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

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Contents

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
m^{-1}	reciprocal metre	wave number
s	time	second
$m\,s^{-1}$	velocity	metre per second
kg	mass	kilogram
s^{-1}	frequency	hertz
$V\,m^{-1}$	electric field strength	volt per meter
$A\,m^{-2}$	electric current density	ampere per square metre
$F\,m^{-1}$	permittivity	farad per metre
$H\,m^{-1}$	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
$\boldsymbol{B}$		Basis of the Cartesian space $\in \mathbb{R}^3$
$\mathbf{u}_x$		Unitary vector of basis $\boldsymbol{B} \in \mathbb{R}$
$\mathbf{u}_y$		Unitary vector of basis $\boldsymbol{B} \in \mathbb{R}$
$\mathbf{u}_z$		Unitary vector of basis $\boldsymbol{B} \in \mathbb{R}$
$\mathbf{E}$		3D electric field vector $\in \mathbb{C}^3$
$\mathbf{E}_x$	$V\,m^{-1}$	Electric field strength along $\mathbf{u}_x \in \mathbb{C}$
$\mathbf{E}_y$	$V\,m^{-1}$	Electric field strength along $\mathbf{u}_y \in \mathbb{C}$
$\mathbf{E}_z$	$V\,m^{-1}$	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 $\in \mathbb{C}^3$

$\mathbf{J}_{HD,x}$	$\mathrm{A\,m^{-2}}$	Component of hydrodynamic electric current density along $\mathbf{u}_x \in \mathbb{C}$
$\mathbf{J}_{HD,y}$	$\mathrm{A\,m^{-2}}$	Component of hydrodynamic electric current density along $\mathbf{u}_y \in \mathbb{C}$
$\mathbf{J}_{HD,z}$	$\mathrm{A\,m^{-2}}$	Component of hydrodynamic electric current density along $\mathbf{u}_z \in \mathbb{C}$
ε_0	$\mathrm{F\,m^{-1}}$	Permittivity constant $\in \mathbb{R}$
ε_{loc}	$\mathrm{F\,m^{-1}}$	Permittivity of the local response $\in \mathbb{C}$
μ_0	$\mathrm{H\,m^{-1}}$	Permeability constant $\in \mathbb{R}$
ν_F	$\mathrm{m\,s^{-1}}$	Fermi velocity $\in \mathbb{R}$
β		Fermi velocity proportionality constant $\in \mathbb{R}$
ω_p	$\mathrm{s^{-1}}$	Plasma frequency of the free electron gas $\in \mathbb{R}$
ω	$\mathrm{s^{-1}}$	Angular frequency of the propagating wave $\in \mathbb{R}$
t	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 $\mathbf{u}_z \in \mathbb{R}$
λ	m	Wavelenght of the incident light $\in \mathbb{R}$
k	$\mathrm{m^{-1}}$	Wave number of the incident light $\in \mathbb{R}$
i		Imaginary unit $\in \mathbb{C}$
$\mathbf{r}$		Displacement vector in 3D space $\in \mathbb{R}$
$\varnothing()$	m	Diameter operator (length of the largest diameter in a geometry) $\in \mathbb{R}$
e		Exponential operator
∇		Gradient operator
$\times$		Cross product operator
$\cdot$		Dot product operator
Ω		Finite 3D meshed volume
$\partial\Omega$		2D meshed boundary
DtN		Dirichlet to Neumann operator

1.3 Abbreviations and Acronyms

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

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 SPDFMsoftware system. Arrows are used to demonstrate the data flow between the system and the other components.

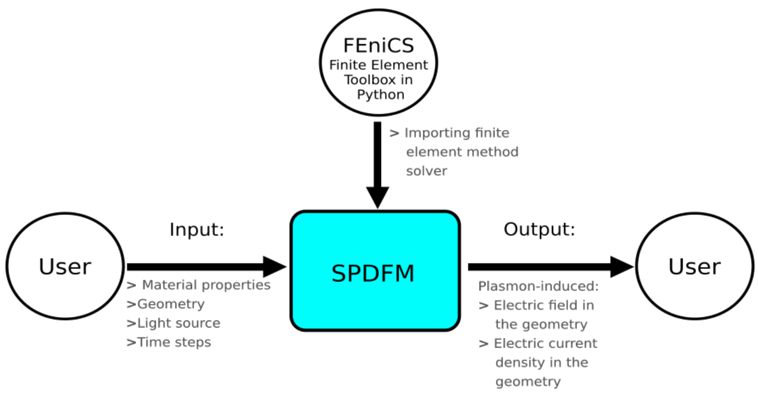


Figure 1: System Context

- 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 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 $\boldsymbol{B}$=\{$\mathbf{u}_x$, $\mathbf{u}_y$, $\mathbf{u}_z$\} and origin of O. For any arbitrary point in this space, such as R=(x,y,z), the displacement vector $\mathbf{r}$ is:

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

- **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 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: Ω, 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 Ω and outer environment.

PS4: As (Ω) is impenetrable, the interaction between incident beam and the object only takes place at the boundary which results in T4.

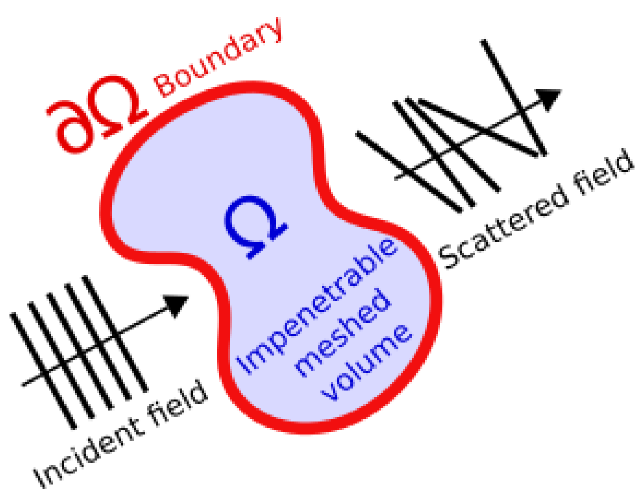


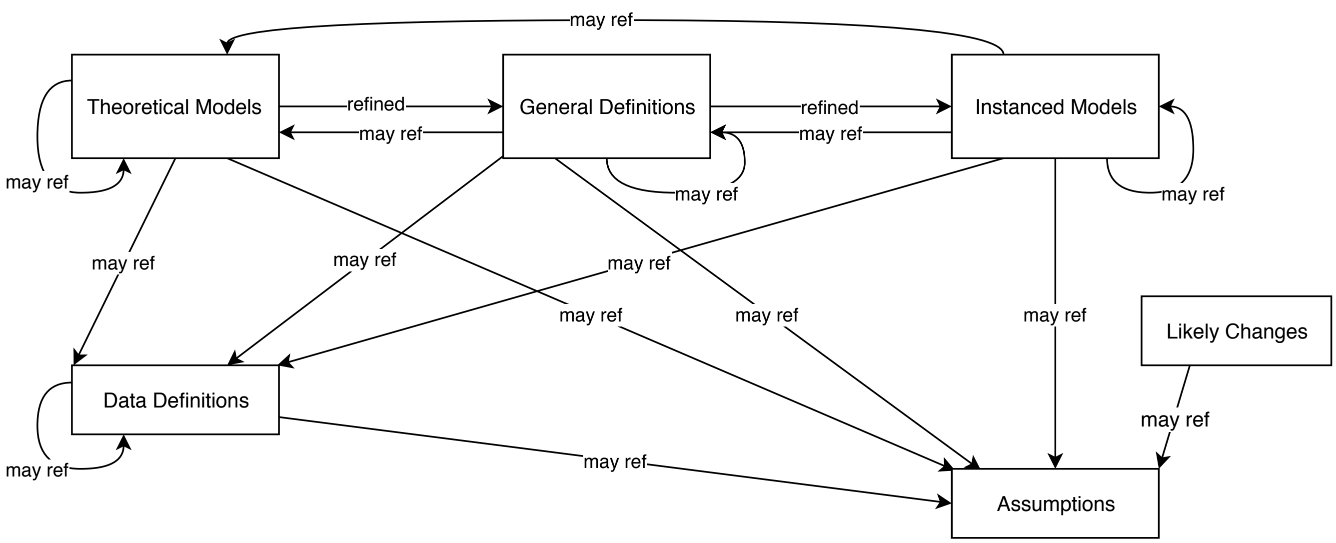
Figure 2: Schematic illustration of a meshed volume (Ω) with

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, $\mathbf{p}.\mathbf{d} = 0$.

A5: The wavelength of the incident field (light source) is in the range of infrared to ultraviolet.

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	**Electric field of a propagating plane wave (light source)**
Equation	$$\mathbf{E}_i = \mathbf{p}\ cos(k\mathbf{d}.\mathbf{r} - \omega t) - i\ sin(k\mathbf{d}.\mathbf{r} - \omega t) \quad (2)$$
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 ω (s^{-1}). The calculated electric field is a 3D vector field.
Source	Monk et al. (2003), section 1.3
Ref. By	DD1, IM1

Number	T2
Label	**Nonlocal hydrodynamic current density ($\mathbf{J}_{HD}$) formula**
Equation	$$\frac{\partial^2}{\partial t^2}\mathbf{J}_{HD}(\mathbf{r},t) + \gamma\frac{\partial}{\partial t}\mathbf{J}_{HD}(\mathbf{r},t) - \beta^2\nabla^2\mathbf{J}_{HD}(\mathbf{r},t) = \varepsilon_0\omega_p^2\frac{\partial}{\partial t}\mathbf{E}(\mathbf{r},t) \qquad (3)$$
Description	The above partial differential equation represents the relationship between hydrodynamic electric current density vector $\mathbf{J}_{HD}(\mathbf{r},t)$ and electric field vector $\mathbf{E}(\mathbf{r},t)$ in time and space domain. This equation is derived from the definition electric current density vector and discussed in detail in Hiremath et al. (2012). Both $\mathbf{J}_{HD}(\mathbf{r},t)$ and $\mathbf{E}(\mathbf{r},t)$ are in $\mathbb{C}^3$. In this equation γ (plasmon damping term (s^{-1}) $\in \mathbb{R}$), β (Fermi velocity ($\mathrm{m\,s}^{-1}$) $\in \mathbb{R}$), and ω_p (plamsa frequency, (s^{-1}) $\in \mathbb{R}$) are material properties that depend on the chosen medium to study. ε_0 (permittivity constant ($\mathrm{F\,m}^{-1}$) $\in \mathbb{R}$) is a constant with value of $8.85418781 * 10^{-12}$ $\mathrm{F\,m}^{-1}$.
Source	Hiremath et al. (2012)
Ref. By	GD1, DD3, IM2

Number	T3
Label	**Nonlocal hydrodynamic form of curl-curl equation of electric field (E)**
Equation	$$\nabla \times [\frac{1}{\mu_0}\nabla \times \mathbf{E}(\mathbf{r},t)] + \varepsilon_0\varepsilon_{loc}\frac{\partial^2}{\partial t^2}\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t) \quad (4)$$
Description	Above partial differential equation, similar to equation 3, shows the relationship between $\mathbf{E}(\mathbf{r}$,t) (electric field vector $\in \mathbb{C}$) and hydrodynamic electric current density vector $\mathbf{J}_{HD}(\mathbf{r},t)$. However, equation 4 is derived from Maxwell's equations, the approach is explained in detail in Hiremath et al. (2012). In this equation μ_0 (permeability constant with value of $1.256637062 * 10^{-6}$ $\mathrm{H\,m^{-1}}$) and ε_0 (permittivity constant with value of $8.85418781{*}10^{-12}$ $\mathrm{F\,m^{-1}}$) are constants. ε_{loc} is permeability of the medium ($\varepsilon_{loc} \in \mathbb{C}$, $\mathrm{F\,m^{-1}}$).
Source	Hiremath et al. (2012)
Ref. By	GD2, IM2

Number	T4
Label	**General boundary condition for the nonlocal hydrodynamic system**
Equation	$$\begin{cases} \int_{\Omega}((\nabla \times \phi).(\mu_0^{-1}\nabla \times \mathbf{E}) - \omega^2 \phi \epsilon_{local}\mathbf{E}_i)dV + \int_{\partial\Omega} \phi.DtN(\mathbf{E})dA \\ \quad -i\omega \int_{\Omega} \phi.\mathbf{J}_{HD}dV = -\int_{\partial\Omega} \phi.(n \times (\mu_0^{-1}\nabla \times \mathbf{E}_i))dA + \int_{\partial\Omega} \phi.DtN(\mathbf{E}_i)dA \\ \\ n.\mathbf{J}_{HD} = 0 \quad on\ \partial\Omega \end{cases} \tag{5}$$
Description	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 **n** is the unit normal vector of the surface of the meshed volume ($\partial\Omega boundary$), ϕ in an arbitrary test vector function in the meshed geometry (Ω domain), ε_{loc} is permeability of the medium ($\varepsilon_{loc} \in \mathbb{C}$, $\mathrm{F\,m^{-1}}$), $\mathbf{E}_i$ is the electric field of the incident light source, and ω (s^{-1}) is the angular frequency of the light source. DtN is the Dirichlet to Neumann boundary condition which is discussed in detail in Monk et al. (2003). The lower equation is also seen in 7 and indicates that electric current only propagates on the surface of the mesh geometry (Ω).
Source	Hiremath et al. (2012), Monk et al. (2003)
Ref. By	DD2,IM2

4.2.3 General Definitions

Number	GD1
Label	**Weak formulation of the hydrodynamic current density**
SI Units	The SI unit for $\lvert\mathbf{J}\rvert$ is $\mathrm{A\,m^{-1}}$
Equation	$-\int_{\Omega}\beta^2(\nabla.\psi)(\nabla.\mathbf{J}_{HD})dV+\omega(\omega+i\gamma)\int_{\Omega}\psi.\mathbf{J}_HDdV-i\omega\omega_p^2\int_{\Omega}\psi.\varepsilon_0\mathbf{E}dV=0$
Description	The weak formulation is a notation that is adopted for the finite element methods. Derivation of above equation is discussed in Hiremath et al. (2012). This equation is a different notation of equation 3 which is known as weak formulation.
Source	Hiremath et al. (2012)
Ref. By	T2, IM2, DD2

Number	GD2
Label	**Weak formulation of the hydrodynamic electric field**
SI Units	$\mathrm{W\,m^{-2}}$
Equation	$\int_{\Omega}((\nabla\times\phi).(\mu_0^{-1}\nabla\times\mathbf{E})-\omega^2\phi.\epsilon_{local}\mathbf{E})dV+\int_{\partial\Omega}\phi.(\mathbf{n}\times(\mu_0^{-1}\nabla\times\mathbf{E}))dA=i\omega\int_{\Omega}\phi.\mathbf{J}_{HD}dV$
Description	The weak formulation is a notation that is adopted for the finite element methods. Derivation of above equation is discussed in Hiremath et al. (2012). 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	**Incident electric field wave number**
Symbol	k
SI Units	m^{-1}
Equation	$k = \frac{2\pi}{\lambda}$
Description	λ is the wavelength of a given wave (m). k is Wave number that indicates the number of waves (cycles) per unit distance.
Sources	https://en.wikipedia.org/wiki/Wavenumber
Ref. By	IM1, T1

Number	DD2
Label	**Meshed geometry**
Symbol	$\Omega + \partial\Omega$
SI Units	dimensionless
Equation	N/A
Description	Ω 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 Ω
Sources	N/A
Ref. By	IM2, T4, GD1, GD2

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

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

Number	IM2
Label	**Forming weak formulation of hydrodynamic equations**
Input	γ, ν_f, ε_0 , ω_p, μ_0, ε_{local}, $\mathbf{E}_i$, Ω, $\partial\Omega$, Δt, t_{final}
Output	$\mathbf{J}_{HD}(\mathbf{r}, t)$, $\mathbf{E}(\mathbf{r}, t)$
Description	γ is the surface plasmon damping coefficient (s^{-1}). β is the fermi velocity ($\mathrm{m\,s^{-1}}$). This material property is used for calculating Fermi velocity proportionality coefficient β using equation **??** (3). ε_0 is permittivity constant ($\mathrm{F\,m^{-1}}$). ω_p is the plasma frequency of the target material ($\mathrm{s^{-1}}$). μ_0 is the permeability constant ($\mathrm{H\,m^{-1}}$). ε_{local} is the local permittivity ($\mathrm{F\,m^{-1}}$). $\mathbf{E}_i$ is the electric field of the incident light in $\mathbb{C}$, which is obtained in IM1. Using above values, and weak form of equations T2 and T3, (GD1 and GD2) and the boundary conditions in T4 forms a system of equation that FEniCS can solve using finite element method and obtains the electric current density $\mathbf{J}_H D(\mathbf{r}, t)$ and electric field $\mathbf{E}(\mathbf{r}, t)$ on the meshed geometry. $$\begin{cases} -\int_\Omega \beta^2(\nabla.\psi)(\nabla.\mathbf{J}_{HD})dV + \omega(\omega+i\gamma)\int_\Omega \psi.\mathbf{J}_H D dV - \\ i\omega\omega_p^2 \int_\Omega \psi.\varepsilon_0 \mathbf{E} dV = 0 \\ \\ \int_\Omega((\nabla\times\phi).(\mu_0^{-1}\nabla\times\mathbf{E}) - \omega^2\phi.\epsilon_{local}\mathbf{E})dV + \\ \int_{\partial\Omega}\phi.(\mathbf{n}\times(\mu_0^{-1}\nabla\times\mathbf{E}))dA = i\omega\int_\Omega \phi.\mathbf{J}_{HD}dV \\ \\ \int_\Omega((\nabla\times\phi).(\mu_0^{-1}\nabla\times\mathbf{E}) - \omega^2\phi\epsilon_{local}\mathbf{E}_i)dV + \int_{\partial\Omega}\phi.DtN(\mathbf{E})dA \\ -i\omega\int_\Omega\phi.\mathbf{J}_{HD}dV = -\int_{\partial\Omega}\phi.(n\times(\mu_0^{-1}\nabla\times\mathbf{E}_i))dA + \int_{\partial\Omega}\phi.DtN(\mathbf{E}_i)dA \\ \\ n.\mathbf{J}_{HD} = 0 \quad on\ \partial\Omega \end{cases} \quad (6)$$
Sources	Hiremath et al. (2012)
Ref. By	IM1, IM3, T3, T2, GD1, GD2

Number	IM3
Label	**Finding amplitude of the fields in the domain**
Input	$\mathbf{J}_{HD}(\mathbf{r}, t)$, $\mathbf{E}(\mathbf{r}, t)$
Output	$\|\mathbf{J}_{HD}(\mathbf{r}, t)\|$, $\|\mathbf{E}(\mathbf{r}, t)\|$
Description	After FEniCS solving the equation system 6, as $\mathbf{J}_{HD}(\mathbf{r}, t)$, and $\mathbf{E}(\mathbf{r}, t)$ are in $\mathbb{C}$ having the magnitude of the variables are more desirable for post processing.
Sources	Monk et al. (2003)
Ref. By	IM2

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.

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.

Table 1: Input Variables

Var	Physical Constraints	Software Constraints	Typical Value	Uncertainty
$\mathbf{p}$	$\lvert\mathbf{p}\rvert = 1, \mathbf{p} \in \mathbb{R}^3, \mathbf{p}.\mathbf{d} = 0$	$\lvert\mathbf{p}\rvert = 1, \mathbf{p} \in \mathbb{R}^3, \mathbf{p}.\mathbf{d} = 0$	$(1, 0, 0)$	N/A
$\mathbf{d}$	$\lvert\mathbf{d}\rvert = 1, \mathbf{d} \in \mathbb{R}^3, \mathbf{p}.\mathbf{d} = 0$	$\lvert\mathbf{d}\rvert = 1, \mathbf{d} \in \mathbb{R}^3, \mathbf{p}.\mathbf{d} = 0$	$(0, 1, 0)$	N/A
λ	$\lambda > 0, \lambda \in \mathbb{R}$	$\lambda > 0, \lambda \in \mathbb{R}$	$4 * 10^{-7}m$	N/A
ω	$\omega \geqslant 0, \omega \in \mathbb{R}$	$\omega \geqslant 0, \omega \in \mathbb{R}$	1 THz	N/A
δt	$\delta t \geqslant 0, t \in \mathbb{R}$	$t_{min} < \delta t < t_{max}$	$10^{-14}s$	N/A
$\varnothing(\Omega)$	$\varnothing(\Omega) > 0$	$\varnothing(\Omega)_{\mathrm{min}} \leq \varnothing(\Omega) \leq \varnothing(\Omega)_{\mathrm{max}}$	$20 * 10^{-9}$ m	N/A
t_{final}	$t_{final} > 0$	$t_{min} < t_{final} < t_{max}$, $t_{final} \geqslant \delta t$	$10^{-12}s$	N/A

Table 2: Specification Parameter Values

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

5.1 Functional Requirements

R1: Provide the user with instructions to input required data or parameters (IM1, IM2).

R2: Verify the format of the inputs for setting up the light source; $\mathbf{p}$ and $\mathbf{d}$ to be unite vectors in $\mathbb{R}^3$, $\mathbf{p}.\mathbf{d} = 0$, λ and ω and δt to be scalars in $\mathbb{R}$ where $\lambda > 0$, $\omega \geqslant 0$, and $\delta t \geqslant 0$ (IM1).

R3: Calculate the electric field of the light source ($\mathbf{E}_i$) (IM1).

R4: Verify the format of the inputs γ, ν_f, ε_0, ω_p, and μ_0 to be scalars in $\mathbb{R}$ and ε_{local} to be a scalar in $\mathbb{C}$ (IM2).

R5: Verify that all data inputs for Ω are of the correct dimensionality and composed of Real numbers (IM2).

R6: Verify that all data inputs for Ω are of the correct dimensionality and composed of Real numbers (IM2).

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 toolboxes (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: 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

LC4: 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.

LC5: 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 (A8).

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 4 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 5 shows the dependencies of instance models, requirements, and data constraints on each other. Table 3 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

	A1	A2	A3	A4	A5	A6	A7	A8
T1				X	X			X
T2	X	X	X				X	
T3	X	X	X					
T4	X				X	X		
GD1	X	X	X					
GD2	X	X	X					
DD1					X			
DD2		X						
DD3								
IM1				X	X			X
IM2	X	X	X	X	X	X	X	X
IM3	X	X	X	X	X	X	X	X
LC1				X	X			X
LC2	X	X						
LC3	X		X					

Table 3: Traceability Matrix Showing the Connections Between Assumptions and Other Items

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.

	T1	T2	T3	T4	GD1	GD2	DD1	DD2	DD3	IM1	IM2	IM3
T1	X			X			X			X	X	X
T2		X		X	X			X			X	X
T3			X	X		X					X	X
T4	X	X	X	X			X	X	X	X	X	X
GD1		X			X			X	X		X	X
GD2			X			X		X			X	X
DD1	X			X			X			X	X	X
DD2				X	X	X		X			X	X
DD3		X			X				X		X	X
IM1	X			X			X			X	X	X
IM2	X	X	X	X	X	X	X	X	X	X	X	X
IM3	X	X	X	X	X	X	X	X	X	X	X	X

Table 4: Traceability Matrix Showing the Connections Between Items of Different Sections

	IM1	IM2	IM3	4.2.6	R??	R??
IM1		X				X
IM2	X			X		X
IM3						X
R1	X					
R2	X					
R3	X					
R4	X					
R5	X					
R6		X				
R??		X				
R??		X				
R??		X				
R??		X	X			

Table 5: Traceability Matrix Showing the Connections Between Requirements and Instance Models

9 Values of Auxiliary Constants

$\varepsilon_0 = 8.8541878128 * 10^{-12} \mathrm{F\,m^{-1}}$
$\mu_0 = 1.256637062 * 10^{-6}\ \mathrm{H\,m^{-1}}$

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