Commercial Software vs. LAMMPS

I've put together some results comparing the performance of LAMMPS and (COMMERCIAL SOFTWARE) for a test problem involving the tumbling of particles in a couple of rotating drum mixers. In each case, 2 seconds was run to settle the particles and get the drum up to speed so that the operation would effectively be steady state. Timing was then recorded over the next 5 seconds. The LAMMPS jobs were run on one of our clusters, while (COMMERCIAL SOFTWARE) was run on my personal workstation. The machines are fairly comparable in performance. I did replace the interactions in LAMMPS to match those of (COMMERCIAL SOFTWARE) as closely as I can to make sure the comparison was fair. The normal forces do match exactly, but I don't know how (COMMERCIAL SOFTWARE) computes the tangential overlap, so there is still some difference in the tangential interaction. The bulk results were identical between the platforms, however, as determined by looking at the shape of the top surface of the particle bed.

Problem setup # 1:

- Material setup (both particles and drum)
  - o ν = 0.3
  - o G = 1 MPa
  - o ρ = 1000 kg/m^3
  - o CoR = 0.5
  - o μ_s = 0.5
  - o μ_r = 0.0
- Particle size = 6.204 mm radius (1 g net mass)
- Drum:
  - o Radius = 700 mm
  - o Thickness = 300 mm (periodic boundary)
  - o Rotation rate = 30 rpm
- 100,000 particles
- dt = 0.0001 sec (15% Tr)

Results #1 – timings given in seconds; * indicates that the processor allotment was assigned along the axis of the cylinder, effectively ensuring that each processor had a similar number of particles.

	# cores	Periodic	Periodic*
(COMMERCIAL SOFTWARE)	**8**	**2182**	
LAMMPS	**8**	**1347**	**679**
LAMMPS	**16**	**880**	**375**
LAMMPS	**32**	**456**	**246**

Periodic drum								
	# cores	**1**	**2**	**4**	**8**	**16**	**32**
Speedup	**COMMERCIAL**	**1**	**1.61828**	**2.71783**	**3.9736**		
	LAMMPS	**1**	**1.055782**	**1.58289**	**2.78916**	**4.269318**	**8.23904**
	LAMMPS*	**1**	**1.931976**	**3.64689**	**5.52135**	**9.997333**	**15.2398**
Efficiency	**COMMERCIAL**	**1**	**0.80914**	**0.67946**	**0.4967**		
	LAMMPS	**1**	**0.527891**	**0.39572**	**0.34865**	**0.266832**	**0.25747**
	LAMMPS*	**1**	**0.965988**	**0.91172**	**0.69017**	**0.624833**	**0.47624**

Problem setup # 2:

- Material setup (both particles and drum)
  - o ν = 0.3
  - o G = 1 MPa
  - o ρ = 1000 kg/m^3
  - o CoR = 0.5
  - o μ_s = 0.5
  - o μ_r = 0.0
- Particle size = 6.204 mm radius (1 g net mass)
- Drum:
  - o Radius = 365 mm
  - o Thickness = 1090 mm
  - o Rotation rate = 30 rpm
- 100,000 particles
- dt = 0.0001 sec (15% Tr)

Results #2 – timings given in seconds; * indicates that the processor allotment was assigned along the axis of the cylinder, effectively ensuring that each processor had a similar number of particles.

	# cores	Nonperiodic	Nonperiodic*
(COMMERCIAL SOFTWARE)	8	1987.2	
LAMMPS	8	1202	522.5
LAMMPS	16	646.5	253
LAMMPS	32	354.5	132

Nonperiodic drum							
	# cores:	1	2	4	8	16	32
Speedup	COMMERCIAL	1	1.836735	2.21997	3.16105		
	LAMMPS	1	2.006371	2.11598	3.0129	5.601701	10.2158
	LAMMPS*	1	2.031443	3.87989	6.9244	14.3004	27.4091
Efficiency	COMMERCIAL	1	0.918367	0.55499	0.39513		
	LAMMPS	1	1.003186	0.529	0.37661	0.350106	0.31924
	LAMMPS*	1	1.015722	0.96997	0.86555	0.893775	0.85653

LIGGGHTS 1.0.1 vs. LIGGGHTS 1.0 vs. LAMMPS

# steps	LAMMPS	LIGGGHTS (original, 1.0)	LIGGGHTS (new, 1.0.1)
10000	**89**	**127**	**86**
10000	**103**	**148**	**101**
50000	**519**	**740**	**506**

Results are also consistent. The three data sets below are offset by 0.05 just to show each pattern.