IBM Research, Zürich, 29 September 2017

UNIVERSITAT JAUME I

Accelerating the Solution of Sparse Linear Systems with GPUs

Goran Flegar

Joint work with: Hartwig Anzt, Nicholas Higham, Enrique S. Quintana-Ortí

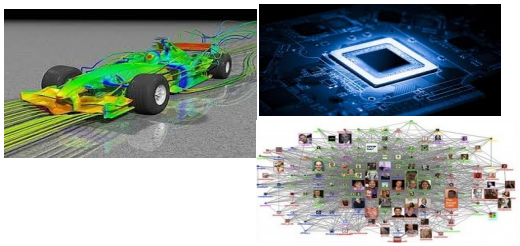
Scan me for slides!

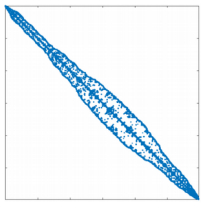
github.com/gflegar/talks/tree/master/ibm_zurich_2017_09

flegar@uji.es

MAGMA-sparse software library

- GPU-accelerated sparse linear algebra library
  - Focus: linear systems





$$Ax = b$$

MAGMA SPARSE

Joint effort: Innovative Computing Lab at University of Tennessee, Knoxvile; Karlsruhe Institute of Technology; Universidad Jaume I

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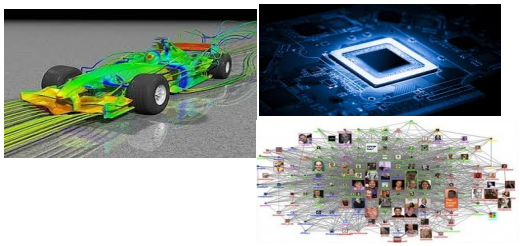

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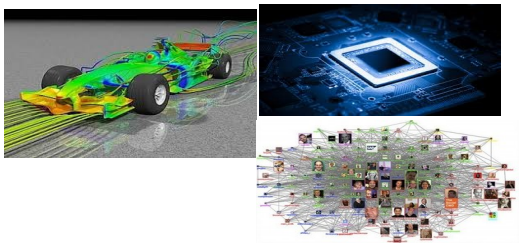

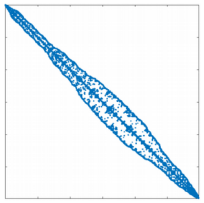

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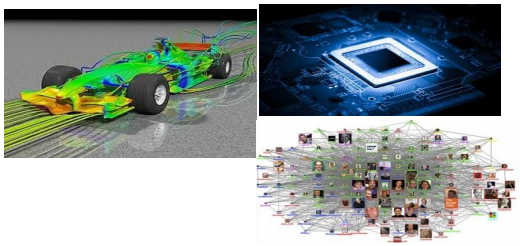

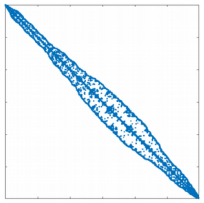

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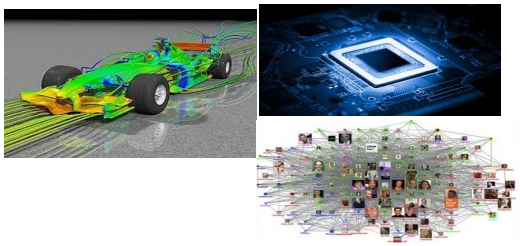

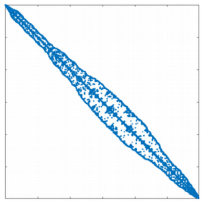

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Preconditioning

$$Ax = b, \;\; A \in \mathbb{R}^{n \times n}$$

Preconditioning

$$Ax = b,\ A \in \mathbb{R}^{n \times n} \longrightarrow M^{-1}Ax = M^{-1}b$$

Replace the original system with an equivalent preconditioned system

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Do not compute the preconditioned system matrix explicitly!

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$$y := M^{-1}z$$

Preconditioner application

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$$A \rightsquigarrow M$$

Preconditioner setup

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Preconditioner setup

Preconditioner application

Trade-off:
faster convergence,
but more work per iteration

Block-Jacobi preconditioning

- Current focus: improve performance for problems with inherent block structure
  - Usually blocks are smaller than 30x30 (blocks can be of different sizes!)

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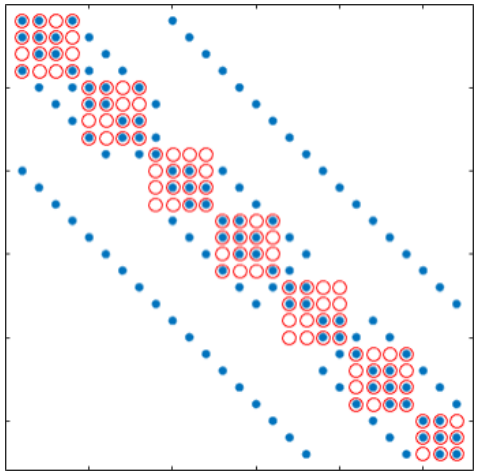

- Block-Jacobi preconditioning
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$$\mathrm{diag}(A) = [D_1, \ldots, D_k]$$
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Benefits of block-Jacobi

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  - Scalar Jacobi preconditioner
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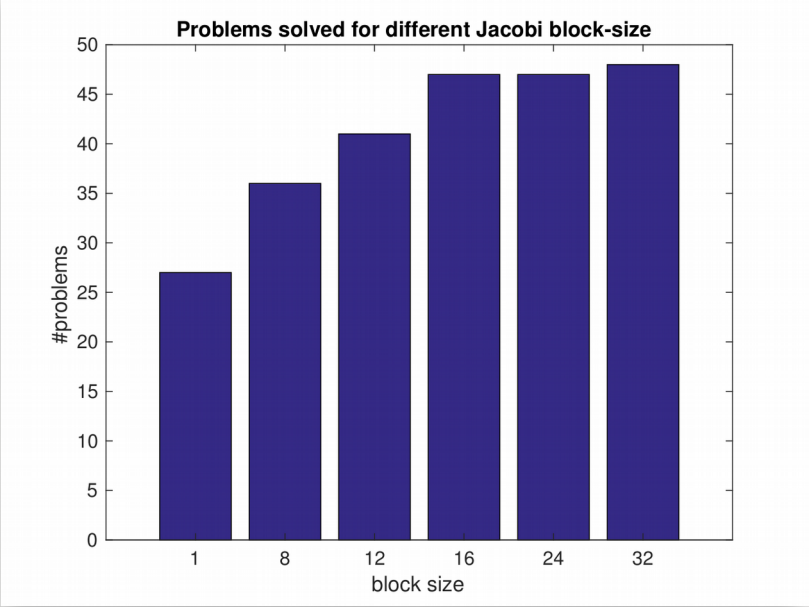

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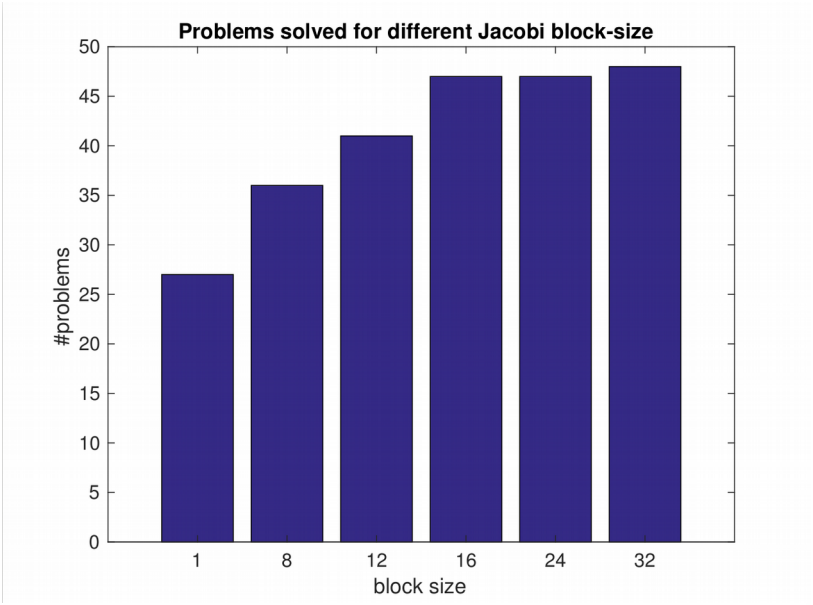

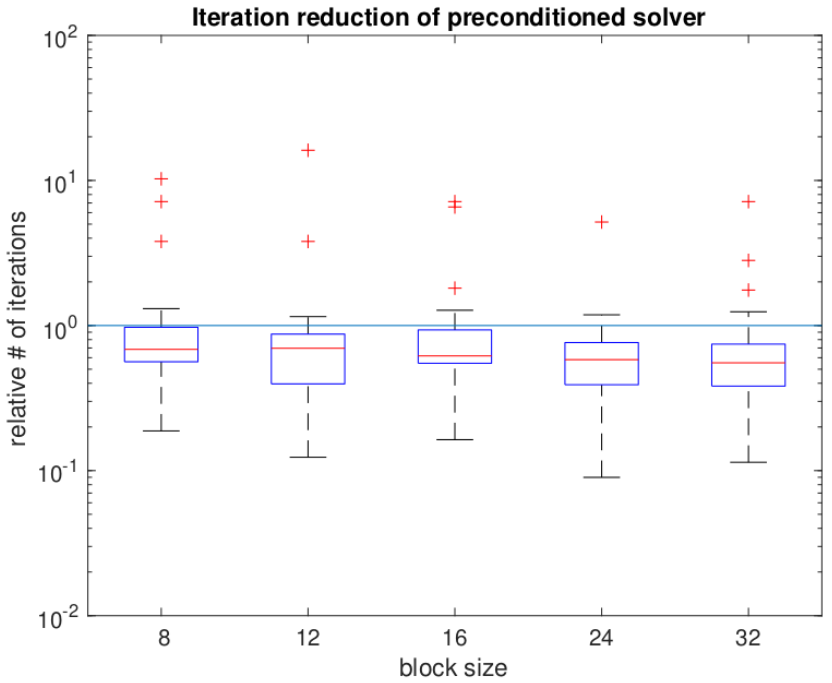

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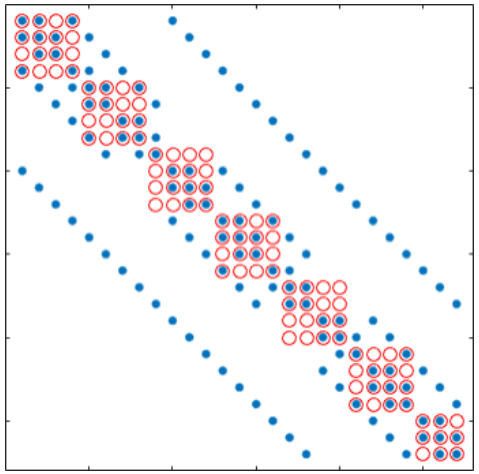

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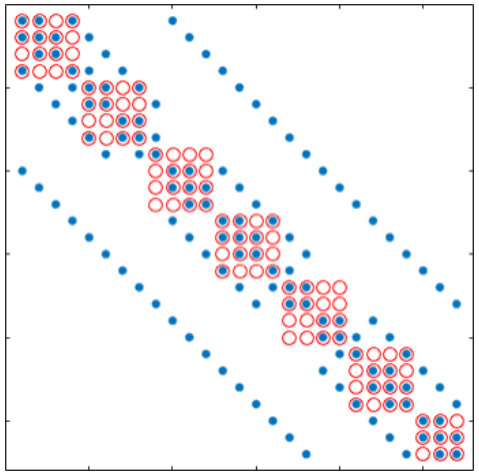

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$$\longrightarrow \widetilde{D}_i := \text{inv}(D_i)$$
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inv = Gauss-Jordan elimination

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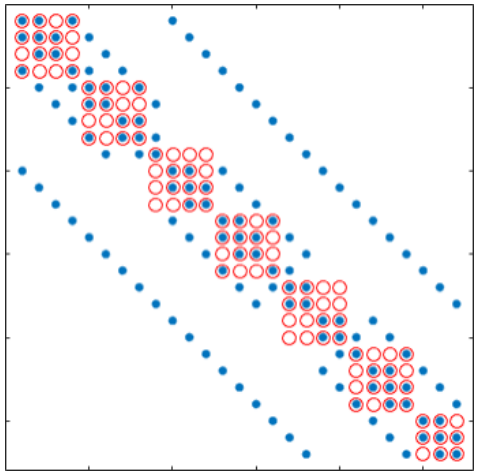

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$$\widetilde{D}_i := \text{inv}(D_i)$$ **Setup**

$$y_i := \widetilde{D}_i z_i$$ **Application**

Inversion-based block-Jacobi

inv = Gauss-Jordan elimination

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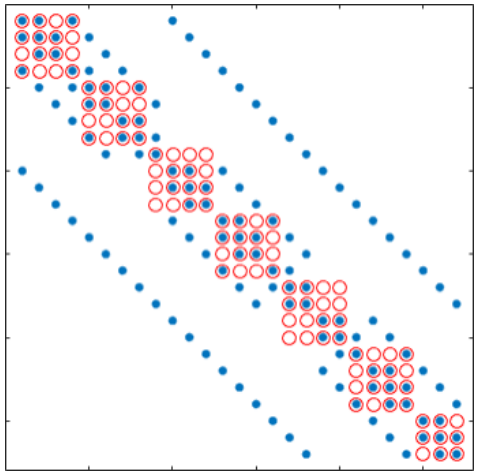

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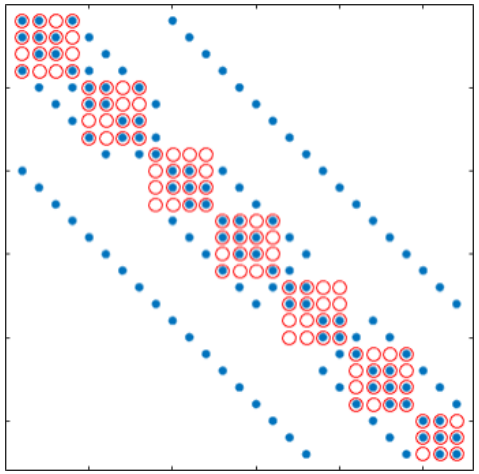

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$$D_i = L_i U_i$$

$$\longrightarrow D_i y_i = z_i \longrightarrow \begin{array}{l} U_i y_i = w_i \\ L_i w_i = z_i \end{array}$$

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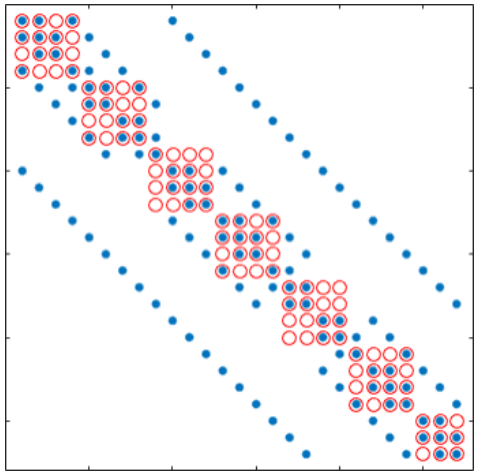

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$$\longrightarrow D_i y_i = z_i \longrightarrow \begin{aligned} U_i y_i &= w_i \\ L_i w_i &= z_i \end{aligned}$$ **Application**

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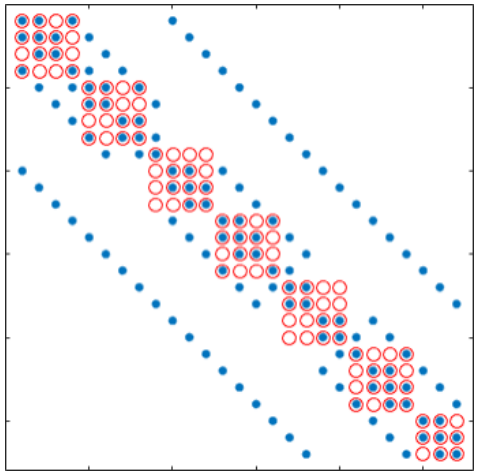

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$$\widetilde{D}_i := \mathrm{gh}_d(D_i)$$

$$z_i := \mathrm{gh}_a(\widetilde{D}_i, y_i)$$

gh = Gauss-Huard decomposition / application

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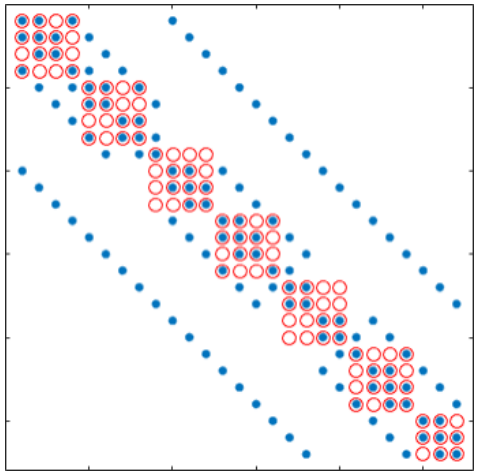

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Decomposition-based block-Jacobi

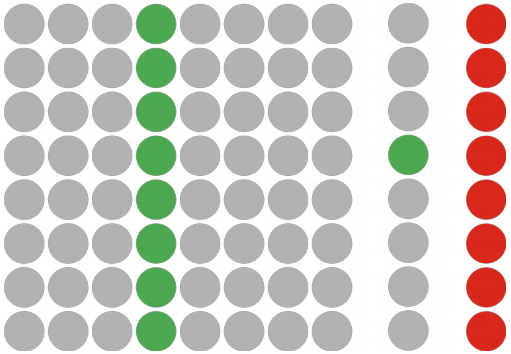
Block-Jacobi setup & application ecosystem

Setup

Application

Gauss-Jordan inversion

Inversion-based
($2n^3 + 2n^2$ FLOPS)
matrix-vector multiply



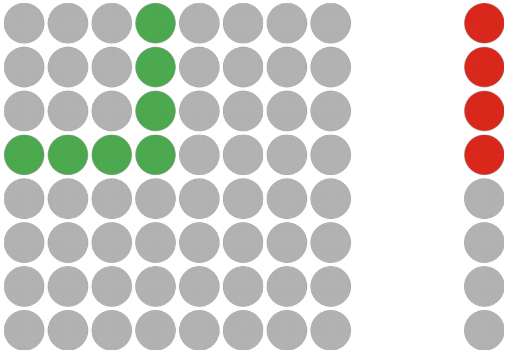
H. Anzt et al. “Batched Gauss-Jordan Elimination for Block-Jacobi Preconditioner Generation on GPUs”, PMAM’17

Gauss-Huard decomposition

LU factorization

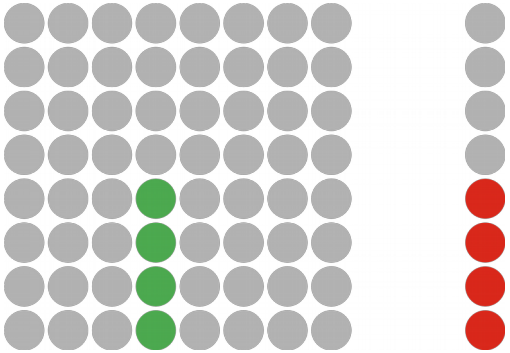
Decomposition-based
($2/3n^3 + 2n^2$ FLOPS)

Gauss-Huard solve



H. Anzt et al. “Variable-Size Batched Gauss-Huard for Block-Jacobi Preconditioning”, ICCS’17

2x triangular solve



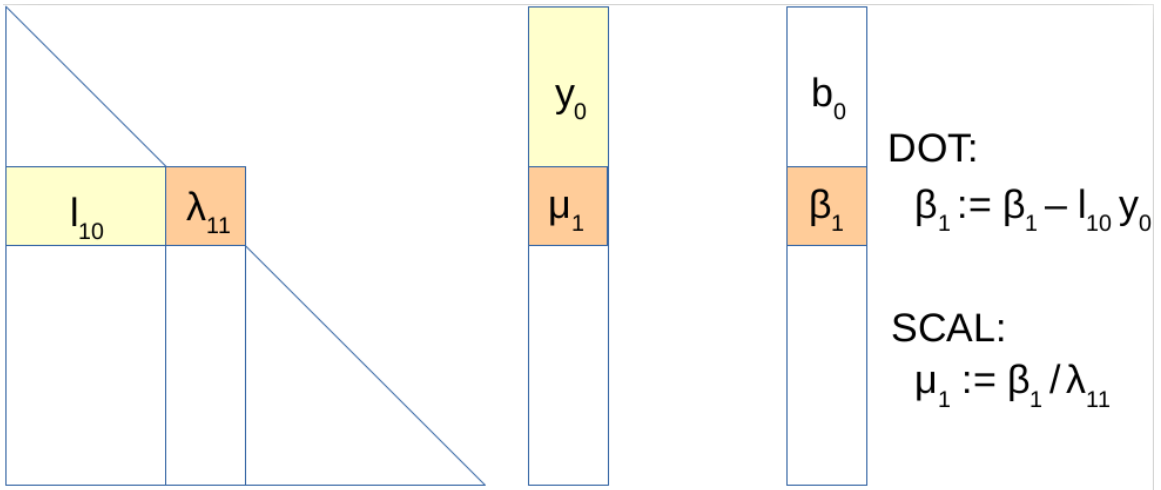
H. Anzt et al. “Flexible-Size Batched LU for Small Matrices and its Integration into Block-Jacobi Preconditioning”, ICPP’17

- read - write

MAGMA-sparse triangular solves

- Use "eager" triangular solves
  - Cast solution vector updates in terms of axpy, not in terms of dot product!

"Lazy" triangular solve



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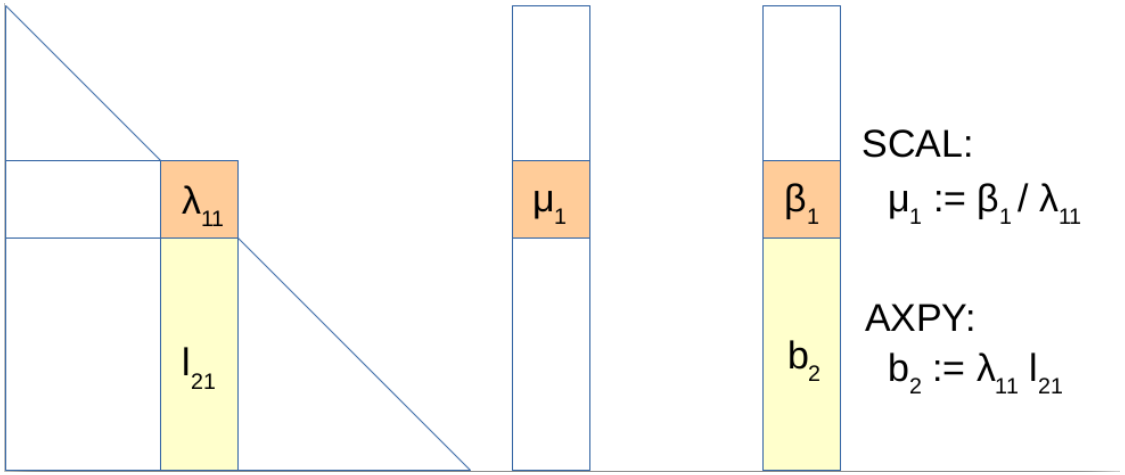

GPU programming 101

- NVIDIA P100 GPU
  - 4.7 TFLOPs DP performance
  - Up to 740 GB/s (1 : 51)
  - 56 SMs x 64 cores = 3584 cores!

source: devblogs.nvidia.com/parallelforall/

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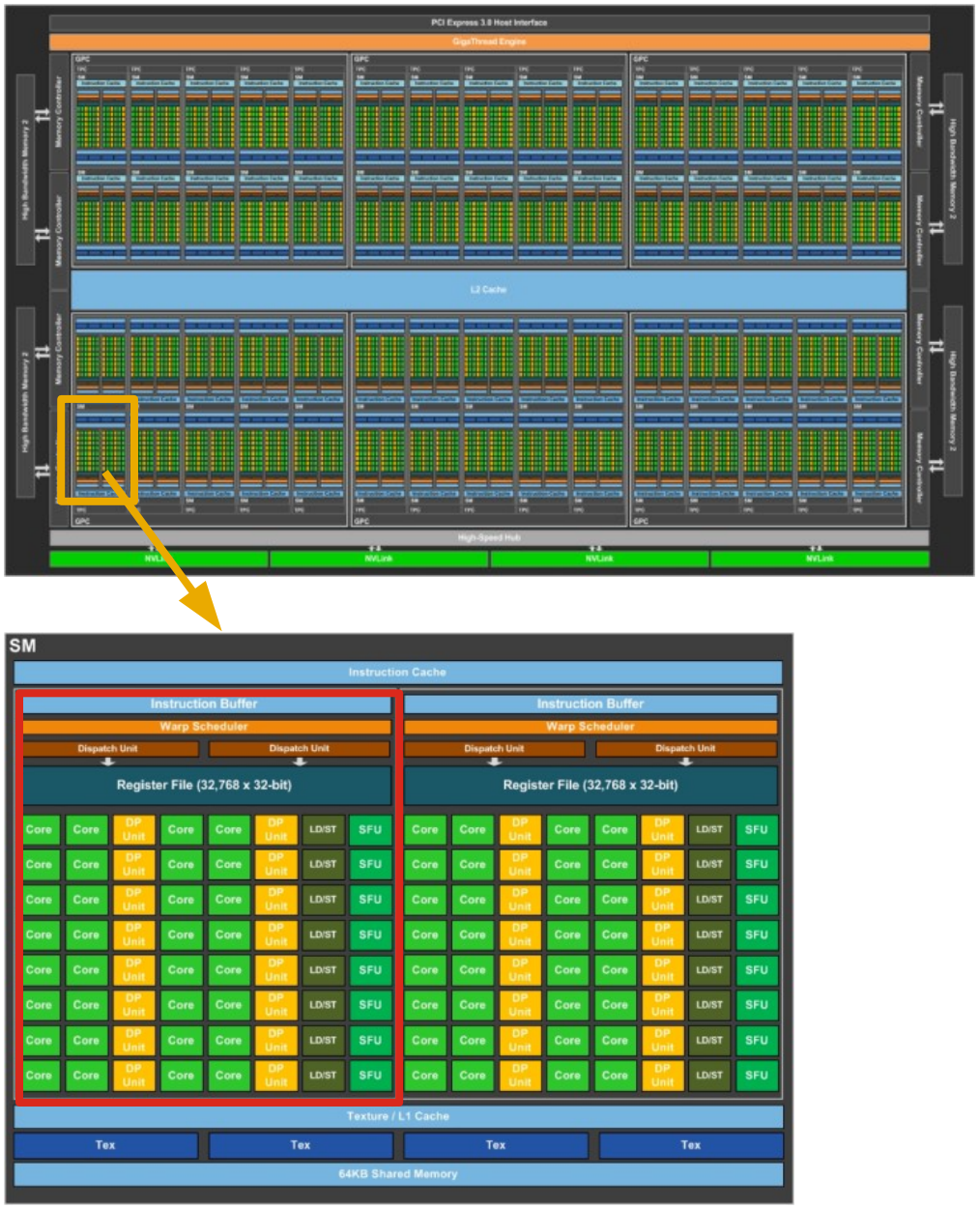
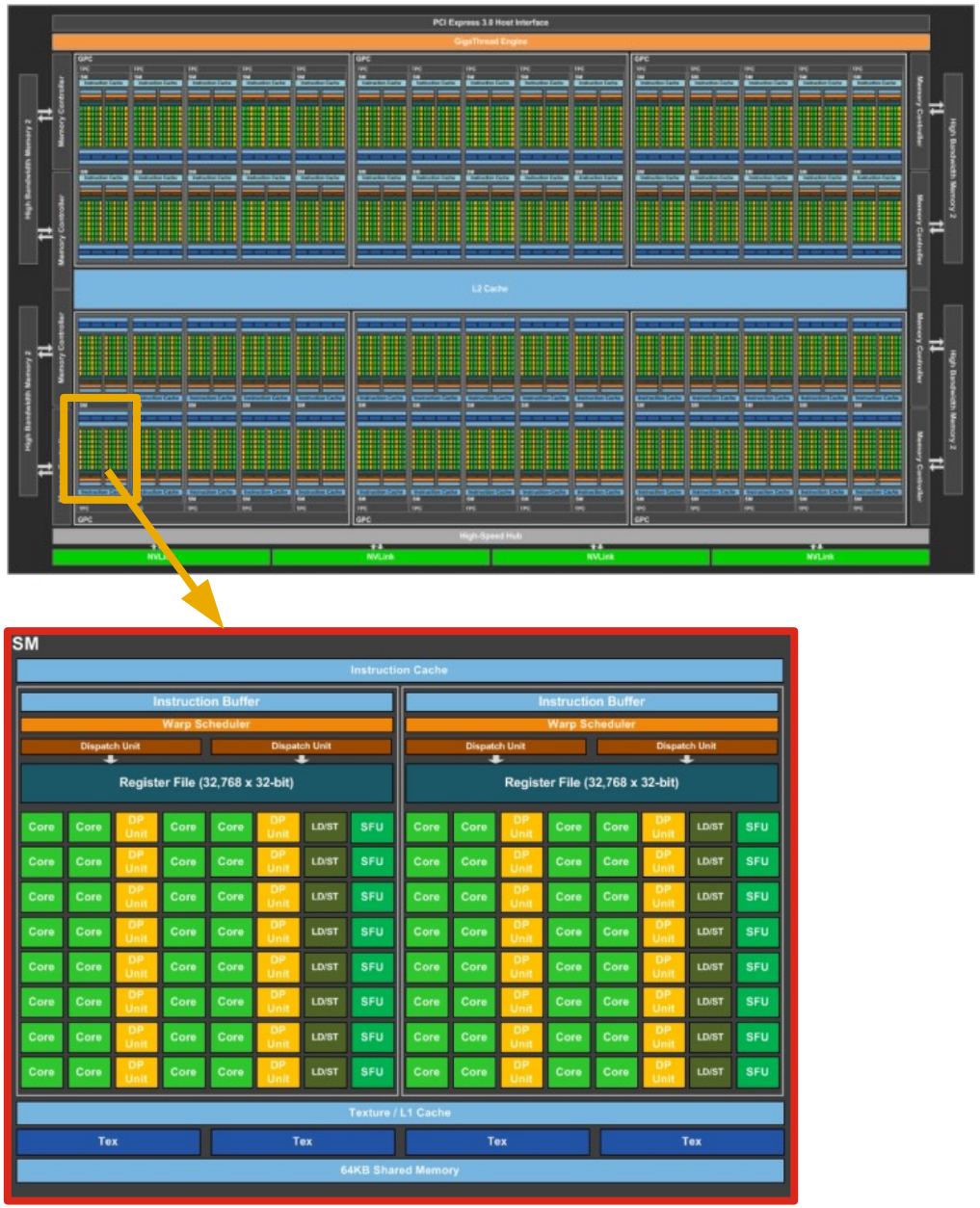
- Hierarchical architecture / programming model:
  - Thread
    - Basic building block, assigned to 1 core
  - Warp
    - Group of 32 threads
    - Perfectly synchronized execution
    - Can share values directly from the registers (1KB / thread)
    - Cannot execute different instructions (warp divergence)



source: devblogs.nvidia.com/parallelforall/

GPU programming 101

- Block
  - Group of several warps (≤ 64)
  - Can be explicitly synchronized
  - Can share data via shared memory (64KB)



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GPU programming 101

- Block
  - Group of several warps (≤ 64)
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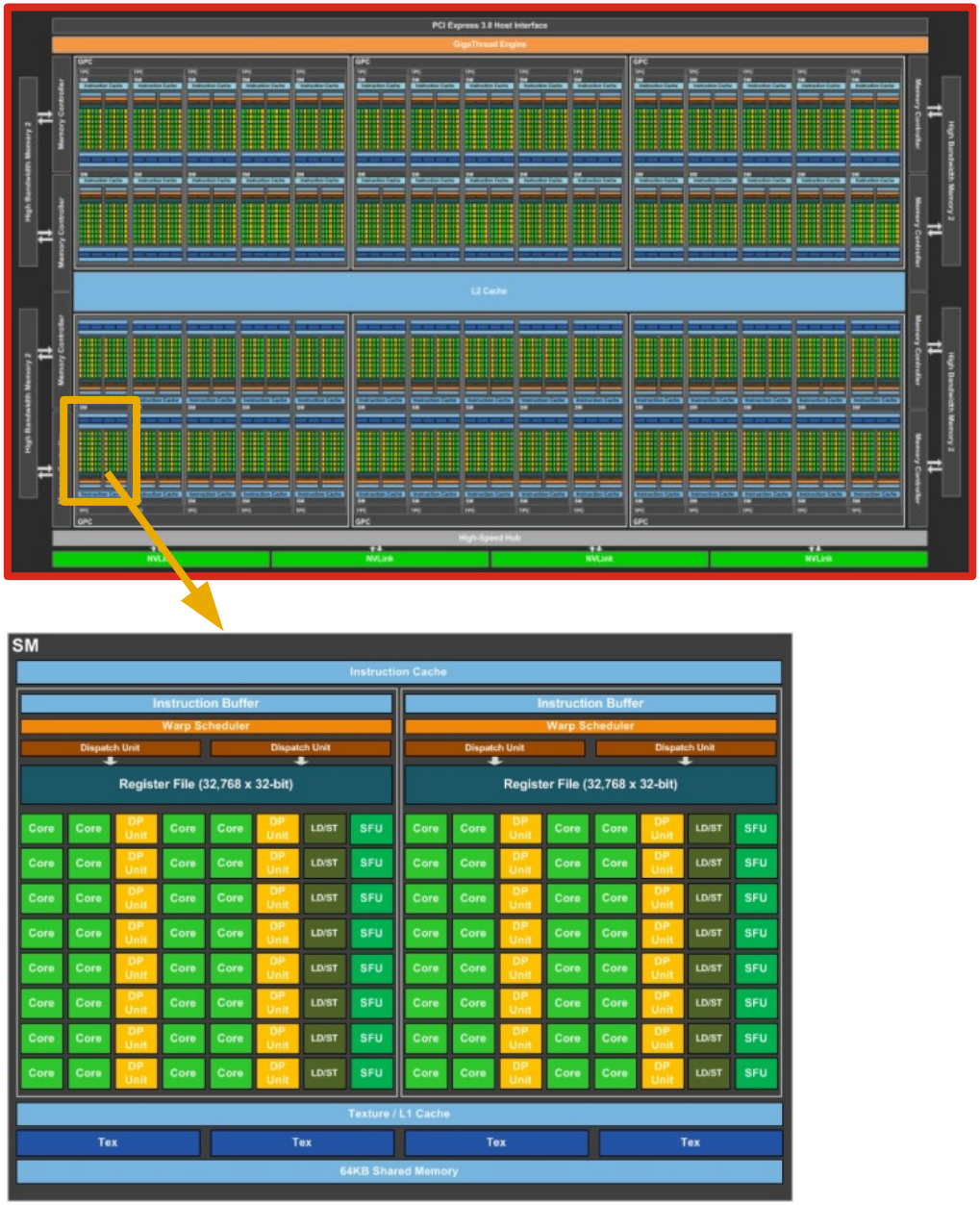
- Grid
  - Group of blocks
  - **Cannot synchronize!**
  - Global memory (12 or 16GB)
  - Simple caches
  - Atomics



source: devblogs.nvidia.com/parallelforall/

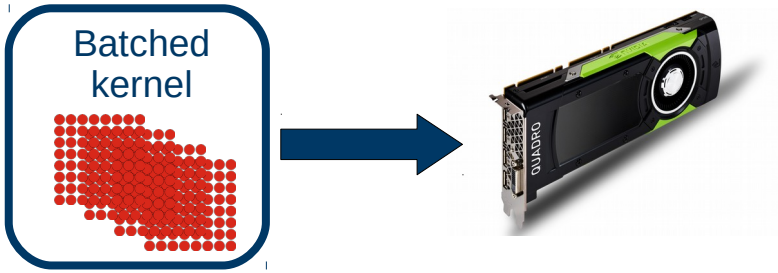
Block-Jacobi preconditioning

Solving 30-by-30 systems in sequence on a GPU with several thousand cores wastes computational resources!

N x GEMM vs batched GEMM comparison:
https://devblogs.nvidia.com/parallelforall/cublas-strided-batched-matrix-multiply

Batched routines

Launch a single kernel which applies an operation to multiple independent data entities in parallel.



** Measured on NVIDIA P100*

Batched routines

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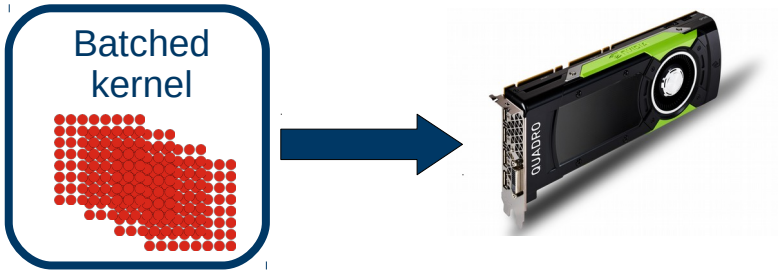

- There is no standard BLAS & LAPACK interface
- Most implementations only support problems of equal sizes
- High performance libraries are not optimized for small blocks
  - cuBLAS batched trsv: ~25 Gflop/s *
  - MAGMA-sparse SpMV: 60 – 90 Gflop/s *

** Measured on NVIDIA P100*

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  - hardware SIMD unit, represented as a group of 32 threads in CUDA

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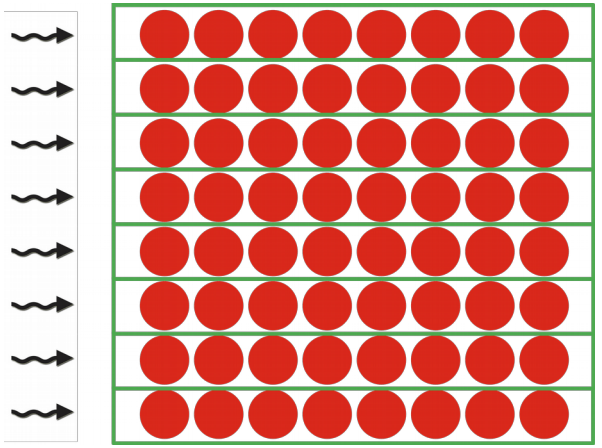
  - keep the entire row (column) in thread's registers
  - Communicate data between rows via warp-shuffles
  - Current implementation: use padding for problems of smaller sizes
  - Future work: multiple smaller problems per warp



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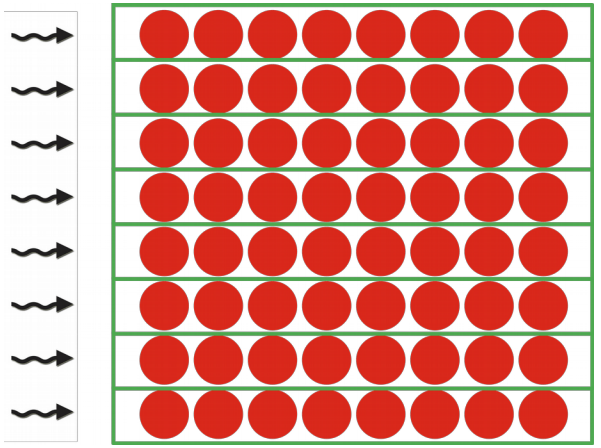
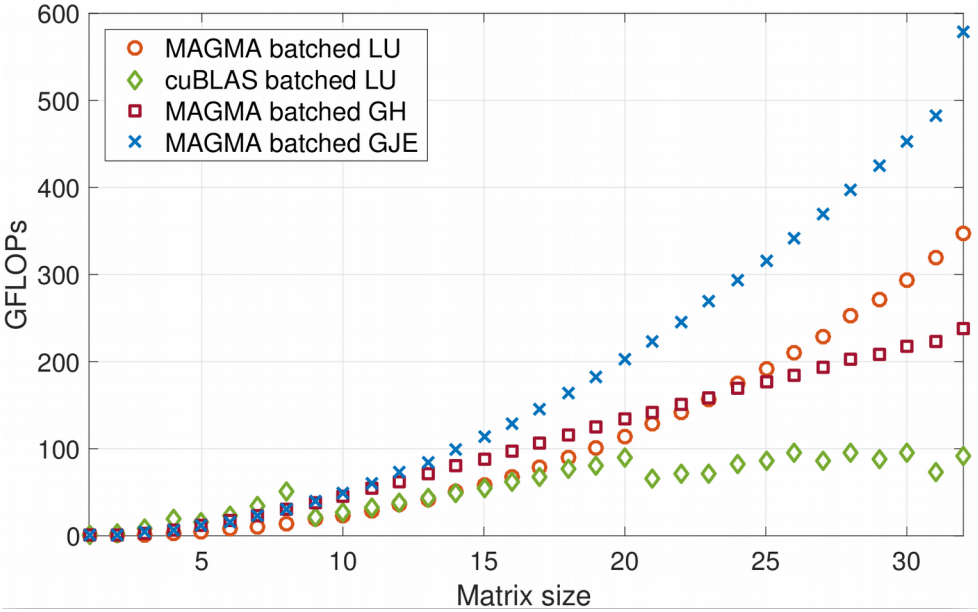
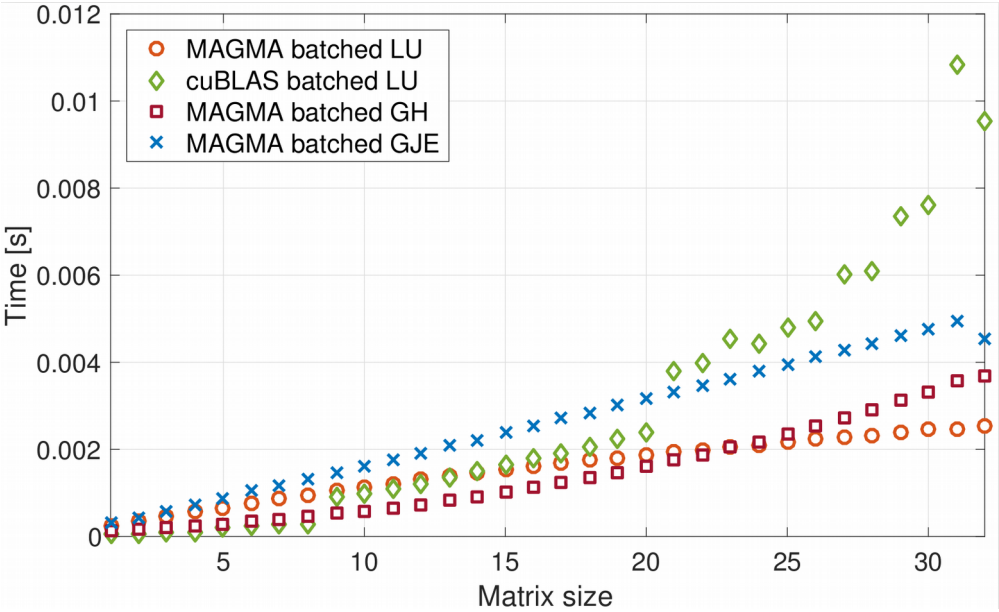


- Use implicit pivoting
  - Do not explicitly swap rows (column), "re-assign" the threads instead

Batched routines performance





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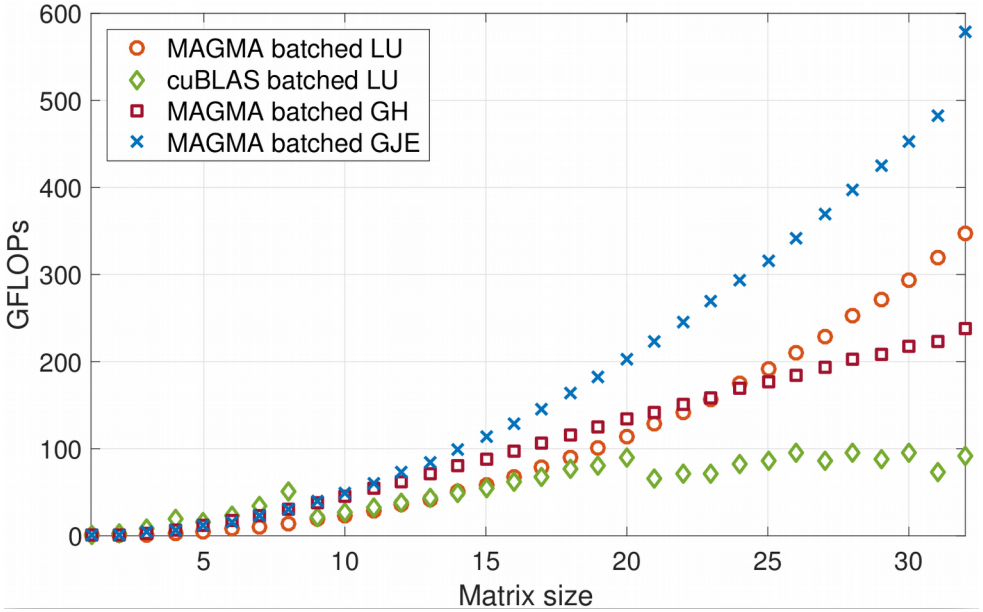
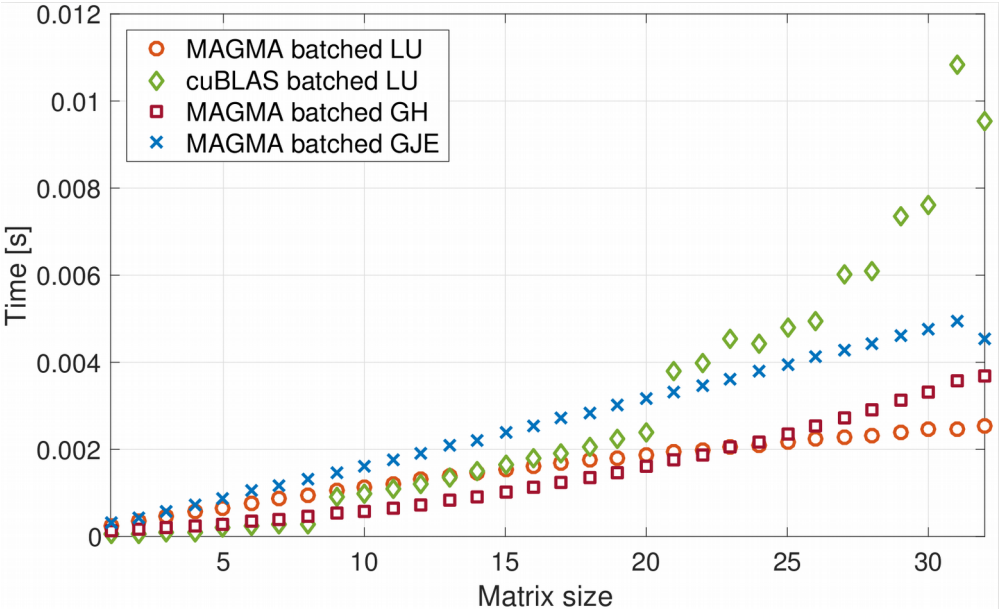
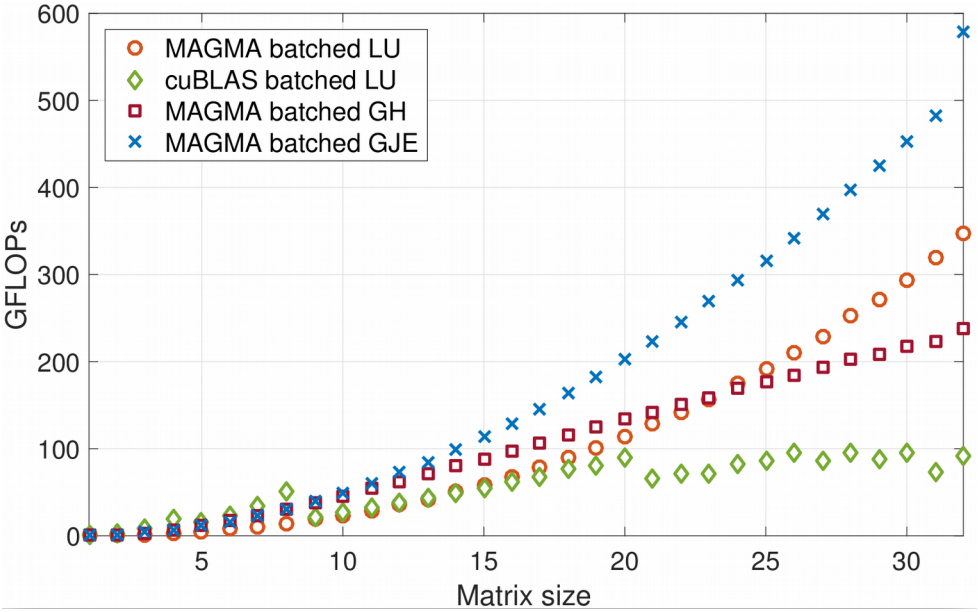


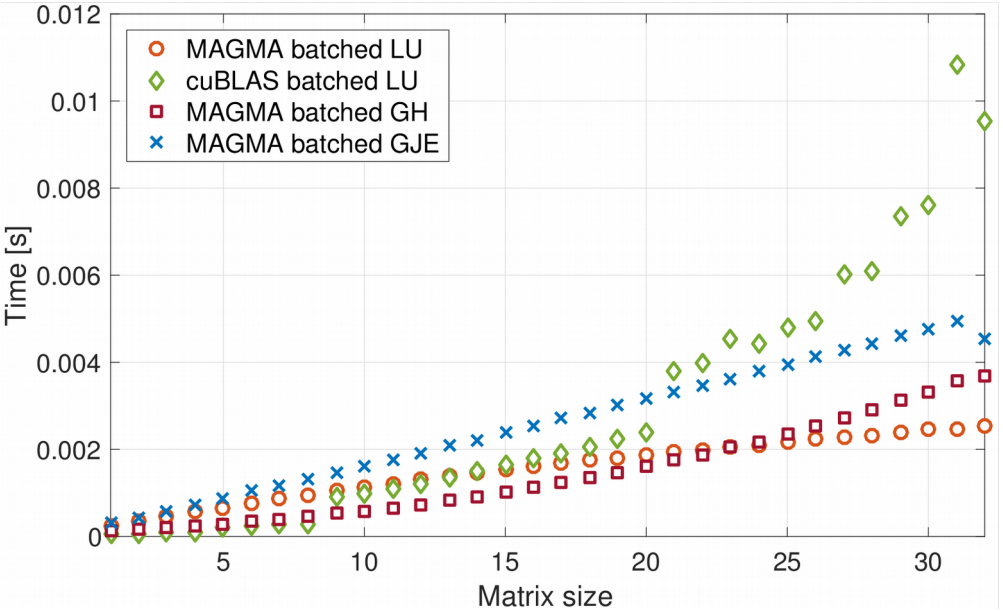


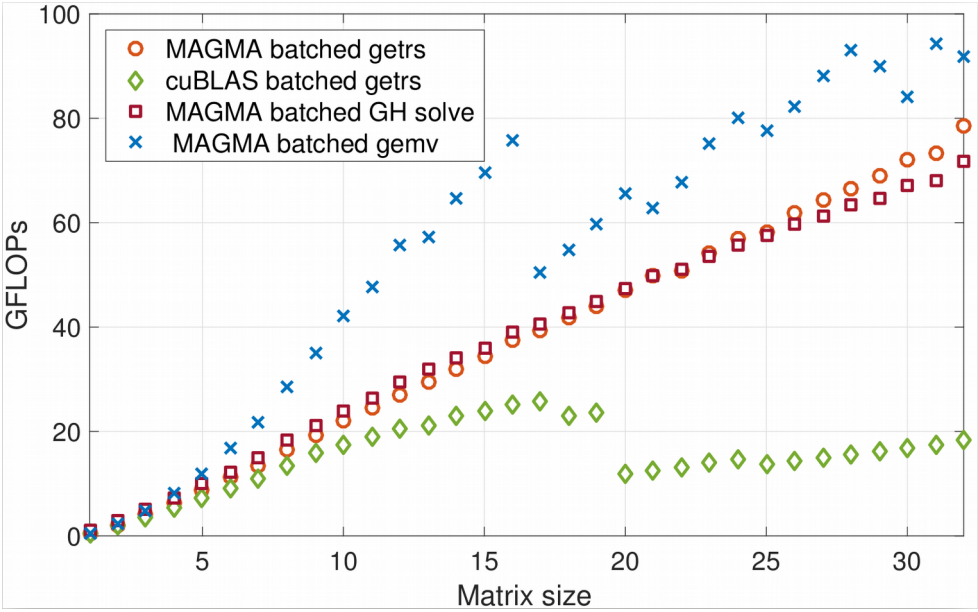
MAGMA-sparse routines can also:

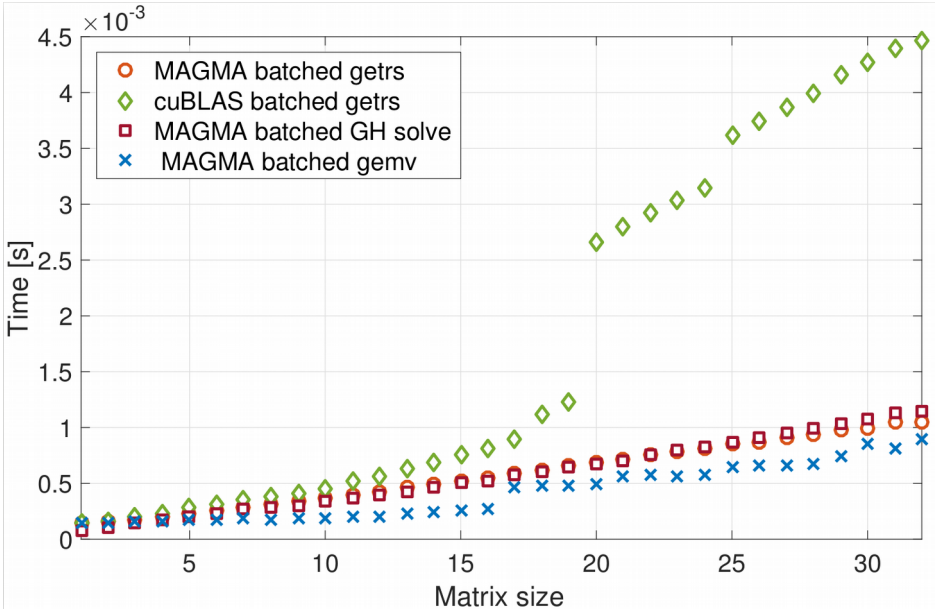
- Handle problems of different sizes
- Integrate diagonal block extraction and diagonal block decomposition / inversion into a single kernel

Batched routines performance



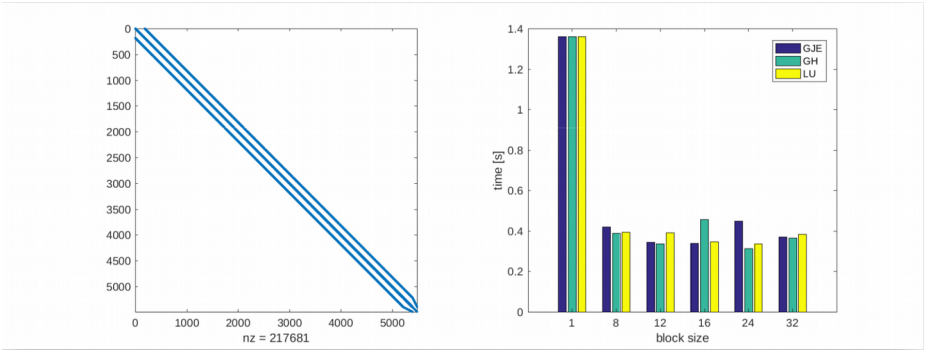




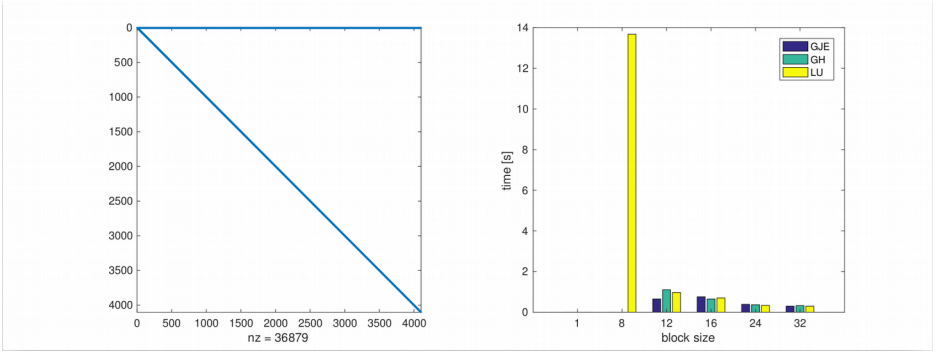


Complete solver runtime

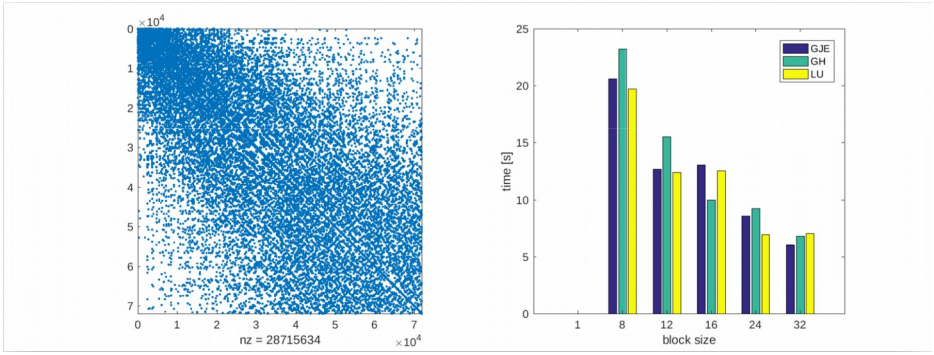
s2rmt3m1



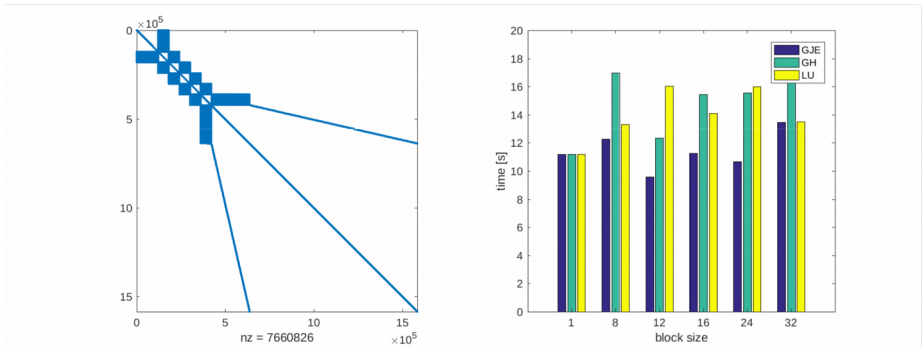
Chebyshev3



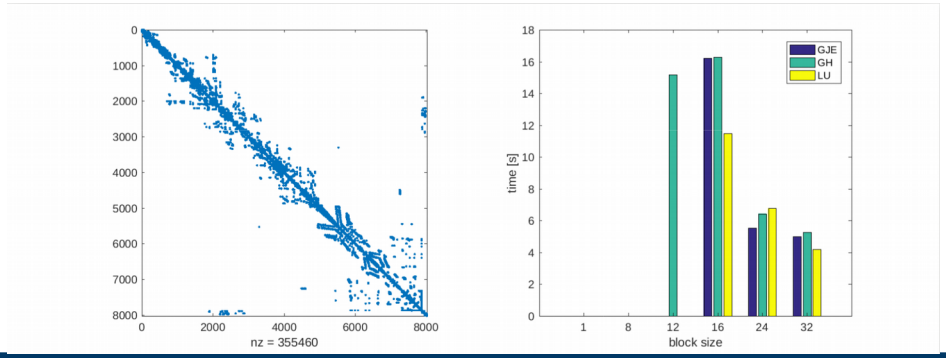
nd24k



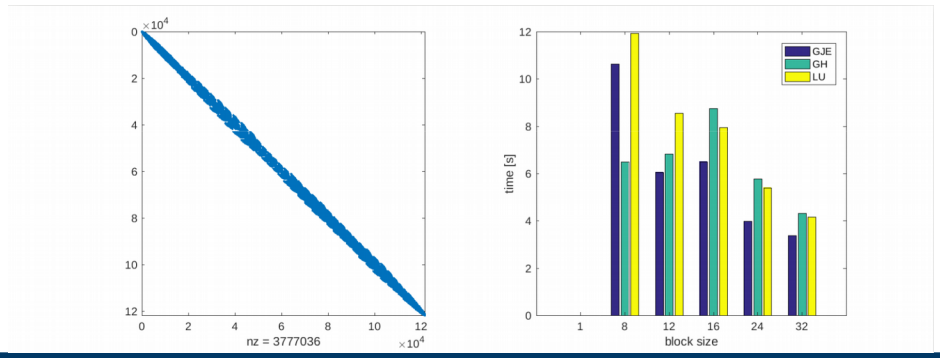
G3_circuit



bcsstk38

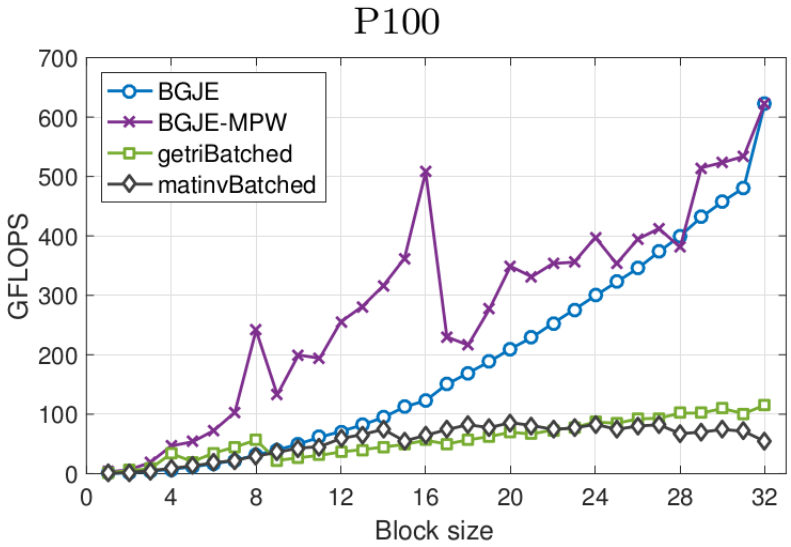


ship_003



Flexible-size batched routines & future research

- Problems can be to small to effectively use one warp
  - Solution: assign multiple problems per warp



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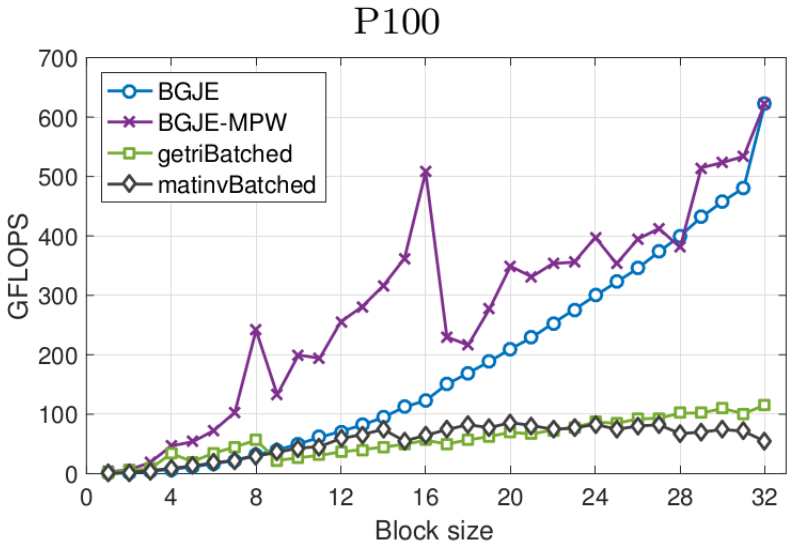
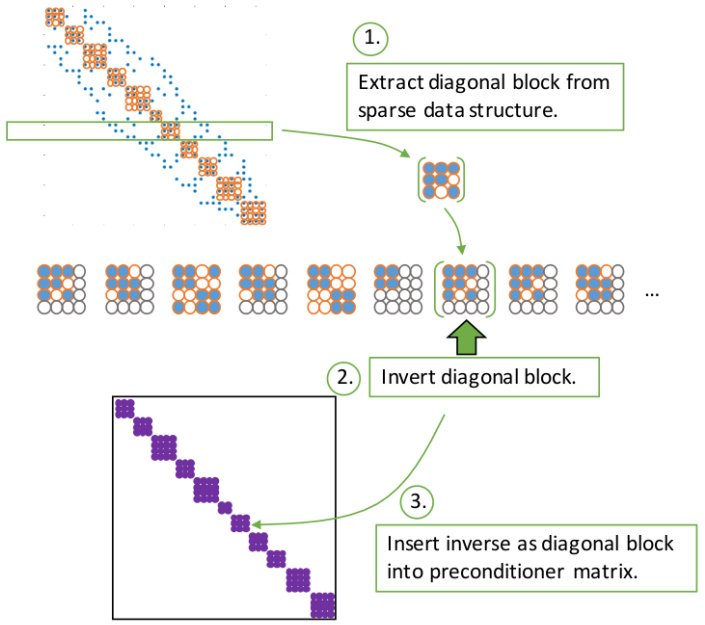


- Allow batches where problems are of different sizes (flexible-size)
  - How to combine this with multiple problems per warp?
    - Remember: entire warp executes the same instruction!
    - Current solution: padding



Adaptive precision block-Jacobi

Preconditioner is an approximation of the system matrix

- Applying a preconditioner inherently carries an error
- For block-Jacobi the relative error of z is usually around 0.01 – 0.1

$$z := M^{-1}y \approx A^{-1}y$$

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Adaptive precision in inversion-based block-Jacobi:

- All computation is done in double precision
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Assuming the preconditioner block is relatively well conditioned

- The error is determined by the product of u, and the condition number
- Choose the precision for each block **independently,** such that at least 1 digit of the result is correct

Experimental results

Determining the precision:

$$\begin{cases} \text{fp16} & \text{if } 0 < \kappa_1(D_i) \leq 10^2, \\ \text{fp32} & \text{if } 10^2 < \kappa_1(D_i) \leq 10^6, \text{ and} \\ \text{fp64} & \text{otherwise,} \end{cases}$$

* Prototype implementation in MATLAB,
Results on 63 matrices from SuiteSparse

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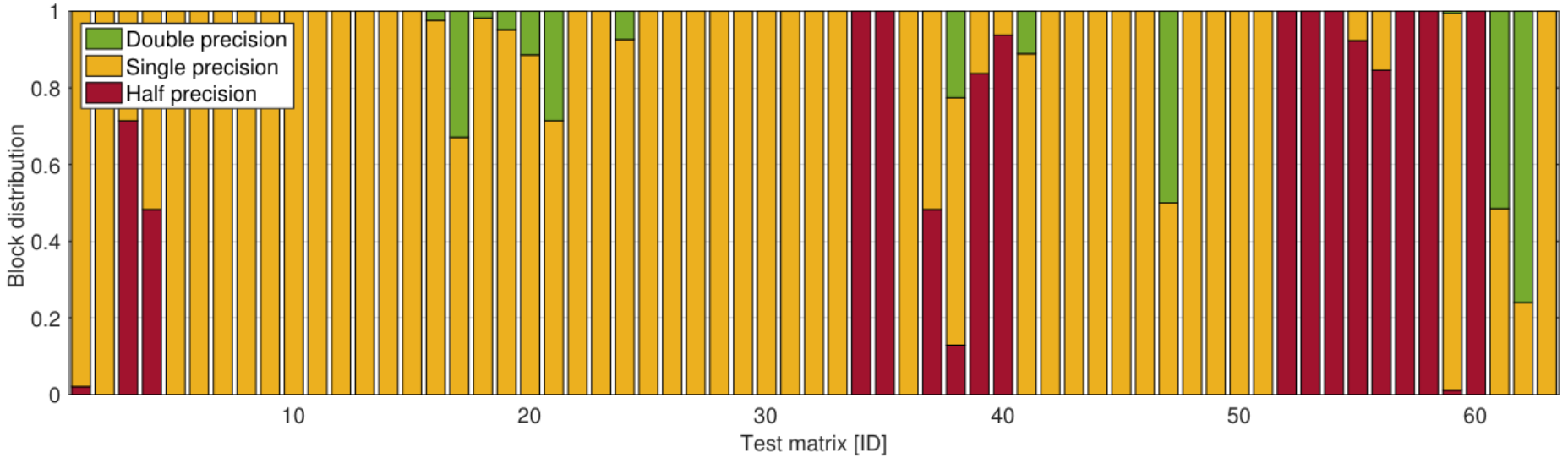
% of diagonal blocks stored in each precision *:



Usually < 5% iteration increase for reaching convergence

Energy efficiency of adaptive precision block-Jacobi

Memory access is an order of magnitude more expensive than computation! [Shalf 2013]

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Energy model assumptions:

- Accessing 1 bit of data has a cost of 1 (energy unit)
- Disregard energy cost of arithmetic operations
- Total energy cost of each iteration:

$$\underbrace{14n \cdot \text{fp64}}_{\text{vector memory transfers}} + \underbrace{(2n + n_z) \cdot \text{fp64} + (n + n_z) \cdot \text{int32}}_{\text{CSR-SpMV memory transfers}} + \underbrace{2n \cdot \text{fp64} + \sum_{i=1}^{N} m_i^2 \cdot \text{fpxx}_i}_{\text{preconditioner memory transfers}}$$

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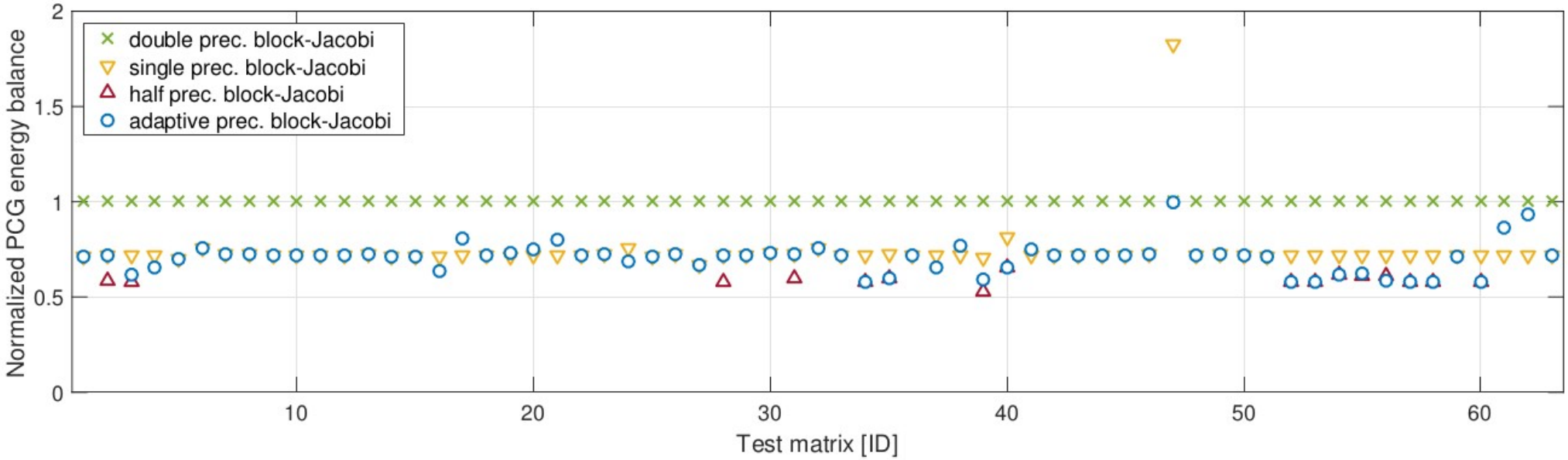
Predicted energy savings of adaptive precision block-Jacobi:



Thank you! Questions?

All functionalities are part of the MAGMA-sparse project.

MAGMA SPARSE

ROUTINES	BiCG, BiCGSTAB, Block-Asynchronous Jacobi, CG, CGS, GMRES, IDR, Iterative refinement, LOBPCG, LSQR, QMR, TFQMR
PRECONDITIONERS	ILU / IC, Jacobi, ParILU, ParILUT, Block Jacobi, ISAI
KERNELS	SpMV, SpMM
DATA FORMATS	CSR, ELL, SELL-P, CSR5, HYB

http://icl.cs.utk.edu/magma/

Scan me for slides!

github.com/gflegar/talks/tree/master/ibm_zurich_2017_09

This research is based on a cooperation between Hartwig Anzt (Karlsruhe Institute of Technology), Jack Dongarra (University of Tennessee), Nicholas Higham (University of Manchester), Goran Flegar and Enrique S. Quintana-Ortí (Universidad Jaume I).

Karlsruher Institut für Technologie

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