Overview



•What is gpvdm/theoretical overview?

Installing gpvdm

•Running simple simulations

- •Your first gpvdm simulation
- •Changing electrical parameters

•Optical simulations and the materials database

•Perovskite solar cells and time domain simulations

•OFET simulations and finite difference meshing.

•The position of carriers in energy space and dumping to disk.

Meshing and dumping

Meshing and dumping





Now you should be able to see the electrical finite difference mesh





•On a mesh point click 'Set/Unset energy slice dump' this will turn on dumping of the trap population at a given mesh point.

•Click '**Set/Unset verbose electrical solver dumping**', this will *turn off* the outputting files like Ec.dat, Ev.dat, Fn.dat etc...

•Click on another mesh point and select '**Set/Unset dumping 1D slice**', this will turn on the dumping of the trap population across the device.

Your window should now look like this..





•We have turned off dumping of Ec.dat, Ev.dat etc...., and are going to be dumping the distribution of trap states along the blue line, and at the green point.

https://www.gpvdm.com





•From the *output tab* open the snapshot window.



•Then make sure npt_map.dat is selected this is a slice through the device in position/energy space. Along the blue dots below.



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Select energy_slice_nt.dat, to show the trap population at a given point.





•You can step through the simulation as a function of time/voltage.



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You can turn on/off other output files through configure \rightarrow configure \rightarrow output files



8	Configure (https://www.gpvdm.com)	↑ _ □ X
Output files Detailed dump control		1 Help
Plot bands etc	OFF	True/Fal
Dump from newton solver	OFF	True/Fals
Dump dynamic	OFF	True/Fals
Dump fx domain data	OFF	True/Fals
Time of pause	0.0	s
Dump optical information	OFF	True/Fals
Dump optics verbose	OFF	True/Fals
Print newton error	OFF	True/Fals
Print solver convergence		True/Fals
Write newton solver convergence to dis	k OFF	True/Fals
Print poisson solver convergence	OFF	True/Fals
Dump PL spectra	OFF	True/Fals
Dump zip files	OFF	True/Fals
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