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Accelerating MCAE with GPUs

Information Sciences Institute

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15 Sept 2010

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Outline

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MCAE Sparse Solver Bottleneck

Review of Multifrontal Method

Adding a GPU

Performance Results

Future Directions

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MCAE

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Mechanical Computer Aided Engineering

- ISVs ABAQUS, ANSYS, LS-DYNA, & NASTRAN
- GOTS Alegra, ALE3D, CTH, & ParaDYN

Broad range of capabilities

- Static analysis
- Vibration analysis
- Crash analysis

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Defense Examples

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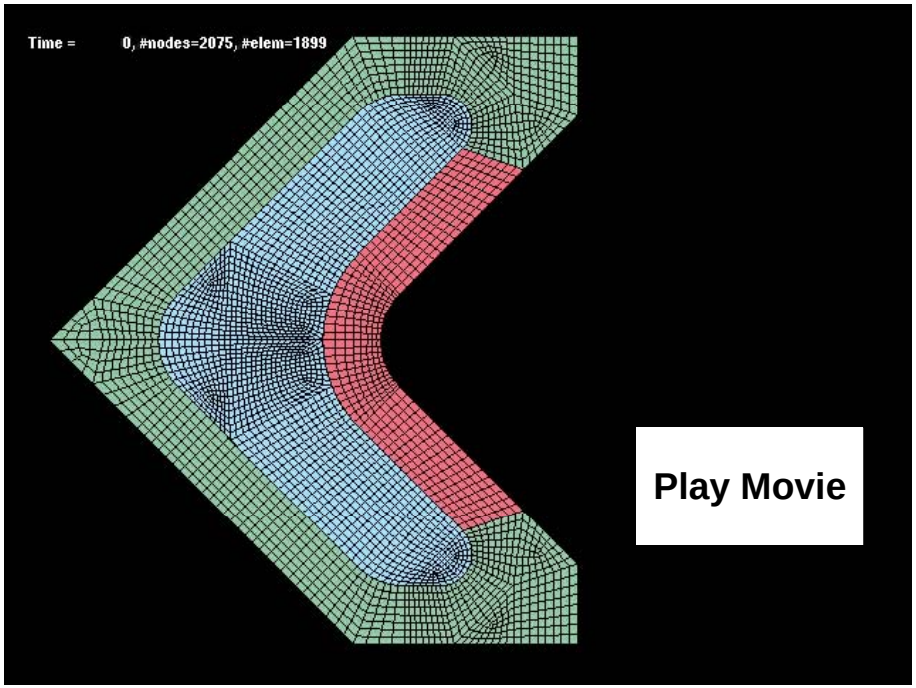

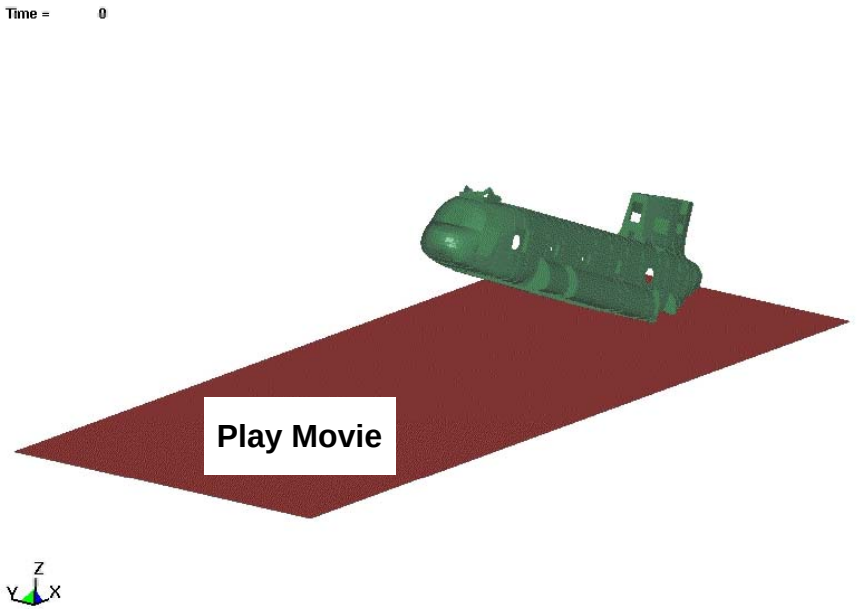

Shaped charge
Courtesy FEA Info & LSTC

CH47 Landing
Courtesy FEA Info & Boeing

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Computational Bottleneck

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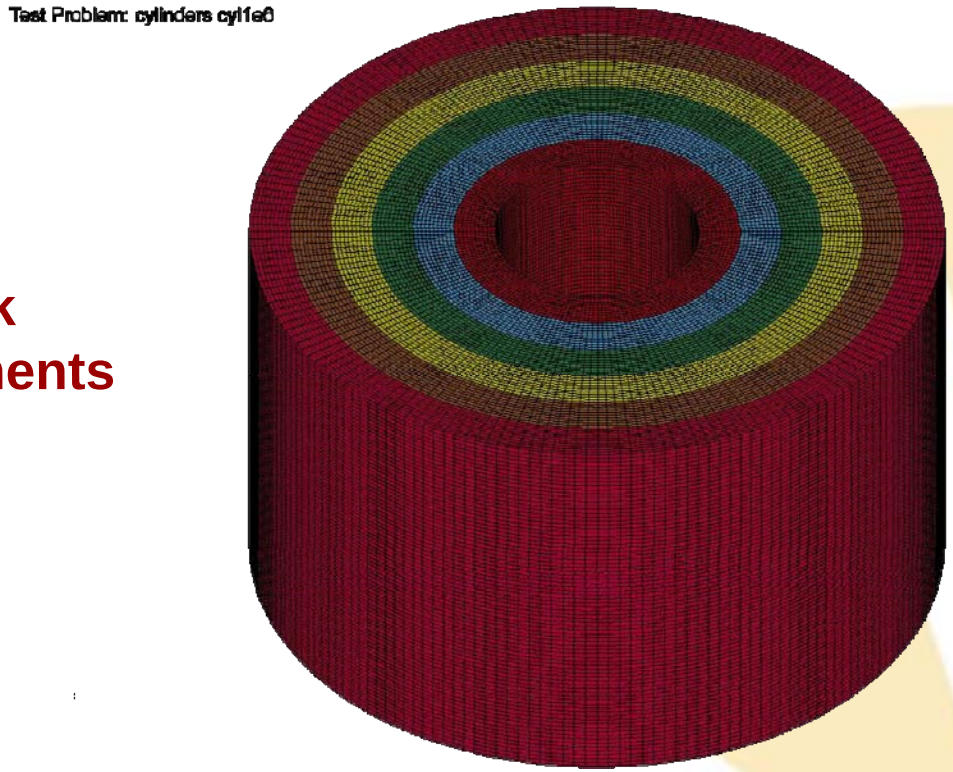
Total time	**2057 sec.**	
Linear solver	**1995 sec.**	**97%**
Factorization	**1981 sec.**	**96%**

AWE benchmark
230K 3D Finite Elements
Courtesy LSTC



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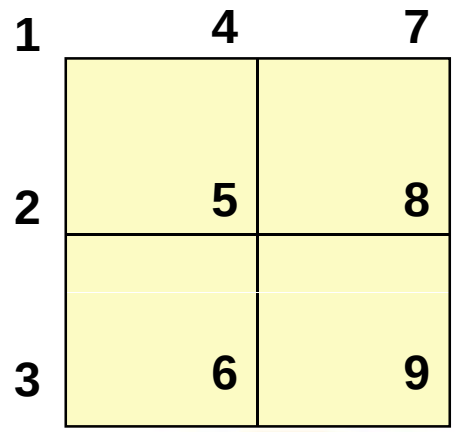
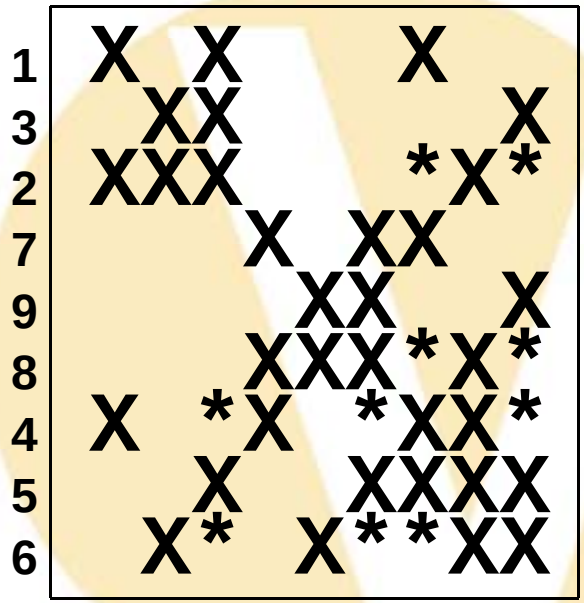
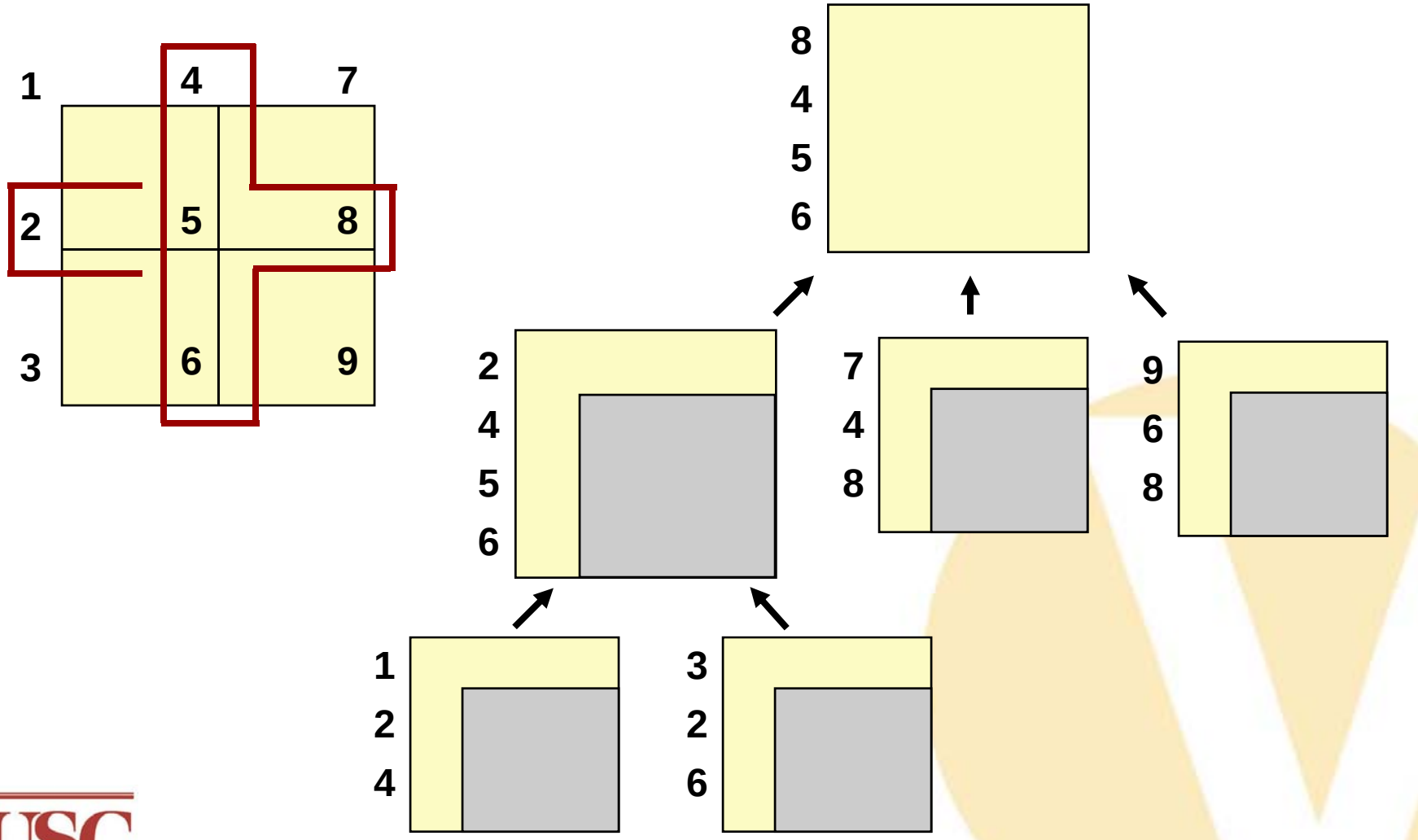
Toy Sparse Matrix

```
      do 4 k = 1, 9
        do 1 i = k + 1, 9
          a(i, k) = a(i,k) / a(k,k)
1       continue
        do 3 j = k + 1, 9
          do 2 i = k + 1, 9
            a(i,j) = a(i,j) -
     1                 a(i,k) *
     2                 a(k,j)
2         continue
3       continue
4     continue
```





Multifrontal View of the Toy Matrix



Duff and Reid, ACM TOMS 1983

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A Real Problem : “Hood”

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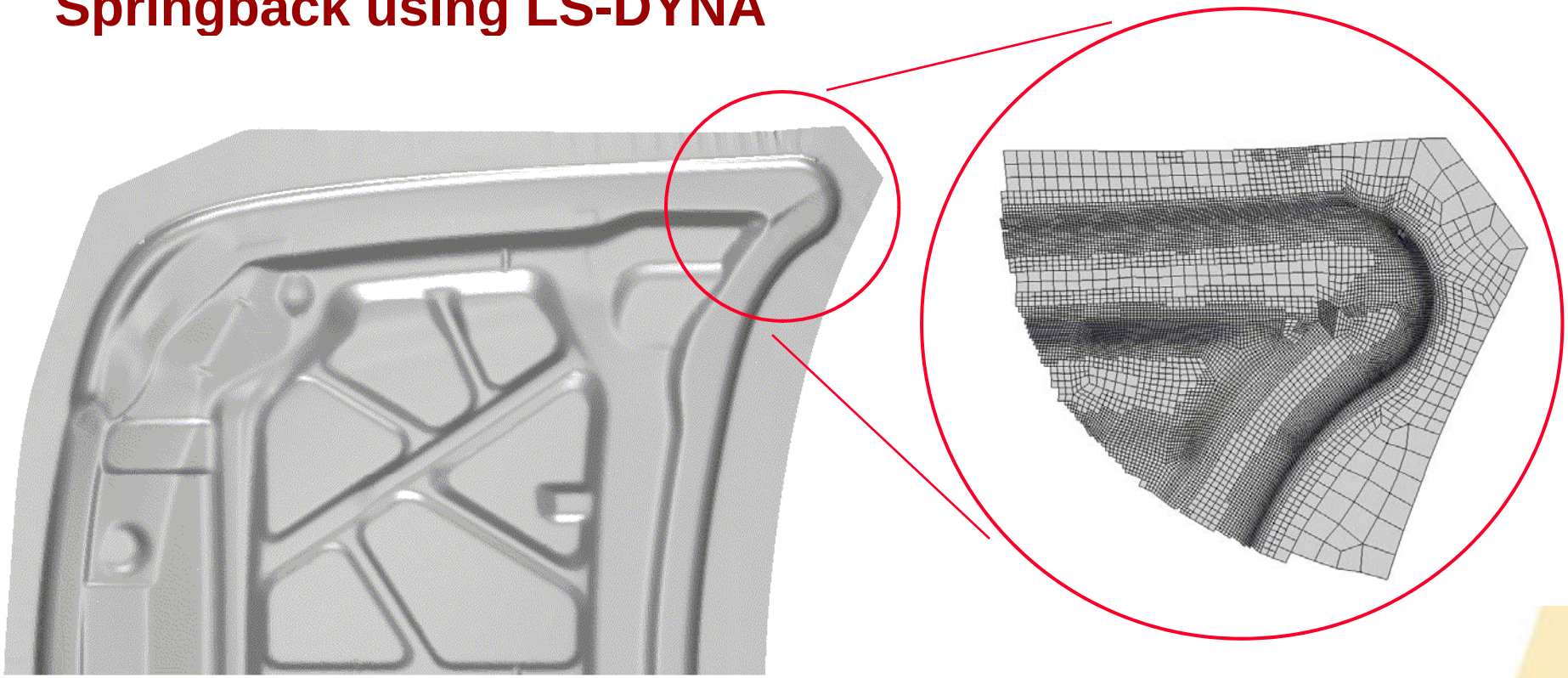
Automotive Hood Inner Panel Springback using LS-DYNA



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“Hood” Elimination Tree

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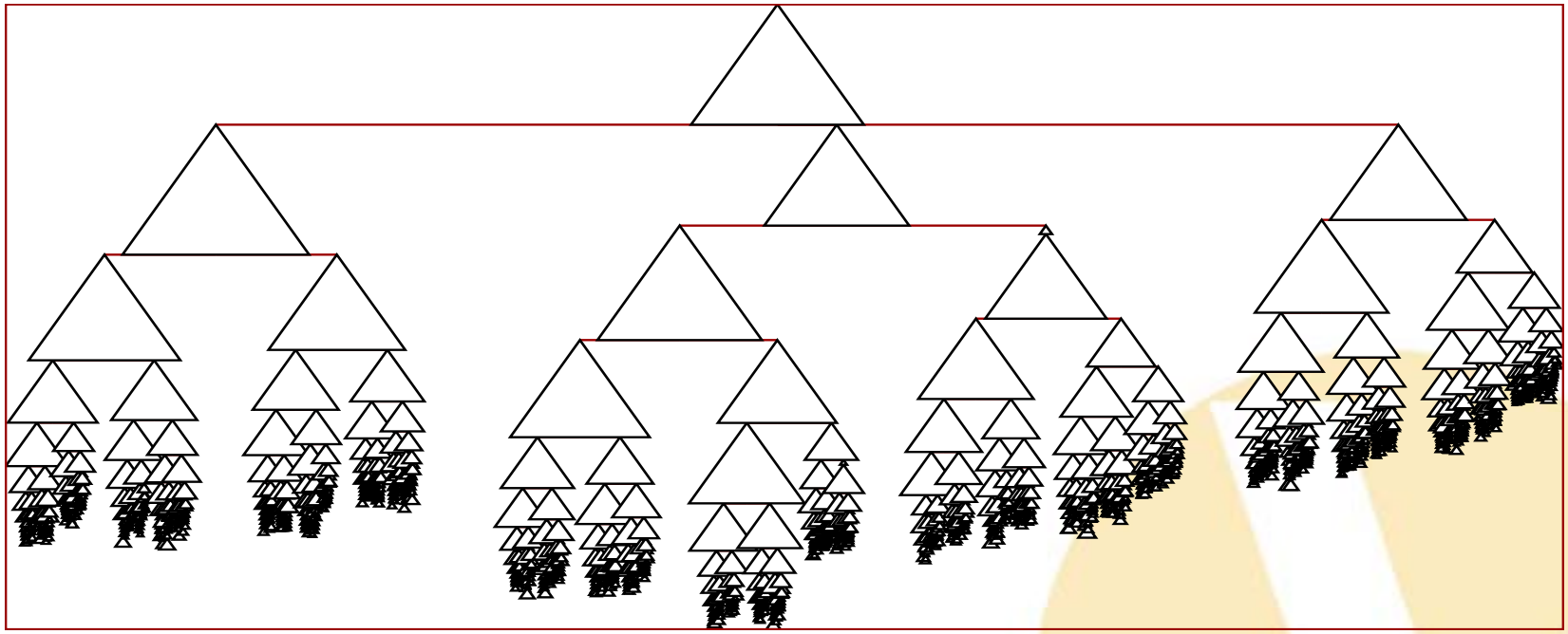

Each frontal matrix’s triangle scaled by operations required to factor it.

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Two Sources of Concurrency

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Concurrency within frontal matrices

- Small P => column wrap
- Large P => 2D (ala LINPACK benchmark)

Concurrency across elimination tree

- Frontal matrices only dependent on children
- “Subtree – subcube” typically used
- Limits communication

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Shared Memory Concurrency

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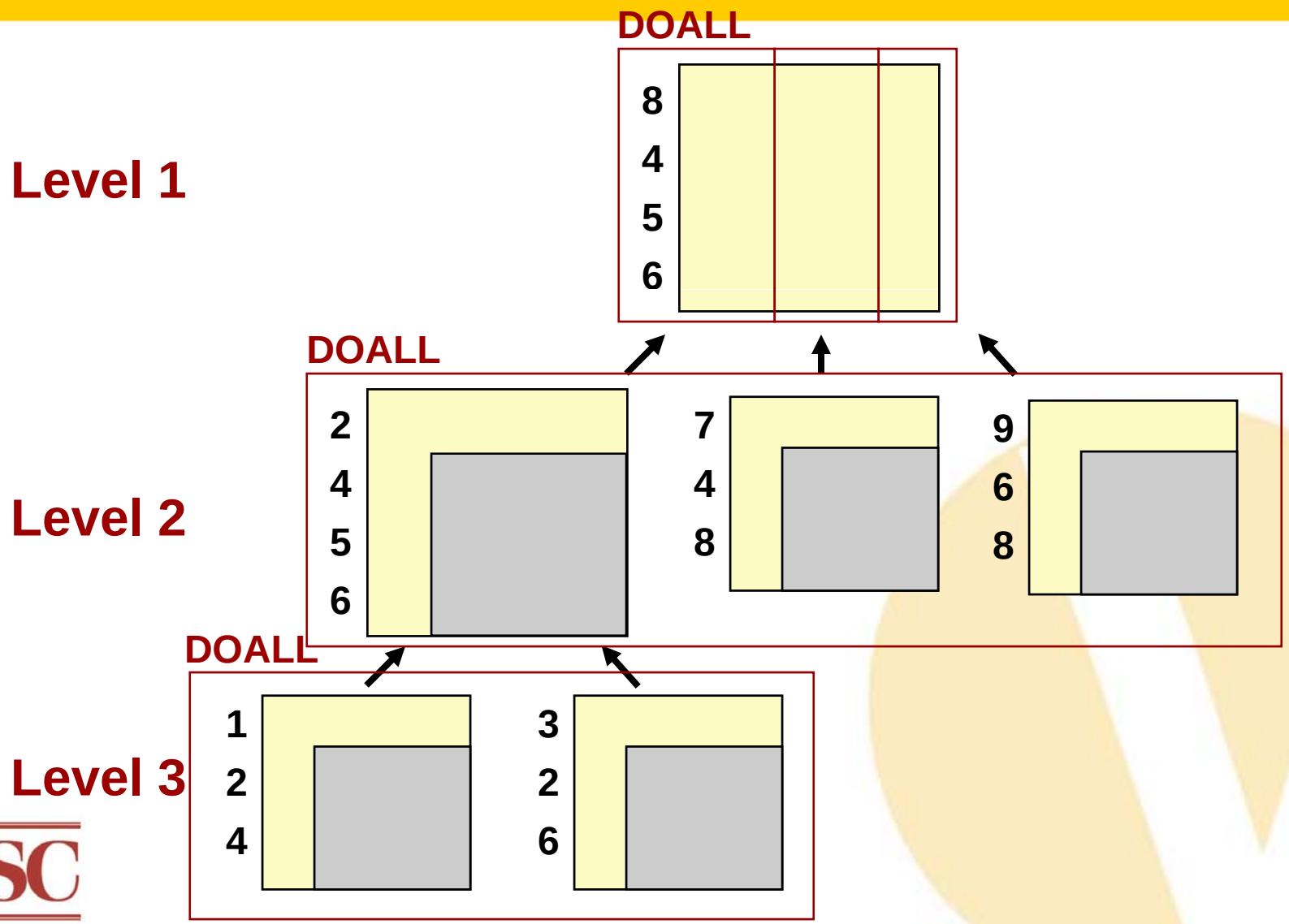

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Why Explore GPUs?

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Ubiquitous, cheap, high performance!

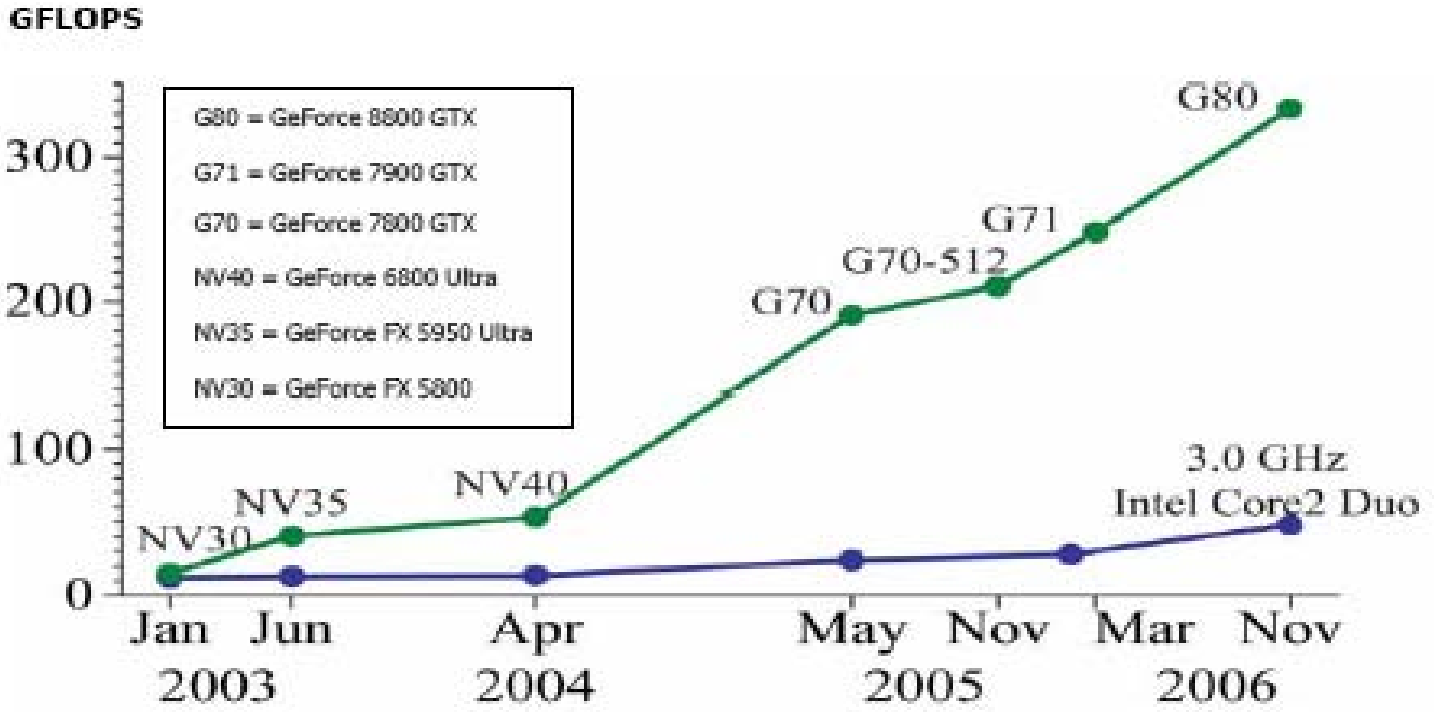

Figure 1-1. Floating-Point Operations per Second for the CPU and GPU

Courtesy NVIDIA

GPU Architecture

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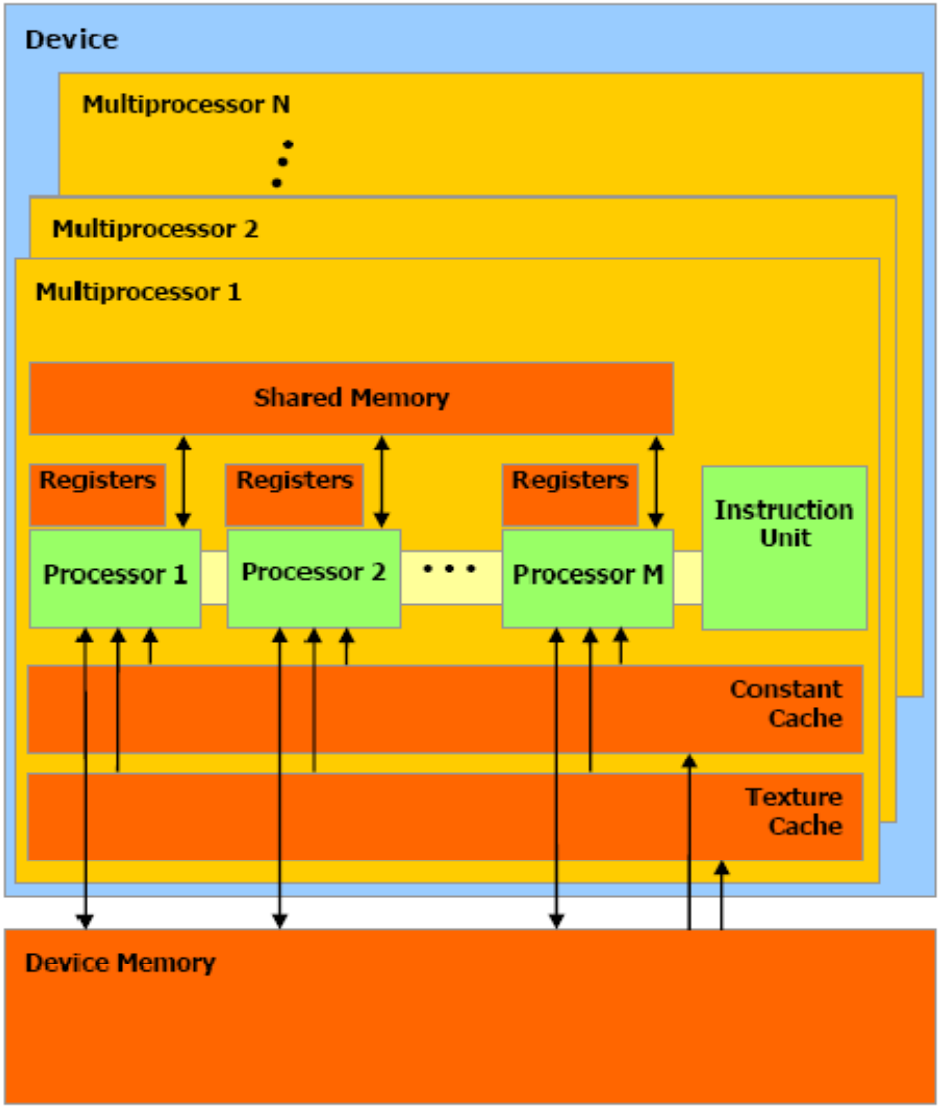
Multiple SIMD cores

Multithreaded
- **O(1000) per GPU**

Banked shared memory
- **16 Kbytes C1060**
- **48 Kbytes C2050**

Simple thread model
- **Only sync at host**



A set of SIMD multiprocessors with on-chip shared memory.

Figure 3-1. Hardware Model

Courtesy NVIDIA

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Fortran vs CUDA

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```
do j = jl, jr
  do i = jr + 1, ld
    x = 0.0
    do k = jl, j - 1
      x = x + s(i, k) * s(k, j)
    end do
    s(i, j) = s(i, j) - x
  end do
end do
```

```
ip=0;
for (j = jl; j <= jr; j++) {
  if(ltid <= (j-1)-jl){
    gpulskj(ip+ltid) = s[IDXS(jl+ltid,j)];
    }
  ip = ip + (j - 1) – jl + 1;
  }

__syncthreads();

for (i  = jr + 1 + tid; i <= ld;
     i += GPUL_THREAD_COUNT) {
  for (j = jl; j <= jr; j++) {
    gpuls(j-jl,ltid) = s[IDXS(i,j)];
    }
  ip=0;
  for (j = jl; j <= jr; j++) {
    x = 0.0f;
    for (k = jl; k <= (j-1); k++) {
      x  = x  + gpuls(k-jl,ltid) * gpulskj(ip);
      ip = ip + 1;
      }
      gpuls(j-jl,ltid) -= x;
    }
  for (j = jl; j <= jr; j++) {
    s[IDXS(i,j)] = gpuls(j-jl,ltid);
    }
  }
```

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Initial Experiment

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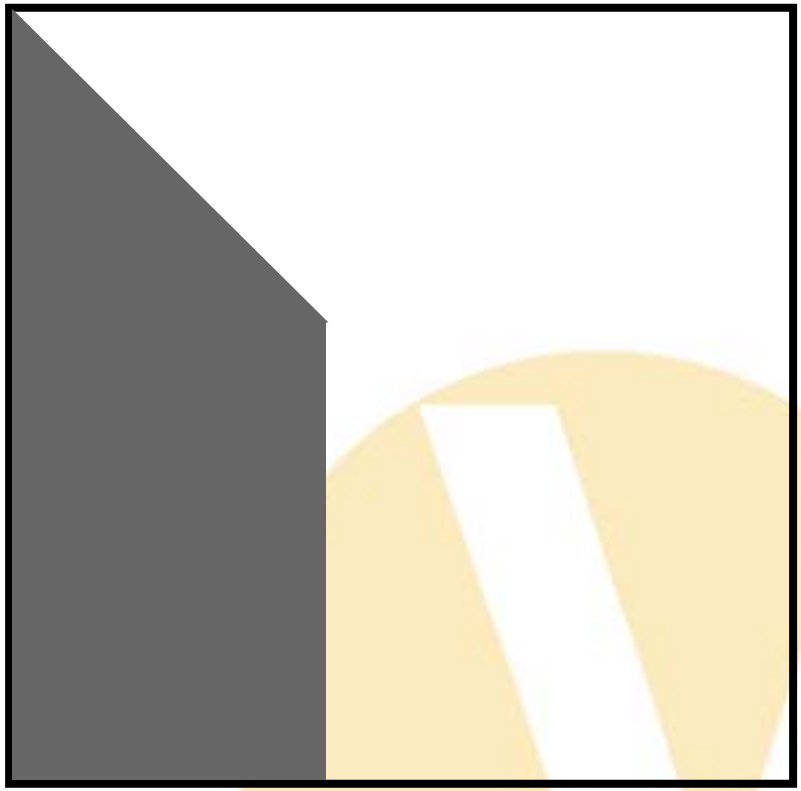
Assemble frontal matrix on host CPU

Initialize by sending panel of assembled frontal matrix

Only large frontal matrices due to high cost of sending data to and from GPU



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Eliminate panels

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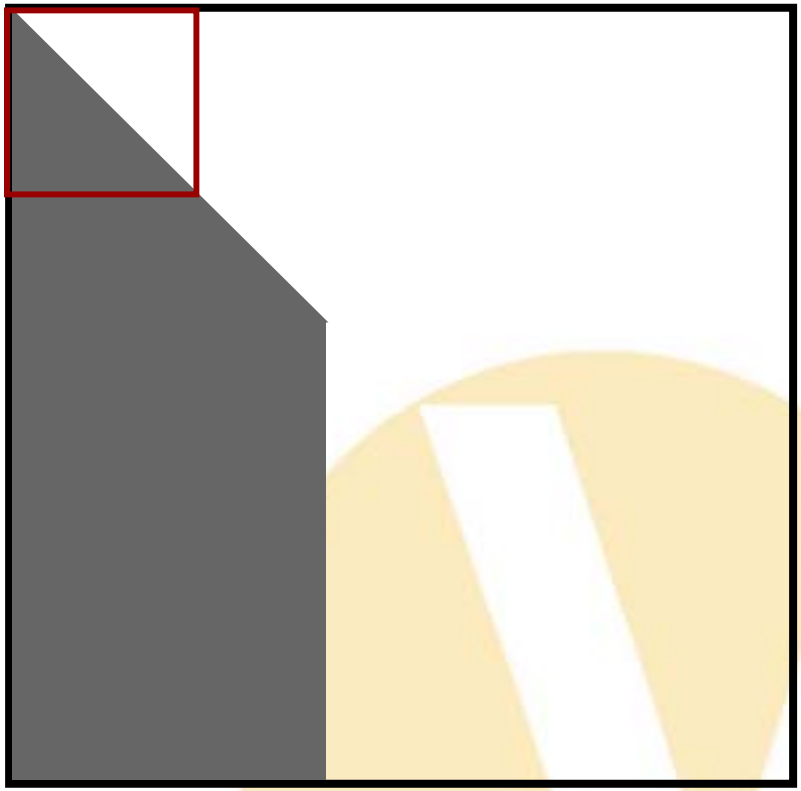
Factor diagonal block

Note: host is faster, but its better to avoid data transfer



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Eliminate panels

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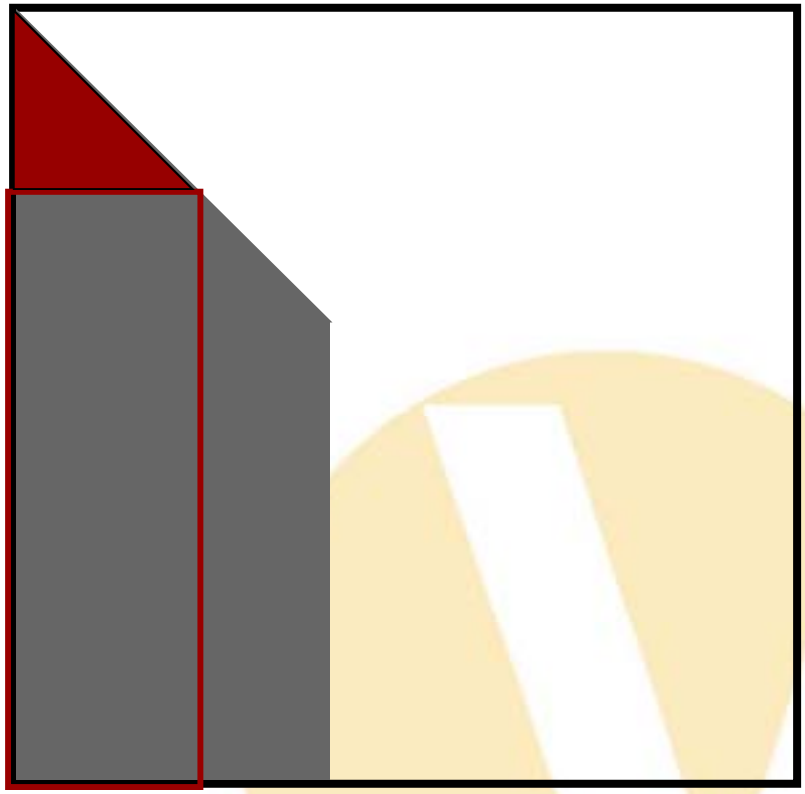
Eliminate off-diagonal panel

Earlier CUDA code



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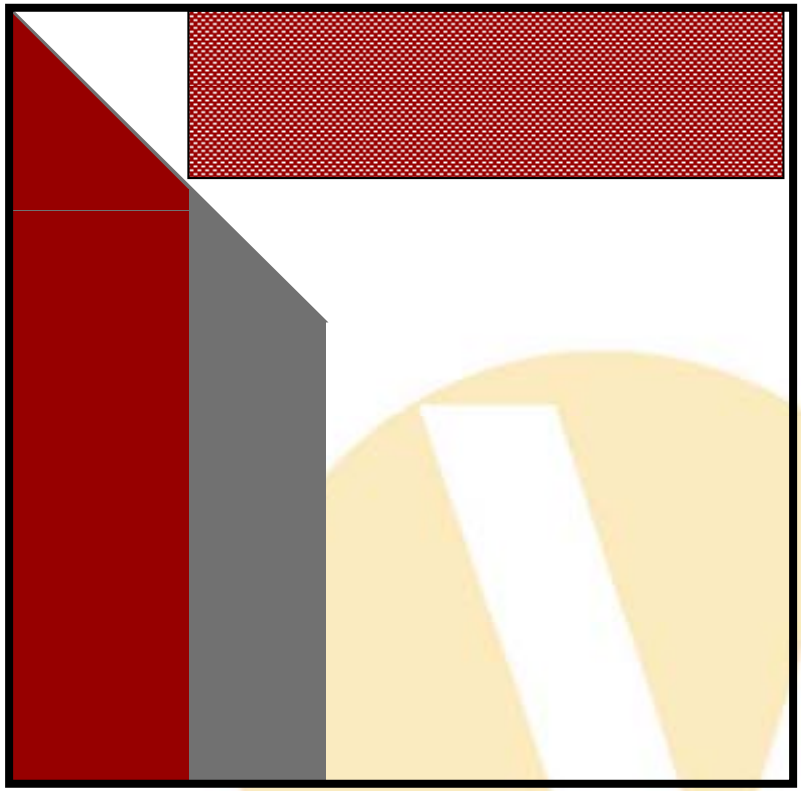
Fill Upper Triangle



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Update Schur Complement

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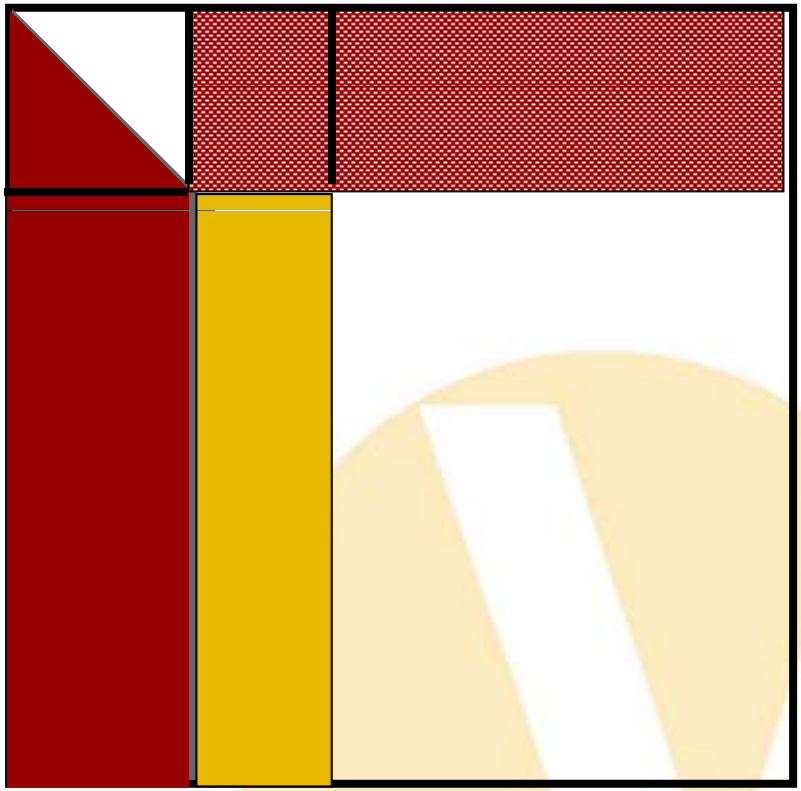
Update panels with DGEMM

DGEMM is extremely fast!

We've observed >100 GFlop/s
Tesla C2050 (i4r8)



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Update Schur Complement

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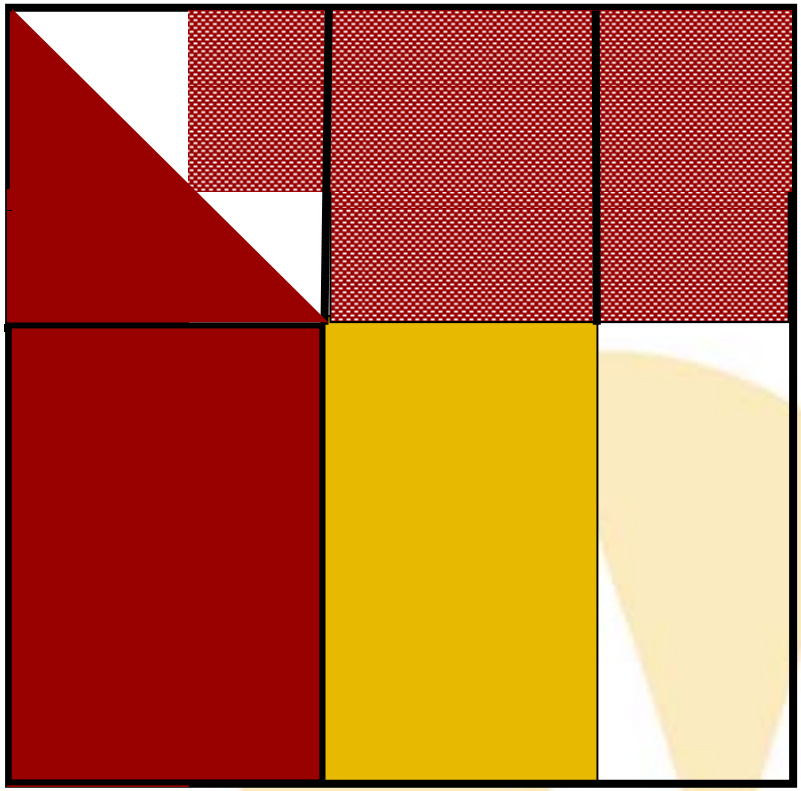
Wider panels in Schur complement

DGEMM is even faster



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Return Entire Frontal Matrix

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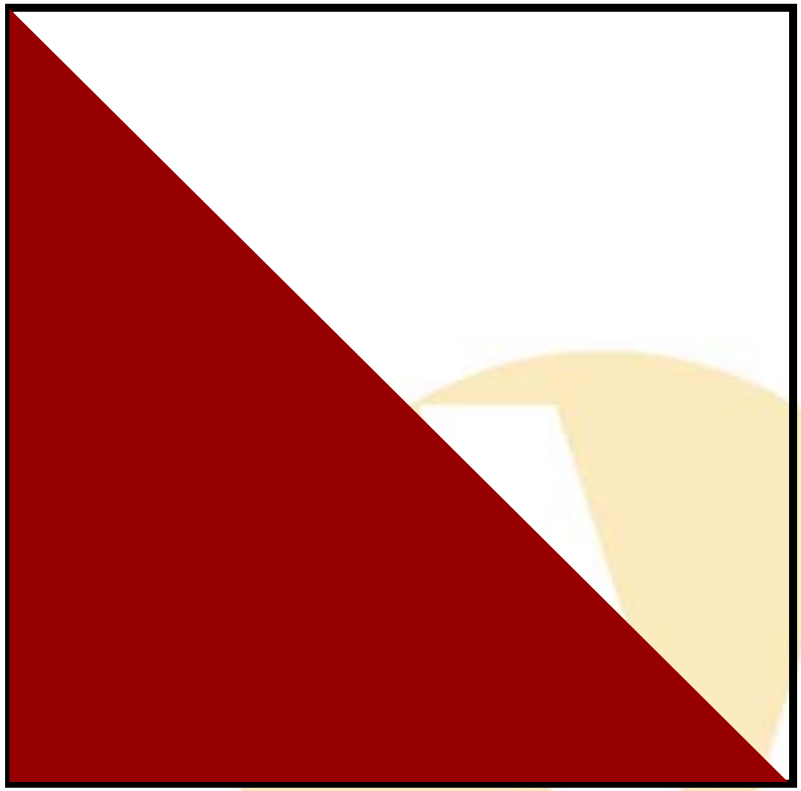
Return error if diagonal of 0.0 encountered or pivot threshold exceeded

Otherwise complete frontal matrix is returned

Schur complement added to initial values on host CPU



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Factoring a Frontal Matrix Timing on C1060 (i4r4)

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Method Name	GPU msec	%GPU time
Copy data to and from GPU	201.0	32.9%
Factor 32x32 diagonal blocks	42.6	7.0%
Eliminate off diagonal panels	37.0	6.1%
Update with SGEMM	330.6	54.1%
Total time	611.4	100.0%

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Calibrating Expectations
Dense Kernel Performance

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Intel Nehalem Host

2 sockets * 4 cores * {4,2} ALUs * 2.6 GHz

We get ~80 GFlop/s (r4) and 53 GFlop/s (r8)

NVIDIA Tesla C1060

30 processors * {8,1} ALUs * 1.3 GHz

We get 170 GFlop/s (r4)

NVIDIA Tesla C2050 (aka, Fermi)

28 processors * {16,8} ALUs * 1.15 GHz

We get 97 GFlop/s (r8)

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Kernel Performance (i4r8) C2050 vs 8 Nehalem Cores

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Upper GPU, lower CPU - red means GPU is faster

		Update	Order	
Degree	1024	2048	3072	4096
512	N/A 22.8	23.5 47.0	32.3 49.9	42.0 51.5
1024	22.3 43.2	42.5 48.1	57.0 50.5	66.7 51.8
1536	36.2 42.2	55.5 49.0	68.8 49.9	77.3 52.0
2048	47.9 46.8	66.6 49.8	78.2 51.2	86.1 52.2
2560	57.0 48.0	73.9 50.3	83.6 51.5	91.5 52.0
3072	65.6 49.0	80.1 50.8	89.0 51.4	97.4 52.6

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What goes on GPU?

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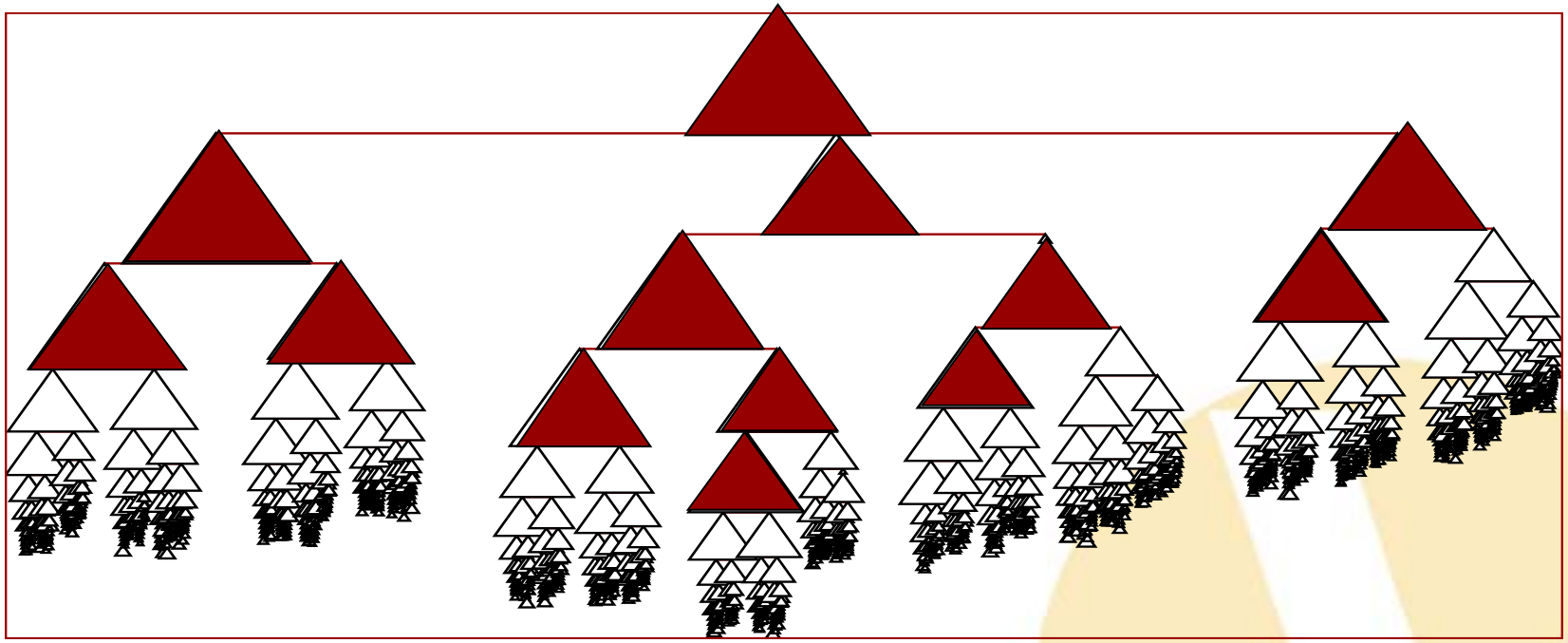

Handful of large supernodes near the root of the tree

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Computational Bottleneck

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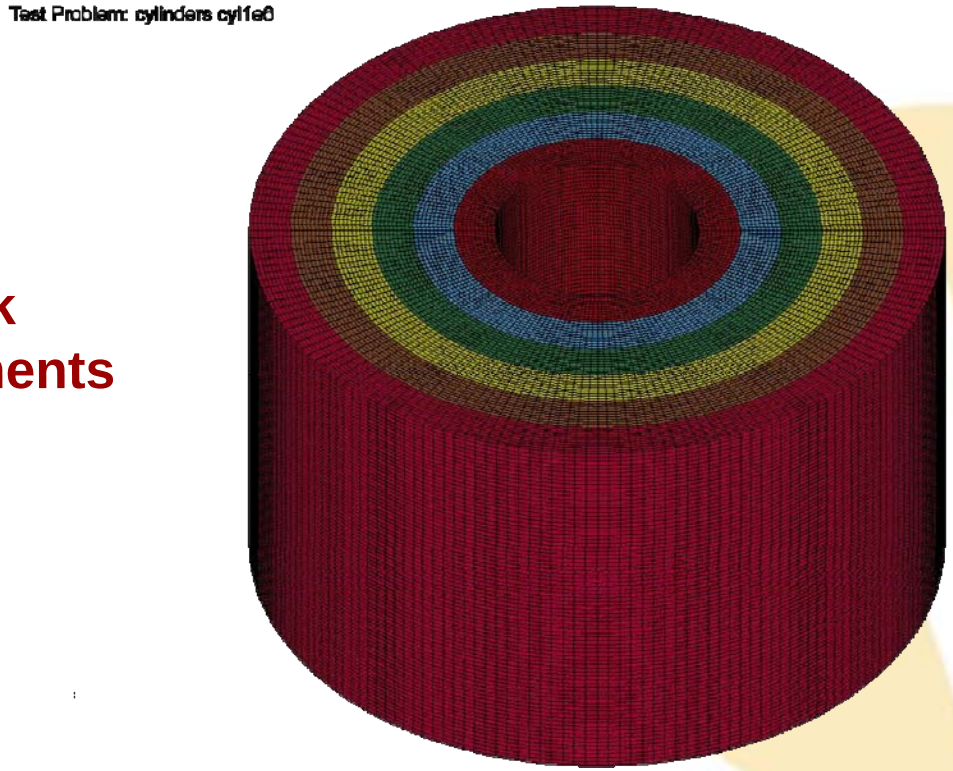
Total time	**2057 sec.**	
Linear solver	**1995 sec.**	**97%**
Factorization	**1981 sec.**	**96%**
Suitable for GPU?		**88%**



AWE benchmark
230K 3D Finite Elements
Courtesy LSTC

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Number of Supernodes & Factor Operations in Tree

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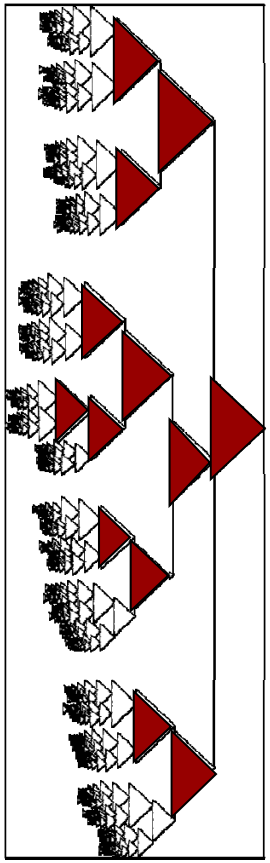

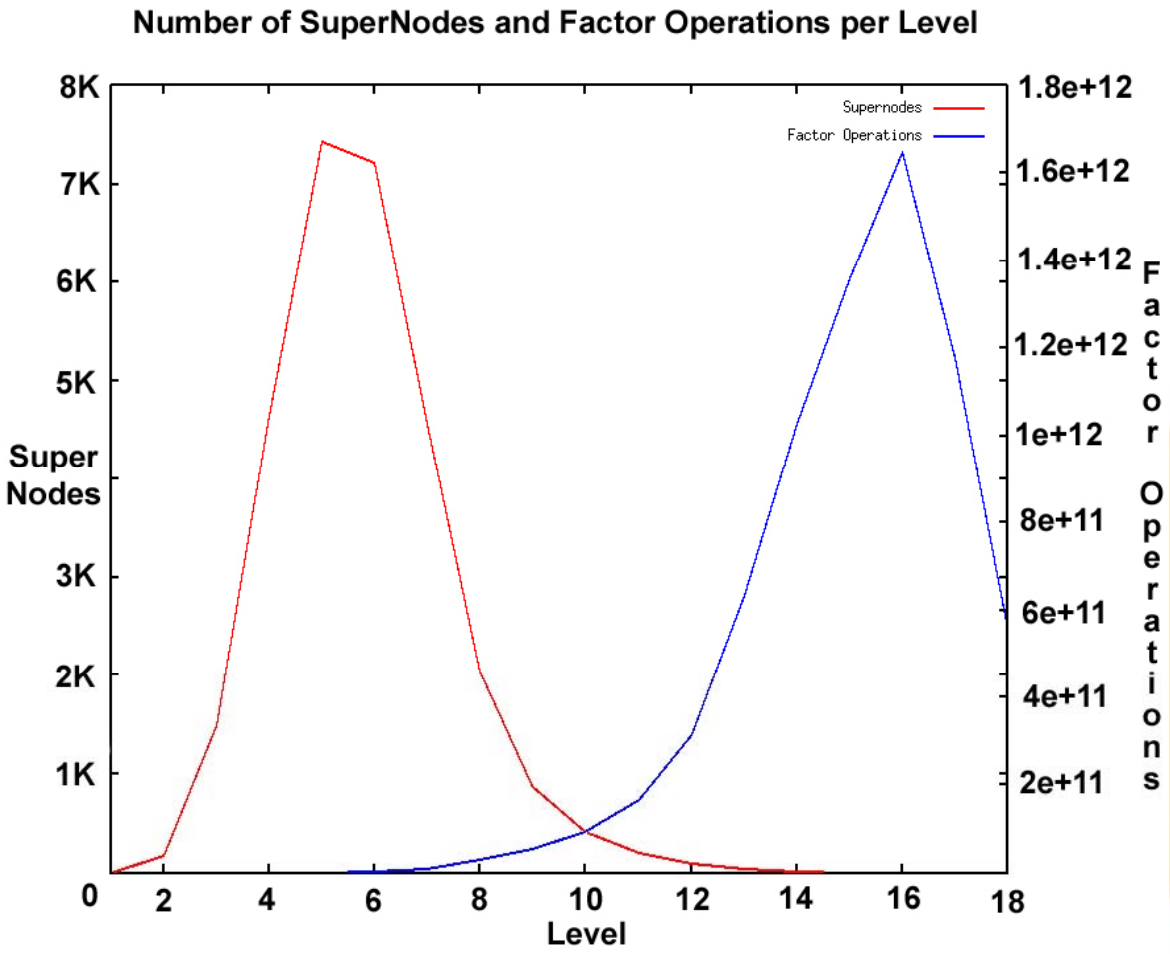

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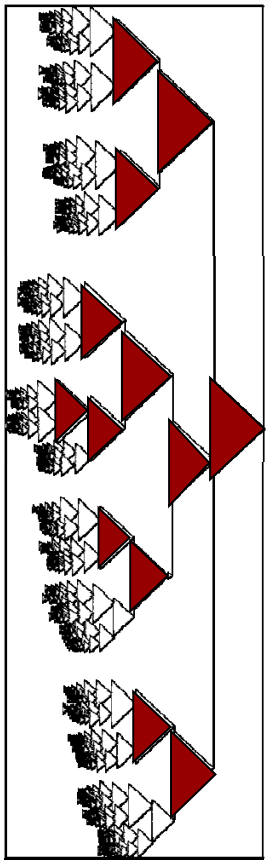
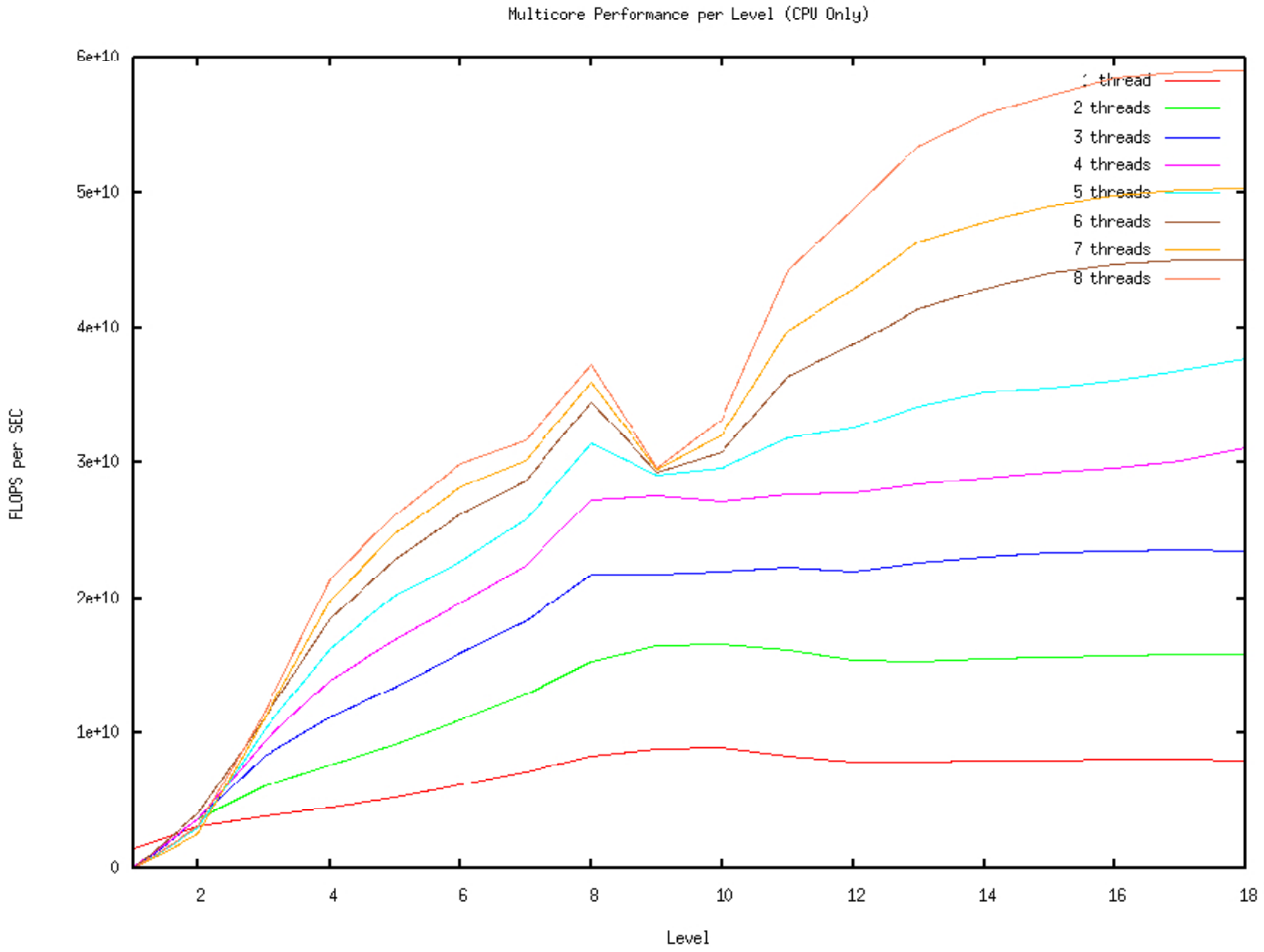
Multicore Performance (i4r4) vs. the Elimination Tree





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LS-DYNA Implicit CPU vs. CPU & GPU (i8r8)

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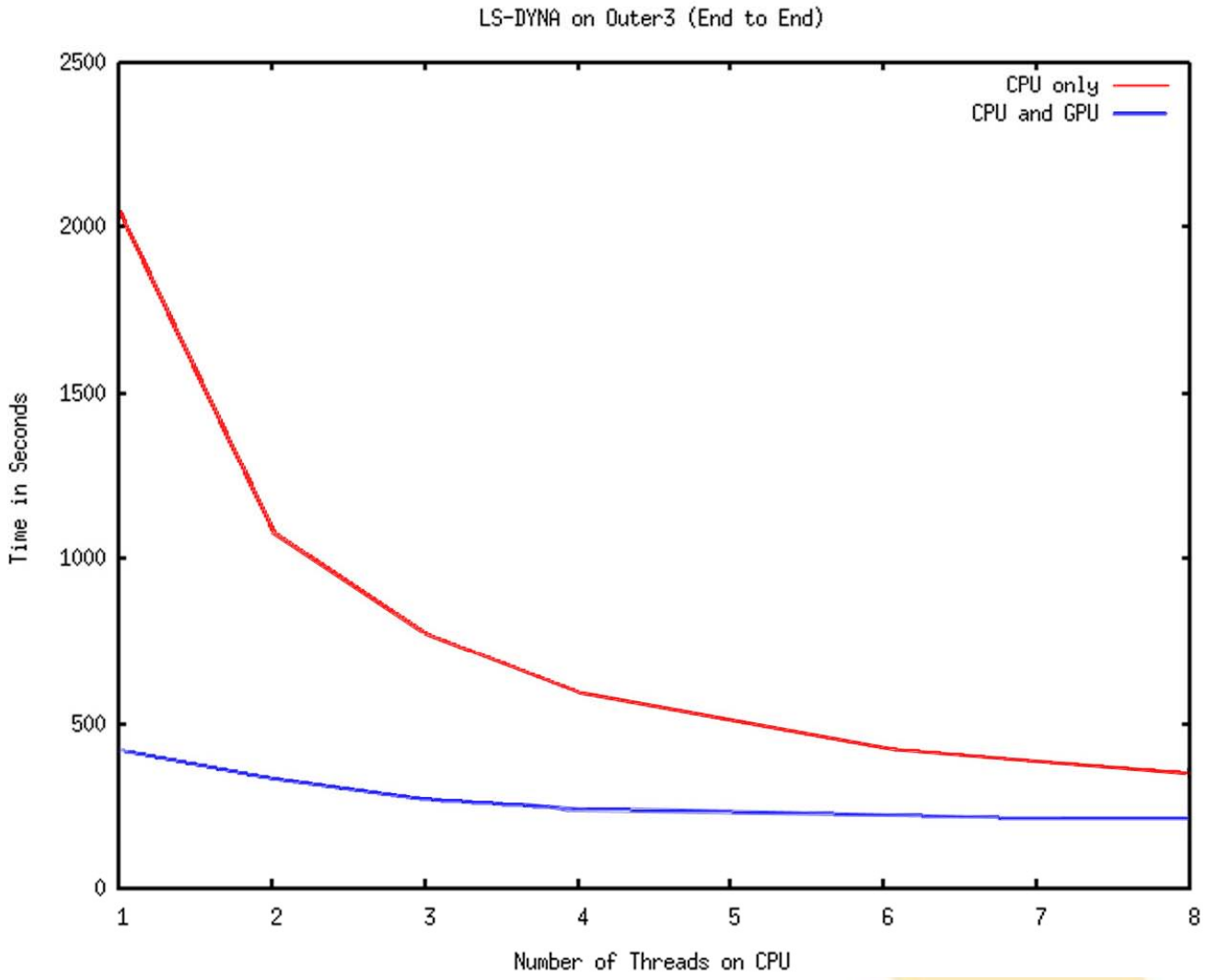

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Near-term Future Bigger Problems

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- Problems that don't fit in GPU memory
  - Out-of-core to host memory?
- Performance Optimization
  - Better NVIDIA libraries
  - Re-optimize our CUDA kernel
  - Overlap computation & communication
- Pivoting for numerical stability
- Distributed memory (e.g., MPI)
  - One GPU per Supernode
  - Kernel with MPI and GPUs

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CUBLAS 3.2 is Faster

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CUBLAS 3.2 based on UTK's MAGMA

We've seen:

- **SGEMM 398 Gflop/s**
- **DGEMM 231 Gflop/s**

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Longer-term Future Smaller Problems

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- Factor smaller frontal matrices on GPU
  - Maintain real stack on GPU
  - Assemble initial values on GPU
- If the entire matrix fits on the GPU
  - Forward and back solves
  - Exploit GDRAM memory B/W

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Summary

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- **Factoring large frontal matrices on Nvidia C2050**
  - **Sped up LS-DYNA implicit**
  - **Another factor of 2X likely**
  - **Explicit will be much harder**
- **Similar results for other implicit MCAE codes**
  - **BCSLIB-GPU too**
- **ISVs slowly to come to market**
  - **Modest speedup**
  - **Support and pricing issues**

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