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Scalable Multi-Coloring Preconditioning for Multi-core CPUs and GPUs

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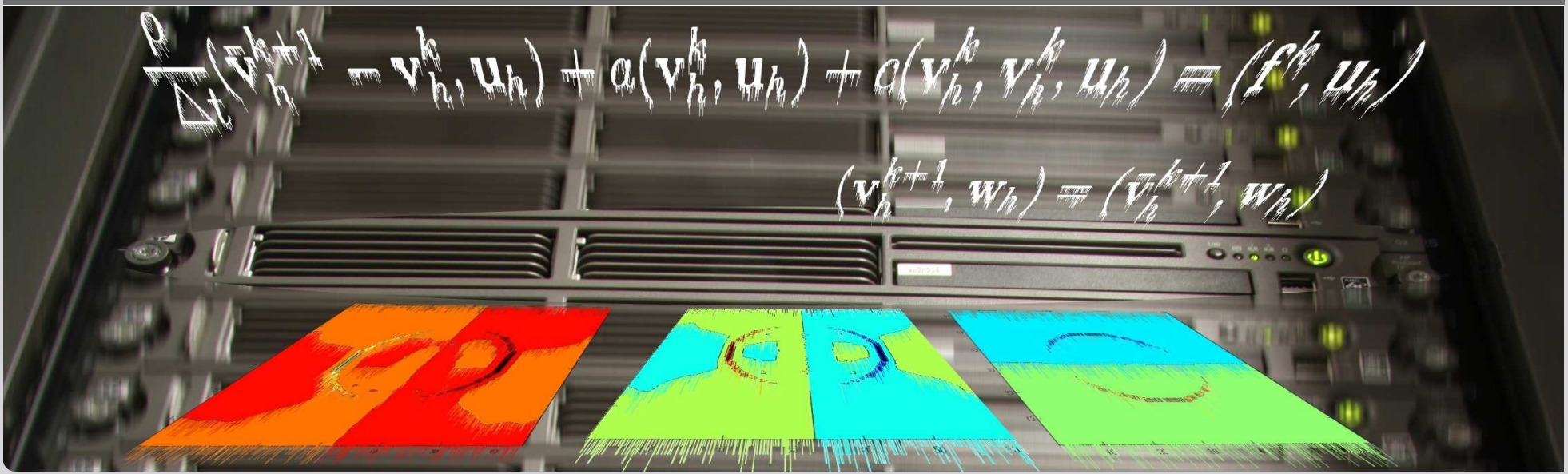
Engineering Mathematics and Computing Lab (EMCL)[1] / SRG New Frontiers in High Performance Computing[2]



Emerging Multi-/Many-core Technologies

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Sea change in hardware technologies and programming paradigms

- Exponentially increasing core counts
- Multi-level and fine-grained parallelism
- Deeply nested hierarchical memory sub-systems
- Heterogeneous platforms

Programming Challenges

MPI, OpenMP, CUDA, OpenCL, Ct, IBM Cell SDK, PGAS, ...

Urgent Questions:

- Portability, Flexibility, Scalability!
- How to adapt algorithms and numerical schemes?
- How to develop hardware-aware methodologies?

Linear Solvers and Preconditioners

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We want to solve $Ax = b$ on a node-level parallel system:

Most iterative linear solvers can be performed in parallel

Krylov subspace methods: CG, GMRES, ...
Splitting methods: Jacobi, Richardson, ...
Projection methods: Chebyshev, ...

All underlying routines are parallelizable:

- Vector operations (BLAS 1): scalar product, norm and vector updates are data parallel routines
- Sparse matrix-vector multiplications (sparse BLAS 2) are data parallel routines with irregular memory access patterns

Linear Solvers and Preconditioners

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The preconditioner influences the condition number of the linear system and decreases the number of iterations

Goal: Provide an efficient, flexible, and scalable preconditioner suitable for multi-core CPUs, GPUs, and other coprocessors

In each step of the solver an additional linear system has to be solved

$$Mz = r$$

In our test scenario we are using a Conjugate Gradient (CG) solver and a Symmetric Gauss-Seidel (SGS) preconditioner of type

$$M = (D + L)D^{-1}(D + R),$$

where $A = D + L + R$ with L lower-triangular, R upper-triangular, and D diagonal.

Solving the Preconditioning Equation

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- Sequential scheme
  - Gauss Elimination / Incomplete LU
    - **Pros:** *very easy to implement*
    - **Cons:** *not parallel; PCIe bottleneck (i.e. not suitable for GPUs)*
- Parallel schemes
  - Jacobi preconditioner
    - **Pros:** *very simple and very easy to implement*
    - **Cons:** *does often not improve the condition number of the system*
  - Block-Jacobi-type preconditioner
    - **Pros:** *simple and easy to implement*
    - **Cons:** *small sequential task, not scalable (decoupling the system)*
  - Algebraic Multigrid
    - **Pros:** *good improvements, scalable*
    - **Cons:** *complex, mostly sequential setup step*
  - Multi-coloring reordering
    - **Pros:** *fast, scalable, better cache utilization*
    - **Cons:** *requires a pre-processing step*

Multi-coloring Algorithm

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The goal is to color (label) the nodes of the sparse matrix (graph) in a way that there are no two adjacent nodes having the same color and the number of colors is as small as possible.

for i=1,...,N Set Color(i)=0; (where N=#nodes)
for i=1,...,N Set Color(i)=min(k>0:k!=Color(j) for j $\in$ Adj(i));

where $\mathrm{Adj}(i) = \{j \neq i | a_{i,j} \neq 0\}$ are the adjacents to node i.

- Parallel approach: block decomposition
- Diagonal blocks of size $b_k \times b_k$ are diagonal matrices with multi-coloring!
- Degrees of parallelism are $b_k = N/B$, where N is the number of unknowns in the system and B is the number of colors

Solving the Block-decomposed System

- Crucial point: Inversion of matrices D_i on block-diagonal
- Main goal of multi-coloring: obtain only diagonal elements in the block-diagonal matrices D_i
- SpMV dominates the algorithm: good scalability and high degree of parallelism
- The number of SpMV operations is $B(B-1)$
- The algorithm is bandwidth-bound !

$$x_i := D_i^{-1}(r_i - \sum_{j=1}^{i-1} L_{i,j}x_j) \text{ for } i = 1,\ldots,B$$

$$y_i := D_i^{-1}x_i \text{ for } i = 1,\ldots,B$$

$$z_i := D_i^{-1}(y_i - \sum_{j=1}^{B-i} R_{i,j}z_{i+j}) \text{ for } i = B,\ldots,1$$

D_1	R_{11}	R_{12}	R_{13}
L_{21}	D_2	R_{21}	R_{22}
L_{31}	L_{32}	D_3	R_{31}
L_{41}	L_{41}	L_{41}	D_4

Hardware Configurations

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Host				Device			
CPU	MEM [GB]	BW [GB/s]	H2D [GB/s]	GPU	MEM [GB]	BW [GB/s]	D2H [GB/s]
2x Intel Xeon 4c (E5450) 8 cores	16	8c: 6.14 1c: 2.62	Pa: 1.92 Pi: 5.44	Tesla T10 S1070	4x4	BT: 71.8 daxpy: 83.1 ddot: 83.3	Pa: 1.55 Pi: 3.77
1x Intel Core2 2c (6600) 2 cores	2	2c: 3.28 1c: 3.08	Pa: 1.76 Pi: 2.57	GTX 480	1.5	BT: 108.6 daxpy: 135.0 ddot: 146.7	Pa: 1.38 Pi: 1.82
1x Intel Core i7 4c (920) 4 cores	6	4c: 12.07 1c: 5.11	Pa: 5.08 Pi: 5.64	GTX 280	1.0	BT: 111.5 daxpy: 124.3 ddot: 94.8	Pa: 2.75 Pi: 5.31

Table: CPU and GPU system configuration: Pa/Pi = Pageable/Pinned memory, H2D = host-to-device, D2H = device-to-host, 1c/2c/4c/8c = 1/2/4/8 core(s)

Test Matrices

Name	Description of the problem	#rows	#non-zeros	#colors	#block-SpMV in MCSGS
g3 circuit	Circuit simulation	1585478	7660826	4	12
L2D 4M	FEM - Q1 Laplace 2D	4000000	19992000	2	2
s3dkq4m2	FEM - Cylindrical shells	90449	4820891	24	552

Table: Description and properties of test matrices

Impact of Preconditioning

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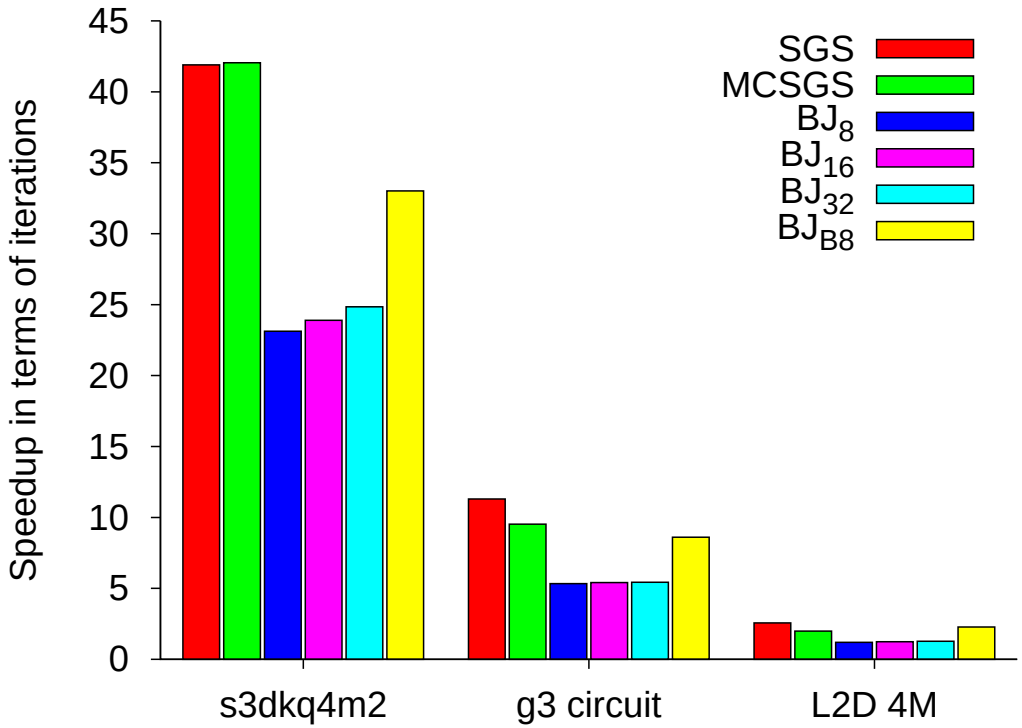
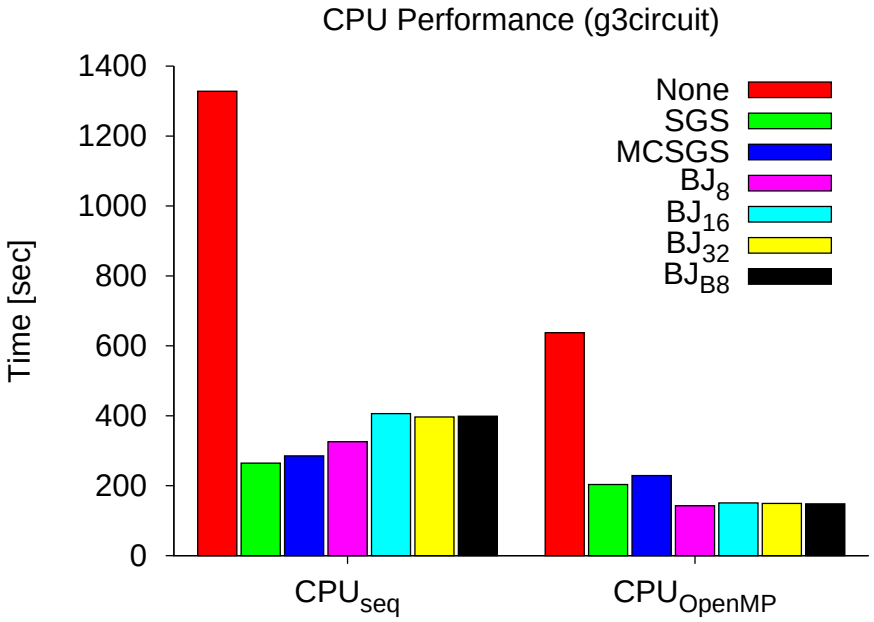
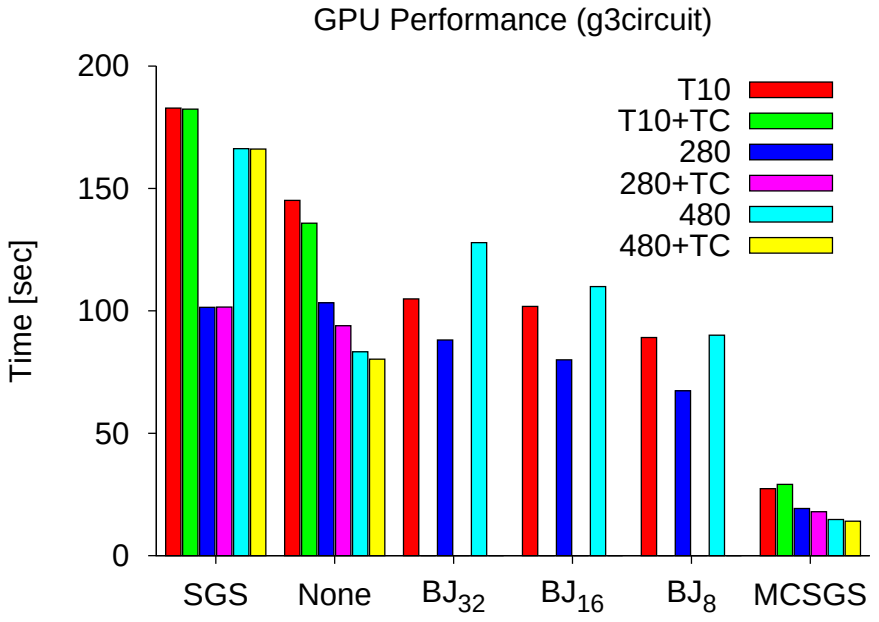
Reduction of number of iterations:



Speedup by preconditioning: ratio of necessary number of iterations of the unpreconditioned system to the necessary number of iterations of the preconditioned system

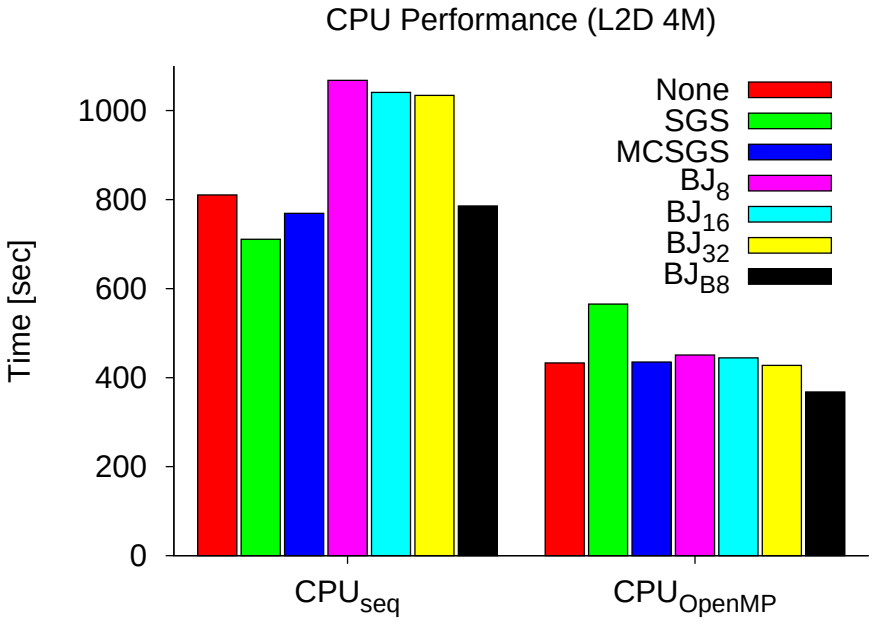
Problem 1: Circuit simulation

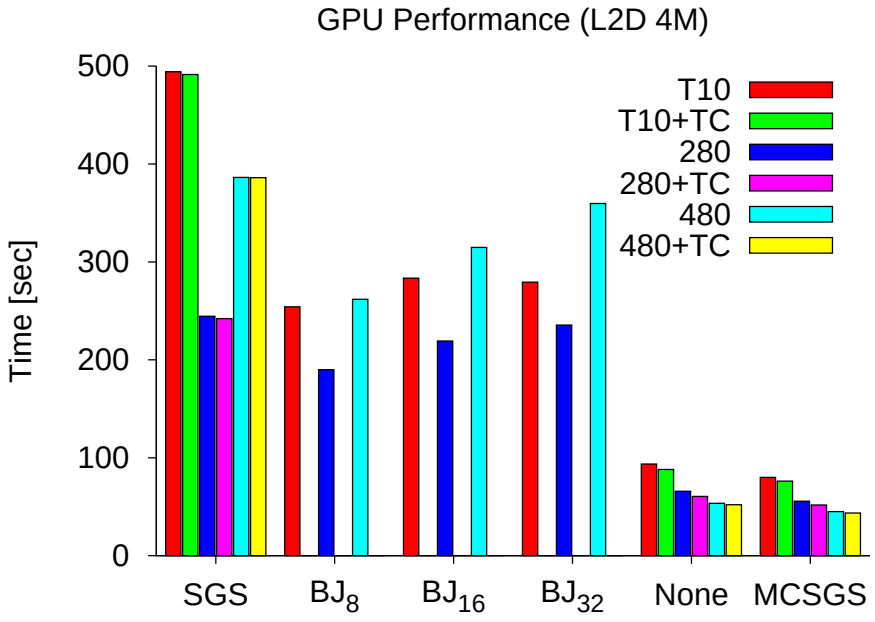




- Matrix color decomposition is imbalanced
- The solver behaves according to platform-specific bandwidth
- The best CPU performance is BJ since the cores are optimized for executing large sequential codes; on the GPU MCSGS is superior

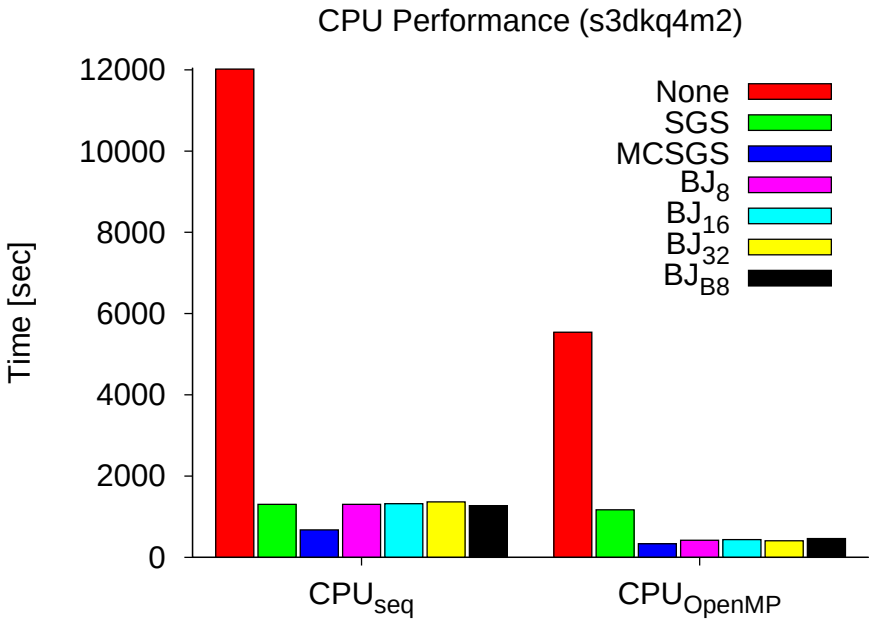
Problem 2: Laplace on regular grids

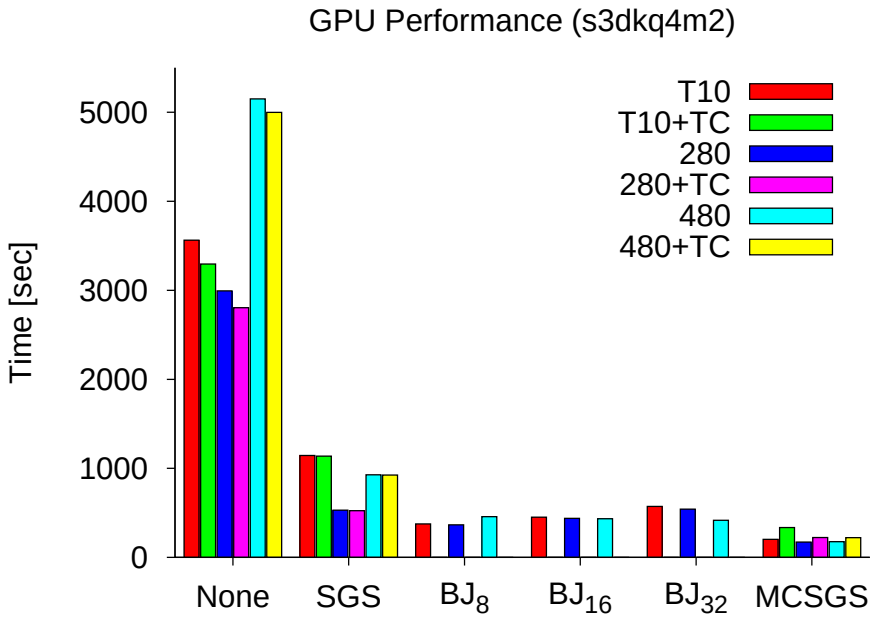




- The matrix color decomposition is balanced
- The solver behaves according to platform-specific bandwidth
- SGS - single core bandwidth utilization and PCIe for the GPU
- Small number of SpMV for MCSGS / texture caching on GPU improves performance

Problem 3: FEM - Cylindrical shells





- The matrix is comparably small: #rows = 90449
- Due to the small matrix size the function calls on the GPU (latency) have a significant impact on the total run time
- Very good cache utilization for MCSGS on the CPU
- Large number of SpMV for MCSGS / impact of texture caching on GPU

Conclusion

- The multi-coloring SGS scheme provides a parallel and scalable preconditioner
- Applicable on multi-core CPUs and GPUs
- Out-of-the box solution for general deployment
- Convincing performance for all test scenarios
- Improved cache utilization
- No bottlenecks due to PCIe connection
- No sequential parts

HiFlow^3

Our preconditioner is part of the ImpLAtoolbox of the HiFlow^3 open source parallel finite element package. It will be available on **http://www.hiflow3.org**

Contact and Acknowledgements

Further Information

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- http://www.emcl.kit.edu
- http://www.hiflow3.org

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Thank you for your attention!