Dear. Dr. Tranchida

We tries some simple 2D example with SPIN package. Can you please check the following in/out put data and let us know your ideas.

In your paper we see,

Massively parallel symplectic algorithm for coupled magnetic spin dynamics and molecular dynamics

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> In each case, the thermostatted degrees of freedom stayed at the target temperature for the duration of the simulation. And the non-thermostated degrees of freedom relaxed from their initial temperature to the thermostatted temperature due to the spin–lattice coupling of the dynamics. In both cases the re-

We performed some test calculations

Case 1 :

```
fix             langevin all langevin 200 200 0.1 365
fix             3 all nve/spin lattice moving
```

Due to "fix 3" we expected to see a change in the magnetization of the system in the z direction. The fourth column in the table oppsite:

Step	Time	v_magnorm	v_magz	c_out_temp	KinEng	PotEng
0	0	0.33333333	0.33333333	0	0	-1822.7476
10	0.002	0.33333333	0.33333333	3.5790389	0.55468987	-1822.7451
20	0.004	0.33333333	0.33333333	7.1441238	1.1072171	-1822.7258
30	0.006	0.33333333	0.33333333	10.237599	1.586653	-1822.6747
40	0.008	0.33333333	0.33333333	13.29194	2.0600236	-1822.58
50	0.01	0.33333333	0.33333333	16.008878	2.4811026	-1822.4315
60	0.012	0.33333333	0.33333333	18.015175	2.7920442	-1822.2261
70	0.014	0.33333333	0.33333333	19.955255	3.0927236	-1821.9682
80	0.016	0.33333333	0.33333333	21.422322	3.3200938	-1821.6598
90	0.018	0.33333333	0.33333333	22.790869	3.5321953	-1821.3097
100	0.02	0.33333333	0.33333333	23.395925	3.6259686	-1820.9336
110	0.022	0.33333333	0.33333333	24.330784	3.7708559	-1820.5525
120	0.024	0.33333333	0.33333333	24.844552	3.850481	-1820.1686
130	0.026	0.33333333	0.33333333	25.458135	3.9455759	-1819.7967
140	0.028	0.33333333	0.33333333	26.055084	4.0380928	-1819.4489
150	0.03	0.33333333	0.33333333	26.843732	4.1603197	-1819.1259
160	0.032	0.33333333	0.33333333	27.847128	4.3158291	-1818.827
170	0.034	0.33333333	0.33333333	29.303358	4.5415198	-1818.5604
180	0.036	0.33333333	0.33333333	30.779305	4.7702664	-1818.3263
190	0.038	0.33333333	0.33333333	32.474984	5.0330677	-1818.113
200	0.04	0.33333333	0.33333333	34.028836	5.2738882	-1817.9133
210	0.042	0.33333333	0.33333333	35.31115	5.4726249	-1817.7143
220	0.044	0.33333333	0.33333333	36.453691	5.6496992	-1817.5145
230	0.046	0.33333333	0.33333333	37.399993	5.7963599	-1817.3186
240	0.048	0.33333333	0.33333333	39.428755	6.1107833	-1817.1168
250	0.05	0.33333333	0.33333333	40.543823	6.2835998	-1816.8944
260	0.052	0.33333333	0.33333333	41.614836	6.4495885	-1816.6577
270	0.054	0.33333333	0.33333333	42.216928	6.5429026	-1816.4184
280	0.056	0.33333333	0.33333333	43.876083	6.8000432	-1816.1811
290	0.058	0.33333333	0.33333333	44.769375	6.9384883	-1815.9446
300	0.06	0.33333333	0.33333333	45.966234	7.1239809	-1815.7209
310	0.062	0.33333333	0.33333333	46.023523	7.1328597	-1815.513
320	0.064	0.33333333	0.33333333	46.710889	7.2393896	-1815.3296
330	0.066	0.33333333	0.33333333	48.163861	7.4645756	-1815.1745
340	0.068	0.33333333	0.33333333	49.58907	7.6854585	-1815.0419
350	0.07	0.33333333	0.33333333	50.606391	7.843126	-1814.9248
360	0.072	0.33333333	0.33333333	51.400057	7.9661307	-1814.8271
370	0.074	0.33333333	0.33333333	53.292183	8.2593778	-1814.7401
380	0.076	0.33333333	0.33333333	54.903581	8.509117	-1814.6549
390	0.078	0.33333333	0.33333333	56.112933	8.6965459	-1814.564
400	0.08	0.33333333	0.33333333	56.562682	8.7662493	-1814.4741
410	0.082	0.33333333	0.33333333	57.926595	8.9776325	-1814.3822
420	0.084	0.33333333	0.33333333	59.470408	9.2168971	-1814.2752
430	0.086	0.33333333	0.33333333	61.021955	9.4573604	-1814.1382

But we only saw a change in the system magnetization in the z direction when using the following command:

Case 2 :

```
fix             3 all nve/spin lattice moving
fix             langevin all langevin 100 100 0.1 365
fix             2 all langevin/spin 100 0.01 21
```

By entering the command "fix 2 all langevin / spin 100 0.1 21", the change in magnetization begins.

The conclusion we reached was that for efficient spin-lattice coupling the "fix 1 all nve / spin lattice moving" command alone could not stimulate magnons. And for example, to work at a temperature of 100 K, you must give temperature to the spins, interaction with the lattice alone does not stimulate the spins

To me this seems in conflict with what you mentioned in the paper.

Step	Time	v_magnorm	v_magz	c_out_temp	KinEng	PotEng
0	0	0.33333333	0.33333333	0	0	-1822.7476
10	0.002	0.33315321	0.33315228	3.5790389	0.55468987	-1822.7148
20	0.004	0.33297397	0.33297166	7.144124	1.1072172	-1822.6636
30	0.006	0.33281744	0.33281512	10.2376	1.5866531	-1822.5865
40	0.008	0.33262966	0.33262649	13.291942	2.060024	-1822.4586
50	0.01	0.33245984	0.33245582	16.008884	2.4811034	-1822.284
60	0.012	0.33228395	0.33228033	18.015184	2.7920457	-1822.0464
70	0.014	0.33210723	0.33210294	19.955271	3.092726	-1821.7599
80	0.016	0.33198148	0.33197576	21.422345	3.3200974	-1821.435
90	0.018	0.33184307	0.33183532	22.790901	3.5322003	-1821.0604
100	0.02	0.33164088	0.33163338	23.395965	3.6259748	-1820.6569
110	0.022	0.3315058	0.33149752	24.330835	3.7708637	-1820.2536
120	0.024	0.33129133	0.33128273	24.844615	3.8504909	-1819.834
130	0.026	0.33102328	0.33101356	25.458212	3.9455878	-1819.42
140	0.028	0.33084422	0.33083733	26.055171	4.0381063	-1819.0408
150	0.03	0.33067338	0.3306605	26.843833	4.1603355	-1818.6897
160	0.032	0.33050318	0.33049032	27.847238	4.3158461	-1818.3601
170	0.034	0.33033708	0.33032137	29.303475	4.541538	-1818.0737
180	0.036	0.33021389	0.33020214	30.779414	4.7702833	-1817.8192
190	0.038	0.3300257	0.33001197	32.47507	5.033081	-1817.5846
200	0.04	0.32982555	0.32980541	34.028919	5.2739011	-1817.3533
210	0.042	0.32969331	0.32966707	35.311228	5.4726371	-1817.1357
220	0.044	0.32955973	0.32953491	36.453756	5.6497093	-1816.9101
230	0.046	0.3294775	0.32944693	37.400051	5.7963688	-1816.7017
240	0.048	0.32942018	0.32938766	39.428818	6.1107931	-1816.4852
250	0.05	0.32927663	0.32925189	40.543882	6.283609	-1816.2442
260	0.052	0.32913816	0.32911728	41.614899	6.4495983	-1815.9756
270	0.054	0.32887311	0.32885847	42.216996	6.542913	-1815.7004
280	0.056	0.32869646	0.32867841	43.876157	6.8000547	-1815.434
290	0.058	0.32858004	0.32856137	44.769395	6.9384913	-1815.183
300	0.06	0.32848304	0.32846684	45.96624	7.1239819	-1814.94
310	0.062	0.32832632	0.32831451	46.023441	7.1328471	-1814.7047
320	0.064	0.3281634	0.32815026	46.710756	7.239369	-1814.4917
330	0.066	0.32804925	0.3280364	48.163674	7.4645465	-1814.3205
340	0.068	0.32792803	0.3279161	49.588801	7.6854169	-1814.1761
350	0.07	0.32773475	0.32772179	50.60607	7.8430762	-1814.0393
360	0.072	0.32774384	0.32773189	51.399666	7.9660701	-1813.9396
370	0.074	0.32763399	0.32761963	53.29175	8.2593107	-1813.8347
380	0.076	0.32748353	0.32747083	54.90311	8.5090439	-1813.7178
390	0.078	0.32732229	0.32731097	56.112482	8.6964759	-1813.604
400	0.08	0.32719741	0.32718716	56.562224	8.7661783	-1813.4989
410	0.082	0.32712284	0.32710877	57.926096	8.9775552	-1813.3997
420	0.084	0.3271437	0.32713413	59.469977	9.2168304	-1813.3007
430	0.086	0.32712746	0.32712324	61.021542	9.4572964	-1813.1601

In the following, we will examine two other cases:

Case 3 :

```
fix             3 all nve/spin lattice moving
fix             2 all langevin/spin 100 0.01 21
```

Step	Time	v_magnorm	v_magz	c_out_temp	KinEng	PotEng
0	0	0.33333333	0.33333333	0	0	-1822.7476
10	0.002	0.33315321	0.33315228	0.0010168675	0.00015759709	-1822.7174
20	0.004	0.33297397	0.33297166	0.003976006	0.000616213	-1822.686
30	0.006	0.33281744	0.33281512	0.0086112193	0.0013345919	-1822.6607
40	0.008	0.33262966	0.33262649	0.014505438	0.0022480951	-1822.6284
50	0.01	0.33245984	0.33245582	0.021128123	0.0032744981	-1822.6034
60	0.012	0.33228395	0.33228033	0.027882883	0.0043213704	-1822.5723
70	0.014	0.33210723	0.33210294	0.034161059	0.0052943805	-1822.5446
80	0.016	0.33198148	0.33197576	0.039396503	0.0061057848	-1822.5289
90	0.018	0.33184307	0.33183533	0.043116606	0.0066823372	-1822.505
100	0.02	0.33164088	0.33163339	0.044985021	0.0069719096	-1822.4779
110	0.022	0.3315058	0.33149752	0.044832181	0.006948222	-1822.4556
120	0.024	0.33129134	0.33128273	0.04267084	0.006613251	-1822.4196
130	0.026	0.33102329	0.33101356	0.038695177	0.0059970912	-1822.3768
140	0.028	0.33084422	0.33083733	0.033263501	0.0051552742	-1822.3446
150	0.03	0.33067338	0.33066049	0.026866059	0.0041637802	-1822.3156
160	0.032	0.33050316	0.3304903	0.020080835	0.0031121863	-1822.2838
170	0.034	0.33033706	0.33032134	0.0135213	0.0020955704	-1822.2629
180	0.036	0.33021387	0.33020212	0.0077808668	0.0012059014	-1822.2417
190	0.038	0.33002565	0.33001192	0.0033790833	0.00052370018	-1822.2197
200	0.04	0.32982552	0.32980537	0.00071446982	0.00011073062	-1822.1877
210	0.042	0.32969326	0.32966703	2.8319172e-05	4.3889878e-06	-1822.169
220	0.044	0.32955969	0.32953487	0.0013827666	0.0002143052	-1822.1434
230	0.046	0.32947748	0.32944691	0.0046551421	0.00072146749	-1822.1314
240	0.048	0.32942013	0.32938761	0.0095491218	0.0014799507	-1822.1174
250	0.05	0.32927657	0.32925183	0.015621657	0.0024210899	-1822.0998
260	0.052	0.32913815	0.32911727	0.022323213	0.0034597165	-1822.069
270	0.054	0.32887313	0.3288585	0.029047633	0.0045018869	-1822.0341
280	0.056	0.32869647	0.32867842	0.035187085	0.0054533969	-1822.0059
290	0.058	0.32858007	0.32856141	0.040187061	0.0062283078	-1821.9923
300	0.06	0.328483	0.3284668	0.043596472	0.0067567083	-1821.9734
310	0.062	0.32832623	0.32831442	0.045108273	0.0069910116	-1821.9462
320	0.064	0.32816329	0.32815015	0.044586998	0.0069102229	-1821.9166
330	0.066	0.32804912	0.32803627	0.042080742	0.0065217959	-1821.9001
340	0.068	0.32792797	0.32791603	0.037816559	0.0058609205	-1821.8877
350	0.07	0.32773463	0.32772167	0.032179758	0.0049873126	-1821.867
360	0.072	0.3277437	0.32773175	0.025678987	0.0039798042	-1821.864
370	0.074	0.32763393	0.32761958	0.018900308	0.0029292248	-1821.8452
380	0.076	0.32748335	0.32747066	0.012454396	0.0019302185	-1821.8124
390	0.078	0.32732223	0.32731091	0.006921617	0.0010727324	-1821.7887
400	0.08	0.3271974	0.32718716	0.0027999026	0.00043393706	-1821.7729
410	0.082	0.32712288	0.32710881	0.00046007204	7.1303305e-05	-1821.7652
420	0.084	0.32714371	0.32713414	0.00011258663	1.7449004e-05	-1821.7732
430	0.086	0.32712743	0.32712323	0.0017886891	0.00027721625	-1821.7697

Case 4 :

```
fix             3 all nve/spin lattice frozen
fix             2 all langevin/spin 100 0.01 21
```

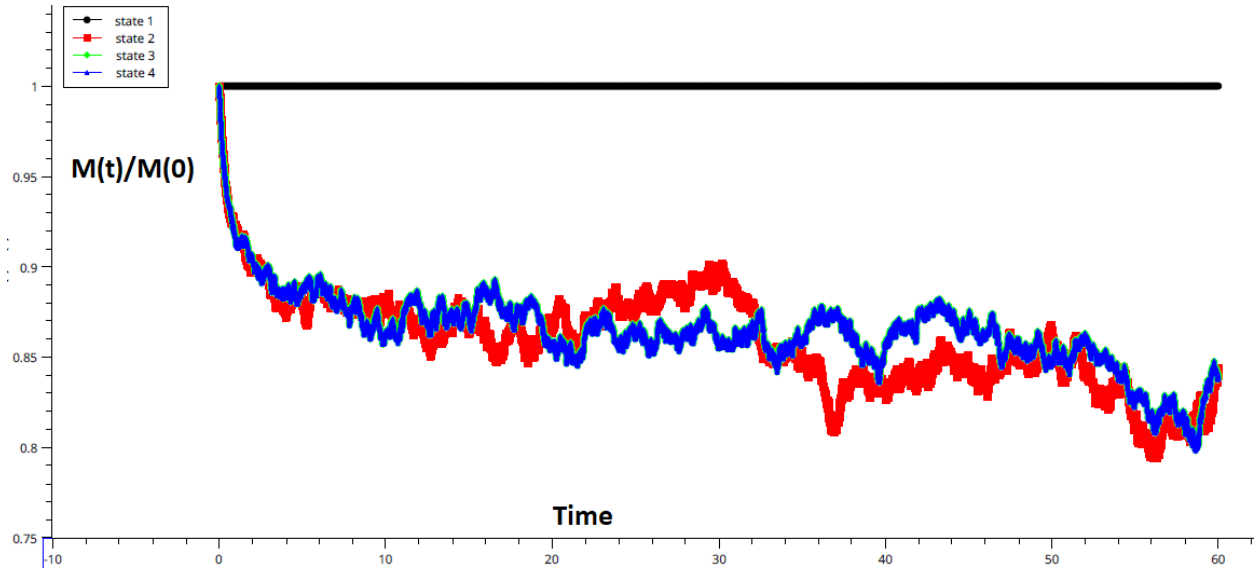
There is no difference between the two. Although in the fourth case we have given up network vibration and in the third case we have considered network vibration.

The Fig can be viewed for better comparison

Step	Time	v_magnorm	v_magz	c_out_temp	KinEng	PotEng
0	0	0.33333333	0.33333333	0	0	-1822.7476
10	0.002	0.33315321	0.33315228	0	0	-1822.7172
20	0.004	0.33297397	0.33297166	0	0	-1822.6854
30	0.006	0.33281744	0.33281512	0	0	-1822.6594
40	0.008	0.33262966	0.33262649	0	0	-1822.6262
50	0.01	0.33245984	0.33245582	0	0	-1822.6001
60	0.012	0.33228395	0.33228033	0	0	-1822.5679
70	0.014	0.33210723	0.33210294	0	0	-1822.5393
80	0.016	0.33198148	0.33197576	0	0	-1822.5228
90	0.018	0.33184307	0.33183533	0	0	-1822.4983
100	0.02	0.33164088	0.33163339	0	0	-1822.4709
110	0.022	0.3315058	0.33149752	0	0	-1822.4487
120	0.024	0.33129134	0.33128273	0	0	-1822.413
130	0.026	0.33102329	0.33101356	0	0	-1822.3708
140	0.028	0.33084422	0.33083733	0	0	-1822.3395
150	0.03	0.33067338	0.33066049	0	0	-1822.3114
160	0.032	0.33050316	0.3304903	0	0	-1822.2807
170	0.034	0.33033706	0.33032134	0	0	-1822.2608
180	0.036	0.33021387	0.33020212	0	0	-1822.2405
190	0.038	0.33002565	0.33001192	0	0	-1822.2192
200	0.04	0.32982552	0.32980537	0	0	-1822.1876
210	0.042	0.32969326	0.32966703	0	0	-1822.169
220	0.044	0.32955969	0.32953487	0	0	-1822.1432
230	0.046	0.32947748	0.32944691	0	0	-1822.1306
240	0.048	0.32942013	0.32938761	0	0	-1822.116
250	0.05	0.32927657	0.32925183	0	0	-1822.0973
260	0.052	0.32913815	0.32911727	0	0	-1822.0655
270	0.054	0.32887313	0.3288585	0	0	-1822.0296
280	0.056	0.32869647	0.32867842	0	0	-1822.0005
290	0.058	0.32858007	0.32856141	0	0	-1821.986
300	0.06	0.328483	0.3284668	0	0	-1821.9667
310	0.062	0.32832623	0.32831442	0	0	-1821.9392
320	0.064	0.32816329	0.32815015	0	0	-1821.9097
330	0.066	0.32804912	0.32803627	0	0	-1821.8936
340	0.068	0.32792797	0.32791603	0	0	-1821.8818
350	0.07	0.32773463	0.32772167	0	0	-1821.862
360	0.072	0.3277437	0.32773175	0	0	-1821.8601
370	0.074	0.32763393	0.32761958	0	0	-1821.8422
380	0.076	0.32748335	0.32747066	0	0	-1821.8105
390	0.078	0.32732223	0.32731091	0	0	-1821.7876
400	0.08	0.3271974	0.32718716	0	0	-1821.7725
410	0.082	0.32712288	0.32710881	0	0	-1821.7651
420	0.084	0.32714371	0.32713414	0	0	-1821.7732
430	0.086	0.32712743	0.32712323	0	0	-1821.7695

Our question is to calculate the spin-lattice interaction of both subnets

Should they reach the desired temperature with the thermostat?



The green and blue diagrams are exactly the same .