LIGGGHTS Benchmarking Study

This document describes a series of benchmarking simulations that were used both to compare LIGGGHTS against a commercial code and to gauge the overall parallelization performance of the code in a variety of situations. The simulations are described below, and the input decks are provided at the end of the document to give the reader some understanding of how these timings were generated. The codes here are not claimed to be the most efficient simulations possible (but hopefully are at least in the ballpark!).

Batch processes

- Bin flow
- Rotating drum
- Couette cylinder
- Plow mixer
- Pin mixer
- Vertical shear mixer
- Ribbon blender
- V-blender
- Auger doser

Continuous processes

- CB mixer #1
- CB mixer #2
- CB mixer #3
- CB mixer #4
- Vibrating conveyor

All LIGGGHTS jobs were run with version 2.2.3 and 2.2.4 on a cluster consisting of 320 nodes with Intel X5670 2.93 GHz chips (12 cores/node) and 24 GB RAM per node. As a result, all jobs were parallelized in increments of 12 cores.

All jobs run with the COMMERCIAL CODE were run on an 8-core Intel X5365 3.0GHz chip workstation with 16 GB RAM.

Bin Flow:

A cylindrical hopper was initially filled with a set of spherical particles which were allowed to settle under the influence of gravity. The bottom of the hopper was then opened and the material was allowed to pour from the hopper. We track the flowrate of material from the hopper as a comparison metric.

	Model 1	Model 2	Model 3
Initial # of particles	300,000	3,000,000	10,000,000
Particle diameter (m)	0.003	0.0014	0.001
Particle density (kg/m^3)	1000	1000	1000
Poisson ratio	0.25	0.25	0.25
Young's modulus (MPa)	25	25	25
Coefficient of restitution	0.5	0.5	0.5
Static friction coefficient	0.2	0.2	0.2
Rolling friction coefficient	0.0	0.0	0.0
Timestep (sec)	10^{-5}	$5x10^{-6}$	$3.33x10^{-6}$
Settling time (sec)	1.5	1.5	1.5
Flow time (sec)	3.0	5.0	2.0

Model parameters for bin flow simulations.

Results

Timings for these simulations are shown in the tables below. (COMMERCIAL CODE) simulations were performed for only model #1 as the other two cases proved to be prohibitively expensive from a computational standpoint to even generate results. We also compare LIGGGHTS simulation with and without dynamic load balancing to gauge the effect on simulation speed in the table below.

Code	# cores	Time for settling (sec)	Time for flow (sec)	Net time (sec)	# particles remaining	Comments
COMMERCIAL CODE	8	32724	92556	125280	215611	
LIGGGHTS 2.2	12	4195	10799	14994	215775	Default options
LIGGGHTS 2.2	24	4039	10500	14539	215676	Default options
LIGGGHTS 2.2	36	3942	9032	12974	215769	Default options
LIGGGHTS 2.2	48	2818	6824	9642	215767	Default options
LIGGGHTS 2.2	60	2433	5448	7881	215789	Default options
LIGGGHTS 2.2	12	2742	6672	9413	215861	Dynamic balancing
LIGGGHTS 2.2	24	1758	4057	5814	215675	Dynamic balancing
LIGGGHTS 2.2	36	1549	3537	5086	215740	Dynamic balancing
LIGGGHTS 2.2	48	1160	2694	3854	215584	Dynamic balancing
LIGGGHTS 2.2	60	996	2253	3249	215695	Dynamic balancing

Simulation timing for bin flow simulations using 300,000 particles

Code	# cores	Time for settling (sec)	Time for flow (sec)	Net time (sec)	# particles remaining	Comments
LIGGGHTS 2.2	12	103924	333500	437424	1378787	Default options
LIGGGHTS 2.2	24	88396	320665	409061	1378631	Default options
LIGGGHTS 2.2	36	85153	278119	363272	1378299	Default options
LIGGGHTS 2.2	48	59076	202588	261664	1379198	Default options
LIGGGHTS 2.2	60	51327	180506	231833	1379284	Default options
LIGGGHTS 2.2	12	69247	214907	284154	1378345	Dynamic balancing
LIGGGHTS 2.2	24	40752	123065	163817	1378569	Dynamic balancing
LIGGGHTS 2.2	36	34372	106290	140662	1378606	Dynamic balancing
LIGGGHTS 2.2	48	24425	76710	101135	1378656	Dynamic balancing
LIGGGHTS 2.2	60	22871	72132	95003	1378668	Dynamic balancing

Simulation timing for bin flow simulations using 3,000,000 particles

Code	# cores	Time for settling (sec)	Time for flow (sec)	Net time (sec)	# particles remaining	Comments
LIGGGHTS 2.2	36	395779	395779	652341	8137542	Dynamic balancing
LIGGGHTS 2.2	48	266060	266060	449551	8137415	Dynamic balancing
LIGGGHTS 2.2	60	250682	250682	424165	8137238	Dynamic balancing

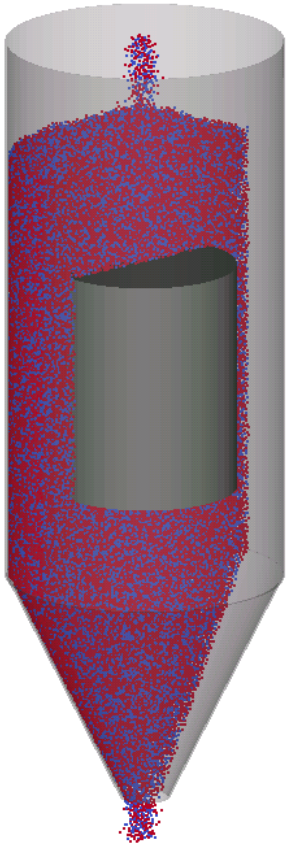
Simulation timing for bin flow simulations using 10,000,000 particles

Based on the results above, we can see that LIGGGHTS offers a significant speed advantage over (COMMERCIAL CODE) for bin flow simulations. For simulations with 300,000 particles, we are able to achieve over 15x speedup as compared to (COMMERCIAL CODE) using default options and running the job on 60 cores. We are able to achieve as much as a 40x speedup (97.5% reduction in simulation time) compared to (COMMERCIAL CODE) by also utilizing dynamic load balancing. This stems from the fact that as the hopper empties, a dead space forms at the top of the bin where there processors are basically being wasted. By rebalancing the processor load, we are able to regain use of all cores and significantly speed up the simulation.

While these simulations do show some speed benefits based on increasing the degree of parallelization, the parallelization efficiency is nowhere near linear. That said, with the large capacity of the rho and nimbus clusters, we have plenty of capacity to parallelize jobs. Also, when dynamic balancing is used, the speedup is more pronounced. For the 3,000,000 particle simulations, using 12 cores, the use of dynamic balancing leads to a ~30% speedup. Using 60 cores, the speedup is over 250%.

Couette cylinder:

A Couette cylinder with axial flow, based on work by Kheiripour et al[1], is depicted in the figure below. The device is intended to look at the rheological behaviour of a granular flow and to permit study of the tendency for material to segregated based on particle size. In these simulations, we have randomly inserted two different particle sizes (particles are otherwise identical) over a one second interval. The stopper at the bottom of the hopper is then pulled and material flows through a periodic z-boundary condition to flow back into the top of the unit. In doing so, the net mass in the system remains constant. Simultaneously, the drum in the center of the unit rotates about its axis, setting up a shearing action inside the cylinder.



	Model 1
# of particles	450,000
Particle diameter (m)	0.0025 / 0.0020
Particle density (kg/m^3)	1000
Poisson ratio	0.25
Young's modulus (MPa)	25
Coefficient of restitution	0.5
Static friction coefficient	0.5
Rolling friction coefficient	0.1
Impeller speed (RPM)	60
Timestep (sec)	6.25×10^{-5}
Settling time (sec)	1.0
Data-gathering time (sec)	30.0
Net simulation time (sec)	31.0

Model parameters for Couette cylinder simulations.

[1] *Study of powder flow patterns in a Couette cell with axial flow using tracers and solid fraction measurements*, M. Kheiripour Langroudi, P. R. Mort, Gi. I. Tardos, Granular Matter, Oct 2011, Vol 13, Iss 5, pp 541-552

Results

Code	# cores	Time for Insertion (sec)	Time for Equilibration (sec)	Net time (sec)	Comments
LIGGGHTS 2.2	12	4935	197212	202148	Default options
LIGGGHTS 2.2	24	3070	117830	120900	Default options
LIGGGHTS 2.2	36	2633	95686	98319	Default options
LIGGGHTS 2.2	48	2230	83627	85856	Default options
LIGGGHTS 2.2	12	4936	173694	178629	Dynamic balancing
LIGGGHTS 2.2	24	3074	91162	94237	Dynamic balancing
LIGGGHTS 2.2	36	2639	75228	77867	Dynamic balancing
LIGGGHTS 2.2	48	2216	60755	62970	Dynamic balancing

Simulation timing for Couette cylinder simulations using 450,000 total particles

Plow Mixer:

A single shaft plow mixer was initially filled with a set of spherical particles which were allowed to settle under the influence of gravity. The set of plows/scrapers and the chopper are then set to rotate for a period of time to equilibrate the system, and then a further period of time is simulated for steady-state data gathering.

	Model 1	Model 2	Model 3
# of particles	15,000	100,000	1,000,000
Particle diameter (m)	0.004	0.0025	0.0012
Particle density (kg/m^3)	1000	1000	1000
Poisson ratio	0.25	0.25	0.25
Young's modulus (MPa)	25	25	25
Coefficient of restitution	0.5	0.5	0.5
Static friction coefficient	0.5	0.5	0.5
Rolling friction coefficient	0.1	0.1	0.1
Impeller speed (RPM)	40	40	40
Chopper speed (RPM)	1200	1200	1200
Timestep (sec)	$4x10^{-5}$	$2x10^{-5}$	$8x10^{-6}$
Settling time (sec)	1.0	2.0	2.0
Equilibration time (sec)	5.0	5.0	5.0
Data-gathering time (sec)	5.0	5.0	5.0
Net simulation time (sec)	11.0	12.0	12.0

Model parameters for plow mixer simulations.

Results

Code	# cores	Time for Insertion (sec)	Time for Equilibration (sec)	Time for Data-Gathering (sec)	Net time (sec)	Comments
COMMERCIAL CODE	4	371	2686	2740	5796	
COMMERCIAL CODE	8	212	1552	1555	3319	
LIGGGHTS 2.2	24	28	637	642	1307	Default options
LIGGGHTS 2.2	36	37	652	642	1331	Default options
LIGGGHTS 2.2	48	32	547	537	1116	Default options

Simulation timing for plow mixer simulations using 15,000 particles

Code	# cores	Time for Insertion (sec)	Time for Equilibration (sec)	Time for Data-Gathering (sec)	Net time (sec)	Comments
COMMERCIAL CODE	8	8424	21492	21564	51480	
LIGGGHTS 2.2	12	911	4578	4628	10118	Default Options
LIGGGHTS 2.2	24	744	2977	2929	6650	Default Options
LIGGGHTS 2.2	36	519	2086	2054	4660	Default Options
LIGGGHTS 2.2	48	389	1758	1741	3888	Default Options
LIGGGHTS 2.2	12	631	3567	3581	7779	Dynamic Balancing
LIGGGHTS 2.2	24	382	2160	2147	4689	Dynamic Balancing
LIGGGHTS 2.2	36	279	1560	1556	3395	Dynamic Balancing
LIGGGHTS 2.2	48	216	1296	1296	2808	Dynamic Balancing

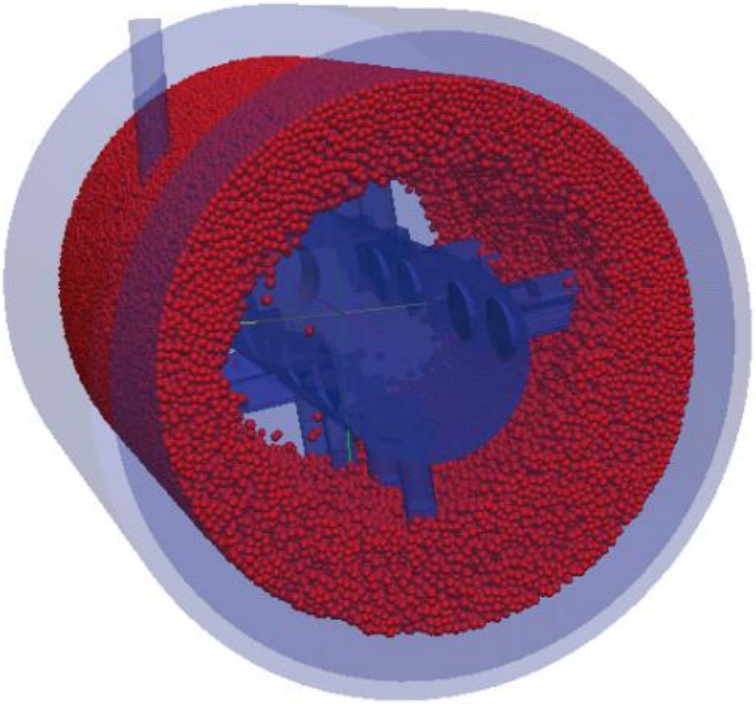
Simulation timing for plow mixer simulations using 100,000 particles

Code	# cores	Time for Insertion (sec)	Time for Equilibration (sec)	Time for Data-Gathering (sec)	Net time (sec)	Comments
LIGGGHTS 2.2	12	17182	76648	77991	171821	Dynamic Balancing
LIGGGHTS 2.2	24	9777	42956	43566	96298	Dynamic Balancing
LIGGGHTS 2.2	36	7042	30158	30486	67686	Dynamic Balancing

Simulation timing for plow mixer simulations using 1,000,000 particles

Pin Mixer:

A single shaft pin mixer was initially filled with a set of spherical particles which were allowed to settle under the influence of gravity. The shaft/pins are then set to rotate for a period of time to equilibrate the system, and then a further period of time is simulated for steady-state data gathering. Note that due to what is believed to be a bug in the current version (2.2.4) of LIGGGHTS, particle insertion fails in some cases when using multiple factories simultaneously. As a result, these simulations used sequential filling operations, necessitating a longer filling and settling time than should be possible.



	Model 1	Model 2
# of particles	83,000	215,000
Particle diameter (m)	0.00275	0.002
Particle density (kg/m^3)	1000	1000
Poisson ratio	0.25	0.25
Young's modulus (MPa)	25	25
Coefficient of restitution	0.5	0.5
Static friction coefficient	0.5	0.5
Rolling friction coefficient	0.1	0.1
Impeller speed (RPM)	1125	1125
Timestep (sec)	$1x10^{-5}$	$1x10^{-5}$
Settling time (sec)	1.5	1.5
Equilibration time (sec)	2.0	2.0
Data-gathering time (sec)	2.0	2.0
Net simulation time (sec)	5.5	5.5

Model parameters for pin mixer simulations.

Results

Code	# cores	Time for Insertion (sec)	Time for Equilibration (sec)	Time for Data-Gathering (sec)	Net time (sec)	Comments
LIGGGHTS 2.2	12	1509	2245	2196	5949	Default Options
LIGGGHTS 2.2	24	999	1381	1350	3730	Default Options
LIGGGHTS 2.2	36	1038	1110	1079	3226	Default Options
LIGGGHTS 2.2	48	815	918	898	2631	Default Options
LIGGGHTS 2.2	12	1521	2096	2066	5683	Dynamic Balancing
LIGGGHTS 2.2	24	987	1234	1225	3445	Dynamic Balancing
LIGGGHTS 2.2	36	1032	1082	1063	3177	Dynamic Balancing
LIGGGHTS 2.2	48	817	897	885	2598	Dynamic Balancing

Simulation timing for pin mixer simulations using 83,000 particles

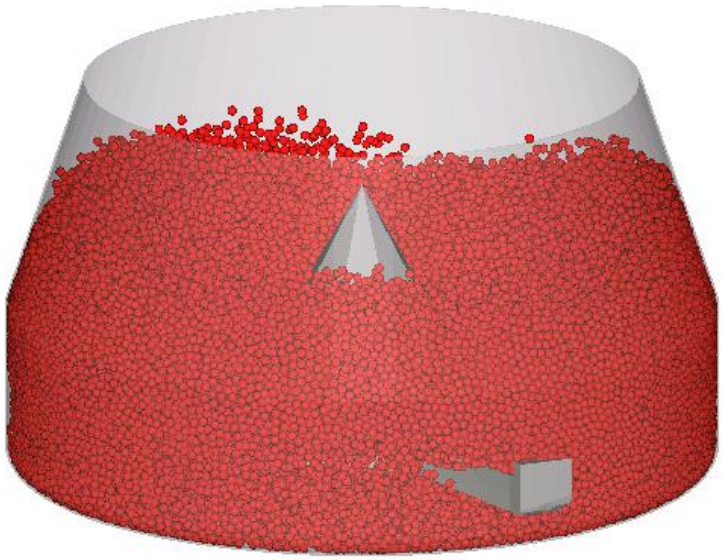
Code	# cores	Time for Insertion (sec)	Time for Equilibration (sec)	Time for Data-Gathering (sec)	Net time (sec)	Comments
LIGGGHTS 2.2	12	4222	6337	6143	10559	Default Options
LIGGGHTS 2.2	24	2697	3283	3156	5980	Default Options
LIGGGHTS 2.2	36	2885	2692	2557	5577	Default Options
LIGGGHTS 2.2	48	2306	2380	2273	4686	Default Options
LIGGGHTS 2.2	12	4293	6307	6214	10599	Dynamic Balancing
LIGGGHTS 2.2	24	2687	2979	2923	5666	Dynamic Balancing
LIGGGHTS 2.2	36	2928	2645	2589	5573	Dynamic Balancing
LIGGGHTS 2.2	48	2298	2211	2176	4509	Dynamic Balancing

Simulation timing for pin mixer simulations using 215,000 particles

As evidenced from the above results, the application of load balancing does not make a significant difference in the overall speed of the simulation. This stems from the simulation domain already being reasonably completely uniformly filled. If the mixer were spinning more slowly to where the particles are residing in the bottom half of the mixer, we can expect load balancing to play a stronger role in speeding up the simulation.

Vertical Shear Mixer:

A vertical high shear mixer was initially filled with a set of spherical particles which were allowed to settle under the influence of gravity. The central blade is then set to rotate for a period of time to equilibrate the system, and then a further period of time is simulated for steady-state data gathering.



	Model 1	Model 2
# of particles	60,000	500,000
Particle diameter (m)	0.002	0.001
Particle density (kg/m^3)	1000	1000
Poisson ratio	0.25	0.25
Young's modulus (MPa)	25	25
Coefficient of restitution	0.5	0.5
Static friction coefficient	0.5	0.5
Rolling friction coefficient	0.1	0.1
Impeller speed (RPM)	180	180
Timestep (sec)	$1x10^{-5}$	$5x10^{-6}$
Settling time (sec)	1.0	1.0
Mixing time (sec)	10.0	7.0
Net simulation time (sec)	11.0	8.0

Model parameters for vertical high shear mixer simulations.

Results

Code	# cores	Time for Insertion (sec)	Time for Mixing (sec)	Net time (sec)	Comments
COMMERCIAL CODE	8	2016	34704	36720	
LIGGGHTS 2.2	12	397	6746	7142	Default Options
LIGGGHTS 2.2	24	226	4859	5086	Default Options
LIGGGHTS 2.2	36	209	3447	3656	Default Options

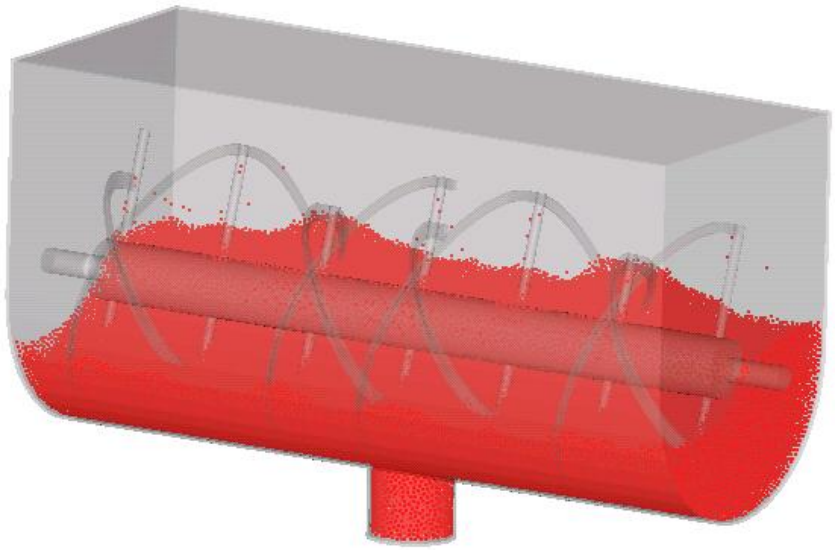
Simulation timing for vertical high shear mixer simulations using 60,000 particles

Code	# cores	Time for Insertion (sec)	Time for Mixing (sec)	Net time (sec)	Comments
COMMERCIAL CODE	8	38520	515631	554151	
LIGGGHTS 2.2	12	7145	80921	88065	Default Options
LIGGGHTS 2.2	24	4242	57888	62130	Default Options
LIGGGHTS 2.2	36	4130	41037	45167	Default Options
LIGGGHTS 2.2	48	3302	36209	39511	Default Options
LIGGGHTS 2.2	12	7137	56768	63905	Dynamic Balancing
LIGGGHTS 2.2	24	4267	39245	43512	Dynamic Balancing
LIGGGHTS 2.2	36	4113	27464	31577	Dynamic Balancing
LIGGGHTS 2.2	48	3314	23442	26756	Dynamic Balancing

Simulation timing for vertical high shear mixer simulations using 500,000 particles

Ribbon blender:

A ribbon blender was initially filled with a set of spherical particles which were allowed to settle under the influence of gravity. The shaft is then set to rotate for a period of time to equilibrate the system, and then a further period of time is simulated for steady-state data gathering.



	Model 1	Model 2
# of particles	60,000	200,000
Particle diameter (m)	0.005	0.003
Particle density (kg/m^3)	1000	1000
Poisson ratio	0.25	0.25
Young's modulus (MPa)	25	25
Coefficient of restitution	0.5	0.5
Static friction coefficient	0.5	0.5
Rolling friction coefficient	0.1	0.1
Shaft speed (RPM)	40	40
Timestep (sec)	3.2×10^{-5}	2.0×10^{-5}
Settling time (sec)	2.0	1.0
Equilibration time (sec)	20.0	15.0
Net simulation time (sec)	22.0	16.0

Model parameters for ribbon blender simulations.

Results

Code	# cores	Time for Insertion (sec)	Time for Mixing (sec)	Net time (sec)	Comments
COMMERCIAL CODE	4	1426	17366	18792	Used timestep of 4.0×10^{-5}
LIGGGHTS 2.2	12	285	6471	6756	Default Options
LIGGGHTS 2.2	24	140	3202	3342	Default Options
LIGGGHTS 2.2	36	97	2338	2435	Default Options

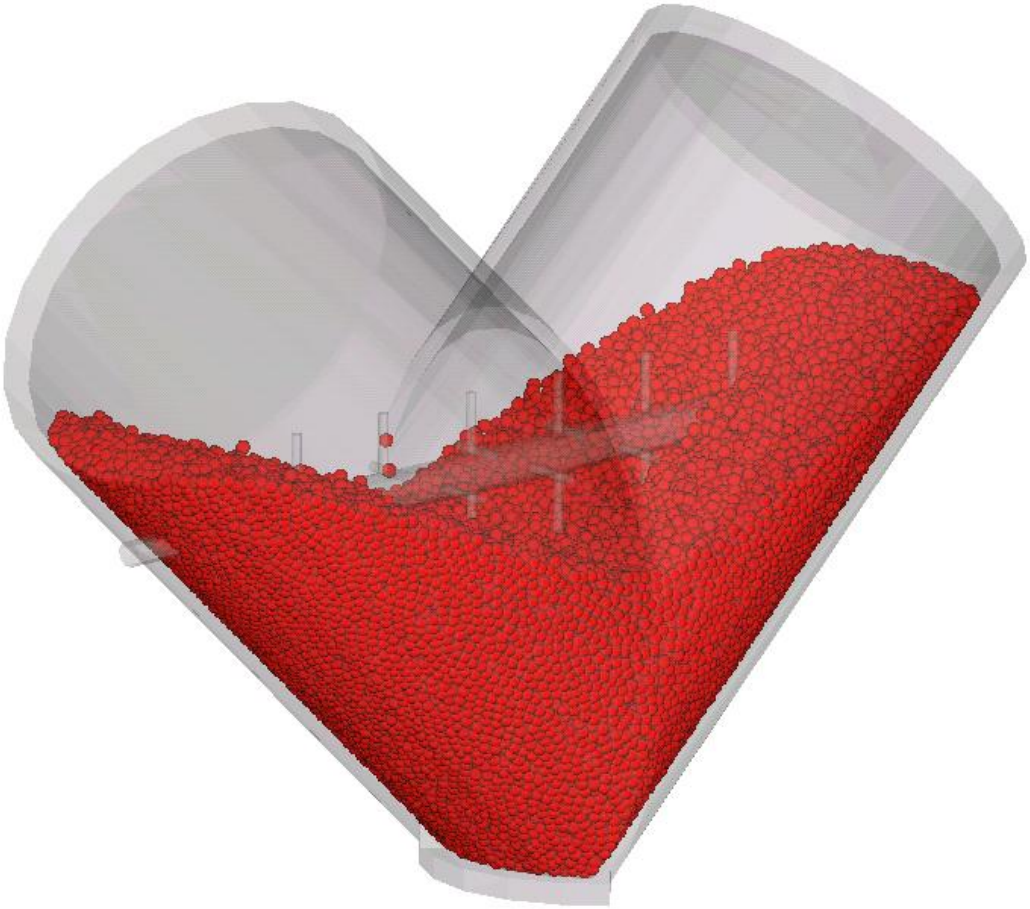
Simulation timing for ribbon blender simulations using 60,000 particles

Code	# cores	Time for Insertion (sec)	Time for Mixing (sec)	Net time (sec)	Comments
COMMERCIAL CODE	4	4860	225540	230400	
LIGGGHTS 2.2	12	939	29687	30626	Default Options
LIGGGHTS 2.2	24	464	14909	15373	Default Options
LIGGGHTS 2.2	36	308	10327	10635	Default Options
LIGGGHTS 2.2	48	326	11668	11994	Default Options
LIGGGHTS 2.2	12	541	17207	17748	Dynamic balancing
LIGGGHTS 2.2	24	300	9655	9955	Dynamic balancing
LIGGGHTS 2.2	36	208	6944	7152	Dynamic balancing
LIGGGHTS 2.2	48	170	5684	5854	Dynamic balancing

Simulation timing for ribbon blender simulations using 200,000 particles

V-blender:

A V-blender was initially filled with a set of spherical particles which were allowed to settle under the influence of gravity. Both the blender and internal impeller are then set to rotate to mix the system.



	Model 1	Model 2
# of particles	50,000	235,000
Particle diameter (m)	0.0025	0.0015
Particle density (kg/m^3)	1000	1000
Poisson ratio	0.25	0.25
Young's modulus (MPa)	25	25
Coefficient of restitution	0.5	0.5
Static friction coefficient	0.5	0.5
Rolling friction coefficient	0.1	0.1
Timestep (sec)	$2x10^{-5}$	$1x10^{-5}$
V-blender speed (RPM)	24	24
Impeller speed (RPM)	2200	2200
Settling time (sec)	1.0	1.0
Equilibration time (sec)	30.0	10.0
Net simulation time (sec)	31.0	11.0

Model parameters for V-blender simulations.

Results

Code	# cores	Time for Insertion (sec)	Time for Mixing (sec)	Net time (sec)	Comments
COMMERCIAL CODE	4	1480	103640	105120	
LIGGGHTS 2.2	12	196	33986	34182	Default Options
LIGGGHTS 2.2	24	334	42062	42396	Default Options
LIGGGHTS 2.2	36	408	40021	40429	Default Options
LIGGGHTS 2.2	12	144	22675	22818	Dynamic balancing
LIGGGHTS 2.2	24	91	15701	15793	Dynamic balancing
LIGGGHTS 2.2	36	106	14213	14318	Dynamic balancing

Simulation timing for V-blender simulations using 50,000 particles

Code	# cores	Time for Insertion (sec)	Time for Mixing (sec)	Net time (sec)	Comments
LIGGGHTS 2.2	12	5537	72563	78100	Default Options
LIGGGHTS 2.2	24	8600	87277	95877	Default Options
LIGGGHTS 2.2	36	11816	88194	100010	Default Options
LIGGGHTS 2.2	48	8366	64099	72465	Default Options
LIGGGHTS 2.2	12	3065	49382	52448	Dynamic balancing
LIGGGHTS 2.2	24	1817	30716	32532	Dynamic balancing
LIGGGHTS 2.2	36	1401	29179	30580	Dynamic balancing
LIGGGHTS 2.2	48	1101	20672	21773	Dynamic balancing

Simulation timing for V-blender simulations using 235,000 particles

The V-blender simulation shows some rather unusual behaviour in terms of parallelization efficiency. Because the simulation uses the complete domain rather inefficiently, the parallelization scheme can significantly affect the speed of the simulation. Increasing the number of cores can actually slow down the simulation in the absence of any sort of load balancing by moving cores into completely empty areas of the simulation domain and thus waste them.

When using load balancing, we see a dramatic improvement in simulation speed as well as scalability with increasing number of cores used.

Auger filler:

An auger filler is a packaging device that is used to deliver a measured amount of granular material into a package. An example of such a unit is pictured below. The auger filler consists of a main hopper with an auger threaded through a straight tubular section at the bottom of the hopper. The auger is connected to a spinner plate that inhibits the flow of material when the auger is at rest. To deliver a dose, the auger is simply spun at some rate for some specified number of turns in order to deliver a desired amount of material.

	Model 1
# of particles	500,000
Particle diameter (m)	0.004
Particle density (kg/m^3)	1000
Poisson ratio	0.25
Young's modulus (MPa)	10
Coefficient of restitution	0.5
Static friction coefficient	
Particle-particle	0.5
Particle-wall	0.2
Rolling friction coefficient	
Particle-particle	0.1
Particle-wall	0.025
Timestep (sec)	$2x10^{-5}$
Auger Rotation rate (RPM)	800
# rotations per dose	3
Net time per dose (sec)	1
Settling time (sec)	5.0
Dosing time (sec)	10.0
Net simulation time (sec)	15.0

Model parameters for auger doser simulations.

Results

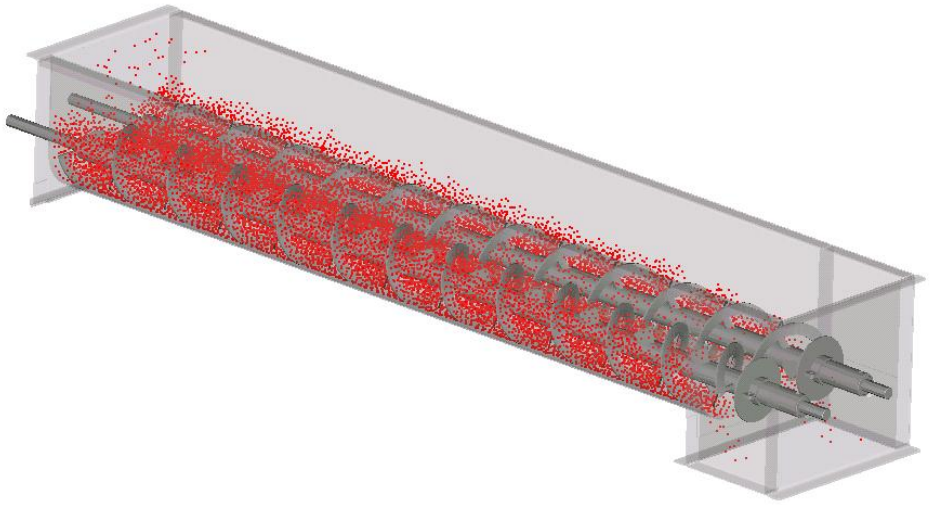
Code	# cores	Fill time (sec)	Dosing time (sec)	Net time (sec)	Holdup (# particles)	Comments
LIGGGHTS 2.2	12	16905	42852	59757	442255	Default Options
LIGGGHTS 2.2	24	22123	58637	80760	442362	Default Options
LIGGGHTS 2.2	36	33928	87656	121584	442233	Default Options
LIGGGHTS 2.2	48	21263	55890	77153	442268	Default Options
LIGGGHTS 2.2	12	12702	38869	51571	442216	Dynamic balancing
LIGGGHTS 2.2	24	8317	28966	37284	442163	Dynamic balancing
LIGGGHTS 2.2	36	8032	27823	35855	442280	Dynamic balancing
LIGGGHTS 2.2	48	5673	18408	24082	442231	Dynamic balancing

Simulation timing for auger filler simulations

Because the particles occupy only a fraction of the entire domain space, the basic domain decomposition is rather inefficient, and owing the increasingly wasted cores on greater parallelization, actually slows the simulation down as more cores are added. As with many other examples in this report, using load balancing allows the simulation to more appropriately assign processors and significantly improves the code performance.

Continuous blending (CB) mixer #1:

A continuous blending bed is simulated in which a stream of particles enters at one end and is continuously blended as it travels down the length of the bed before discharging through a chute at the other end of the unit. We consider different feed rates and different impeller rotation rates. Material is fed into the simulation via a constant mass flowrate stream at one end of the unit, and is removed through a chute at the other end.



	Model 1	Model 2
Feed rate (kg/min)	100	200
Particle radius (m)	0.01	0.01
Particle density (kg/m^3)	1000	1000
Poisson ratio	0.25	0.25
Young's modulus (MPa)	25	25
Coefficient of restitution	0.5	0.5
Static friction coefficient	0.5	0.5
Rolling friction coefficient	0.1	0.1
Timestep (sec)	6.25×10^{-5}	6.25×10^{-5}
Rotation rate (RPM)	40	80
Net simulation time (sec)	480	480
Final holdup (particles)	~24000	~22850

Model parameters for CB mixer #1 simulations.

Results

Code	# cores	Net time (sec)	Holdup (# particles)	Comments
COMMERCIAL CODE	4	381600	25400	
LIGGGHTS 2.2	12	51157	24000	Default Options
LIGGGHTS 2.2	24	52465	23990	Default Options
LIGGGHTS 2.2	36	38712	23990	Default Options
LIGGGHTS 2.2	12	59374	24040	Dynamic balancing
LIGGGHTS 2.2	24	47715	23950	Dynamic balancing
LIGGGHTS 2.2	36	37720	24130	Dynamic balancing

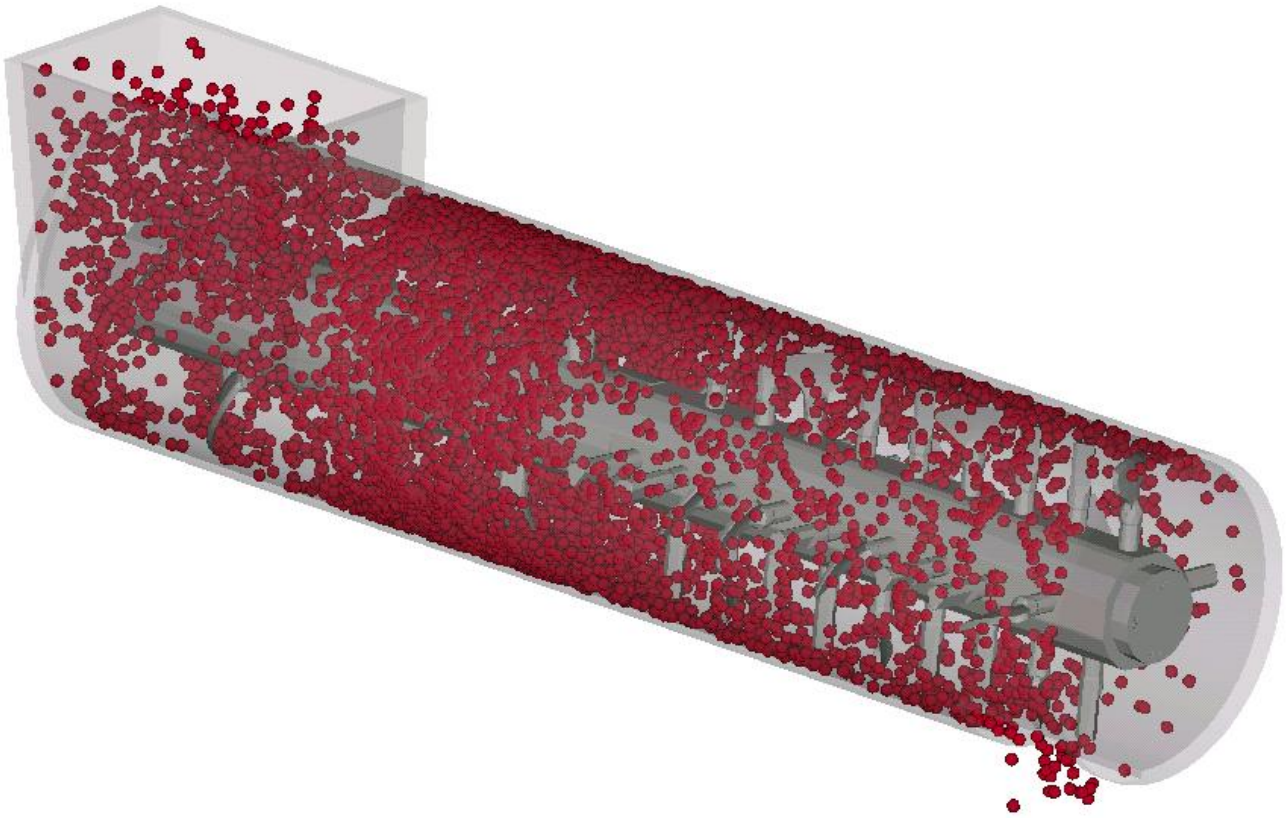
Simulation timing for CB mixer #1 simulations corresponding to Model 1 above

Code	# cores	Net time (sec)	Holdup (# particles)	Comments
COMMERCIAL CODE	4	300600	20950	
LIGGGHTS 2.2	12	48999	22770	Default Options
LIGGGHTS 2.2	24	50295	22900	Default Options
LIGGGHTS 2.2	36	36464	21100	Default Options
LIGGGHTS 2.2	12	57577	22770	Dynamic balancing
LIGGGHTS 2.2	24	45029	22630	Dynamic balancing
LIGGGHTS 2.2	36	34943	22450	Dynamic balancing

Simulation timing for CB mixer #1 simulations corresponding to Model 2 above

Continuous blending (CB) mixer #2:

A different type of CB mixer (from that above) is simulated for different particles sizes. Material is fed into the simulation via a constant mass flowrate stream at one end of the unit, and is removed through a chute at the other end.



	Model 1	Model 2	Model 3
Feed rate (kg/min)	12.9	12.9	12.9
Particle radius (m)	0.005	0.003	0.001
Particle density (kg/m^3)	1000	1000	1000
Poisson ratio	0.25	0.25	0.25
Young's modulus (MPa)	25	25	25
Coefficient of restitution	0.5	0.5	0.5
Static friction coefficient	0.5	0.5	0.5
Rolling friction coefficient	0.1	0.1	0.1
Timestep (sec)	2.5×10^{-4}	2.0×10^{-5}	5.0×10^{-6}
Rotation rate (RPM)	1252	1252	1252
Net simulation time (sec)	30	30	30

Model parameters for CB mixer #2 simulations.

Results

Code	# cores	Net time (sec)	Holdup (# particles)	Comments
COMMERCIAL CODE	8	8748	1678	
LIGGGHTS 2.2	12	8578	2522	Default Options
LIGGGHTS 2.2	24	5584	2477	Default Options
LIGGGHTS 2.2	36	4057	2493	Default Options
LIGGGHTS 2.2	12	14451	2532	Dynamic balancing
LIGGGHTS 2.2	24	12052	2528	Dynamic balancing
LIGGGHTS 2.2	36	10106	2570	Dynamic balancing

Simulation timing for CB mixer #2 simulations corresponding to Model 1 above

Code	# cores	Net time (sec)	Holdup (# particles)	Comments
COMMERCIAL CODE	8	13716	8665	
LIGGGHTS 2.2	12	13787	7635	Default Options
LIGGGHTS 2.2	24	9218	7573	Default Options
LIGGGHTS 2.2	36	6589	7572	Default Options
LIGGGHTS 2.2	12	24720	7523	Dynamic balancing
LIGGGHTS 2.2	24	16559	7465	Dynamic balancing
LIGGGHTS 2.2	36	12697	7606	Dynamic balancing

Simulation timing for CB mixer #2 simulations corresponding to Model 2 above

Code	# cores	Net time (sec)	Holdup (# particles)	Comments
COMMERCIAL CODE	8	2836800	304824	
LIGGGHTS 2.2	12	370874	295236	Default Options
LIGGGHTS 2.2	24	241647	312483	Default Options
LIGGGHTS 2.2	36	173178	309312	Default Options
LIGGGHTS 2.2	12	290054	304845	Dynamic balancing
LIGGGHTS 2.2	24	177543	319269	Dynamic balancing
LIGGGHTS 2.2	36	147945	302679	Dynamic balancing

Simulation timing for CB mixer #2 simulations corresponding to Model 3 above

As discussed above, the use of dynamic load balancing can significantly reduce the computational time for certain simulations. However, care should be exercised in using it. For the first two model cases above, the use of dynamic balancing actually significantly slows the simulation as the time required to actually balance the system is greater than the time saved from the balancing. For the third case, where the number of particles is significantly larger, the balancing operation saves significant time relative to the default operation.

Continuous blending (CB) mixer #3:

In the simulation, material is fed into the unit via a constant mass flowrate stream at one end of the unit, and is removed through a chute at the other end. There are two rotating shafts inside the unit that turn in opposite directions.

	Model 1	Model 2
Feed rate (kg/min)	200	200
Particle radius (m)	0.00635	0.004
Particle density (kg/m^3)	1000	1000
Poisson ratio	0.25	0.25
Young's modulus (MPa)	25	25
Coefficient of restitution	0.5	0.5
Static friction coefficient	0.5	0.5
Rolling friction coefficient	0.1	0.1
Timestep (sec)	$4x10^{-5}$	$2.5x10^{-5}$
Rotation rate shaft 1 (RPM)	100	100
Rotation rate shaft 2 (RPM)	200	200
Net simulation time (sec)	80	100

Model parameters for CB mixer #3 simulations.

Results

Code	# cores	Processor setup	Net time (sec)	Holdup (# particles)	Comments
COMMERCIAL CODE	8		48240	32880	
LIGGGHTS 2.2	12	1x6x2	33269	31330	Default Options
LIGGGHTS 2.2	24	2x6x2	22541	31490	Default Options
LIGGGHTS 2.2	36	2x9x2	17571	31620	Default Options
LIGGGHTS 2.2	48	2x8x3	22563	31990	Default Options
LIGGGHTS 2.2	48	2x12x2	12778	31678	Assigned processors

Simulation timing for CB mixer #3 simulations corresponding to Model 1 above

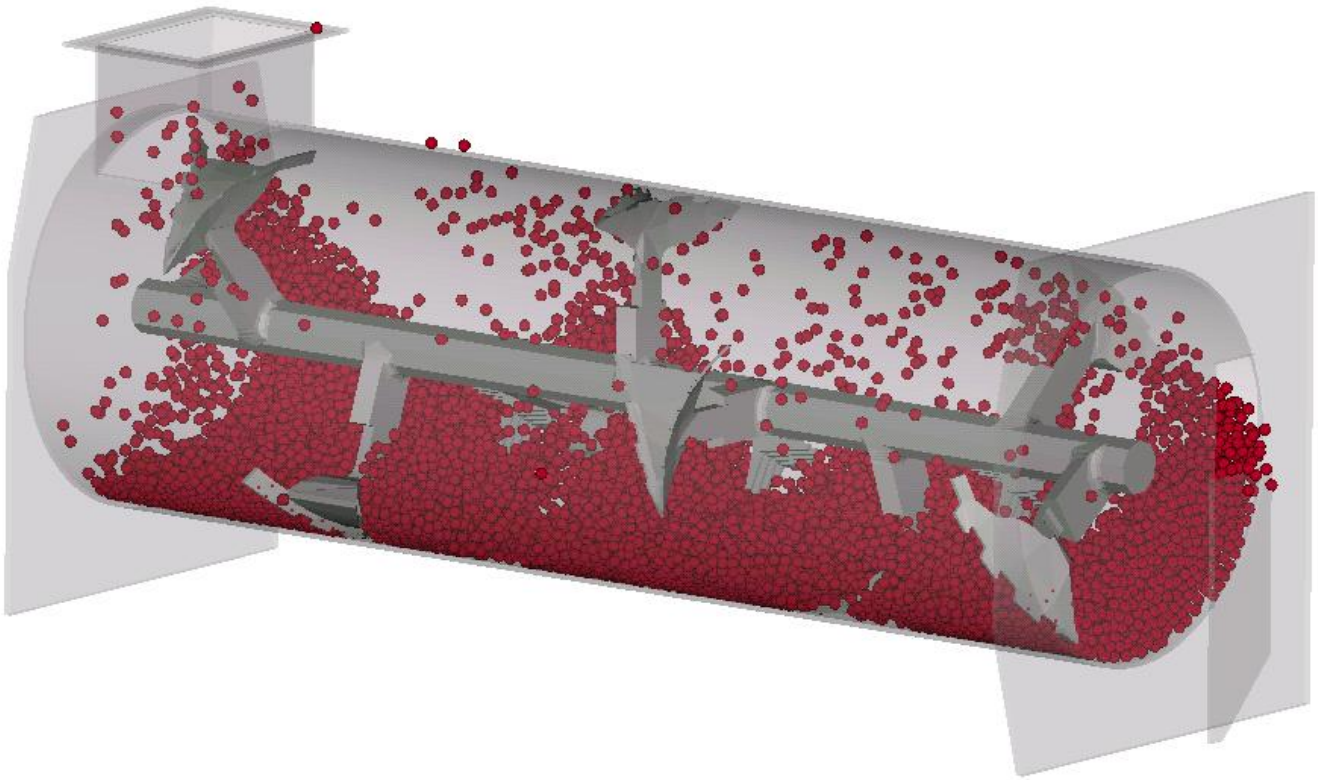
Code	# cores	Processor setup	Net time (sec)	Holdup (# particles)	Comments
LIGGGHTS 2.2	12	1x6x2	133987	126040	Default Options
LIGGGHTS 2.2	24	2x6x2	80117	127210	Default Options
LIGGGHTS 2.2	36	2x9x2	60178	127570	Default Options
LIGGGHTS 2.2	48	2x8x3	82887	128440	Default Options
LIGGGHTS 2.2	48	2x12x2	41446	127900	Assigned processors

Simulation timing for CB mixer #3 simulations corresponding to Model 2 above

Note that due to the feed and exit protrusions in the z-direction, and the fact that the computational domain must be a rectangular box, there are significant volumes of 'dead' space along the top and bottom of the computational domain where no particles can reside. Thus, when we expand to 48 cores and the default parallelization uses three cores in the z-direction, the work load becomes highly imbalanced (two layers of cores have little to do while the third layer does most of the work). By forcing LIGGGHTS to instead split the z-direction into two layers, we are able to more effectively distribute the load and speed up the simulation.

Continuous blending (CB) mixer #4:

In the simulation, material is fed into the unit via a constant mass flowrate stream at one end of the unit, and is removed through a chute at the other end. There is one rotating shaft inside the unit that mixes and conveys material through the unit, along with three high speed choppers along one side of the mixer. The choppers do not affect the particle size distribution within these simulations, but they do affect the particle dynamics and resulting holdup. The discharge rate is controlled by the height of an adjustable weir.



	Model 1	Model 2
Feed rate (kg/min)	140	140
Particle radius (m)	0.01	0.005
Particle density (kg/m^3)	1000	1000
Poisson ratio	0.3	0.3
Young's modulus (MPa)	26	26
Coefficient of restitution	0.4	0.4
Static friction coefficient	0.5	0.5
Rolling friction coefficient	0.1	0.1
Timestep (sec)	6.25×10^{-5}	4.0×10^{-5}
Shaft Rotation rate (RPM)	60	60
Chopper rotation rate (RPM)	2400	2400
Net simulation time (sec)	600	175

Model parameters for CB mixer #4 simulations.

Results

Code	# cores	Net time (sec)	Holdup (# particles)	Comments
LIGGGHTS 2.2	12	142082	43210	Default Options
LIGGGHTS 2.2	24	109479	43321	Default Options
LIGGGHTS 2.2	36	91961	43217	Default Options

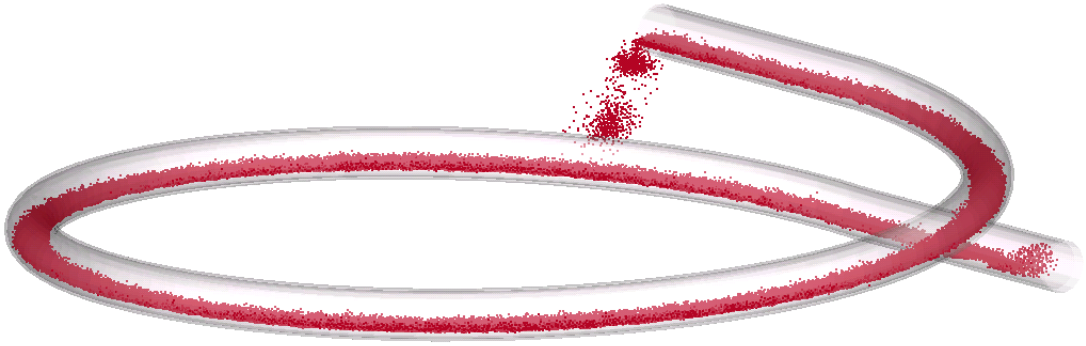
Simulation timing for CB mixer #4 simulations corresponding to Model 1 above

Code	# cores	Net time (sec)	Holdup (# particles)	Comments
LIGGGHTS 2.2	12	207515	354700	Default Options
LIGGGHTS 2.2	24	100740	356000	Default Options
LIGGGHTS 2.2	36	75082	356700	Default Options

Simulation timing for CB mixer #4 simulations corresponding to Model 2 above

Vibrating conveyor

In this problem, we consider the motion of material through a vibrating helical conveyor. Material is fed into the unit via a constant mass flowrate stream at one end of the unit (bottom), and is removed through a chute at the other end (top). Here we consider the dynamics of two different sized particles in a single-loop system.



	Model 1	Model 2
Feed rate (kg/min)	10	10
Particle radius (m)	0.00484	0.002
Particle density (kg/m^3)	1000	1000
Poisson ratio	0.25	0.25
Young's modulus (MPa)	25	25
Coefficient of restitution	0.5	0.5
Static friction coefficient	0.5	0.5
Rolling friction coefficient	0.1	0.1
Timestep (sec)	2.5×10^{-5}	1.0×10^{-5}
Vertical amplitude (m)	0.0071	0.0071
Rotational amplitude (deg)	0.498	0.498
Vibration frequency (Hz)	11.17	11.17
Net simulation time (sec)	480	480

Model parameters for vibrating conveyor simulations.

Results

Code	# cores	Net time (sec)	Holdup (# particles)	Comments
(COMMERCIAL CODE)	8	4356	5460	
LIGGGHTS 2.2	12	2718	5470	Default Options
LIGGGHTS 2.2	24	2247	5460	Default Options
LIGGGHTS 2.2	36	1746	5480	Default Options
LIGGGHTS 2.2	12	3711	5470	Dynamic balancing
LIGGGHTS 2.2	24	2693	5460	Dynamic balancing
LIGGGHTS 2.2	36	2215	5470	Dynamic balancing

Simulation timing for vibrating conveyor simulations corresponding to Model 1 above

Code	# cores	Net time (sec)	Holdup (# particles)	Comments
(COMMERCIAL CODE)	8	257040	64000	
LIGGGHTS 2.2	12	59834	66300	Default Options
LIGGGHTS 2.2	24	73934	66100	Default Options
LIGGGHTS 2.2	36	29831	66400	Default Options
LIGGGHTS 2.2	12	72252	66250	Dynamic balancing
LIGGGHTS 2.2	24	43054	66300	Dynamic balancing
LIGGGHTS 2.2	36	32439	66500	Dynamic balancing

Simulation timing for vibrating conveyor simulations corresponding to Model 2 above

 # Binflow simulation

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.138 0.138 -0.138 0.138 -0.0045 0.43 units box
create_box      2 reg

# Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 2 0.5 0.5 0.5 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 2 0.2 0.175 0.175 0.5

# Contact physics
pair_style      gran/hertz/history
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file hopper.stl type 2 scale 0.001
fix             geometry all wall/gran/hertz/history mesh n_meshes 1 meshes cad1

# Create stopper for funnel using primitive
fix             stopper all wall/gran/hertz/history primitive type 2 zplane 0.0

# Particle insertion
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.0007
fix             pdd all particledistribution/discrete 63243 1 pts 1.0
fix             ins_mesh all mesh/surface file factory.stl type 2 scale 0.001
fix             ins all insert/stream seed 123481 distributiontemplate pdd nparticles 3000000 particlerate 3000000 overlapcheck yes vel
constant 0. 0. -3.0 insertion_face ins_mesh extrude_length 0.02

# Timestep (keep < 20% T_Rayleigh)
timestep        0.000005

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          10000
thermo_modify   lost ignore norm no
compute_modify  thermo_temp dynamic yes

# Run to create a single particle to initiate a dump file and check the timestep
fix             timecheck all check/timestep/gran 1 0.01 0.01
run             1
unfix           timecheck

# Load balancing
fix             lb all balance 0 xyz 10 1.1 out balance.txt

# Fill the hopper
run             300000 upto

# Pull the stopper
unfix           stopper

# Drain the hopper
run             1000000
```

 # Rotating drum example

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.101 0.101 -0.051 0.051 -0.051 0.051 units box
create_box      1 reg

# Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 1 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 1 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 1 0.1

# Contact physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file drum.stl type 1 scale 0.001 curvature 1e-5
fix             drum all wall/gran/hertz/history mesh n_meshes 1 meshes cad1 rolling_friction cdt

# Particle insertion
region          factory block -0.097 0.097 -0.035 0.035 0.030 0.035 units box
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.001
fix             pdd all particledistribution/discrete 12345 1 pts 1.0
fix             ins all insert/rate/region seed 3412 distributiontemplate pdd nparticles 100000 particlerate 200000 insert_every 1000
overlapcheck yes vel constant 0. 0. -2. region factory ntry_mc 10000

# Timestep
timestep        0.000005

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          20000
thermo_modify   lost ignore norm no
compute_modify  thermo_temp dynamic yes

# Check the timestep
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix           ctg

# Load balancing
#fix            lb all balance 0 xyz 10 1.1 out balance.txt

# Run 1 second to fill the drum
run             200000 upto

# Make a dump of particles and the stl file
#dump           dmp all custom 10000 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dmpstl all stl 10000 dump*.stl
#dump           dmpjpg all image 20000 dump*.jpg type type adiam 0.002 axes yes 1 0.01 size 1024 1024

# Rotate the drum
fix             movecad1 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 1. 0. 0. period 1.0

# Run 10 seconds
run             2000000
```

 # Couette cylinder simulation

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f p
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.078 0.078 -0.078 0.078 -0.1524 0.306 units box
create_box      2 reg

# Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 2 0.5 0.5 0.5 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 2 0.5 0.5 0.5 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 2 0.1 0.1 0.1 0.1

# Contact physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file outer_cylinder.stl type 1 scale 0.001 curvature 1e-5
fix             cad2 all mesh/surface file inner_cylinder.stl type 1 scale 0.001 curvature 1e-5
fix             cad3 all mesh/surface file funnel.stl type 1 scale 0.001 curvature 1e-5
fix             cad4 all mesh/surface file plate.stl type 1 scale 0.001 curvature 1e-5
fix             geometry all wall/gran/hertz/history mesh n_meshes 4 meshes cad1 cad2 cad3 cad4 rolling_friction cdt

# Particle insertion
fix             pts1 all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.00125
fix             pts2 all particletemplate/sphere 1 atom_type 2 density constant 1000 radius constant 0.00100
fix             pdd all particledistribution/discrete 12345 2 pts1 0.5 pts2 0.5
fix             ins_mesh all mesh/surface file factory.stl type 1 scale 0.001
fix             ins all insert/stream seed 123481 distributiontemplate pdd nparticles 450000 particlerate 900000 overlapcheck yes vel
constant 0. 0. -3.0 insertion_face ins_mesh extrude_length 0.02

# Timestep
timestep        0.00000625

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          8000
thermo_modify   lost ignore norm no
compute_modify  thermo_temp dynamic yes

# Set up restarts
#restart        12500 restart.1 restart.2

# Check timestep
fix             timecheck all check/timestep/gran 1 0.01 0.01
run             1
unfix           timecheck

# Run 1.0 sec to insert and settle particles
run             160000 upto

# Dump output
#dump           dmp all custom 16000 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dumpstl all stl 16000 dump*.stl
#dump           dmp2 all custom 16000 dump.txt type x y z radius

# Load balancing
fix             lb all balance 0 xyz 10 1.1 out balance.txt
group           large type 1
group           small type 2
```

```
# Remove the stopper and start the rotation
unfix                   geometry
fix                     geometry all wall/gran/hertz/history mesh n_meshes 3 meshes cad1 cad2 cad3 rolling_friction cdt
fix                     movecad all move/mesh mesh cad2 rotate origin 0. 0. 0. axis 0. 0. 1. period 1.

# Run 30  sec
run                     4800000
```

 # Plow mixer example

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes
#processors     6 4 1

# Declare domain
region          reg block -0.205 0.205 -0.310 0.01 -0.205 0.205 units box
create_box      1 reg

# Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 1 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 1 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 1 0.1

# Contact physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file housing.stl type 1 scale 0.001 move 0 0 0 rotate axis 0 1 0 angle -90 curvature 1e-5
fix             cad2 all mesh/surface file shaft.stl type 1 scale 0.001 curvature 1e-5
fix             cad3 all mesh/surface file chopper.stl type 1 scale 0.001 move 0 0.0101015 0 rotate axis 0 1 0 angle -90 curvature 1e-5
fix             mixer all wall/gran/hertz/history mesh n_meshes 3 meshes cad1 cad2 cad3

# Particle insertion
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.0012
fix             pdd all particledistribution/discrete 634718 1 pts 1.0
region          factory block -0.1 0.1 -0.27 -0.07 0.09 0.11 units box
fix             ins all insert/rate/region seed 324123 distributiontemplate pdd nparticles 1000000 &
                particlerate 1000000 insert_every 1000 overlapcheck yes vel constant 0. 0. -2.0 region &
                factory ntry_mc 10000

# Timestep
timestep        0.000008

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          6250
thermo_modify   norm no #lost ignore
compute_modify  thermo_temp dynamic yes

# Check time step
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix           ctg

fix             lb all balance 0 xyz 10 1.1 out balance.txt

# Run 2 seconds to insert the particles
run             250000 upto

# Make a dump of particles and the stl files
#dump           dmp all custom 2500 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dumpstl all stl 2500 dump*.stl

# Rotate the impeller
fix             movecad1 all move/mesh mesh cad2 rotate origin 0. 0. 0. axis 0. 1. 0. period 1.5  # 40 RPM
fix             movecad2 all move/mesh mesh cad3 rotate origin -0.06703 -0.145 -0.08595 axis 0.06703 0. 0.08595 period 0.05
        #1200 RPM

# Run 5 seconds equilibration
```

```
run                     625000

# Run 5 seconds data gathering
run                     625000
```

 # Vertical high shear mixer example

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.17 0.17 -0.17 0.17 -0.003 0.19 units box
create_box      1 reg

#Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 1 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 1 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 1 0.1

# Physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file container.stl type 1 scale 1.0 move -0.1625948 -0.1970097 0 curvature 1e-5
fix             cad2 all mesh/surface file top_lid.stl type 1 scale 1.0 move -0.1625948 -0.1970097 0 curvature 1e-5
fix             cad3 all mesh/surface file blade.stl type 1 scale 0.001 curvature 1e-5
fix             mixer all wall/gran/hertz/history mesh n_meshes 3 meshes cad1 cad2 cad3 rolling_friction cdt

# Particle insertion
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.001
fix             pdd all particledistribution/discrete 634718 1 pts 1.0
fix             ins_mesh all mesh/surface file factory.stl type 1 scale 0.001
fix             ins all insert/stream seed 321412 distributiontemplate pdd nparticles 500000 particlerate 500000 overlapcheck yes vel
constant 0. 0. -1.0 insertion_face ins_mesh extrude_length 0.03

# Timestep
timestep        0.000005

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          20000
thermo_modify   norm no #lost ignore
compute_modify  thermo_temp dynamic yes

# Run 1 step to initialize dump file and check time step
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix           ctg

# Run 1 second to insert the particles
run             200000 upto
unfix           ins

# Load balancing
fix             lb all balance 0 z 10 1.1 out balance.txt

# Make a dump of particles and the stl file
#dump           dmp all custom 20000 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dumpstl all stl 20000 dump*.stl

# Rotate central shaft
fix             movecad1 all move/mesh mesh cad3 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.33333        # 180 RPM

# Run 2 seconds to equilibrate
run             400000
```

```
# Run 5 seconds to equilibrate
run                     1000000
```

 # Ribbon blender simulation

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.187 0.187 -0.525 0.525 -0.269 0.289 units box
create_box      1 reg

# Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 1 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 1 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 1 0.1
#fix            m6 all property/global cohesionEnergyDensity peratomtypepair 1 61817

# Contact physics
pair_style      gran/hertz/history rolling_friction cdt  # Hertz with cohesion
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file Ribbon-Blender-Frame.STL type 1 scale 0.001 curvature 1e-5
fix             cad2 all mesh/surface file Ribbon-Blender-Shaft.STL type 1 scale 0.001 curvature 1e-5
fix             geometry all wall/gran/hertz/history mesh n_meshes 2 meshes cad1 cad2 rolling_friction cdt

# Particle insertion
region          factory block -0.15 0.15 -0.43 0.43 0.24 0.26 units box
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.003
fix             pdd all particledistribution/discrete 14127 1 pts 1.0
fix             ins all insert/rate/region seed 12341 distributiontemplate pdd nparticles 200000 particlerate 300000 insert_every 1000
overlapcheck yes vel constant 0. 0. -2.0 region factory ntry_mc 10000

# Timestep
timestep  0.00002

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          2500
thermo_modify   lost ignore norm no
compute_modify  thermo_temp dynamic yes

# Run 1 step to initiate dump file and check the timestep
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix           ctg

# Load balancing
fix             lb all balance 0 xyz 10 1.1 out balance.txt

# Insert the particles - 1 sec
run             50000 upto

# Rotate the shaft
fix             movecad1 all move/mesh mesh cad2 rotate origin 0. 0. 0. axis 0. 1. 0. period -1.5# 40 RPM
#fix            movecad2 all move/mesh mesh cad3 rotate origin 0. 0. 0. axis 0. 1. 0. period -1.5# 40 RPM

# Make a dump of particles and the stl file
#dump           dmp all custom 10 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dumpstl all stl 10 dump*.stl

# Run to 15 sec to equilibrate system
run             750000
```

 # V-blender mixer example

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.28 0.28 -0.28 0.28 -0.28 0.28 units box
create_box      2 reg

# Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 2 0.5 0.5 0.5 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 2 0.5 0.5 0.5 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 2 0.1 0.1 0.1 0.1

# Contact physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file V-blender.stl type 1 scale 0.001 curvature 1e-5 #rotate axis 1 0 0 angle 90
fix             cad2 all mesh/surface file V-blender-shaft.stl type 1 scale 0.001 move 0. 0. -0.07 curvature 1e-5 #-0.08806 0 0 rotate axis
1 0 0 angle 90

# Use the imported mesh as granular wall
fix             mixer all wall/gran/hertz/history mesh n_meshes 2 meshes cad1 cad2 rolling_friction cdt

# Particle insertion
region          factory1 cylinder z 0 -0.125 0.05 0.01 0.03 units box
region          factory2 cylinder z 0  0.125 0.05 0.01 0.03 units box
fix             pts1 all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.0015
fix             pts2 all particletemplate/sphere 1 atom_type 2 density constant 1000 radius constant 0.0015
fix             pdd1 all particledistribution/discrete 634718 1 pts1 1.0
fix             pdd2 all particledistribution/discrete 562363 1 pts2 1.0
fix             ins1 all insert/rate/region seed 123481 distributiontemplate pdd1 nparticles 117500 particlerate 186000 &
                insert_every 1000 overlapcheck yes vel constant 0.  2.0 -2.0 region factory1 ntry_mc 1000
fix             ins2 all insert/rate/region seed 958238 distributiontemplate pdd2 nparticles 117500 particlerate 186000 &
                insert_every 1000 overlapcheck yes vel constant 0. -2.0 -2.0 region factory2 ntry_mc 1000

# Timestep
timestep  0.00001

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          1000
thermo_modify   norm no lost ignore
compute_modify  thermo_temp dynamic yes

# Run to create a single particle to initiate a dump file and check the timestep
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix           ctg

# Make a dump file of particle positions and stl files
#dump           dmp all custom 1000 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dumpstl all stl 1000 dump*.stl

# Load balancing
#fix            lb all balance 0 xyz 10 1.1 out balance.txt

# Run 1 second for particle insertion
run             100000 upto
```

```
# Rotating the V-blender and impeller
fix             movecad1 all move/mesh mesh cad1 rotate origin 0. 0. -0.07 axis 0. 1. 0. period 2.5                  # 24 RPM - V
fix             movecad2 all move/mesh mesh cad2 rotate origin 0. 0. -0.07 axis 0. 1. 0. period -0.027272727        # -2200 RPM - shaft

# Run 100 seconds
run             10000000
```

 # Auger doser simulation

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.35 0.35 -0.35 0.35 -0.25 0.66 units box
create_box      2 reg

# Material and interaction properties
fix             m1 all property/global youngsModulus peratomtype 1.0e7 1.0e7
fix             m2 all property/global poissonsRatio peratomtype 0.25 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 2 0.5 0.5 0.5 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 2 0.5 0.2 0.2 0.2
fix             m5 all property/global coefficientRollingFriction peratomtypepair 2 0.1 0.025 0.025 0.025

# Physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff      * *

# Time step
timestep        0.00002

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file auger.stl type 1 scale 0.001 curvature 1e-5
fix             cad2 all mesh/surface file funnel.stl type 1 scale 0.001 curvature 1e-5
fix             cad3 all mesh/surface file collector_funnel.stl type 2 scale 0.001 move 0.0 0.0 0.075 curvature 1e-5
fix             geometry all wall/gran/hertz/history mesh n_meshes 3 meshes cad1 cad2 cad3 rolling_friction cdt

# Particle insertion
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.002
fix             pdd all particledistribution/discrete 12345 1 pts 1.0
fix             ins_mesh all mesh/surface file factory.stl type 1 scale 0.001
fix             ins all insert/stream seed 123481 distributiontemplate pdd nparticles 500000 massrate 33.51032 &
                overlapcheck yes vel constant 0. 0. -1.0 insertion_face ins_mesh extrude_length 0.05

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          2500
thermo_modify   lost ignore norm no
compute_modifythermo_temp dynamic yes

# Run to create a single particle to initiate a dump file
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix           ctg

# Load balancing
fix             lb all balance 0 xyz 10 1.1

run             250000 upto

# Make a dump of particles and the stl file
dump            dmp all custom 2500 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
dump            dumpstl all stl 2500 dump*.stl

# Iteration 1
fix             movecad1 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
run             11250
unfix           movecad1
run             38750

# Iteration 2
fix             movecad2 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
```

```
run             11250
unfix           movecad2
run             38750

# Iteration 3
fix             movecad3 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
run             11250
unfix           movecad3
run             38750

# Iteration 4
fix             movecad4 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
run             11250
unfix           movecad4
run             38750

# Iteration 5
fix             movecad5 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
run             11250
unfix           movecad5
run             38750

# Iteration 6
fix             movecad6 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
run             11250
unfix           movecad6
run             38750

# Iteration 7
fix             movecad7 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
run             11250
unfix           movecad7
run             38750

# Iteration 8
fix             movecad8 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
run             11250
unfix           movecad8
run             38750

# Iteration 9
fix             movecad9 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
run             11250
unfix           movecad9
run             38750

# Iteration 10
fix             movecad10 all move/mesh mesh cad1 rotate origin 0. 0. 0. axis 0. 0. 1. period 0.075
run             11250
unfix           movecad10
run             38750
```

 # CB Mixer #1 simulation

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.320 0.320 -1.960 1.460 -0.290 0.335 units box
create_box      1 reg

# Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 1 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 1 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 1 0.1

# Contact physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file trough2.stl type 1 scale 0.001 curvature 1e-5
fix             cad2 all mesh/surface file left_shaft2.stl type 1 scale 0.001 curvature 1e-5
fix             cad3 all mesh/surface file right_shaft2.stl type 1 scale 0.001 curvature 1e-5
fix             mixer all wall/gran/hertz/history mesh n_meshes 3 meshes cad1 cad2 cad3 rolling_friction cdt

# Timestep (keep < 20% T_Rayleigh)
timestep        0.00003125

# Particle insertion
region          factory block -0.225 0.225 -1.650 -1.450 0.3 0.33 units box
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.005
fix             pdd all particledistribution/discrete 14127 1 pts 1.0
fix             ins all insert/rate/region seed 132412 distributiontemplate pdd nparticles 10000000 &
                massrate 1.66666667 insert_every 1000 overlapcheck yes vel constant 0. 0. -1. &
                region factory ntry_mc 10000

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          1600
thermo_modify   lost ignore norm no
compute_modify  thermo_temp dynamic yes

# Rotate the shafts
fix             movecad1 all move/mesh mesh cad2 rotate origin -0.1369 0. -0.0462 axis 0. 1. 0. period 1.5      # 40 RPM
fix             movecad2 all move/mesh mesh cad3 rotate origin  0.1369 0. -0.0462 axis 0. 1. 0. period -1.5     # 40 RPM

# Run to create a single particle to initiate a dump file and check the timestep
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix ctg

# Define the dump files for the particles and the geometry
#dump           dmp all custom 5000 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dumpstl all stl 5000 dump*.stl

# Load balancing
fix             lb all balance 0 xyz 10 1.1 out balance.txt

# Run to 300 sec to equilibrate system
run             3840000 upto
```

 # CB Mixer #2 simulation

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.165 0.205 -0.025 1.275 -0.165 0.255 units box
create_box      1 reg

#Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 1 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 1 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 1 0.1

# Contact physics
pair_style      gran/hertz/history
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file housing_meshed.stl type 1 scale 0.001 curvature 1e-5
fix             cad2 all mesh/surface file shaft_meshed.stl type 1 scale 0.001 curvature 1e-5
fix             cad3 all mesh/surface file lid.stl type 1 scale 0.001 curvature 1e-5
fix             mixer all wall/gran/hertz/history mesh n_meshes 3 meshes cad1 cad2 cad3 rolling_friction cdt

# Particle insertion
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.001
fix             pdd all particledistribution/discrete 14127 1 pts 1.0
region          factory block 0.005 0.179 0.015 0.305 0.200 0.220 units box
fix             ins all insert/rate/region seed 83472 distributiontemplate pdd nparticles 10000000 massrate 0.215 overlapcheck yes vel
constant 0. 0. -1.0 insert_every 1000 region factory ntry_mc 1000

# Timestep
timestep        0.000005

# Thermo settings
thermo_style    custom step atoms ke
thermo          10000
thermo_modify   lost ignore norm no
compute_modify  thermo_temp dynamic yes

# Rotate shaft
fix             movecad1 all move/mesh mesh cad2 rotate origin 0. 0. 0. axis 0. 1. 0. period 0.0479233                    # 1252
RPM

# Check time step
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix           ctg

# Make a dump of particles and the stl file
#dump           dmp all custom 1000 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dumpstl all stl 1000 dump*.stl

# Load balancing
fix             lb all balance 0 xyz 10 1.1 out balance.txt

# Run 30 seconds
run             6000000 upto
```

 # CB Mixer #3 simulation

```
# Preliminaries
units           si
atom_style      sphere
boundary        f f f
newton          off
communicate     single vel yes
processors      2 12 2

# Declare domain
region          reg block -0.340 0.650 -0.11 3.16 -0.520 0.555 units box
create_box      1 reg

#Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 1 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 1 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 1 0.1

# Contact physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff      * *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file housing.stl type 1 scale 0.001 curvature 1e-5
fix             cad2 all mesh/surface file left_shaft.stl type 1 scale 0.001 curvature 1e-5
fix             cad3 all mesh/surface file right_shaft.stl type 1 scale 0.001 move 0.3937 0 0 curvature 1e-5
fix             cad4 all mesh/surface file lid.stl type 1 scale 1.0 curvature 1e-5
fix             mixer all wall/gran/hertz/history mesh n_meshes 4 meshes cad1 cad2 cad3 cad4 rolling_friction cdt

# Particle insertion
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.004
fix             pdd all particledistribution/discrete 14127 1 pts 1.0
region          factory block 0.123 0.402 0.038 0.317 0.450 0.500 units box
fix             ins all insert/rate/region seed 2341324 distributiontemplate pdd nparticles 20000000 massrate 3.3333 insert_every 1000
overlapcheck yes vel constant 0. 0. -1.0 region factory ntry_mc 10000

# Timestep
timestep        0.000025

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          10000
thermo_modify   lost ignore norm no
compute_modify  thermo_temp dynamic yes

# Rotate shafts
fix             movecad1 all move/mesh mesh cad2 rotate origin 0. 0. 0. axis 0. 1. 0. period -0.6# 100 RPM
fix             movecad2 all move/mesh mesh cad3 rotate origin 0.3937 0. 0. axis 0. 1. 0. period 0.3        # 200 RPM

# Check timestep
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix           ctg

# Make a dump of particles and the stl file
#dump           dmp all custom 50000 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dumpstl all stl 1 dump*.stl

# Run to 100 sec to equilibrate system
run             4000000 upto
```

 # CB Mixer #4 simulation

```
# Preliminaries
units           si
atom_style      sphere
atom_modify     map array
boundary        f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.05 2.04 -0.40 0.45 -0.48 0.61 units box
create_box      1 reg

# Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.6e7
fix             m2 all property/global poissonsRatio peratomtype 0.3
fix             m3 all property/global coefficientRestitution peratomtypepair 1 0.4
fix             m4 all property/global coefficientFriction peratomtypepair 1 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 1 0.1

# Contact physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff      * *

# Timestep
timestep        0.00004

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file housing.stl type 1 scale 0.001 curvature 1e-5
fix             cad2 all mesh/surface file shaft.stl type 1 scale 0.001 curvature 1e-5
fix             cad3 all mesh/surface file chopper1.stl type 1 scale 0.001 curvature 1e-5
fix             cad4 all mesh/surface file chopper2.stl type 1 scale 0.001 curvature 1e-5
fix             cad5 all mesh/surface file chopper3.stl type 1 scale 0.001 curvature 1e-5
fix             mixer all wall/gran/hertz/history mesh n_meshes 5 meshes cad1 cad2 cad3 cad4 cad5 rolling_friction cdt

# Particle insertion
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.005
fix             pdd all particledistribution/discrete 14127 1 pts 1.0
region          factory block 0.05 0.25 -0.15 0.05 0.4 0.5 units box
fix             ins all insert/rate/region seed 1234123 distributiontemplate pdd nparticles 10000000 massrate 2.33333 overlapcheck yes
insert_every 1000 vel constant 0. 0. -4.0 region factory ntry_mc 1000

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          10000
thermo_modify   lost ignore norm no
compute_modify  thermo_temp dynamic yes

# Run to create a single particle to initiate a dump file and check the timestep
fix             ctg all check/timestep/gran 1 0.01 0.01
run             1
unfix           ctg

# Rotate the impeller and choppers
fix             movecad1 all move/mesh mesh cad2 rotate origin 0.000 0. 0. axis 1. 0.000 0. period 1.0              # 60 RPM
fix             movecad2 all move/mesh mesh cad3 rotate origin 0.625 0. 0. axis 0. 0.866 -0.5 period -0.025     # 2400 RPM
fix             movecad3 all move/mesh mesh cad4 rotate origin 1.125 0. 0. axis 0. 0.866 -0.5 period -0.025     # 2400 RPM
fix             movecad4 all move/mesh mesh cad5 rotate origin 1.625 0. 0. axis 0. 0.866 -0.5 period -0.025     # 2400 RPM

# Make a dump of particles and the stl file
#dump           dmp all custom 10000 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dumpstl all stl 10000 dump*.stl
#restart        40000 cc.restart.1 cc.restart.2

# Run to 600 sec to equilibrate system
run             10000000 upto
```

 # Vibrating conveyor

```
# Preliminaries
units           si
atom_style      sphere
boundary f f f
newton          off
communicate     single vel yes

# Declare domain
region          reg block -0.855 0.855 -0.855 0.855 -0.28 0.052 units box
#region         reg block -0.855 0.855 -0.855 0.855 -0.270 0.50 units box
create_box      1 reg

# Material properties and interactions
fix             m1 all property/global youngsModulus peratomtype 2.5e7
fix             m2 all property/global poissonsRatio peratomtype 0.25
fix             m3 all property/global coefficientRestitution peratomtypepair 1 0.5
fix             m4 all property/global coefficientFriction peratomtypepair 1 0.5
fix             m5 all property/global coefficientRollingFriction peratomtypepair 1 0.1

# Contact physics
pair_style      gran/hertz/history rolling_friction cdt
pair_coeff* *

# Integrator
fix             integrate all nve/sphere

# Gravity
fix             grav all gravity 9.81 vector 0.0 0.0 -1.0

# Import mesh from cad:
fix             cad1 all mesh/surface file conveyor_pilot_single_loop.stl type 1 scale 0.001 curvature 1e-5
fix             geometry all wall/gran/hertz/history mesh n_meshes 1 meshes cad1

# Particle insertion
fix             pts all particletemplate/sphere 1 atom_type 1 density constant 1000 radius constant 0.002
fix             pdd all particledistribution/discrete 634718 1 pts 1.0
fix             factory all mesh/surface file factory.stl type 1 scale 0.001
fix             ins all insert/stream seed 123412 distributiontemplate pdd nparticles 10000000 massrate 0.166666667 overlapcheck yes
vel constant 1. 0. 0. insertion_face factory extrude_length 0.02

# Timestep
timestep   0.00001

# Thermo settings
thermo_style    custom step atoms ke cpu
thermo          10000
thermo_modify   norm no lost ignore
compute_modify  thermo_temp dynamic yes

# Coupled motion - linear and rotational vibration to create a screw like motion
fix             wiggle all move/mesh mesh cad1 wiggle amplitude 0. 0. 0.007094 period 0.089552
fix             riggle all move/mesh mesh cad1 riggle origin 0. 0. 0. axis 0. 0. 1. period 0.089552 amplitude 0.553071

# Run 1 step to check timestep and initialize the dump file
fix             timecheck all check/timestep/gran 1 0.01 0.01
run             1
unfix           timecheck

# Make a dump of particles and the stl file
#dump           dmp all custom 200 dump.1 id type type x y z ix iy iz vx vy vz fx fy fz omegax omegay omegaz radius
#dump           dmpstl all stl 200 dump*.stl
#dump           dmpvtk all mesh/vtk 200 dump*.vtk id owner vel

# Run 60 seconds
run             6000000 upto
```