

Assuming all dual-issue.

Assuming that only Mul/Adds can be simultaneous

Assuming SIMD only issuable on alternating cycles, otherwise

Movss can be sent out on dual-issue

SIMD Stuff Starts executing on n/n+1

Data dependencies account for weirdness

Assuming SIMD Adder can Subtract

Instruction	Issue	Execute
<b>.nb302_single_loop:</b>		
mov edx, [esp + nb302_innerjjnr]	1	2
mov eax, [edx]	1	3
add dword ptr [esp + nb302_innerjjnr], 4	2	3
mov esi, [ebp + nb302_pos]	2	3
lea eax, [eax + eax*2]	3	4
xorps xmm3, xmm3	3	5
xorps xmm4, xmm4	5	7
xorps xmm5, xmm5	7	9
movss xmm3, [esi + eax*4]	9	10
movss xmm4, [esi + eax*4 + 4]	9	10
movss xmm5, [esi + eax*4 + 8]	10	11
movlps xmm6, [esi + eax*4 + 12]	11	13
movss xmm7, [esi + eax*4 + 20]	13	14
movhps xmm6, [esi + eax*4 + 24]	14	16
movss xmm2, [esi + eax*4 + 32]	16	17
shufps xmm6, xmm6, 216 ;# constant 11011000	17	19
unpcklps xmm7, xmm2	19	21
movaps xmm0, [esp + nb302_ixO]	21	23
movaps xmm1, [esp + nb302_iyO]	23	25
movaps xmm2, [esp + nb302_izO]	25	27
movlhps xmm3, xmm6	27	29
shufps xmm4, xmm6, 228 ;# constant 11100100	29	31
shufps xmm5, xmm7, 68 ;# constant 01000100	31	33
movaps [esp + nb302_jxO], xmm3	33	35
movaps [esp + nb302_jyO], xmm4	35	37
movaps [esp + nb302_jzO], xmm5	37	39
subps xmm0, xmm3	39	41
subps xmm1, xmm4	41	43
subps xmm2, xmm5	43	45
movaps [esp + nb302_dxOO], xmm0	45	47
movaps [esp + nb302_dyOO], xmm1	47	49
movaps [esp + nb302_dzOO], xmm2	49	51
mulps xmm0, xmm0	51	53
mulps xmm1, xmm1	53	55
mulps xmm2, xmm2	55	57 *Simul
addps xmm0, xmm1	55	57
addps xmm0, xmm2	57	59
rsqrtps xmm1, xmm0	60	62
movaps xmm2, xmm1	63	65

mulps xmm1, xmm1	65	67
movaps xmm3, [esp + nb302_three]	67	69
mulps xmm1, xmm0	69	71 *Data Dependence
subps xmm3, xmm1	71	74
mulps xmm3, xmm2	75	77
mulps xmm3, [esp + nb302_half] ;# rinv iO - j water	78	79
movaps xmm1, xmm3	80	82
mulps xmm1, xmm0	83	85
movaps xmm0, xmm3	85	87
mulps xmm1, [esp + nb302_tsc]	87	89
movhlps xmm2, xmm1	90	92
cvttps2pi mm6, xmm1	92	94
cvttps2pi mm7, xmm2	94	96
cvtpi2ps xmm3, mm6	96	98
cvtpi2ps xmm2, mm7	98	100
movlhps xmm3, xmm2	101	103
subps xmm1, xmm3	104	106
movaps xmm2, xmm1	107	109
mulps xmm2, xmm2	110	112
pslld mm6, 2	113	114 *Dual
pslld mm7, 2	113	114
movd ebx, mm6	115	116 *Dual Move
movd ecx, mm7	115	116
psrlq mm7, 32	116	117
movd edx, mm7	116	118
mov esi, [ebp + nb302_VFtab]	117	118
movlps xmm5, [esi + ebx*4]	118	120
movlps xmm7, [esi + ecx*4]	120	122
movhps xmm7, [esi + edx*4] ;# got half coulomb table	122	125 *Have to Wait
movaps xmm4, xmm5	123	125
shufps xmm4, xmm7, 136 ;# constant 10001000	125	127
shufps xmm5, xmm7, 221 ;# constant 11011101	127	129
movlps xmm7, [esi + ebx*4 + 8]	129	131
movlps xmm3, [esi + ecx*4 + 8]	131	133
movhps xmm3, [esi + edx*4 + 8] ;# other half of coulomb table	133	135
movaps xmm6, xmm7	135	137
shufps xmm6, xmm3, 136 ;# constant 10001000	137	139
shufps xmm7, xmm3, 221 ;# constant 11011101	139	141
mulps xmm6, xmm1	141	143
mulps xmm7, xmm2	143	145 *Simul
addps xmm5, xmm6	143	145
addps xmm5, xmm7	145	147
mulps xmm7, [esp + nb302_two]	147	149
xorps xmm3, xmm3	151	153
movss xmm3, [esp + nb302_qqOO]	153	155
movhps xmm3, [esp + nb302_qqOH]	155	157
addps xmm7, xmm6	157	159
addps xmm7, xmm5 ;# xmm7=FF	159	161
mulps xmm5, xmm1 ;# xmm5=eps*Fp	161	163 *Simul

addps xmm5, xmm4 ;# xmm5=VV	161	163
mulps xmm5, xmm3 ;# vcoul=qq*VV	163	165
mulps xmm3, xmm7 ;# fijC=FF*qq	165	167 *Simul
addps xmm5, [esp + nb302_vctot]	165	167
movaps [esp + nb302_vctot], xmm5	167	169
xorps xmm2, xmm2	169	
mulps xmm3, [esp + nb302_tsc]	171	173 *Simul
subps xmm2, xmm3	171	173
mulps xmm0, xmm2	173	175
movaps xmm1, xmm0	175	177
movaps xmm2, xmm0	177	179
mulps xmm0, [esp + nb302_dxOO]	179	181
mulps xmm1, [esp + nb302_dyOO]	181	183
mulps xmm2, [esp + nb302_dzOO]	183	185
xorps xmm3, xmm3	185	187
xorps xmm4, xmm4	187	189
xorps xmm5, xmm5	189	191
subps xmm3, xmm0	191	193
subps xmm4, xmm1	193	195
subps xmm5, xmm2	195	197
movaps [esp + nb302_fjxO], xmm3	197	199
movaps [esp + nb302_fjyO], xmm4	199	201
movaps [esp + nb302_fjzO], xmm5	201	203
addps xmm0, [esp + nb302_fixO]	203	205
addps xmm1, [esp + nb302_fiyO]	205	207
addps xmm2, [esp + nb302_fizO]	207	209
movaps [esp + nb302_fixO], xmm0	209	211
movaps [esp + nb302_fiyO], xmm1	211	213
movaps [esp + nb302_fizO], xmm2	213	215
movaps xmm0, [esp + nb302_ixH1]	215	217
movaps xmm1, [esp + nb302_iyH1]	217	219
movaps xmm2, [esp + nb302_izH1]	219	221
movaps xmm3, [esp + nb302_ixH2]	221	223
movaps xmm4, [esp + nb302_iyH2]	223	225
movaps xmm5, [esp + nb302_izH2]	225	227
subps xmm0, [esp + nb302_jxO]	227	229
subps xmm1, [esp + nb302_jyO]	229	231
subps xmm2, [esp + nb302_jzO]	231	233
subps xmm3, [esp + nb302_jxO]	233	235
subps xmm4, [esp + nb302_jyO]	235	237
subps xmm5, [esp + nb302_jzO]	237	239
movaps [esp + nb302_dxH1O], xmm0	239	241
movaps [esp + nb302_dyH1O], xmm1	241	243
movaps [esp + nb302_dzH1O], xmm2	243	245
movaps [esp + nb302_dxH2O], xmm3	245	247
movaps [esp + nb302_dyH2O], xmm4	247	249
movaps [esp + nb302_dzH2O], xmm5	249	251
mulps xmm0, xmm0	251	253
mulps xmm1, xmm1	253	255

mulps xmm2, xmm2	255	257
mulps xmm3, xmm3	257	259
mulps xmm4, xmm4	259	261
mulps xmm5, xmm5	261	263 *Simul
addps xmm0, xmm1	261	263
addps xmm4, xmm3	263	265
addps xmm0, xmm2	265	267
addps xmm4, xmm5	267	269
movaps [esp + nb302_rsqrH2O], xmm4	269	271
rsqrtps xmm1, xmm0	271	273
rsqrtps xmm5, xmm4	273	275
movaps xmm2, xmm1	275	277
movaps xmm6, xmm5	277	279
mulps xmm1, xmm1	279	281
mulps xmm5, xmm5	281	283
movaps xmm3, [esp + nb302_three]	283	285
movaps xmm7, xmm3	285	287
mulps xmm1, xmm0	287	289
mulps xmm5, xmm4	289	291 *Simul
subps xmm3, xmm1	289	291
subps xmm7, xmm5	291	293
mulps xmm3, xmm2	293	295
mulps xmm7, xmm6	295	297
mulps xmm3, [esp + nb302_half] ;# rinv H1 - j water	297	299
mulps xmm7, [esp + nb302_half] ;# rinv H2 - j water	299	301
movaps [esp + nb302_rinvH2O], xmm7	301	303
movaps xmm1, xmm3	303	305
mulps xmm1, xmm0	305	307
movaps xmm0, xmm3	307	309
mulps xmm1, [esp + nb302_tsc]	309	311
movhlps xmm2, xmm1	311	313
cvttps2pi mm6, xmm1	313	315
cvttps2pi mm7, xmm2	315	317
cvtpi2ps xmm3, mm6	317	319
cvtpi2ps xmm2, mm7	319	321
movlhps xmm3, xmm2	321	323
subps xmm1, xmm3	323	325
movaps xmm2, xmm1	325	327
mulps xmm2, xmm2	327	329
pslld mm6, 2	329	330 *Dual
pslld mm7, 2	329	330
movd ebx, mm6	330	331
movd ecx, mm7	330	331
psrlq mm7, 32	331	332
movd edx, mm7	331	333
movlps xmm5, [esi + ebx*4]	333	335
movlps xmm7, [esi + ecx*4]	335	337
movhps xmm7, [esi + edx*4] ;# got half coulomb table	337	339
movaps xmm4, xmm5	339	341

shufps xmm4, xmm7, 136 ;# constant 10001000	341	343
shufps xmm5, xmm7, 221 ;# constant 11011101	343	345
movlps xmm7, [esi + ebx*4 + 8]	345	347
movlps xmm3, [esi + ecx*4 + 8]	347	349
movhps xmm3, [esi + edx*4 + 8] ;# other half of coulomb table	349	351
movaps xmm6, xmm7	351	353
shufps xmm6, xmm3, 136 ;# constant 10001000	353	355
shufps xmm7, xmm3, 221 ;# constant 11011101	355	357
mulps xmm6, xmm1	357	359
mulps xmm7, xmm2	359	361 *Simul
addps xmm5, xmm6	359	361
addps xmm5, xmm7	361	363
mulps xmm7, [esp + nb302_two]	363	365
xorps xmm3, xmm3	365	367
movss xmm3, [esp + nb302_qqOH]	367	368
movhps xmm3, [esp + nb302_qqHH]	378	380
addps xmm7, xmm6	380	381
addps xmm7, xmm5 ;# xmm7=FF	382	384
mulps xmm5, xmm1 ;# xmm5=eps*Fp	384	386 *Simul
addps xmm5, xmm4 ;# xmm5=VV	384	386
mulps xmm5, xmm3 ;# vcoul=qq*VV	386	388
mulps xmm3, xmm7 ;# fijC=FF*qq	388	390 *Simul
addps xmm5, [esp + nb302_vctot]	388	390
movaps [esp + nb302_vctot], xmm5	390	392
xorps xmm1, xmm1	392	394
mulps xmm3, [esp + nb302_tsc]	394	396
mulps xmm3, xmm0	396	398 *Simul
subps xmm1, xmm3	396	398
movaps xmm0, xmm1	398	400
movaps xmm2, xmm1	400	402
mulps xmm0, [esp + nb302_dxH1O]	402	404
mulps xmm1, [esp + nb302_dyH1O]	404	406
mulps xmm2, [esp + nb302_dzH1O]	406	408
movaps xmm3, [esp + nb302_fjxO]	408	410
movaps xmm4, [esp + nb302_fjyO]	410	412
movaps xmm5, [esp + nb302_fjzO]	412	414
subps xmm3, xmm0	414	416
subps xmm4, xmm1	416	418
subps xmm5, xmm2	418	420
movaps [esp + nb302_fjxO], xmm3	420	422
movaps [esp + nb302_fjyO], xmm4	422	424
movaps [esp + nb302_fjzO], xmm5	424	426
addps xmm0, [esp + nb302_fixH1]	426	428
addps xmm1, [esp + nb302_fiyH1]	428	430
addps xmm2, [esp + nb302_fizH1]	430	432
movaps [esp + nb302_fixH1], xmm0	432	434
movaps [esp + nb302_fiyH1], xmm1	434	436
movaps [esp + nb302_fizH1], xmm2	436	438
movaps xmm0, [esp + nb302_rinvH2O]	438	440

movaps xmm1, [esp + nb302_rsqrH2O]	440	442
mulps xmm1, xmm0	442	444
mulps xmm1, [esp + nb302_tsc]	444	446
movhlps xmm2, xmm1	446	448
cvttps2pi mm6, xmm1	448	450
cvttps2pi mm7, xmm2	450	452
cvtpi2ps xmm3, mm6	452	454
cvtpi2ps xmm2, mm7	454	456
movlhps xmm3, xmm2	456	458
subps xmm1, xmm3	458	460
movaps xmm2, xmm1	460	462
mulps xmm2, xmm2	462	464
pslld mm6, 2	464	466
pslld mm7, 2	464	466
movd ebx, mm6	466	468
movd ecx, mm7	466	468
psrlq mm7, 32	468	470
movd edx, mm7	468	470
movlps xmm5, [esi + ebx*4]	470	472
movlps xmm7, [esi + ecx*4]	472	474
movhps xmm7, [esi + edx*4] ;# got half coulomb table	474	476
movaps xmm4, xmm5	476	478
shufps xmm4, xmm7, 136 ;# constant 10001000	478	480
shufps xmm5, xmm7, 221 ;# constant 11011101	480	482
movlps xmm7, [esi + ebx*4 + 8]	482	484
movlps xmm3, [esi + ecx*4 + 8]	484	486
movhps xmm3, [esi + edx*4 + 8] ;# other half of coulomb table	486	488
movaps xmm6, xmm7	488	490
shufps xmm6, xmm3, 136 ;# constant 10001000	490	492
shufps xmm7, xmm3, 221 ;# constant 11011101	492	494
mulps xmm6, xmm1	494	496
mulps xmm7, xmm2	496	498 *Simul
addps xmm5, xmm6	496	498
addps xmm5, xmm7	498	500
mulps xmm7, [esp + nb302_two]	500	502
xorps xmm3, xmm3	502	504
movss xmm3, [esp + nb302_qqOH]	504	505
movhps xmm3, [esp + nb302_qqHH]	506	507
addps xmm7, xmm6	508	510
addps xmm7, xmm5 ;# xmm7=FF	510	512
mulps xmm5, xmm1 ;# xmm5=eps*Fp	512	514 *Simul
addps xmm5, xmm4 ;# xmm5=VV	512	514
mulps xmm5, xmm3 ;# vcoul=qq*VV	514	516
mulps xmm3, xmm7 ;# fijC=FF*qq	516	518 *Simul
addps xmm5, [esp + nb302_vctot]	516	518
movaps [esp + nb302_vctot], xmm5	518	520
xorps xmm1, xmm1	520	522
mulps xmm3, [esp + nb302_tsc]	522	524
mulps xmm3, xmm0	524	526 *Simul

subps xmm1, xmm3	524	526
movaps xmm0, xmm1	526	528
movaps xmm2, xmm1	528	530
mulps xmm0, [esp + nb302_dxH2O]	530	532
mulps xmm1, [esp + nb302_dyH2O]	532	534
mulps xmm2, [esp + nb302_dzH2O]	534	536
movaps xmm3, [esp + nb302_fjxO]	536	538
movaps xmm4, [esp + nb302_fjyO]	538	540
movaps xmm5, [esp + nb302_fjzO]	540	542
subps xmm3, xmm0	542	544
subps xmm4, xmm1	544	546
subps xmm5, xmm2	546	548
mov esi, [ebp + nb302_faction]	548	549
movaps [esp + nb302_fjxO], xmm3	549	551
movaps [esp + nb302_fjyO], xmm4	551	553
movaps [esp + nb302_fjzO], xmm5	553	555
addps xmm0, [esp + nb302_fixH2]	555	557
addps xmm1, [esp + nb302_fiyH2]	557	559
addps xmm2, [esp + nb302_fizH2]	559	561
movaps [esp + nb302_fixH2], xmm0	561	563
movaps [esp + nb302_fiyH2], xmm1	563	565
movaps [esp + nb302_fizH2], xmm2	565	567
movlps xmm0, [esi + eax*4]	567	569
movlps xmm1, [esi + eax*4 + 12]	569	571
movhps xmm1, [esi + eax*4 + 24]	571	573
movaps xmm3, [esp + nb302_fjxO]	573	575
movaps xmm4, [esp + nb302_fjyO]	575	577
movaps xmm5, [esp + nb302_fjzO]	577	579
movaps xmm6, xmm5	579	581
movaps xmm7, xmm5	581	583
shufps xmm6, xmm6, 2 ;# constant 00000010	583	585
shufps xmm7, xmm7, 3 ;# constant 00000011	585	587
addss xmm5, [esi + eax*4 + 8]	587	589
addss xmm6, [esi + eax*4 + 20]	589	591
addss xmm7, [esi + eax*4 + 32]	591	593
movss [esi + eax*4 + 8], xmm5	593	594
movss [esi + eax*4 + 20], xmm6	593	594
movss [esi + eax*4 + 32], xmm7	594	595
movaps xmm5, xmm3	595	597
unpcklps xmm3, xmm4	597	599
unpckhps xmm5, xmm4	599	601
addps xmm0, xmm3	601	603
addps xmm1, xmm5	603	605
movlps [esi + eax*4], xmm0	605	607
movlps [esi + eax*4 + 12], xmm1	607	609
movhps [esi + eax*4 + 24], xmm1	609	611
dec dword ptr [esp + nb302_innerk]	611	612
jz .nb302_updateouterdata	611	612

jmp .nb302\_single\_loop

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