CUDA for Real-Time Multigrid Finite Element Simulation of Soft Tissue Deformations

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Motivation

- Real-time physics-based simulation of deformable objects
  - Various applications in medical surgery training and planning
- Finite element method (FEM) in combination with a geometric multigrid solver
  - Physics-based material constants
  - Mathematically sound
  - Easy handling of boundaries
  - Linear-time complexity of the solver in the number of unknowns
- Goal: Exploit the GPU's massive computing power and memory bandwidth to significantly increase simulation update rates / increase FE resolution

Take-Away

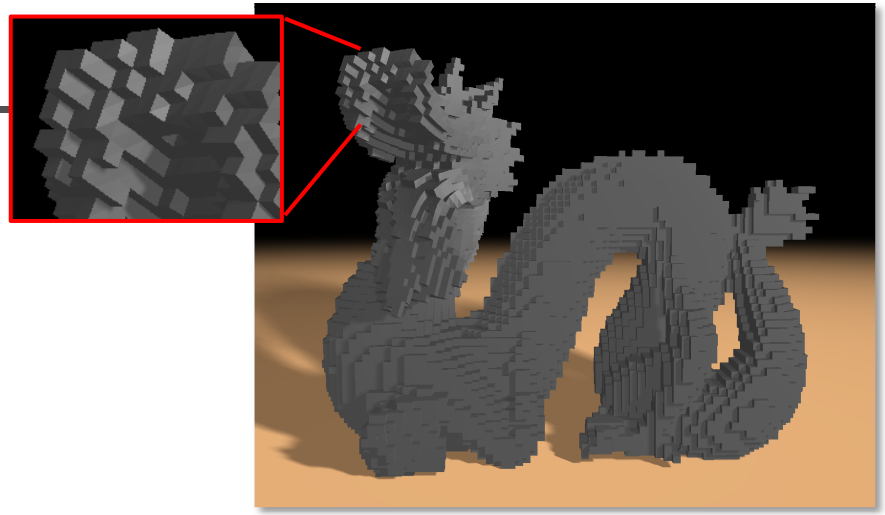
- First fully GPU-based geometric multigrid solver for real-time FEM simulation of deformable objects (linear elasticity, co-rotated strain)
  - Matrix-free FEM and multigrid formulation suited for the GPU
  - Highly efficient CUDA implementation
    - Data structures, memory layout, parallelization
  - Detailed performance analysis
    - Up to 27x faster than 1 CPU core / 4x faster than 8 CPU cores
    - Up to 56 GFLOPS (single) / 34 GFLOPS (double precision) *(sustained performance)*
    - Up to 88 GB/s memory throughput *(sustained performance)*
    - Simulation rates:
      - 120 time steps/sec for 12,000 hexahedral elements
      - 11 time steps/sec for 269,000 hexahedral elements

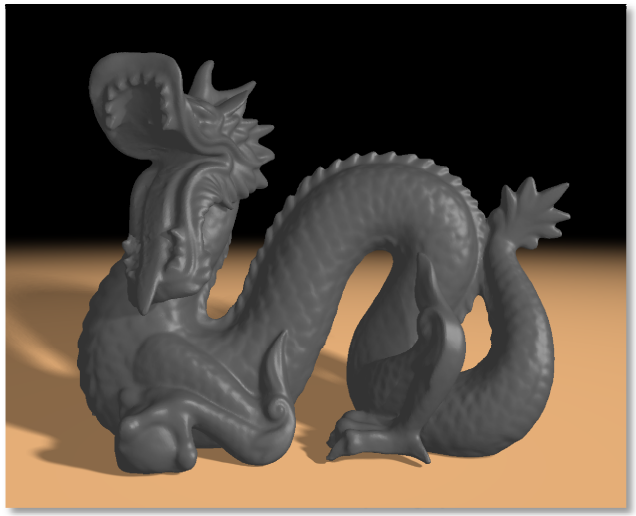
Deformable Objects on the GPU

- Architecture of the NVIDIA Fermi GPU
  - 15 multiprocessors, each with 32 CUDA cores (ALUs) for integer- and floating-point arithmetic operations
  - GPU executes thousands of threads in parallel
- Requirements for an algorithm to run *efficiently* on the GPU
  - Restructure algorithm to expose fine-grained parallelism (one thread per data element)
  - Avoid execution divergence of threads in the same warp
  - Choose memory layouts which enable coalescing of device memory accesses
  - Only threads in the same thread block can communicate and be synchronized efficiently (global synchronization only via separate kernel calls)
  - Very limited resources (registers, shared memory) per thread

Our Approach

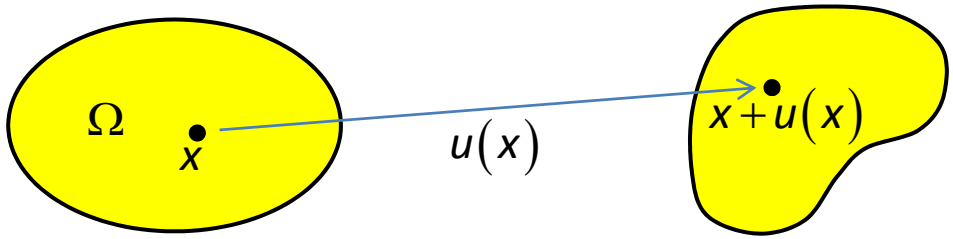
- Hexahedral (tri-linear) finite elements on a uniform Cartesian grid
- Linear elasticity, co-rotated strain
- Geometric multigrid solver
- CUDA API to flexibly access all resources on the graphics card
- Advantages:
  - Numerical stencil of regular shape enables efficient GPU implementation
  - FE model and multigrid hierarchy generation is easy and fast
  - Only one pre-computed element stiffness matrix (greatly reduces memory requirements)





Elasticity & FEM

- Deformation of an object is described by a displacement field $u : \Omega \to \mathbb{R}^3$



Undeformed configuration Deformed configuration

- u is determined by minimizing the functional (potential energy)

$$E(u) = \frac{1}{2}\int_{\Omega} \varepsilon^T \sigma \, dx - \int_{\Omega} f^T u \, dx \to \min$$

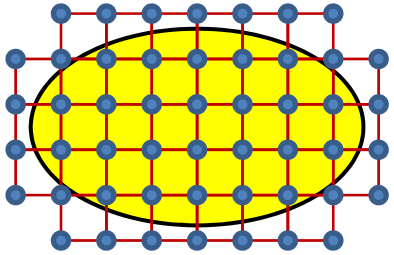
ε : Strain

σ : Stress

f : External forces

Elasticity & FEM

- For the numerical solution, *u* and *f* are discretized by
  - a finite element decomposition of the object's domain (regular hexahedra) and
  - a nodal basis formed by the elements' shape functions (tri-linear interpolation)



$$u(x) = \sum_{\text{Nodes } i} u_i \varphi_i(x)$$

u_i : Displacement at Node *i*

φ_i : Basis function for Node *i*

- For a single element, the functional is minimized by solving a linear system

$$E^e(u^e) = \frac{1}{2}\int_\Omega (u^e)^T B^T D B u^e \, dx - \int_\Omega (f^e)^T u^e \, dx \rightarrow \min$$

$$\Leftrightarrow \underbrace{B^T D B}\, u^e = f^e$$

K^e : Element stiffness matrix

u^e : Linearized u_i

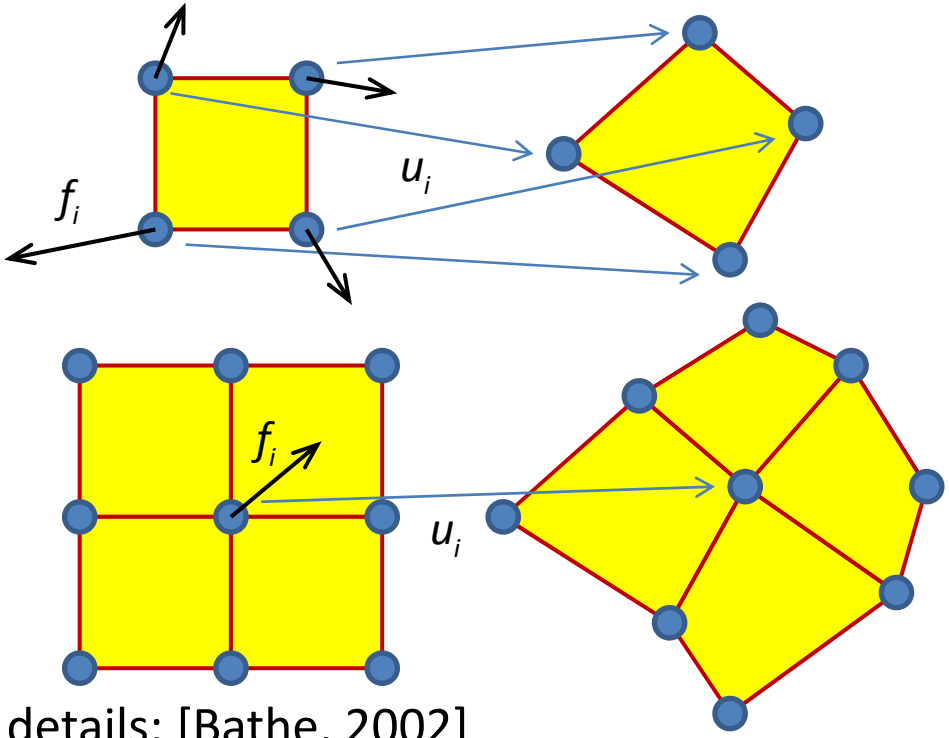
f^e : Linearized f_i

B : Strain matrix

D : Material law

Elasticity & FEM

- The global system of equations is assembled from the individual elements by considering sharing of vertices



Per element

$K^e u^e = f^e$

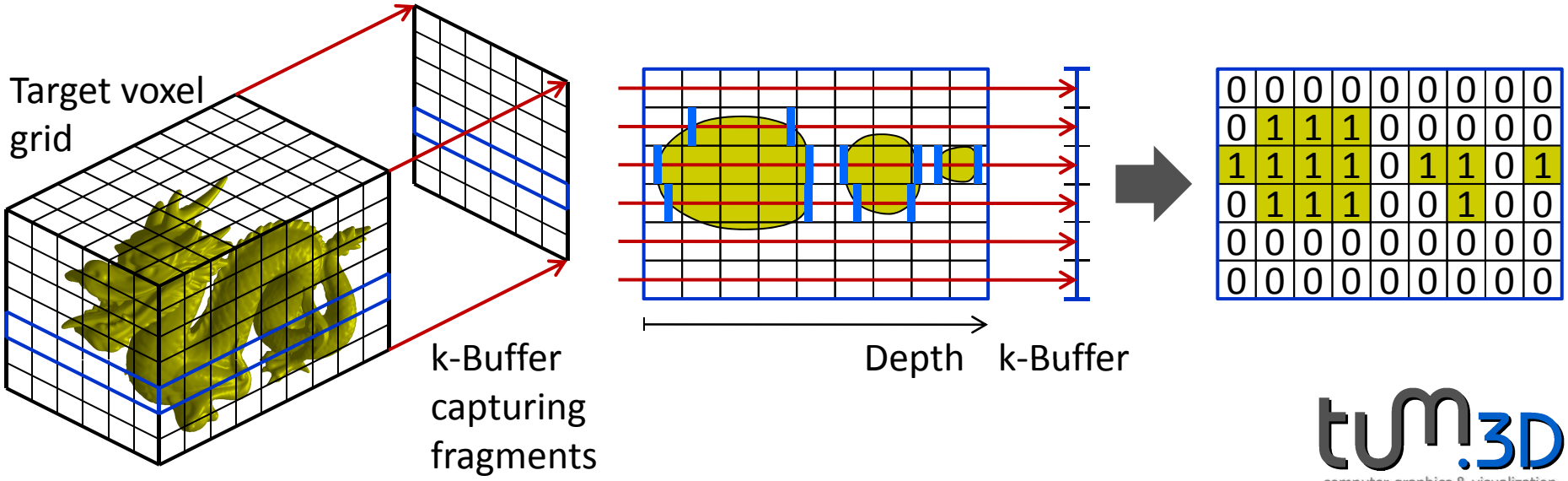
Sharing of u_i and f_i

$Ku = f$

- For more details: [Bathe, 2002]

Finite Element Discretization

- Hexahedral finite element discretization on a uniform Cartesian grid
  - Easily obtained from a surface triangle mesh by voxelization
    - A voxel is classified as “inside” iff the voxel’s center is inside the object
    - The “inside” voxels correspond to the finite elements



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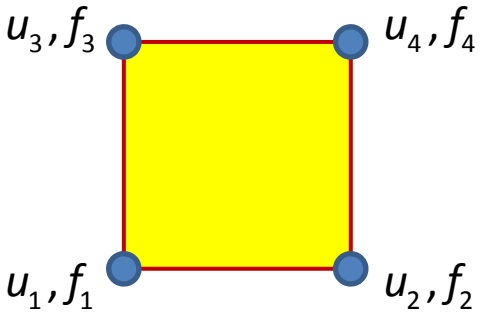
Per-Element Equations (static)

- Per-element equations

$$\sum_{j=1}^{8} K_{ij} u_j = f_i \quad , \quad i = 1,\ldots,8$$

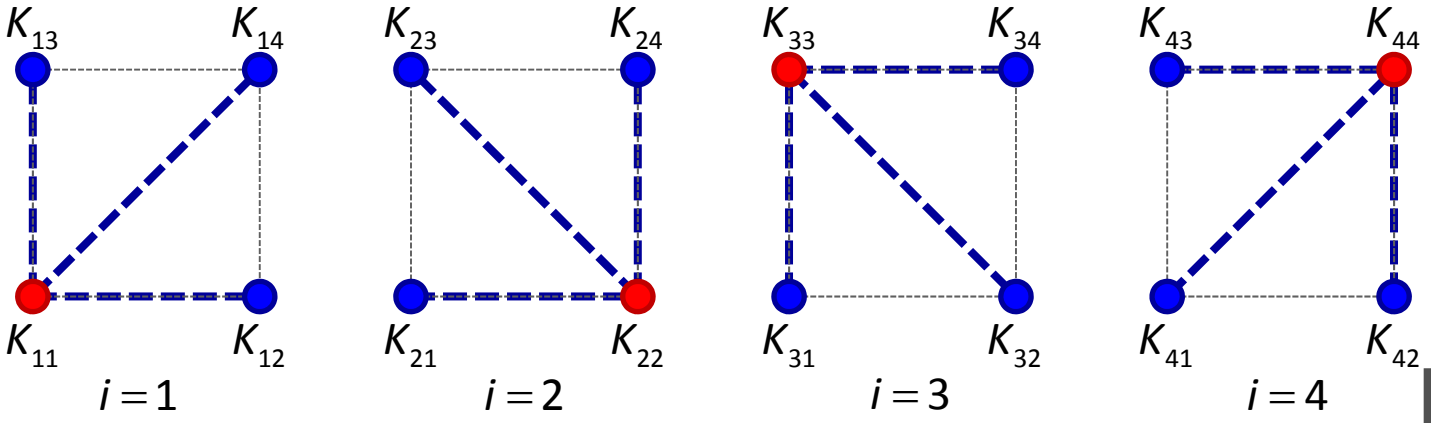
u_i : Displacements

f_i : Forces



e is now omitted

K : Element stiffness matrix consisting of 8x8 3x3-matrix coefficients



Per-Element Equations (co-rotated, static)

- Co-rotated strain

Rotate forces from initial into current configuration

Rotate displacements back into initial configuration

$$\sum_{j=1}^{8} RK_{ij}\left(R^T\left(p_j^0+u_j\right)-p_j^0\right)=f_i \quad , \quad i=1,\ldots,8$$

$$\sum_{j=1}^{8} \underbrace{RK_{ij}R^T}_{\hat{A}_{ij}} u_j = \underbrace{f_i-\sum_{j=1}^{8} RK_{ij}\left(R^T p_j^0-p_j^0\right)}_{\hat{b}_i}$$

R : Element rotation

p_j^0 : Undeformed vertex positions

Linear strain

Linear, co-rotated strain

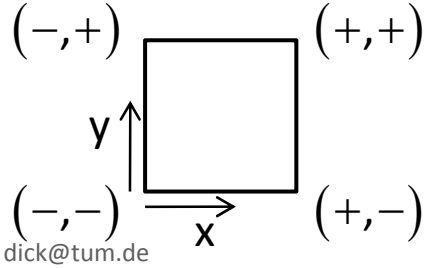
- R is obtained by polar decomposition of the element's average deformation gradient (5 iterations)

$$R_0 = I_3 + \frac{1}{4}\sum_{i=1}^{8} u_i^{old}\left(\pm\frac{1}{a},\pm\frac{1}{b},\pm\frac{1}{c}\right)$$

$$R_{n+1} = \frac{1}{2}\left(R_n + \left(R_n^{-1}\right)^T\right)$$

a, b, c : Edge lengths of hexahedral element

Signs :



Per-Element Equations (co-rotated, dynamic)

- Dynamics

$$\sum_{j=1}^{8}\left(M_{ij}\ddot{u}_j + C_{ij}\dot{u}_j + \hat{A}_{ij}u_j\right) = \hat{b}_i \quad , \quad i = 1,\ldots,8$$

M: Mass matrix

C : Damping matrix

- Newmark time integration

$$\dot{u}_i = \frac{2}{dt}\left(u_i - u_i^{old}\right) - \dot{u}_i^{old} \quad , \quad \ddot{u}_i = \frac{4}{dt^2}\left(u_i - u_i^{old} - \dot{u}_i^{old}dt\right) - \ddot{u}_i^{old}$$

dt: Time step length

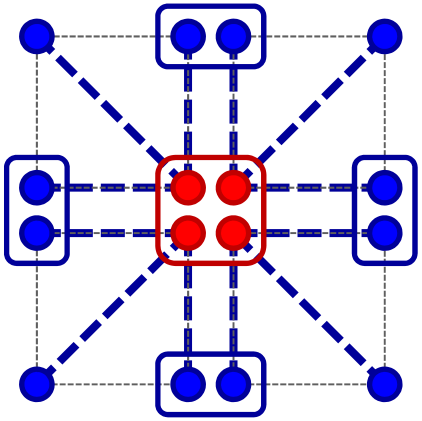
$$\sum_{j=1}^{8}\underbrace{\left(\frac{4}{dt^2}M_{ij} + \frac{2}{dt}C_{ij} + \hat{A}_{ij}\right)}_{A_{ij}}u_j = \underbrace{\hat{b}_i + \sum_{j=1}^{8}\left[M_{ij}\left(\frac{4}{dt^2}\left(u_j^{old} + \dot{u}_j^{old}dt\right) + \ddot{u}_j^{old}\right) + C_{ij}\left(\frac{2}{dt}u_j^{old} + \dot{u}_j^{old}\right)\right]}_{b_i}$$

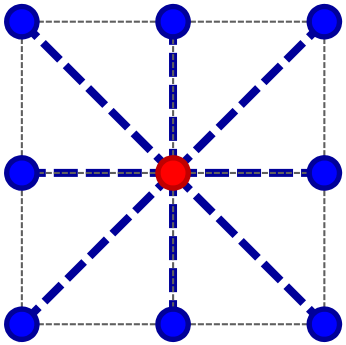
- Mass proportional damping: $C_{ij} = \alpha M_{ij}$
- Mass lumping: $M_{ii} = m_i I_3$, $M_{ij} = 0$ for $i \neq j$

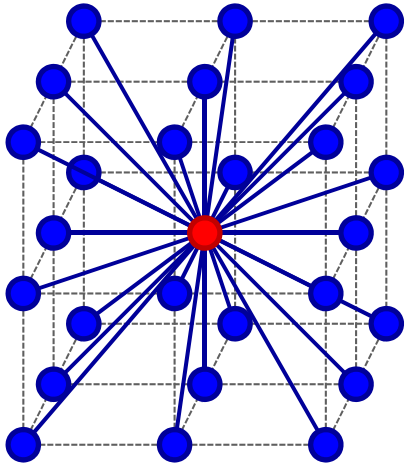
mass of vertex i (1/8 element mass)

Per-Vertex Equations

- Per-vertex equations: Add stencil coefficients of shared vertices







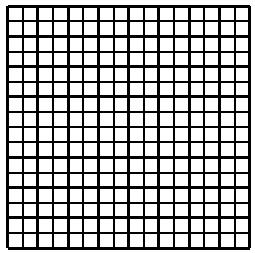
- Stencil on a 3^3 domain of adjacent vertices: 27 3x3-matrix coefficients

$$\sum_{i=(-1,-1,-1)^T}^{(1,1,1)^T} A_i^x u_{x+i} = b_x$$

- Dirichlet boundary conditions: Replace equation by $I_3 u_x = 0$ and in the other equations set the respective coefficient A_i corresponding to this vertex to 0

Geometric Multigrid

- Solve $A^h u^h = b^h$, current approximate solution v^h

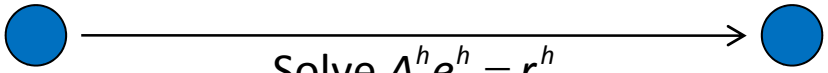


Ω^h

Relax $A^h v^h \approx b^h$

Residual $r^h = b^h - A^h v^h$

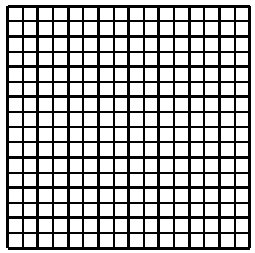
Correct $v^h \leftarrow v^h + e^h$



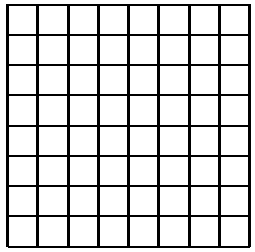
Solve $A^h e^h = r^h$

Geometric Multigrid

- Solve $A^h u^h = b^h$, current approximate solution v^h



Ω^h



Ω^{2h}

Relax $A^h v^h \approx b^h$ — Pre-smoothing

Residual $r^h = b^h - A^h v^h$

Restrict

$r^{2h} = R_h^{2h} r^h$

Solve $A^{2h} e^{2h} = r^{2h}$

Interpolate

$e^h = I_{2h}^h e^{2h}$

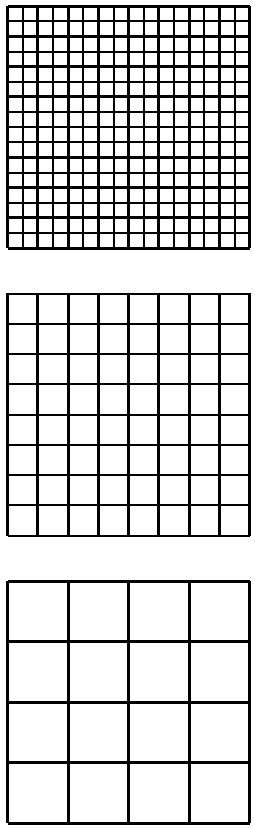
Correct $v^h \leftarrow v^h + e^h$

Relax $A^h v^h \approx b^h$ — Post-smoothing

Coarse grid correction

Geometric Multigrid

- Solve $A^h u^h = b^h$, current approximate solution v^h



Ω^h

Ω^{2h}

Ω^{4h}

Relax $A^h v^h \approx b^h$ — Pre-smoothing

Residual $r^h = b^h - A^h v^h$

Restrict

$r^{2h} = R_h^{2h} r^h$

Multigrid V-Cycle

Coarsest Grid Solver

Relax $A^h v^h \approx b^h$ — Post-smoothing

Correct $v^h \leftarrow v^h + e^h$

Coarse grid correction

Interpolate

$e^h = I_{2h}^h e^{2h}$

Linear time complexity in the number of unknowns

Variational Properties of Multigrid

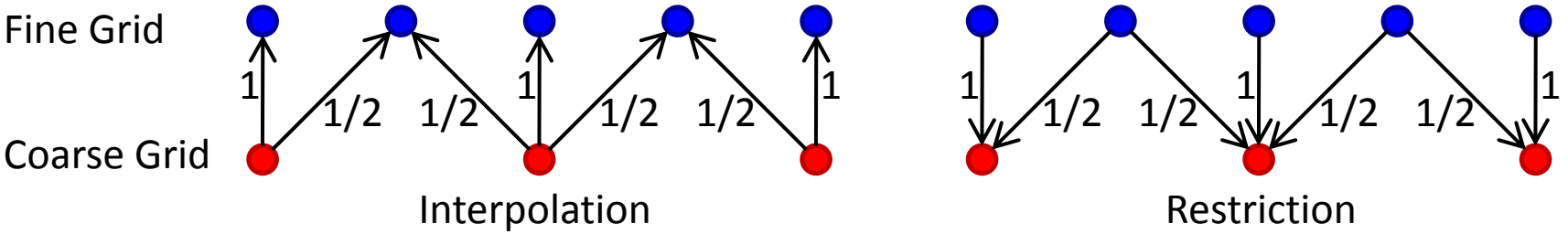
- Selection of transfer operators and coarse grid operators:

  I_{2h}^{h} : Tri-linear interpolation

  $R_h^{2h} = \left(I_{2h}^{h}\right)^T$ ← Restriction is transpose of interpolation

  $A^{2h} = R_h^{2h} A^h I_{2h}^{h}$ ← Galerkin-based coarsening

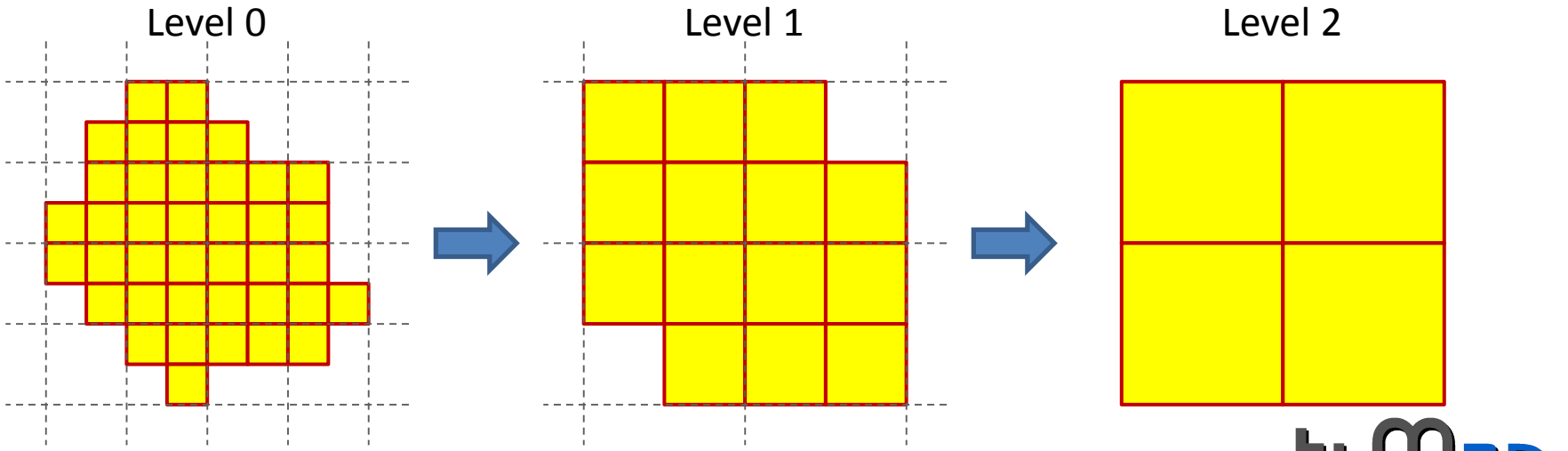
1D Example:



- In the finite element context, these choices naturally arise from the variational principle
  - Coarse grid correction minimizes the functional

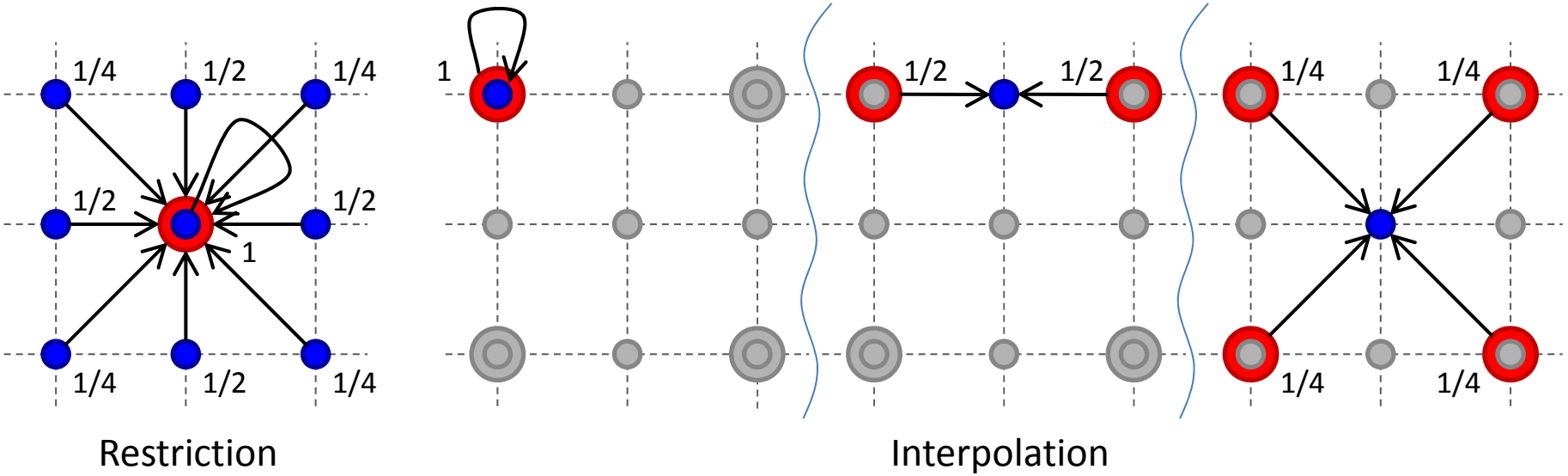
Multigrid Hierarchy

- The Cartesian grid enables to efficiently construct a nested multigrid hierarchy
  - Grids are successively built from fine to coarse levels
  - With each coarser level the cell size is doubled
  - A cell is created if it covers at least one cell on the previous finer level



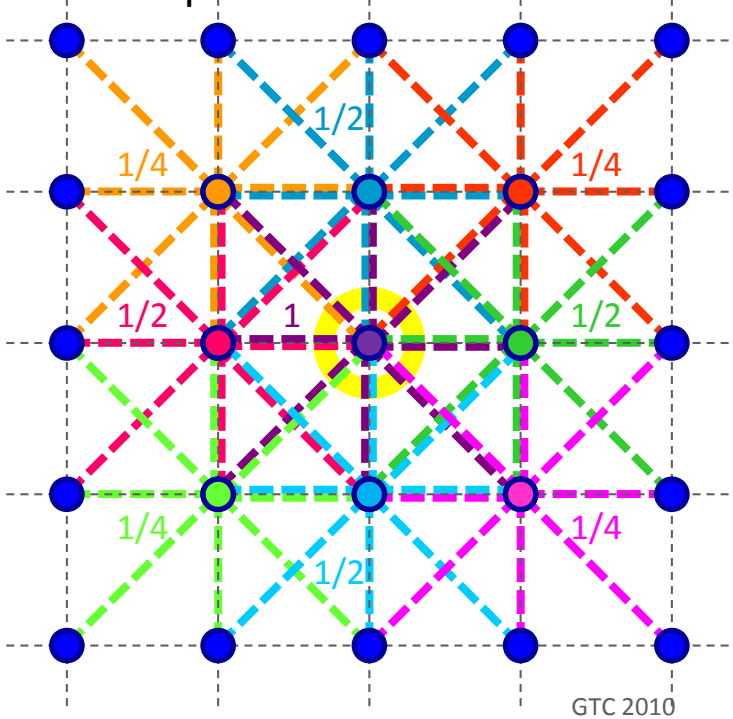
Matrix-Free Multigrid Formulation

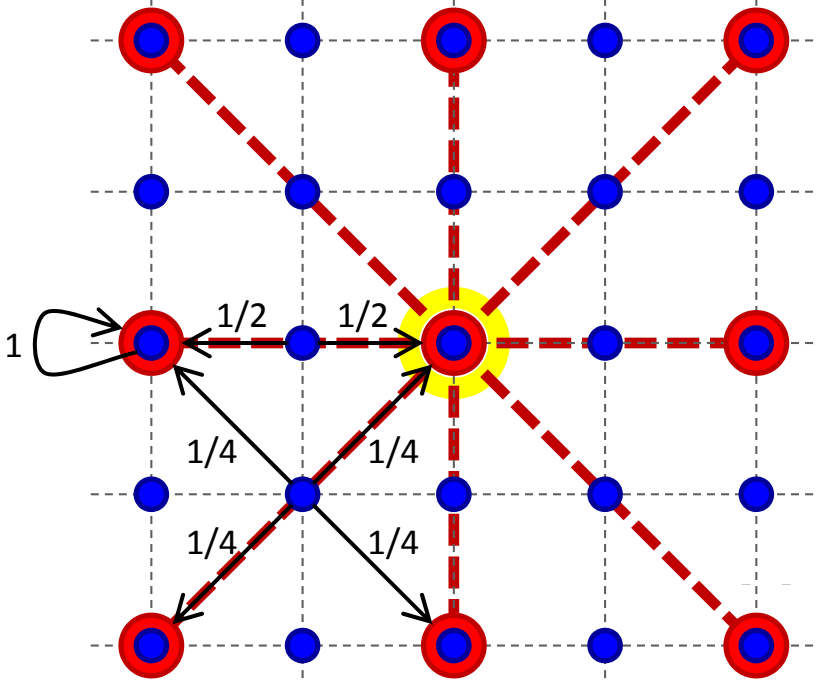
- Restriction and Interpolation
  - Weights are implicitly determined by the location of the vertices



Matrix-Free Multigrid Formulation

- Construction of coarse grid equations $A^{2h} = R_h^{2h} A^h I_{2h}^h$
  - Restriction: Linear combination of 3^3 fine grid equations leads to a 5^3 stencil
  - Interpolation: Substitution of fine grid unknowns reduces the stencil to a 3^3 domain





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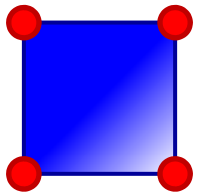
Data Structures – FE Model Topology

- Index-based representation of FE model and multigrid hierarchy
  - Finite elements and vertices are enumerated and accessed via indices
  - Typically requires significantly less memory than an index-free representation using a rectangular domain with implicit neighborhood relationships
  - Indices are represented by 32-bit integers
  - A special index value of -1 indicates “void” elements/vertices

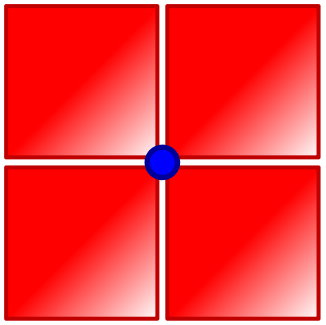
We store:

- For each finite element:



8 indices of incident vertices

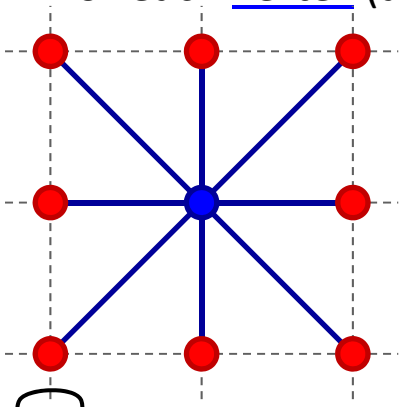
- For each simulation level vertex:



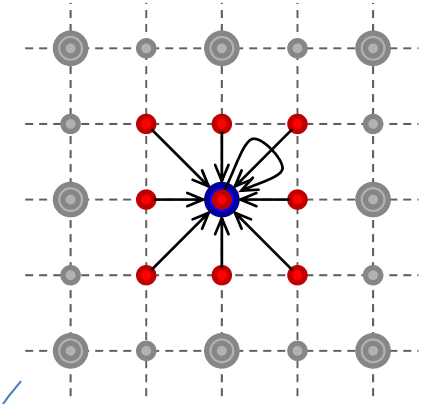
8 indices of incident elements

Data Structures – FE Model Topology

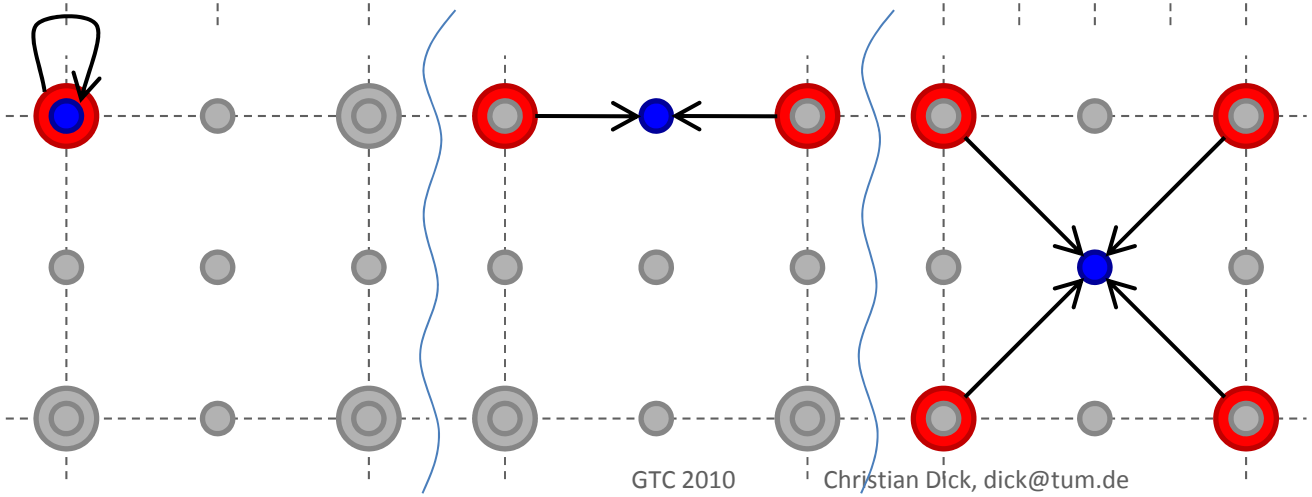
- For each vertex (all multigrid levels):



27 indices of neighbor vertices (on the same level), i.e. the 3^3 domain of the numerical stencil



27 indices of vertices which restrict to the considered vertex (on the next finer level)



Up to 8 indices of vertices which the considered vertex interpolates from (on the next coarser level)

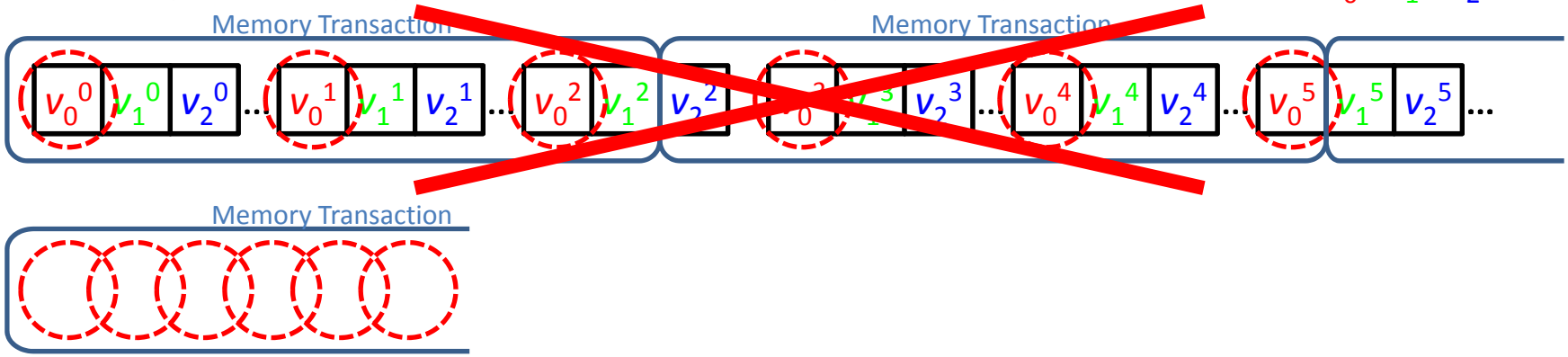
Data Structures – Simulation

- For each finite element:
  - Elastic modulus E
  - Element rotation R
  - Density ρ
- For each simulation level vertex:
  - Vertex position p^0 in undeformed state
  - Is the vertex fixed?
  - Force vector f
  - Displacement vector u^{old} of previous time step and its first and second derivatives $\dot{u}^{old}$,$\ddot{u}^{old}$
- For each vertex (all multigrid levels):
  - 27 3x3 matrix coefficients A_i
  - Right hand side vector b
  - Displacement vector u
  - Residual vector r

GPU-friendly Memory Layout

- Coalescing of device memory accesses
  - Fermi GPU fetches contiguous blocks of 128 bytes aligned at 128-byte boundaries
  - Threads in a warp should access successive memory addresses
- General parallelization strategy: One CUDA thread per vertex/finite element

  Arrays with multiple scalar components (up to 243) per data element (v_0^i, v_1^i, v_2^i, …)



- Store arrays such that their scalar components are grouped into separate memory blocks

CUDA Kernels (1)

In each time step:

- (1) Re-assemble system of equations to consider current element rotations

  - Computation of element rotations
  - Assembly of simulation level equations (1)
  - Assembly of simulation level equations (2) (Forces and dynamics)
  - Assembly of coarse grid equations

- (2) Solve system of equations by performing multigrid V-cycles (next slide)

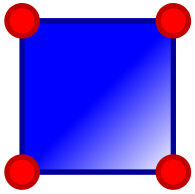
CUDA Kernels (2)

- (2) Solve system of equations by performing multigrid V-cycles

```
for (int c = 0; c < numVCycles; c++) // Perform numVCycles V-cycles per time step
{
    for (int ℓ = 0; ℓ < numLevels-1; ℓ++) // Going down in the V-cycle from fine to coarse grids (level 0 is the finest)
    {
        for (int i = 0; i < numPreSmoothSteps; i++) { Gauss-Seidel relaxation on level ℓ }
        Computation of residual on level ℓ
        Restriction of residual from level ℓ to level ℓ+1
    }
    CG solver for coarsest level (i.e., level numLevels-1)
    for (int ℓ = numLevels-2; ℓ >= 0; ℓ--) // Going up in the V-cycle from coarse to fine grids
    {
        Interpolation of error from level ℓ+1 to level ℓ and coarse grid correction
        for (int i = 0; i < numPostSmoothSteps; i++) { Gauss-Seidel relaxation on level ℓ }
    }
}
```

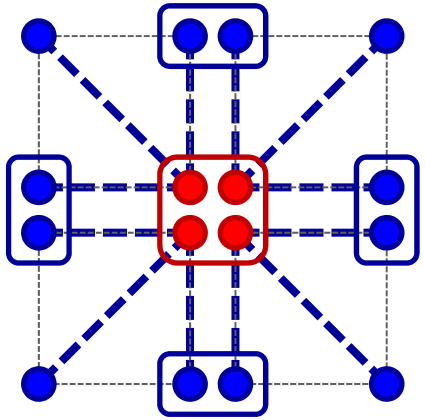
Computation of Element Rotations

- 1 CUDA thread per finite element
- *Algorithm:*
  - Fetch indices of element's vertices
  - Fetch displacement vectors *u* at these vertices
  - Compute deformation gradient
  - Compute element rotation *R* by iterative polar decomposition
  - Store element rotation *R*



Assembly of Simulation Level Equations (1)

- 1 CUDA thread per simulation level vertex
- A single generic element stiffness matrix K^0 is stored in constant memory
  - A specific element stiffness matrix K is obtained by scaling with the element's elastic modulus E: $K = EK^0$
- *Algorithm:*
  - Host: Initialize global memory with 0
  - If vertex is fixed: Store equation $I_3 u = 0$
  - Else: Iterate over the incident elements of the vertex
    - Fetch element index
    - Fetch element rotation R and elastic modulus E
    - Iterate over element's vertices
      - Accumulate the per-vertex equation in global memory;
        Skip LHS part of a vertex's contribution if the vertex is fixed

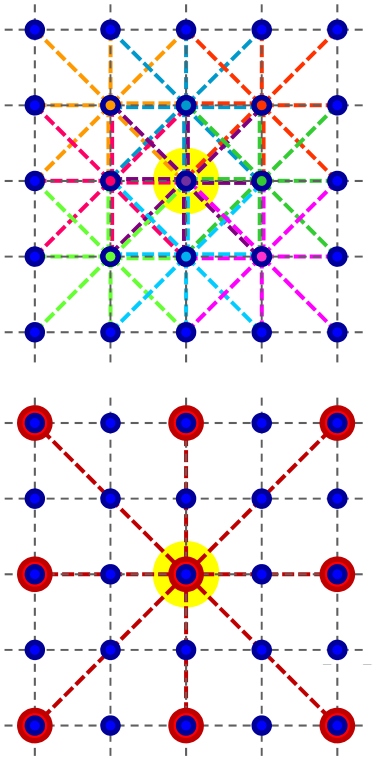


Assembly of Simulation Level Equations (2)

- 1 CUDA thread per simulation level vertex
- *Algorithm:*
  - If the vertex is not fixed:
    - Fetch $u, u^{old}, \dot{u}^{old}, \ddot{u}^{old}$
    - Update $\ddot{u}^{old}, \dot{u}^{old}, u^{old}$ and store in global memory
    - Fetch force vector f
    - Fetch indices of incident elements
    - Fetch densities ρ of incident elements and compute vertex mass
    - Add the contributions of the external force and of the dynamics to the equation in global memory

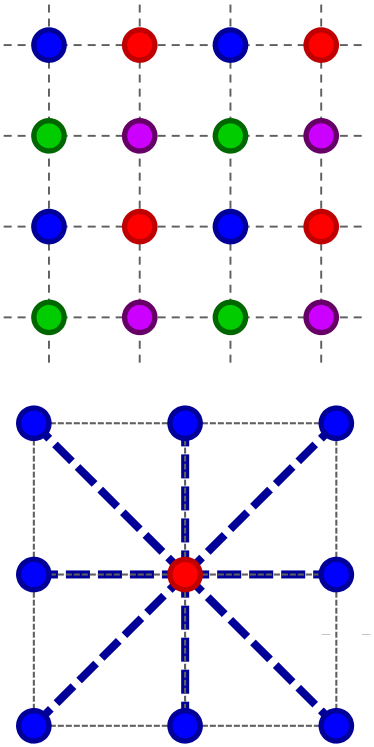
Assembly of Coarse Grid Equations

- 9 CUDA threads per vertex (each thread computes one of the nine components of all 3x3 matrix coefficients of the stencil)
- Stencil is accumulated in 27 registers and finally written to global memory
- *Algorithm:*
  - Iterate over 5^3 domain
    - Accumulate contributions of the 27 stencils at current position (restriction)
    - Distribute result to 3^3 stencil (interpolation)
- Code had to be manually unrolled to achieve optimal performance



Gauss-Seidel Relaxation

- Multi-color Gauss-Seidel relaxation by partitioning the vertices into 8 subsets
  - Vertices in each subset can be relaxed in parallel, but subsets must be processed sequentially: The kernel is called once for each subset
- 1 CUDA thread per vertex of the respective subset
- *Algorithm:*
  - Fetch RHS vector *b*
  - Iterate over the 3^3 domain of neighbor vertices
    - Fetch index of neighbor vertex
    - Fetch displacement vector *u* at this vertex
    - Fetch 3x3 matrix coefficient A_i
    - Accumulate contributions
  - Relax equation and store new displacement vector *u* in global memory

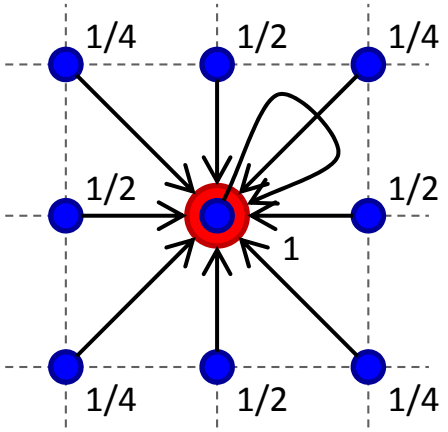


Computation of Residual

- 1 CUDA thread per vertex
- Similar to Gauss-Seidel relaxation, however now all vertices can be processed in parallel with a single kernel call

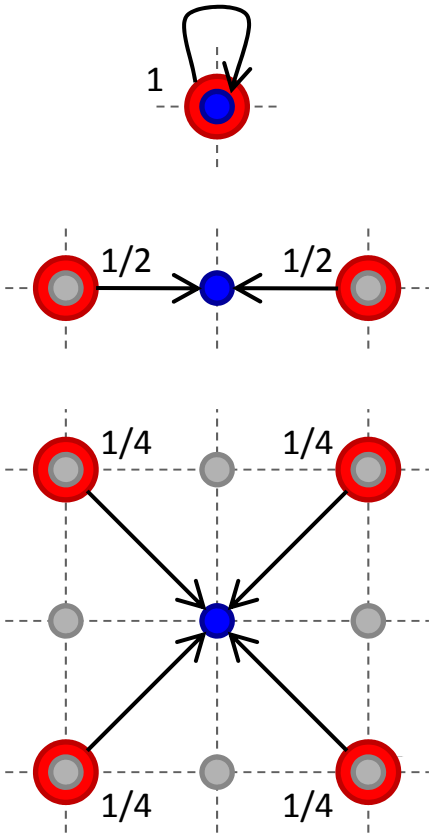
Restriction of Residual

- 1 CUDA thread per vertex
- *Algorithm:*
  - Iterate over the 27 vertices which restrict to this vertex
    - Fetch index of vertex
    - Fetch residual *r* at this vertex
    - Accumulate weighted residual
  - Store accumulated residual as right hand side vector *b* in global memory
  - Initialize displacement vector *u* with 0



Interpolation of Error and Coarse Grid Corr.

- 1 CUDA thread per vertex
- *Algorithm:*
  - Iterate over the up to 8 vertices which this vertex interpolates from
    - Fetch index of vertex
    - Fetch displacement vector *u* at this vertex
    - Accumulate weighted displacement vector
  - Add accumulated displacement vector to the displacement vector *u* in global memory (coarse grid correction)

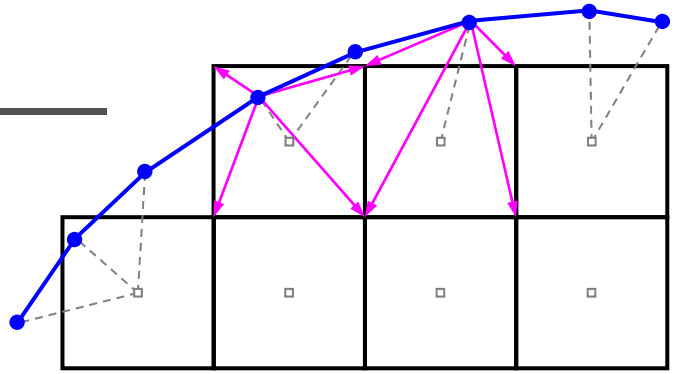


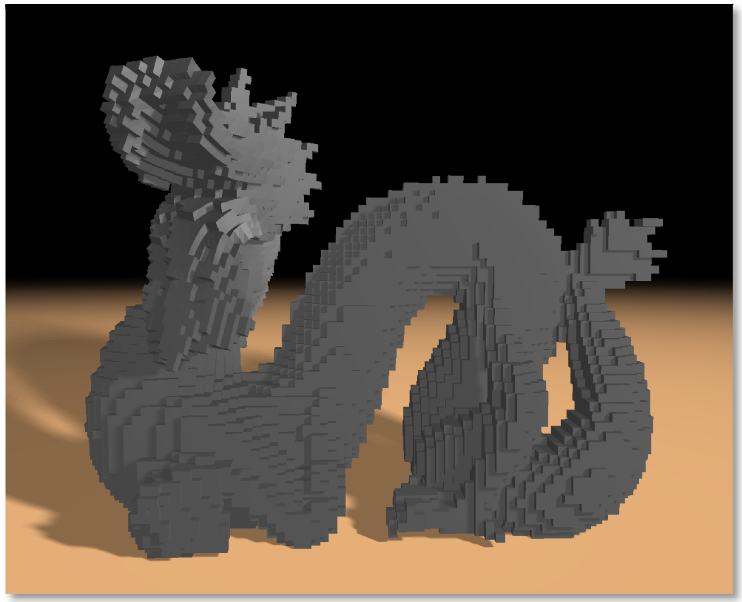
Solver for the Coarsest Level

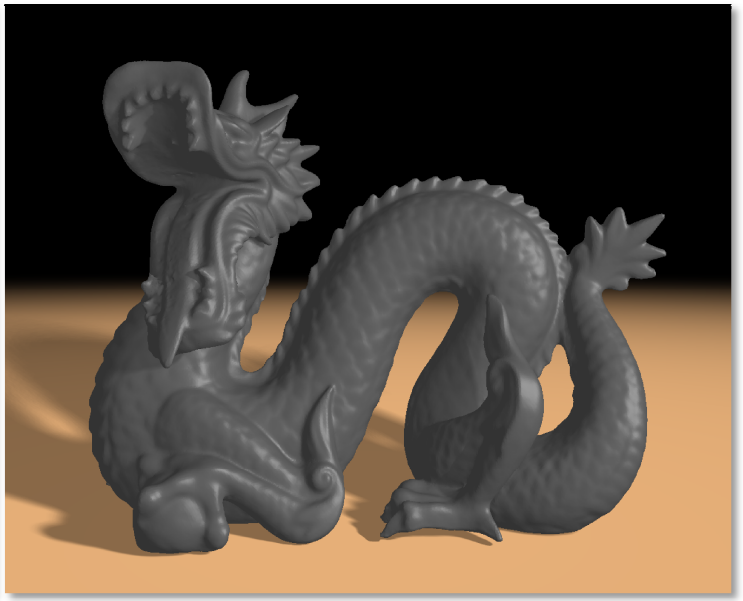
- Conjugate gradient (CG) solver with Jacobi pre-conditioner (inverse diagonal)
- Runs on a single multiprocessor (using a single thread block) to avoid global synchronization via separate kernel calls
- 1 CUDA thread per vertex
- Number of unknowns is limited by the maximum number of threads per block and by the size of the shared memory
  - Number of multigrid levels is chosen such that the number of vertices on the coarsest grid is ≤ 512

Rendering

- High resolution render surfaces
  - Each vertex is bound to nearest finite element
  - Deformed vertex positions are determined by tri-linear interpolation/extrapolation



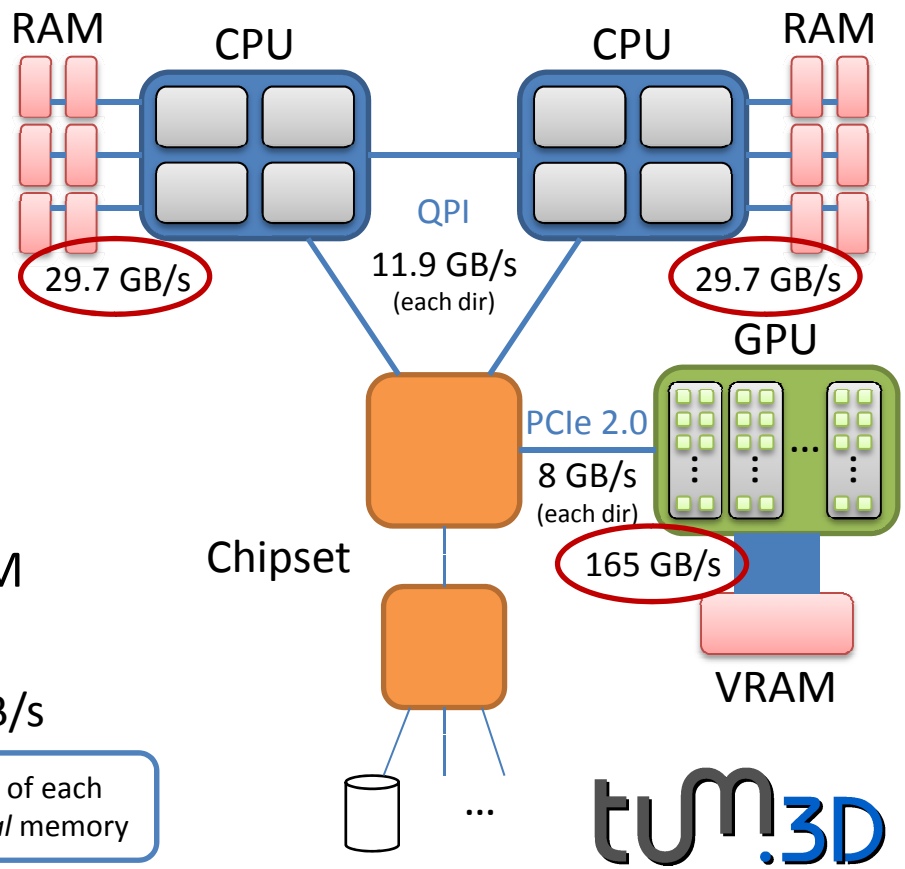




Performance – Test System

- 2x Intel Xeon X5560 2.8 GHz (3.2 GHz)
  - 4 cores per CPU
- 48 GB DDR3 1333 MHz, triple channel
  - NUMA architecture*
  - Theoretical memory bandwidth: 29.7 GB/s (per CPU)
  - Theoretical QPI bandwidth: 11.9 GB/s (each direction)
- NVIDIA GTX 480 (“Fermi”), 1.5 GB VRAM
  - 15 multiprocessors, 480 CUDA cores
  - Theoretical memory bandwidth: 165 GB/s

*For the parallelized CPU implementation, the coefficients of each per-vertex equation are stored in the respective CPU’s *local* memory



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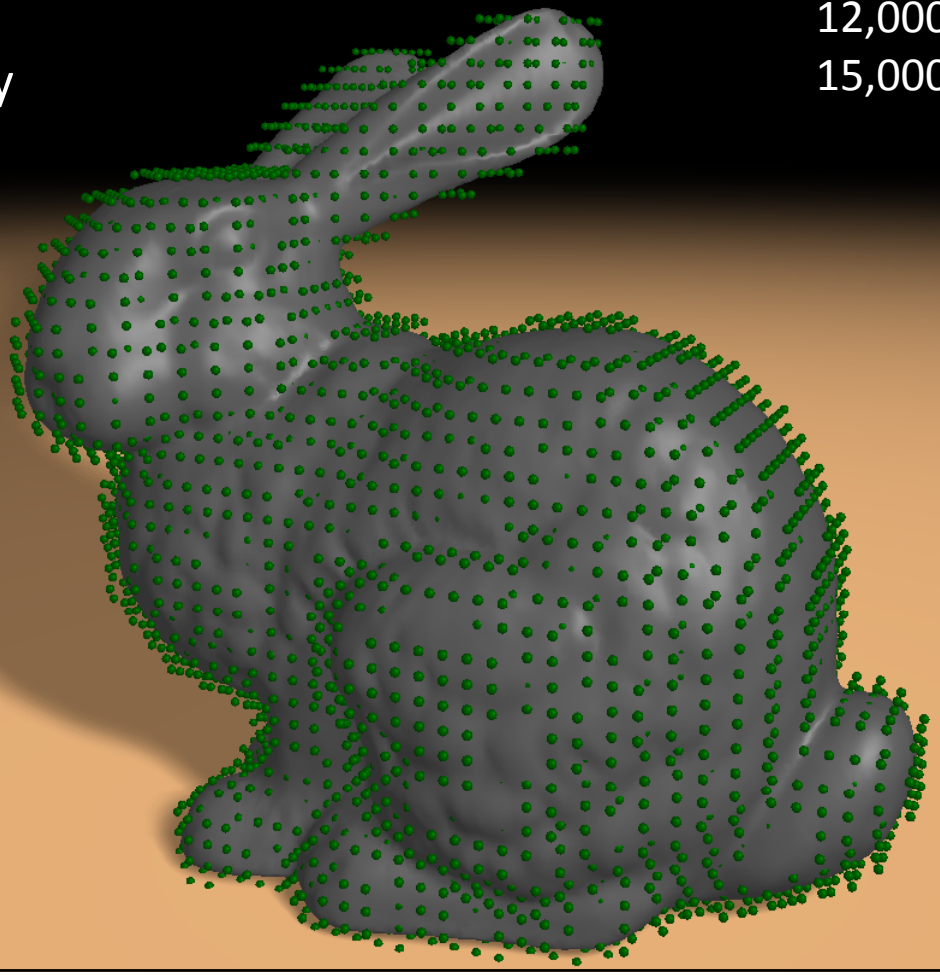
Performance – Test Model

- Stanford Bunny

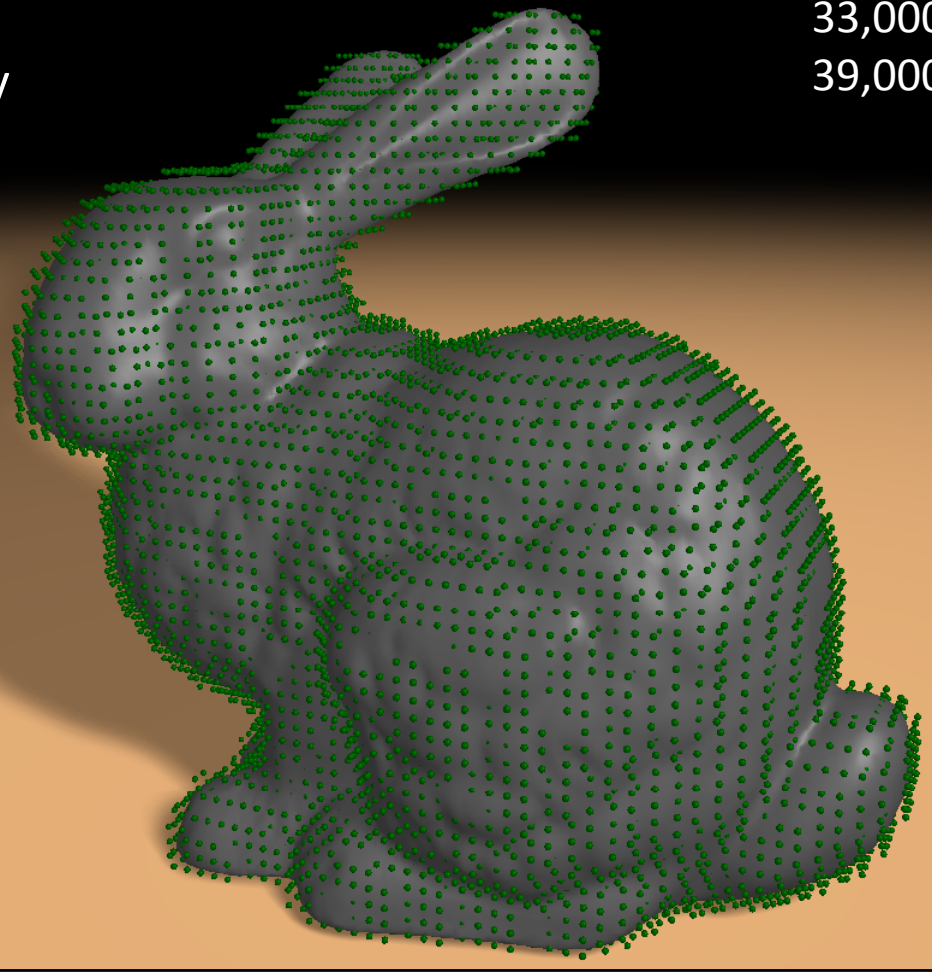
12,000 Elements
15,000 Vertices



Performance – Test Model

- Stanford Bunny

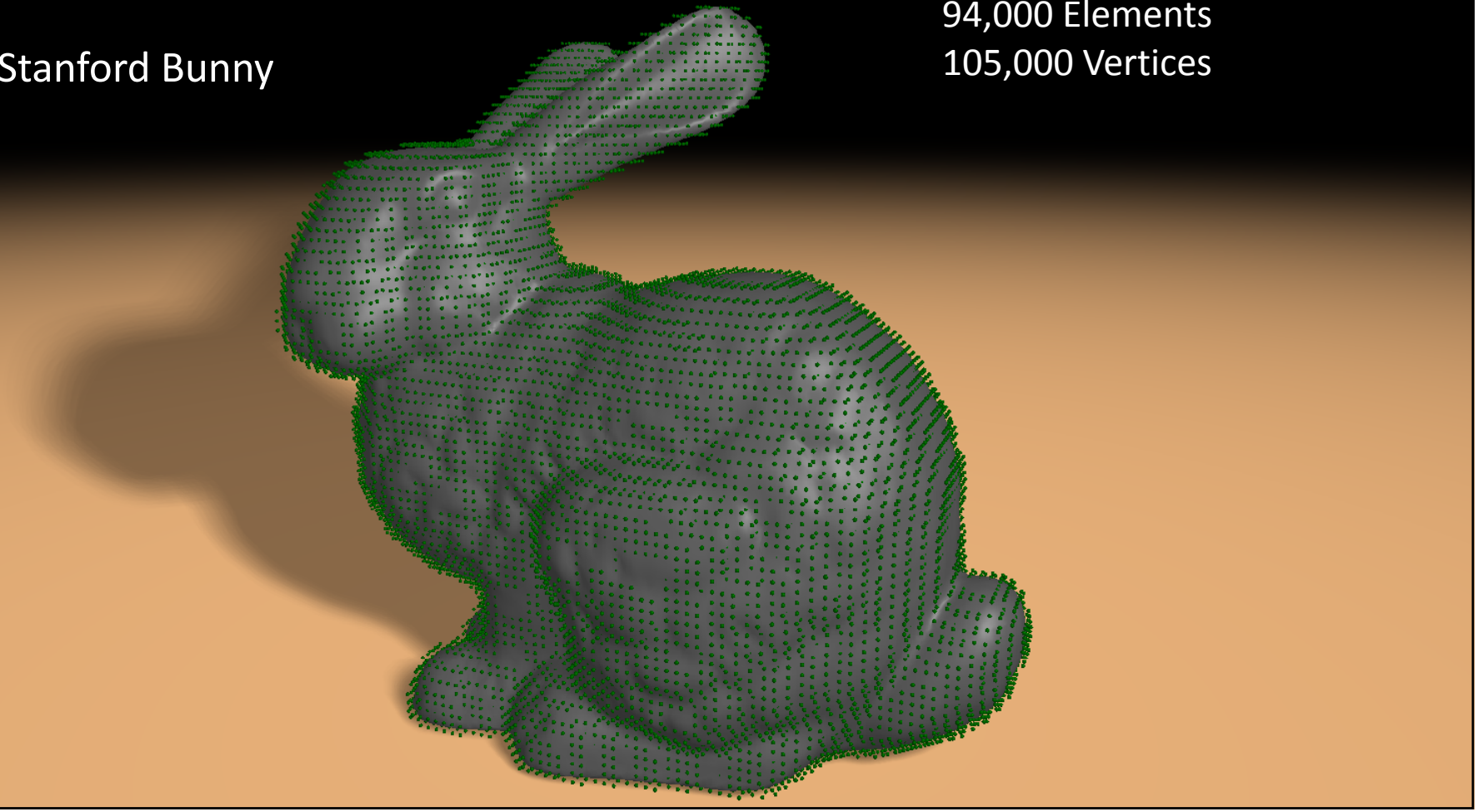
33,000 Elements
39,000 Vertices



Performance – Test Model

- Stanford Bunny

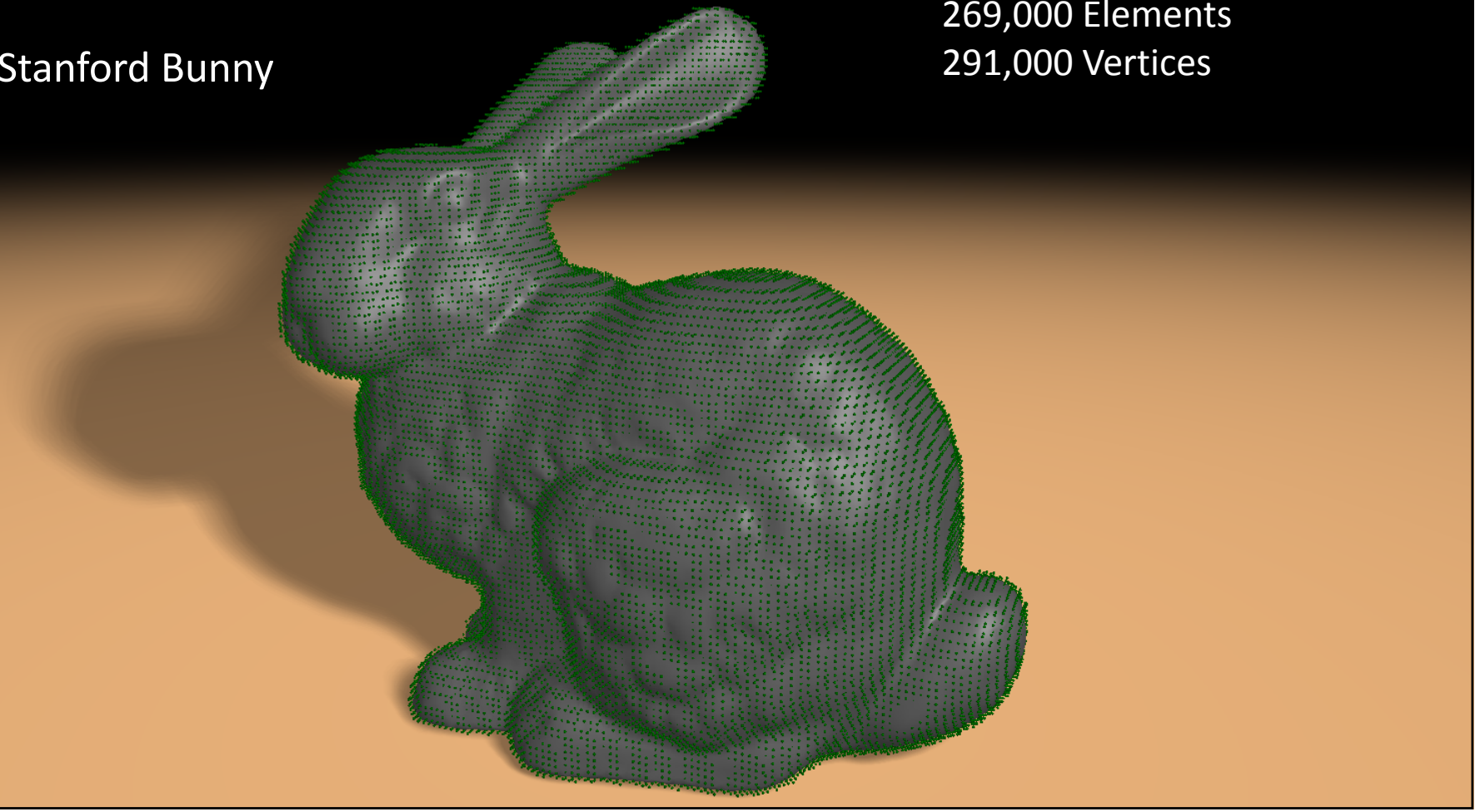
94,000 Elements
105,000 Vertices



Performance – Test Model

- Stanford Bunny

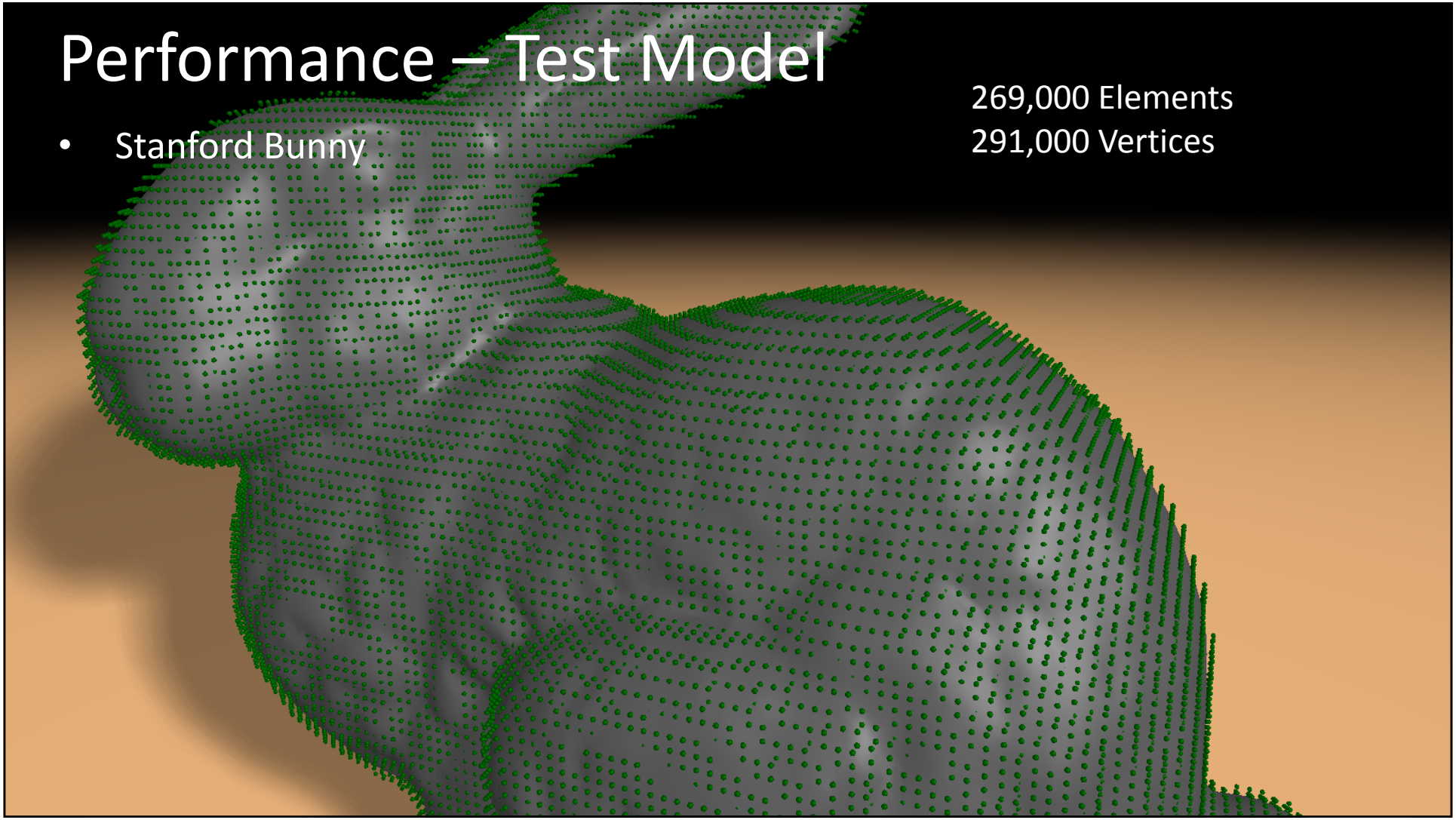
269,000 Elements
291,000 Vertices



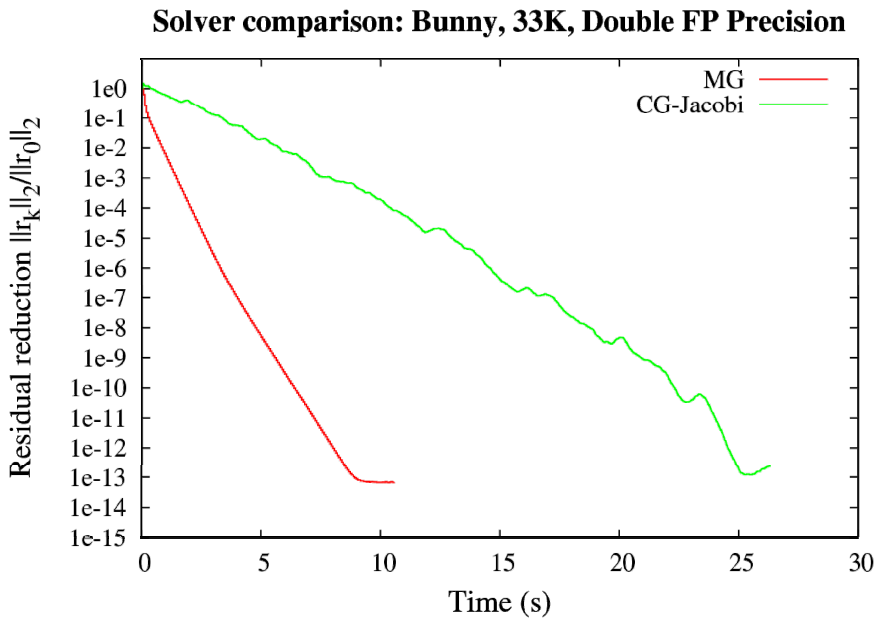
Performance – Test Model

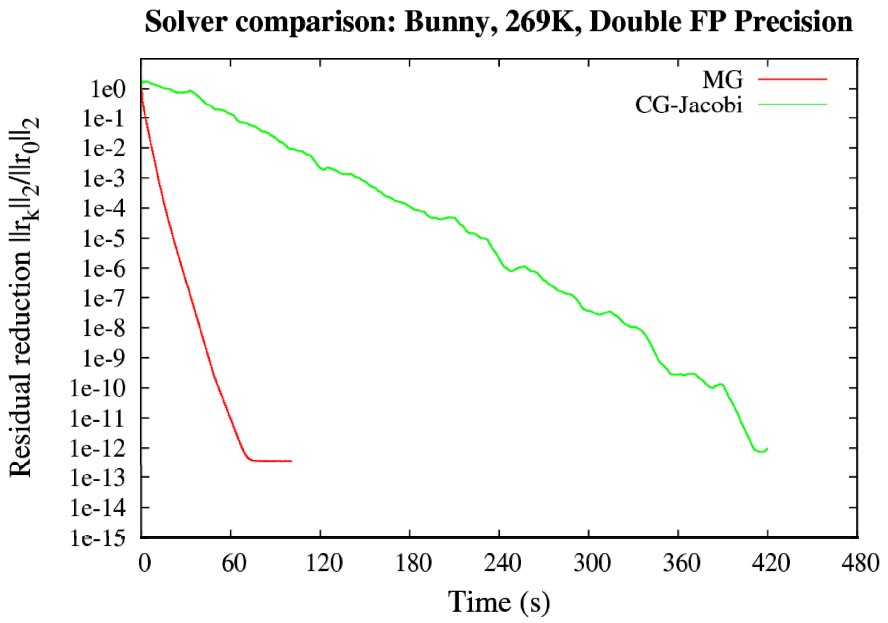
- Stanford Bunny

269,000 Elements
291,000 Vertices



Performance – Solver Convergence

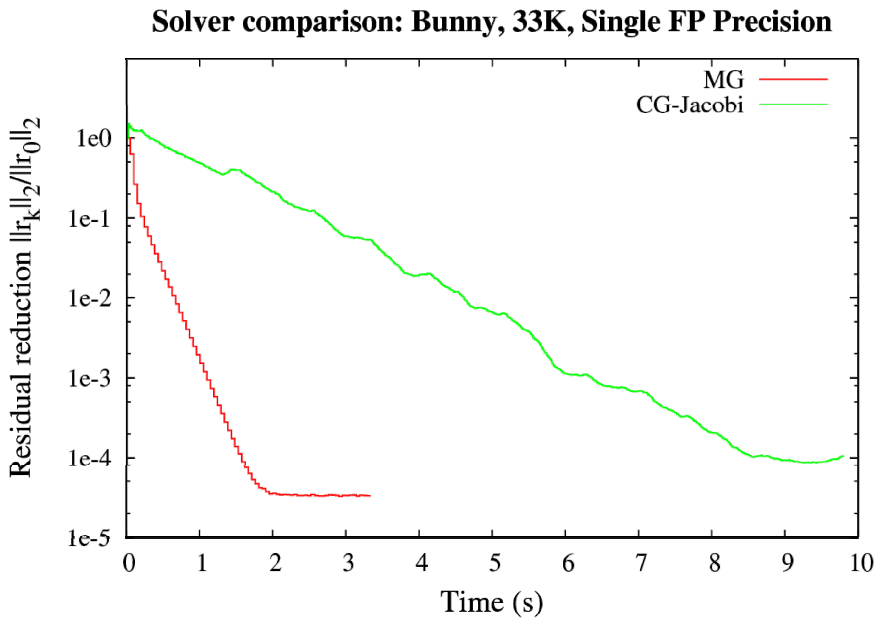


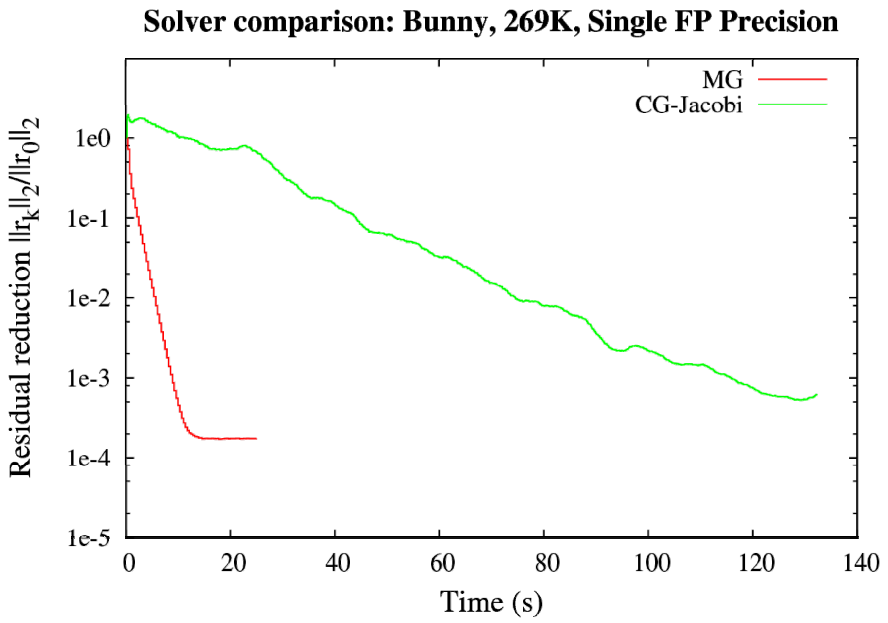


Timings were obtained on the CPU using 1 core

$E = 10^6 Pa$, $\nu = 0.3$, $\rho = 10^5 kg/m^3$, $dt = 50ms$, hexahedra edge length $= 2.8mm$ and $1.4mm$

Performance – Solver Convergence

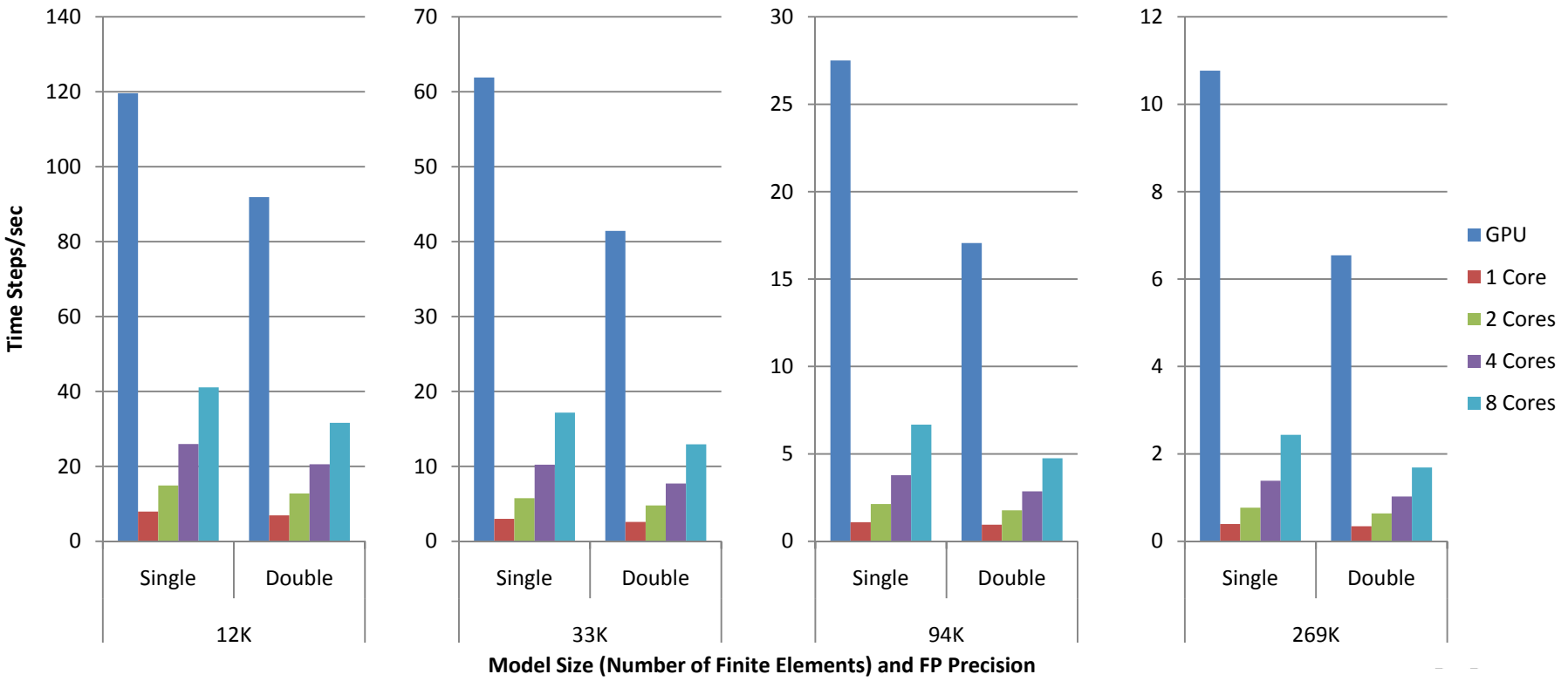




Timings were obtained on the CPU using 1 core

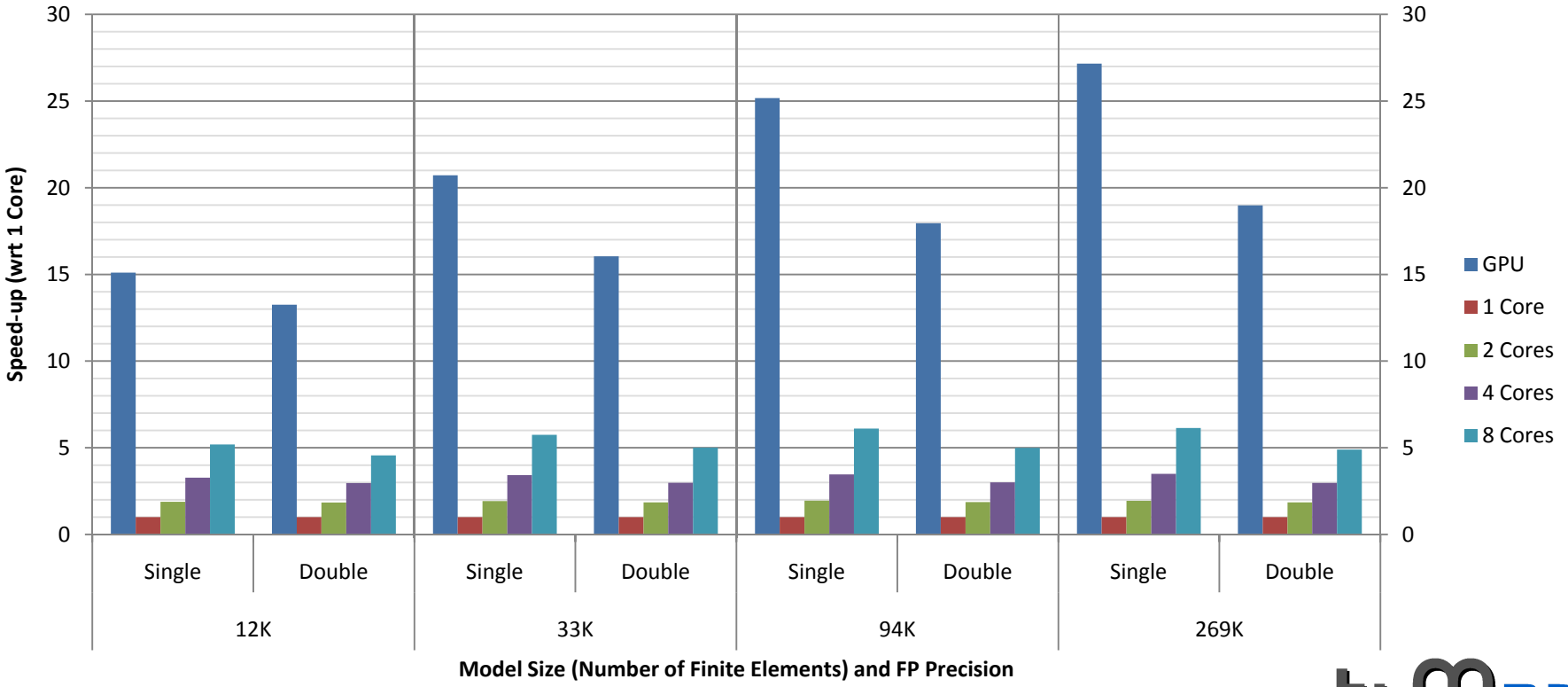
$E = 10^6 Pa$, $\nu = 0.3$, $\rho = 10^5 kg / m^3$, $dt = 50ms$, hexahedra edge length $= 2.8mm$ and $1.4mm$

Performance – Simulation Time Steps/sec



Each time step includes the re-assembly of the per-vertex equations (simulation level + coarse grids) for the co-rotational strain formulation and 2 multigrid V-cycles, each with 2 pre- and 1 post-smoothing Gauss-Seidel steps

Performance – Speed-up



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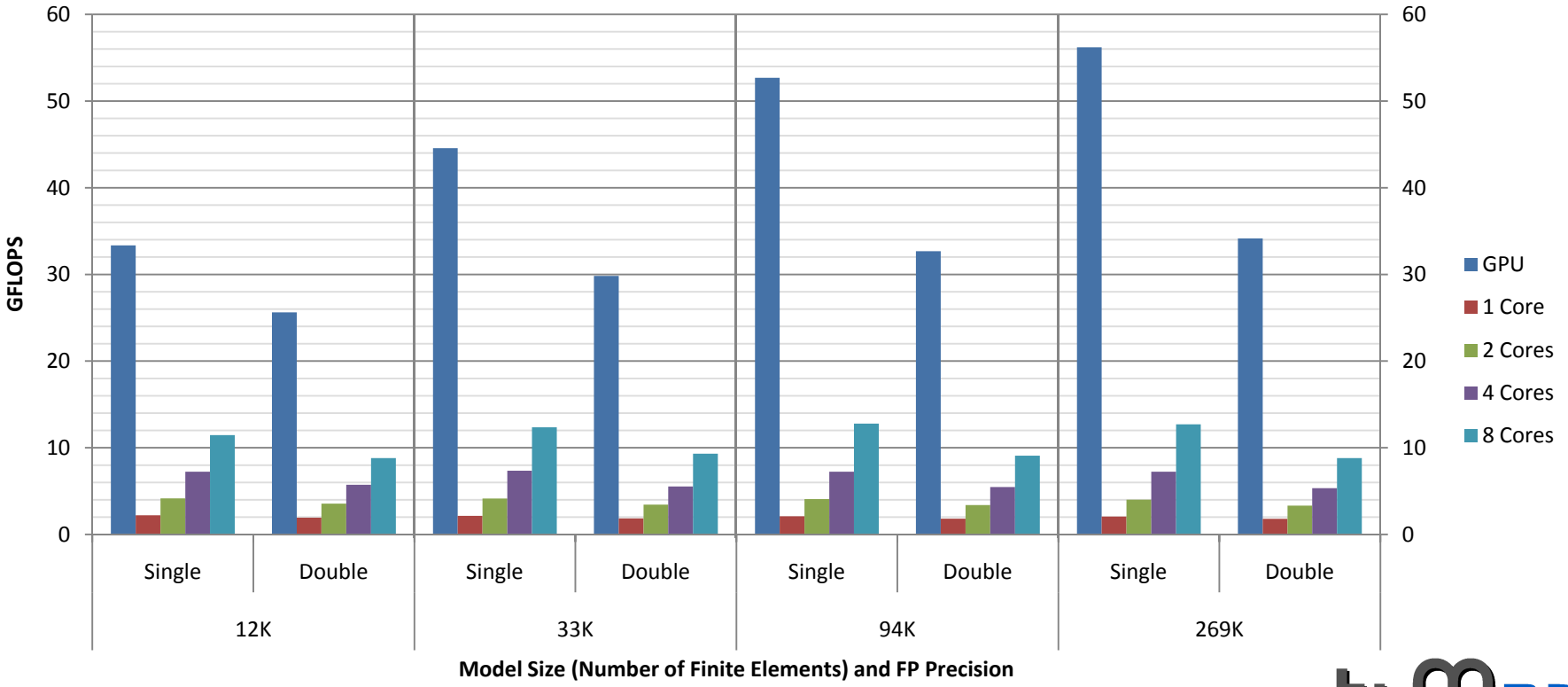
Performance – Costs per Finite Element

- Amortized costs per finite element per time step (Bunny 269K elements)

Kernel	FLOPs	%	Bytes R/W		%	GPU Timings %	
			Single	Double		Single	Double
Computation of element rotations	470	2	160	300	1	0	1
Assembly of simulation level equations (1)	10000	51	6600	13000	23	33	30
Assembly of simulation level equations (2)	32	0	140	270	0	0	0
Assembly of coarse grid equations	3200	17	5100	10000	18	24	21
Gauss-Seidel relaxation	6 x 660	20	6 x 1800	6 x 3500	39	27	33
Computation of residual	2 x 620	6	2 x 1800	2 x 3500	13	11	12
Restriction of residual	2 x 210	2	2 x 580	2 x 1000	4	1	1
Interpolation of error and coarse grid corr.	2 x 39	0	2 x 200	2 x 350	1	2	1
CG solver on coarsest level	2 x 3	0	2 x 1	2 x 1	0	1	1
Total (per finite element per time step)	19000		28000	54000			

2 V(2,1)-cycles per time step

Performance – GFLOPS *(sustained)*



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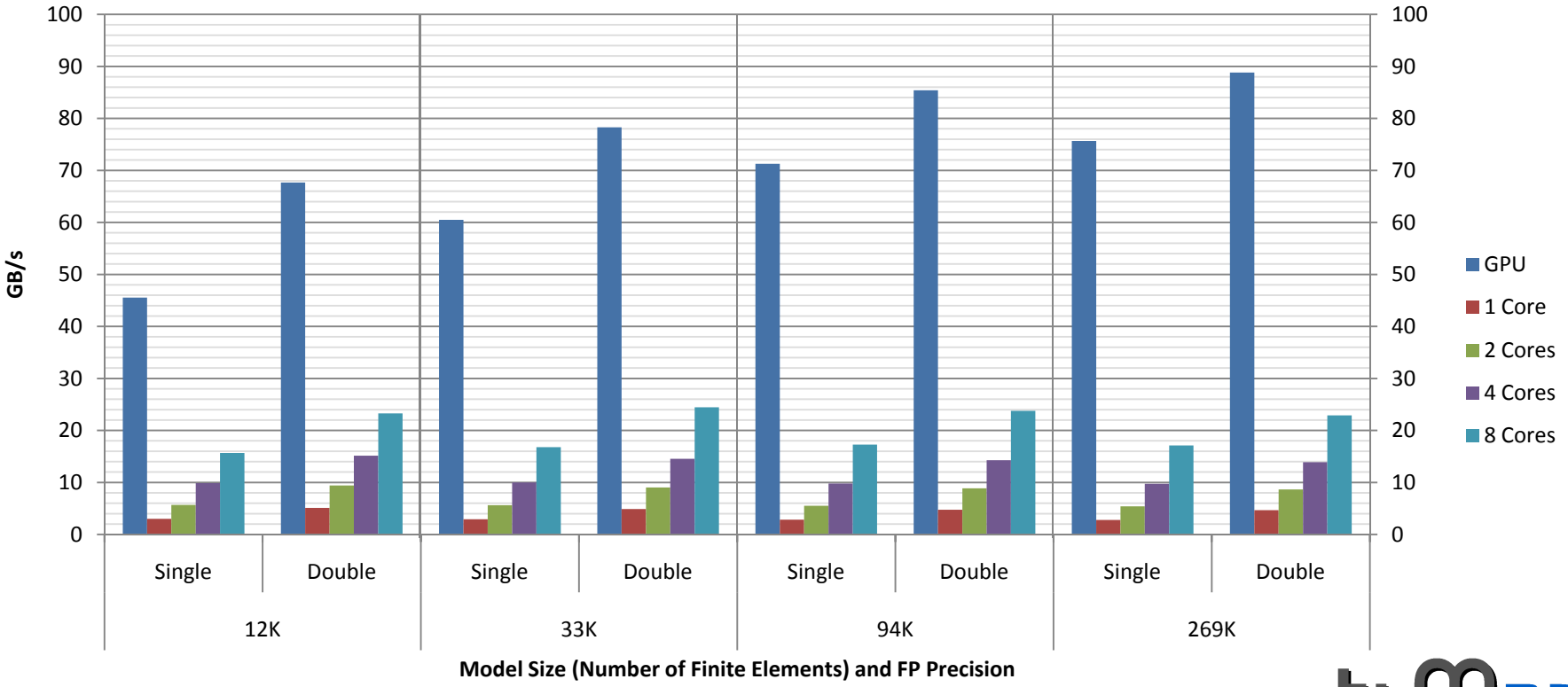
Performance – Memory Throughput *(sustained)*



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Conclusion and Future Work

- Real-time FEM simulation of deformable objects enabled by a fully GPU-based geometric multigrid solver
  - Hexahedral finite elements on a uniform Cartesian grid, co-rotational strain
  - Regular shape of stencil enables GPU-friendly parallelization and memory accesses
  - Performance is boosted by the GPU's compute power and memory bandwidth
    - Up to 27x faster than 1 CPU core / 4x faster than 8 CPU cores
    - Up to 56 GFLOPS (single) / 34 GFLOPS (double precision) *(sustained performance)*
    - Up to 88 GB/s memory throughput *(sustained performance)*
    - Real-time/interactive simulation rates:
      120 time steps/sec for 12,000 elements, 11 time steps/sec for 269,000 elements
- Future work
  - GPU-based collision detection
  - Parallelization on multiple GPUs

Thanks for your attention!

- http://wwwcg.in.tum.de/Research/Publications/CompMechanics

C. Dick, J. Georgii, R. Westermann. A Real-Time Multigrid Finite Hexahedra Method for Elasticity Simulation using CUDA. Technical Report, July 2010.

Demo Executables

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