# LIGGGHTS performance evaluation

# Common elements

- Contact model – Hertz-Mindlin with history
  - Includes tangential damping
  - No cohesion
- All codes run on 8 cores unless otherwise noted

# Angle of Repose

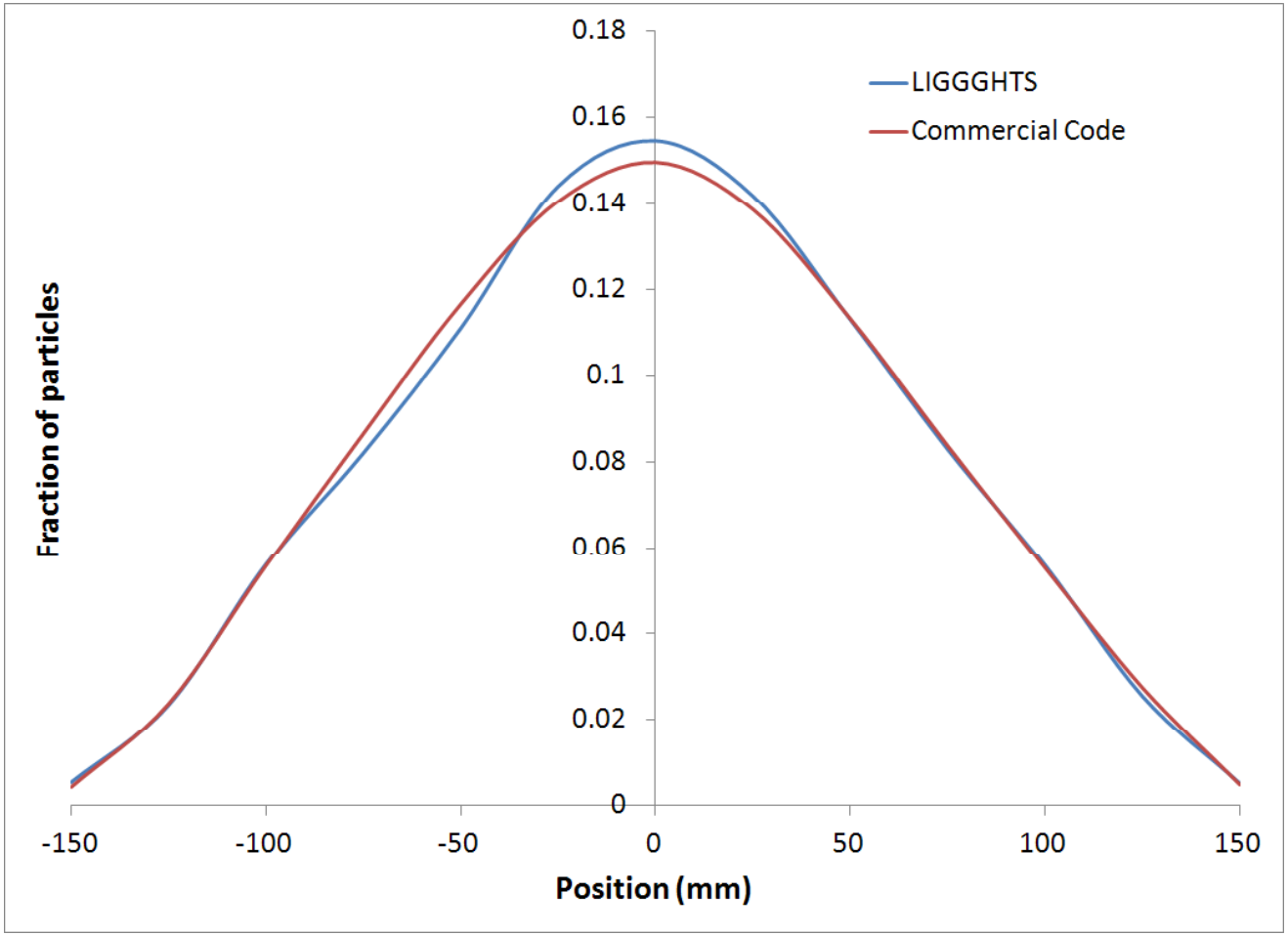
3500 monodisperse spheres poured into a narrow slot (30 cm long by 2 cm wide) to create a 2-D heap

Codes compared by mapping the particles beds

# Angle of Repose

| Simulation properties | | | |
|---|---|---|---|
| | Young's modulus | $2.5 \times 10^{8}$ | Pa |
| | Poisson ratio | 0.25 | |
| | Coefficient restitution | 0.25 | |
| | Coefficient friction | 0.5 | |
| | $\Delta t$ | $5 \times 10^{-6}$ | sec |
| | Particle diameter | 4 | mm |
| | Density | 1000 | $kg/m^3$ |
| | # particles | 3500 | |
| | | | |
| | | | |
| | Commercial code | 2574 | sec |
| | LIGGGHTS | 315 | sec |

# Angle of Repose



# Flow through a Funnel

10000 monodisperse spheres poured into a conical funnel w/ stopper

Stopper then pulled to release particles.

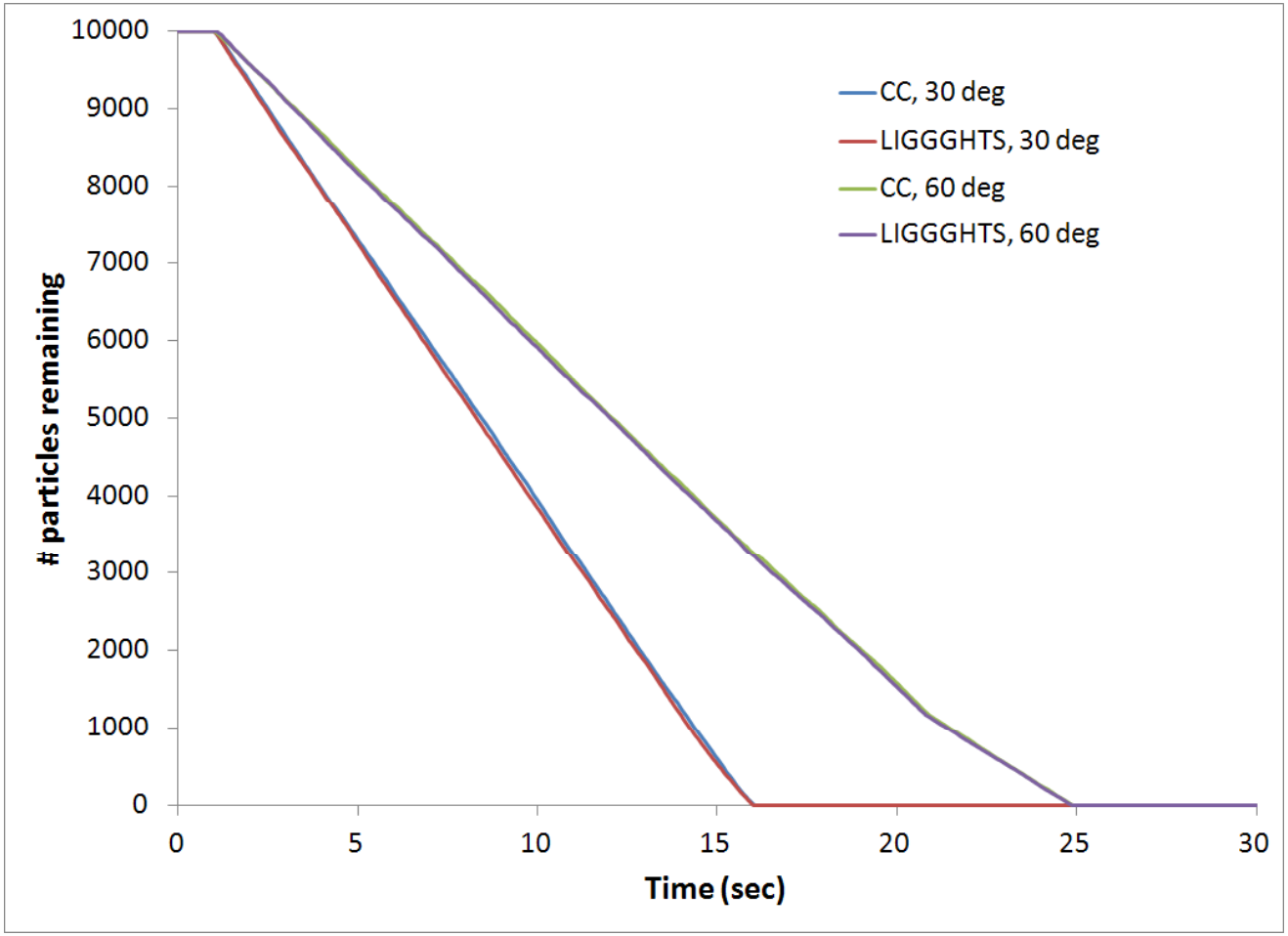
Two different funnels considered – $30^o$ and $60^o$ pitch

Codes compared by measuring flow rates

# Flow through a Funnel

| Simulation properties | | | |
|---|---|---|---|
| | Young's modulus | $2.5 \times 10^{6}$ | Pa |
| | Poisson ratio | 0.25 | |
| | Coefficient restitution | 0.5 | |
| | Coefficient friction | 0.5 | |
| | $\Delta t$ | $1 \times 10^{-4}$ | sec |
| | Particle diameter | 10 | mm |
| | Density | 1000 | $kg/m^3$ |
| | # particles | 10000 | |
| | | | |
| | | | |
| | Commercial code | 1239 | sec |
| | LIGGGHTS | 271 | sec |

# Flow through a Funnel



# Flow through a Funnel (2)

100000 monodisperse spheres poured into a conical funnel w/ stopper

Stopper then pulled to release particles.

Funnel pitch = $30^{o}$

Computational time recorded for 30 sec of simulation time beyond the pull of the stopper

# Flow through a Funnel (2)

| Simulation properties | | | |
|---|---|---|---|
| | Young's modulus | $2.5 \times 10^{6}$ | Pa |
| | Poisson ratio | 0.25 | |
| | Coefficient restitution | 0.5 | |
| | Coefficient friction | 0.5 | |
| | $\Delta t$ | $1 \times 10^{-4}$ | sec |
| | Particle diameter | 10 | mm |
| | Density | 1000 | $kg/m^3$ |
| | # particles | 100000 | |

# Flow through a Funnel (2)

| Timing comparison | | | |
|---|---|---|---|
| | Commercial code (8 cores) | 10.9 | hours |
| | | | |
| | LIGGGHTS | | |
| | 8 cores | 2.00 | hours |
| | 16 cores | 1.44 | hours |
| | 24 cores | 1.47 | hours |
| | 32 cores | 1.09 | hours |
| | 64 cores | 0.85 | hours |
| | | | |
| | | | |
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| | | | |
| | | | |

# Continuous Blending Mixer

Stream of monodisperse spheres poured onto a continuous blending mixer at 1 kg/sec

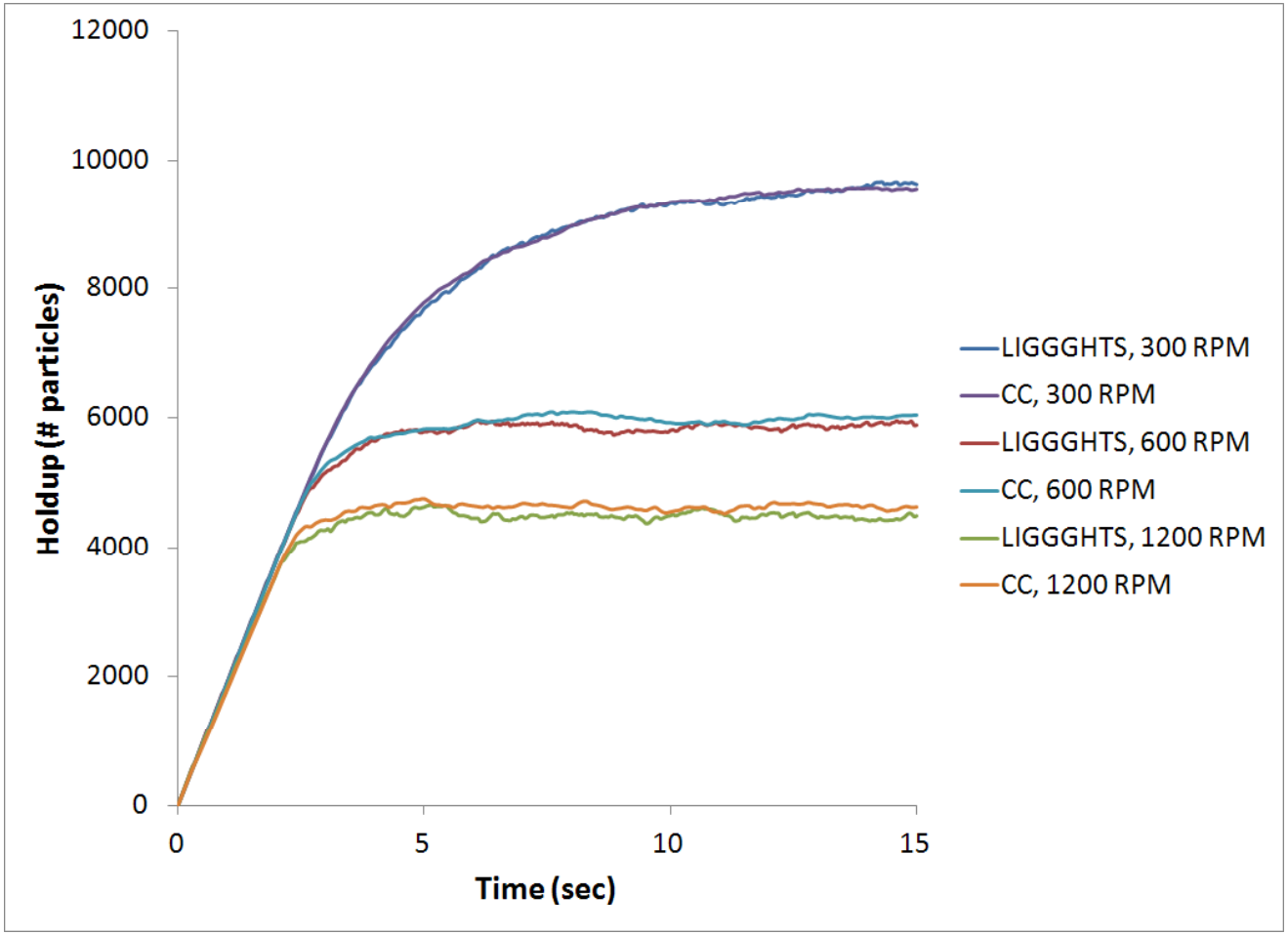
Mixer shaft rotated at 300 RPM, 600 RPM, 1200 RPM.

Codes compared by measuring holdup

# Continuous Blending Mixer

| Simulation properties | | | |
|---|---|---|---|
| | Young's modulus | $2.5 \times 10^{8}$ | Pa |
| | Poisson ratio | 0.25 | |
| | Coefficient restitution | 0.5 | |
| | Coefficient friction | 0.5 | |
| | $\Delta t$ | $1 \times 10^{-5}$ | sec |
| | Particle diameter | 10 | mm |
| | Density | 1000 | $kg/m^3$ |
| | Pour rate | 1 | kg/sec |
| | | | |
| | | | |
| | Commercial code | 3.5 | hrs |
| | LIGGGHTS | 11.1 | hrs |

# Continuous Blending Mixer



# Segregation Test

Equal masses of two different diameter spheres poured into a narrow slot (30 cm long by 2 cm wide) to create a 2-D heap

- 4000 of diameter 2 mm
- 32000 of diameter 1 mm

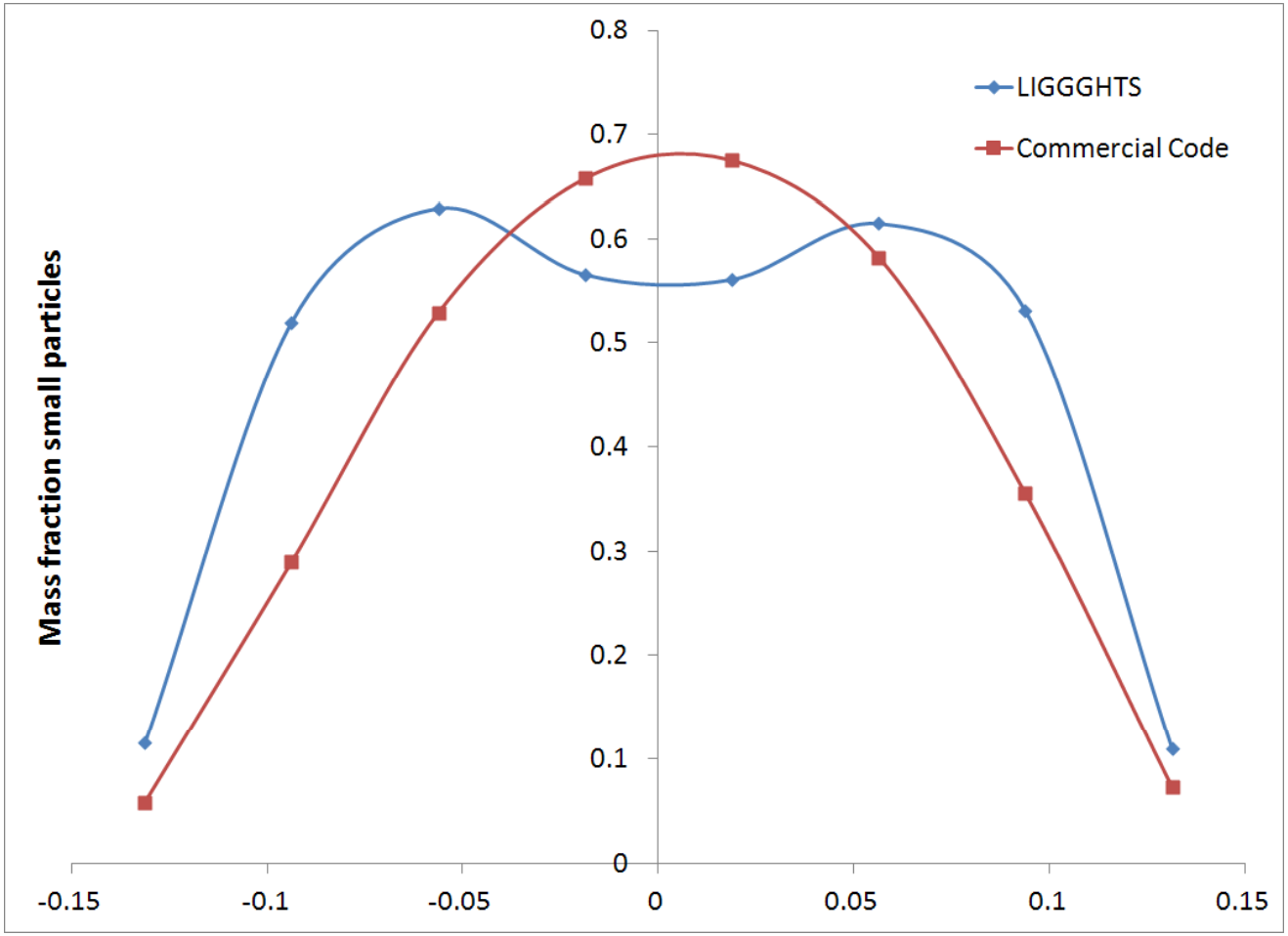
Particles poured for 8 seconds, then settled for 2 additional seconds

Codes compared by mapping the particles beds

# Segregation Test

| Simulation properties | | | |
|---|---|---|---|
| | Young's modulus | $2.5 \times 10^{8}$ | Pa |
| | Poisson ratio | 0.25 | |
| | Coefficient restitution | 0.25 | |
| | Coefficient friction | 0.5 | |
| | $\Delta t$ | $4 \times 10^{-6}$ | sec |
| | Particle diameter | 2 / 4 | mm |
| | Density | 1000 | $kg/m^3$ |
| | # particles (total) | 36000 | |
| | | | |
| | | | |
| | Commercial code (6 proc) | ~22 | hrs |
| | LIGGGHTS (8 proc) | 2.2 | hrs |

# Segregation Test



# Remaining tests

- Multiple materials
  - e.g. particle flow through a funnel in which particle-particle and particle-funnel interactions are different
- Multiple particle sizes
  - Need to understand the segregation test results
- Cohesion
- Particle shapes