

# Advanced settings

## Parallelization

The number of threads can be controlled using the command `<Maximum_Number_of_Threads>`

```
<Simulation_Parameter>
...
<Maximum_Number_of_Threads>12</Maximum_Number_of_Threads>
...
</Simulation_Parameter>
```

For optimal performances, we recommended that `<Maximum_Number_of_Threads>` does not exceed the number of **physical** cores (when hyperthreading is activated, the number of physical cores is half the one on logical processors).

## Parallization in case of combined Temperature-Voltage sweep

In the case where a combined Temperature-Voltage sweep is used, there are two levels of parallelization. The first is at the level of the command `<Threads>` in the `<SweepParameters>` section.

```
<SweepParameters>
  <SweepType>Temperature-Voltage</SweepType>
  ...
  <Threads>6</Threads> <!-- Parallelization for Temperature-Voltage sweep -->
</SweepParameters>
```

The second level of parallelization occurs in the `<Simulation_Parameter>` section:

```
<Simulation_Parameter>
...
<Maximum_Number_of_Threads>2</Maximum_Number_of_Threads>
...
</Simulation_Parameter>
```

In this example, the total number of threads will be `<Threads>* <Maximum_Number_of_Threads> = 6*2 = 12`.

## Contributions of individual scattering processes

The following command allow to display self-energies and spectral functions for some specific mechanisms, like e.g. scattering due to optical phonons:

```
<Scattering>
```

```
...  
<Separate_Scattering>yes</Separate_Scattering>  
...  
</Scattering>
```

This command is only for analysis purpose, and has no influence on the other calculated quantities. It only involves an additional calculation of self-energies and Green's functions. In each basis folder, a folder with the name of the scattering process will appear, containing the retarded self-energy and the spectral function arising only from the specific scattering mechanism. Hence this spectral function gives the contribution to broadening of an individual scattering process.

## Asymmetric interface roughness

It is possible to specify asymmetric interface roughness using the following command (note: this feature is currently not working due to syntax changes).

```
<Interface_Roughness>  
  
<InterfaceAutoCorrelationType> 0 </InterfaceAutoCorrelationType>  
<Correlation_Length_in_XY unit="nm"> 8 </Correlation_Length_in_XY>  
  
<Asymmetric_Interfaces> yes </Asymmetric_Interfaces>  
<Amplitude_in_Z_Left> 0.1 </Amplitude_in_Z_Left>  
<Amplitude_in_Z_Right> 0.2 </Amplitude_in_Z_Right>  
  
</Interface_Roughness>
```

## Output format for 2D plots

By default, 2D plots are output in a [VTK format](#) (files with a .vtr extension). [Gnuplot](#) files are also generated (in a file explorer, double click on the file to generate the gnuplot figure).

In addition, to output 2D plots in a [AVS/Express format](#) (.fld extension), the following command "<FLD\_format>" can be added in the <Output> section of the input file.

The following commands can be used to control the output formats:

```
<Output>  
...  
<VTK_format>yes</VTK_format>  
<FLD_format>yes</FLD_format>  
<Gnuplot_format>yes</Gnuplot_format>  
...  
</Output>
```

## Scaling 1D wavefunctions

In order to scale the output of the square of the wavefunctions (1D plots), the following command can be used:

```
<Output>
...
<ScaleWaveFunction>0.1</ScaleWaveFunction>
...
</Output>
```

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