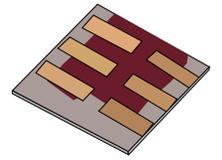
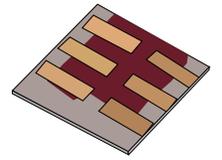


Overview



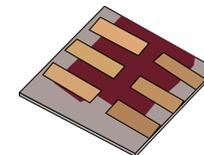
- What is gpvdm/theoretical overview?
- Installing gpvdm
- Running simple simulations
 - Your first gpvdm simulation
 - Changing electrical parameters
- Optical simulations and the materials database
- Perovskite solar cells and time domain simulations
- OFET simulations and finite difference meshing.
- The position of carriers in energy space and dumping to disk.
- Simulation OLEDs with gpvdm
- Closing remarks**

Things I've not covered/ working together...



- gpvdm can do quite a few other things like simulate PL/EL spectra, IS, IMPS, import FDTD data etc.. but I've either not had time to cover this in this tutorial or the features are not robust enough to release.
- gpvmd is a work in progress if you want a feature added it does not have let me know..... and please include me in your paper/collaboration ;). I am always after new experimental partners/collaborations

Fitting to experiment..



•Fitting complex data sets to experiment is a pain due to high CPU demand/number of parameters So I have built quite a lot of code to do the fitting on a cluster of 100 CPUs.

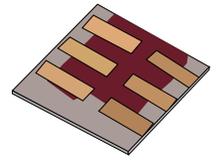
•I've released the code but it is a pain to use, **SO: If you want to fit the model to data sets, I recommend you talk to me and see if I can do it for you.**

number	type	name	ip	cpus	max_cpus	sock	load	load0	last_seen
0	slave	node001	10.0.0.1	8	8	5	8	0.790000	1
1	slave	node008	10.0.0.8	12	12	7	12	1.030000	0
2	slave	node005	10.0.0.5	8	8	6	8	0.560000	0
3	slave	node002	10.0.0.2	8	8	10	8	1.080000	1
4	master	gpvdm_master	10.154.55.33	0	0	8	0	0.350000	1543332532

n	name	done	status	target	ip	copystate	start	force_stop	stop	cpus	pid
0	job0	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.1/200	10.0.0.1	0	10.0.0.1	0	2018/11/27-15:28:43	2	24128
1	job1	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.1/400	10.0.0.1	0	10.0.0.1	0	2018/11/27-15:28:43		
2	job2	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.1/600	10.0.0.1	0	10.0.0.1	0	2018/11/27-15:28:43		
3	job3	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.1/800	10.0.0.1	0	10.0.0.1	0	2018/11/27-15:28:43		
4	job4	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.1/1000	10.0.0.8	0	10.0.0.8	0	2018/11/27-15:28:43		
5	job5	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.2/200	10.0.0.8	0	10.0.0.8	0	2018/11/27-15:28:43		
6	job6	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.2/400	10.0.0.8	0	10.0.0.8	0	2018/11/27-15:28:43		
7	job7	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.2/600	10.0.0.8	0	10.0.0.8	0	2018/11/27-15:28:43		
8	job8	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.2/800	10.0.0.8	0	10.0.0.8	0	2018/11/27-15:28:43		
9	job9	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.2/1000	10.0.0.8	0	10.0.0.8	0	2018/11/27-15:28:43		
10	job10	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.4/200	10.0.0.5	0	10.0.0.5	0	2018/11/27-15:28:43		
11	job11	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.4/400	10.0.0.5	0	10.0.0.5	0	2018/11/27-15:28:43		
12	job12	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.4/600	10.0.0.5	0	10.0.0.5	0	2018/11/27-15:28:43		
13	job13	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.4/800	10.0.0.5	0	10.0.0.5	0	2018/11/27-15:28:43		
14	job14	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.4/1000	10.0.0.2	0	10.0.0.2	0	2018/11/27-15:28:43		
15	job15	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.8/200	10.0.0.2	0	10.0.0.2	0	2018/11/27-15:28:43		
16	job16	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.8/400	10.0.0.2	0	10.0.0.2	0	2018/11/27-15:28:43		
17	job17	0	1	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.8/600	10.0.0.2	0	10.0.0.2	0	2018/11/27-15:28:43		
18	job18	0	0	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.8/800	-	0	-	0	-	-	2
19	job19	0	0	/home/rod/t/data_sets/merck_new_fit/non_symetric1/0.8/1000	-	0	-	0	-	-	2
20	job20	0	0	/home/rod/t/data_sets/merck_new_fit/non_symetric1/1.0/200	-	0	-	0	-	-	2
21	job21	0	0	/home/rod/t/data_sets/merck_new_fit/non_symetric1/1.0/400	-	0	-	0	-	-	2
22	job22	0	0	/home/rod/t/data_sets/merck_new_fit/non_symetric1/1.0/600	-	0	-	0	-	-	2
23	job23	0	0	/home/rod/t/data_sets/merck_new_fit/non_symetric1/1.0/800	-	0	-	0	-	-	2
24	job24	0	0	/home/rod/t/data_sets/merck_new_fit/non_symetric1/1.0/1000	-	0	-	0	-	-	2



Road map...



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- Two immediate things I'm working on:
 - Ray tracing of complex surfaces
 - Better FDTD