TASK-BASED SPARSE DIRECT SOLVER FOR SYMMETRIC INDEFINITE SYSTEMS

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Rutherford Appleton Laboratory

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Where A is a large, sparse and symmetrically-structured matrix

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- SpLDLT: for symmetric systems:
  - positive-definite (LL^T)
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- SpLDLT: for symmetric systems:
  - positive-definite (LL^T)
  - indefinite (LDL^T)
- SpLU: for unsymmetric (LU) systems

Heterogenous CPU-GPU systems

Heterogeneous CPU-GPU architectures have been increasingly popular in the HPC community over the past few years:

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- ▼ Limited memory available on the device (16GB on V100)
- ▼ CPU $\leftrightarrow$ GPU memory transfer potentially slow
  e.g. PCIe 10$\times$ slower than NVLink but still common

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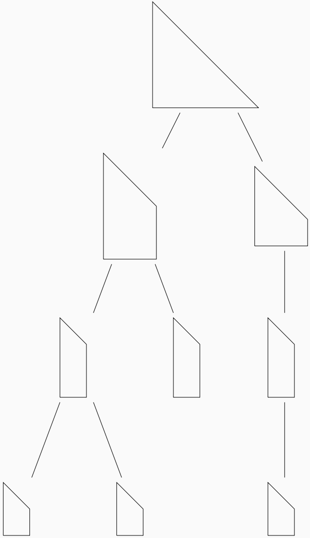
Sparse direct methods: parallelism

The multifrontal factorization is achieved with a topological traversal of the elimination tree:

1. Assemble the contributions from the descendant
2. Factor the column associated with the current node
3. Form the contribution blocks



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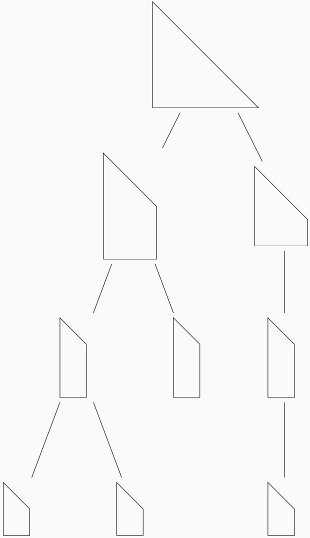
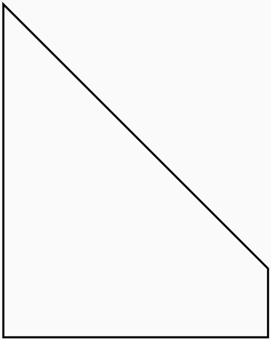
For the factorization and the solve phases, the sources of parallelism in the *elimination tree* include:

- Tree parallelism: nodes in independent branches can be processed concurrently
- Node parallelism: when a node is large enough, it may be processed in parallel



MULTIFRONTAL FACTORIZATION FOR MULTICORE CPUS

Dense Cholesky factorization on multicore CPUs



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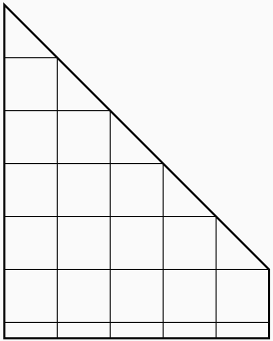

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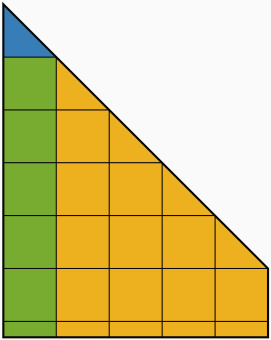

Factor diagonal block $A_{kk} = L_{kk} L_{kk}^T$

Apply pivots $L_{ik} = A_{ik} L_{kk}^{-T}$

Update trailing sub-matrix $A_{ij} -= L_{ik} L_{jk}^T$

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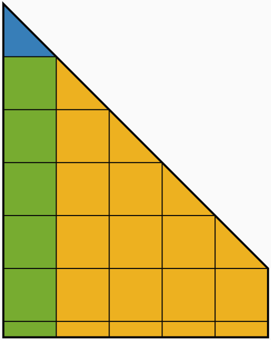

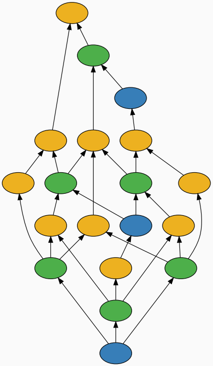

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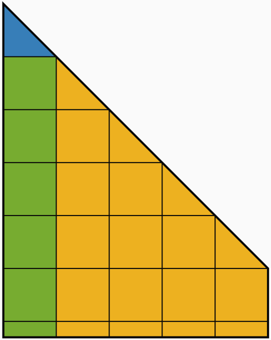

Indefinite systems: small diagonal elements and/or large off-diagonal elements might cause a lose of accuracy

Factor	diagonal block $A_{kk} = L_{kk} L_{kk}^T$
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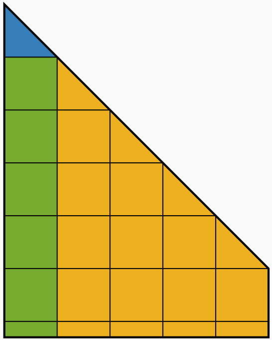

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$\Longrightarrow$ avoid it by using pivoting

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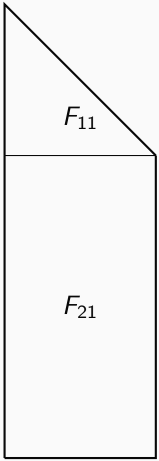
Pivoting strategies

Two main pivoting strategies for the LDL^T factorization:



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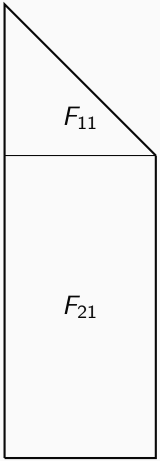

- Threshold Partial Pivoting (TPP)
  - ▲ Ensures that $|l_{ij}| < u^{-1}$ for some threshold u
  - ▼ Requires global communication on each columns
  - ○ Used in `HSL_MA97`

Numerically robust but hard to parallelize

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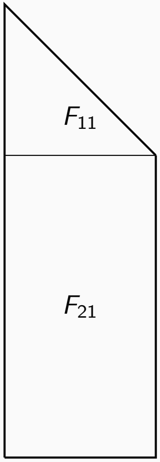

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  Numerically robust but hard to parallelize

- Supernode Bunch-Kaufmann (SBK)
  - ▲ Performs pivoting in only within F_{11} using Bunch-Kaufmann algorithm
  - ▼ Requires the use of a pivots perturbation strategy
  - ○ Scaling and ordering techniques may be used to alleviate this problem
  - ○ Used in `PARDISO`

  Plenty of parallelism but potentially unstable

A Posteriori Threshold Pivoting

A Posteriori Threshold Pivoting (APTP) strategy: improve the parallelism of TPP while preserving numerical stability of the factorization

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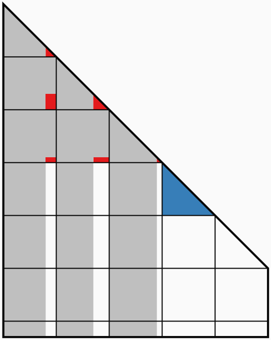

- Factor diagonal block using complete pivoting

```
do k = 1, nblk
  ! Factor diagonal block
  call Factor(A(k,k):RW, nelim_k)

end do
```

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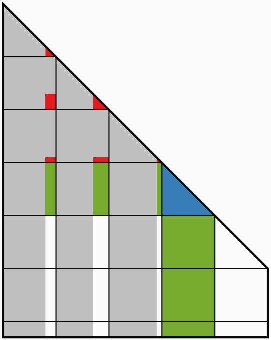

- Apply pivots in parallel using speculative execution

```
do k = 1, nblk
  ! Factor diagonal block
  call Factor(A(k,k):RW, nelim_k)
  ! Compute factors sub-diagonal on blocks
  do j = k+1, mblk
    call ApplyN(A(k,j):RW, A(k,k):R, nelim_k)
  end do
  ! Compute factors left-diagonal on blocks
  do j = 1, k-1
    call ApplyT(A(k,j):RW, A(k,k):R, nelim_k)
  end do









end do
```

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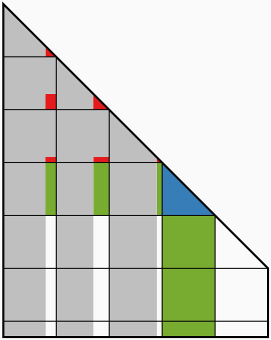

- Determine the number of successfully eliminated pivots w.r.t threshold u^{-1}

```
do k = 1, nblk
  ! Factor diagonal block
  call Factor(A(k,k):RW, nelim_k)
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  do j = k+1, mblk
    call ApplyN(A(k,j):RW, A(k,k):R, nelim_k)
  end do
  ! Compute factors left-diagonal on blocks
  do j = 1, k-1
    call ApplyT(A(k,j):RW, A(k,k):R, nelim_k)
  end do
  ! Compute nelim_k
  call Adjust(A(:,k):R, nelim_k)
end do
```

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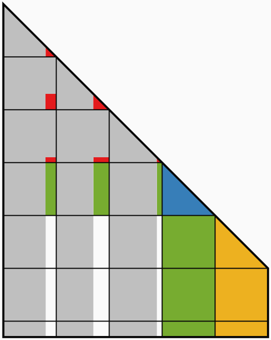

- Update blocks in the trailing sub-matrix

```
do k = 1, nblk
  ! Factor diagonal block
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  do j = k+1, mblk
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  end do
  ! Compute factors left-diagonal on blocks
  do j = 1, k-1
    call ApplyT(A(k,j):RW, A(k,k):R, nelim_k)
  end do
  ! Compute nelim_k
  call Adjust(A(:,k):R, nelim_k)
  ! Update trailing sub-matrix
  do j = k, nblk
    do i = j, mblk
      call UpdateNN(A(i,k):R, A(j,k):R, A(i,j):RW,
                    nelim_k)
    end do
  end do
end do
```

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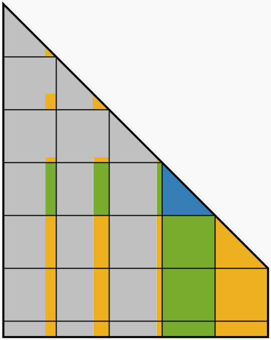

- Update uneliminated and failed entries in the left-diagonal blocks

```
do k = 1, nblk
  ! Factor diagonal block
  call Factor(A(k,k):RW, nelim_k)
  ! Compute factors sub-diagonal on blocks
  do j = k+1, mblk
    call ApplyN(A(k,j):RW, A(k,k):R, nelim_k)
  end do
  ! Compute factors left-diagonal on blocks
  do j = 1, k-1
    call ApplyT(A(k,j):RW, A(k,k):R, nelim_k)
  end do
  ! Compute nelim_k
  call Adjust(A(:,k):R, nelim_k)
  ! Update trailing sub-matrix
  do j = k, nblk
    do i = j, mblk
      call UpdateNN(A(i,k):R, A(j,k):R, A(i,j):RW,
                    nelim_k)
    end do
  end do
  ! Update uneliminated entries on left-diagonal
  ! blocks
  do j = 1, k-1
    do i = j, k-1
      call UpdateTT(A(k,i):R, A(k,j):R, A(i,j):RW,
                    nelim_k)
    end do
    do i = k, mblk
      call UpdateTT(A(i,k):R, A(k,j):R, A(i,j):RW,
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    end do
  end do
end do
```

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   - ▼ Backups of entries $\Longrightarrow$ increased memory footprint
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2. Failed-in-place approach: keep the failed columns in place:
   - ▲ Dramatically reduce data movement
   - ▼ Failed entries must be kept up-to-date $\Longrightarrow$ Reduced granularity

Parallel multifrontal factorization for multicore CPUs

SpLDLT implements a multifrontal factorization using a Sequential Task Flow (STF) model

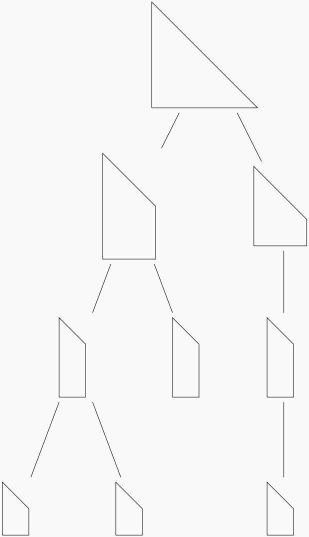
```
do n = 1, nnodes ! Topologically ordered
   ! Allocate memory
   call activate(front(n));
   ! Assemble fully-summned columns
   call assemble(front(n), children(n));
   ! Compute factors
   call factor(front(n));
   ! Assemble contribution block
   call assemble_contrib(front(n), children(n));
end do

! Wait for completion of submitted tasks
call task_wait_for_all();
```

- `assemble`
  1. Allocate memory (fully-summed and contribution blocks)
  2. Assemble contributions from children nodes into fully-summed columns
- `factor` Factorize the fully-summed columns and form the contribution blocks
- `assemble_contrib` Assemble contributions from children nodes into contribution blocks

MULTIFRONTAL FACTORIZATION FOR GPU DEVICES

Multifrontal factorization for GPU devices



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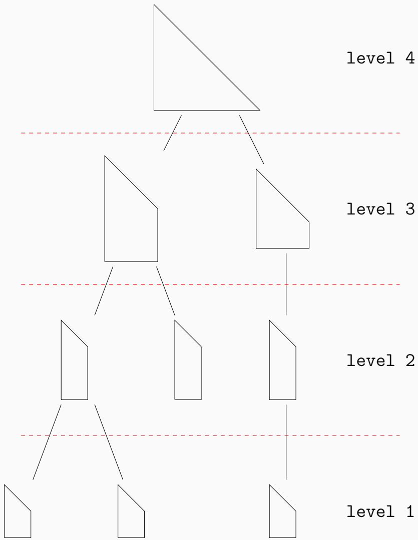

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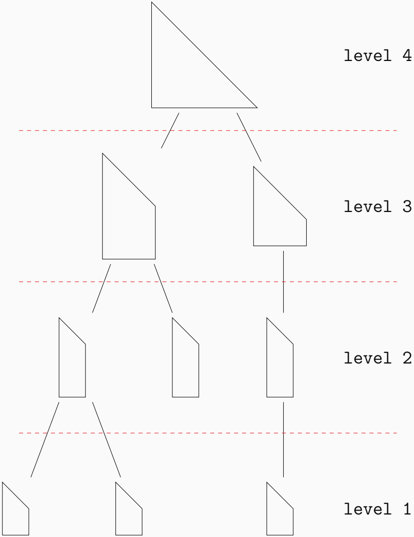


```
do lvl = 1, nlevels
   ! Allocate memory
   call activate_lvl(fronts(lvl))
   ! Assemble fully-summned columns
   call assemble_lvl(fronts(lvl), child(lvl))
   ! Compute factors
   call factor_lvl(fronts(lvl))
   ! Assemble contribution block
   call assemble_cb_lvl(fronts(lvl), child(lvl))
end do
```

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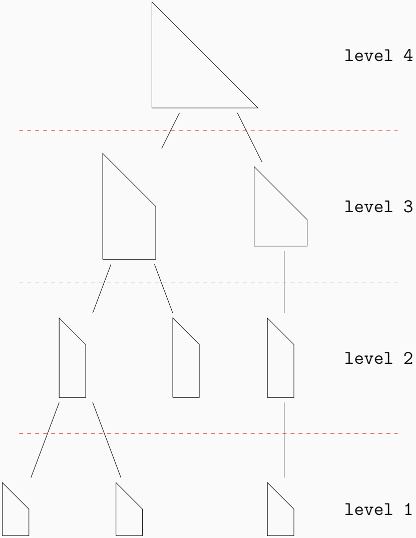


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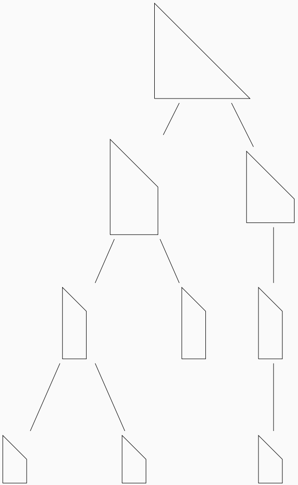
   ! Assemble contribution block
   call assemble_cb_lvl(fronts(lvl), child(lvl))
end do
```

```
chol_gpu: do jj = 1, n(lvl), nb
   do kk = jj, jj+nb, ib
      ! Factor inner panel
      call potrf_gpu_batched(lvlnodes(kk))
      ! Update inner panel
      call syrk_gpu_batched(lvlnodes(kk))
      ! Update trailing submatrix
   end do
   call syrk_gpu_batched(lvlnodes(jj), &
        lvlnodes(jj+nb))
end do chol_gpu
```

HETEROGENEOUS CPU-GPU MULTIFRONTAL FACTORIZATION

Heterogeneous CPU-GPU multifrontal factorization



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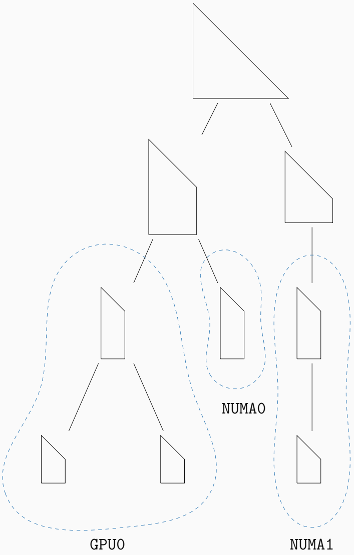
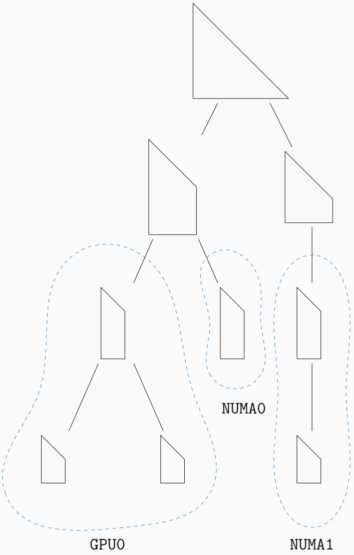


- Partition the assembly tree between NUMA regions and GPU devices

Heterogeneous CPU-GPU multifrontal factorization



- Partition the assembly tree between NUMA regions and GPU devices
- balance $= \dfrac{\max_i(w_i \quad)}{\frac{1}{n_{\mathrm{res}}}\sum_j(w_j \quad)}$

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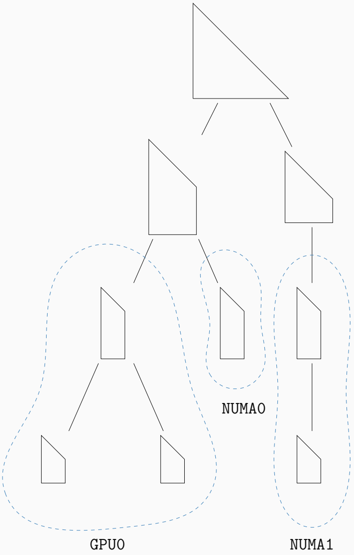

- Partition the assembly tree between NUMA regions and GPU devices
- balance $= \frac{\max_i (w_i/\alpha_i)}{\frac{1}{n_{\text{res}}}\sum_j (w_j/\alpha_j)}$
  - $\alpha_i = 1.0$ for NUMA regions
  - $\alpha_i = Perf_{GPU}/Perf_{CPU}$ for GPU devices

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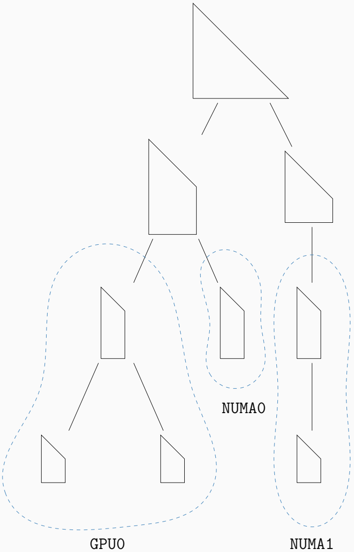

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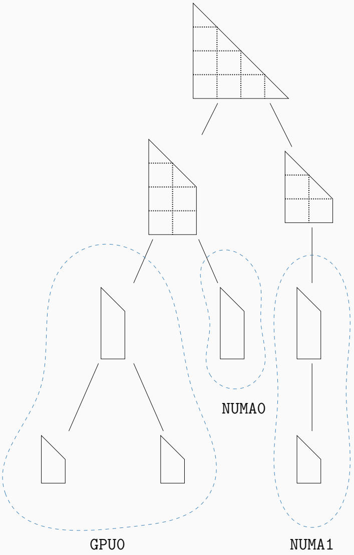
  - $\alpha_i = Perf_{GPU}/Perf_{CPU}$ for GPU devices
- Within subtree:
  - NUMA partition: task-based factorization
  - GPU partition: batched factorization

Heterogeneous CPU-GPU multifrontal factorization



- Partition the assembly tree between NUMA regions and GPU devices
- balance $= \frac{\max_i(w_i/\alpha_i)}{\frac{1}{n_{\text{res}}}\sum_j(w_j/\alpha_j)}$
  - $\alpha_i = 1.0$ for NUMA regions
  - $\alpha_i = Perf_{GPU}/Perf_{CPU}$ for GPU devices
- Within subtree:
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  - GPU partition: batched factorization
- Root partition: use task-based factorization where tasks run either on a CPU core or in a GPU stream

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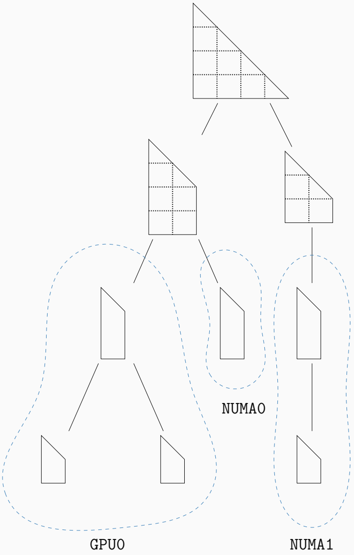

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SpLDLT implementation details:

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▲ Exploitation of data locality within each subtree

▲ Reduce the impact of the cost for the CPU $\leftrightarrow$ GPU memory transfers

NUMERICAL EXPERIMENTS

Numerical experiments

Experimental setup:

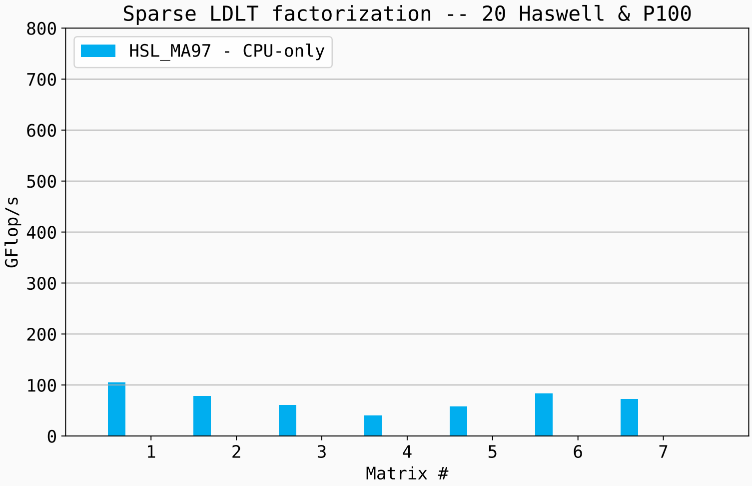
- 20 cores Intel Haswell machine (2 x E5-2695 v3)
- 1 NVIDIA Pascal P100
- 64 GB of RAM
- GNU compilers 7.1.0 with flags "-g -O2 -march=native"
- Intel MKL BLAS 11.3.1
- Metis 4.0.3

Numerical experiments: Sparse LDL^T factorization

#	Problem	n $\times 10^3$	$nz(A)$ $\times 10^6$	$nz(L)$ $\times 10^6$	*flops* $\times 10^9$
1	Oberwolfach/t3dh	79.17	2.22	50.60	70.10
2	Lin/Lin	256.00	1.01	126.00	285.00
3	PARSEC/H2O	67.02	2.22	234.00	1290.00
4	GHS_indef/sparsine	50.00	0.80	207.00	1390.00
5	PARSEC/Ge99H100	112.98	4.28	669.00	7070.00
6	PARSEC/Ga10As10H30	113.08	3.11	690.00	7280.00
7	PARSEC/Ga19As19H42	133.12	4.51	823.00	9100.00

- HSL_MA97: multifrontal solver from the HSL library (CPU-only)
- PARDISO: supernodal solvers part of the MKL library (CPU-only)
- SpLDLT: our new solver, part of the SyLVER package (CPU-GPU)

Numerical experiments: Sparse LDL^T factorization



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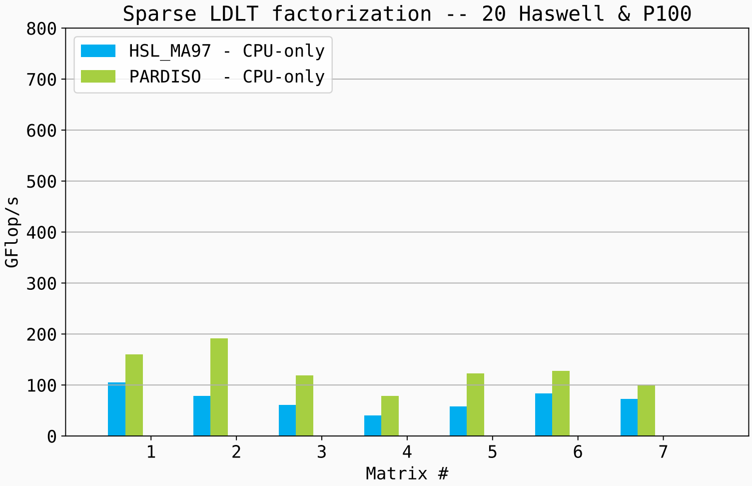

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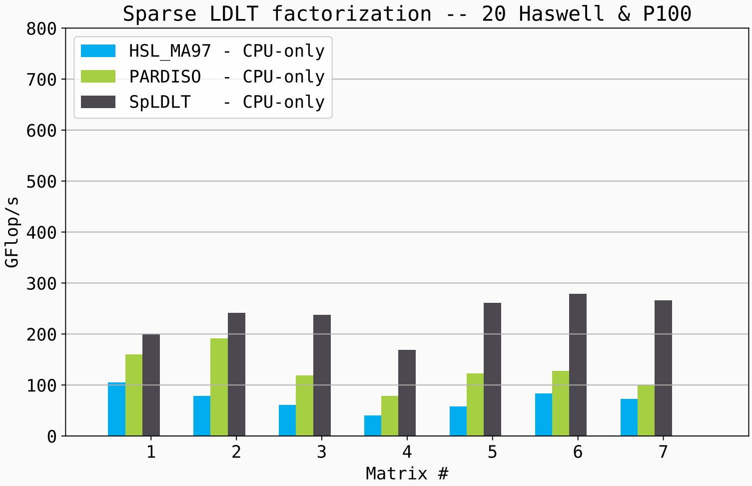
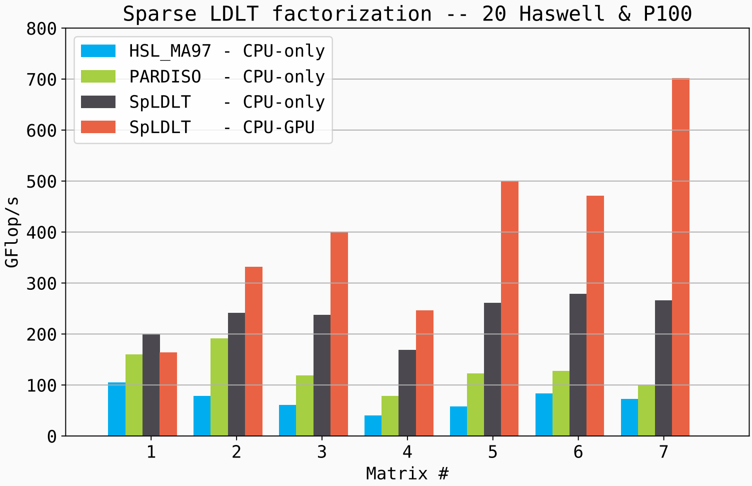


- CPU-only SpLDLT code is up to $\times 3$ faster compared to PARDISO

Numerical experiments: Sparse LDL^T factorization



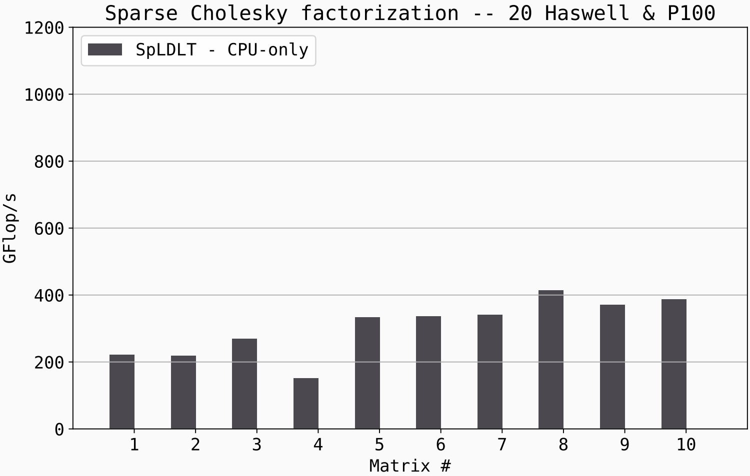
- CPU-only SpLDLT code is up to $\times 3$ faster compared to PARDISO
- Heterogeneous CPU-GPU SpLDLT code is up to $\times 3$ faster compared to CPU-only version

Numerical experiments: Sparse Cholesky factorization

#	Problem	n $\times 10^3$	$nz(A)$ $\times 10^6$	$nz(L)$ $\times 10^6$	$flops$ $\times 10^9$
1	Koutsovasilis/F1	344	13.6	173.7	218.8
2	Oberwolfach/boneS10	915	28.2	278.0	281.6
3	ND/nd12k	36.0	7.1	116.5	505.0
4	ND/nd24k	72.0	14.4	321.6	2054.4
5	Janna/Flan_1565	1565	59.5	1477.9	3859.8
6	Oberwolfach/bone010	987	36.3	1076.4	3876.2
7	GHS_psdef/audikw_1	944	39.3	1242.3	5804.1
8	Janna/Fault_639	639	14.6	1144.7	8283.9
9	Janna/Hook_1498	1498	31.2	1532.9	8891.3
10	Janna/Emilia_923	923	21.0	1729.9	13661.1

- SpLDLT: our new solver, part of the SyLVERpackage (CPU-GPU)

Numerical experiments: Sparse Cholesky factorization



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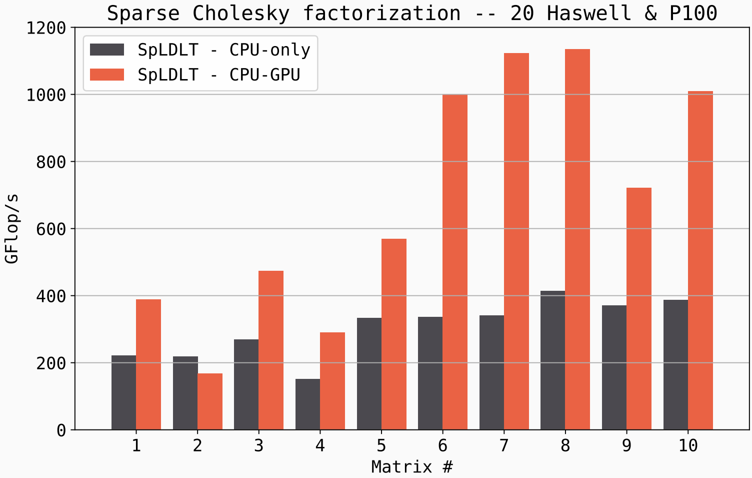

Conclusions and future work

- Our sparse LDL^T factorization with APTP on multicore compares favourably with the state of the art solvers
- Using StarPU allows us GPU devices along with the multicores
- SpLDLT offers better numerical robustness compared to SBK like strategies

- We adapted the APTP pivoting to LU factorization..
- ..integrating it within SpLU using the same tree partitioning strategy as for SpLDLT

Thanks for listening!

Questions?