpose of this document is to provide a detailed description of functional and the non-functional requirements of the Surface Plasmon Dynamics Finite Method (SPDFM) software. The theoretical models on which the requirements are based on are also described to provide the context of each instance model.

### 2.2 Scope of Requirements

The scope of requirements for the software SPDFM is limited to the realization of GS 1 which measures the 3D plasmon-enhanced electric field on the condition that user provide sufficient environmental parameters. SPDFM is for the moment limited to the study of isotropic, nonmagnetic, dielectric environments under uniform illumination of an electromagnetic wave.

### 2.3 Characteristics of Intended Reader

The intended reader of this work should have a minimum knowledge in mathematics and electrodynamics at undergraduate level. More specifically, for knowledge of partial differential equations, the reader can look at [Boyce and DiPrima \(2012\)](#), for electromagnetism [Griffiths \(1962\)](#) is suggested, and for near-field optics the reader should be familiar with the concept of surface plasmons which can be found in [Maier \(2007\)](#). Moreover, a basic knowledge in finite element method is recommended for deeper understanding of this document; look at [Monk et al. \(2003\)](#).

### 2.4 Organization of Document

The document follows the organizational scheme laid out by [Smith and Lai \(2005\)](#) and [Smith et al. \(2007\)](#).

### 3 General System Description

This section provides general information about the system. It identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints.

#### 3.1 System Context

Figure 1 shows the system context. Circles represent the external entities outside the software, in this case the user and the FEniCS toolbox. The blue rectangle represents the SPDFM software system. Arrows are used to demonstrate the data flow between the system and the other components.

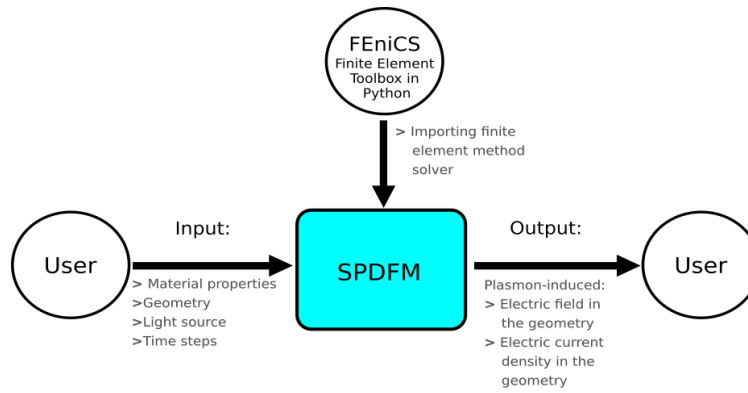


Figure 1: System Context

- User Responsibilities:
  - Provide the sufficient and correct data to the program.
  - Be aware of impacts of user inputs on the quality of the output.
  - Judge the correctness and accuracy of the data.
  - Use required hardware and devices for interacting with software.
- FEniCS toolbox Responsibilities:
  - Calculate the solution to the provided system of equations and mesh by SPDFM.
- SPDFM Responsibilities:
  - Inform user of their responsibilities in using SPDFM
  - Read input files and inform user if the file formats are wrong or information are missing.



- Interact with FEniCS toolbox.
- Display the calculated data.
- Export data in the correct format(s).

### 3.2 User Characteristics

The end user of SPDFM should have a relatively strong background in Physics (Electromagnetism, and light/mater interaction) and Mathematics (PDEs) at graduate level to be able to deeply understand the data represented and properly utilize the software. Failing to properly interact with SPDFM has fatal impact on the output that can lead to some physical misinterpretations. A general familiarity with programming and finite element method is expected.

### 3.3 System Constraints

SPDFMsoftware must be able to read .msh files for meshed environment import, and .csv file for the material properties import to be able to setup the numerical calculations system.

## 4 Specific System Description

This section first presents the problem description, which gives a high-level view of the **problem** to be solved. This is followed by the solution characteristics specification, which presents the **assumptions**, **theories**, **definitions** and finally the **instance models**.

### 4.1 Problem Description

SPDFM is intended to calculate the 3D electric field and current density dynamics generated by surface plasmons in a plasmonic material.

#### 4.1.1 Terminology and Definitions

[This section is expressed in words, not with equations. It provide the meaning of the different words and phrases used in the domain of the problem. The terminology is used to introduce concepts from the world outside of the mathematical model The terminology provides a real world connection to give the mathematical model meaning. —TPLT]

This subsection provides a list of terms that are used in the subsequent sections and their meaning, with the purpose of reducing ambiguity and making it easier to correctly understand the requirements:

- **3D Cartesian coordinate system:** An orthonormal system with a basis of  $\mathbf{B}=\{\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z\}$  and origin of  $O$ . For any arbitrary point in this space, such as  $R=(x,y,z)$ , the

displacement vector  $\mathbf{r}$  is:

$$\forall(x, y, z) \in \mathbb{R}^3 : \mathbf{r} = x\mathbf{u}_x + y\mathbf{u}_y + z\mathbf{u}_z \quad (1)$$

- **Mesh:** A network of coordinates in 3D Cartesian space that subdivides an environment or a geometry into smaller subspace.
- **Surface plasmon:** Collective oscillation of the free electron density on the surface of a conductive material due to the interaction with an electromagnetic of an incident photon or a swift electron beam.
- **Plasmonic materials:** materials such as nobel metals that have surface plasmonic properties.

#### 4.1.2 Physical System Description

[The purpose of this section is to clearly and unambiguously state the physical system that is to be modelled. Effective problem solving requires a logical and organized approach. The statements on the physical system to be studied should cover enough information to solve the problem. The physical description involves element identification, where elements are defined as independent and separable items of the physical system. Some example elements include acceleration due to gravity, the mass of an object, and the size and shape of an object. Each element should be identified and labelled, with their interesting properties specified clearly. The physical description can also include interactions of the elements, such as the following: i) the interactions between the elements and their physical environment; ii) the interactions between elements; and, iii) the initial or boundary conditions. —TPLT]

The physical system of SPDFM, as shown in Figure 2, includes the following elements:

- PS1: An incident field (as assumed in A4 is a propagating plane wave).
- PS2:  $\Omega$ , a 3D meshed volume (as assumed in A6 this body is impenetrable to the incident field).
- PS3:  $\partial\Omega$ , a boundary, which forms a 2D interface between  $\Omega$  and outer environment.
- PS4: As ( $\Omega$ ) is impenetrable, the interaction between incident beam and the object only takes place at the boundary which results in T??. This interaction affects the charge distribution on the surface of the.

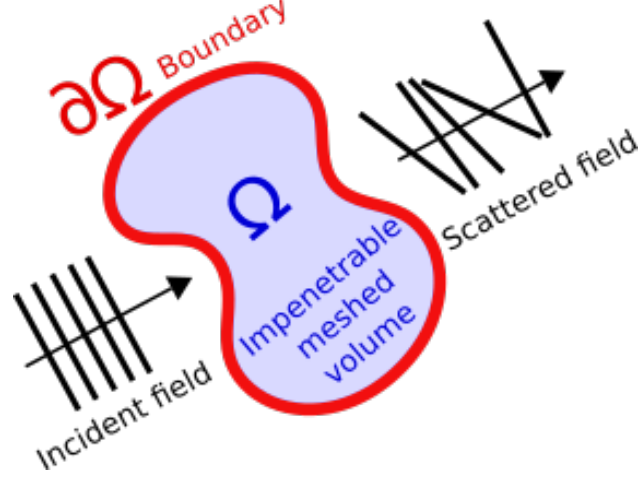


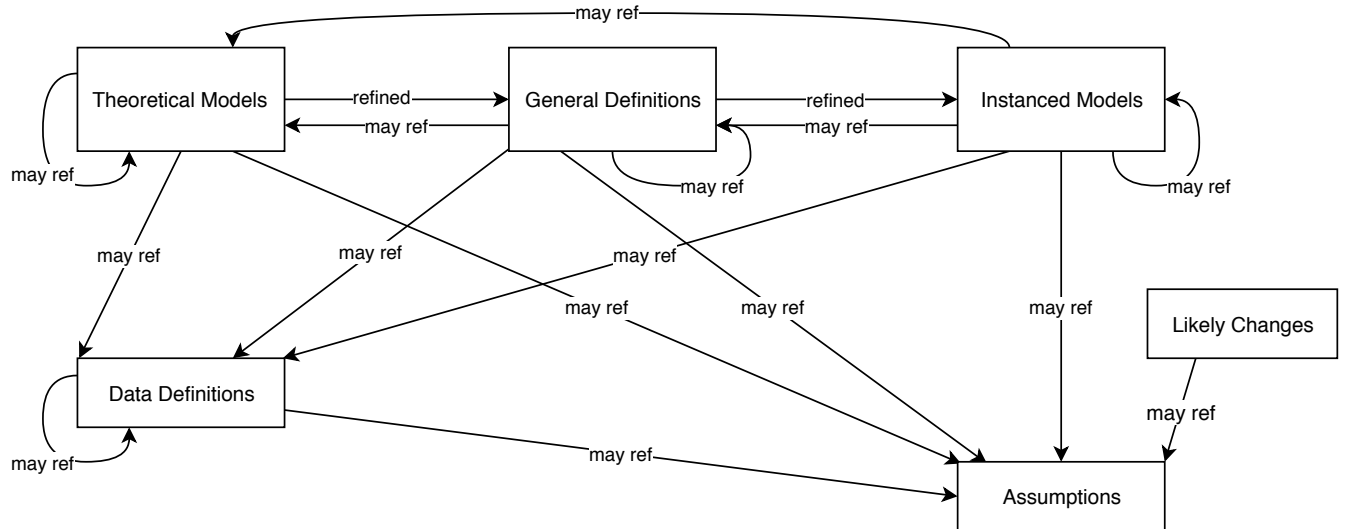
Figure 2: Schematic illustration of a meshed volume ( $\Omega$ ) with

#### 4.1.3 Goal Statements

Given a meshed geometry with corresponding material properties (permittivity, fermi velocity, plasma frequency), and an incident field, the goal statement is:

GS1: Calculating the plasmon-induced electric vector field dynamics and electric current density in the 3D geometry.

## 4.2 Solution Characteristics Specification



The instance models that govern SPDFM are presented in Subsection 4.2.5. The information to understand the meaning of the instance models and their derivation is also presented, so

that the instance models can be verified.

#### 4.2.1 Assumptions

- A1: Surface plasmon relations are governed by nonlocal hydrodynamic models and all physical assumptions in [Hiremath et al. \(2012\)](#) are valid.
- A2: As SPDFM uses nonlocal hydrodynamic Drude physics the size of the meshed geometry is between 10 nm to 100 nm ([Hiremath et al. \(2012\)](#))).
- A3: The dielectric medium is nonmagnetic.
- A4: The incident field (light source) is a plane wave with polarization vector of  $\mathbf{p}$  propagating towards direction  $\mathbf{d}$ , therefore,  $\mathbf{p} \cdot \mathbf{d} = 0$ .
- A5: The wavelength of the incident field (light source) is in the range of infrared to ultra-violet.
- A6: The dielectric medium is impenetrable to the incident field.
- A7: Surface charges propagate along the surface.
- A8: The time domain that surface plasmon activities are studies in the software is ranged from femtoseconds to microseconds.

#### 4.2.2 Theoretical Models

This section focuses on the general equations and laws that SPDFM is based on.

Number	T1
Label	<b>Electric field of a propagating plane wave (light source)</b>
Equation	$\mathbf{E}_i = \mathbf{p}e^{i(k\mathbf{r} \cdot \mathbf{d} - \omega t)} \quad (2)$
Description	The above equation calculates the electric field of a propagating plane wave (the light source) with a nonzero polarity vector $\mathbf{p}$ , with wave number $k$ ( $m^{-1}$ ), with unit direction vector of $\mathbf{d}$ , and angular frequency of $\omega$ ( $s^{-1}$ ). The calculated electric field is a 3D vector field.
Source	<a href="#">Monk et al. (2003)</a> , section 1.3
Ref. By	DD1, IM1

Number	T2
Label	<b>Nonlocal hydrodynamic current density (<math>\mathbf{J}_{HD}</math>) formula</b>
Equation	$\frac{\partial^2}{\partial t^2} \mathbf{J}_{HD}(\mathbf{r}, t) + \gamma \frac{\partial}{\partial t} \mathbf{J}_{HD}(\mathbf{r}, t) - \beta^2 \nabla^2 \mathbf{J}_{HD}(\mathbf{r}, t) = \varepsilon_0 \omega_p^2 \frac{\partial}{\partial t} \mathbf{E}(\mathbf{r}, t) \quad (3)$
Description	<p>The above partial differential equation represents the relationship between hydrodynamic electric current density vector <math>\mathbf{J}_{HD}(\mathbf{r}, t)</math> and electric field vector <math>\mathbf{E}(\mathbf{r}, t)</math> in time and space domain. This equation is derived from the definition electric current density vector and discussed in detail in <a href="#">Hiremath et al. (2012)</a>. Both <math>\mathbf{J}_{HD}(\mathbf{r}, t)</math> and <math>\mathbf{E}(\mathbf{r}, t)</math> are in <math>\mathbb{C}^3</math>.</p> <p>In this equation <math>\gamma</math> (plasmon damping term (<math>\text{s}^{-1}</math>) <math>\in \mathbb{R}</math>), <math>\beta</math> (Fermi velocity (<math>\text{m s}^{-1}</math>) <math>\in \mathbb{R}</math>), and <math>\omega_p</math> (plasma frequency, (<math>\text{s}^{-1}</math>) <math>\in \mathbb{R}</math>) are material properties that depend on the chosen medium to study.</p> <p><math>\varepsilon_0</math> (permittivity constant (<math>\text{F m}^{-1}</math>) <math>\in \mathbb{R}</math>) is a constant with value of <math>8.85418781 * 10^{-12} \text{ F m}^{-1}</math>.</p>
Source	<a href="#">Hiremath et al. (2012)</a>
Ref. By	GD1, DD3, IM2

Number	T3
Label	<b>Nonlocal hydrodynamic form of curl-curl equation of electric field (<b>E</b>)</b>
Equation	$\nabla \times \left[ \frac{1}{\mu_0} \nabla \times \mathbf{E}(\mathbf{r}, t) \right] + \varepsilon_0 \varepsilon_{loc} \frac{\partial^2}{\partial t^2} \mathbf{E}(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{J}(\mathbf{r}, t) \quad (4)$
Description	<p>Above partial differential equation, similar to equation 3, shows the relationship between <math>\mathbf{E}(\mathbf{r}, t)</math> (electric field vector <math>\in \mathbb{C}</math>) and hydrodynamic electric current density vector <math>\mathbf{J}_{HD}(\mathbf{r}, t)</math>. However, equation 4 is derived from Maxwell's equations, the approach is explained in detail in Hiremath et al. (2012).</p> <p>In this equation <math>\mu_0</math> (permeability constant with value of <math>1.256637062 * 10^{-6} \text{ H m}^{-1}</math>) and <math>\varepsilon_0</math> (permittivity constant with value of <math>8.85418781 * 10^{-12} \text{ F m}^{-1}</math>) are constants.</p> <p><math>\varepsilon_{loc}</math> is permeability of the medium (<math>\varepsilon_{loc} \in \mathbb{C}, \text{ F m}^{-1}</math>).</p>
Source	Hiremath et al. (2012)
Ref. By	GD2, IM2

Number	T4
Label	<b>General boundary condition for the nonlocal hydrodynamic system</b>
Equation	$\begin{cases} \int_{\Omega} ((\nabla \times \phi) \cdot (\mu_0^{-1} \nabla \times \mathbf{E}) - \omega^2 \phi \epsilon_{local} \mathbf{E}_i) dV + \int_{\partial\Omega} \phi \cdot DtN(\mathbf{E}) dA \\ -i\omega \int_{\Omega} \phi \cdot \mathbf{J}_{HD} dV = - \int_{\partial\Omega} \phi \cdot (n \times (\mu_0^{-1} \nabla \times \mathbf{E}_i)) dA + \int_{\partial\Omega} \phi \cdot DtN(\mathbf{E}_i) dA \\ n \cdot \mathbf{J}_{HD} = 0 \text{ on } \partial\Omega \end{cases} \quad (5)$
Description	<p>The upper equation is known as the weak formulation of the boundary condition on the electric field in a nonlocal hydrodynamic system. In this equation <math>\mathbf{n}</math> is the unit normal vector of the surface of the meshed volume (<math>\partial\Omega_{boundary}</math>), <math>\phi</math> in an arbitrary test vector function in the meshed geometry (<math>\Omega</math> domain), <math>\epsilon_{loc}</math> is permeability of the medium (<math>\epsilon_{loc} \in \mathbb{C}</math>, <math>\text{F m}^{-1}</math>), <math>\mathbf{E}_i</math> is the electric field of the incident light source, and <math>\omega</math> (<math>s^{-1}</math>) is the angular frequency of the light source.</p> <p><math>DtN</math> is the Dirichlet to Neumann boundary condition which is discussed in detail in <a href="#">Monk et al. (2003)</a>.</p> <p>The lower equation is also seen in <a href="#">8</a> and indicates that electric current only propagates on the surface of the mesh geometry (<math>\Omega</math>).</p>
Source	<a href="#">Hiremath et al. (2012)</a> , <a href="#">Monk et al. (2003)</a>
Ref. By	DD2,IM2

### 4.2.3 General Definitions

Number	GD1
Label	<b>Weak formulation of the hydrodynamic current density</b>
SI Units	The SI unit for $ \mathbf{J} $ is $\text{A m}^{-1}$
Equation	$-\int_{\Omega} \beta^2 (\nabla \cdot \psi) (\nabla \cdot \mathbf{J}_{HD}) dV + \omega(\omega + i\gamma) \int_{\Omega} \psi \cdot \mathbf{J}_H dV - i\omega\omega_p^2 \int_{\Omega} \psi \cdot \epsilon_0 \mathbf{E} dV = 0$
Description	The weak formulation is a notation that is adopted for the finite element methods. Derivation of above equation is discussed in <a href="#">Hiremath et al. (2012)</a> . This equation is a different notation of equation 3 which is known as weak formulation.
Source	<a href="#">Hiremath et al. (2012)</a>
Ref. By	T2, IM2, DD2

Number	GD2
Label	<b>Weak formulation of the hydrodynamic electric field</b>
SI Units	$\text{W m}^{-2}$
Equation	$\int_{\Omega} ((\nabla \times \phi) \cdot (\mu_0^{-1} \nabla \times \mathbf{E}) - \omega^2 \phi \cdot \epsilon_{local} \mathbf{E}) dV + \int_{\partial\Omega} \phi \cdot (\mathbf{n} \times (\mu_0^{-1} \nabla \times \mathbf{E})) dA = i\omega \int_{\Omega} \phi \cdot \mathbf{J}_{HD} dV$
Description	The weak formulation is a notation that is adopted for the finite element methods. Derivation of above equation is discussed in <a href="#">Hiremath et al. (2012)</a> . This equation is a different notation of equation 4 which is known as weak formulation.
Source	Citation here
Ref. By	T3, IM2, DD2

### Detailed derivation of simplified rate of change of temperature

### 4.2.4 Data Definitions

This section collects and defines all the data needed to build the instance models. The dimension of each quantity is also given.



Number	DD1
Label	<b>Incident electric field wave number</b>
Symbol	$k$
SI Units	$m^{-1}$
Equation	$k = \frac{2\pi}{\lambda}$
Description	$\lambda$ is the wavelength of a given wave (m). $k$ is Wave number that indicates the number of waves (cycles) per unit distance.
Sources	<a href="https://en.wikipedia.org/wiki/Wavenumber">https://en.wikipedia.org/wiki/Wavenumber</a>
Ref. By	IM1, T1

Number	DD2
Label	<b>Meshed geometry</b>
Symbol	$\Omega + \partial\Omega$
SI Units	dimensionless
Equation	N/A
Description	$\Omega$ is the 3D set of coordinate that shape a volume together and $\partial\Omega$ is a set of coordinates in 3D space that form the interface of $\Omega$
Sources	N/A
Ref. By	IM2, T4, GD1, GD2

Number	DD3
Label	Fermi velocity proportionality coefficient
Symbol	$\beta$
SI Units	$m^{-1}$
Equation	$\beta^2 = \frac{3}{5}\nu_f^2$
Description	$\nu_f$ is the Fermi velocity of electron in the medium ( $ms^{-1}$ )
Sources	<a href="#">Hiremath et al. (2012)</a>
Ref. By	GD1, T2, IM2

Number	DD4
Label	<b>Heat flux out of coil</b>
Symbol	$q_C$
SI Units	$W\ m^{-2}$
Equation	$q_C(t) = h_C(T_C - T_W(t))$ , over area $A_C$
Description	$T_C$ is the temperature of the coil ( $^{\circ}C$ ). $T_W$ is the temperature of the water ( $^{\circ}C$ ). The heat flux out of the coil, $q_C$ ( $W\ m^{-2}$ ), is found by assuming that Newton's Law of Cooling applies (A??). This law (GD??) is used on the surface of the coil, which has area $A_C$ ( $m^2$ ) and heat transfer coefficient $h_C$ ( $W\ m^{-2}\ ^{\circ}C^{-1}$ ). This equation assumes that the temperature of the coil is constant over time (A??) and that it does not vary along the length of the coil (A??).
Sources	Citation here
Ref. By	IM??

#### 4.2.5 Instance Models

This section transforms the problem defined in Section 4.1 into one which is expressed in mathematical terms. It uses concrete symbols defined in Section 4.2.4 to replace the abstract symbols in the models identified in Sections 4.2.2 and 4.2.3.

Number	IM1
Label	<b>Setting up the light source</b>
Input	$\mathbf{p}, \mathbf{d}, \lambda, \omega$ The input must satisfy: $\mathbf{p} \cdot \mathbf{d} = 0$
Output	$\mathbf{E}_i$
Description	<p><math>\mathbf{p}</math> is the 3D polarity vector of the light source (<math>\mathbf{p}=(p_x, p_y, p_z)</math>, <math>\mathbf{p} \in \mathbb{R}^3</math>).</p> <p><math>\mathbf{d}</math> is the 3D unite direction vector of the propagation of the incident light (<math>\mathbf{d} = (d_x, d_y, d_z)</math>, <math>\mathbf{d} \in \mathbb{R}^3</math>).</p> <p><math>\lambda</math> is the wavelength of the light source (m).</p> <p><math>k=\frac{2\pi}{\lambda}</math> is the wave number of the propagating wave (<math>\text{m}^{-1}</math>).</p> <p><math>\omega</math> is the angular frequency of the light source and can accept any positive value and zero (<math>\text{s}^{-1}</math>).</p> <p><math>\mathbf{E}_i</math> is the 3D electric vector field calculated using Equation 2 in T1 (<math>\mathbf{E}_i = (E_x, E_y, E_z)</math>, <math>\mathbf{E}_i \in \mathbb{C}^3</math>).</p>
Sources	Monk et al. (2003)
Ref. By	T1, DD1

Number	IM2
Label	<b>Forming weak formulation of hydrodynamic equations</b>
Input	$\gamma, \nu_f, \varepsilon_0, \omega_p, \mu_0, \varepsilon_{local}, \mathbf{E}_i, \Omega, \partial\Omega, \Delta t, t_{final}$
Output	$\mathbf{J}_{HD}(\mathbf{r}, t), \mathbf{E}(\mathbf{r}, t)$
Description	<p><math>\gamma</math> is the surface plasmon damping coefficient (<math>s^{-1}</math>).</p> <p><math>\beta</math> is the fermi velocity (<math>m s^{-1}</math>). This material property is used for calculating Fermi velocity proportionality coefficient <math>\beta</math> using equation ?? (3).</p> <p><math>\varepsilon_0</math> is permittivity constant (<math>F m^{-1}</math>).</p> <p><math>\omega_p</math> is the plasma frequency of the target material (<math>s^{-1}</math>).</p> <p><math>\mu_0</math> is the permeability constant (<math>H m^{-1}</math>).</p> <p><math>\varepsilon_{local}</math> is the local permittivity (<math>F m^{-1}</math>).</p> <p>Using above values, equations 3 and 4 can be formed that show the relationship between electric current density <math>\mathbf{J}_{HD}(\mathbf{r}, t)</math> and electric field <math>\mathbf{E}(\mathbf{r}, t)</math>; <math>\mathbf{J}_{HD}(\mathbf{r}, t), \mathbf{E}(\mathbf{r}, t) \in \mathbb{C}^3</math>.</p> <p><math>\mathbf{E}_i</math> is the incident electric field calculated at IM1</p> <p><math>\Omega</math> and <math>partial\Omega</math> are respectively the meshed domain and the boundary of it. Therefore,</p> <p>For solving the hydrodynamic equations for electric current density (<math>\mathbf{J}_{HD}(\mathbf{r}, t)</math>), and electric field (<math>\mathbf{E}(\mathbf{r}, t)</math>), a system of partial differential equations consisting of equations ??, 4 presented in T2 and T3 plus their boundary conditions in equation system 5 in T4 needs to be solved for a desired geometry. For doing so, this system of equations and a meshed geometry are handed to the FEniCS finite element solver. This toolbox</p>
Sources	Citation here
Ref. By	IM??

### Derivation of ...

[The derivation shows how the IM is derived from the TMs/GDs. In cases where the derivation cannot be described under the Description field, it will be necessary to include this subsection. —TPLT]

#### 4.2.6 Input Data Constraints

Table 1 shows the data constraints on the input output variables. The column for physical constraints gives the physical limitations on the range of values that can be taken by the variable. The column for software constraints restricts the range of inputs to reasonable values. The software constraints will be helpful in the design stage for picking suitable algorithms. The constraints are conservative, to give the user of the model the flexibility to experiment with unusual situations. The column of typical values is intended to provide a feel for a common scenario. The uncertainty column provides an estimate of the confidence with which the physical quantities can be measured. This information would be part of the input if one were performing an uncertainty quantification exercise.

The specification parameters in Table 1 are listed in Table 2.

Table 1: Input Variables

Var	Physical Constraints	Software Constraints	Typical Value
$\varnothing(\Omega)$	$\varnothing(\Omega) > 0$	$\varnothing(\Omega)_{\min} \leq \varnothing(\Omega) \leq \varnothing(\Omega)_{\max}$	$20 * 10^{-9} \text{ m}$
$t_{final}$	$t_{final} > 0$	$t_{min} < t_{final} < t_{max}$	$10^{-12} \text{ s}$

Table 2: Specification Parameter Values

Var	Value
$\varnothing(\Omega)_{\min}$	$10^{-8} \text{ m}$
$\varnothing(\Omega)_{\max}$	$10^{-7} \text{ m}$
$t_{min}$	$10^{-15}$
$t_{max}$	$10^{-12}$

#### 4.2.7 Properties of a Correct Solution

The correct measured variables must be judged by the user, based on him/herself knowledge. For simple cases user can compare the simulated result with analytical solutions.

## 5 Requirements

This section provides the functional requirements, the business tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is

expected to exhibit.

## 5.1 Functional Requirements

- R1: Provide the user with instructions to input  $\mathbf{p}$  and  $\mathbf{d}$  (IM1).
- R2: Verify the format of the inputs  $\mathbf{p}$  and  $\mathbf{d}$  to be vectors in  $\mathbb{R}^3$  and  $\mathbf{p} \cdot \mathbf{d} = 0$  (IM1).
- R3: Calculate the electric field of the light source  $\mathbf{E}_i$  to setup the light source (IM1).
- R4: Provide the user with instructions to input  $\lambda$ , and  $\omega$  (IM1).
- R5: Verify the format of the inputs  $\mathbf{p}$  and  $\mathbf{d}$  to be scalars in  $\mathbb{R}$  and  $\lambda > 0$  and  $\omega \geq 0$  (IM1).
- R6: Provide the user with instructions to input material properties  $\gamma$ ,  $\nu_f$ ,  $\varepsilon_0$ ,  $\omega_p$ ,  $\mu_0$ ,  $\varepsilon_{local}$ ,  $\Delta t$ , and  $t_{final}$  (IM2).
- R7: Verify the format of the inputs  $\gamma$ ,  $\nu_f$ ,  $\varepsilon_0$ ,  $\omega_p$ , and  $\mu_0$  to be scalars in  $\mathbb{R}$  and  $\varepsilon_{local}$  to be a scalar in  $\mathbb{C}$  (IM2).
- R8: Provide the user with instructions to input meshed domain  $\Omega$  (IM2).
- R9: Verify that all data inputs for  $\Omega$  are of the correct dimensionality and composed of Real numbers (ref2)
- R10: Output  $|J_{HD}|$ ,  $|E|$  on each element of the  $\Omega$  domain (IM??).

## 5.2 Nonfunctional Requirements

- NR 1 : The software should run on a modern desktop computer with a descent CPU and at least 8 GB of RAM.
- NR 2 : The calculated data at each step of the process should be accessible to the user, so that user be able monitor the evolution of the data.
- NR 3 : The user should be able to extract the final data in whatever desirable format.
- NR 4 : The software should be maintainable and expandable by the original programmer and future users.
- NR 5 : The software should function on any operating systems that can run dependant tool-boxes (specifically FEniCS toolbox).

## 6 Likely Changes

- LC1: In the current version of the SPDFM plane wave propagation condition is assumed for the incident electric field (A4). However, as surface plasmons are physically damped harmonic charge oscillations, it is more accurate to study their dynamic after a pulse excitation when they can free damp. Therefore, it is possible that in future more options for the incident electric field will be considered such as pulsed laser illumination.
- LC2: Although SPDFM is formulated around nonlocal hydrodynamic responses of the electric field, by adding quantum formulations for smaller structures and local electrostatic formulations for bigger structures size of the modeled system can be more flexible (A2).
- LC3: As in real media surface can experience skin effect, which means incident electric field have a penetration depth, it is possible to consider this effect in future versions (A6).
- LC4: Although current version of SPDFM is only considering nonmagnetic materials, it is likely to study impact of magnetism on hydrodynamic formalism and add capability of study these materials to the software in the future (A3).

## 7 Unlikely Changes

- LC5: As this software is written for studying surface plasmon activities, this package will expand around this physical phenomenon that takes place in wavelengths ranged from infrared to ultraviolet (A5). Thus, it is less probable that this wavelength range change.
- LC6: As plasmon activities damp within femtoseconds, for studying these system and their interaction with other components in the environment time domains beyond microseconds will not add any useful information. Therefore changing the time domain for calculations in is unlikely (A??).

## 8 Traceability Matrices and Graphs

The purpose of the traceability matrices is to provide easy references on what has to be additionally modified if a certain component is changed. Every time a component is changed, the items in the column of that component that are marked with an “X” may have to be modified as well. Table 3 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 4 shows the dependencies of instance models, requirements, and data constraints on each other. Table 5 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

[You will have to modify these tables for your problem. —TPLT]

	T??	T??	T??	GD??	GD??	DD4	DD??	DD??	DD??	IM??	IM??	IM??	IM??
T??													
T??			X										
T??													
GD??													
GD??	X												
DD4				X									
DD??				X									
DD??													
DD??								X					
IM??					X	X	X				X		
IM??					X		X		X	X			X
IM??		X											
IM??		X	X				X	X	X		X		

Table 3: Traceability Matrix Showing the Connections Between Items of Different Sections

	IM??	IM??	IM??	IM??	4.2.6	R??	R??
IM??		X				X	X
IM??	X			X		X	X
IM??						X	X
IM??		X				X	X
R??							
R??						X	
R??					X		
R??	X	X				X	X
R??	X						
R??		X					
R??			X				
R??				X			
R??			X	X			
R??		X					
R??		X					

Table 4: Traceability Matrix Showing the Connections Between Requirements and Instance Models



	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??
T??	X																		
T??																			
T??																			
GD??		X																	
GD??			X	X	X	X													
DD4							X	X	X										
DD??			X	X						X									
DD??																			
DD??																			
IM??											X	X		X	X	X			X
IM??												X	X			X	X	X	
IM??														X					X
IM??													X					X	
LC??				X															
LC??								X											
LC??									X										
LC??											X								
LC??												X							
LC??															X				

Table 5: Traceability Matrix Showing the Connections Between Assumptions and Other Items

[The traceability matrix is challenging to maintain manually. Please do your best. In the future tools (like Drasil) will make this much easier. —TPLT]

The purpose of the traceability graphs is also to provide easy references on what has to be additionally modified if a certain component is changed. The arrows in the graphs represent dependencies. The component at the tail of an arrow is depended on by the component at the head of that arrow. Therefore, if a component is changed, the components that it points to should also be changed. Figure ?? shows the dependencies of theoretical models, general definitions, data definitions, instance models, likely changes, and assumptions on each other. Figure ?? shows the dependencies of instance models, requirements, and data constraints on each other.

## 9 Values of Auxiliary Constants

$$\varepsilon_0 = 8.8541878128 * 10^{-12} \text{F m}^{-1}$$

$$\mu_0 = 1.256637062 * 10^{-6} \text{H m}^{-1}$$

## References

- William E Boyce and Richard C DiPrima. *Elementary differential equations and boundary value problems*. John Wiley & Sons, Inc. All rights reserved., 2012.
- David J Griffiths. *Introduction to electrodynamics*. Prentice Hall New Jersey, 1962.
- Kirankumar R Hiremath, Lin Zschiedrich, and Frank Schmidt. Numerical solution of non-local hydrodynamic drude model for arbitrary shaped nano-plasmonic structures using nédélec finite elements. *Journal of Computational Physics*, 231(17):5890–5896, 2012.
- Stefan Alexander Maier. *Plasmonics: fundamentals and applications*. Springer Science & Business Media, 2007.
- Peter Monk et al. *Finite element methods for Maxwell’s equations*. Oxford University Press, 2003.
- W. Spencer Smith and Lei Lai. A new requirements template for scientific computing. In J. Ralyté, P. Ågerfalk, and N. Kraiem, editors, *Proceedings of the First International Workshop on Situational Requirements Engineering Processes – Methods, Techniques and Tools to Support Situation-Specific Requirements Engineering Processes, SREP’05*, pages 107–121, Paris, France, 2005. In conjunction with 13th IEEE International Requirements Engineering Conference.
- W. Spencer Smith, Lei Lai, and Ridha Khedri. Requirements analysis for engineering computation: A systematic approach for improving software reliability. *Reliable Computing, Special Issue on Reliable Engineering Computation*, 13(1):83–107, February 2007.