GPU based DEM for bulk particle transport simulations.

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Outline

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- DEM
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- Experimental validation
- Conclusion
Introduction

- Proton: $10^{-13}$ cm
- Nuclei: $10^{-11}$ cm
- Atom: $10^{-8}$ cm
- Molecule: $10^{-7}$ cm
- Grain: 1 cm
- Rocks: 100 cm

**Forces**
- Color (Quarks)
- Strong (residual)
- EM, Weak
- Gravity, EM*

Interaction affected by physical contact

The physical size of the particle does not affect interaction
Discrete Element Method

- Similar force ranges and particle sizes
- Motion of particle depend on the net sum of forces per time step
- Binary contact is assumed to resolve contact forces
- Explicit integration
- Embarrassingly parallel
- Particles are commonly treated as spheres
If only they had simulated...
Some of them did...

- “Large-scale simulations of an experimental device, featuring 440,000 spherical particles”

1. *It is meant to be bulk material simulation!*

2. *Shape, no wonder the Mars rover got stuck.*

• “The DEM simulations in this study required over a month of time on 90 processors, since the contact models are stiff and a small timestep is required.”

DEM limitation

• Particle numbers

Ex. fine sand
$\varnothing \approx 200 \, \mu m$
$1 \, cm^3$

$150 \, 000$ particles

DEM challenges for the geomechanic applications is number of elements

Numbers of particles vs time in DEM papers (CPU)

Clock frequency vs time

Size of transistor vs time

Particulate DEM, A geomechanics Perspectives, O’Sullivan 2011

GPU approach needed if we want to increase particles and model the industrial-scale
Aim

- Provide a GPU based framework that can be used to solve bulk flow problems encountered in engineering industry.

- Run on typical workstations using consumer hardware while being able to efficiently utilize multi GPU configurations.

- Needs to provide physical quantities that are relevant to aid in the design process.

- Needs to be modular in terms of:
  - Collision detection.
  - Collision resolution (physics).

- Allow for accurate particle shape representation when needed.
- Allow for large number of particles to be simulated.
GPU-DEM

Because shape and speed matter!
Collision detection

- Current methods use triangulation/particles, which require thousands of checks to determine collision.
- We employ a ray based approach, which does not require a mesh.

\[ d = \mathbf{n} \cdot (\mathbf{v} - \mathbf{c}) \]

- For higher order surfaces we use analytical expressions.

\[ d = f(\mathbf{v}) \]
• Mathematically only a change in normal implies a new surface.

• Thus surface triangulation is not needed for collision detection, a point and normal is sufficient.

• Justification from DEM community is it is needed for calculating wear, stress/pressure, tallies etc.

• However it is actually only a “virtual” mesh that is needed. Furthermore since they are not intrinsic properties they can be processed in parallel/post with the DEM step.
GPU Data Storage

- SOA approach: 2.6 GB per 10 million particles, unpadded since memory is a premium.

- Spatial binning grid requires 8 bytes per cell (8 GB for a 10m³ area).
  - Largest particle dictates cell size.
  - ~15% 1:2 ratio.
  - Smaller ratio than this requires parameter change so cannot compare.

- Can have a coarser grid to decrease memory usage but performance drops by 2.8X and 15X for a factor of 2 and 4 cell-size reduction.

- World Geometry is split into: macro (cylinder, cone), surface (internal concave) and volume (convex) objects. Stored in constant memory*.

- Objects can rotate and translate imparting the resultant dynamics on particles.

- All objects can deform rigidly in real-time.
GPU Computation

- We split world collision detection into (Kernel_Planar) and (Kernel_Marco) to ensure there is no divergence. We launch kernels per world object in multiple streams.

- NN search using spatial binning, requires the cells to be set using memset after each iteration. This is expensive and also scaled with the domain not particles.

- However, we can run the opposite of the binning kernel, to set bin values to zero. 10X faster than memset and scales with number of particles/distn.

- We only grid the region where particles are contained in for silo/flow problems where the domain moves. (First and last particle hash gives the extent of the region).

- Particle, World and Volume CD are in different streams to allow concurrent execution.

- On a single GPU we can do 32 million particles using 8.7GB memory 0.2 seconds per step. **35 minutes** for **1 second** simulation time. Cundall No = 1.6E8

- Multi-GPU: Brute-force sorting on GPU 0, then send N/k particle to each GPU.+ buffer. Only useful when domain does not change much, eg filling, mass flow. Waiting for Pascal...
GPU Optimizations

• For the past 3 years chose “sensible” algorithms for the GPU.
  • Code is many of times faster than CPU codes, and about 3X faster than comparable GPU codes.
  
  – As always predicting the real world is the essential proof, pushing to 10's of millions of particles started taking time, about 3 days for an industry relevant simulation.

• Although it is a new performance level for DEM, I didn't like waiting.

  – Finally this year after extensive validation (documented in journal publications) that shows good agreement to experiment, new ideas kept on the back burner were implemented.

  – Short story in two weeks got a 4X speed-up! That is more than any full algorithmic changes can yield...
What had to change from typical “particle simulations”.

- Gaming approximates contact duration crudely by impulse calculations
  \[ \mathbf{v}^{\text{new}} = \mathbf{v}^{\text{n}} \pm \mathbf{j}/m, \quad \omega^{\text{new}} = \omega^{\text{n}} \pm \mathbf{I}^{-1} (\mathbf{r} \times \mathbf{j}) \]

- Physics simulations resolves the contact duration from constitutive contact models
  \[ F_{\text{elastic}} = (K_r \delta^m n) \]
  \[ F_{\text{diss}} = -K_D \delta^n \mathbf{v}_{\text{rel}} n \]

- Contact is resolved in a single time-step!
- Contact is resolved over multiple steps!
- Gaming is qualitative and estimates visual acceptable behavior
- Physics simulations are quantitative and estimate physical quantities such as energy, impact and shear and normal forces
DEM vs Experiment Spherical Particle Flow
DEM vs Experiment Polyhedra Particle Flow

(a) T=1.0

(b) T=0.5

(c) T=0.5

(d) T=2.0

(e) T=1.0

(f) T=1.0

(g) T=1.0

(h) T=1.5

(i) T=1.5

(j) T=1.5

(k) T=2.5

(l) T=1.5

(m) T=1.5

(n) T=2.5

(o) T=1.5

(p) T=2.5
Flow rates DEM vs Experiment
Flow rates Spheres vs Polyhedra

(a) Flow rates comparison graph for different materials and angles. The graph shows the percentage discharged over time for spheres and polyhedra with various angles.

(b) Polyhedra arching temporarily causes stop start flow. The image shows polyhedra arching in a system, leading to a temporary stop in flow.

(c) Polyhedra (corn) stable arch causing flow to stop. The image illustrates a stable arch formed by polyhedra, which prevents flow.

[CSIR Logo]
Spherical particle flow at the industrial scale

Cross-sectional views of hopper flow patterns at several simulation time (0, 10, 20 and 30s) for silo 2 (16777216 particles, 20 mm diameter)
Why do we need more particles?
Latest LIGGGHTS benchmark
http://www.cfdem.com/media/DEM/benchmarks/LIGGGHTS_Benchmarks.pdf

10 Million Particles, 60 Cores: 1 second = 46 hours
Cost $16000 For just the CPUs! *(Price at launch in 2013)= $ 96000

GPU 242X Faster, 27X Cheaper

Blaze-DEM GPU benchmark
10 Million Particles, 1 GTX 980 : 1 second = 0.19 hours
Cost $600

Because the future is now!
Thank you for your time.


