

dielectric rho和H no tiling版
本merge

罗海文

12.27

bug1-提交脚本参数问题

- -priv_size=32
- 之前报告说MAX_ALLOCATE_SIZE的值小于priv_size就行所以一直没有怀疑是脚本参数的问题

bug2-不能用malloc-thread_allocate

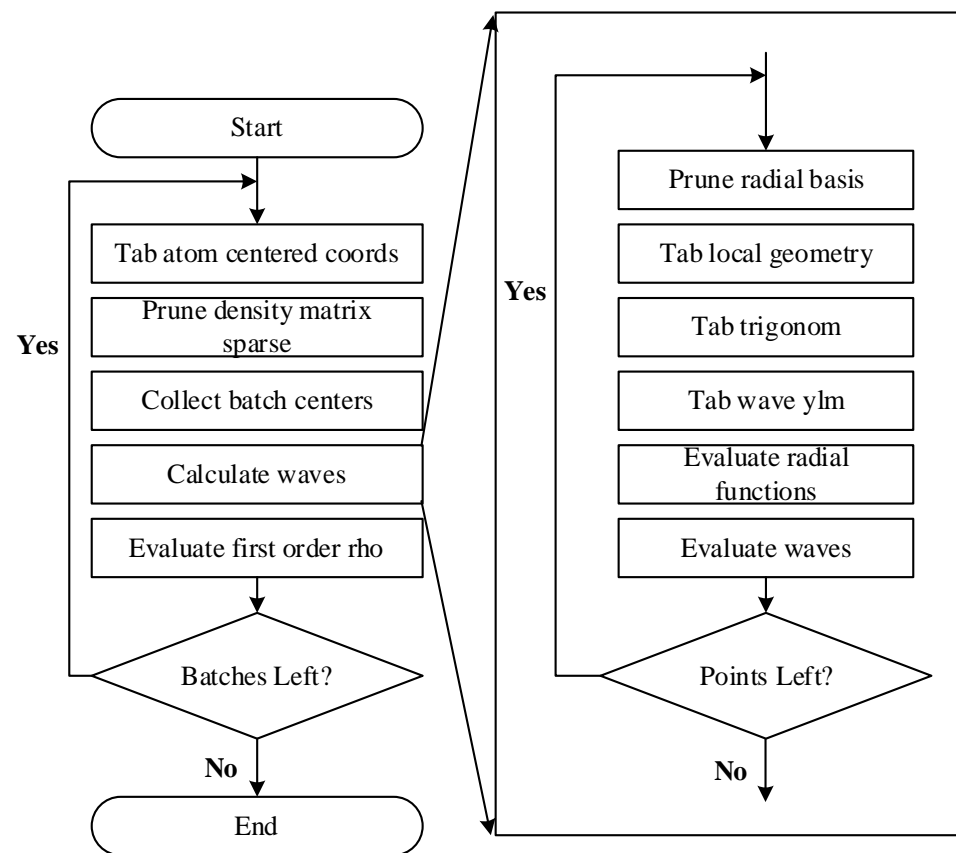
测试结果-rho

rho	fortran	fortran_xmath	c	no_tiling	tiling	tiling_tab_atom
Si 2						
n_100_mini	2.64-0.89	2.19-0.35	2.92-1.02	2.21-0.11	2.23-0.16	1.85-0.12
n_100_rt_mini	4.66-1.61	3.60-0.59	5.11-1.44	3.39-0.13	3.07-0.21	3.04-0.18
n_100_rt_tier1	152.33-56.40	86.55-3.61	136.47-53.94	84.23-1.29	wrong	wrong
n_100_tier1	34.66-16.29	19.32-1.12	34.97-15.80	20.29-0.47	19.95-0.41	18.06-0.39
n_100_tier2	161.68-63.17	99.23-3.93	156.24-62.56	99.98-1.36	wrong	wrong
n_100_tier3	482.14-160.20	343.64-14.92	501.14-172.93	wrong	wrong	wrong
n_200_tier1	26.54-16.53	11.14-0.92	26.56-16.56	10.63-0.41	10.28-0.36	10.24-0.35
n_300_tier1	25.250-17.45	8.95-0.86	27.63-19.52	8.49-0.46	8.23-0.44	8.26-0.42
Si 16						
n_100_mini	22.47-9.10	17.17-2.93	22.64-7.91	16.58-1.11	15.39-0.97	15.26-0.81
n_100_rt_mini	34.77-11.09	28.45-4.78	34.43-10.73	25.57-1.72	25.37-1.54	25.21-1.29
n_100_rt_tier1	out of memory	out of memory	out of memory	out of memory	out of memory	out of memory
n_100_tier1	282.34-121.60	168.64-9.09	280.07-118.32	168.44-3.47	168.08-3.19	168.62-3.02
n_100_tier2	out of memory	out of memory	out of memory	out of memory	out of memory	out of memory
n_100_tier3	out of memory	out of memory	out of memory	out of memory	out of memory	out of memory
n_200_tier1	222.89-130.95	99.57-7.48	223.52-130.04	10.64-0.38	98.78-2.58	98.25-2.42
n_300_tier1	210.62-137.55	80.42-7.05	209.55-137.11	8.49-0.46	wrong	wrong
RBD	233.25	27.29				

测试结果-H

H	fortran	fortran_xmath	c	no_tiling	tiling	tiling_tab_atom	tiling_tab_atom_mpe_reduction
Si 2							
n_100_mini	0.83	0.33	1.45	0.18	0.25	0.23	
n_100_rt_mini	1.42	0.55	2.15	0.62	1.11	0.93	
n_100_rt_tier1	26.36	4.53	44.75	5.21	wrong	wrong	
n_100_tier1	6.15	1.27	9.94	1.15	1.15	1.13	
n_100_tier2	43.64	4.92	85.54	4.24	wrong	wrong	
n_100_tier3	164.44	18.1	269.91	wrong	wrong	wrong	
n_200_tier1	12.04	0.89	24.6	0.85	0.78	0.76	
n_300_tier1	16.92	0.79	27.88	0.79	0.75	0.72	
Si 16							
n_100_mini	7.53	2.78	11.26	7.95	7.54	6.17	
n_100_rt_mini	10.71	4.58	15.37	13.71	12.73	10.17	
n_100_rt_tier1	out of memory	out of memory	out of memory	out of memory	out of memory	out of memory	
n_100_tier1	43.32	10.31	73.94	19.29	18.42	16.29	
n_100_tier2	out of memory	out of memory	out of memory	out of memory	out of memory	out of memory	
n_100_tier3	out of memory	out of memory	out of memory	out of memory	out of memory	out of memory	
n_200_tier1	102.91	7.27	177.45	0.78	15.65	13.12	
n_300_tier1	131.38	6.45	215.03	out of memory	wrong	wrong	
RBD	235.36	34.92					

流程图-rho小kernel



因为小kernel都上从核了
所以没有区分从核和主核