UPPE-FDTD user documentation

Adam Pacewicz

Contents

Abstract

This report documents how to install and use the UPPE-FDTD electromagnetic simulator.

1 Installation

The software requires the following libraries to run:

1. Qt 5.14.2
2. Qwt 6.1.4
3. FFTW 3.3.8
4. GSL 2.3

2 Simulation Parameters - Input File Syntax

2.1 Introduction

For the convenience of the immediate users of the software, the simulation parameters input file syntax has been designed to closely resemble the one of QuickWave-3D (QW-3D) Simulator's **.pa3* (general parameters) and **.sh3* (circuit shape) files. Section 2.2 contains general background and guidelines on preparing the input file. Section 2.3 includes a table of supported materials and lists their required parameters. Section 2.4 includes a table of simulation keywords and their detailed description. An example input file is provided.

2.2 General Remarks

1. To identify the line containing a particular parameter, an elaborated parser searches for the keywords listed in table 2. To begin with, the first occurrences of the keywords listed in the *Basic* section are searched for, and if found, their corresponding parameters are attempted to be read. Next, if all the reads are successful, the parser searches for at least one complete set of keywords from the *Shape* section and attempts to read their parameters. The simulation cannot start unless all the aforementioned reads are successful. Specifying all other commands is optional, however the simulator will issue errors if their definitions are incomplete or contain obvious errors.

2. The parser issues four kinds of errors:

   - *Syntax error* if the value of the parameter does not belong to the allowed range;
   - *keyword "keyword" not found error* if an obligatory in a given context keyword is not found;
   - *Unequal number of keywords in the SHAPE section error* if the number of keywords for the medium types, their parameters and their number of cells are not equal;
   - *User defined pulse could not be read* if a file with the provided name does not exist, does not contain any data or the data is obviously erroneous.

3. If a user defined excitation is desired, the provided file should contain columnar E field values in the consecutive time steps. Comments are allowed.

4. Comments are preceded with the "#" character and extend to the end of the line. A line is considered to be a comment only if the "#" character is its first non-whitespace character. It is recommended to comment out lines that do not contain relevant text to limit the number of potential errors.

5. Each line which does not start with a "#" character and contains a keyword must begin with either a whitespace or a simulation parameter. Keywords and additional non-whitespace strings must be placed after all parameters in the given line have been enumerated. Parameters must be separated from each other, from keywords and from any additional strings by whitespaces only.
   The keywords on the other hand can be part of a longer non-whitespace string.

6. Two kinds of postprocessings have been provided. *Fourier postprocessing* computes the discrete Fourier transform (DFT) of a signal at specified frequencies, location in the grid, and range of finite-difference time-domain (FDTD) iterations. *Time postprocessing* saves a specified number of signal samples at a specified location and range of FDTD iterations.

7. The parser is case insensitive, i.e. does not distinguish between lowercase and uppercase letters. However, the names of files with postprocessing results saved via the *Save All* option follow the specified capitalization.

8. The convenience keyword *end* has been provided. It performs two functions:
   - if used as the *lumped z-location* parameter, it instructs the simulator to place the load at the end of the defined transmission line;
   - if used as the *itend* parameter, it instructs the simulator to keep performing the postprocessing for as long as possible.

9. If the 1DP or the 1DCP problem type is chosen, the parser will take only the first of the specified media into account. In addition, loads are ignored in these problem types. One-dimensional periodic (1DP) problems are normally used with total field/scatter field (TF/SF) sources, and one-dimensional conditionally periodic (1DCP) problems with a single hard source.

2.3 Table of Media

Table 1: Types of media.

Medium type	keyword	parameters(in order)
Lossless dielectric	diel	ϵ_r, μ_r
Lossy dielectric	ldiel	$\epsilon_r, \mu_r, \sigma$
Lorentz single-pole dispersive	lor1	$\epsilon_\infty, \mu_r, \sigma, \epsilon_s, f_c, f_p$, (optional) frequency unit[1]
Lorentz double-pole dispersive	lor2	$\epsilon_\infty, \mu_r, \sigma, \epsilon_s, f_{c1}, f_{p1}, A_1, f_{c2}, f_{p2}, A_2$, (optional) frequency unit
Lorentz triple-pole dispersive	lor3	$\epsilon_\infty, \mu_r, \sigma, \epsilon_s, f_{c1}, f_{p1}, A_1, f_{c2}, f_{p2}, A_2, f_{c3}, f_{p3}, A_3$, (optional) frequency unit
Kerr and single-pole Raman nonlinear	ker1	$\epsilon_r, \mu_r, \chi^{(3)}, \tau_1, \tau_2, \alpha$, (optional) threshold[2]
Kerr and single-pole Raman nonlinear & Lorentz triple-pole dispersive	lor3ker1	$\epsilon_\infty, \mu_r, \sigma, \epsilon_s, f_{c1}, f_{p1}, A_1, f_{c2}, f_{p2}, A_2, f_{c3}, f_{p3}, A_3$, $\chi^{(3)}, \tau_1, \tau_2, \alpha$, (optional) threshold, (optional) frequency unit
	UPPE	
Kerr and single-pole Raman nonlinear with a constant complex refractive index	`const_n_ker1`	$\mathrm{Re}\, n, \mathrm{Im}\, n, \chi^{(3)}, \tau_1, \tau_2, \alpha$
Kerr and single-pole Raman nonlinear with a step in the constant complex refractive index	`step_n_ker1`	$\mathrm{Re}\, n_1, \mathrm{Im}\, n_1, f_{step}(THz), \mathrm{Re}\, n_2, \mathrm{Im}\, n_2, \chi^{(3)}, \tau_1, \tau_2, \alpha$

[1] If not provided, the frequency unit is assumed to be GHz
[2] If not provided, the threshold is assumed to be equal to 0.01

2.4 Table of Keywords

The following table lists the simulation parameters input file keywords. It is recommended to arrange the keywords in the file in logical sections, as has been shown in the table.

Table 2: Keywords of the simulation parameters file syntax.

Section	**Keyword**	**Description**	**Range**	**Required**
Basic	stability	Courant stability factor	positive floating point number (FPN)	yes
	measure	FDTD cell size physical unit	mm, um, nm	yes
	type	problem type	1D, 1DP, 1DCP	yes

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Table 2 – *Continued from previous page*

Section	Keyword	Description	Range	Required
Shape	size meshpoints medium parameters	cell size number of cells type of medium medium parameters	positive FPN positive integer see table 1 see table 1	yes yes yes yes
Sources	geometry z-location shape file 3 dB amplitude funit centre duration	excitation geometry excitation location pulse shape file name 3 dB band of Gauss spectrum source impedance, amplitude, delay in nanoseconds frequency unit carrier frequency number of carrier periods	point, plane_wave integer from 1 to the total number of cells sine, Gauss, user String positive FPN positive FPN, FPN, positive FPN Hz, kHz, MHz, GHz, THz, PHz positive FPN positive FPN	as first [1] yes if user if Gauss yes unless user unless user unless user
Load	lumped (first occurrence) lumped (second occurrence)	lumped load impedance lumped load location	positive FPN from 1 to the total number of cells or *end* (see section 2.2 item 8)	as first yes
Postprocessings	typeOf name z-location funit fstart itstart itend use	type of postprocessing postprocessing name (default for saved files and plot titles) probe location frequency unit start, step and stop frequency first iteration last iteration whether to repeat the postprocessing	Fourier, time any string terminated with a whitespace and the "*" character from 1 to the total number of cells Hz, kHz, MHz, GHz, THz, PHz positive FPN positive FPN positive FPN positive integer positive integer or *end* 0 if not to repeat, else any other integer number	as first yes yes if Fourier if Fourier yes yes yes

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Table 2 – *Continued from previous page*

Section	**Keyword**	**Description**	**Range**	**Required**
	every	repetition period (in iterations), repetition limit (in iterations)	positive integer, positive integer	yes
Breakpoints	action	the action to be performed	suspend	as first
	iterations	iteration at which the action is taken	positive integer	yes
Timing	code	whether to time the FDTD iterations	0 if not to time, else any other integer number	yes
	period	number of FDTD iterations to be timed periodically	positive integer	if timing
	file	file name to which the results are written	string	if timing

2.5 Postprocessings

2.5.1 Energy conversion efficiency

- conversionEfficiency *typeOfPostprocessing
- test *postprocessing name monitor at a single frequency if just one number is present may be completely empty, in that case do not display the conversion efficiency but just the total energy on the plot
- 0.5 10 *start stop If *start* and *stop* are equal, computations will be performed at a single frequency.

2.6 UPPE - specific keywords

2.6.1 ODE parameters

- 1 *fixedstep

  If 1, the ODE solver step is fixed and given by evolutionstep. If 0, the solver step is chosen adaptively, the first attempt is made with initialintegstep. In most cases, adaptive steps unnecessarily lengthen the simulation.

- rkck *method

  Available methods: `gsl_odeiv2_step_rkf45`, `gsl_odeiv2_step_rkck`, `gsl_odeiv2_step_rk8pd`. The letters after the last underscore constitute the keyword.

[1] If specified, all the other keywords in the section are searched for in lines occurring after this keyword

- 1e-6 *initialintegstep

  Initial integration step. Ignored if fixedstep = 1.

- 1e-4 *tolerance

  ODE solution tolerance. Influences the simulation speed in distance per unit time by itself.

- 3e-6 *evolutionstep

  Evolution step set in the ODE solver. This is the integration step only if fixedStep = 1. After the solver covers this distance, the E and A variables are realigned.

- 0 *fshift

  artificial spectral shift of the signal. fshift = 0 and usegeneral = 1 can be used for testing the general transforms.

- thz *funit

  unit of fshift

- 0 *usegeneral

  If usegeneral = 1, general transforms are used (for a complex signal). If usegeneral = 0, simplified transforms are used (assuming a real signal at the input).

2.7 Exemplary configuration files

2.7.1 UPPE

```
#ODE PARAMETERS
1 *fixedStep
#available methods: gsl_odeiv2_step_rkf45, gsl_odeiv2_step_rkck,
    gsl_odeiv2_step_rk8pd
rkck *method
1e-7 *initialintegstep
1e-8 *tolerance
1e-7 *evolutionstep
0 *fshift
thz *funit
0 *usegeneral

#SOURCES - IR
gauss *excitation pulse shape
thz *funit
ps *tunit
6e8 0 *amplitude & delay
192.307 *centre
0.648 *3dB
6.64 *timeduration
8192 *timepoints

#SOURCES - optical
gauss *excitation pulse shape
thz *funit
ps *tunit
6e8 0 *amplitude & delay
394.614 *centre
0.648 *3dB
```

```
6.64 *timeduration
8192 *timepoints

#SHAPE
lor3ker1 *medium
1.0 1.0 0 3.5 14.5 2641520 1 14.5 1288190 0.015976 145 29521.3 3.99634 1e-21
    5.5 32 1 *parameters
mm *unit of measure
1.5 *size

#BREAKPOINTS
saveAll *action
0 *iterations
UPPE_terahertz_generation *filename

exit *action
0 *iterations
```

2.7.2 FDTD

```
#GENERAL
2.0 *stability factor
um *unit of measure
1d *problem type
12 *maximum number of threads
0 *physical distance

#SOURCES
point *excitation geometry
gauss *excitation pulse shape
1 *excitation z-location
thz *funit
ps *tunit
0 6e8 0 *source impedance, amplitude & delay
192.307 *centre
0.648 *3dB
319 *duration

point *excitation geometry
gauss *excitation pulse shape
1 *excitation z-location
thz *funit
ps *tunit
0 6e8 0 *source impedance, amplitude & delay
394.614 *centre
0.648 *3dB
638 *duration

#SHAPE
0.030 *cell size (for all cells in structure)
lor3ker1 *medium
1.0 1.0 0 3.5 14.5 2641520 1 14.5 1288190 0.015976 145 29521.3 3.99634 3e-20 5.5
    32 1 0 *parameters
60000 *meshpoints

#POSTPROCESSINGS
spectrogram *typeOf postprocessing
spectrogram_THz *postprocessing name
```

```
2 0.1 20 *start step end
5e4 0 5e4 *loc_start loc_step loc_end
thz *anyunit

#TIMIING
0 *code

#BREAKPOINTS
saveAll *action
0 *iterations
FDTD_terahertz_generation *filename

exit *action
0 *iterations
```

3 Graphical User Interface Manual

3.1 Introduction

The graphical user interface (GUI) of the developed simulator has been created according to the multiple document interface (MDI) paradigm, in which the main application window manages sub-windows in its central area. The software is based in part on the work of the Qt Widgets for Technical Applications (Qwt) project (http://qwt.sf.net) and the Qt project (http://www.qt.io).

3.2 Main Application Window

Running the executable opens the main application window (fig. 1).

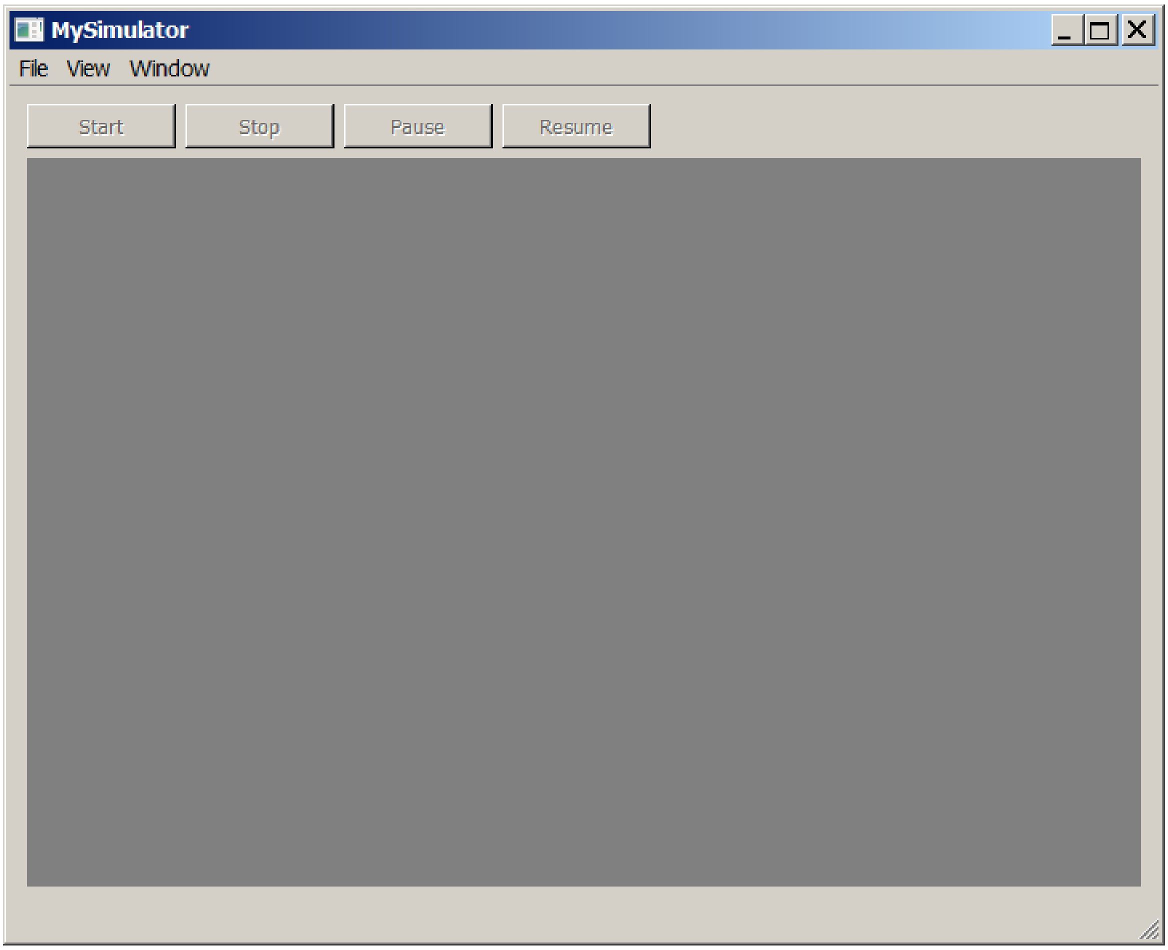

Figure 1: Main application window.

The dialog, from which the user chooses the simulation parameters input file, can be opened via the keyboard shortcut *Ctrl+L* or the *File-¿Load* menu option (see section 3.4). If the file is successfully parsed, the start button will become active and the full path to the loaded file will be visible in the status bar. Once started, the simulation can be stopped (aborted), paused and resumed at any time via the corresponding buttons. The number of executed FDTD iterations is shown in the status bar, and is refreshed every second. Stopping the simulation requires additional user confirmation. It is possible to automatically start the simulation immediately after the application is run if the full path of a simulation parameters input file is provided in the *Settings.txt* file, which must be placed in the same directory as the executable. The beginning of the first non-empty line of *Settings.txt* must contain a non-zero integer number.
Its second non-empty line must contain the absolute file path.

3.3 UPPE-specific information

Bottom right corner: First number: distance covered in 1s Second number: total distance covered so far in m.

3.4 Application Menus

The application menus are shown in fig. 2.

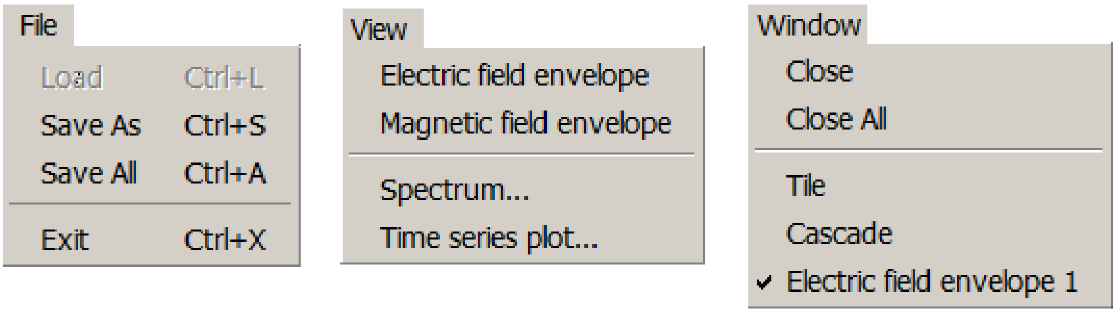

Figure 2: Application menus.

3.4.1 File Menu

- *Load* opens the file dialog so that the simulation parameters input file can be chosen for loading. Active only if no simulation is running.
- *Save As* opens the file dialog so that the simulation results that pertain to the active subwindow (see section 3.4.2) can be saved to a text file under a chosen name.
- *Save All* creates a folder in the current directory with the a name containing the current date and time and saves all simulation results to text files in the created folder. The file names are the subwindow plot titles.
- *Exit* exits the application. The user is asked for confirmation if a simulation is running.

3.4.2 View Menu

Starting the simulation enables the view menu options, by which the simulation results can be visualized in plot subwindows, which all follow the layout shown in fig. 3. It can be chosen whether or not to refresh a results subwindow via the *Refresh* checkbox. The refresh rate expressed in FDTD iterations can be specified in the adjacent text box.

- *Electric field envelope* displays the spatial distribution of the electric field along the full length of the FDTD model. The envelope lines (marked in blue in fig. 3) can be drawn and hidden via the keyboard shortcut *Shift+E* and refreshed via the *E* key.
- *Magnetic field envelope* displays the spatial distribution of the magnetic field along the full length of the FDTD model. The envelope lines can be drawn as described in the previous item.
- *Spectrum* and *Time series plot* display selection dialogs containing the names of the previously defined postprocessings (see fig. 4). The results of the selected postprocessings are displayed in separate subwindows. Multiple selections are allowed. If only one postprocessing of either type has been specified, the corresponding results subwindow is displayed with the omission of the selection dialog.

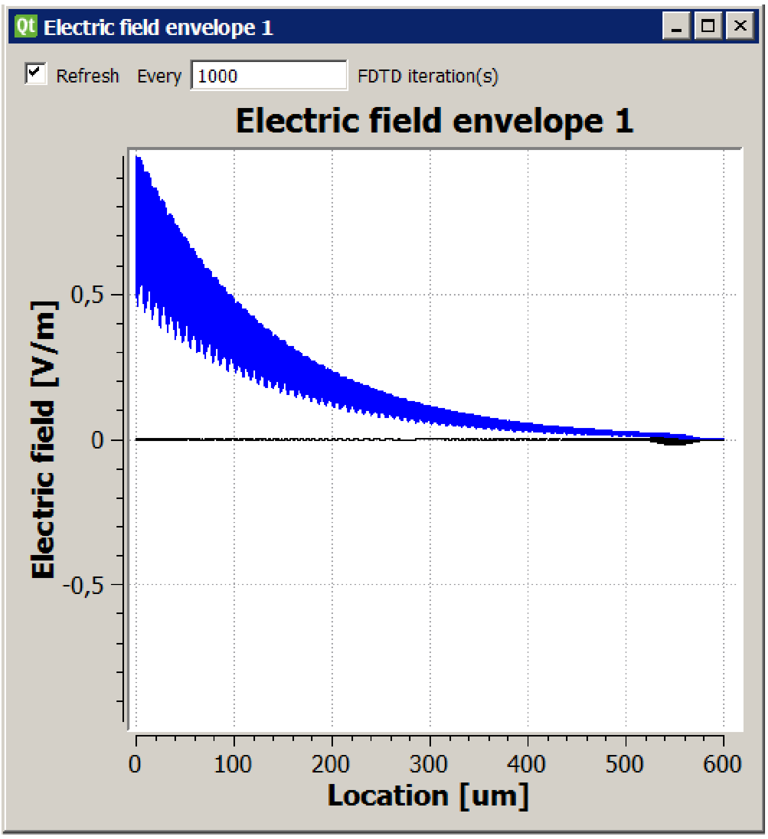

Figure 3: Simulation results subwindow of the electric field spatial distribution of a Gaussian pulse (black) propagating in a linear dispersive medium. Field envelope line is marked in blue.

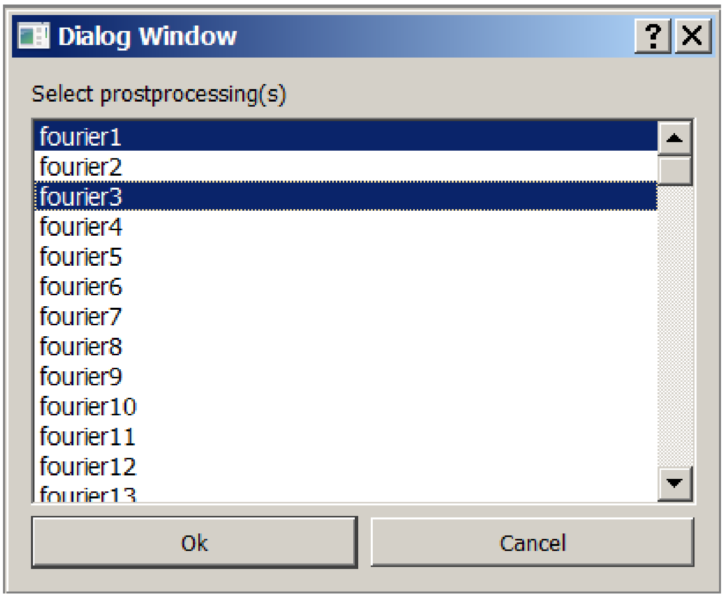

Figure 4: Postprocessings selection dialog.

3.4.3 Window Menu

- *Close* closes the active subwindow.
- *Close All* closes all subwindows.
- *Tile* places the currently displayed subwindows next to each other.
- *Cascade* layers the currently displayed subwindows on top of each other.

3.5 Output files

The UPPE method provides the following output files:

- The time-domain input signal
- The input spectrum
- The output time-domain signal
- The output spectrum

The FDTD method provides the following output files:

- Electric field in space
- Magnetic field in space
- Defined time- and frequency-probes

References

[1] Weisstein, Eric W. "Cubic Formula." From MathWorld–A Wolfram Web Resource, `https://mathworld.wolfram.com/CubicFormula.html`

[2] Sergey Khashin, PhD. Solution of cubic and quartic equations C++. `http://math.ivanovo.ac.ru/dalgebra/Khashin/poly/index.html`