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UNIVERSITAT JAUME I

How to Solve a Linear System

Goran Flegar

Hartwig Anzt, Yen-Chen Chen, Terry Cojean, Jack Dongarra, Nick Higham, Pratik Nayak, Enrique S. Quintana-Ortí, Mike Tsai

Scan me for slides!

github.com/gflegar/talks/tree/master/cmu_pittsburgh_2018_11

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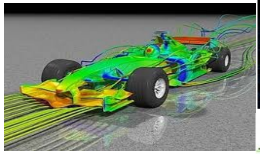
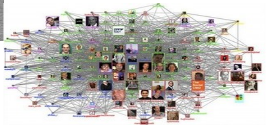
Sources of linear systems

- 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





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  - Krylov-subspace based linear solvers
    - SpMV
    - BLAS-1 operations
  - Sparse matrix formats & SpMV
    - accelerate each iteration of the solver
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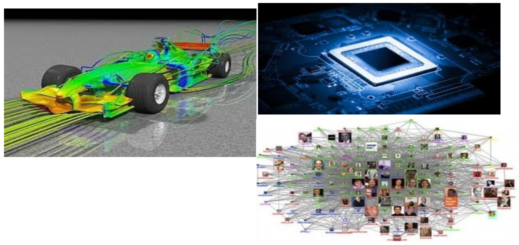
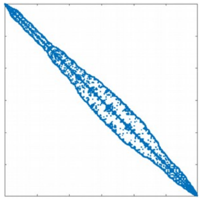
    - reduce the number of iterations





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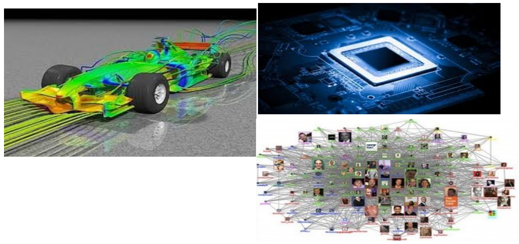

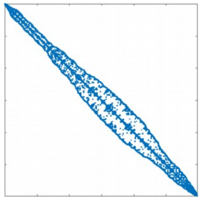

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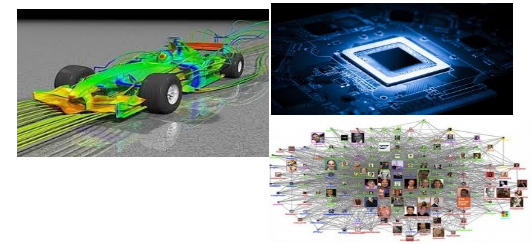

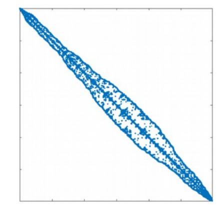

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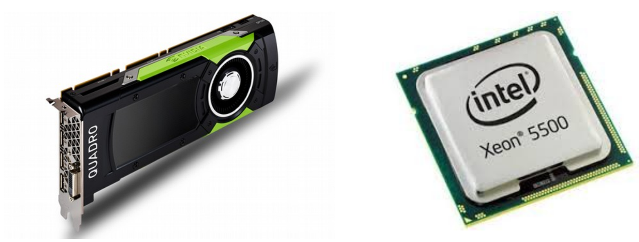
Ginkgo



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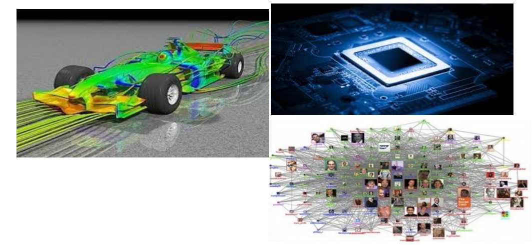

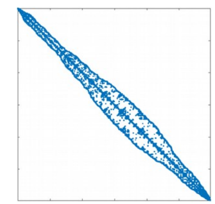

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Ginkgo

The Ginkgo library

- Linear operator algebra library:
  - Matrix formats, preconditioners, (Krylov) solvers

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

THE UNIVERSITY OF TENNESSEE KNOXVILLE

Karlsruher Institut für Technologie

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The Ginkgo library

- Linear operator algebra library:
  - Matrix formats, preconditioners, (Krylov) solvers
- Goals:
  - Backends for various devices (executors)
  - Easy composability – even when using building blocks from a different category (e.g. using a matrix or a solver as a preconditioner)
  - Easy extensibility
  - Support for matrix-free methods

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Core idea

Matrix-vector product

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Preconditioner

$$x = M^{-1}b$$

$$M \approx A$$

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All of them can be expressed as:

- applications of linear operators* (LinOp)

$$L : \mathbb{F}^m \to \mathbb{F}^n$$

* can be realized as a (non-linear) approximation

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All of them can be expressed as:

- applications of linear operators* (LinOp)
- (non-linear) transformations applied to linear operators (Factory)

$$L : \mathbb{F}^m \to \mathbb{F}^n$$
$$\Phi : \mathbb{L}^{mn}(\mathbb{F}) \to \mathbb{L}^{kl}(\mathbb{F})$$

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Example

- Solving a symmetric positive definite linear system using the conjugate gradient (CG) solver, preconditioned with a block-Jacobi (BJ) preconditioner, with a system matrix stored in CSR format

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1. Read the system matrix operator, right hand side and initial guess from file, standard input, or use existing data from the application

$$\mathrm{A}_{\mathrm{CSR}} \;\; \mathrm{b}_{\mathrm{D}} \;\; \mathrm{x}_{\mathrm{D}}$$

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4. Generate the solver operator from the system matrix using the solver factory (preprocessing needed for the solver and preconditioner)

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$$\mathrm{S}_{\mathrm{A}} = \mathrm{CG}_{\mathrm{BJ}}(\mathrm{A}_{\mathrm{CSR}})$$

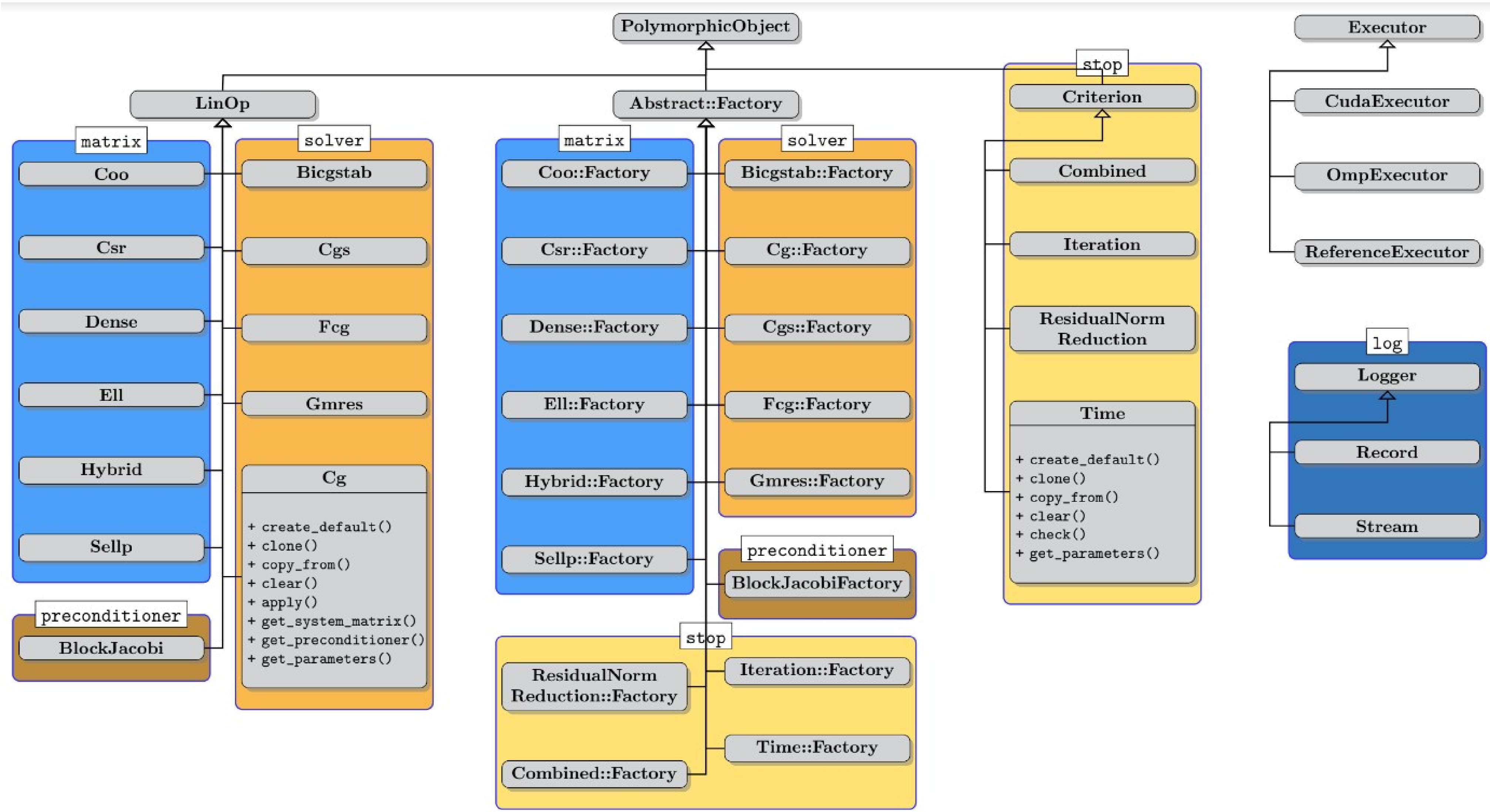
5. Solve the system (actual computation)

$$\mathrm{x}_{\mathrm{D}} = \mathrm{S}_{\mathrm{A}} \mathrm{b}_{\mathrm{D}}$$

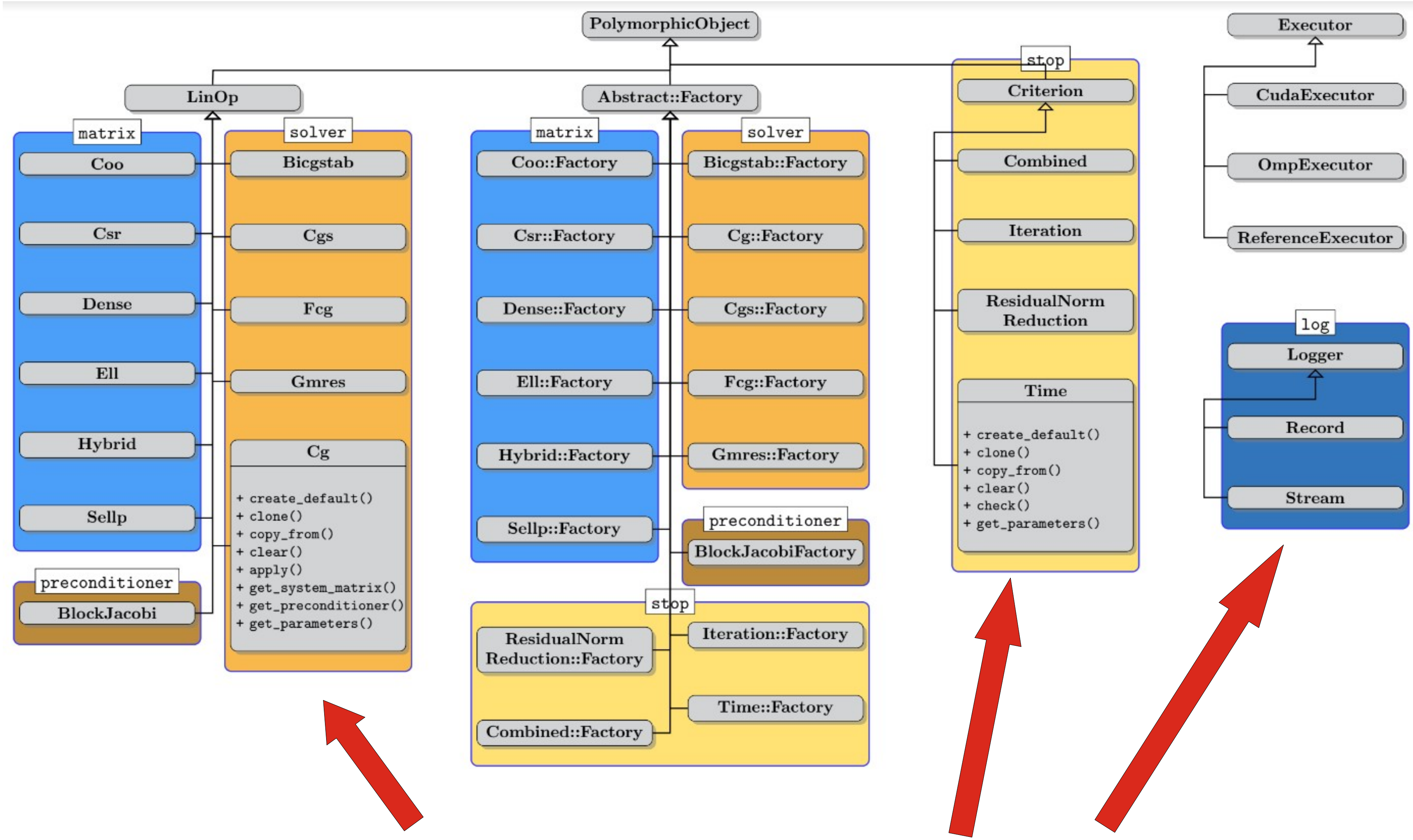
Example source code

```cpp
int main() {
  // Instantiate a CUDA executor
  auto gpu = gko::CudaExecutor::create(0, gko::OmpExecutor::create());
  // Read data
  auto A = gko::read<gko::matrix::Csr<>>(std::cin, gpu);
  auto b = gko::read<gko::matrix::Dense<>>(std::cin, gpu);
  auto x = gko::read<gko::matrix::Dense<>>(std::cin, gpu);
  // Create the solver
  auto solver = gko::solver::Cg<>::build()
    .with_preconditioner(
      gko::preconditioner::Jacobi<>::build().with_max_block_size(32).on(gpu))
    .with_criteria(
        gko::stop::Iteration::build().with_max_iters(20u).on(gpu),
        gko::stop::ResidualNormReduction<>::build()
          .with_reduction_factor(1e-15).on(gpu))
    .on(gpu);
  // Solve system
  solver->generate(give(A))->apply(lend(b), lend(x));
  // Write result
  write(std::cout, lend(x));
}
```

Library features



Library features: extensibility



users can provide new matrices, solvers, preconditioners, stopping criteria, loggers

Without recompiling the library!

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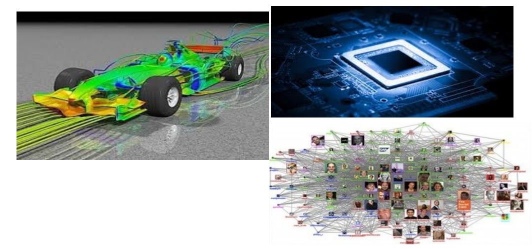

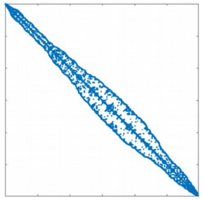

$$Ax = b$$

Ginkgo

Preconditioning

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

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

Replace the original system with an
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$$M \approx A \qquad M^{-1} \text{ easy to compute}$$

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$$\cancel{M^{-1}A}$$

Do not compute the preconditioned system matrix explicitly!

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Preconditioner setup

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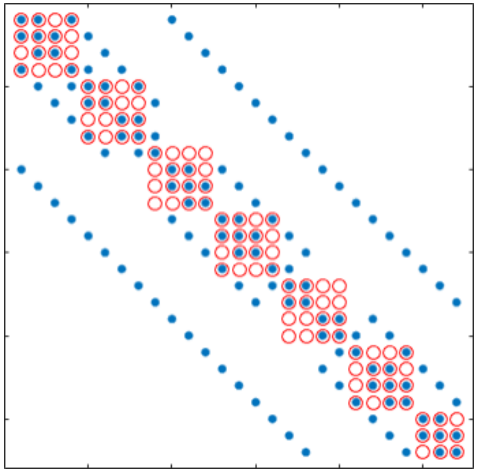
Generation via factory

Linear operator application

Ginkgo linear operator abstraction

Example: Block-Jacobi preconditioning



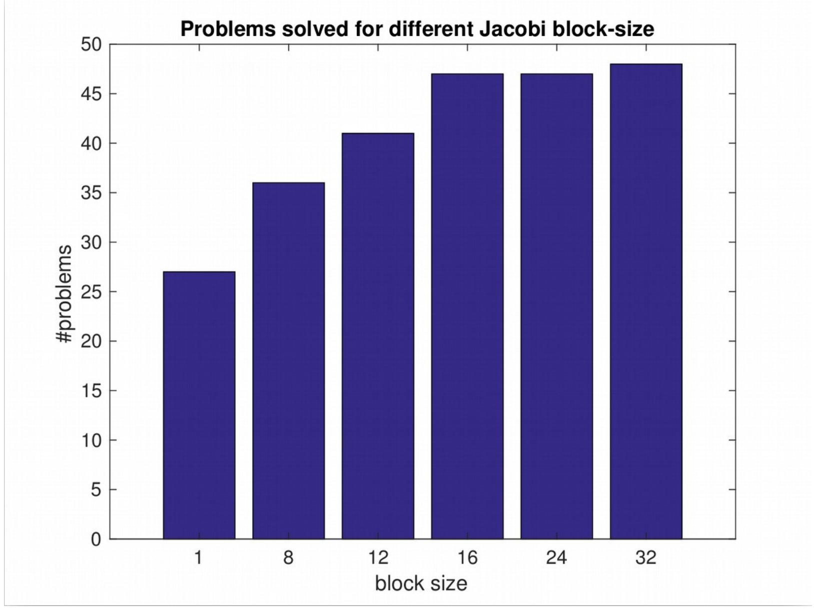
- Block-Jacobi preconditioning
  - Use only diagonal blocks for approximation

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

Anzt, Dongarra, Flegar, Quintana-Ortí, *Variable-size batched Gauss–Jordan elimination for block-Jacobi preconditioning on graphics processors, ParCo*

Benefits of block-Jacobi

- 56 matrices from SuiteSparse with inherent block structure
- MAGMA-sparse open source library
  - IDR solver
  - Supervariable agglomeration
    - Detects block structure of the matrix
- Improves the robustness of the solver



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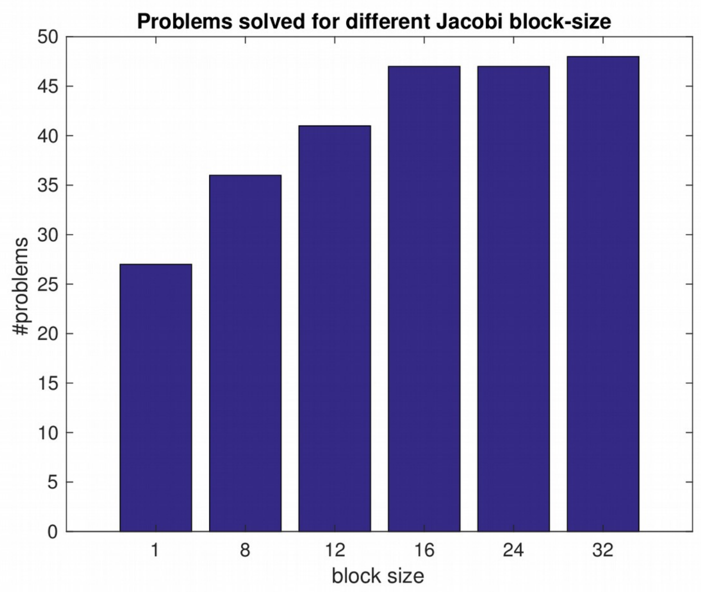
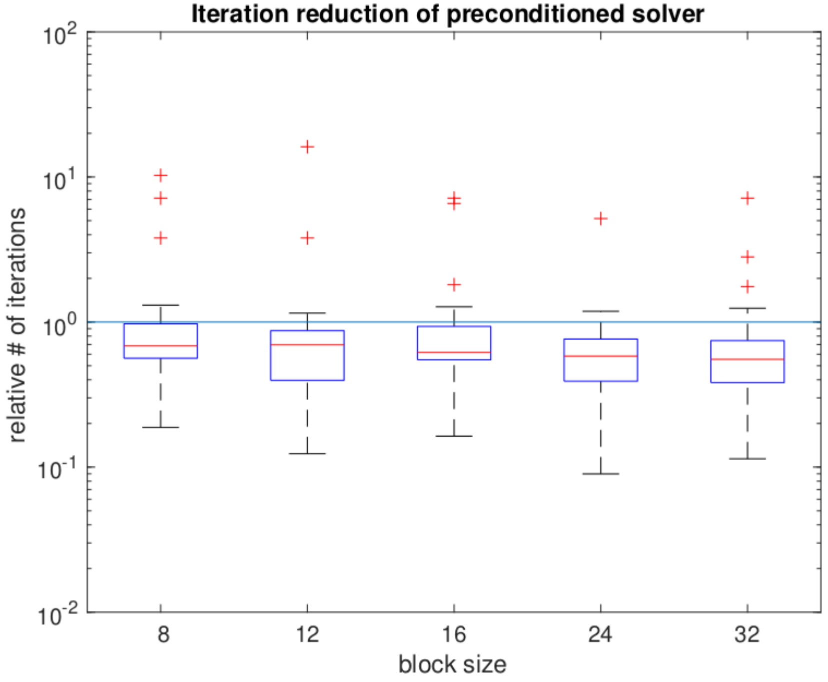
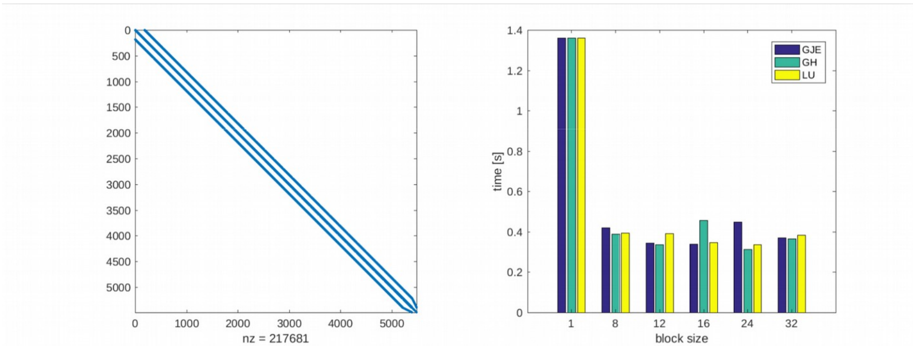


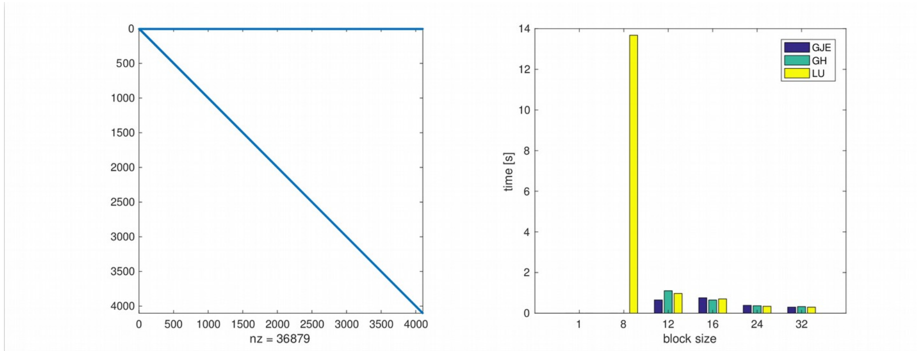


Complete solver runtime

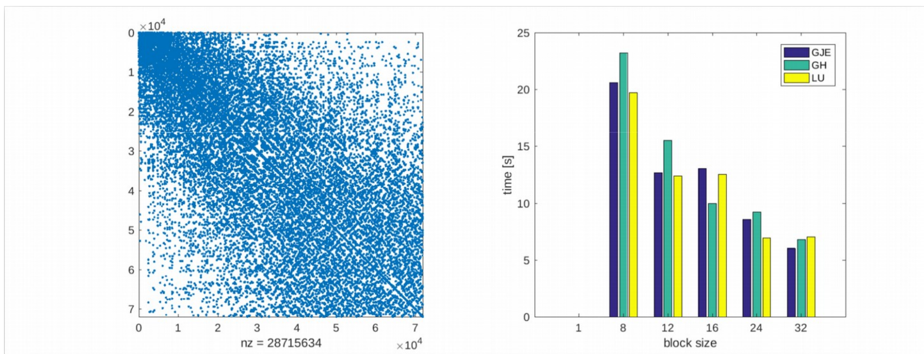
s2rmt3m1



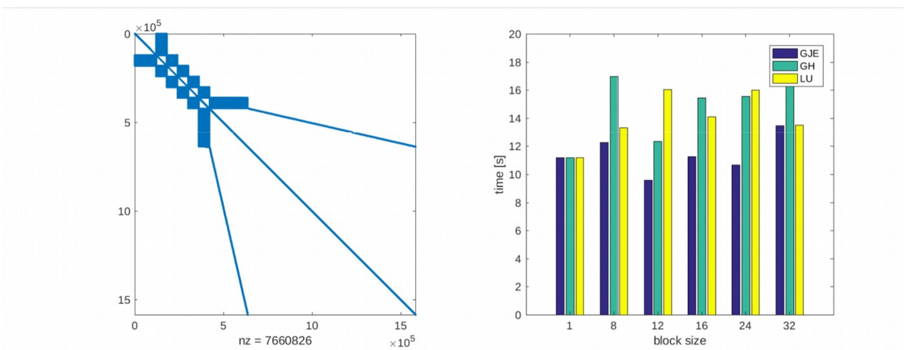
Chebyshev3



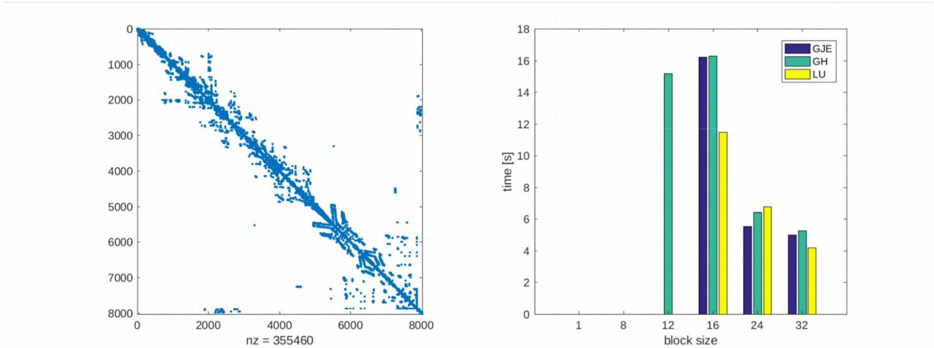
nd24k



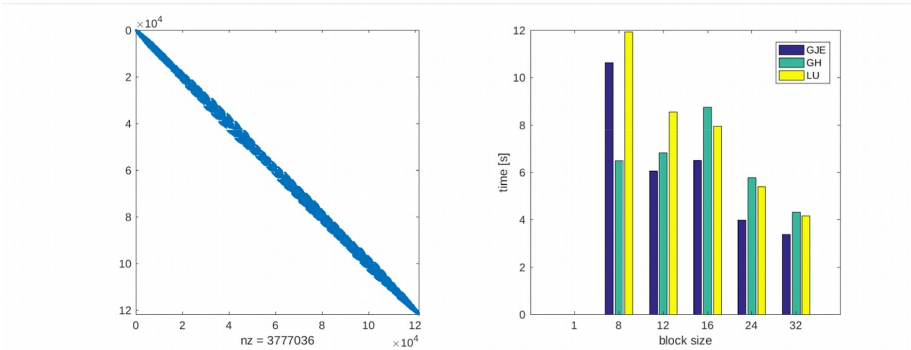
G3_circuit



bcsstk38



ship_003



Current Research: 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
- 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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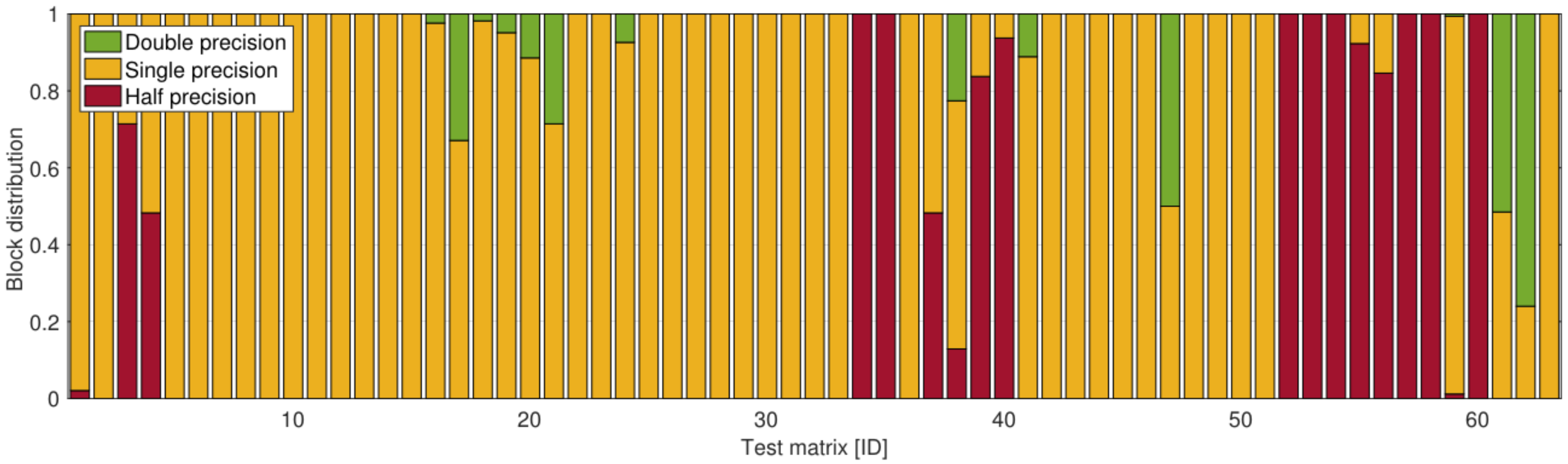
% of diagonal blocks stored in each precision *:



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

Experimental results

Determining the precision:

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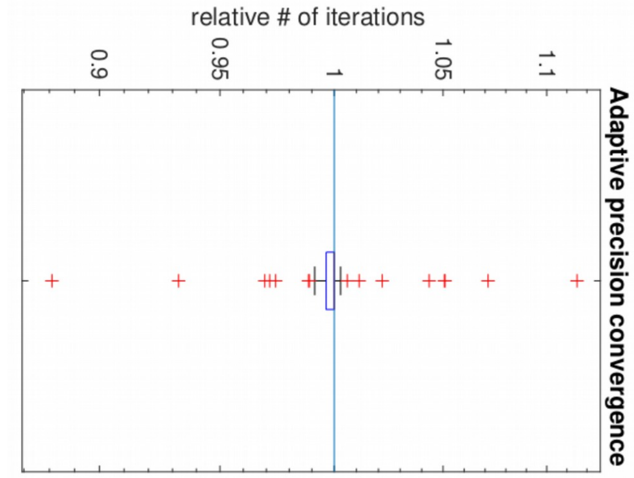
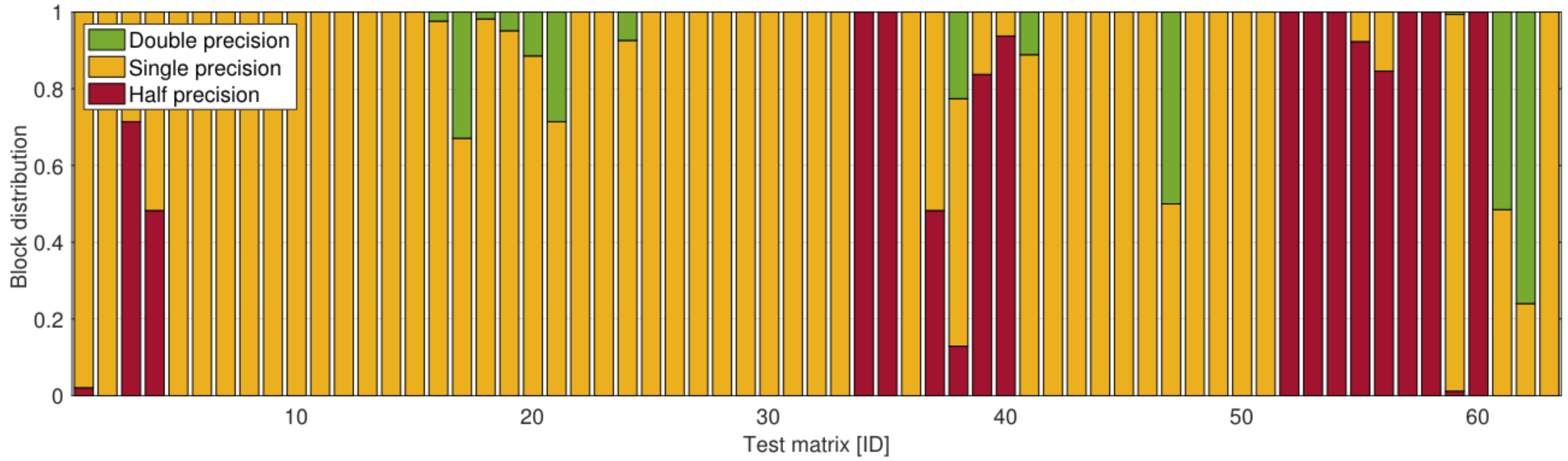


Usually < 5% iteration increase

% of diagonal blocks stored in each precision *:



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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:

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

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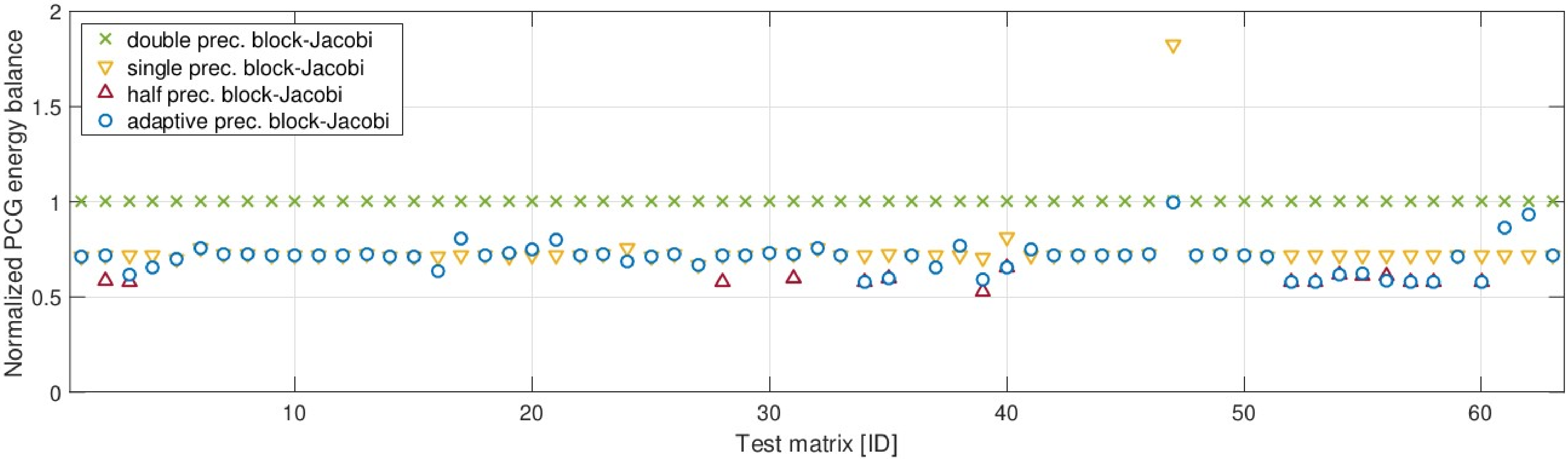
Predicted energy savings of adaptive precision block-Jacobi:



Overflow and underflow

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Overflow and underflow

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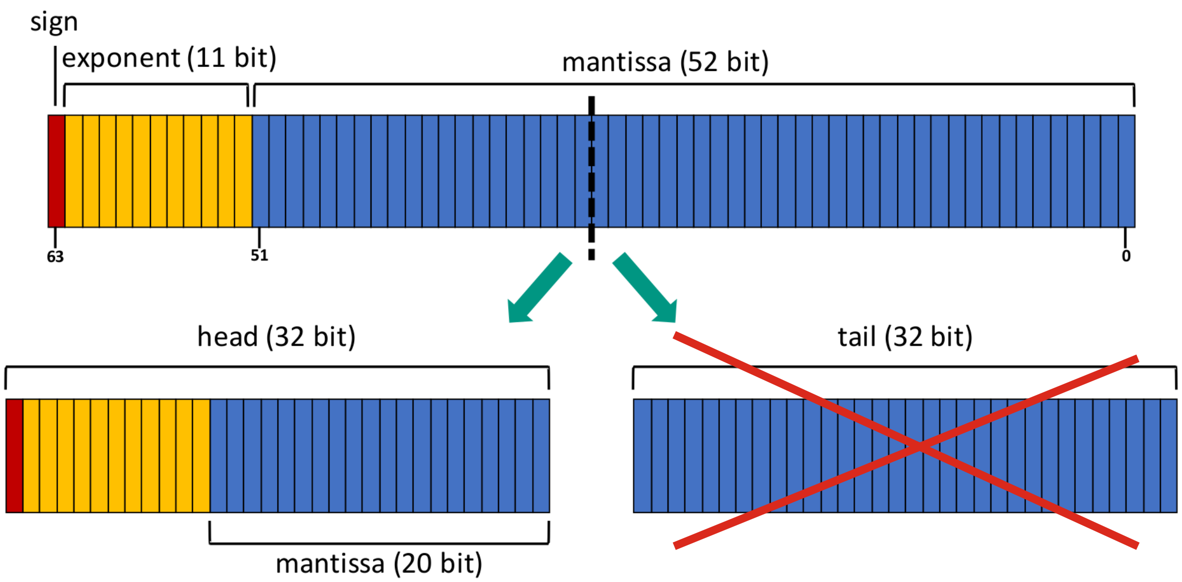
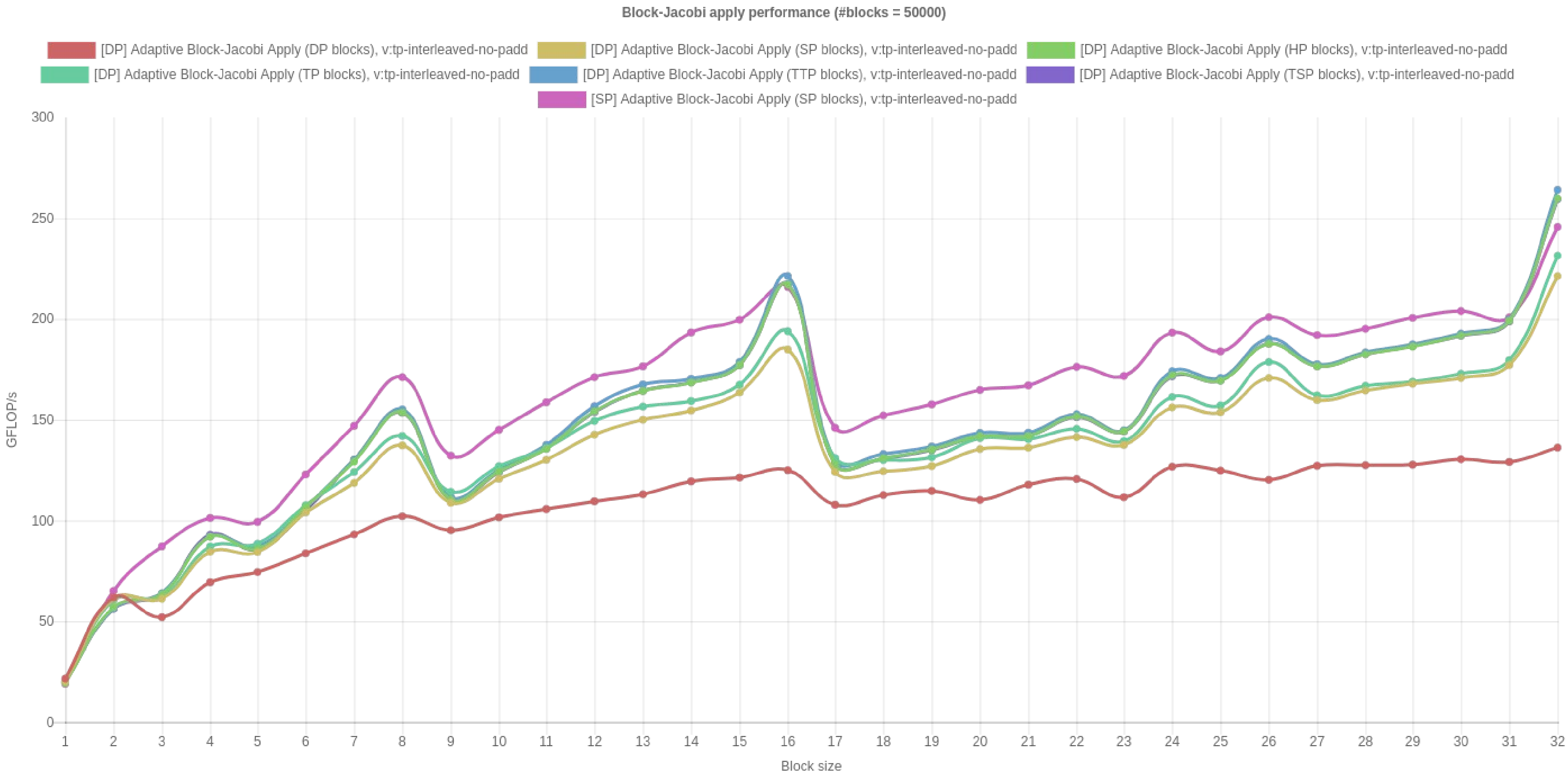
- Two possible solutions:
  1. Check the condition number of the low precision block to verify there were no catastrophic overflows or underflows.
  2. Use a custom storage format that preserves the number of exponent bits:

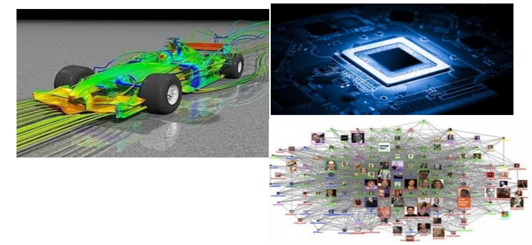


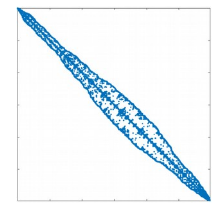
Initial GPU implementation



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
  - Preconditioners
    - reduce the number of iterations
  - Special hardware (e.g. GPUs)
  - Probably not a good idea to implement everything from scratch…
  - Use a library instead: Ginkgo





$$Ax = b$$

Ginkgo

Sparse matrix formats

3.2	0	1.2	0
0	0	0.4	0
2.7	1.3	0	4.1
0.1	0	0	2.7

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0	0	1	2	2	2	3	3	row
0	2	2	0	1	3	0	3	column

COO

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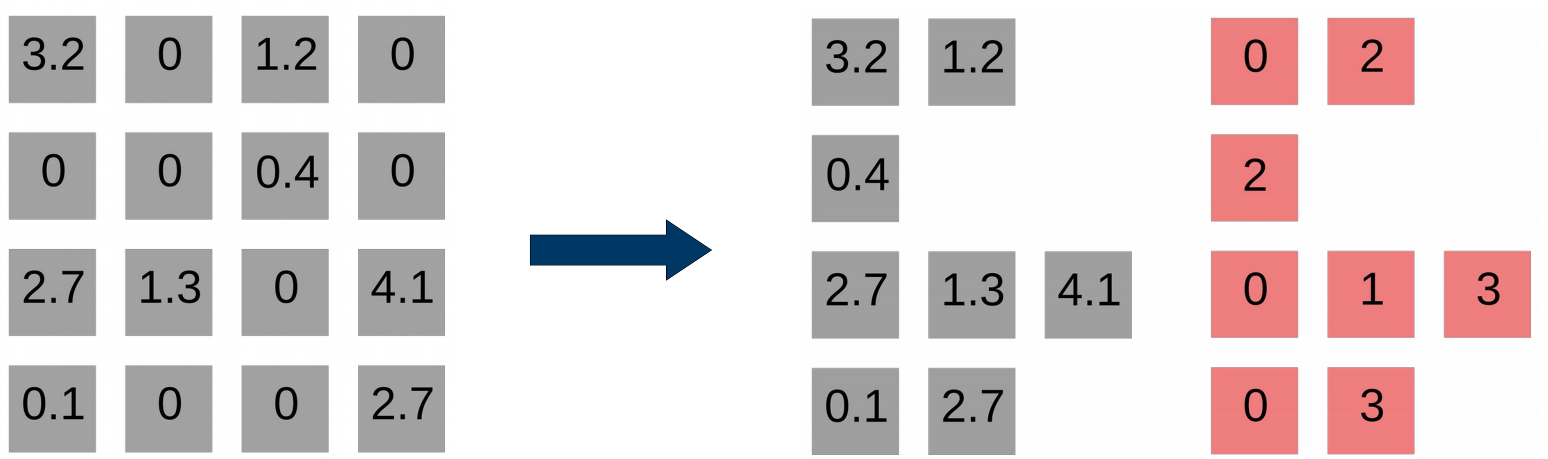

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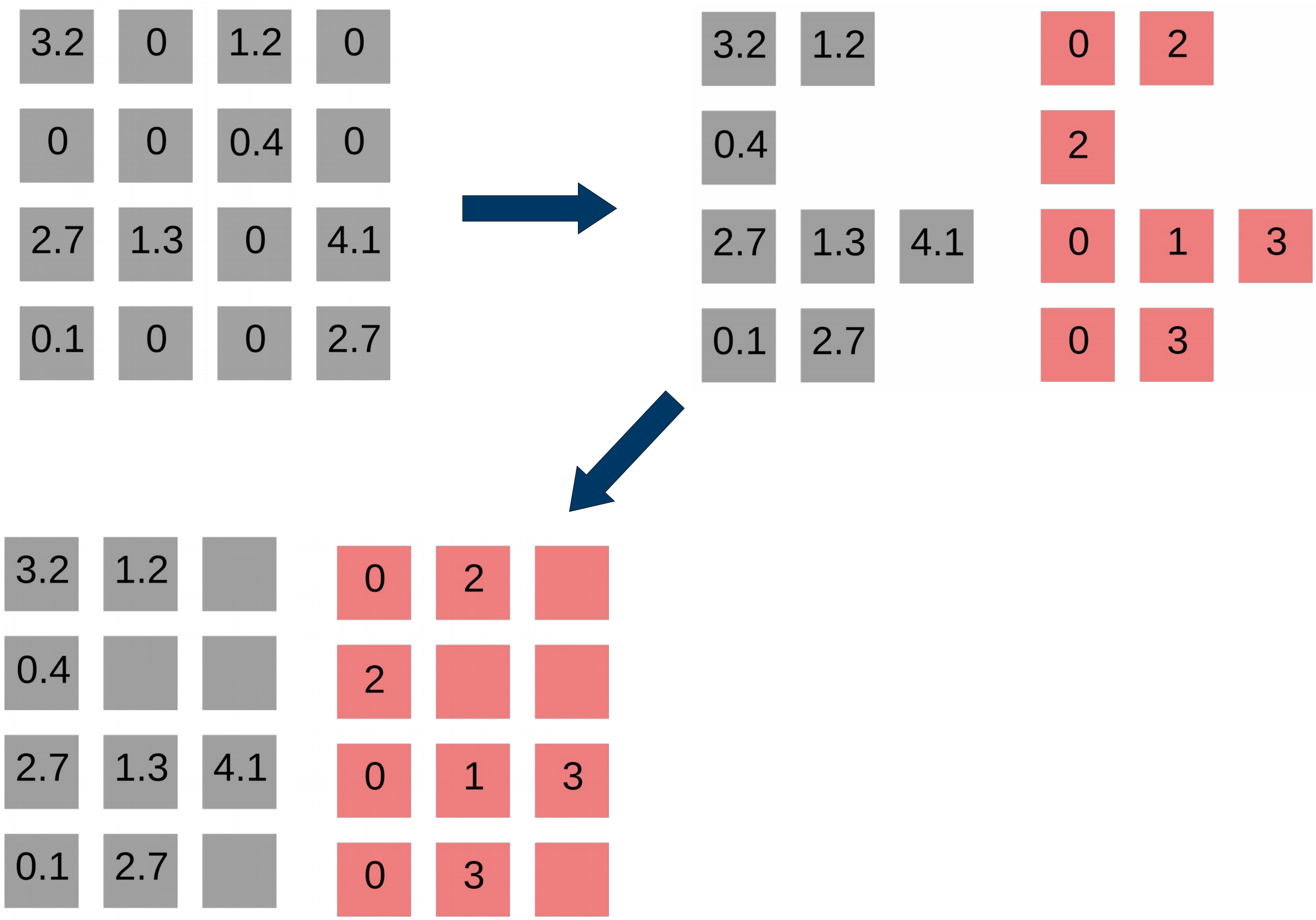

ELL

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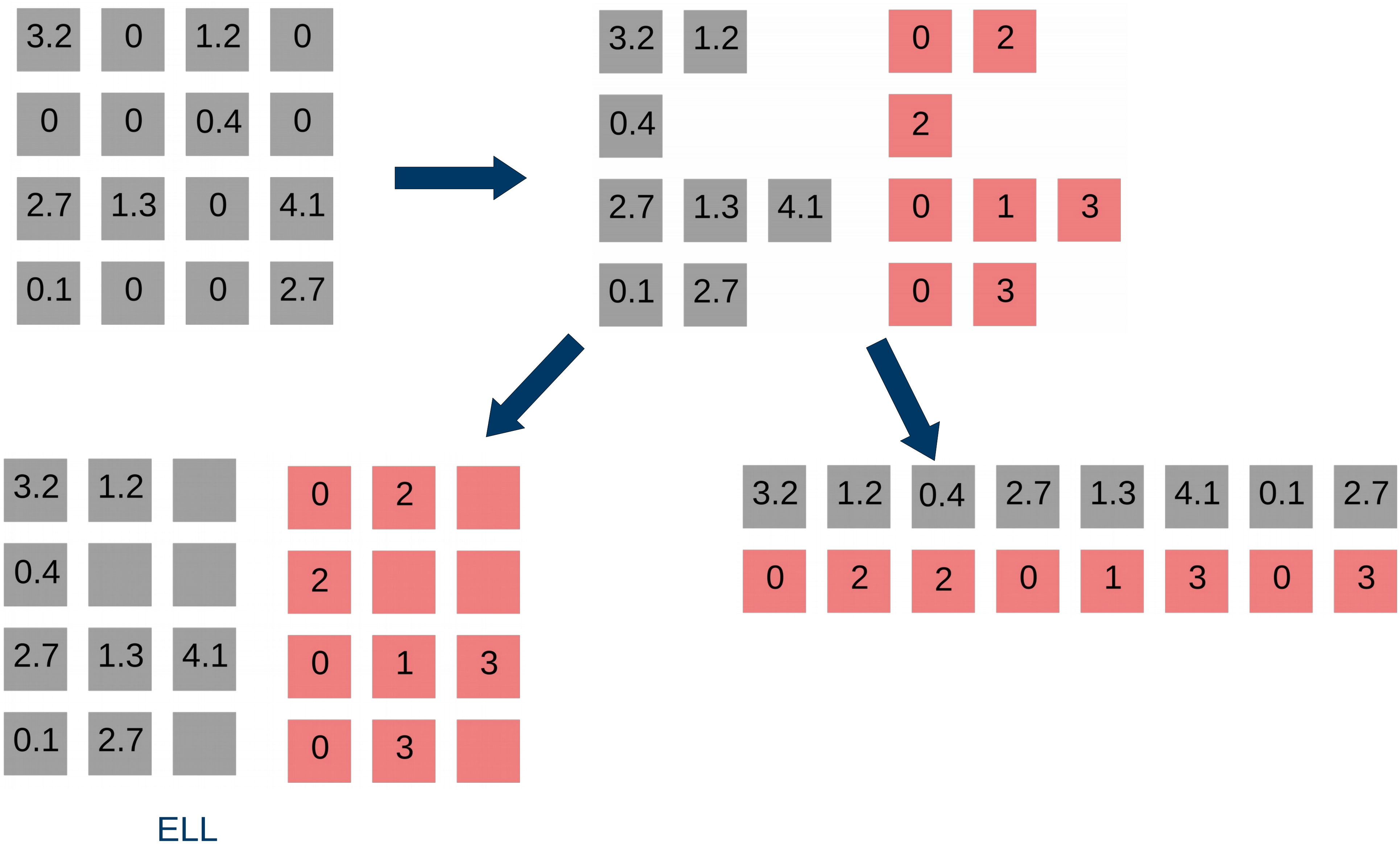

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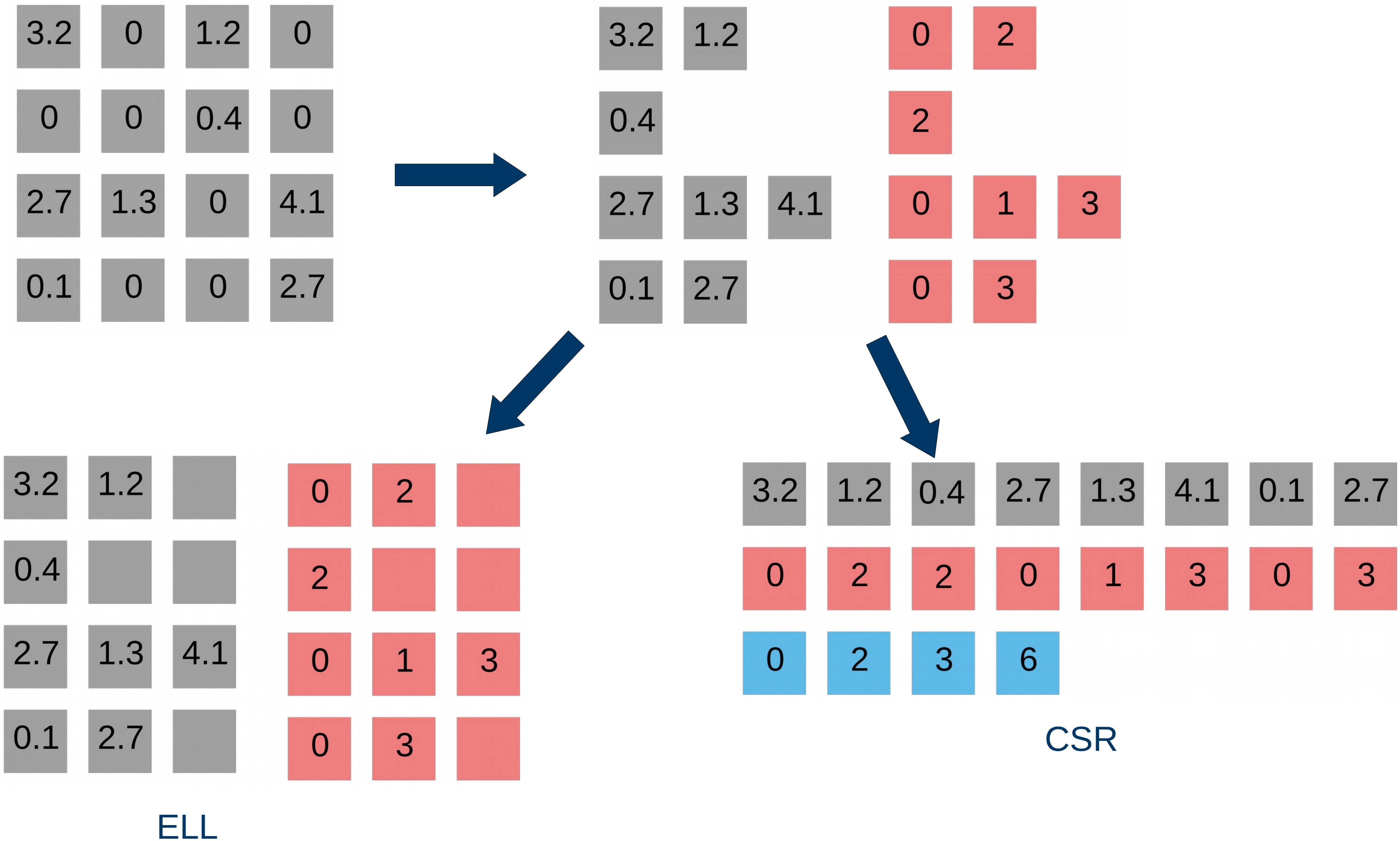

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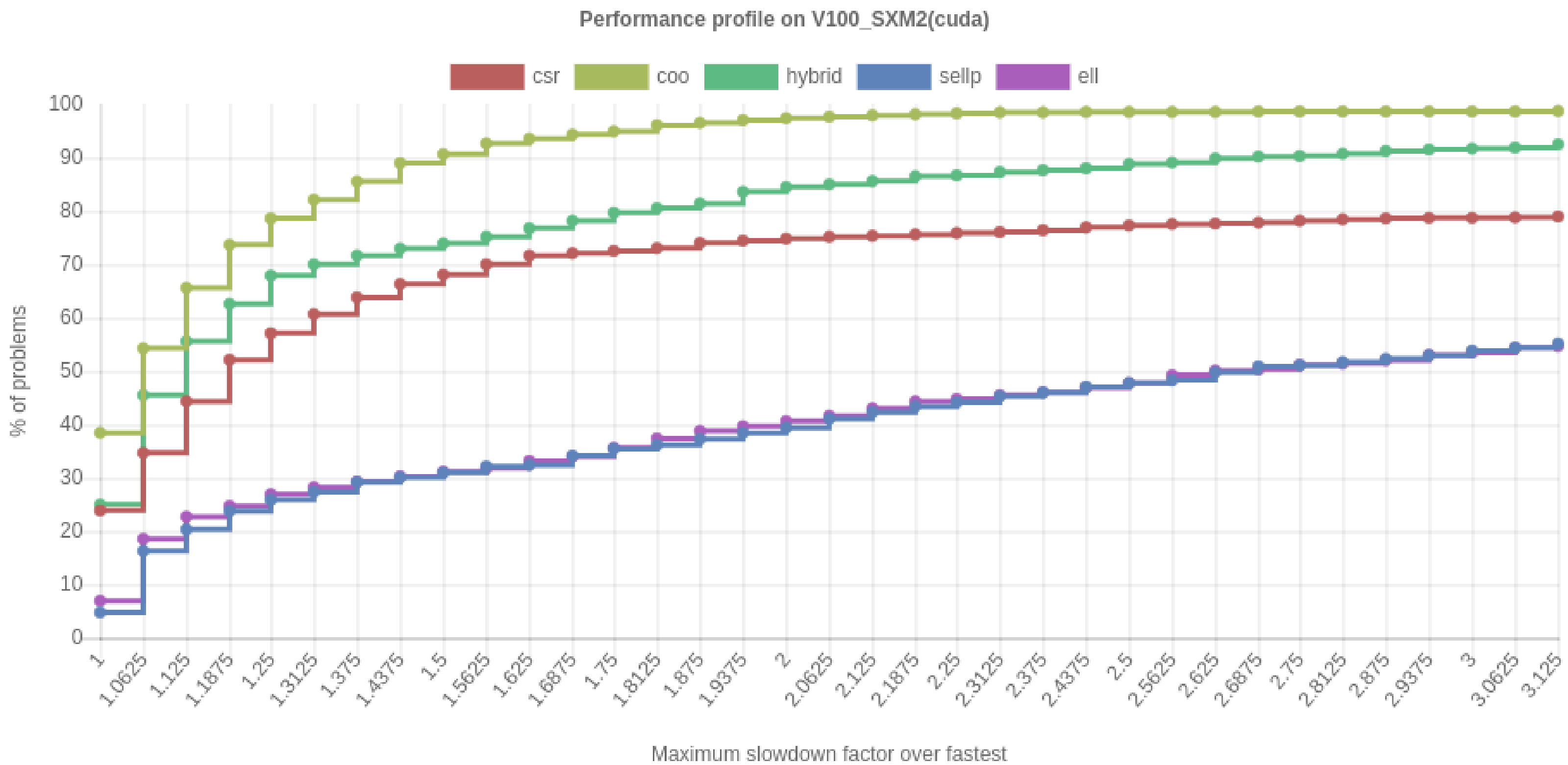
0	2	2	0	1	3	0	3
0	2	3	6				

CSR

“Standard” approach

First things first

THERE IS NO “BEST” SPARSE MATRIX FORMAT / SpMV ALGORITHM



CSR SpMV

3.2	1.2	0.4	2.7	1.3	4.1	0.1	2.7	Values (val)
0	2	2	0	1	3	0	3	Column indexes (colidx)
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$$y := Ax$$

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Bell & Garland '08
- parallelize outer loop

~ cuSPARSE SpMV

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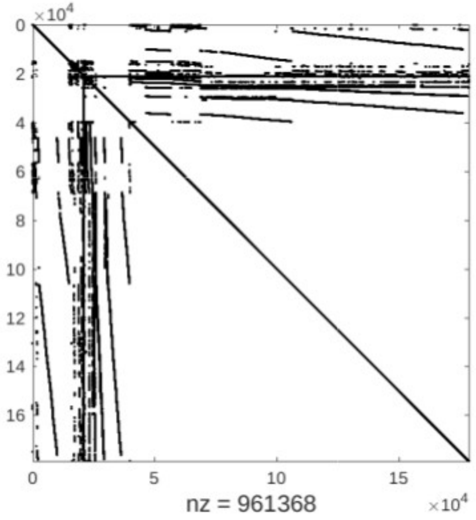
Load imbalance!

Example

Freescale/transient



Example

* GTX 1080

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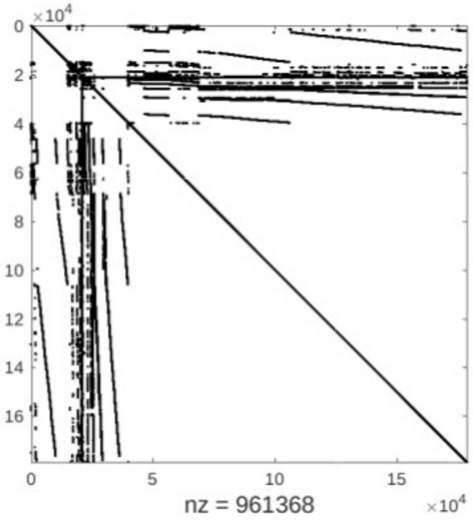

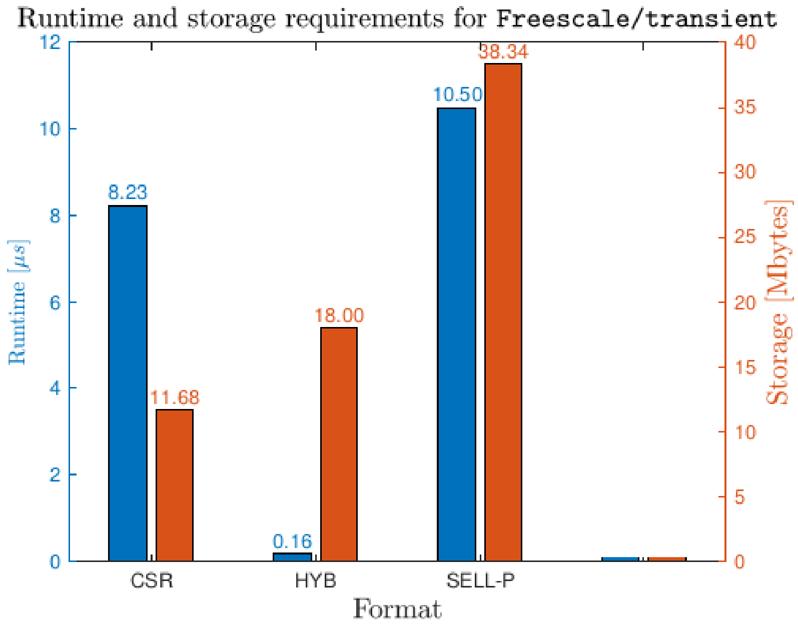

Can we do better than HYB using CSR?

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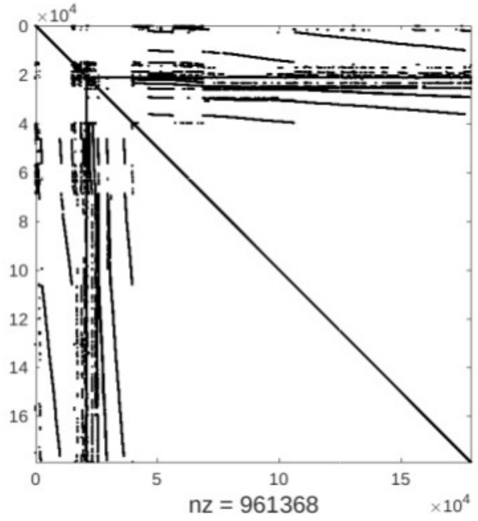

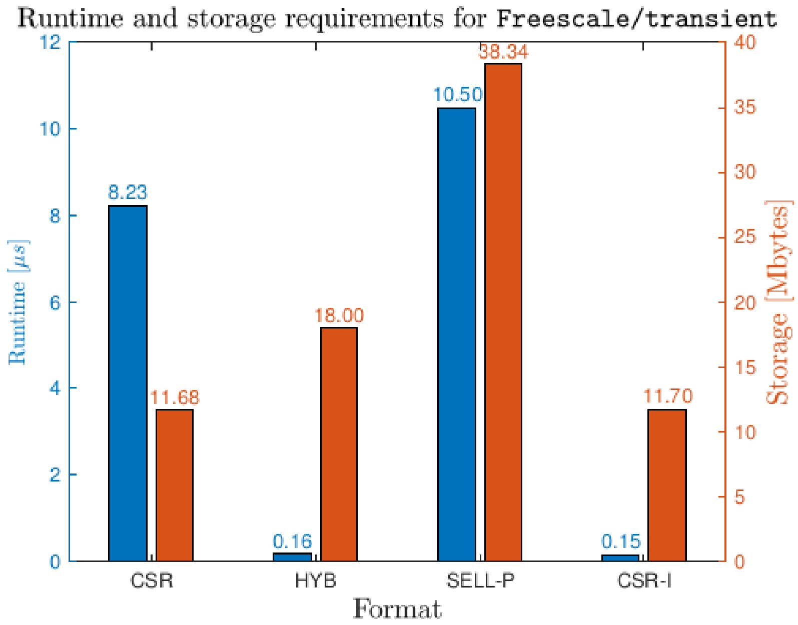

55x speedup

Can we do better than HYB using CSR?

YES!

Flegar, Anzt, *Overcoming Load Imbalance for Irregular Sparse Matrices,* IA3'17

Flegar, Quintana-Ortí, *Balanced CSR Sparse Matrix-Vector Product on Graphics Processors,* Euro-Par'17

How to do it

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- Accumulate partial result in the registers

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Precompute starting value of “row” for each thread.

Getting good performance on GPUs

CUDA thread = 1 lane of a 32-wide SIMD unit (warp)

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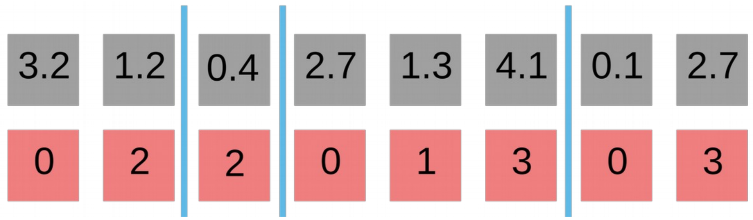

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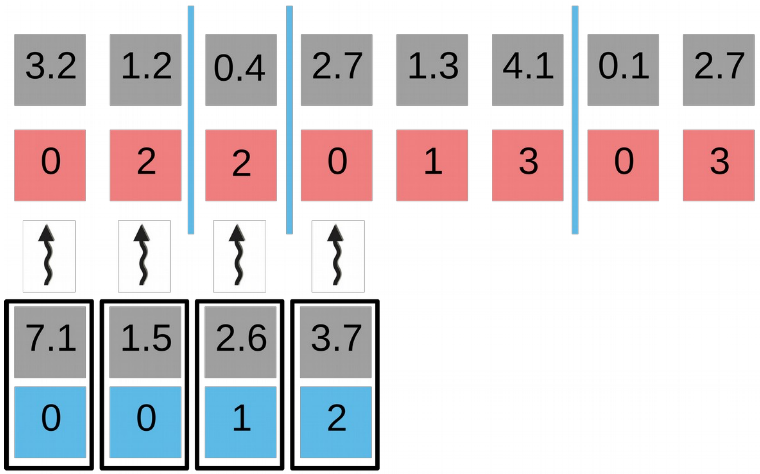

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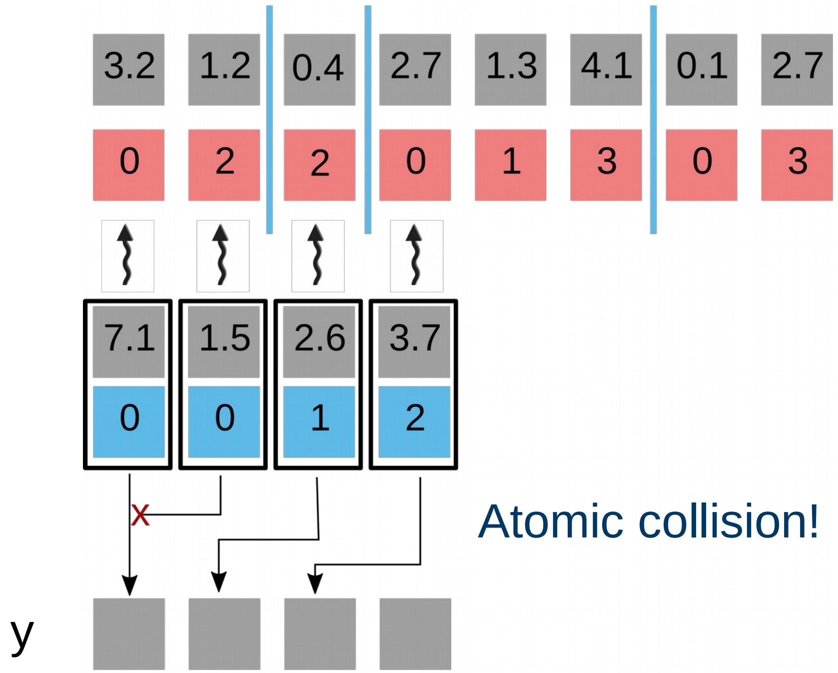
Assign one warp per chunk.



Atomic collision!

Getting good performance on GPUs

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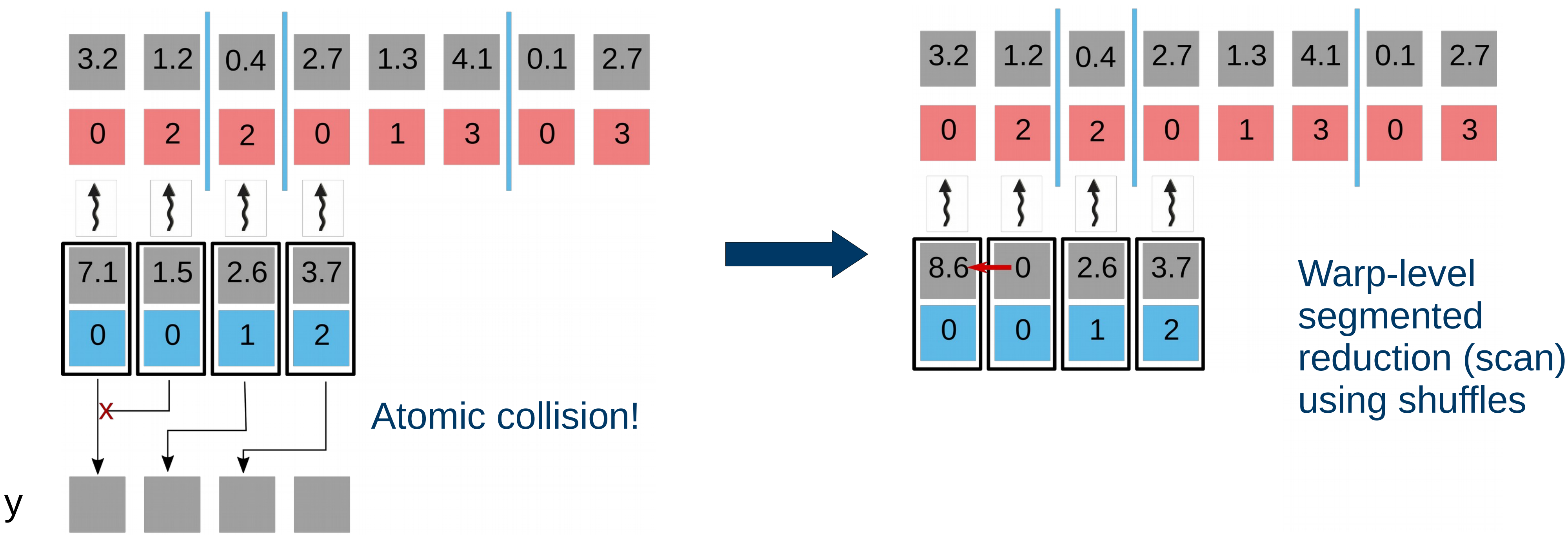

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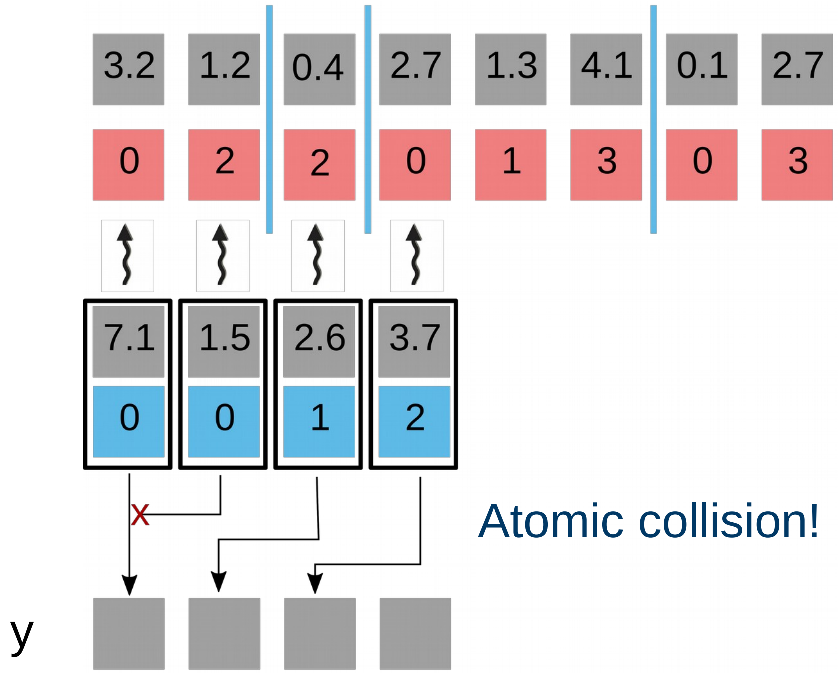

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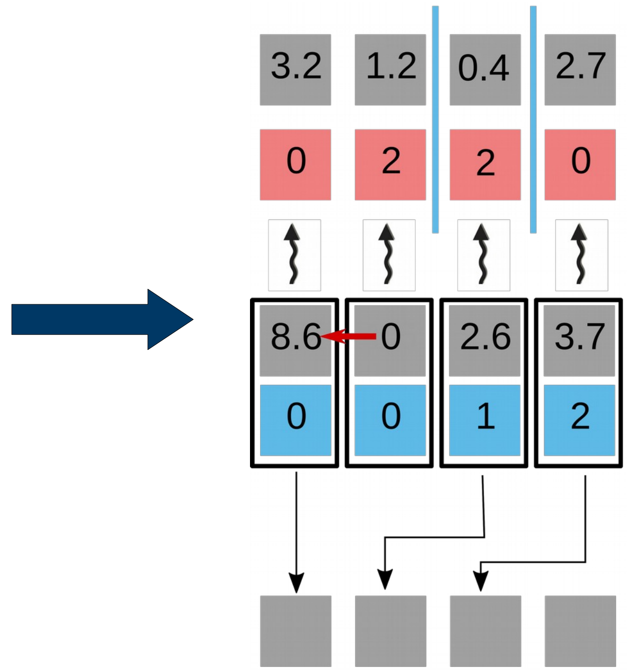
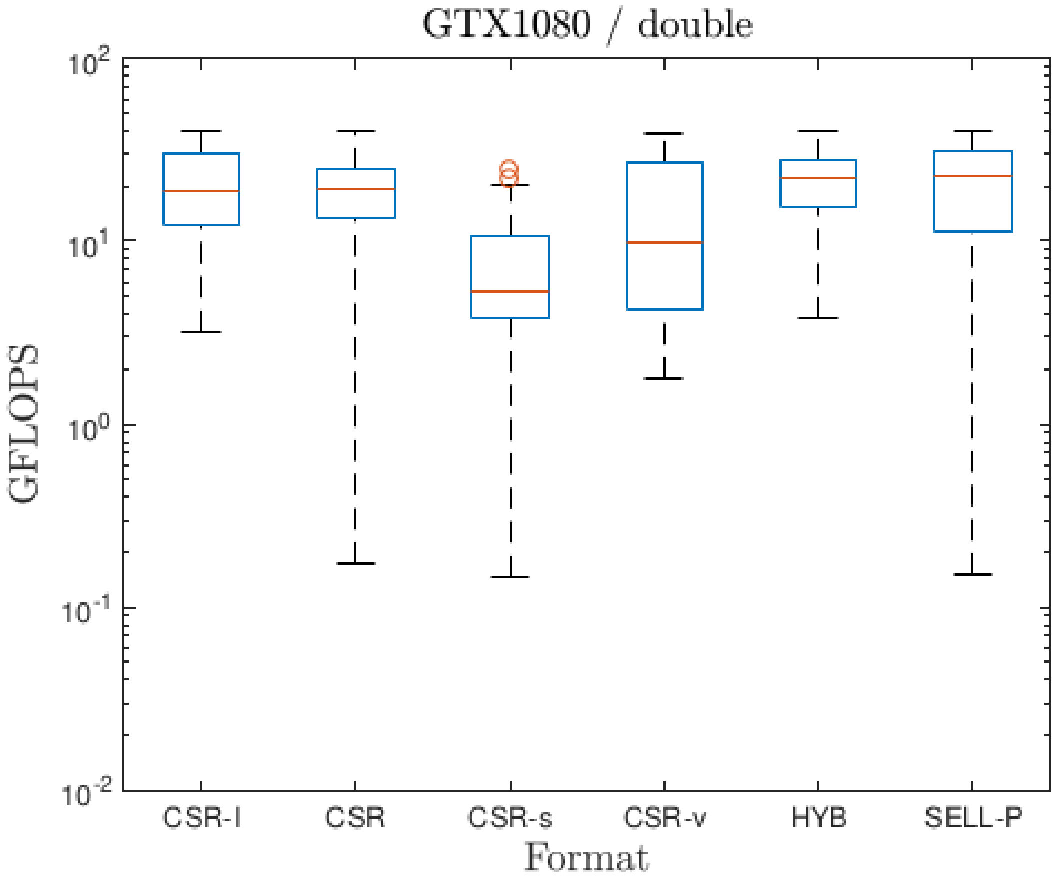


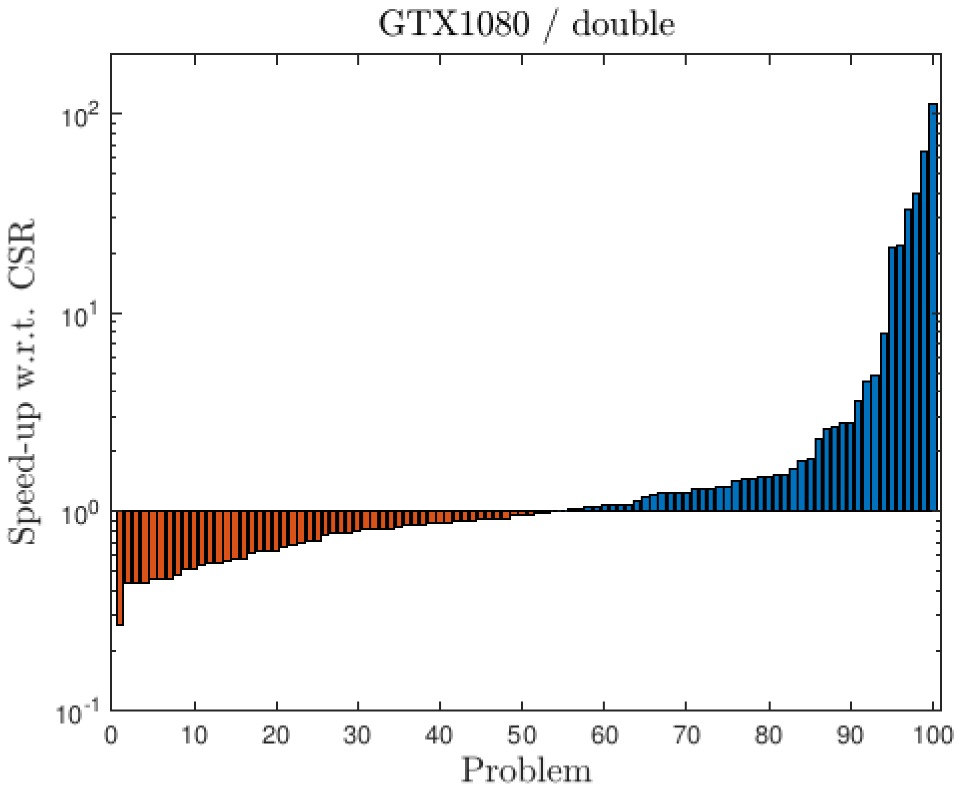
Warp-level segmented reduction (scan) using shuffles

Performance of CSR-I

100 matrices from SuiteSparse



Speed-up / slowdown over cuSPARSE CSR



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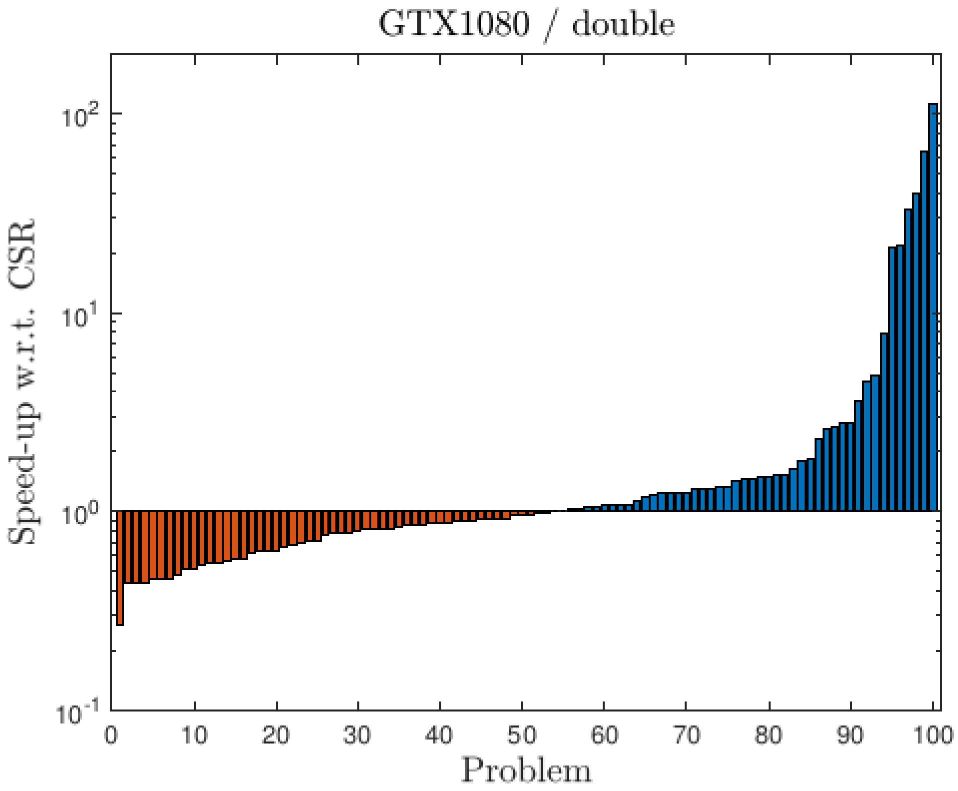

No format conversion!

- try both, and use the fastest later on!
- sometimes 1 cuSPARSE SpMV = 100 CSR-I SpMVs

Choosing the winner a priori

CSR-I designed for irregular patterns

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How to measure irregularity?

Deviation of row lengths from the mean.

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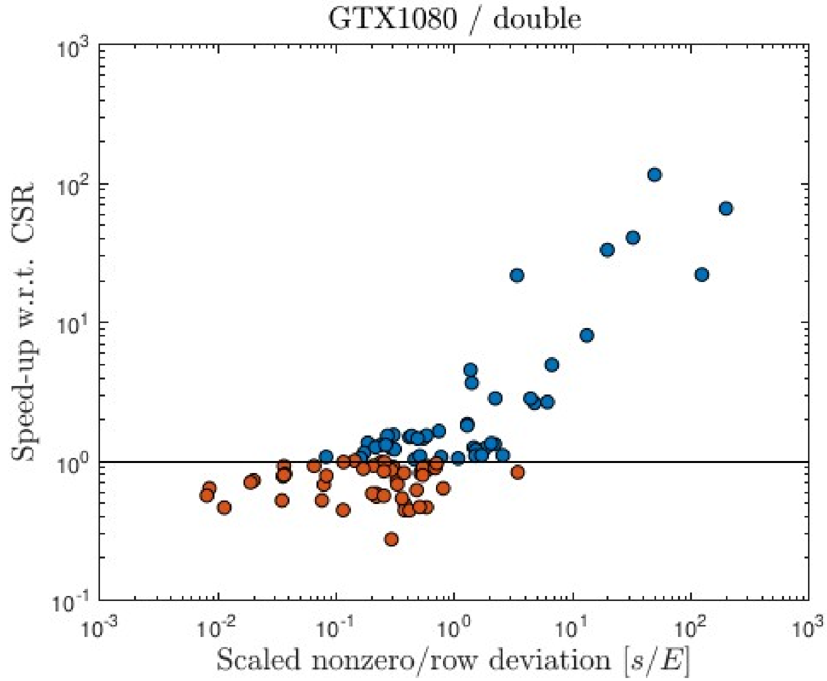
Scatter plot of speedup vs normalized std. dev.



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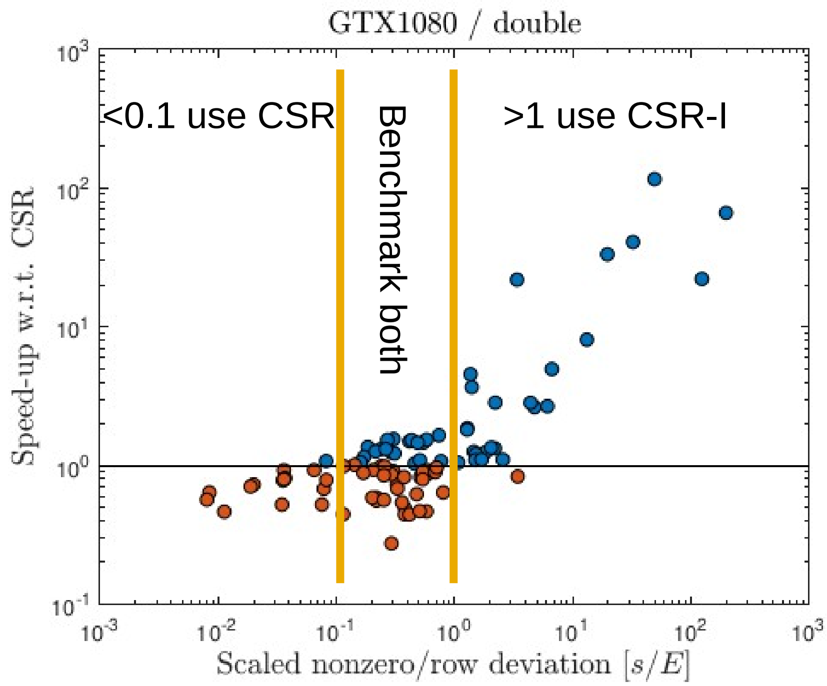
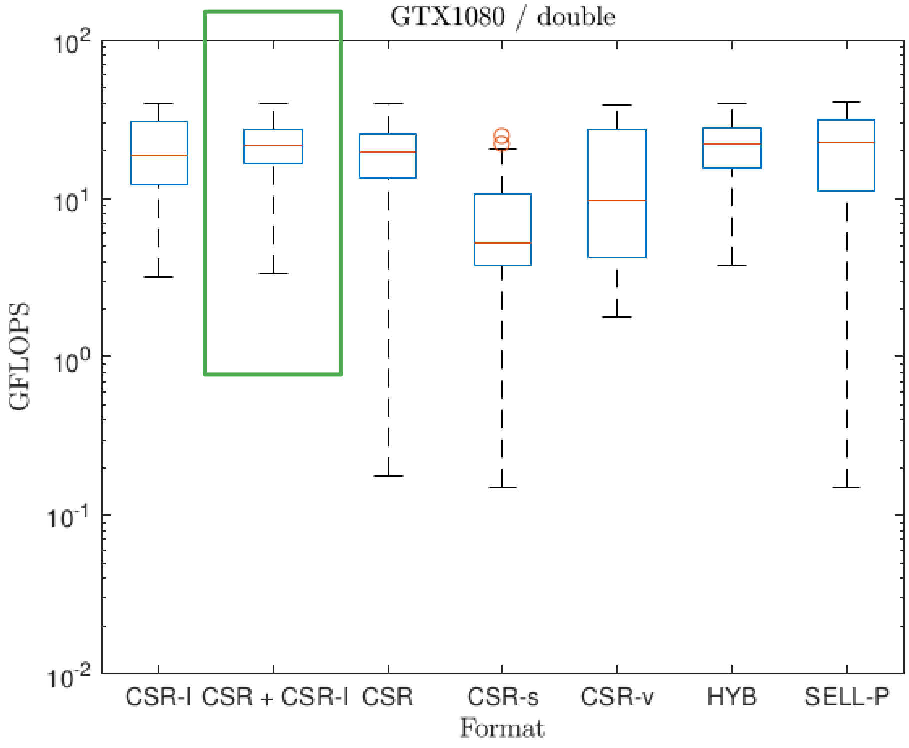


Combining both approaches



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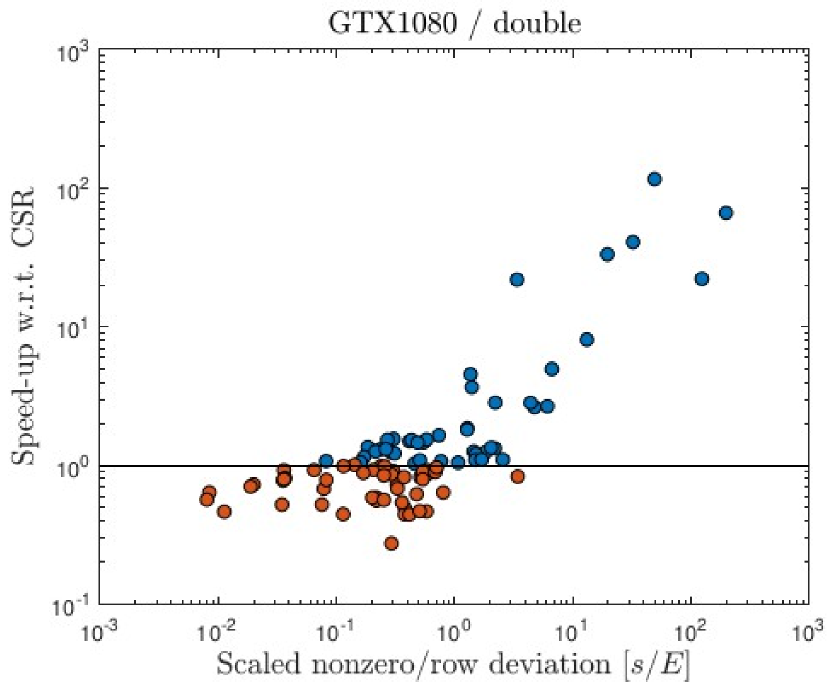

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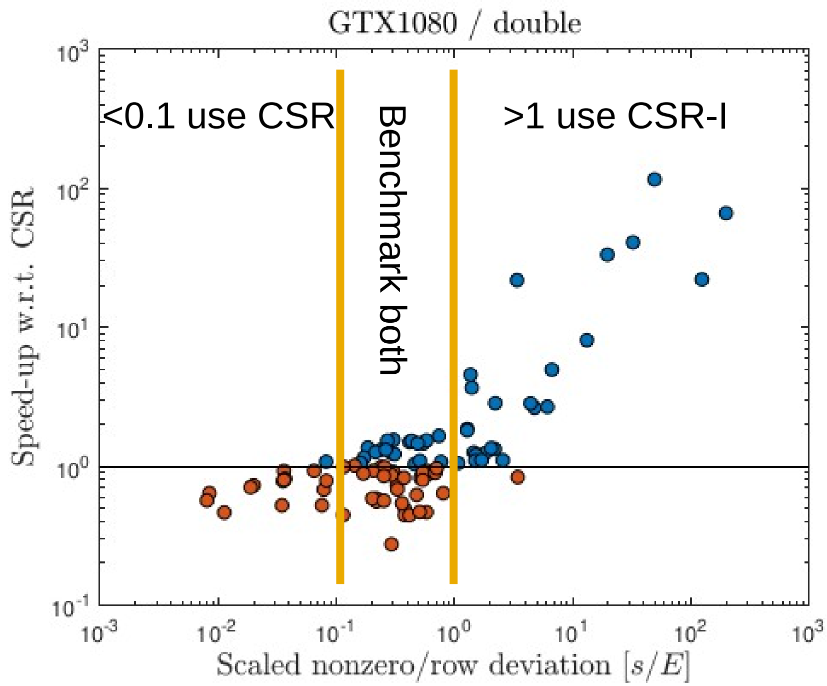

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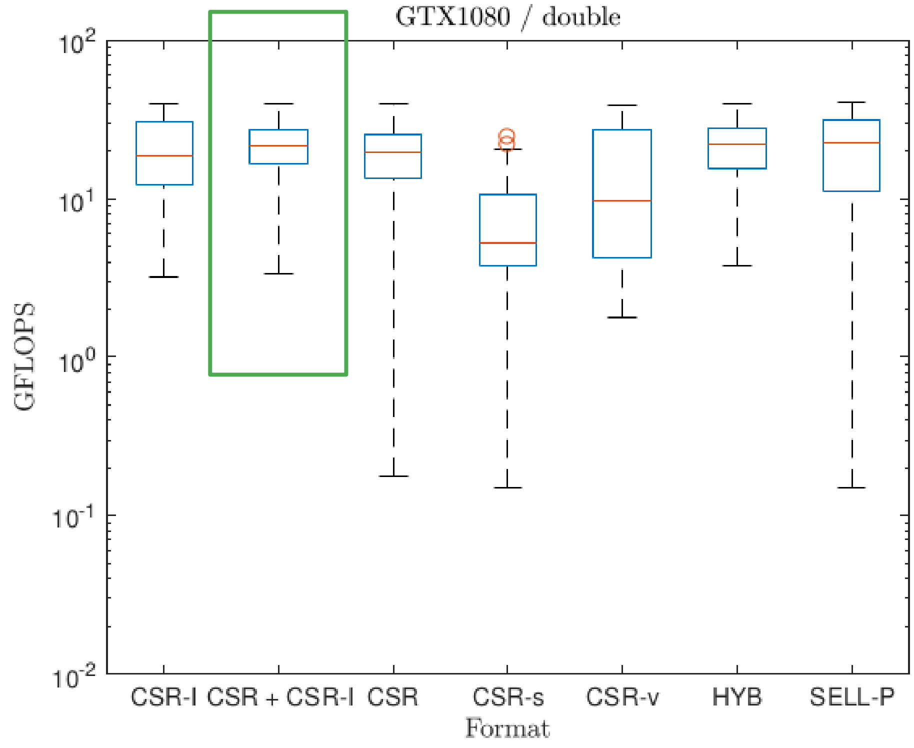
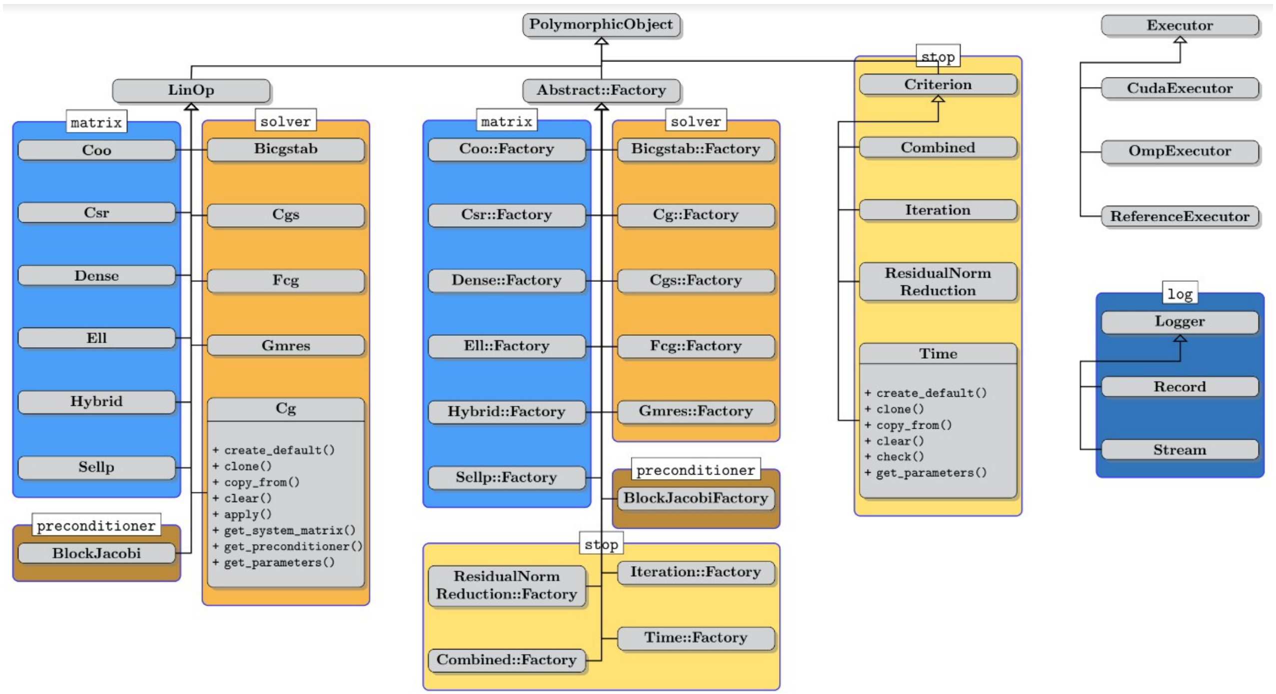


Outlook



Choosing the correct combination of

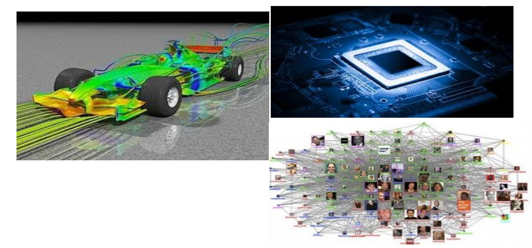
matrix format solver preconditioner

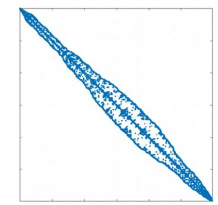
… requires expert knowledge or significant trial and error.

Design a tool that does it (semi-)automatically?

Thank you! Questions?

- Krylov-subspace based linear solvers
  - Performance depends on SpMV and Preconditioners
- Sparse matrix formats & SpMV
  - There is no “holy grail” - best format depends on the problem
- Preconditioners
  - Accelerate the solution of the solver
  - Only an approximation, can use lower precision storage
- Do not implement from scratch, use a library. For example:





$$Ax = b$$

Ginkgo

- github.com/ginkgo-project/ginkgo
- Open source license (BSD-3)
- Modern C++
- High performance GPU backend
- reference CPU implementation
- High performance CPU backend on the way

Slides:

github.com/gflegar/talks/tree/master/cmu_pittsburgh_2018_11