KIT, Karlsruhe, 12 June 2019

UNIVERSITAT JAUME I

Block-Jacobi preconditioning in Ginkgo

Goran Flegar

flegar@uji.es

Introduction

- I’m assuming we are all familiar with:
  - Iterative solution of linear systems
    - Why it’s useful
    - Operations within Krylov solvers (BLAS 1, SpMV, preconditioning)
  - Preconditioning
    - Replacing the original system with the preconditioned system
    - Changes needed within the Krylov solver to incorporate preconditioning

Block-Jacobi preconditioning

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  - Usually blocks are smaller than 30x30 (blocks can be of different sizes!)

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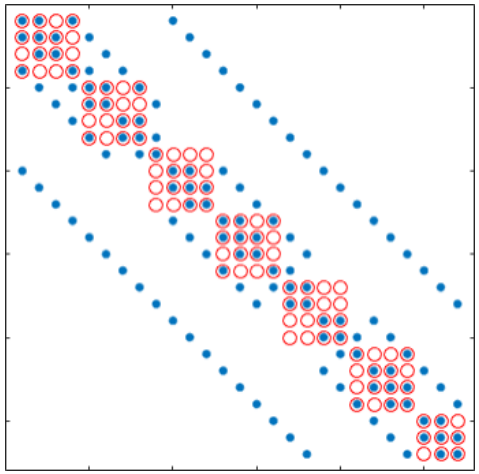

- Block-Jacobi preconditioning
  - Use only diagonal blocks for approximation

$$\mathrm{diag}(A) = [D_1, \ldots, D_k]$$
$$M := \mathrm{diag}(D_1, \ldots, D_k)$$

Benefits of block-Jacobi

- 56 matrices from SuiteSparse
- MAGMA-sparse open source library
  - IDR solver
  - Scalar Jacobi preconditioner
  - Supervariable agglomeration
    - Detects block structure of the matrix

M. Goetz and H. Anzt, "Machine Learning-Aided Numerical Linear Algebra: Convolutional Neural Networks for the Efficient Preconditioner Generation," 2018 IEEE/ACM 9th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (scalA), Dalla, TX, USA, 2018, pp. 49-56.

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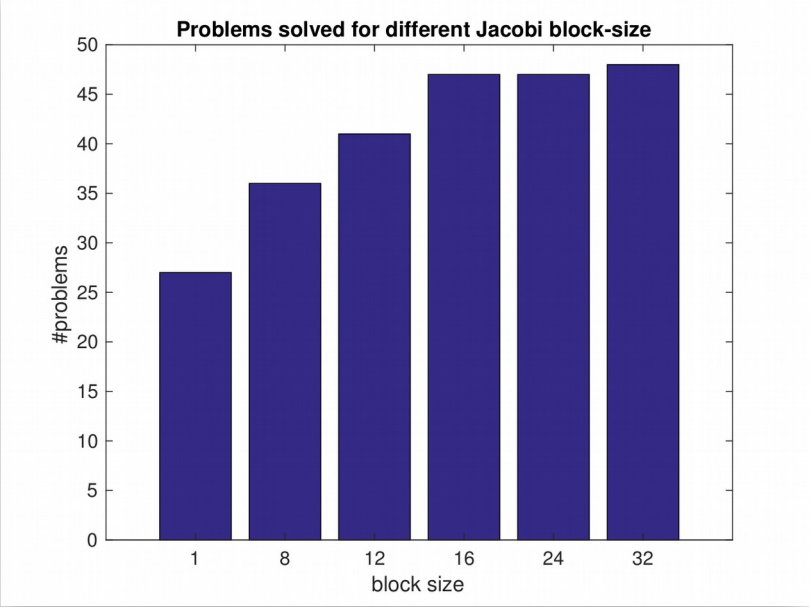

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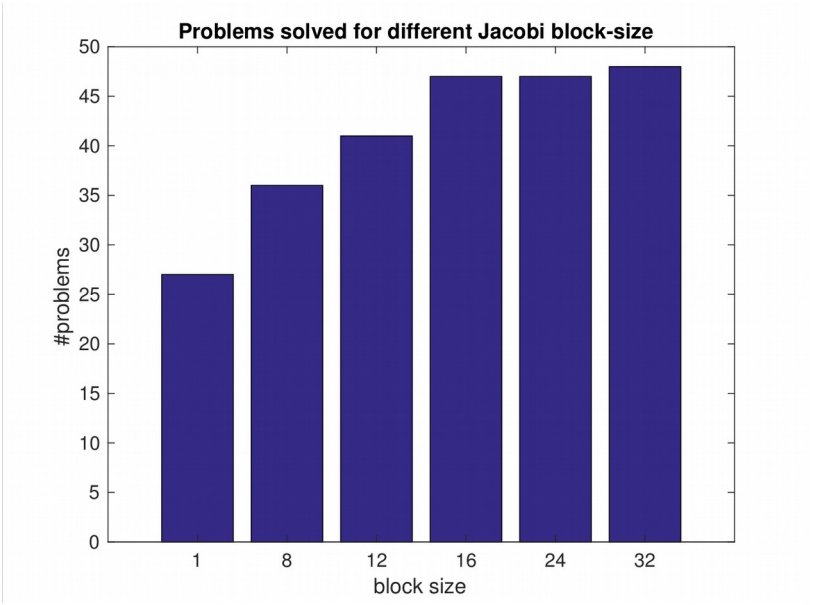
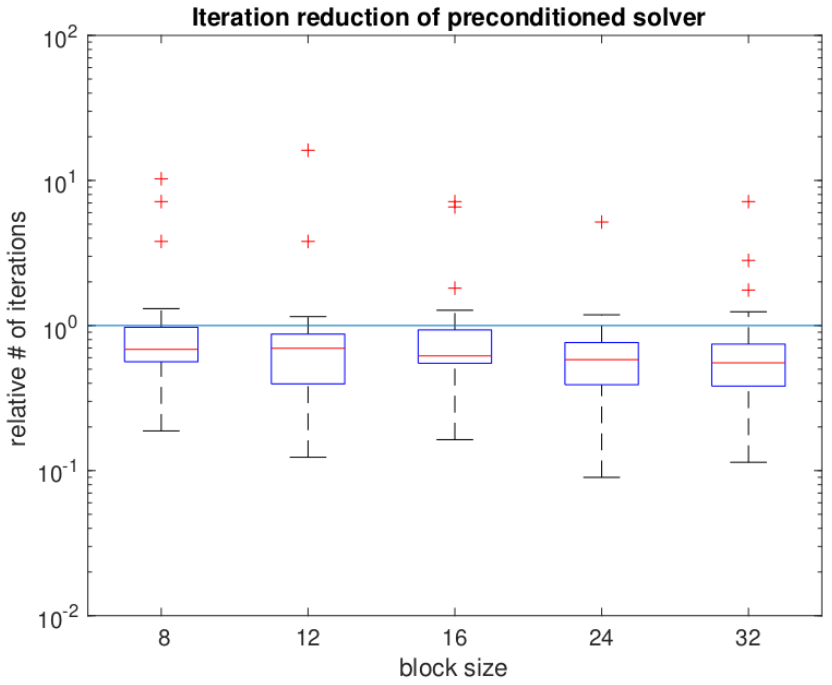
- Improves convergence of the solver





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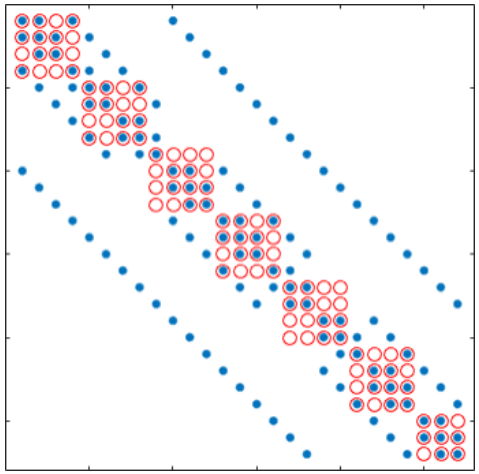

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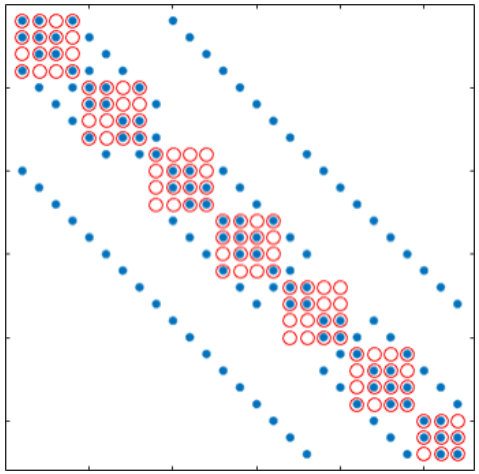

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inv = Gauss-Jordan elimination

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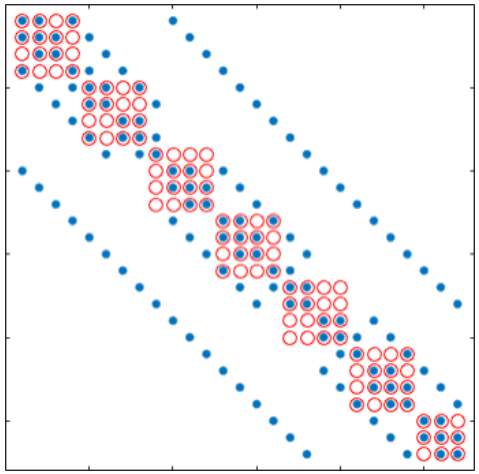

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$$\widetilde{D}_i := \text{inv}(D_i)$$ **Setup**

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

Inversion-based block-Jacobi

inv = Gauss-Jordan elimination

Block-Jacobi preconditioning

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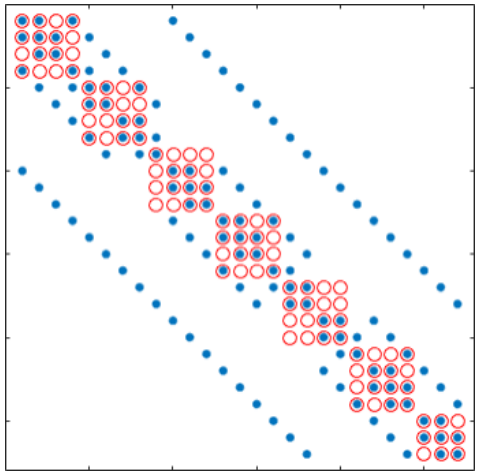

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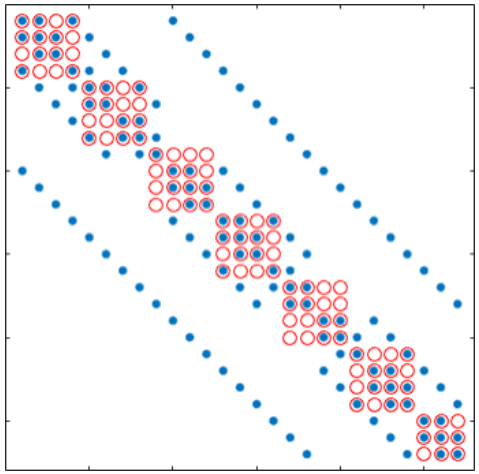

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$$D_i = L_i U_i$$

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

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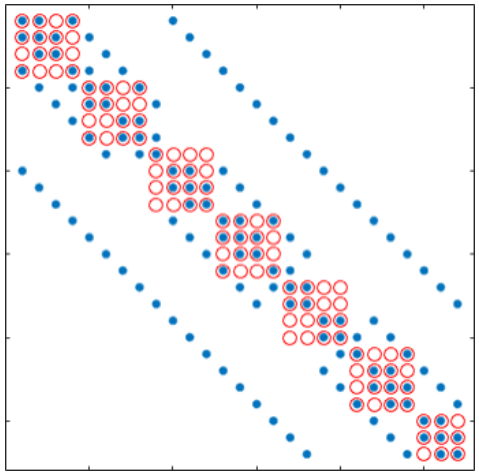

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$$D_i = L_i U_i$$ **Setup**

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

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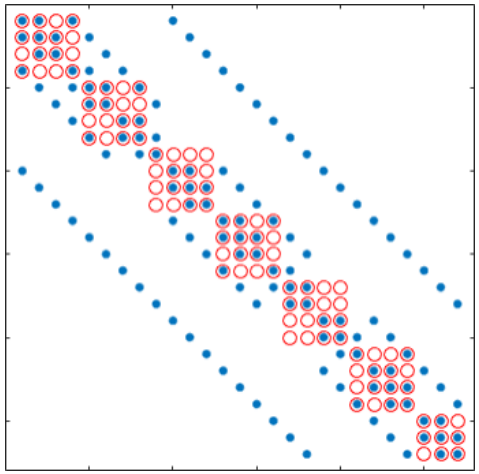

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gh = Gauss-Huard decomposition / application

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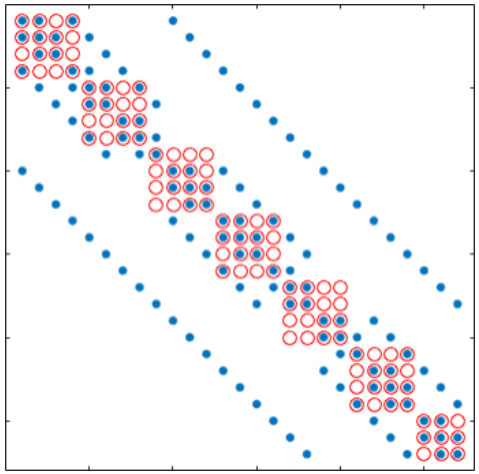

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Decomposition-based block-Jacobi

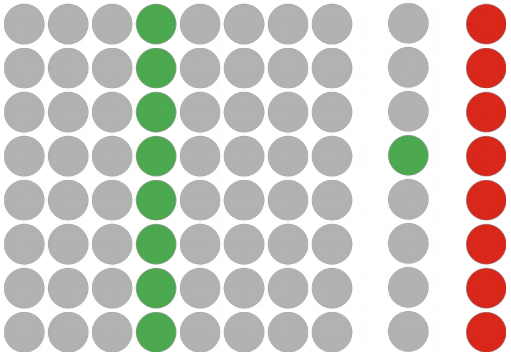
Block-Jacobi setup & application ecosystem

Setup

Application

Gauss-Jordan inversion

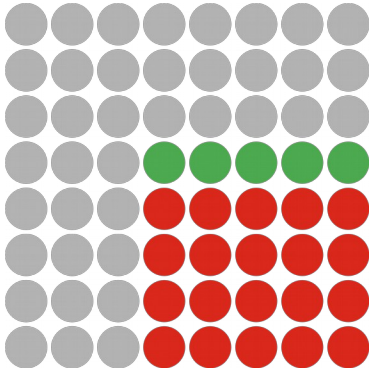
Inversion-based
($2n^3 + 2n^2$ FLOPS)
matrix-vector multiply



H. Anzt et al. “Variable-size batched Gauss–Jordan elimination for block-Jacobi preconditioning on graphics processors”, ParCo’19

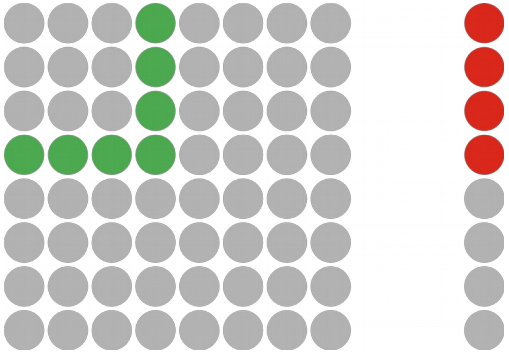
Gauss-Huard decomposition

LU factorization



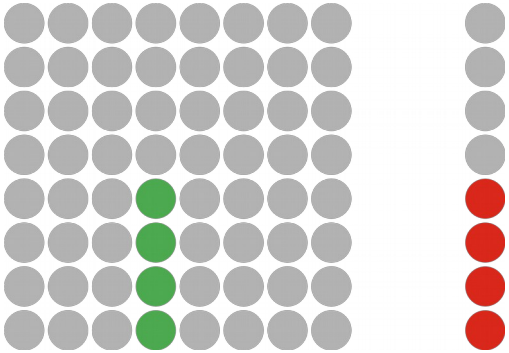
Decomposition-based
($2/3n^3 + 2n^2$ FLOPS)

Gauss-Huard solve



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

2x triangular solve



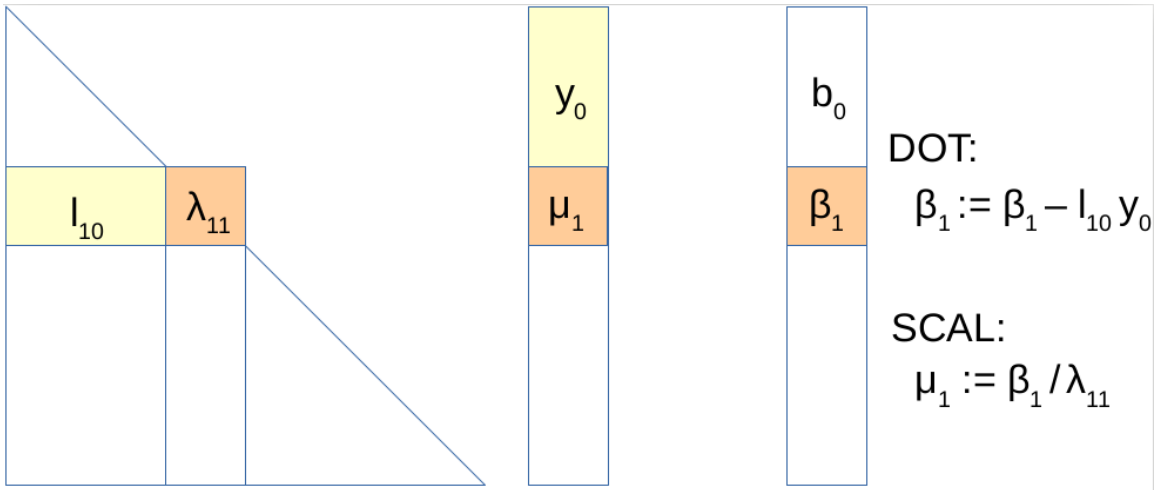
H. Anzt et al. “Flexible-Size Batched LU for Small Matrices and its Integration into Block-Jacobi Preconditioning”, ICPP’17

- read - write

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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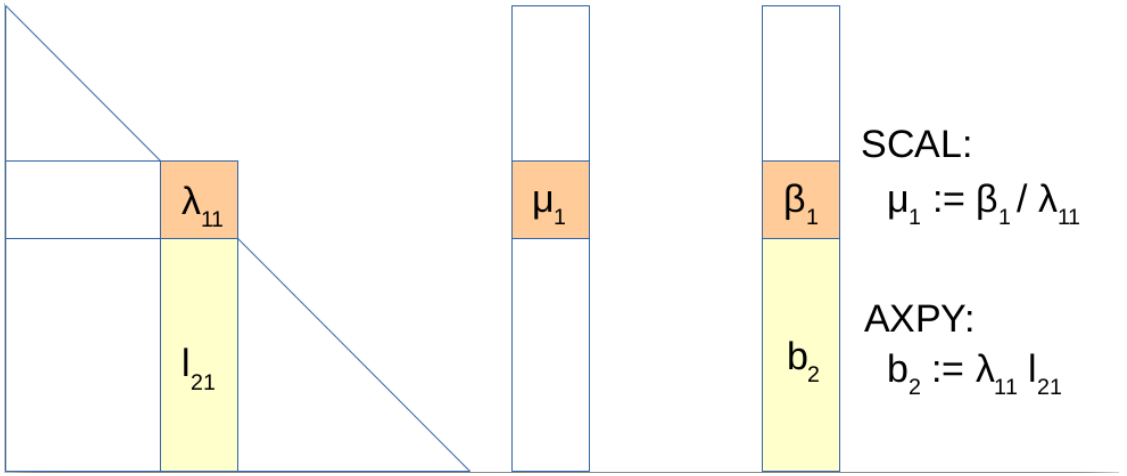
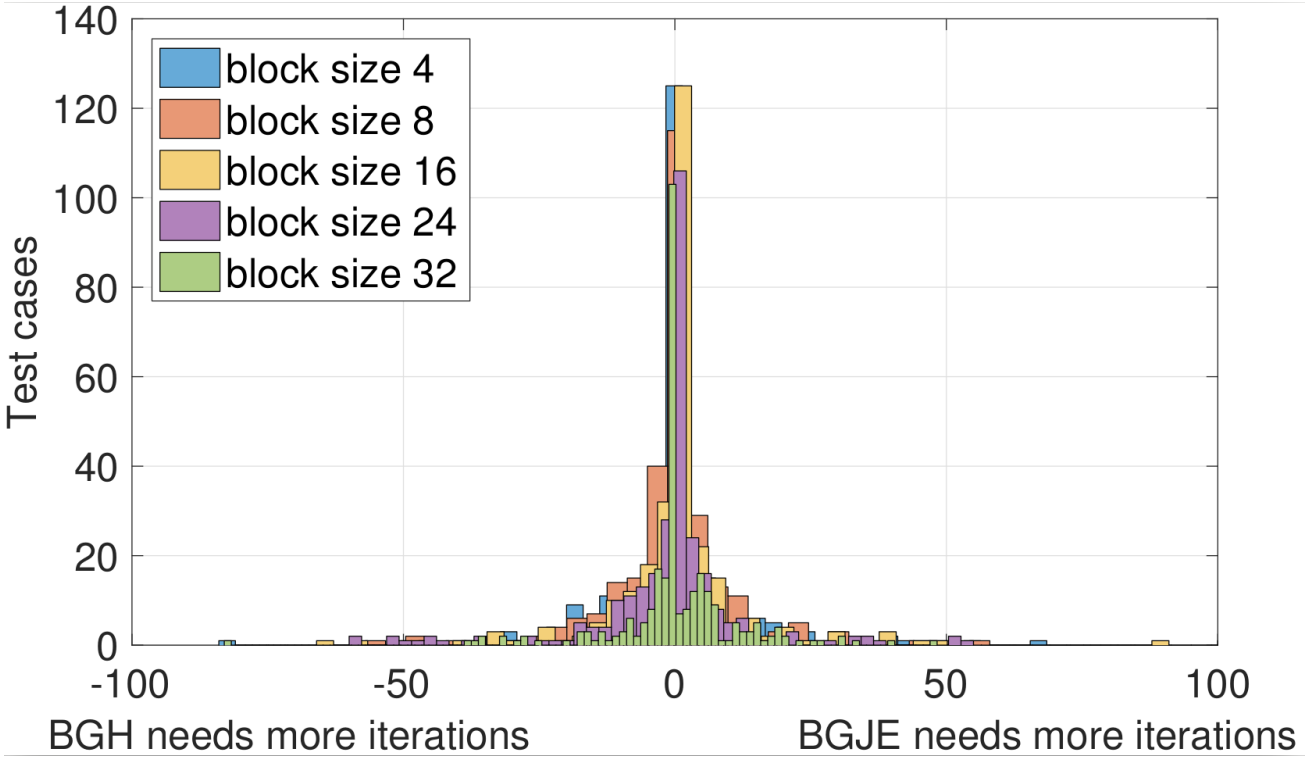


No signs of instability in practice



Batched inversion and decomposition

- Assign one warp to each problem
  - hardware SIMD unit, represented as a group of 32 threads in CUDA

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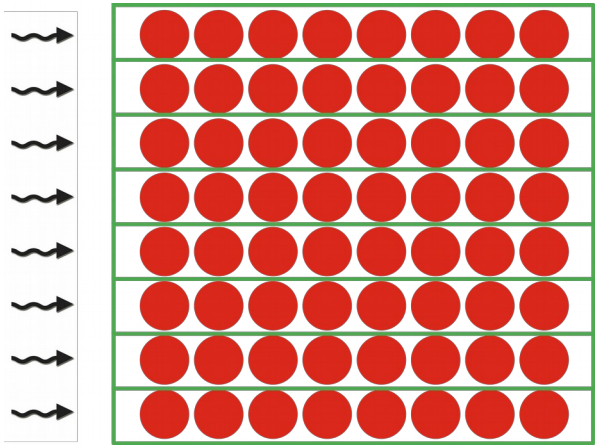
- Process each row (column) by a single thread
  - Able to support problems of size up to 32-by-32
  - Keep the entire row (column) in thread's registers
  - Communicate data between rows via warp-shuffles
  - Current implementation: use padding for problems of smaller sizes
  - Future work: multiple smaller problems per warp



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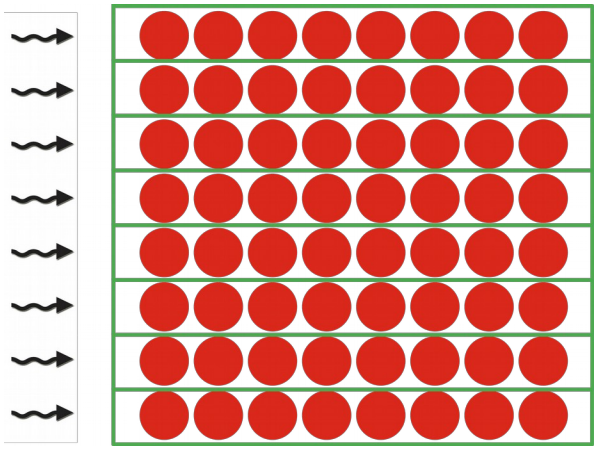
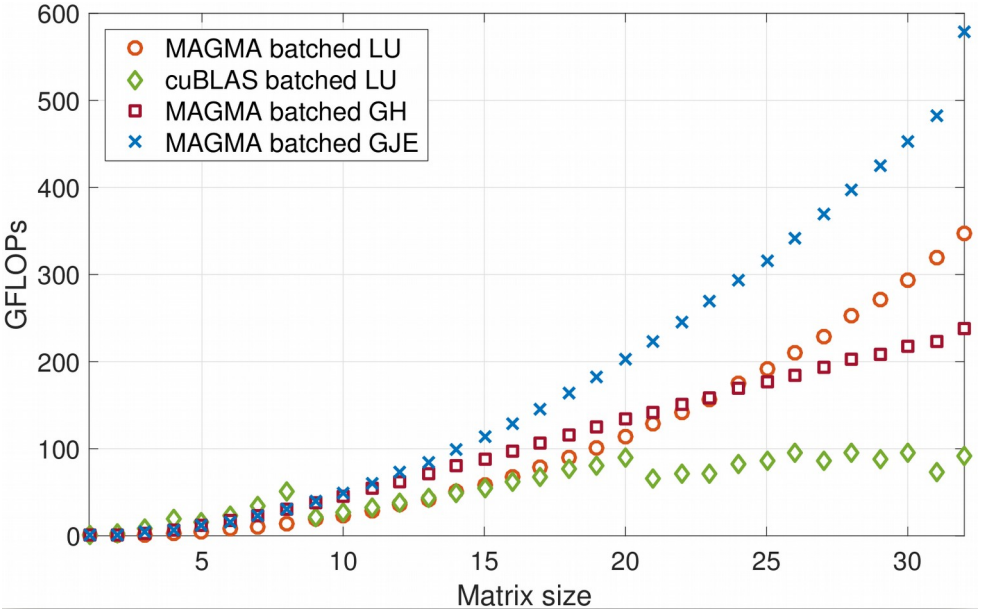
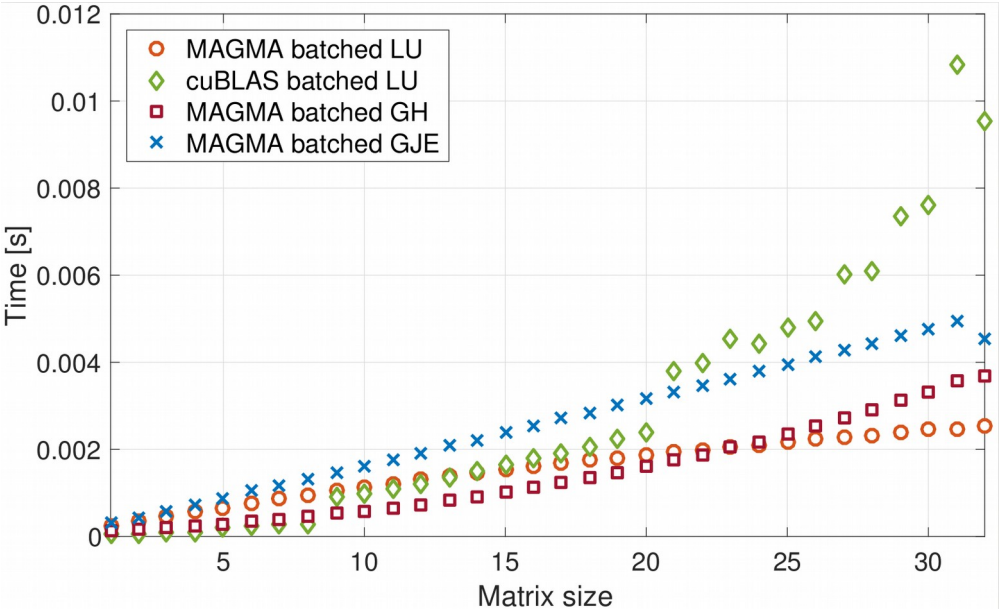


- Use implicit pivoting
  - Do not explicitly swap rows (column), "re-assign" the threads instead

Batched routines performance





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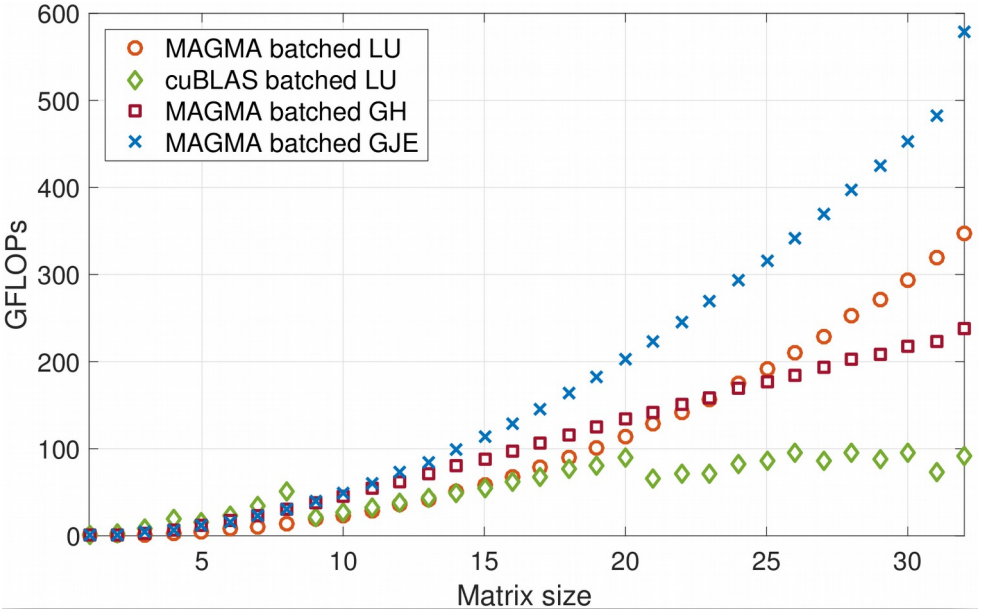
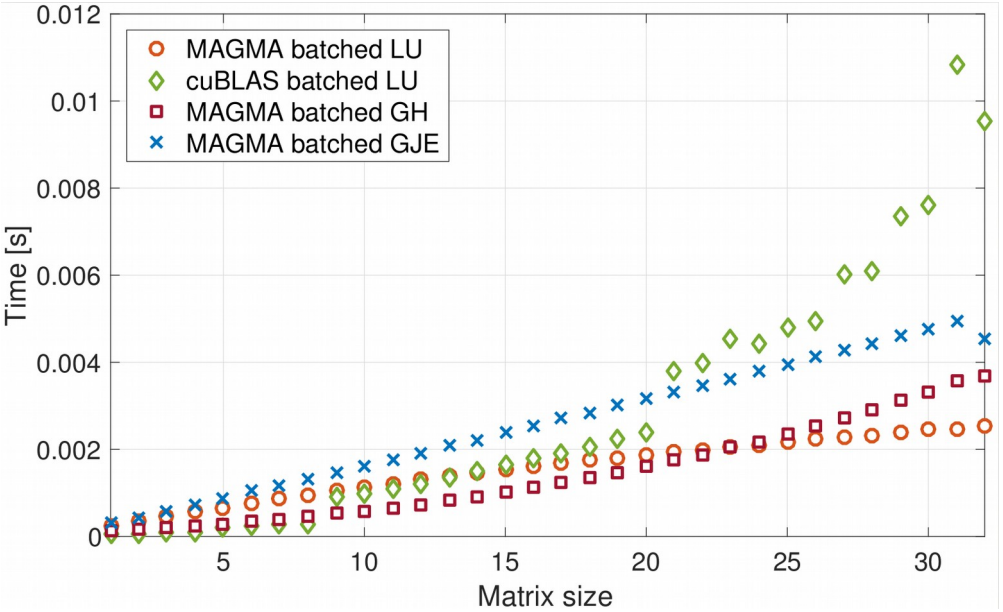
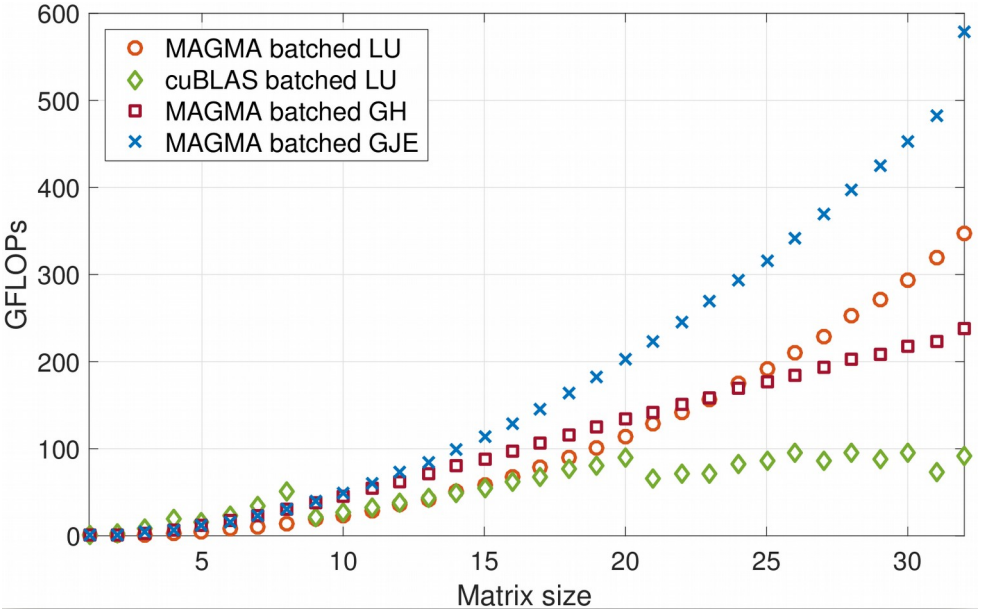


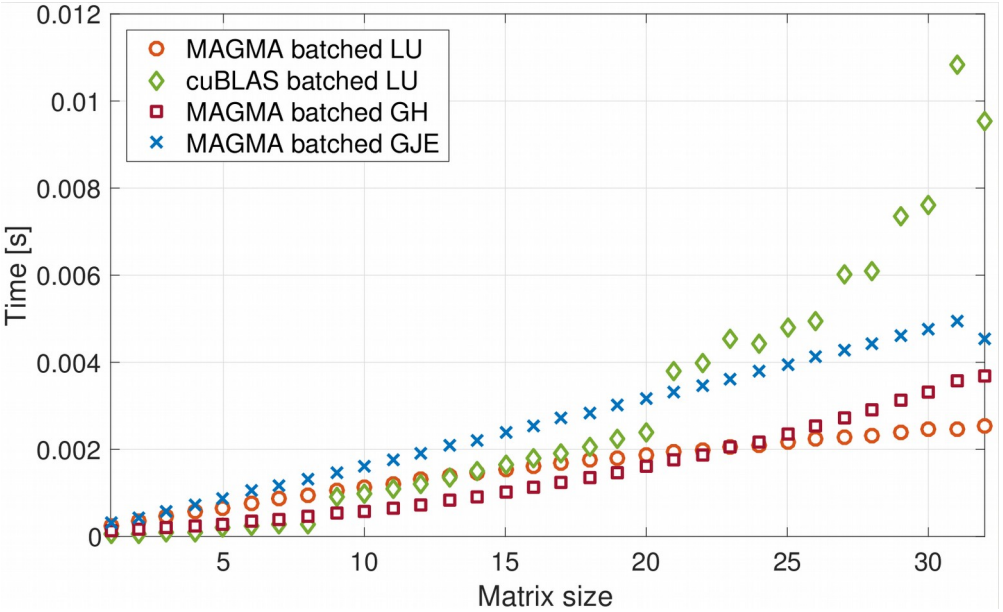


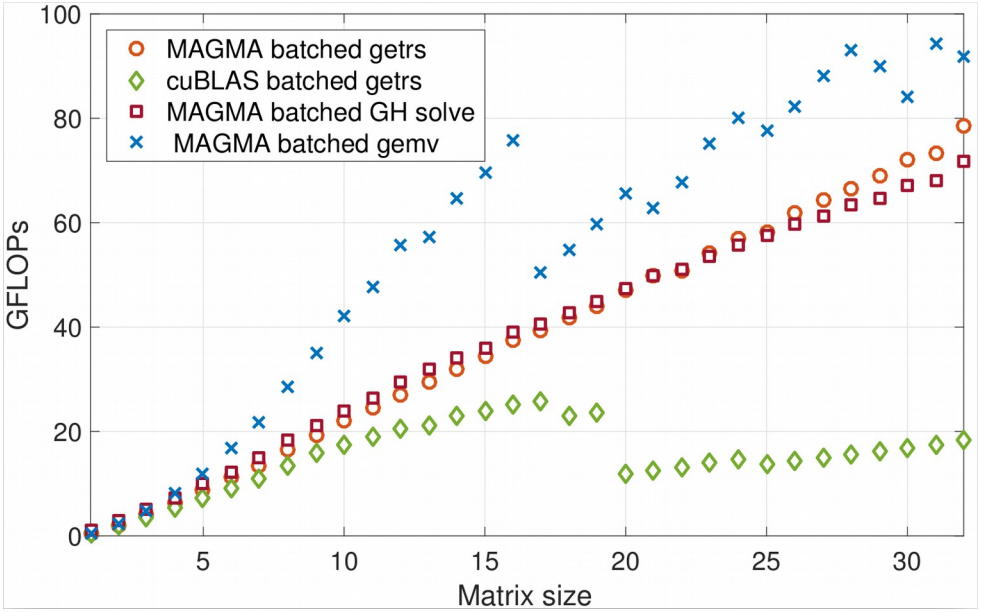
MAGMA-sparse routines can also:

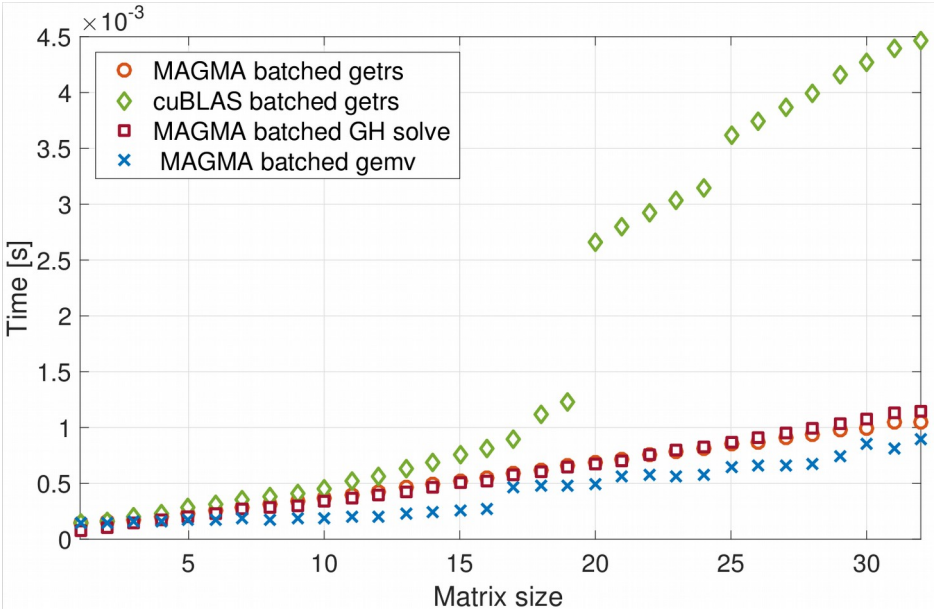
- Handle problems of different sizes
- Integrate diagonal block extraction and diagonal block decomposition / inversion into a single kernel

Batched routines performance



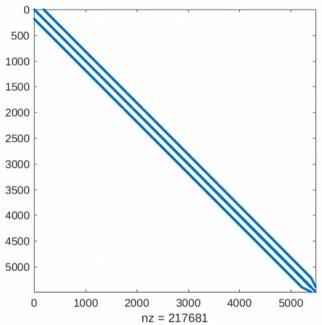


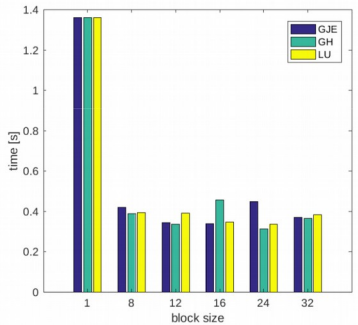




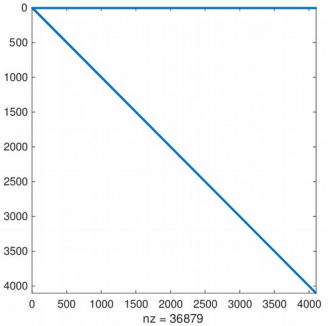
Complete solver runtime

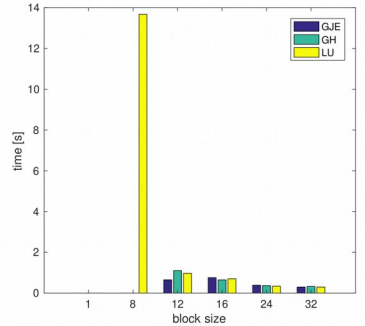
s2rmt3m1



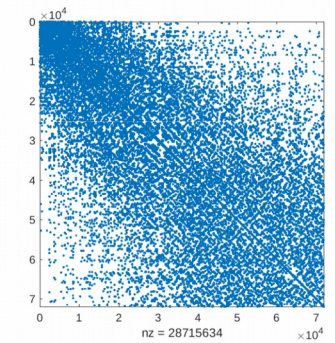


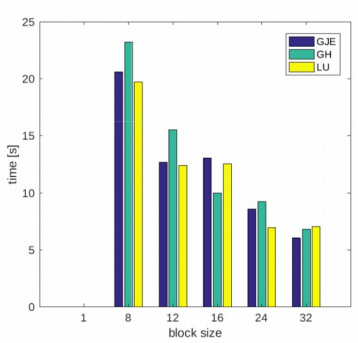
Chebyshev3



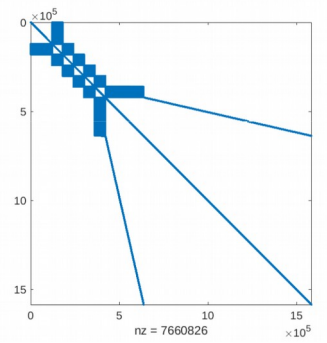


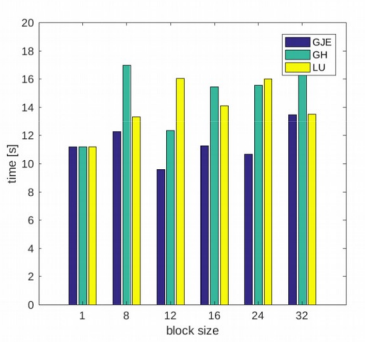
nd24k



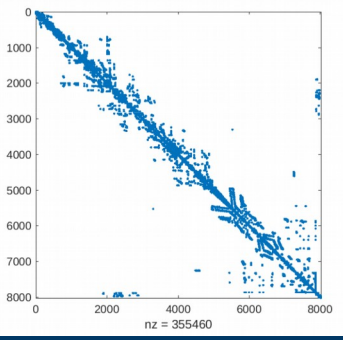


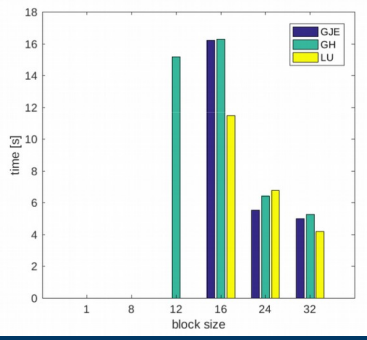
G3_circuit



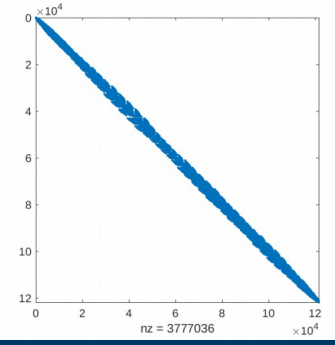


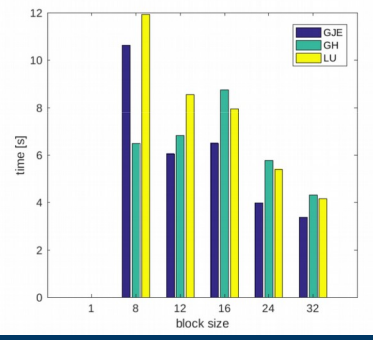
bcsstk38





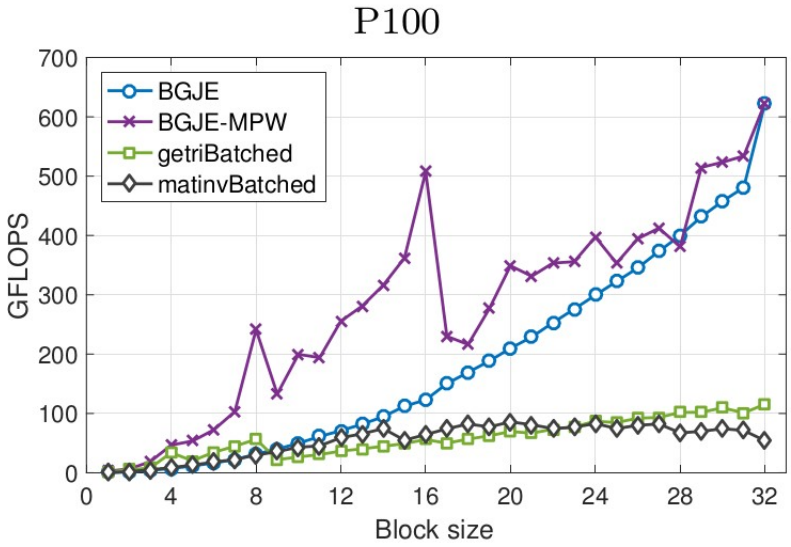
ship_003





Flexible-size batched routines

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



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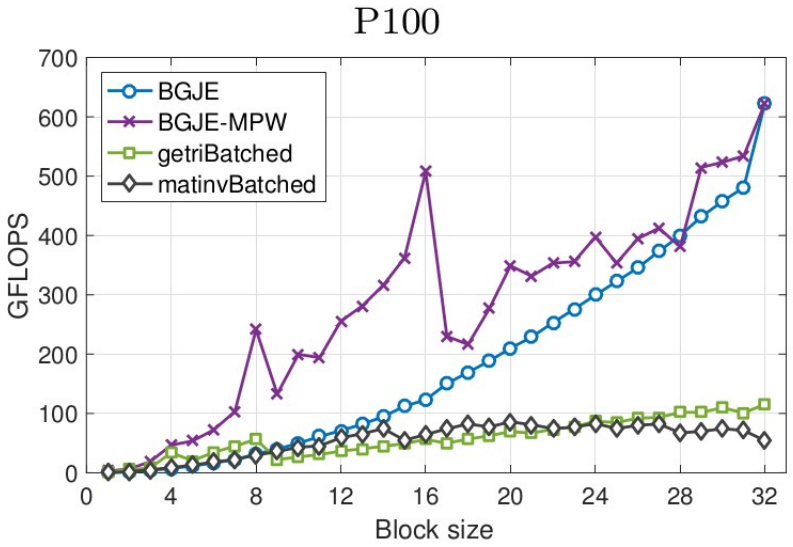
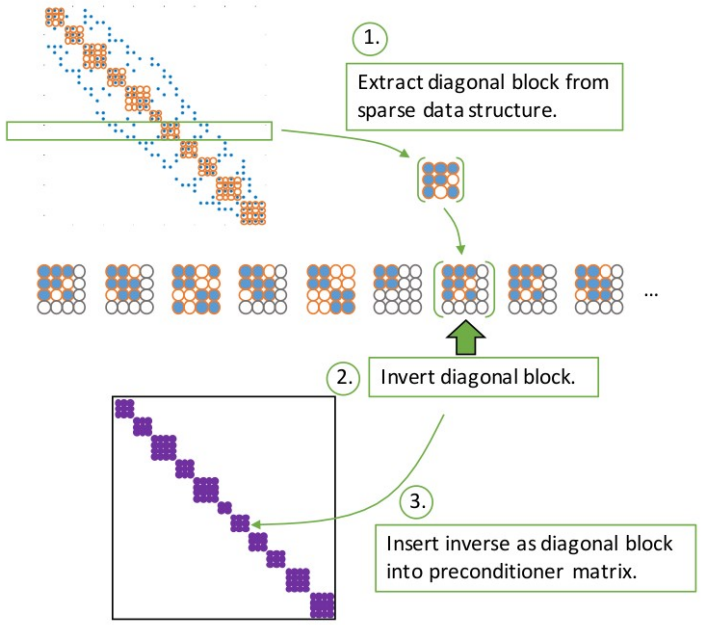


- Allow batches where problems are of different sizes (flexible-size)
  - How to combine this with multiple problems per warp?
    - Remember: entire warp executes the same instruction!
    - Current solution: padding



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

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

Anzt, et al. "Adaptive precision in block-Jacobi preconditioning for iterative sparse linear system solvers." Concurrency and Computation: Practice and Experience 31.6 (2019): e4460.

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- All computation is done in double precision
- Preconditioner matrix is stored in lower precision, with roundoff error “u”
- Error bound:

$$\frac{||\delta z_i||}{||z_i||} \lesssim (c_i \kappa(D_i) u_d + u)\kappa(D_i)$$

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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:

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

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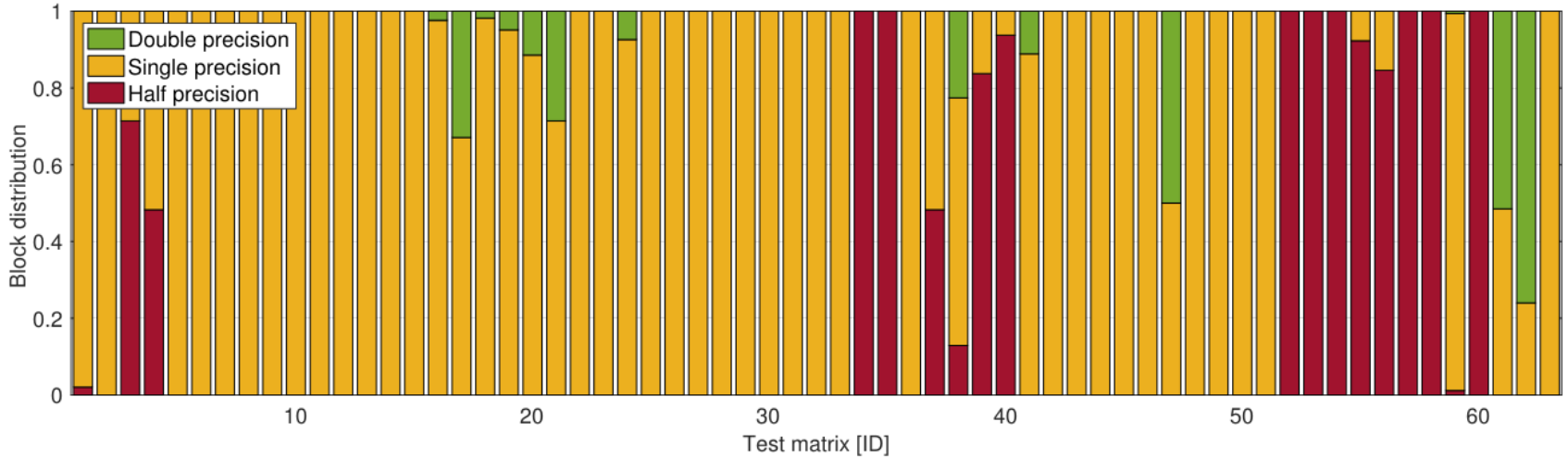
% of diagonal blocks stored in each precision *:



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Results on 63 matrices from SuiteSparse

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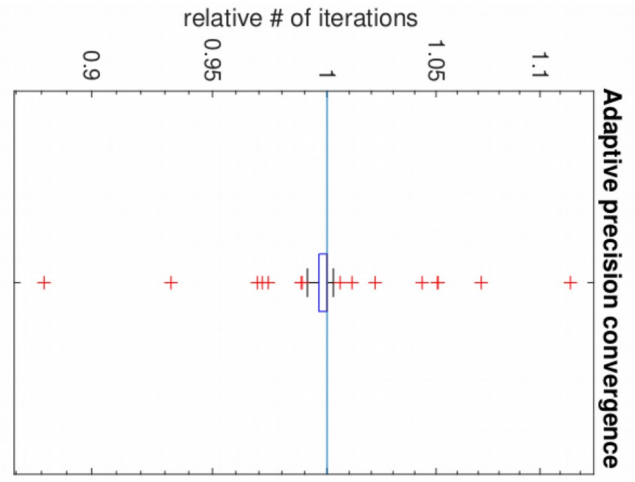

Usually < 5% iteration increase

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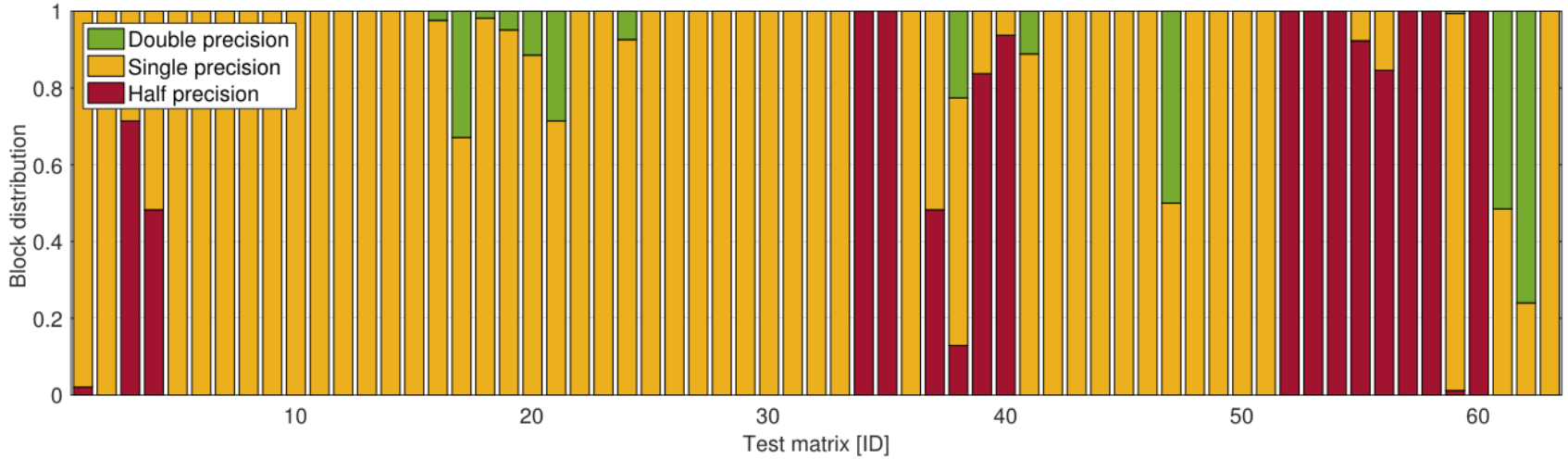

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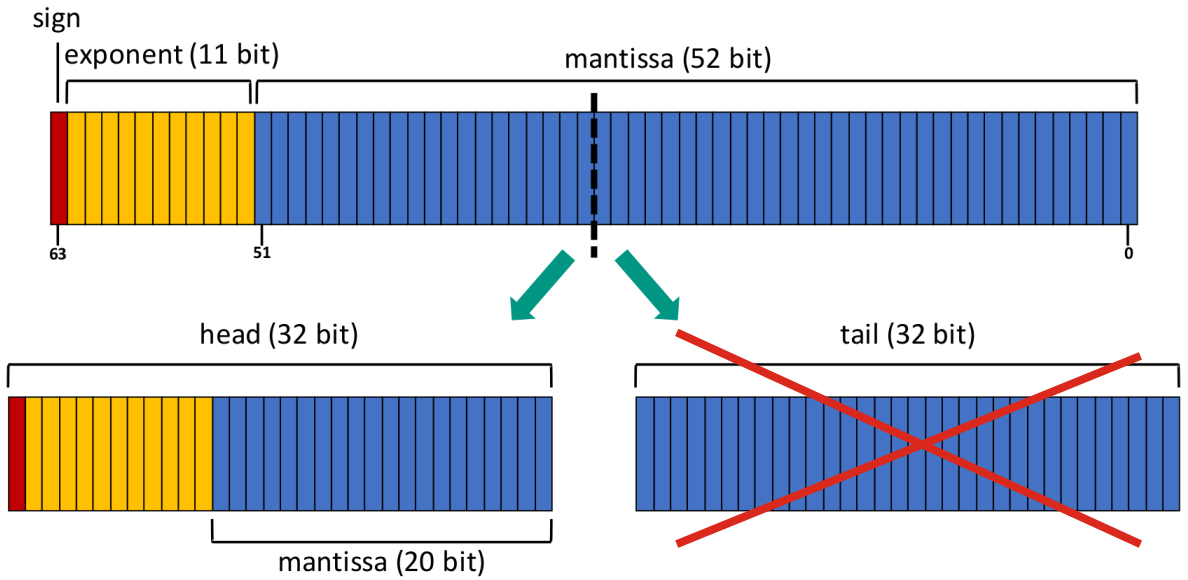
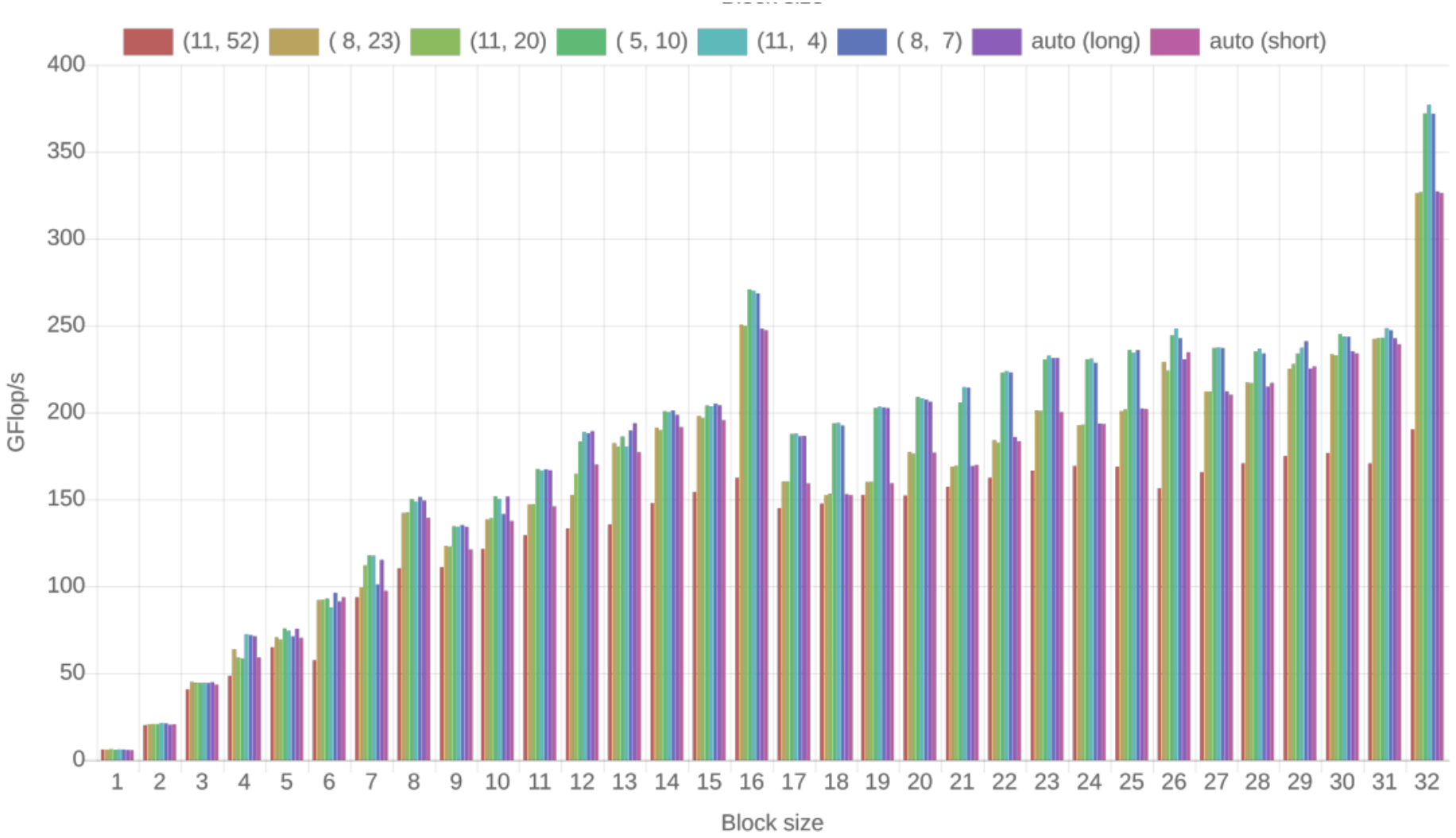
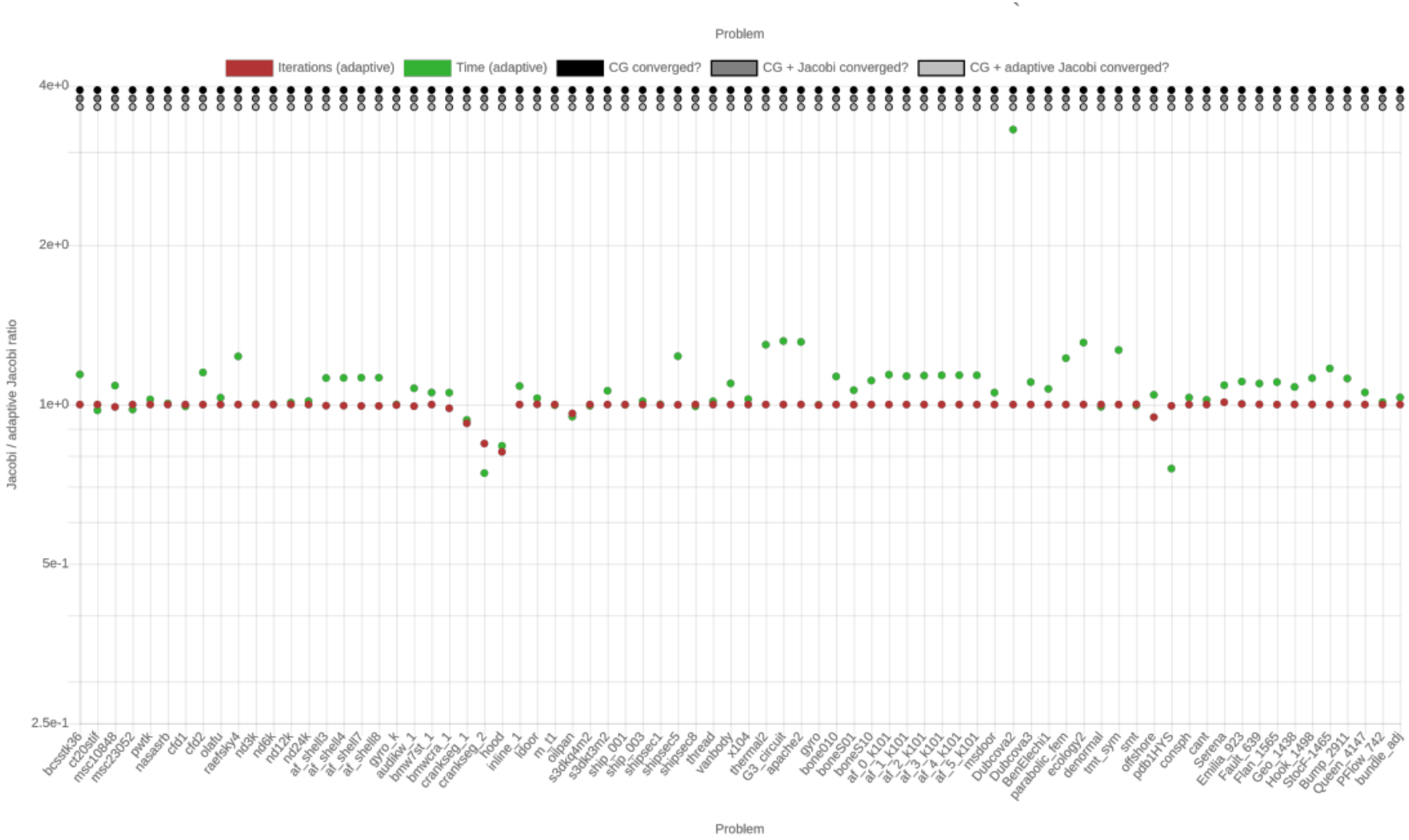


Preconditioner application performance



Time-to-solution, adaptive- vs full-precision BJ



Summary

- Employ inherently parallel preconditioning schemes on accelerator hardware
- Trade more computation for better access patterns
- Take advantage of large register field of NVIDIA GPUs
- Avoid data exchange by “renaming” CUDA threads
- Take advantage of low precision to accelerate preconditioner application
- Independently select precision for each subproblem to preserve preconditioner quality

KIT, Karlsruhe, 12 June 2019

UNIVERSITAT JAUME I

Linear systems, Ginkgo

flegar@uji.es

Sources of linear systems

- Real-world problem transformed into a linear system via:
  - PDE discretizations, graph representations
  - Large number of unknowns (1M+, full matrix 8TB)
  - Most matrix elements are zero
- Possible approach: iterative methods
  - Krylov-subspace based linear solvers
    - SpMV
    - BLAS-1 operations
  - Sparse matrix formats & SpMV
    - accelerate each iteration of the solver
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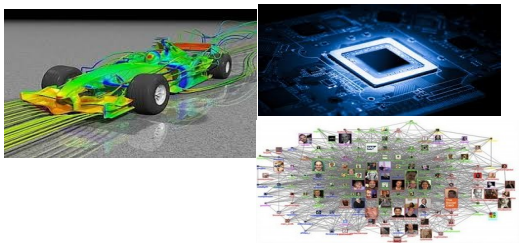
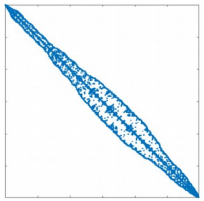
    - reduce the number of iterations





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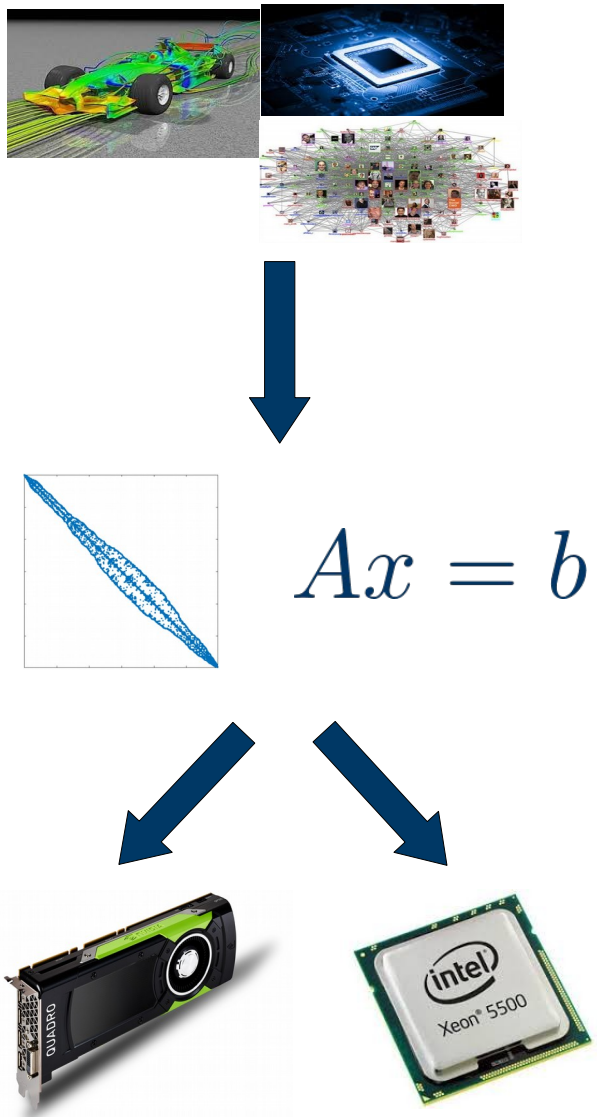

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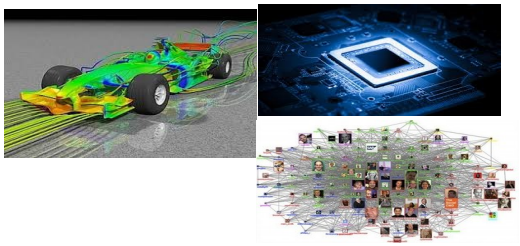
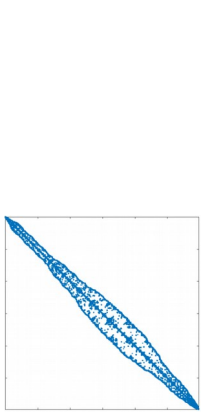
  - Use a library instead: Ginkgo





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Ginkgo

KIT, Karlsruhe, 12 June 2019

UNIVERSITAT JAUME I

Preconditioning

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Preconditioner application

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Preconditioner setup

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