



**ENABLING COMPUTATIONAL DYNAMICS IN
DISTRIBUTED COMPUTING ENVIRONMENTS USING
A HETEROGENEOUS COMPUTING TEMPLATE**

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Report Documentation Page

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GOAL OF OUR WORK...

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- Use High Performance Computing (HPC) to simulate the dynamics of real-life engineering mechanical systems at unprecedented levels of accuracy
- HPC hardware targeted:
 - Cluster of CPUs and GPUs (accelerators)
 - More than 100 CPU cores, tens of GPU cards, tens of thousands of GPU cores



Talk Overview

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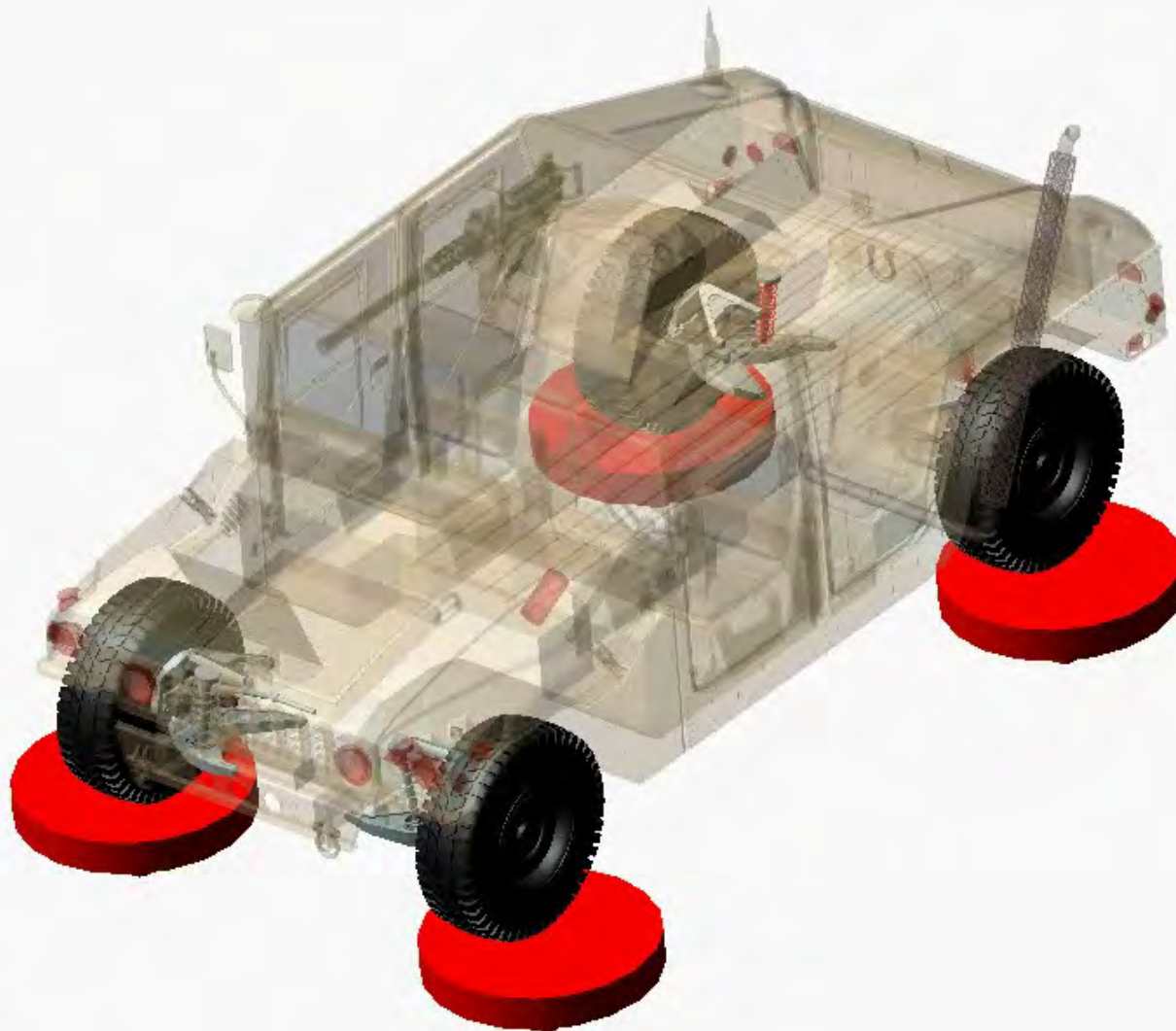
MODELING AND SIMULATION, TESTING AND VALIDATION

- Overview of the engineering problems of interest
- Large-scale Multibody Dynamics
 - Problem formulation, solution method, and parallel implementation
- Overview of Heterogeneous Computing Template (HCT)
- Numerical Experiments
- Conclusions

Computational Multibody Dynamics

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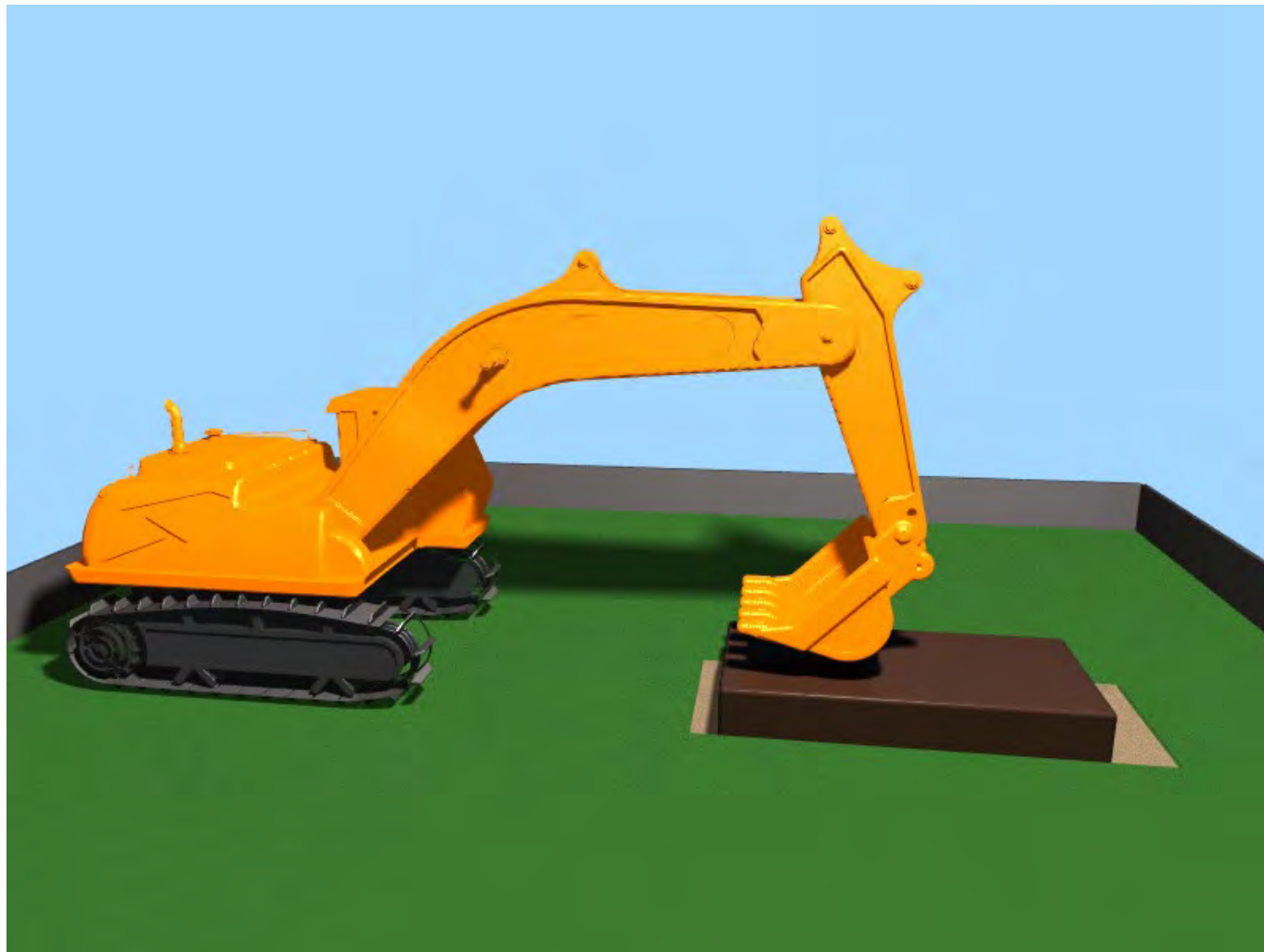


Multi-Physics...

Fluid-Solid Interaction: Navier-Stokes + Newton-Euler.

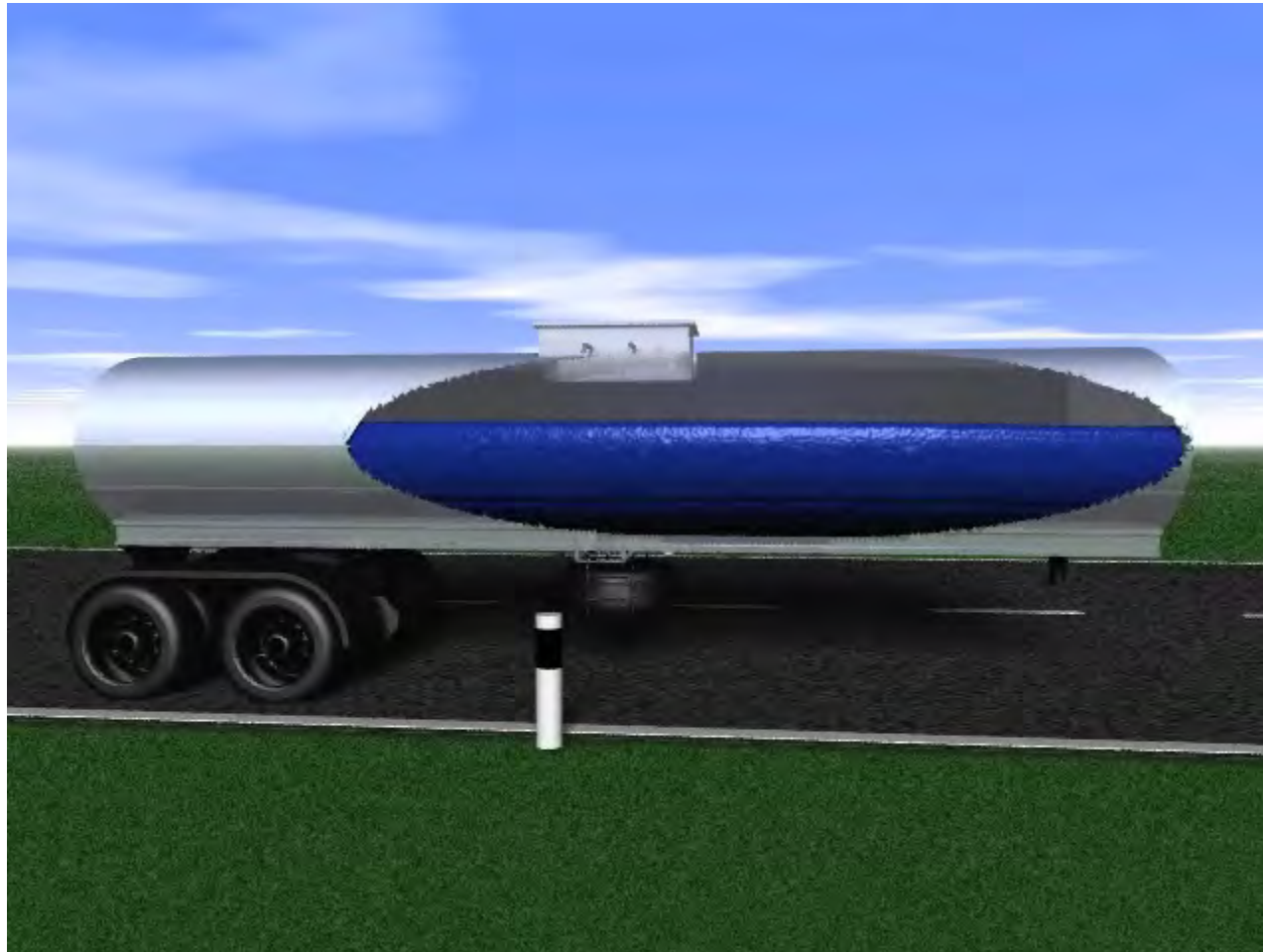
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Computational Dynamics

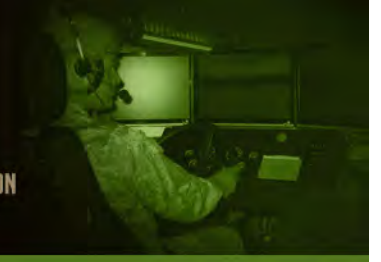
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Rover Mobility on Granular Terrain

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- Wheeled/tracked vehicle mobility on granular terrain
- Also interested in scooping and loading granular material

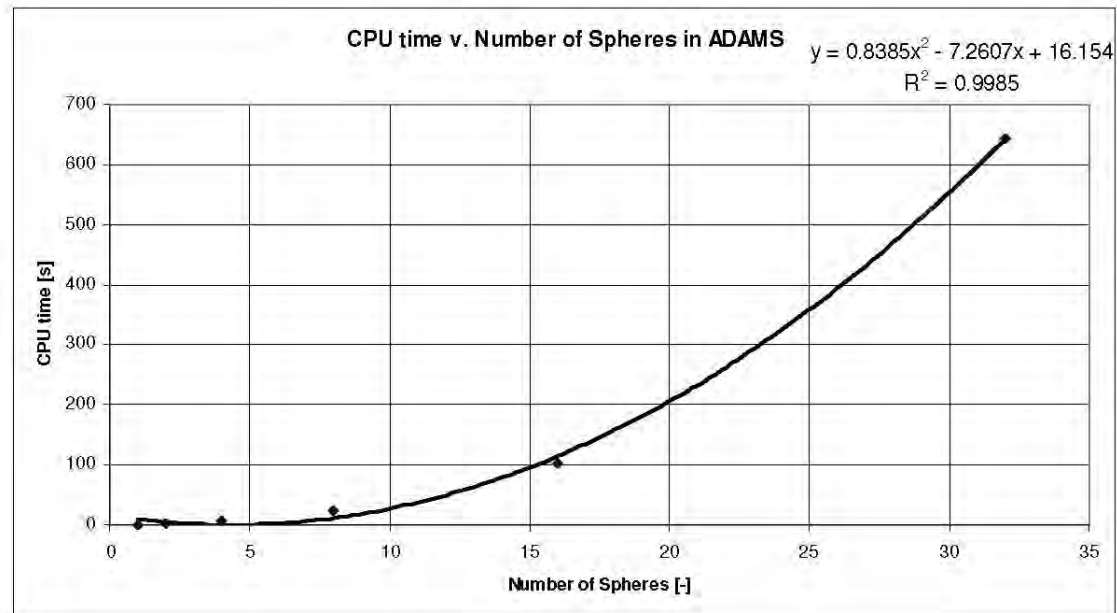


Frictional Contact Simulation [Commercial Solution]

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- Model Parameters:
 - Spheres: 60 mm diameter and mass 0.882 kg
 - Forces: smoothing with stiffness of 1E5, force exponent of 2.2, damping coefficient of 10.0, and a penetration depth of 0.1
 - Simulation length: 3 seconds





Frictional Contact: Two Different Approaches

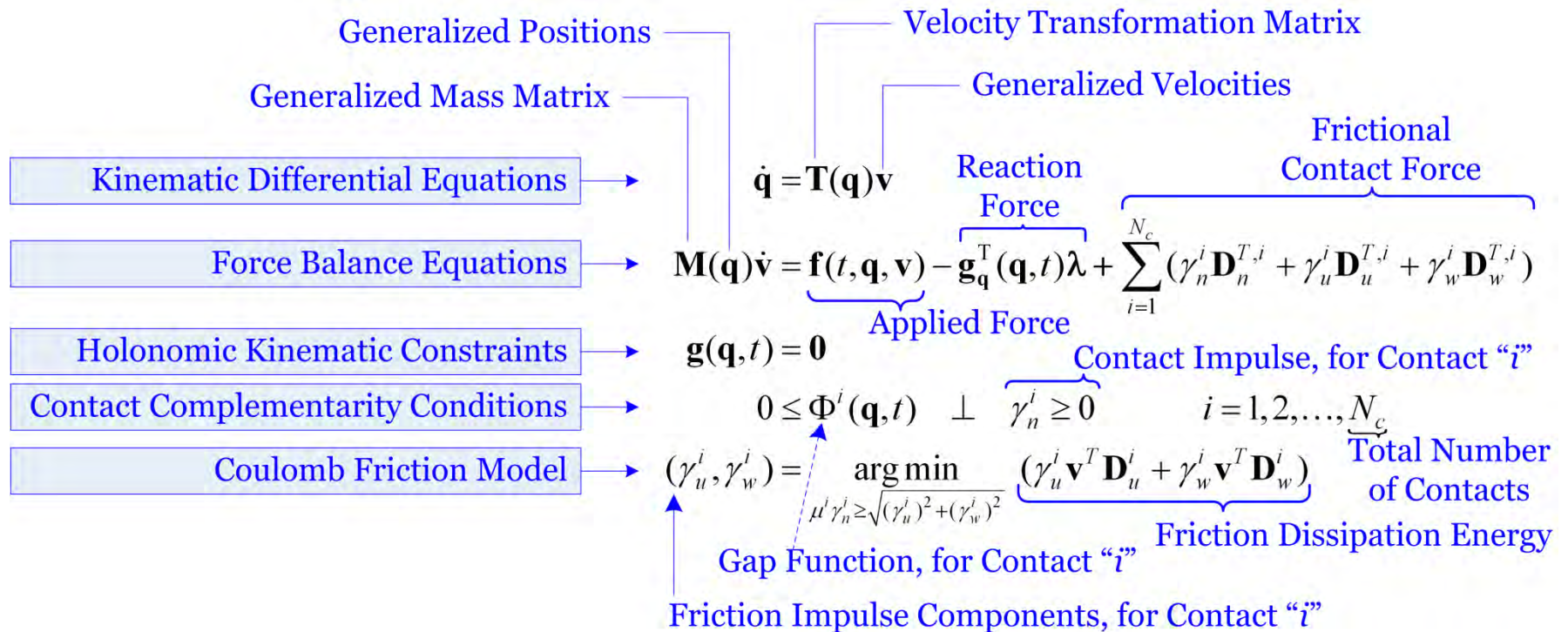
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- Discrete Element Method (DEM) - draws on a “smoothing” (penalty) approach
 - Lots of heuristics
 - Slow
 - General purpose
 - Used in ADAMS
- DVI-based (Differential Variational Inequalities)
 - A set of differential equations combined with inequality constraints
 - Fast (stable for significantly larger integration step-sizes)
 - Less general purpose
 - Used widely in computer games



The Modeling Component

Equations of Motion Multibody Dynamics



Traditional Discretization Scheme

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positions $\mathbf{q}^{(l+1)} = \mathbf{q}^{(l)} + h\mathbf{L}(\mathbf{q}^{(l)})\mathbf{v}^{(l+1)}$

time step index

Mass Mat. $\mathbf{M}(\mathbf{v}^{(l+1)} - \mathbf{v}^l) = hf(t^{(l)}, \mathbf{q}^{(l)}, \mathbf{v}^{(l)}) + \sum_{i \in \mathcal{A}(q^{(l)}, \delta)} (\gamma_{i,n} \mathbf{D}_{i,n} + \gamma_{i,u} \mathbf{D}_{i,u} + \gamma_{i,w} \mathbf{D}_{i,w})$

speeds

Applied Forces

Reaction impulses

$i \in \mathcal{A}(q^{(l)}, \delta) : 0 \leq \frac{1}{h} \Phi_i(\mathbf{q}^{(l)}) + \mathbf{D}_{i,n}^T \mathbf{v}^{(l+1)} \perp \gamma_n^i \geq 0,$

Complementarity Condition

Stabilization term $(\gamma_{i,u}, \gamma_{i,w}) = \underset{\mu_i \gamma_{i,n} \geq \sqrt{\gamma_{i,u}^2 + \gamma_{i,w}^2}}{\text{argmin}} \mathbf{v}^T (\gamma_{i,u} \mathbf{D}_{i,u} + \gamma_{i,w} \mathbf{D}_{i,w}).$

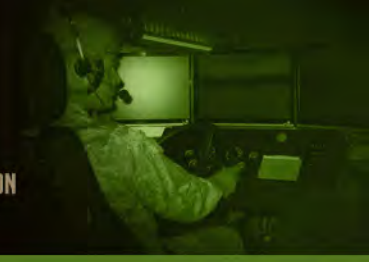
Coulomb 3D friction model

(Stewart & Trinkle, 1996)

Relaxed Discretization Scheme

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$$\mathbf{q}^{(l+1)} = \mathbf{q}^{(l)} + h\mathbf{L}(\mathbf{q}^{(l)})\mathbf{v}^{(l+1)}$$

$$\mathbf{M}(\mathbf{v}^{(l+1)} - \mathbf{v}^l) = h\mathbf{f}(t^{(l)}, \mathbf{q}^{(l)}, \mathbf{v}^{(l)}) + \sum_{i \in \mathcal{A}(q^{(l)}, \delta)} (\gamma_{i,n} \mathbf{D}_{i,n} + \gamma_{i,u} \mathbf{D}_{i,u} + \gamma_{i,w} \mathbf{D}_{i,w})$$

$$i \in \mathcal{A}(q^{(l)}, \delta) : 0 \leq \frac{1}{h} \Phi_i(\mathbf{q}^{(l)}) + \mathbf{D}_{i,n}^T \mathbf{v}^{(l+1)} - \mu^i \sqrt{(\mathbf{v}^T \mathbf{D}_{i,u})^2 + \mathbf{v}^T \mathbf{D}_{i,w})^2} \perp \gamma_n^i \geq 0,$$

Relaxation Term

$$(\gamma_{i,u}, \gamma_{i,w}) = \underset{\mu^i \gamma_{i,n} \geq \sqrt{\gamma_{i,u}^2 + \gamma_{i,w}^2}}{\operatorname{argmin}} \mathbf{v}^T (\gamma_{i,u} \mathbf{D}_{i,u} + \gamma_{i,w} \mathbf{D}_{i,w}).$$

(Anitescu & Tasora, 2008)

The Cone Complementarity Problem [CCP]

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- Overall approach assume the form of a Cone Complementarity Problem (CCP)

- Introduce the convex hypercone...

$$\Upsilon = \left(\bigoplus_{i \in \mathcal{A}(\mathbf{q}^l, \epsilon)} \mathcal{FC}^i \right)$$

- ... and its polar hypercone:

$$\Upsilon^\circ = \left(\bigoplus_{i \in \mathcal{A}(\mathbf{q}^l, \epsilon)} \mathcal{FC}^{i^\circ} \right)$$

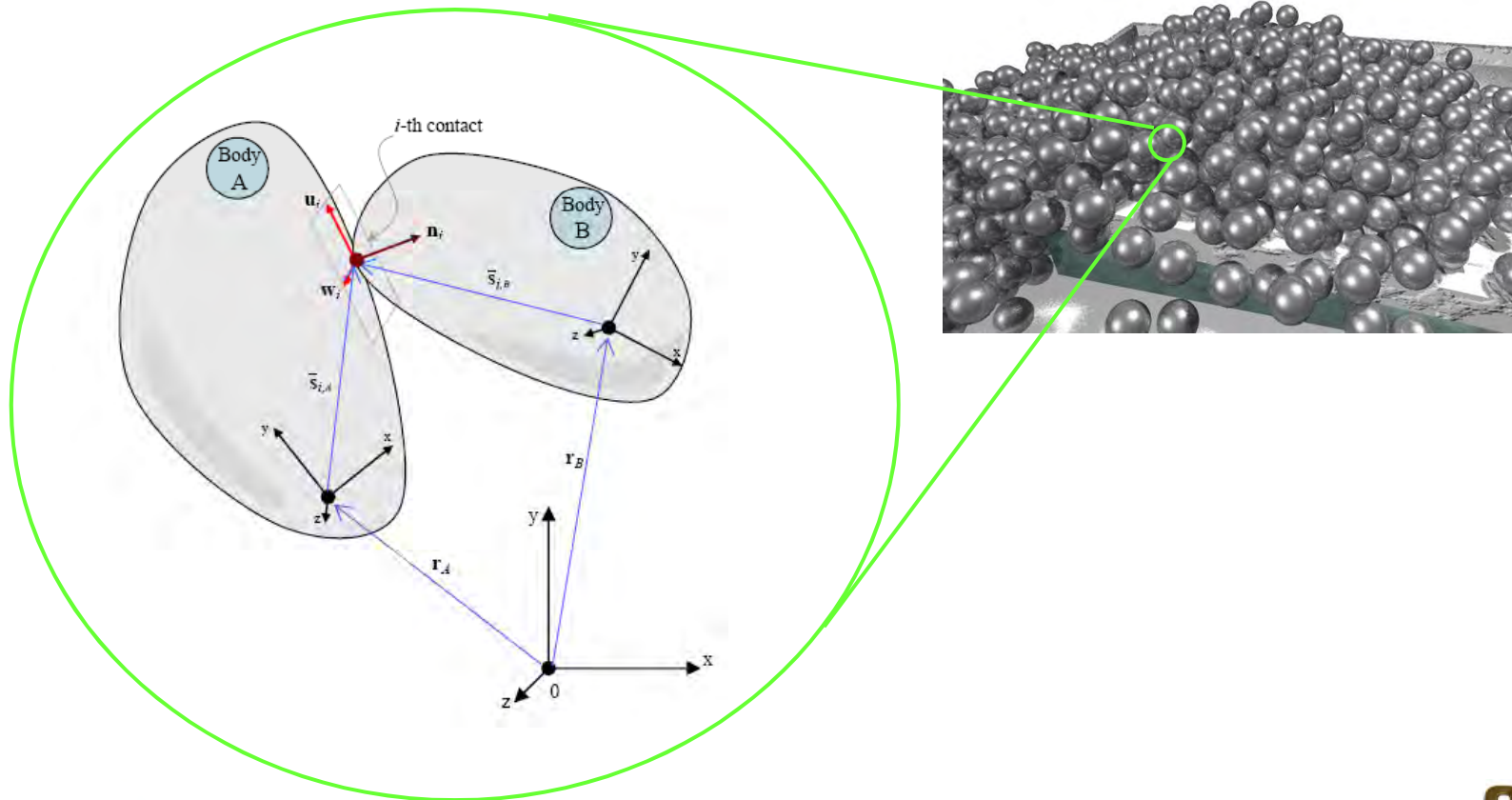
$\mathcal{FC}^i \in \mathbb{R}^3$ represents friction cone associated with i^{th} contact

CCP assumes following form: Find γ such that

$$\gamma \in \Upsilon \perp -(\mathbf{N}\gamma + \mathbf{d}) \in \Upsilon^\circ$$



- Numerical solution can leverage parallel computing

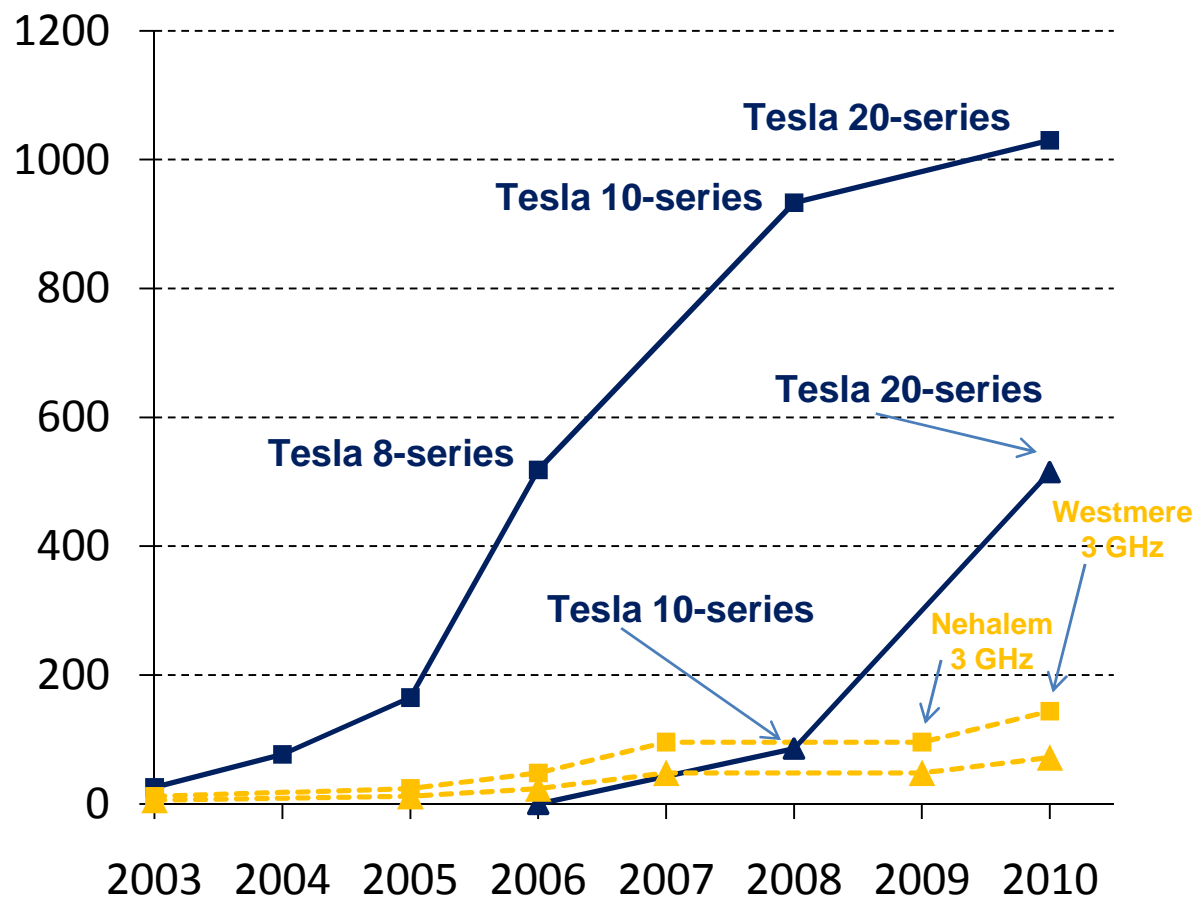


CPU vs. GPU – Flop Rate [GFlop/Sec]

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CPU – in orange
GPU – in blue

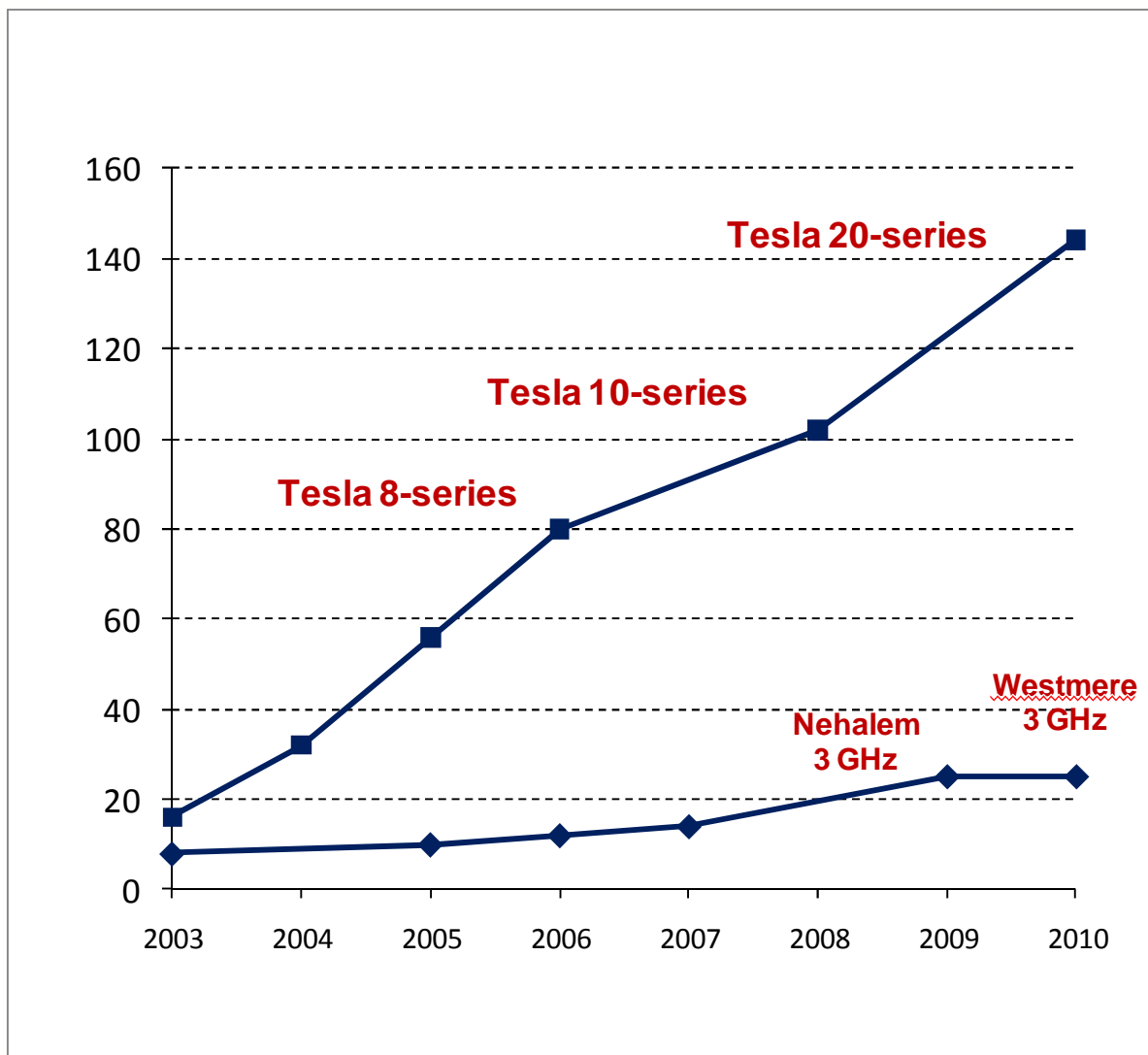
□ Single Precision
△ Double Precision



CPU vs. GPU— Memory Bandwidth [GB/sec]

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Mixing 40,000 Spheres on the GPU

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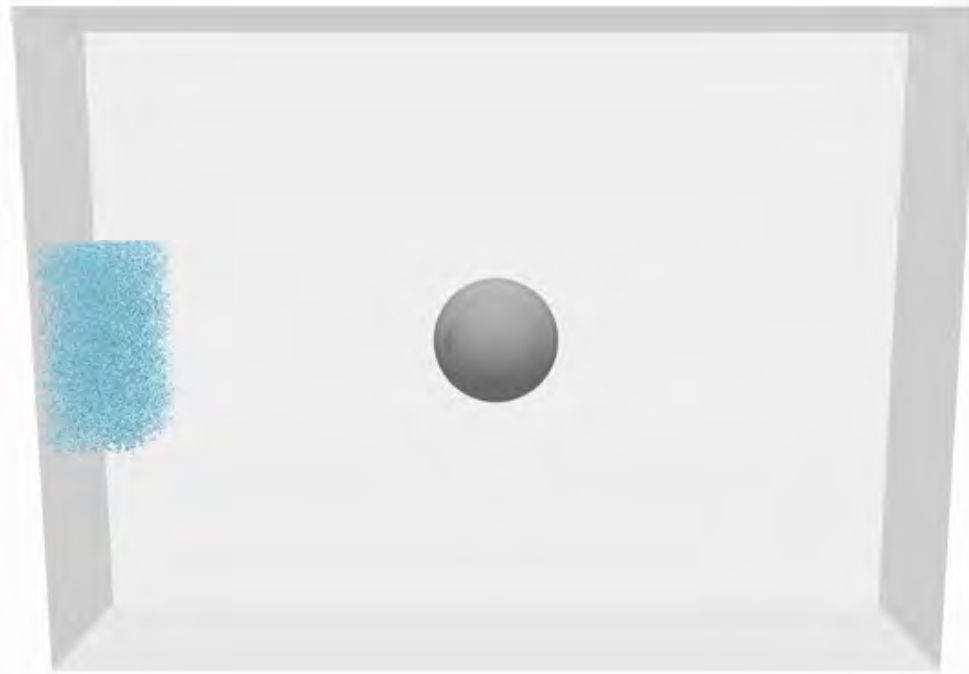
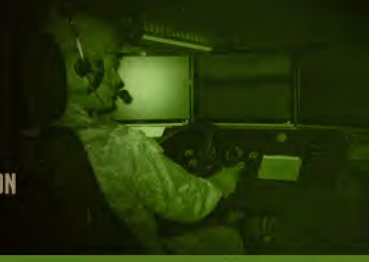
300K Spheres in Tank [parallel on the GPU]

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1.1 Million Rigid Spheres [parallel on the GPU]

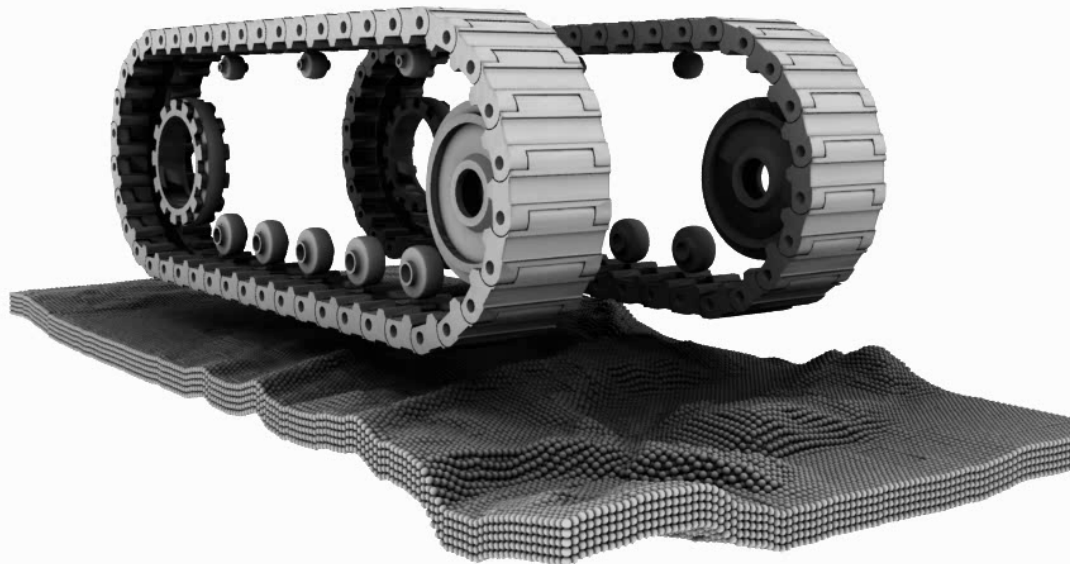
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Computational dynamics

Tracked vehicle mobility

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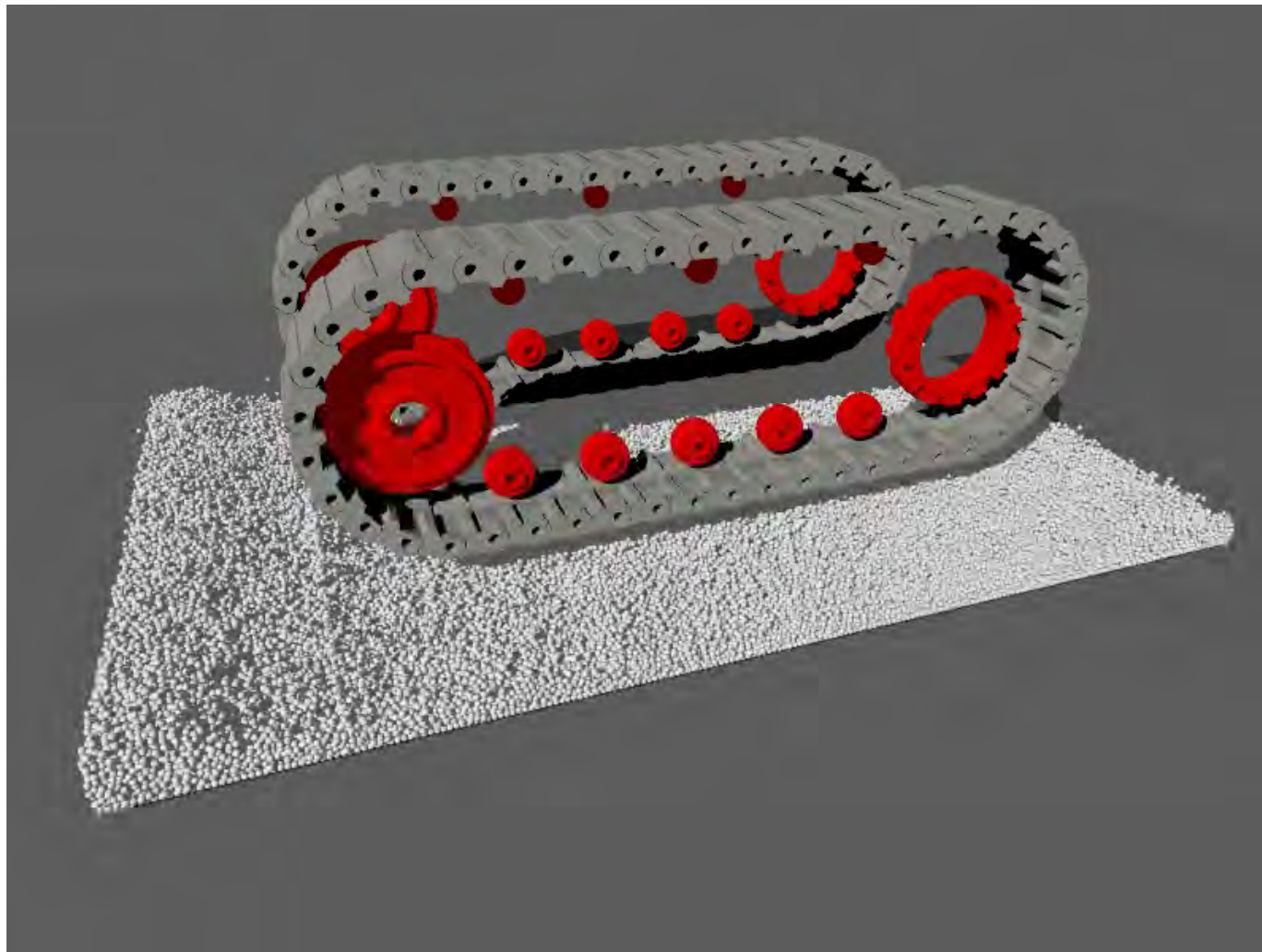
Simulation Setup:

- Driving speed: 1.0 rad/sec
- Length: 12 seconds
- Time step: 0.005 sec
- Computation time: 18.5 hours
- Particle radius: .027273 m
- Terrain: 284,715 particles

Track Simulation

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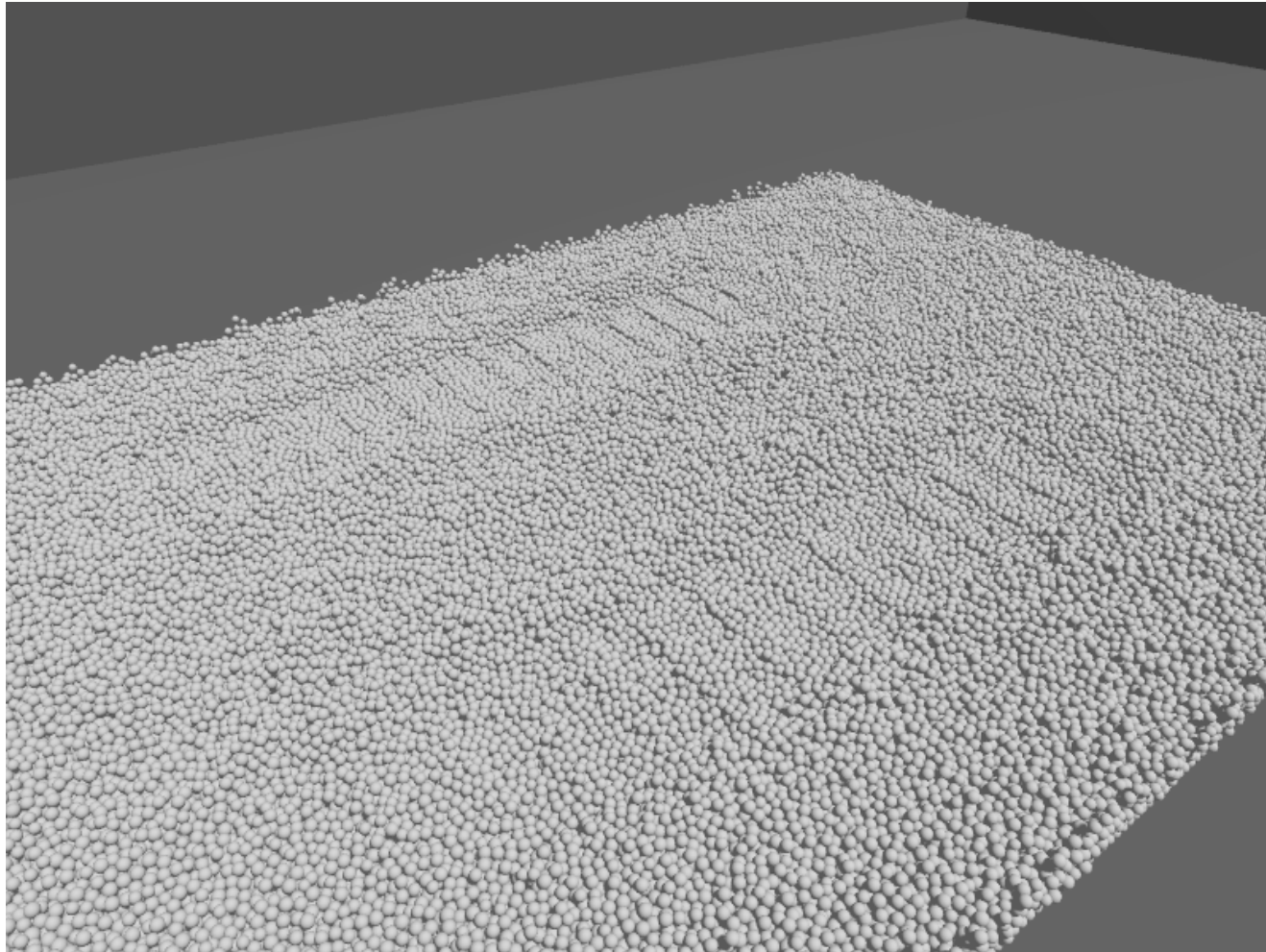
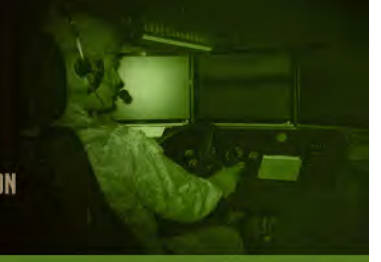
Parameters:

- Driving speed: 1.0 rad/sec
- Length: 10 seconds
- Time step: 0.005 sec
- Computation time: 17.8 hours
- Particle radius: $.025 \pm .0025$ m
- Terrain: 467,100 particles

Track Footprint

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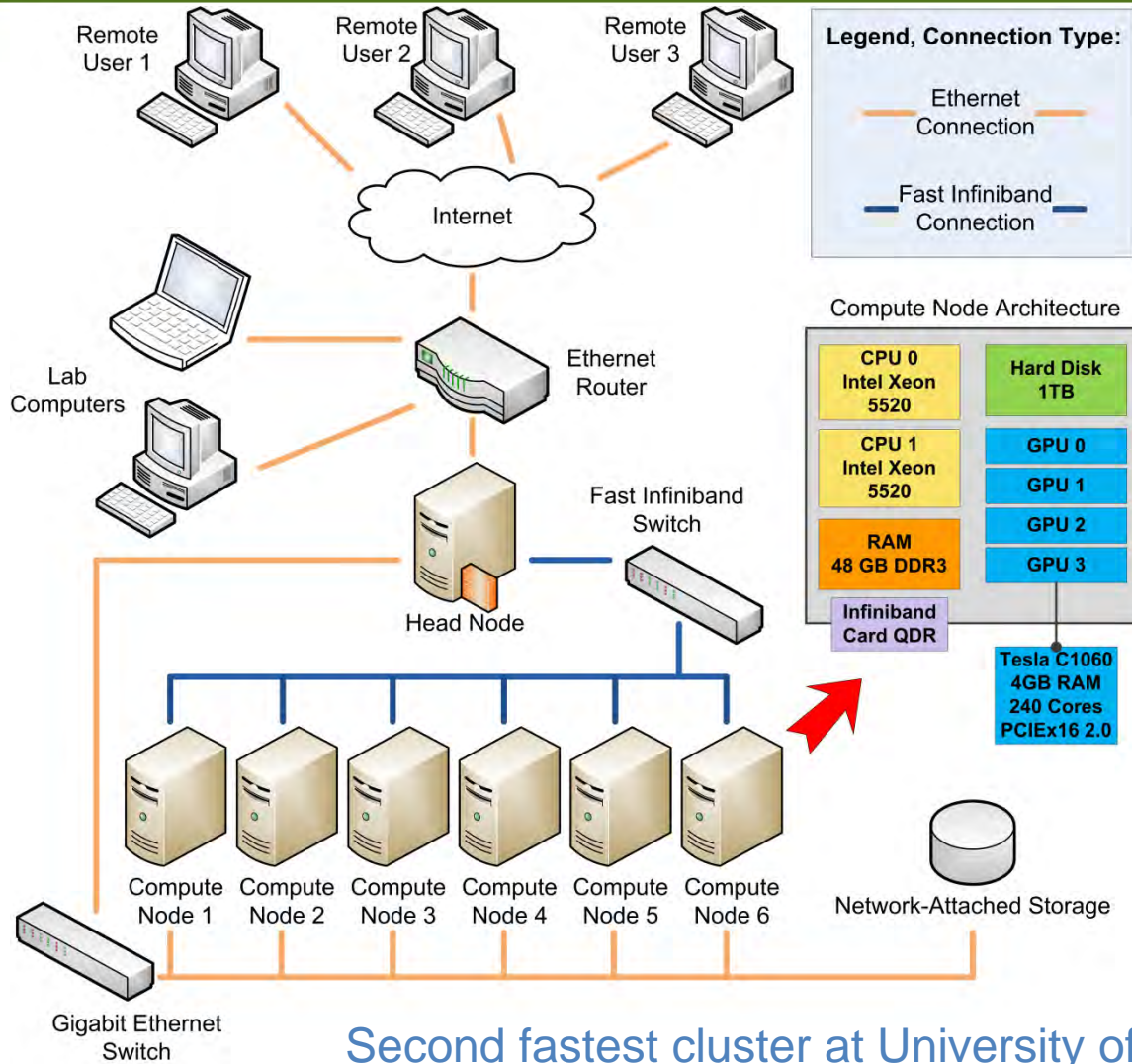


A Heterogeneous Computing Template for Computational Dynamics

Heterogeneous Cluster

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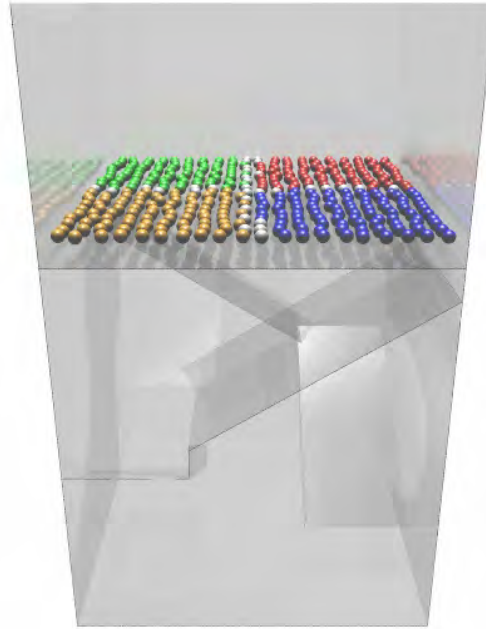


Second fastest cluster at University of Wisconsin-Madison

Computation Using Multiple CPUs [DEM solution]

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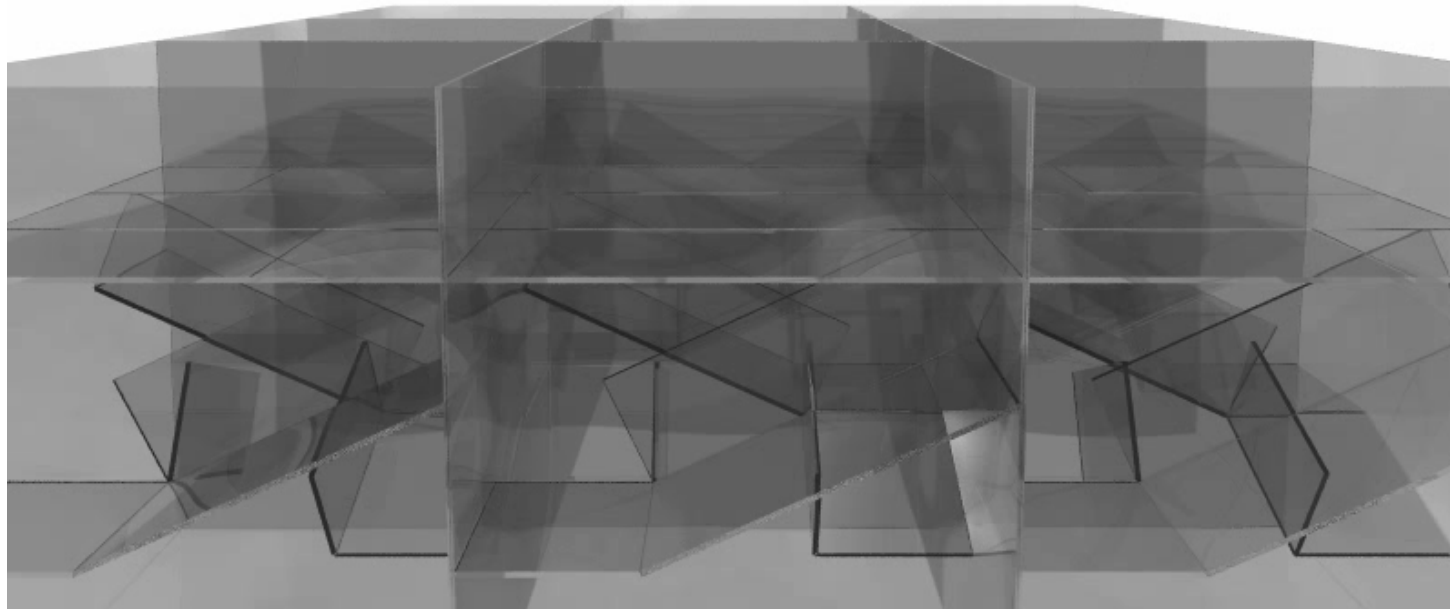
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Computation Using Multiple CPUs
[DEM solution]

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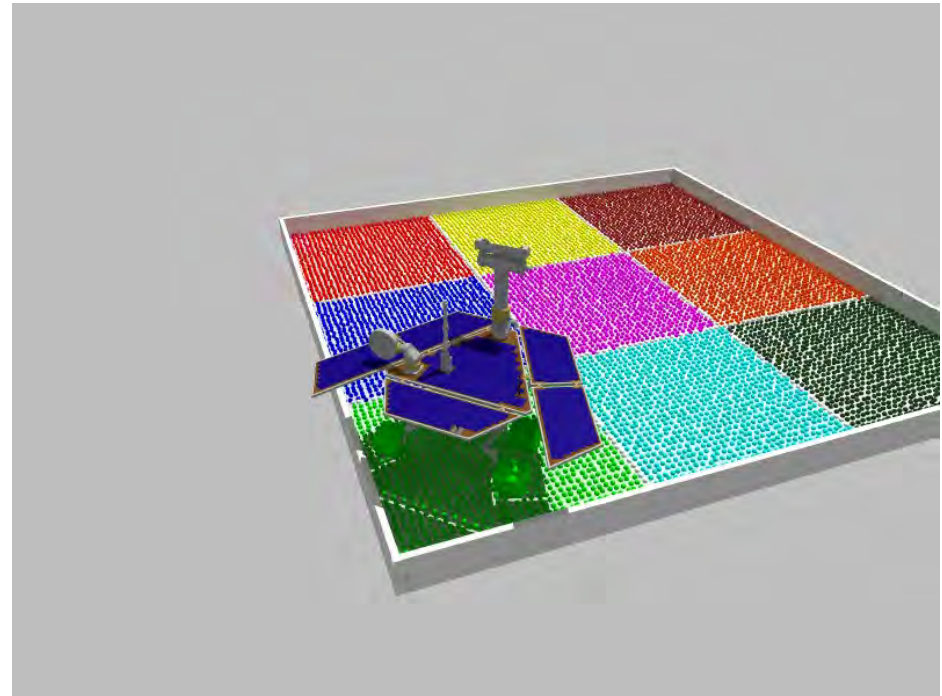
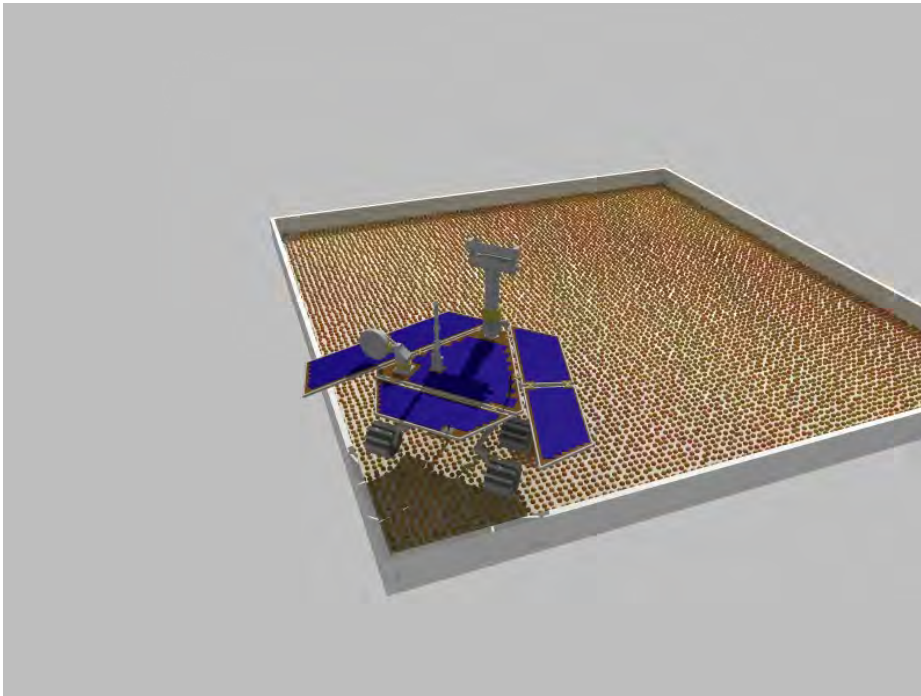
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Computation Using Multiple CPUs [DEM solution]

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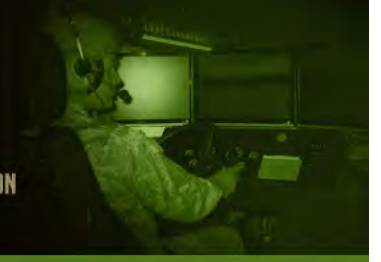
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Computation Using Multiple CPUs [DEM solution]

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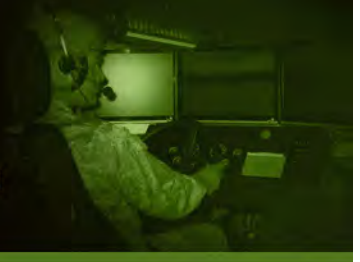


Simulation of MRAP impacted by debris



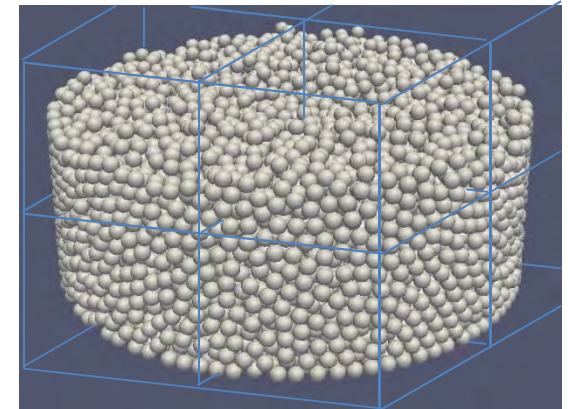
Heterogeneous Computing Template Five Major Components

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- Computational Dynamics requires

- Domain decomposition
- – Proximity computation
- Inter-domain data exchange
- – Numerical algorithm support
- Post-processing (visualization)



- HCT represents the library support and associated API that capture this five component abstraction



Searching for Better Methods

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- Frictionless case (bound constraints in place)
 - Gauss-Jacobi (CE)
 - Projected conjugate gradient (ProjCG)
 - Gradient projected conjugate gradient (GPCG)
 - **Gradient projected MINRES (GPMINRES)**
- Friction case (cone constraints - ongoing)
 - Newton's Method for large bound-constrained problems
 - Uses re-parameterization to handle friction cones (replace with bound constraints)

Numerical Experiments

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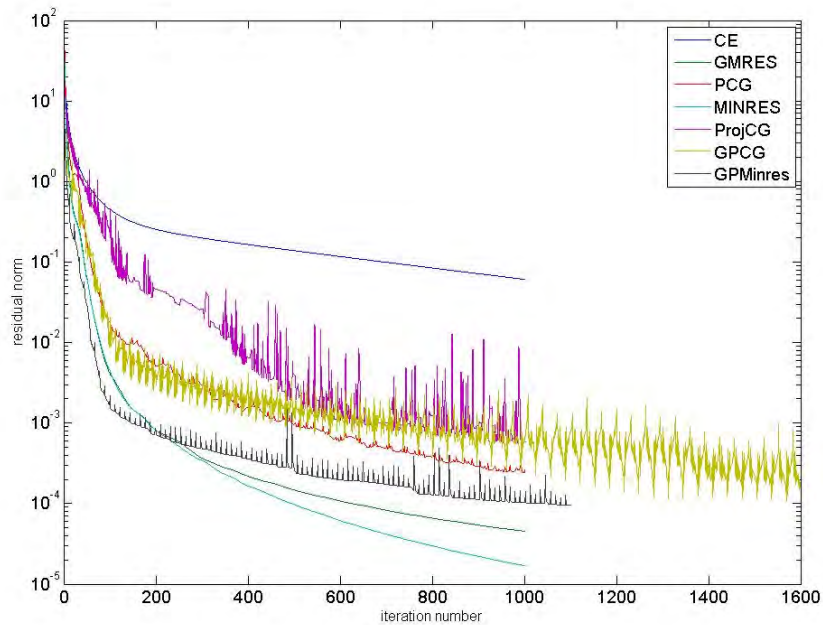


- Test Problem: 40,000 bodies \rightarrow 157,520 contacts
- Frictionless

Test Problem (MATLAB)

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Method	Iterations	Final Residual Norm	γ_{\min}	γ_{\max}	Time [sec]
CE	1000	6.11×10^{-2}	0.0	2.0598	1849.5
ProjCG	1002	5.6344×10^{-4}	0.0	2.2286	1235.6
GPCG	1600	1.0675×10^{-4}	0.0	2.6349	382.3644
GPCGMinres	1100	9.5239×10^{-5}	0.0	2.3090	238.0744
PCG	1000	2.4053×10^{-4}	-1.1116	2.5254	27.9686
GMRES	1000	4.5315×10^{-5}	-1.1635	2.5227	736.3007
MINRES	1000	1.6979×10^{-5}	-1.1316	2.5253	41.5790



Proximity Computation



GPU Collision Detection (CD)

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- 30,000 feet perspective:
 - Carry out spatial partitioning of the volume occupied by the bodies
 - Place bodies in bins (cubes, for instance)
 - Follow up by brute force search for all bodies touching each bin
 - Embarrassingly parallel

Example: Ellipsoid-Ellipsoid CD

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$$\mathbf{d} = \mathbf{P}_1 - \mathbf{P}_2 = \left(\frac{1}{2} \mathbf{M}_1 + \frac{1}{2} \mathbf{M}_2\right) \mathbf{c} + (\mathbf{b}_1 - \mathbf{b}_2)$$

$$\frac{\partial \mathbf{d}}{\partial_i} = \frac{\partial \mathbf{P}_1}{\partial_i} - \frac{\partial \mathbf{P}_2}{\partial_i}, \quad \frac{\partial^2 \mathbf{d}}{\partial_i \partial_j} = \frac{\partial^2 \mathbf{P}_1}{\partial_i \partial_j} - \frac{\partial^2 \mathbf{P}_2}{\partial_i \partial_j}$$

$$\frac{\partial \mathbf{P}}{\partial_i} = \left(\frac{1}{2} \mathbf{M} - \frac{1}{8} \mathbf{M} \mathbf{c} \mathbf{c}^T \mathbf{M}\right) \frac{\partial \mathbf{c}}{\partial_i}$$

$$\begin{aligned} \frac{\partial^2 \mathbf{P}}{\partial_i \partial_j} = & \left(-\frac{1}{8} \mathbf{M} + \frac{3}{32} \mathbf{M} \mathbf{c} \mathbf{c}^T \mathbf{M}\right) \mathbf{c}^T \mathbf{M} \frac{\partial \mathbf{c}}{\partial_j} \frac{\partial \mathbf{c}}{\partial_i} \\ & - \frac{1}{8} \left[\left(\mathbf{c}^T \mathbf{M} \frac{\partial \mathbf{c}}{\partial_i}\right) \mathbf{M} + \mathbf{M} \mathbf{c} \left(\frac{\partial \mathbf{c}}{\partial_i}\right)^T \mathbf{M} \right] \frac{\partial \mathbf{c}}{\partial_j} \\ & + \left(\frac{1}{2} \mathbf{M} - \frac{1}{8} \mathbf{M} \mathbf{c} \mathbf{c}^T \mathbf{M}\right) \frac{\partial^2 \mathbf{c}}{\partial_i \partial_j} \end{aligned}$$

$$\varepsilon: \frac{x^2}{r_1^2} + \frac{y^2}{r_2^2} + \frac{z^2}{r_3^2} = 1$$

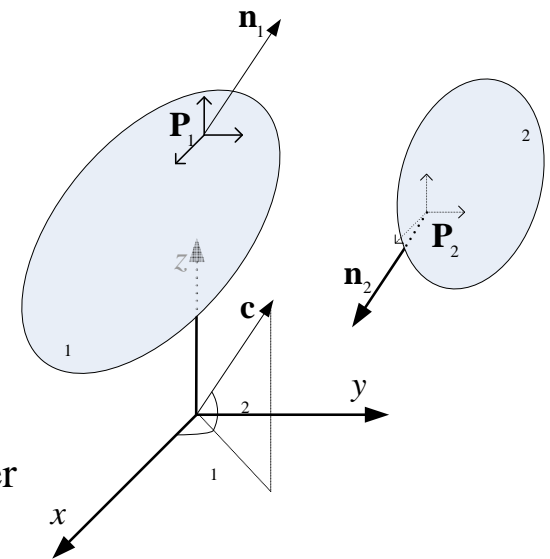
A : Rotation Matrix

$$\mathbf{M} = \mathbf{A} \mathbf{R}^2 \mathbf{A}^T$$

$$\mathbf{R} = \text{diag}(r_1, r_2, r_3)$$

b : Translation of ellipsoids center

$$^2 = \frac{1}{4} \mathbf{n}^T \mathbf{M} \mathbf{n}$$



$$\mathbf{d} = \mathbf{P}_1 - \mathbf{P}_2$$

$$\min_{\alpha_1, \alpha_2} \|d(\alpha_1, \alpha_2)\|^2$$

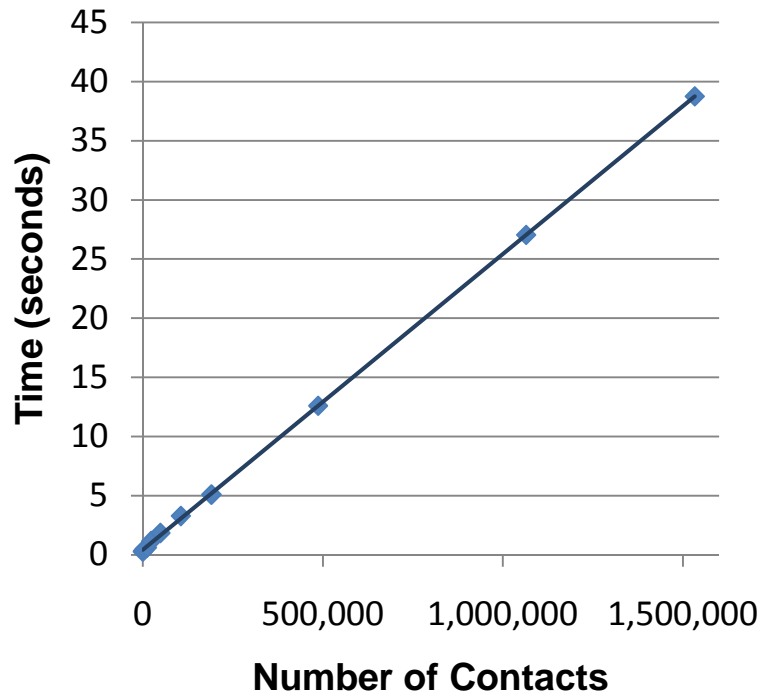
Ellipsoid-Ellipsoid CD: Results

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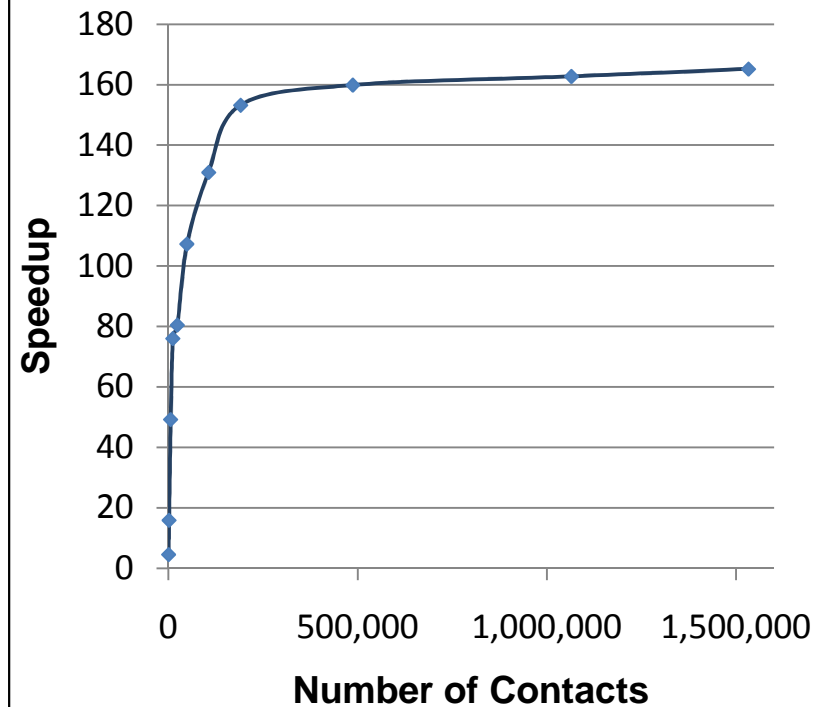
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Time vs. Number of Contacts

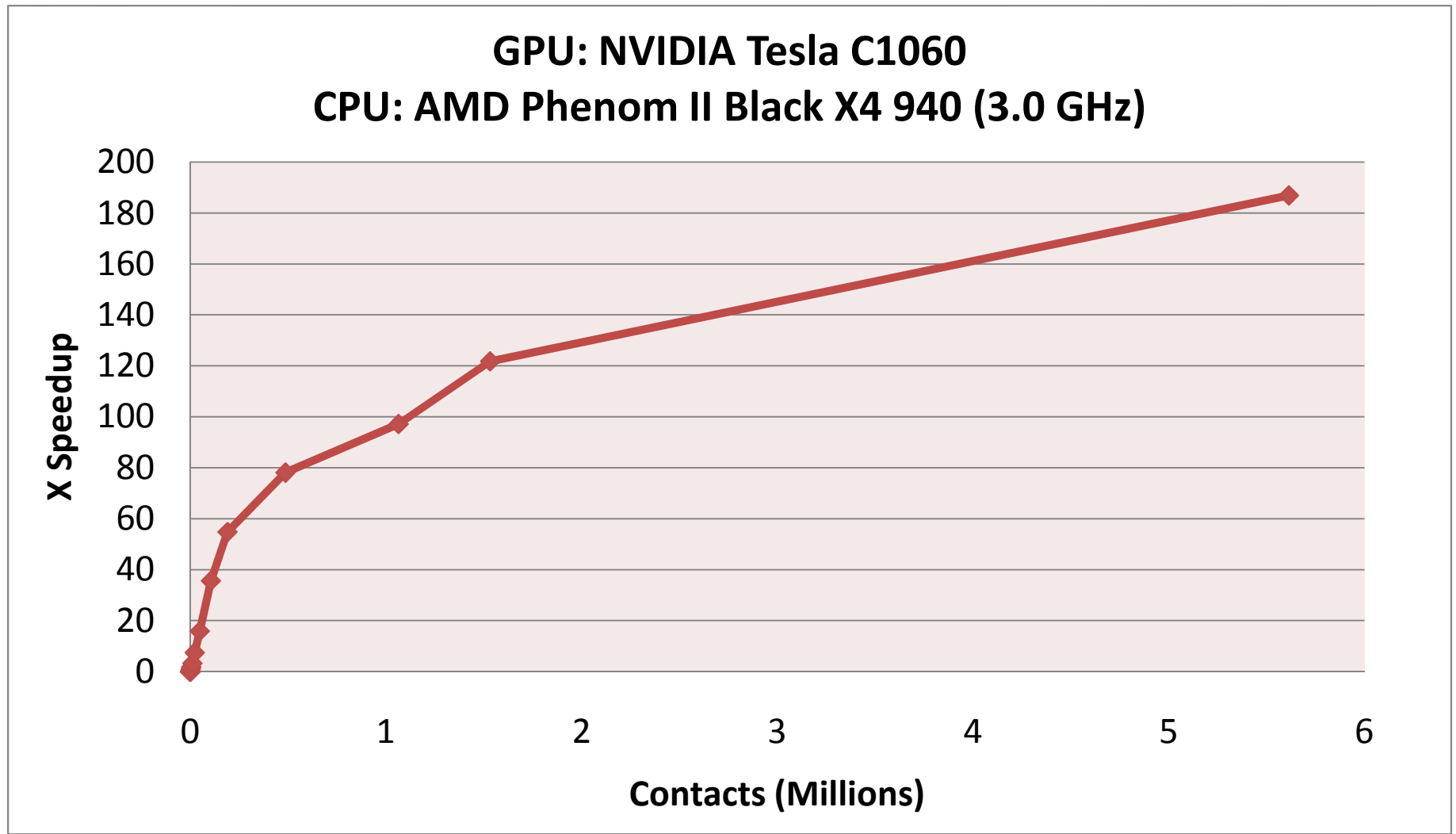
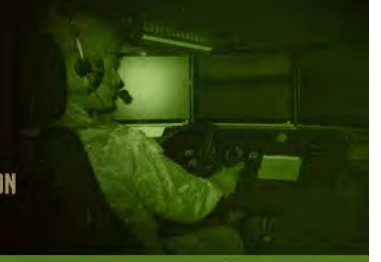


Speedup - GPU vs. CPU



Speedup GPU vs. CPU (sequential Bullet) [results reported are for spheres]

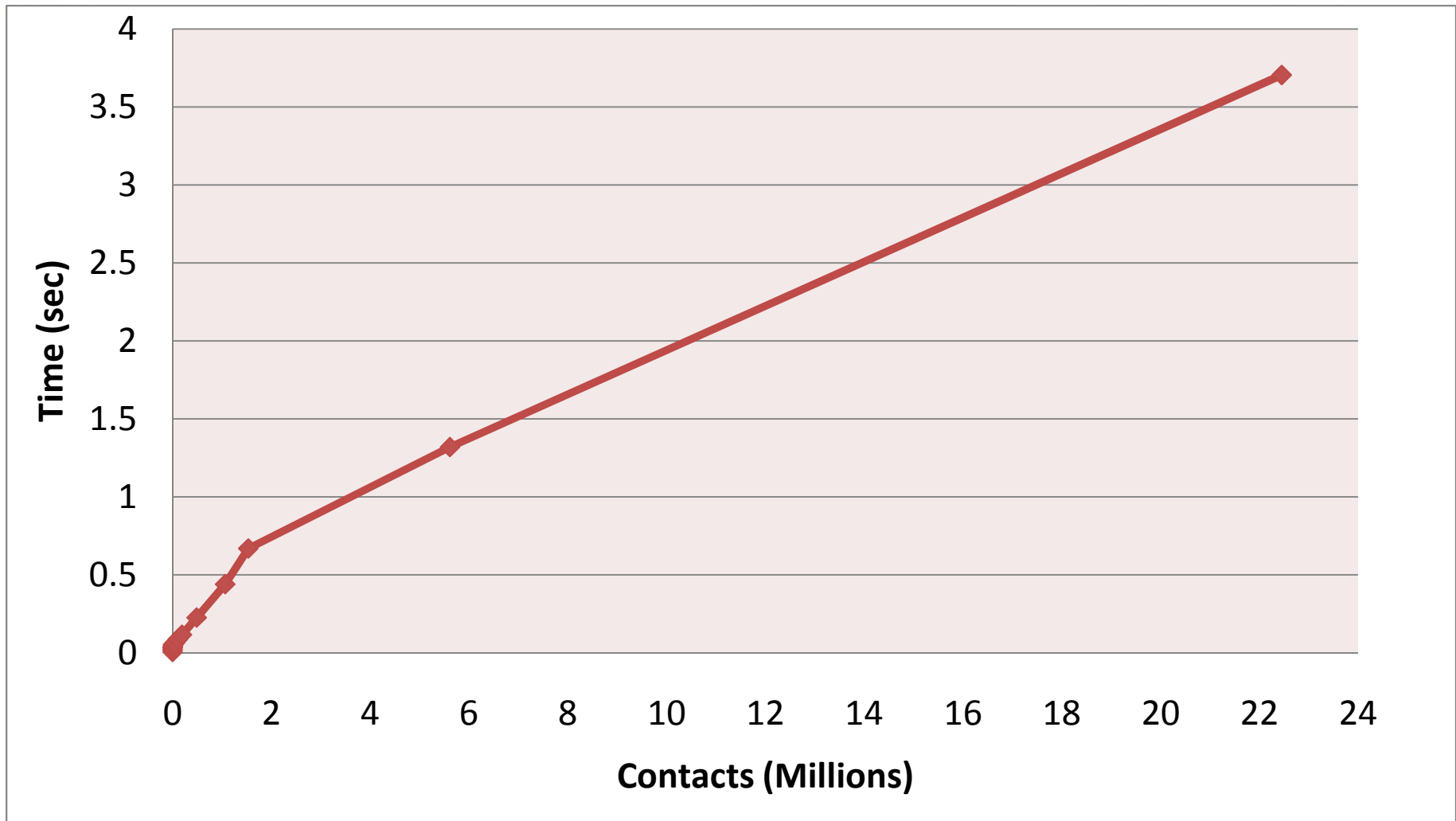
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Parallel Implementation: Number of Contacts vs. Detection Time [results reported are for spheres]

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Multiple-GPU Collision Detection

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Assembled Quad GPU Machine



Processor: AMD Phenom II X4 940 Black

Memory: 16GB DDR2

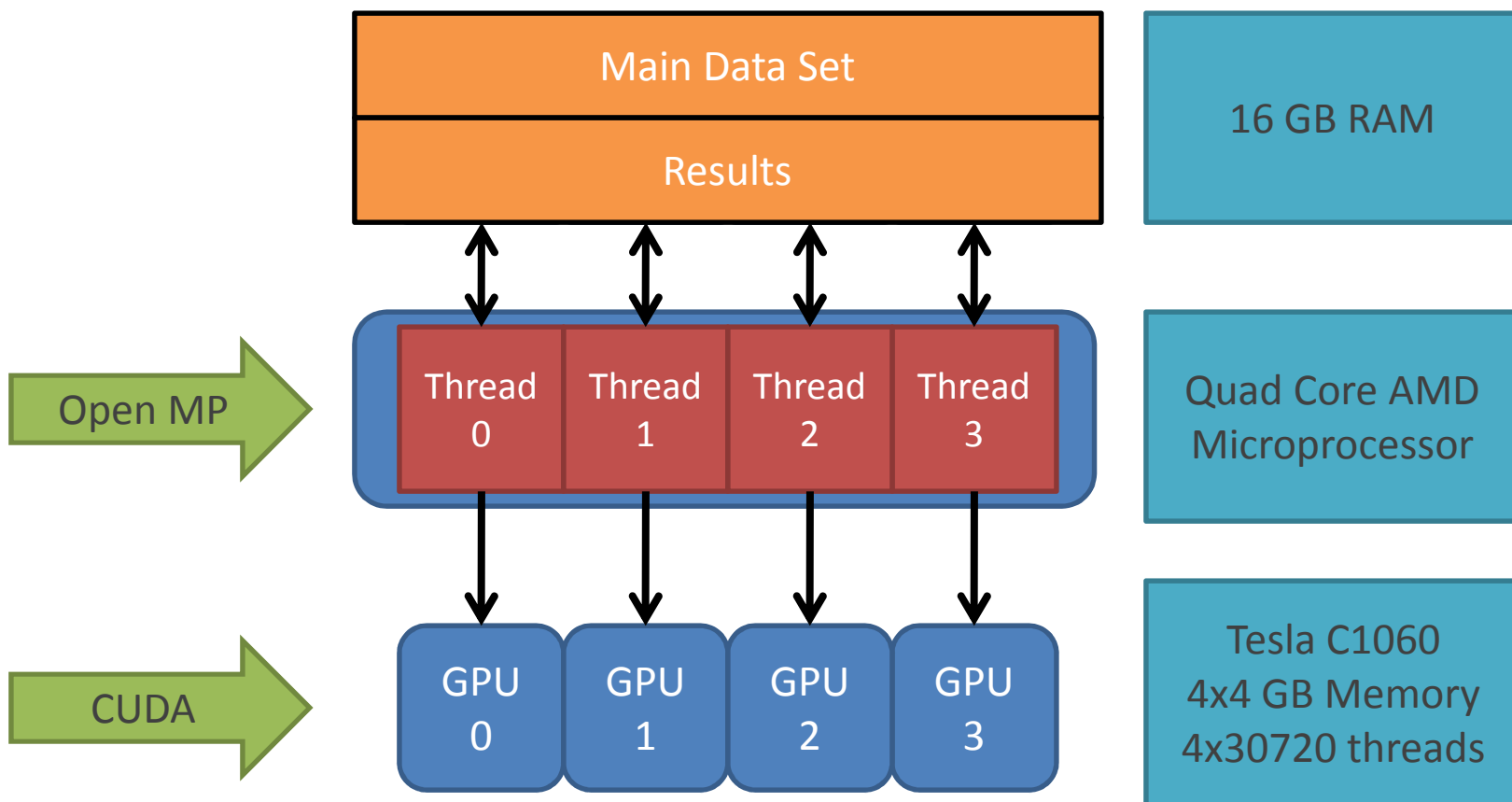
Graphics: 4x NVIDIA Tesla C1060

Power supply 1: 1000W

Power supply 2: 750W

SW/HW Setup

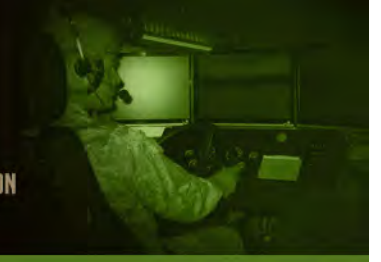
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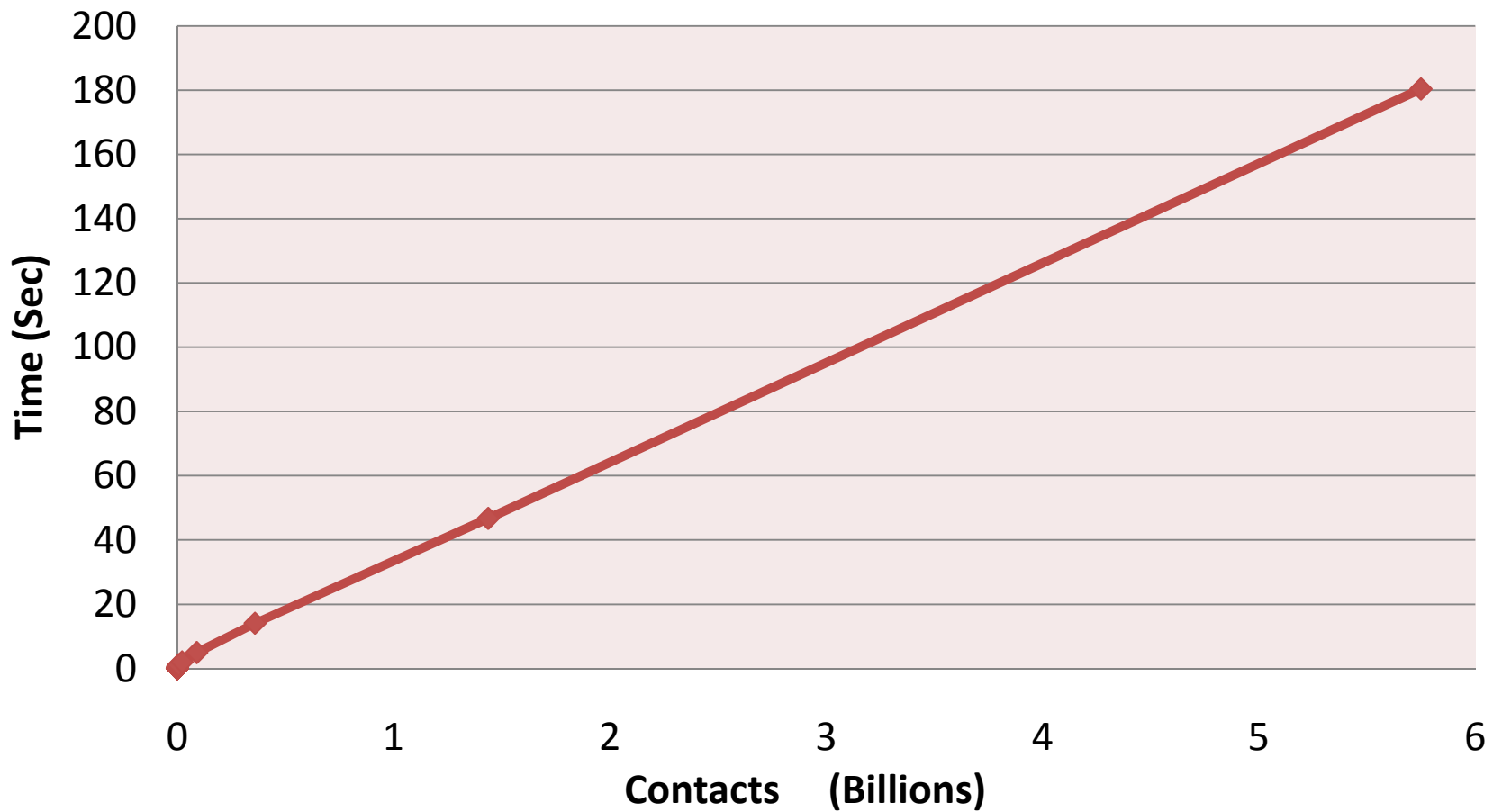
Results – Contacts vs. Time

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Quad Tesla C1060 Configuration



Conclusions

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- HPC will soon enable simulation of billion-body problems
 - Tremendous advances in compute power over the last five years
- Our work: Heterogeneous Computing Template (HCT)
 - HCT draws on symbiosis of CPU + GPU computing
- Accomplishments to date
 - Billion body parallel collision detection
 - Large scale parallel solution of cone complementarity problem
 - Early validation results encouraging



Ongoing/Future Work

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- Validation efforts: at CAT, US Army, and JPL
- Massively parallel linear algebra for solution of CCP problem
 - Preconditioned gradient projected Krylov method
- Parallel collision detection for complex geometries
- Multiphysics:
 - Fluid-solid interaction
 - Cohesion
 - Electrostatics



Thank You.