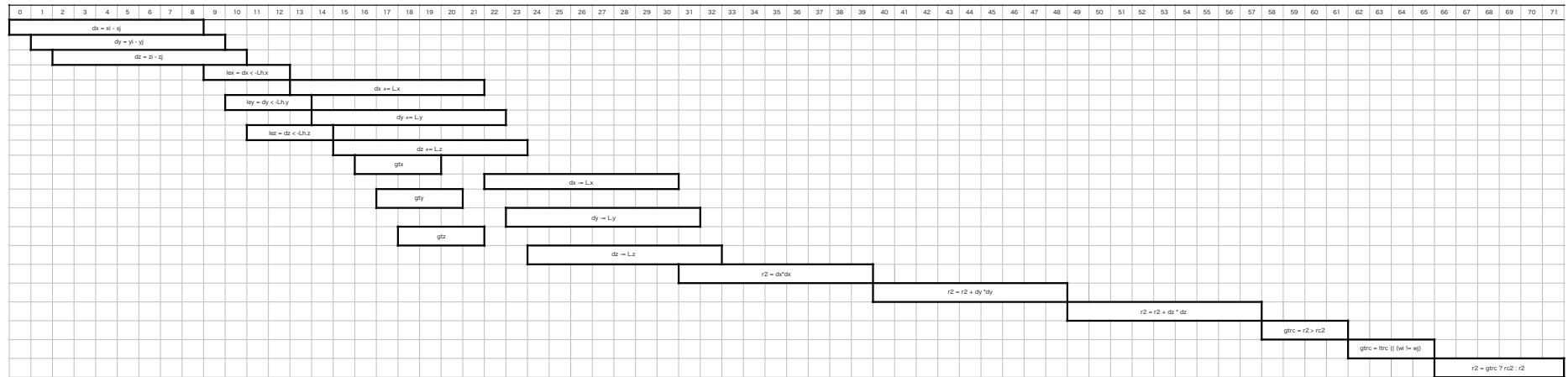


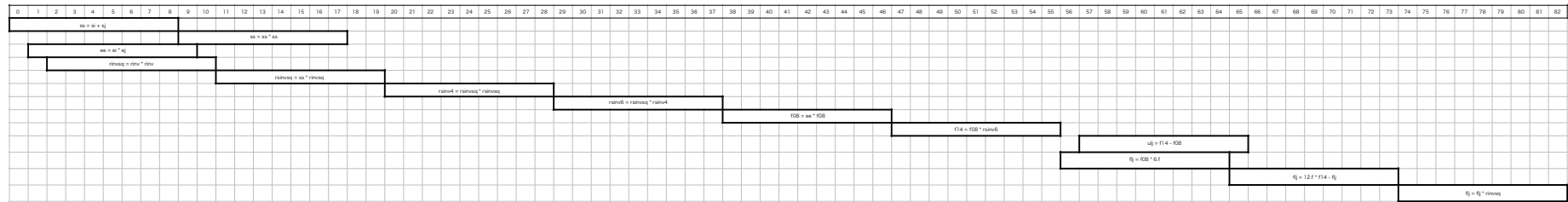
r²計算ループ



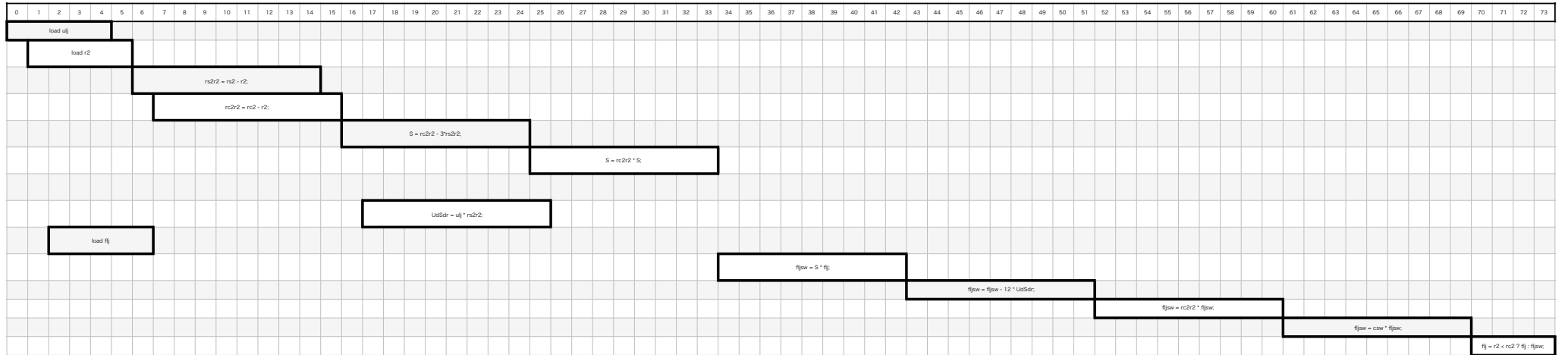
1/r計算ループ

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48			
rsqrte																																																			
				h = r2 * rinu																																															
													h = 1 - h * rinu																																						
																						poly = 0.5 + 3/8 * h																													
																																poly = h * poly																			
																																rinu = rinu + rinu * poly																			

Li相互作用計算ループ



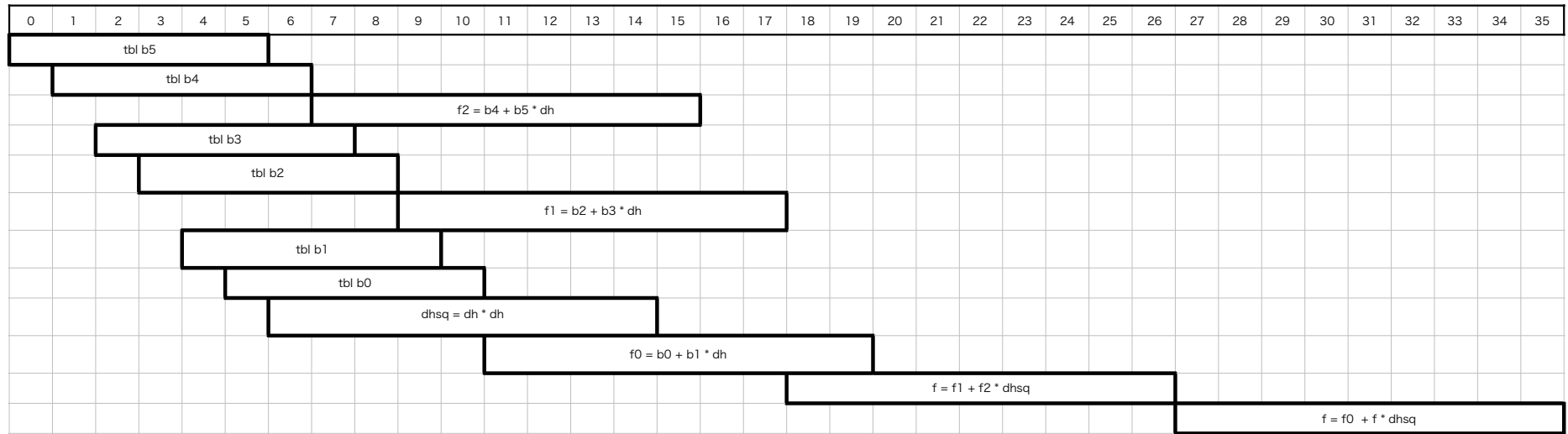
スイッチング関数適用ループ



区間決定ループ

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37				
rb2 = r2 * b2																																									
									idx = rb2 + COMP																																
													idx = idx >> 23																												
																	idx = idx & 0xf																								
																					y = idx << 23																				
																									y = y - COMP																
																																	dh = y + rb2								

多項式計算ループ



静電相互作用計算ループ

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
qq = qi * qj																												
	f = f*f																											
										f = qq * f																		
		rinvsq = rinv * rinv																										
											rinvcb = rinvsq * rinv																	
																				f = f * rinvcb								

足しこみループ

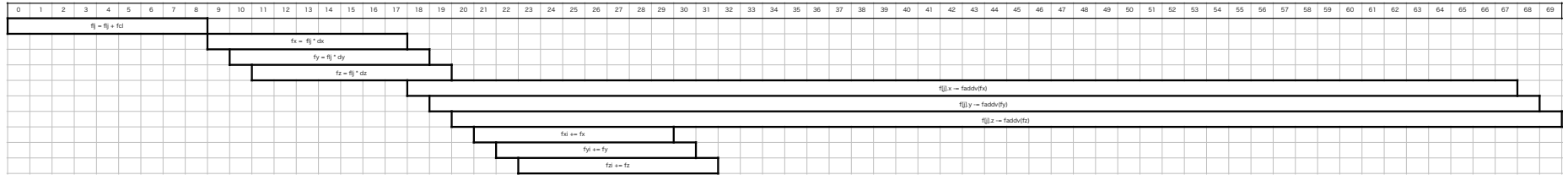


表1

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51
tbl b5																																																			
tbl b4																																																			
						f = b5 + b4 * dh																																													
tbl b3																																																			
							f = b3 + f * dh																																												
tbl b2																																																			
										f = b2 + f * dh																																									
tbl b1																																																			
													f = b1 + f * dh																																						
tbl b0																																																			
																f = b0 + f * dh																																			

