Simulation output

For each simulation run, a new output folder is created in the simulation output folder. The created folder has the name of the input file. In addition date-time is added to the folder name if the option is selected in Options→Expert settings of nextnanomat (this option is recommended in order to avoid overwritten existing output data). The created output folder contains:

- the **input file** (.xml) and the **material database** (.xml).
- a folder '**Input**' which gives material parameters used in the calculation.
- a folder **Strain** (only if the strain option is activated).
- a folder **Polarization** if pyroelectric and/or piezoelectric effects are considered.
- a folder '**Init_Electron_Modes**' where the results of the initial Schrödinger solution is reported.
- a **folder for each parameter step**. In particular, in case of voltage sweep, the name of the folder is the potential drop per period.
- Several files related to the sweep made. For a voltage sweep, it contains plots of physical quantities (current, gain,…) as a function of the applied voltage.
- a **log file** is created at the end of the simulation, containing all the information displayed during the simulation.

'Input' folder

The folder `Input/` contains all information that is input to the simulation such as material parameters.

- `AlloyContent.dat`
  alloy concentration \$x\$ vs. position for ternary materials such as `Al(x)Ga(1-x)As`
- `BandEdge_conduction.dat`
  conduction band edge \$E_{\rm c}\$ including shift due to strain vs. position in units of [eV]
- `BandEdges.dat`
  conduction band edge \$E_{\rm c}\$ and valence band edge \$E_{\rm v}\$ vs. position in units of [eV]
- `BandGap.dat`
  energy band gap \$E_{\rm gap}\$ vs. position in units of [eV]
- `DeformationPotential_ConductionBand.dat`
  conduction band deformation potential vs. position
- `EffectiveMass.dat`
  effective conduction band mass \$m_{\rm c}\$ vs. position in units of [m0]
- `ElasticConstants.dat`
  elastic constants \$c_{ij}\$ vs. position in units of [GPa]
- `EpsOptic.dat`
  optical dielectric constant \$\epsilon(\infty)\$ vs. position
- `EpsStatic.dat`
  static dielectric constants \$\epsilon(0)\$ vs. position
- `LatticeConstants.dat`
  lattice constants \$a\$ vs. position in units of [nm]
- `MaterialDensity.dat`
  material density vs. position in units of [kg/m^3]

- `PhononEnergy_LO.dat`
  longitudinal optical (LO) phonon energy in units of [eV]
- `PiezoConstants.dat`
  piezoelectric constants e_{ij} in units of [C/m^2]
- `PyroConstants.dat`
  pyroelectric polarization P_z (spontaneous polarization) in units of [C/m^2] (wurtzite only)
- `VelocityOfSound.dat`
  sound velocity in units of [m/s]

Strain

If the strain option is activated, a folder `Strain/` is created containing the strain tensor components ϵ_{ij} which are dimensionless.

- `Strain_CrystalSystem.dat`
  This file contains the strain tensor components with respect to the crystal coordinate system.
- `Strain_Simulation.dat`
  This file contains the strain tensor components with respect to the simulation coordinate system.

If the crystal has not been rotated, both files contain identical values.

Piezo and pyroelectric polarization

The folder `Polarization/` contains the piezoelectric and pyroelectric polarization if these options are activated.

- `PiezoChargeDensity.dat`
  This file contains the piezoelectric charge density due to strain. If the strain is zero, the piezoelectric charge density is zero.
- `PyroChargeDensity.dat`
  This file contains the pyroelectric charge density due to spontaneous polarization. Pyroelectric charge density only exists for wurtzite but not for zinc blende materials.

Initial electronic states

The folder `Init_Electr_Modes/` contains 3 different folders corresponding to 3 different sets of basis states. They are calculated at the first step of the calculation, before the NEGF calculation. These 3 sets of states are basis of the reduced Hilbert space obtained after applying the energy cut-off <Energy_Range_Axial>.

These states are displayed for a default voltage of <Energy_Range_Axial>/2. This voltage at which the states are visualized can be modified by the input file command:

```
<Simulation_Parameter>
```

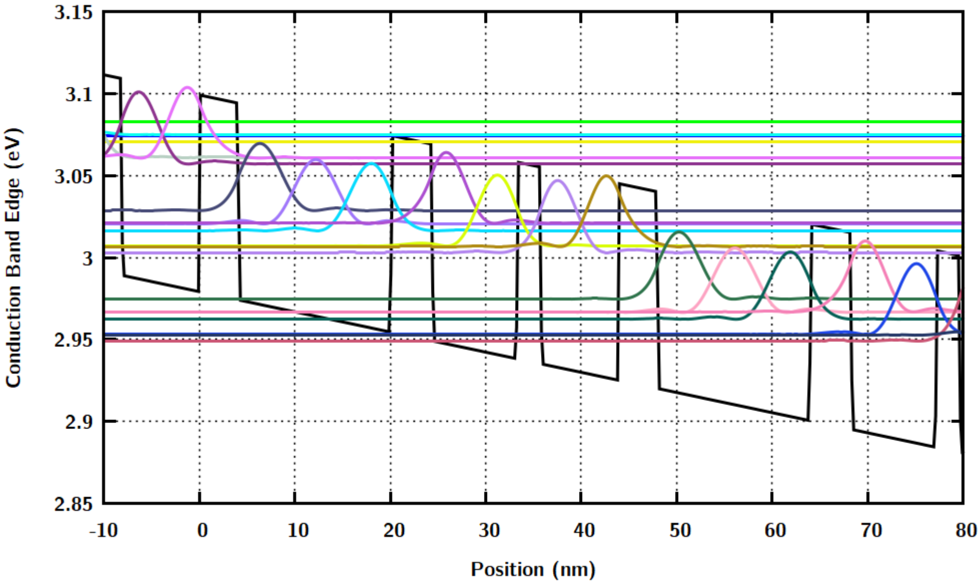
```
  ...
  <Bias_for_initial_Electronic_Modes
unit="meV">54</Bias_for_initial_Electronic_Modes>
  ...
</Simulation_Parameter>
```

'Reduced Real Space' modes

The 'reduced real space' modes are eigenstates of the position operator in the reduced Hilbert space (i.e. after the energy cut-off). Because of the energy cut-off, these states are spatially extended instead of being δ functions. This basis set is the one which is used in the NEGF calculation. It does not depend on the applied voltage. However, this basis has generally little use in terms of physical interpretation.

The folder `Init_Electr_Modes/ReducedRealSpace/` contains:

- `ReducedRealSpaceModes.dat`
  This file contains the conduction band edge and the square of the wave functions (shifted in energy) with respect to the heterostructure coordinate position.
  3 periods are displayed. (p0) means period 0 (left period), (p1) means period 1 (central period), and p2 period 2 (right period). The numbers of states displayed in equal to 3 times the number of states per period, that is the number of selected minibands.

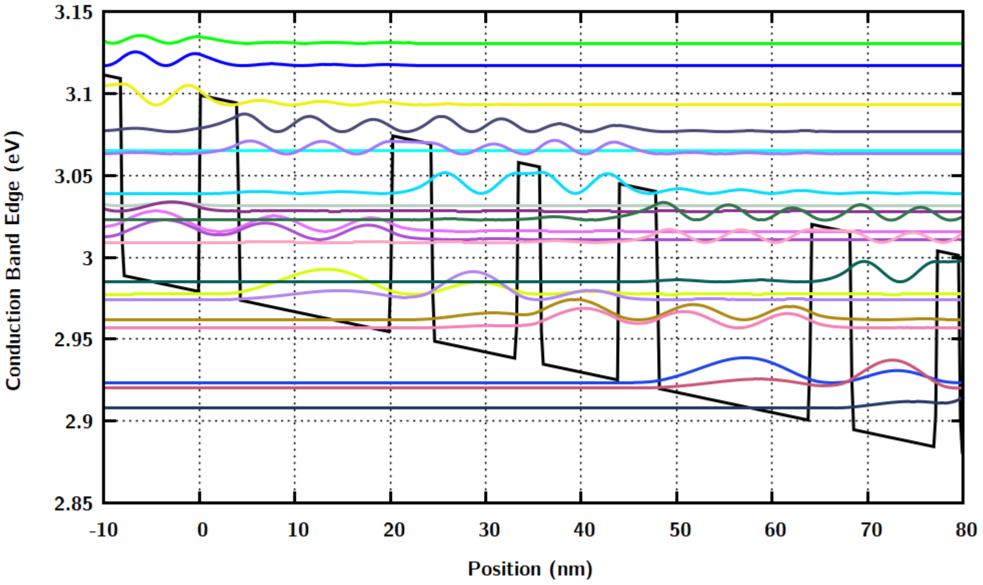


- `ReducedRealSpaceModesOn.dat`
  Same as in `ReducedRealSpaceModes.dat` but the vanishing parts of the wavefunctions are not shown.
- `H0ReducedRealSpace_nobias.mat` gives the expression of the Hamiltonian in this basis when no external bias voltage is applied.
- `H0ReducedRealSpace_nobias.mat` gives the expression of the Hamiltonian in this basis with an applied external voltage.

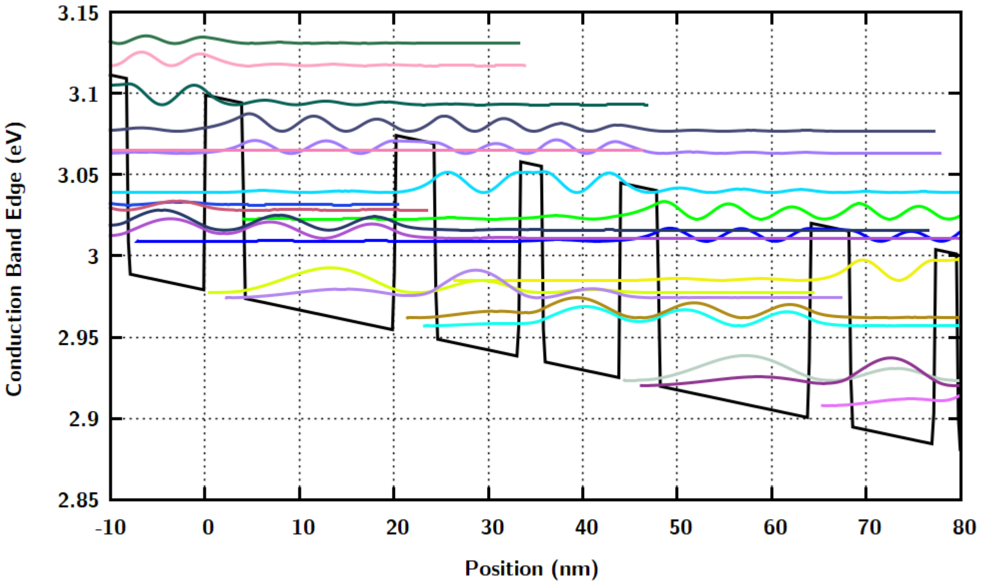
Wannier-Stark states

The Wannier-Stark states correspond to the eigenstates of the Schrödinger equation without accounting for Poisson equation (i.e. electrostatic mean-field).
It contains:

- `Wannier-Stark_States.dat` shows the conduction band edge and the probability densities of the eigenstates of the Wannier-Stark states. Schrödinger equation.



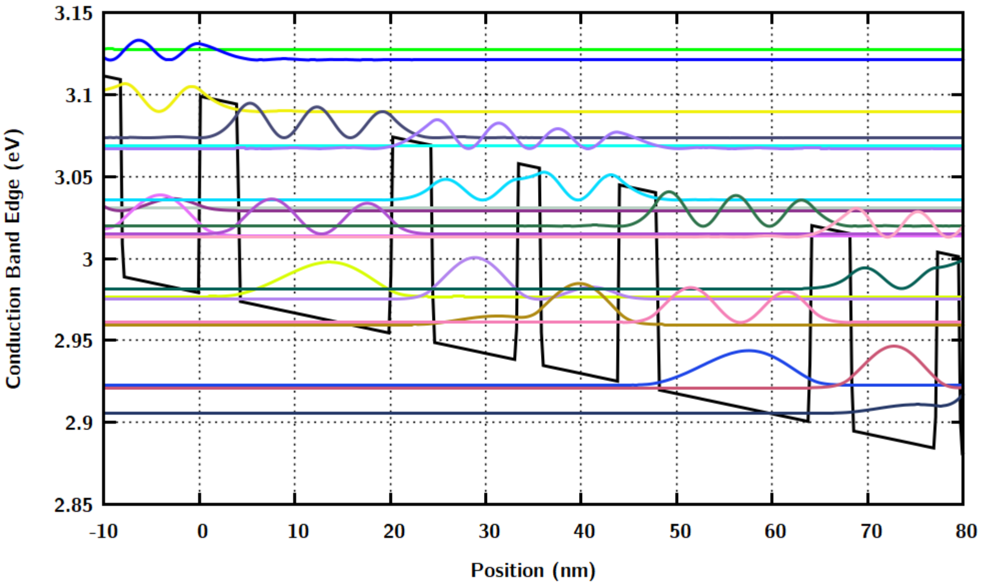
- `Wannier-Stark_levelsOn.dat`. Same than `Wannier-Stark_States.dat` except that points where the probability density is almost zero are omitted.



- `WannierStark_H0.mat` gives the Hamiltonian in the Wannier-Stark basis.
- `Dipoles.mat` gives the dipoles elements (i.e. matrix elements of the position operator).
- `Oscillator_Strength.mat` gives the oscillator strengths.

'Tight-binding' states

The Tight-binding folder contains data only if one or several `<Analysis_Separator>` are defined in the input file. The tight-binding basis corresponds to piecewise solution of the Schrödinger equation between these separators.



In-plane discretization

The file `Lateral_spectrum.dat` gives the energy discretization for the states used to describe the 2-Dimensional (2D) motion in the directions (x,y) perpendicular to the heterostructure. The lateral motion is discretized using cylindrical boundary conditions, and the corresponding eigenstates are Bessel funcitons.
x axis: `Lateral state index`
y axis: `order of Bessel (zero index)-1 of Bessel` `Relative Energy (meV)`.

Simulation output for each voltage

For each voltage or temperature step, the following files are produced as a result of the NEGF calculation:

- `CarrierDensity.dat`
  This file contains the electron density in [10^{18} cm^{-3}] as a function of position [nm].
- `Conduction_BandEdge.dat`
  This file contains the calculated heterostructure conduction band edge profile $E_{\rm c}^\prime$ as a function of position in units of [eV]. It includes the mean field electrostatic potential $|\phi\rangle$ (which is in units of [V]), $E_{\rm c}^\prime = E_{\rm c} - e \phi$.
- `Convergence.txt`
  This file contains values for
  - convergence factor: convergence factor for the lesser Green's function $\mathbf{G}^<$, which corresponds to the relative variation between the last two consecutive Green's

    functions. Should be the closest as possible from 0.
    - current convergence factor: convergence factor for the current density, which corresponds to the relative variation of the last two consecutive current density values. Should be the closest as possible from 0.
    - number of iterations
    - normalization of lesser Green's function $\mathbf{G}^<$
    - sum normalised spectral function: should be the closest as possible from 1.
- `NO-CONVERGENCE.txt`
  This file is generated instead if the calculation did not converge.

- `CurrentDensity.dat`
  This file contains the current density in [A/cm^2] as a function of position [nm].

- `Current-miscellaneous.txt`
  This file contains general information on the simulation.
    - the current density in [A/cm^2]
    - the average electron velocity in [nm/ps]
    - the time taken for one electron to travel through one period in [ps]
    - the electric field in [kV/cm]
    - the doping sheet density per period in [cm^{-2}]
    - the 3D doping density averaged over one period in [cm^{-3}]
    - the effective electronic temperature in [Kelvin]. This is only an effective temperature as electrons are not in thermal equilibrium, which is obtained by averaging the kinetic energy for the in-plane motion.

- `Electrostatic-Potential.dat`
  This file contains the mean field electrostatic potential ϕ (in [V]) as a function of position. The electrostatic potential ϕ is the solution of the Poisson equation and has been calculated self-consistently.

Output in basis sets (ReducedRealSpace, WannierStark, TightBinding)

3 folders are created to output physical quantities in the 3 different basis sets (`Reduced Real Space`, `Wannier-Stark`, and `Tight-Binding`).

For each basis set, the folder contains:

- the probability density $\vert \Psi_i(z) \vert^2$ for the each state Ψ_i. Each level is shifted accordingly to its energy
- the wavefunction $\Psi_i(z)$ in the file `Wavefunctions.dat`
- the population (i.e. the probability of occupation) in each level Ψ_i
- `DensityMatrix_Real.mat` displays the real part of the density matrix. The labelling is made accordingly to the one of the wavefunctions $\Psi_i(z)$, so that the matrix element (i,j) corresponds to the real part of $\langle \Psi_i \vert \rho \vert \Psi_j \rangle$, where ρ is the density matrix. Note that the diagonal element (i,i) is equal to the population of the level Ψ_i.
- `DensityMatrix_Real.mat` displays the imaginary part of the density matrix.
- `SpectralFunctions.dat` shows the diagonal part of the spectral function, i.e. the energy-resolved density of states (DOS).
- `CarrierDistribution_Energy.dat` shows the energy-resolved populations in each state.

2D plots

The folder `2D_Plots_Position-nm_Energy-eV/` contains files where the x axis is position in [nm] and the y axis is energy in units of [eV]. Note that these 2D plots show 2 QCL periods although only 1 period is simulated.

- `DOS_energy_resolved.vtr` / `*.gnu` / `*.fld`
  This file contains the energy-resolved local density of states ${\rm LDOS}(x,E)$ as a function of position and energy. The units are [eV^{-1} nm^{-1}]).

The local density of states is related to the spectral function. It shows the available states for the electrons at $k_\parallel = 0$.

- `CarrierDensity_energy_resolved.vtr` / `*.gnu` / `*.fld`
  This file contains the energy-resolved electron density $n(x,E)$ as a function of position and energy. The units are [cm^{-3} eV^{-1}]. The energy-resolved electron density is related to the Green's function $\mathbf{G}^<$ (“G lesser”).
- `CurrentDensity_energy_resolved.vtr` / `*.gnu` / `*.fld`
  This file contains the energy-resolved current density $j(x,E)$ as a function of position and energy. The units are [A cm^{-2} eV^{-1}].

Gain

The folder `Gain/` contains files where the x axis is position in [nm] and the y axis is photon energy $E_{\rm ph}$ in units of [eV]. Note that these 2D plots show 2 QCL periods although only 1 period is simulated.

- `Energy-Resolved_Gain_Simple-Approximation.fld` / `*.coord` / `*.dat`
  This file contains the energy-resolved intensity gain $G(x,E_{\rm ph})$ as a function of position and photon energy $E_{\rm ph}$. The units are [cm^{-1} nm^{-1}]. (Note that the units of the nextnano.MSB code are [eV^{-1} cm^{-1}].

- `Gain_Simple-Approximation.dat`
  This file contains the gain obtained without the self-consistent calculation.
  The x axis is energy in units of [meV].
  The y axis is the gain in units of [1/cm]. A negative value of gain corresponds to absorption.

- `Gain_SelfConsistent.dat`
  This file contains the intensity gain obtained with the self-consistent calculation.
  The x axis is energy in units of [meV].
  The y axis is the gain in units of [1/cm].

A negative value of gain corresponds to absorption.

Note that the gain output is only done for the voltages specified in the input file.

```
<!-- Calculate gain only between the following values of
     potential drop per period in order to save CPU time -->
     <Vmin unit="mV"> 160 </Vmin>
     <Vmax unit="mV"> 400 </Vmax>
```

Green's functions

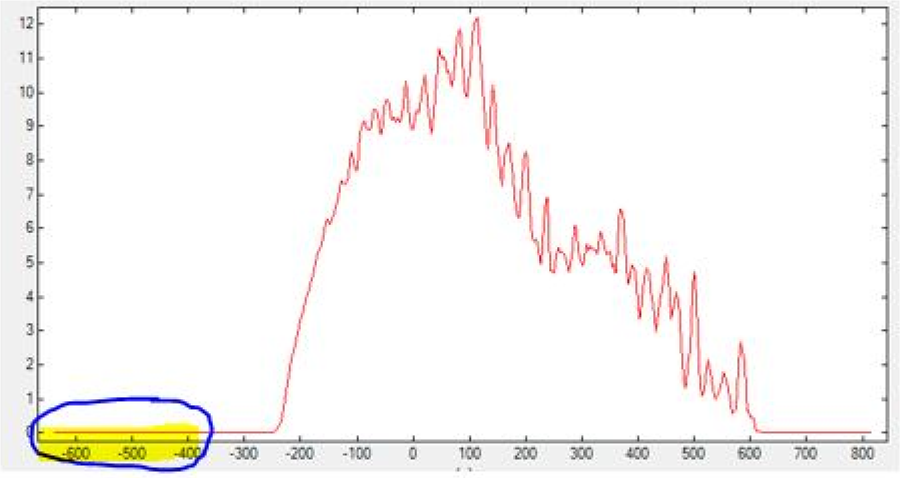
The folder `GreenFunctions/` contains information on the Green's functions.

The **electron density** $n(x,E_x)$ is related to the lesser Green's function $\mathbf{G}^<$ (“G lesser”): $$n(x,E_x) = - \frac{{\rm i}}{2\pi} \mathbf{G}(x,x^\prime=x,E_x)$$

- `GreenLesser_All.dat`
  lesser Green's function $\mathbf{G}^<$
  This file contains the sum over **<u>all</u>** the diagonal (i.e. $x=x^\prime$) lesser Green's functions (sum over one period) as a function of energy E_x.
- `GreenLesser_Z.dat`
  lesser Green's function $\mathbf{G}^<$
  This file contains the lesser Green's function $\mathbf{G}^<$ (i.e. density $n(E)$) for each mode space used in the calculation.

The **local density of states** $\rho(x,E_x)$ is related to the spectral function $\mathbf{A}$: $$\rho(x,E_x) = \frac{1}{2\pi} \mathbf{A}(x,x^\prime=x,E_x)$$ $\mathbf{A}$ is defined as $\mathbf{A} = {\rm i} (\mathbf{G}^{\rm R} - \mathbf{G}^{{\rm R}\dagger}) = - 2 {\rm Im}(\mathbf{G}^{\rm R})$. $\mathbf{G}^{\rm R}$ is the retarded Green's function.

- `GreenSpectral_All.dat`
  This file contains the sum over all the spectral functions (sum over one period) as a function of energy E_x.
  Example: In the figure below, for instance, one can see that <`Emin_shift unit="meV"`> can be increased (by 200 meV) to reduce the calculation time. Essentially, the energy range of the Green's functions is altered by adjusting <`Emin_shift unit=meV`> and <`Emax_shift unit=meV`>.



- `GreenSpectral_Z.dat`
  This file contains the spectral function for each mode space used in the calculation.

Density matrix

The folder `DensityMatrix/` contains the density matrix ρ which is a complex quantity and it is dimensionless. The trace of the density matrix equals 1. In our case, the trace is 1 if we sum over one period. The state labels (state i, period j) are specified in the complex density matrix. $$\rho(i,j) = \rho({\rm state},{\rm period})$$

- `DensityMatrix_complex.mat`
  This file contains the density matrix.
  The x axis contains real and imaginary value.
  The y axis is number of periods.
- `DensityMatrix_RealPart_AbsoluteValue.mat`
  This file contains the absolute value of the real part of the density matrix.
  The x axis contains absolute value of the imaginary part.
  The y axis is number of periods.
- `DensityMatrix_ImaginaryPart_AbsoluteValue.mat`
  This file contains the absolute value of the imaginary part of the density matrix.
  The x axis contains absolute value of the real part.
  The y axis is number of periods.

Output files for voltage sweep

For each simulation, the following files are produced.

- `Energy_WannierStarkStates.dat`
  This file contains the energy levels of the Wannier-Stark states ("E_1 = Energy of level 1", "E_2 = Energy of level 2",…) as a function of voltage, i.e. potential drop per period in units of [mV].
- `Gain_vs_Voltage.dat` and `Gain_vs_EField.dat`
  These files contain the intensity gain as a function of voltage or electric field respectively.
  The x axis is the potential drop per period [mV] (or electric field [kV/cm]).
  The y axis contains the maximum gain in [1/cm] and the photon energy for maximum gain [meV] (or photon frequency in [THz]).0
- `Current_vs_Voltage.dat` and `Current_vs_EField.dat`
  These files contain current-voltage characteristics, i.e. the current density in units of [A/cm^2] as a function of voltage (i.e. potential drop per period in units of [mV]) or electrif field in [kV/cm]. The current is the average of the file `Current-Density.dat`.

Combined temperature-voltage sweep

a combined temperature-voltage sweep can be done using the keyword `Temperature-Voltage` in the field <SweepType> of <`SweepParameters`> (see the example of code below). In this case, the simulation can be parallelized. <`Threads`> defines the number of parallel threads. Its optimal value should be the number of CPU cores available (if the available memory is sufficient). Within each parallel temperature sweep, a serial voltage sweep is performed.

```
<SweepParameters>
    <SweepType>Temperature-Voltage</SweepType>
    <MinV> 50</MinV>
    <MaxV> 60</MaxV>
    <DeltaV> 2</DeltaV>
    <MinT> 25</MinT>
    <MaxT> 300</MaxT>
    <DeltaT> 25</DeltaT>

    <Threads>12</Threads> <!-- Parallelization for Temperature-Voltage sweep
-->
</SweepParameters>
```

Note that for such voltage-temperature sweep, `<Maximum_Number_of_Threads>` in `<Simulation_Parameter>` should be set to 1. (A combined parallelization will result in lower performances.)

```
<Simulation_Parameter>
  ...
  <Maximum_Number_of_Threads>1</Maximum_Number_of_Threads>
</Simulation_Parameter>
```

At the end of the simulation, current and gain maps can be displayed. `Gain_map.fld` gives the maximum gain at each (voltage,temperature) point. `Max_Gain_frequency.fld` gives the map of the corresponding photon energy for which the gain is maximum.

Folder view:

Gain map (V,T):

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