AttoGram Instructions

A) GENERAL INFORMATION

I) Representation of the spectrogram files

Spectrograms that can be loaded and processed with AttoGram, are stored in `.spec` files. The `.spec` files are ASCII files with a particular structure, graphically represented in Figure 1. The first line contains two integers: the number of columns $N\tau$ and the number of rows $N\varepsilon$ of the spectrogram. The following $N\varepsilon$ lines contain the matrix representation of the spectrogram. The line immediately following the spectrogram matrix contains two integers: 1 and $N\tau$. The following $N\tau$ lines contain a vector representation of the delay axis. The line immediately following the delay vector contains two integers: 1 and $N\varepsilon$. The following $N\varepsilon$ lines contain a vector representation of the spectral axis. The following lines in the `.spec` file consist of of 100 carriage return and line-feed characters, followed by the integer 3, the last character in the file.

```
Nτ         Nε
M[1][1]    M[2][1]    ...  M[Nτ][1]
M[1][2]    M[2][2]    ...  M[Nτ][2]
  ⋮           ⋮        ⋱     ⋮
M[1][Nε]   M[2][Nε]   ...  M[Nτ][Nε]
1          Nτ
D[1]
D[2]
  ⋮
D[Nτ]
1          Nε
F[1]
F[2]
  ⋮
F[Nτ]
(100 carriage returns and line feeds)
3
```

Figure 1 Spectrogram file

II) Physical units

AttoGram assumes the following units for the physical quantities:

- time in femtoseconds (fs)
- frequency in petahertz (PHz)
- energy in electron volts (eV)
- electric field in atomic units (a.u.)
- vector potential, given by $E=-\partial A/\partial t$, in atomic units (a.u.)

If the "streaking" radio button is checked, the vertical axis of the spectrogram is represented in eV; if the FROG radio button is checked, then the spectrogram's vertical axis corresponds to frequency in PHz, i.e. **the ordinary frequency $\nu = \omega/2\pi$, not the angular frequency ω.**

III) Representation of 1-D quantities

Complex time-domain quantities (i.e. pulse and gate) loaded into AttoGram are stored in ASCII format, and can be represented using matrices with two or three columns. The first column is always time (in fs). If only two columns are given to AttoGram, then it transforms the real-valued signal $f(t)$, stored in the second column, into an analytical signal with modulus $|f(t)|$ and phase $\varphi(t)$: $f_A(t)=|f(t)|\, e^{i\varphi(t)}$. If the complex time domain profile is given in three columns, then AttoGram assumes that the second and third columns correspond to the real and imaginary parts of the analytical signal: $f_A(t)=f_R(t)+i\, f_I(t)$. If the complex time domain profile is given in more than three columns, all columns beyond the third are ignored.

For real-valued time domain quantities (i.e. the vector potential of the streaking field), only two columns are required. If the real-valued time domain quantity is given in more than two columns, all columns beyond the second are ignored.

AttoGram outputs temporal and spectral quantities in five columns. Temporal profiles $f(t)$ and spectral profiles $g(\nu)$ ($\nu=\omega/2\pi$) are represented with five columns:

(A) temporal profile columns:	t (fs)	Re[f(t)]	Im[f(t)]	$\|f$(t)$\|$	arg[f(t)]
(B) spectral profile columns:	ν (PHz)	Re[$g(\nu)$]	Im[$g(\nu)$]	$\|g(\nu)\|$	arg[$g(\nu)$]

Table 1: Representation of 1-D quantities

B) SIMULATE

The SIMULATE tab is for calculating a spectrogram from a pulse and a vector potential (if the streaking radio button is checked), or from a pulse and a gate (if the FROG radio button is checked). The pulse, gate and vector potential are loaded by clicking on the respective buttons (pulse..., gate... and vector potential...). The location of the spectrogram can be set by clicking on the spectrogram... button. The delay and spectral ranges, as well as the number of delay and spectral points can be set in the corresponding text boxes.

Additionally, the spectrogram can be spectrally centered at a user-defined central energy/frequency. Clicking on the estimate button will extract the central energy/frequency from the pulse.

When all parameters are set, clicking on the CALCULATE SPECTROGRAM button will yield a spectrogram, shown in the upper right false color plot. This spectrogram, along with the relevant data, is stored in the user-specified directory. If no directory was specified, the spectrogram is stored in the same directory as the pulse.

Several files are created by clicking on the CALCULATE SPECTROGRAM button. For a streaking spectrogram, they consist of:

- crab_spectrogram.spec: the calculated streaking spectrogram file in a format that can then be processed by the retrieval algorithm (Figure 1);
- crab_trace.txt: a matrix-only representation of the spectrogram (i.e. without delay and spectral information);
- crab_pars.txt: the spectral and delay parameters used for calculating the spectrogram;
- crab_pulse.txt: the complex pulse used for calculating the spectrogram;
- crab_vecpot.txt: the vector potential used for calculating the spectrogram;
- crab_spectrum.txt: the spectrum of the pulse (in PHz);
- delays.txt: a vector of delay values (in fs), corresponding to the horizontal axis of the spectrogram;
- energies.txt: a vector of energy values (in eV), corresponding to the horizontal axis of the spectrogram;

and for a FROG spectrogram, they are:

- frog_spectrogram.spec: the calculated FROG spectrogram file in a format that can then be processed by the retrieval algorithm (Figure 1);
- frog_trace.txt: a matrix-only representation of the spectrogram (i.e. without delay and spectral information);
- frog_pars.txt: the spectral and delay parameters used for calculating the spectrogram;
- frog_pulse.txt: the complex pulse used for calculating the spectrogram;
- frog_gate.txt: the complex gate used for calculating the spectrogram;
- frog_spectrum.txt: the spectrum of the pulse (in PHz);
- delays.txt: a vector of delay values (in fs), corresponding to the horizontal axis of the spectrogram;
- frequencies.txt: a vector of frequency values (in PHz), corresponding to the horizontal axis of the spectrogram;

The current state of the SIMULATE tab can be saved to a .spa file by clicking on FILE→save parameters. The state of the SIMULATE tab can then be restored by reloading the .spa file (FILE→load parameters). Images of the pulse, vector potential, gate and spectrogram can be saved to a .bmp file by clicking on the corresponding export... button.

C) PARAMETERS

The PARAMETERS tab is for loading a spectrogram and guesses for the pulse, gate or vector potential into AttoGram, and setting the static formatting parameters for the retrieval (i.e. the parameters that are to remain fixed for the entire retrieval). The spectrogram, pulse, gate and vector potential guesses can be loaded by clicking on the spectrogram..., pulse..., gate... and vector potential... buttons respectively. Their pictures can be exported as `.bmp` files by clicking on the corresponding export… button. If the delay convention used in recording the spectrogram is not the one used by AttoGram, the spectrogram can be inverted with respect to the delay axis by clicking on the invert delay checkbox. Inverting the spectrogram with respect to the delay axis is equivalent to time-reversing and conjugating the pulse and gate.

Prior to the retrieval, the spectrogram can be cropped by either setting the spectral and delay limits in the textboxes to the left, or by dragging a rectangle with the left mouse button over the appropriate region of the false color plot on the upper right corner. The coordinates of the cursor are displayed above the upper right corner of the false color plot. After releasing the left mouse button, the delay and spectral limits of the rectangle are immediately displayed in the textboxes to the left, as well as updated values for the delay and spectral samples, and the central energy of the spectrogram if the streaking radio button is checked. In the case of streaking, the central energy is required in order to properly calculate the vector potential from the gate.

The time sample of the retrieval can also be adjusted. After loading a spectrogram, it is by default just the reciprocal of the spectral range of the spectrogram. It can be changed in the corresponding textbox prior to the retrieval. Prior to the retrieval, AttoGram will readjust the spectral range of the spectrogram according to the chosen time sample. Because of the discrete Fourier transform requirements, choosing a finer time sample will result in a spectrogram represented over a larger spectral range. Therefore, choosing a time sample smaller than the default value could potentially require more energy samples to faithfully pre-format the spectrogram prior to the retrieval.

The retrieval algorithm can accept guesses for the pulse, gat or vector potential. Such guesses can be loaded into AttoGram by clicking on the pulse…, gate… or vector potential… buttons respectively. Naturally, if the FROG radio button is checked, then the vector potential option disappears and only a guess for the gate can loaded. If no guesses are given, then the retrieval algorithm uses 0 for the initial pulse, and 1 for the initial gate. The RESET buttons at the bottom of the PARAMETERS tab are used to re-initialize the pulse and gate to their default initial values (0 and 1 respectively).

The combined state of the PARAMETERS and RETRIEVAL tabs can be saved to a `.lpa` file by clicking on FILE→save parameters. The state of both tabs can then be restored by reloading the .lpa file (FILE→load parameters).

D) RETRIEVAL

The RETRIEVAL tab displays the real time LSGPA retrieval from the spectrogram that was loaded in the PARAMETERS tab. The retrieval is started by clicking on the START LSGPA button. The top left false color plot shows the original spectrogram, formatted according to the parameters set in the PARAMETERS tab. The top center false color plot shows the currently retrieved spectrogram, and the top right plot shows the RMS deviation Δ between the two spectrograms:

$$\Delta = \sqrt{\frac{\sum_{i,j} \left| S_{ij}^{(O)} - \beta S_{ij}^{(R)} \right|^2}{N_\varepsilon N_\tau}}, \qquad (1)$$

where the normalization factor β is chosen to minimize the figure of merit Δ. The bottom left and right plots show the currently retrieved pulse and gate/vector potential, respectively.

The RETRIEVAL tab contains additional parameters that can be adjusted during the retrieval. At the top of the tab, there are four boxes that contain integer values. The accuracy box determines the number of iterations of the least-squares method at each iteration of the retrieval algorithm. Choosing a larger value increases the accuracy of the pulse and gate pair retrieved after every iteration and can help the algorithm to converge. The iterations box sets the total number of iterations of the retrieval algorithm. The write interval and display interval boxes set the frequency at which results are written to the hard disk, and displayed in the RETRIEVAL tab, respectively.

It is possible to choose whether or not to optimize the pulse or the gate/vector potential. This can be done by clicking on the optimize checkbox located below the corresponding plots. When the optimize box is un-checked, the corresponding quantity will not change from iteration to iteration.

It happens sometimes that the retrieved pulse is not exactly centered at zero time. Clicking on the CENTER button will center the pulse in time, and will shift the gate and vector potential accordingly.

If the spectrogram loaded in to AttoGram does not strictly consist of a pure spectrogram, as given by the form:

$$S(\omega,\tau) = \left| \int_{-\infty}^{\infty} P(t) G(t+\tau) e^{i\omega t} dt \right|^2, \qquad (2)$$

then the retrieved gate will exhibit fine oscillations a scale equal to the time sample. As discussed in [1], these oscillations are unphysical, and can be removed by increasing the number in the gate cleaning box, at the bottom right corner of the RETRIEVAL tab.

Clicking on the **STOP LSGPA** button will save the current results of the retrieval to the same directory as the original spectrogram, and the retrieved pulse and gate/vector potential are plotted in the bottoms plots in the PARAMETERS tab – they can be used as the guesses for the next retrieval. There are a good number of files created upon termination of the retrieval. They contain all the pertinent information about the retrieved quantities:

- !!delays.txt: a vector corresponding to the delay axes of the matrices contained in !!initial_trace.txt, !!measured_trace.txt and !!retrieved_trace.txt;
- !!delays_full.txt: a vector corresponding to the delay axes of the matrices contained in !!initial_trace_full.txt, !!measured_trace_full.txt and !!retrieved_trace_full.txt;
- !!energies.txt: a vector corresponding to the energy axes of the matrices contained in !!initial_trace.txt, !!measured_trace.txt, !!retrieved_trace.txt, !!initial_trace_full.txt, !!measured_trace_full.txt and !!retrieved_trace_full.txt;
- !!frog_error: a matrix with three columns, representing the convergence of the algorithm -- the first column is the iteration number, the second column is the RMS deviation between the original and retrieved spectrograms (cf. equation(1)), and the third column is the relative change in the FROG error.
- !!initial_spectrogram.spec: contains a spectrogram calculated from the guessed pulse and gate/vector potential;
- !!initial_spectrogram_full.spec: a delay-interpolated version of !!initial_spectrogram.spec;
- !!initial_trace.txt: contains the spectrogram matrix of !!initial_spectrogram.spec;
- !!initial_trace_full.txt: contains the spectrogram matrix of !!initial_spectrogram_full.spec;
- !!measured_spectrogram.spec: contains a formatted version of the original spectrogram;
- !!measured_spectrogram_full.spec: a delay-interpolated version of !!measured_spectrogram.spec;
- !!measured_trace.txt: contains the spectrogram matrix of !!measured_spectrogram.spec;
- !!measured_trace_full.txt: contains the spectrogram matrix of !!measured_spectrogram_full.spec;
- !!retrieved_spectrogram.spec: contains the “minimal” spectrogram retrieved by the algorithm (see appendix for details);
- !!retrieved_spectrogram_full.spec: the “complete” version of the retrieved spectrogram, with a delay step equal to the time sample (see appendix for details);
- !!retrieved_trace.txt: contains the spectrogram matrix of !!retrieved_spectrogram.spec;
- !!retrieved_trace_full.txt: contains the spectrogram matrix of !!retrieved_spectrogram_full.spec;
- formatting_pars.txt: contains relevant information about the formatting parameters used for the retrieval, corresponding to the values set in the PARAMETERS tab;
- gate_initial.txt: contains a matrix representing the (complex) guessed gate, the columns are given in Table 1A;
- gate_spectral.txt: contains a matrix representing the retrieved gate in the frequency domain, the columns are given in Table 1B;
- gate_temporal.txt: contains a matrix representing the retrieved gate in the time domain, the columns are given in Table 1A;

- pulse_initial.txt: contains a matrix representing the (complex) guessed pulse, the columns are given in Table 1A;
- pulse_spectral.txt: contains a matrix representing the retrieved pulse in the frequency domain, the columns are given in Table 1B;
- pulse_temporal.txt: contains a matrix representing the retrieved pulse in the time domain, the columns are given in Table 1A;
- `!!retrieved_pulses_spectral_IMAGINARY.txt`, `!!retrieved_pulses_spectral_REAL.txt`, `!!retrieved_pulses_spectral_MODULUS.txt`, `!!retrieved_pulses_spectral_PHASE.txt`, `!!retrieved_pulses_temporal_IMAGINARY.txt`, `!!retrieved_pulses_temporal_REAL.txt`, `!!retrieved_pulses_temporal_MODULUS.txt`, `!!retrieved_pulses_temporal _PHASE.txt`: the columns of the matrices contained in these files represent a version of the complex pulse (in the time and frequency domain) for each delay, see appendix for details
- `!!retrieved_signal_matrix_IMAGINARY.txt`, `!!retrieved_signal_matrix_REAL.txt`, `!!retrieved_signal_matrix_MODULUS.txt`, `!!retrieved_signal_matrix_PHASE.txt`: the matrices contained in these files represent the retrieved signal matrix, which is a complex matrix obtained by inverse Fourier transforming the columns of the complex spectrogram, see appendix for details
- `vector_potential.txt`: contains a matrix representing the temporal profile of the vector potential calculated from the retrieved gate, the first column is time in fs, and the second column is the vector potential, $E=-\partial A/\partial t$, in a.u.;
- `electric_field.txt`: contains a matrix representing the temporal profile of the electric field calculated from the retrieved vector potential, the first column is time in fs, and the second column is the electric field, E, in a.u.;
- `streaking_pulse.txt`: contains a matrix representing the analytical signal of the real electric field contained in `electric_field.txt`, it contains five columns, which are given in Table 1A;
- `measured_trace.bmp`: a bitmap representing the matrix contained in `!!measured_trace.txt`;
- `retrieved_trace.bmp`: a bitmap representing the matrix contained in `!!retrieved_trace.txt`;

E) ABOUT

AttoGram was written in C++ by Justin Gagnon, based on the LSGPA algorithm, developed by Vladislav Yakovlev, Eleftherios Goulielmakis and Justin Gagnon. Acknowledgements go out to Vladislav Yakovlev, Eleftherios Goulielmakis, Ivanka Grguras and Wolfgang Schweinberger for many helpful comments and suggestions on

the program. If you publish results obtained from the use of this program, please cite the paper that describes the LSGPA algorithm:

J. Gagnon, E. Goulielmakis and V. S. Yakovlev, "The accurate FROG characterization of attosecond pulses from streaking measurements", Appl. Phys. B **92**, 25-32 (2008)

APPENDIX

For a given pulse vector $P=(P_1,P_2,...,P_{N_\varepsilon})$ and gate vector $G=(G_1,G_2,...,G_{N_G})$, the elements of the signal matrix are given by

$$S_{ij}=P_j G_{j+L(i-1)},\ i=1...N_\tau,\ j=1...N_\varepsilon \qquad \text{(A1)}$$

where the integer $L=\delta\tau/\delta t$ represents the number of time samples δt contained in a delay step $\delta\tau$ ($L=\delta\tau/\delta t$). Since the time sample satisfies the discrete Fourier transform relation, $\delta\varepsilon\ \delta t=2\pi/N_\varepsilon$, the sampling condition for the spectrogram is $N_\varepsilon\ \delta\varepsilon\ \delta\tau=2\pi L$, where the energy bin size $\delta\varepsilon$ and delay step $\delta\tau$ are expressed in mutually commensurate units (for example, in atomic units). If the energy is measured in eV, and the delay in femtosecond, this relation becomes

$$\mathrm{N}_\varepsilon\ \delta\varepsilon\ \delta\tau=2\times10^{-15}\,\frac{\varepsilon_0\,\hbar}{e\,m_e\,a_0}\,L\approx 0.2418\,L \qquad \text{(A2).}$$

From the definition of the signal matrix (A1), we see that the number of gate points is $N_G=N_\varepsilon+L(N_\tau-1)$, where N_τ is the number of delay points (i.e. the number of columns in the signal matrix). There is a well defined timing relation between the pulse and gate points: element k of the pulse vector corresponds to the same time value as element $k+L(N_\tau-1)/2$ of the gate vector.

The signal matrix, as defined by (A1), can be interpreted as a result of moving the pulse vector along the gate vector, and at each delay recording the composite signal produced by the product of their elements (Figure A1), corresponding to a column of the signal matrix. According to (A1), L-1 time samples are skipped between each column of the signal matrix.

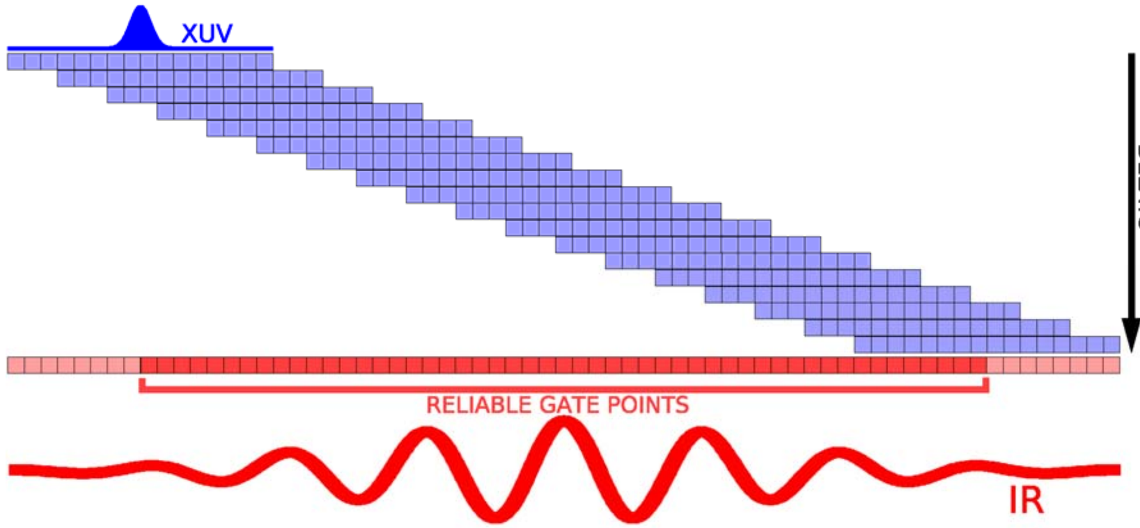

Figure A1 Illustration of the signal matrix

However, if the pulse and gate were properly retrieved by the algorithm without artifacts, then it is possible to calculate from them the "complete" signal matrix, and hence the "complete" spectrogram by shifting the pulse along the gate by exactly one time sample – i.e. assuming a delay step equal to the time sample. Therefore, the complete spectrogram contains the spectra that lie in between the recorded spectra. This is the spectrogram that is contained in the `!!retrieved_trace_full.txt` and `!!retrieved_spectrogram_full.spec files` that are written during the retrieval.