RWTH Aachen, 14 September 2018

How to Solve a Linear System

Goran Flegar

W/: Hartwig Anzt, Yen-Chen Chen, Terry Cojean, Pratik Nayak, Enrique S. Quintana-Ortí, Mike Tsai

Scan me for slides!

github.com/gflegar/talks/tree/master/rwth_aachen_2018_09

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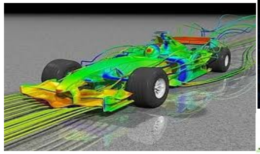
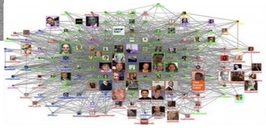
Sources of linear systems

- 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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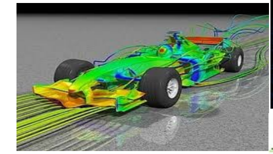

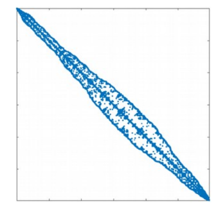

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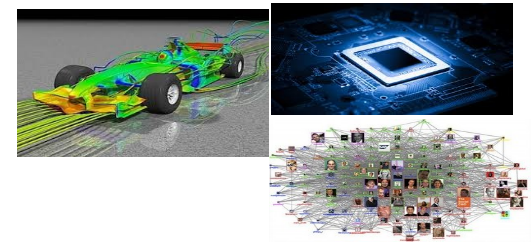

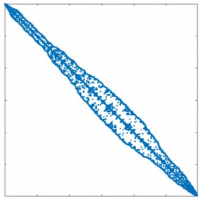

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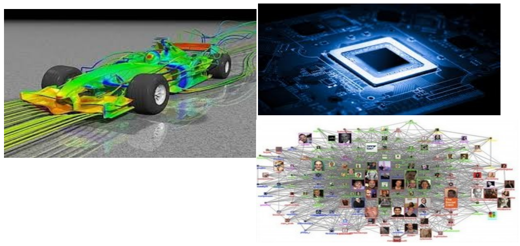

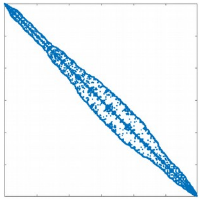

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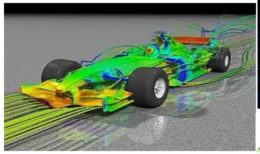

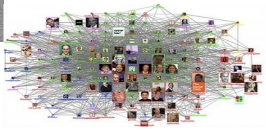

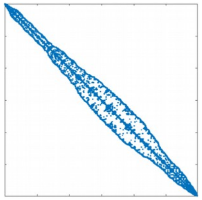

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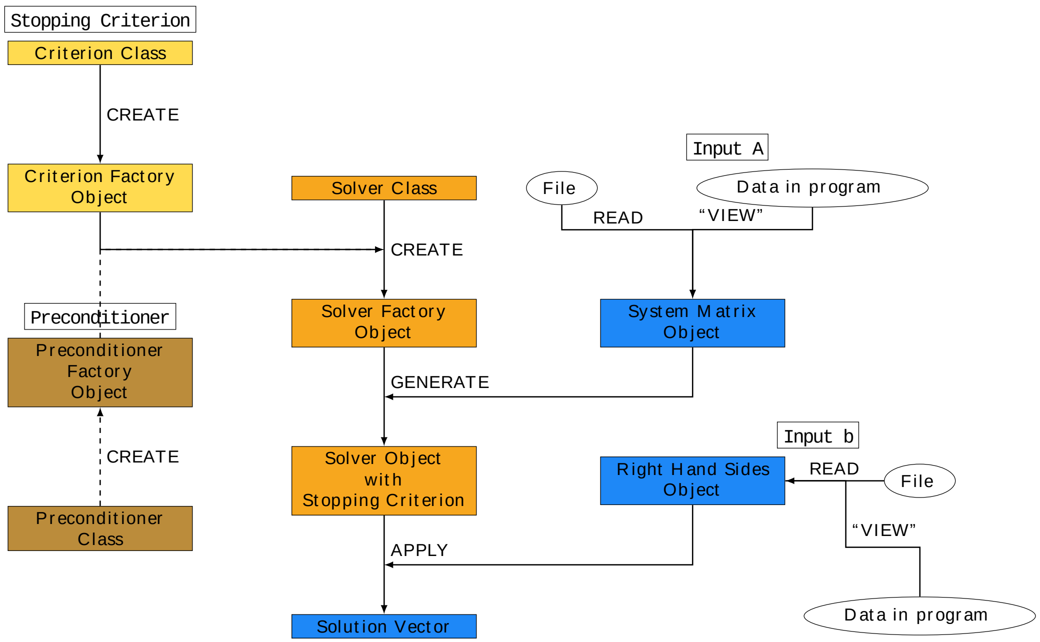
Ginkgo

The Ginkgo library

- Linear operator library
  - Matrices, preconditioners, (Krylov) solvers



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

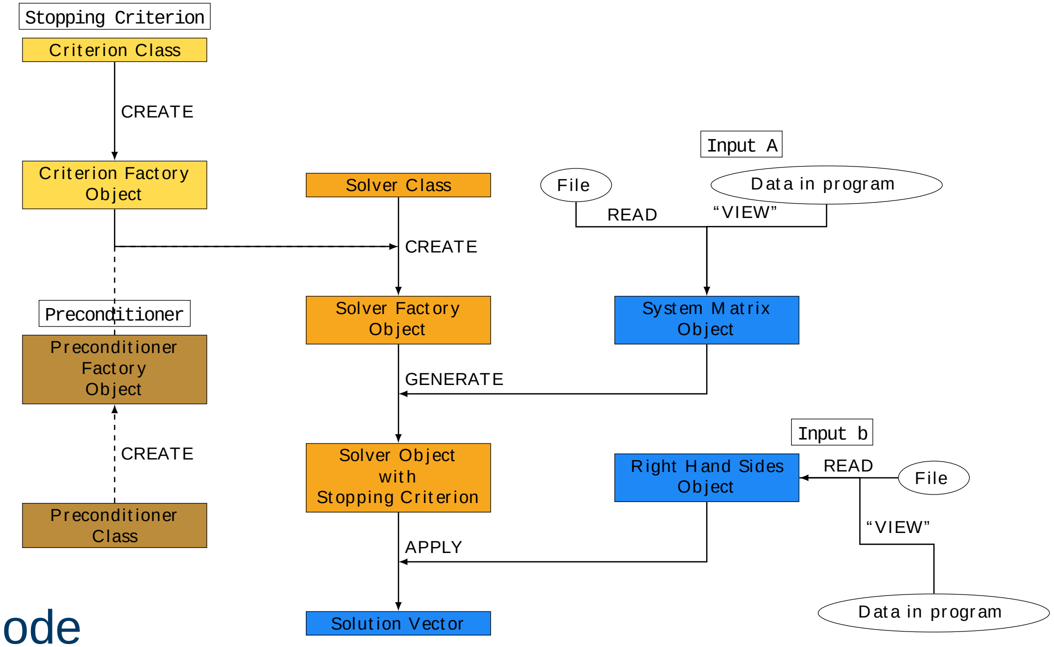
THE UNIVERSITY OF TENNESSEE KNOXVILLE

Karlsruher Institut für Technologie

UNIVERSITAT JAUME I

The Ginkgo library

- Linear operator library
  - Matrices, preconditioners, (Krylov) solvers
- Supports execution on different devices
  - GPU
  - Sequential reference CPU
  - OpenMP under development
  - Plans for multi GPU, CPU + GPU, full node



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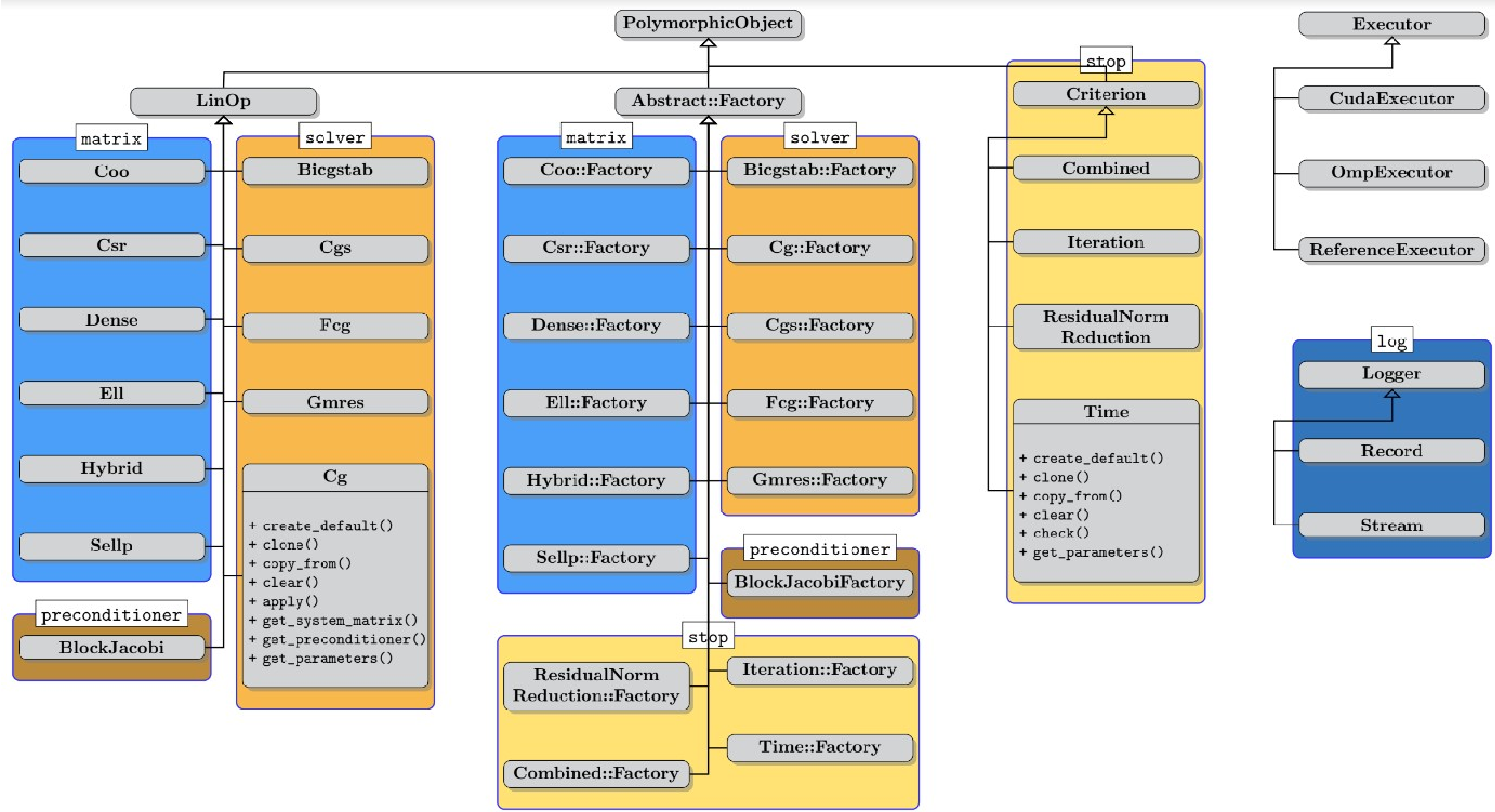
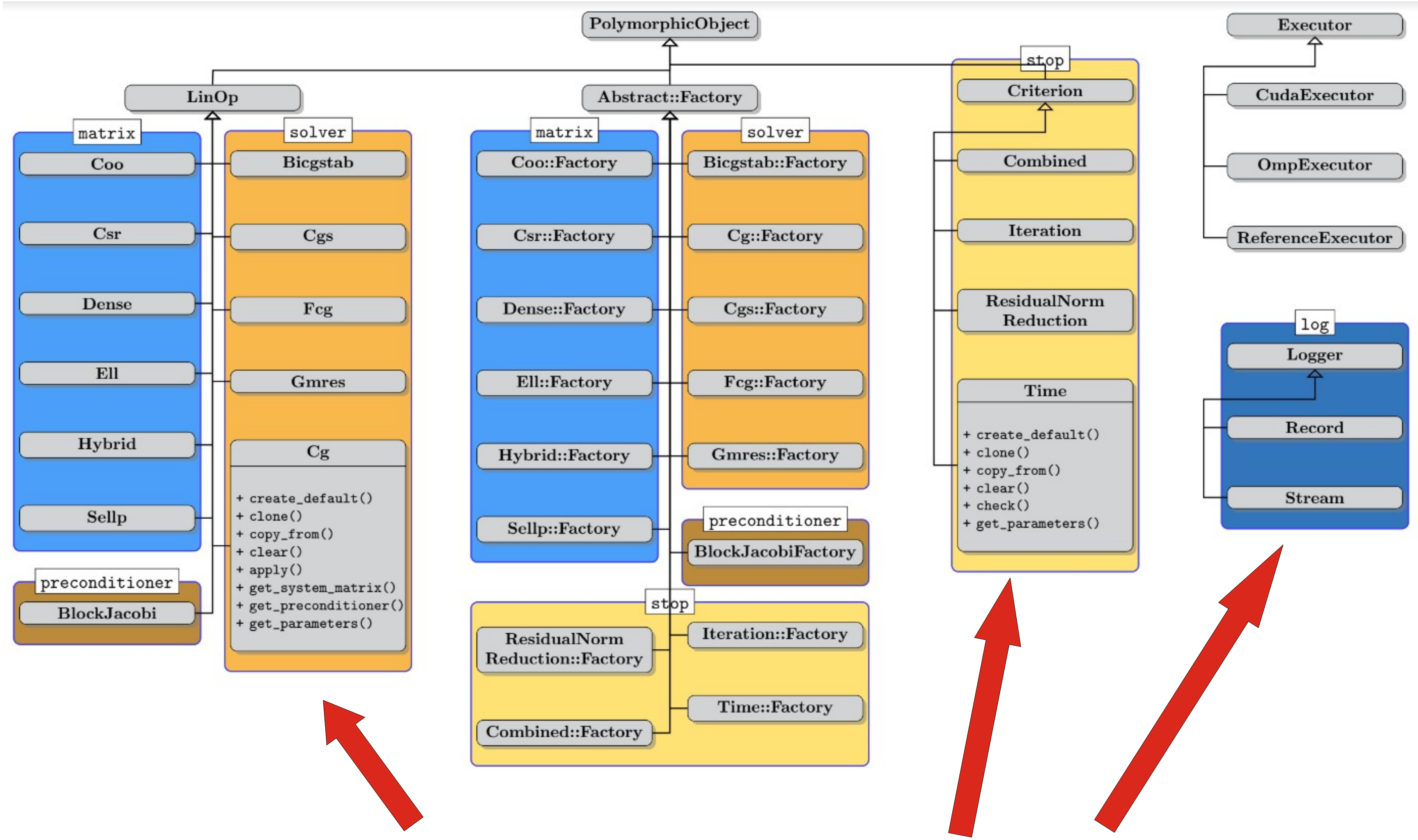
```
int main()
{
  // Instantiate a CUDA executor
  auto exec = gko::CudaExecutor::create(0, gko::OmpExecutor::create());
  // Read data
  auto A = gko::read<gko::matrix::Csr<>>(std::cin, exec);
  auto b = gko::read<gko::matrix::Dense<>>(std::cin, exec);
  auto x = gko::read<gko::matrix::Dense<>>(std::cin, exec);
  // Create the solver
  auto solver = gko::solver::Cg<>::Factory::create()
    .with_preconditioner(
      gko::preconditioner::BlockJacobiFactory<>::create(exec, 32))
    .with_criterion(gko::stop::Combined::Factory::create()
      .with_criteria(
        gko::stop::Iteration::Factory::create()
          .with_max_iters(20u)
          .on_executor(exec),
        gko::stop::ResidualNormReduction<>::Factory::create()
          .with_reduction_factor(1e-15)
          .on_executor(exec))
      .on_executor(exec))
    .on_executor(exec);
  // 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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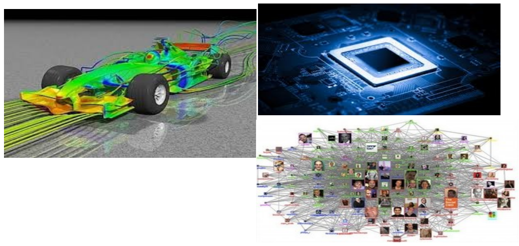

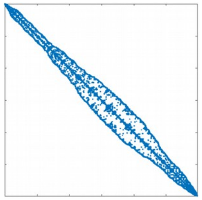

$$Ax = b$$

Ginkgo

Preconditioning

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

Preconditioning

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

Replace the original system with an
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$$\Downarrow$$

$$z := Ax$$

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

Preconditioner application

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Generate the preconditioner matrix, and store it in a form suitable for application

$$\boxed{A \rightsquigarrow M^{-1}} \longrightarrow \begin{array}{c} z := Ax \\ \boxed{y := M^{-1}z} \end{array}$$

Preconditioner setup **Preconditioner application**

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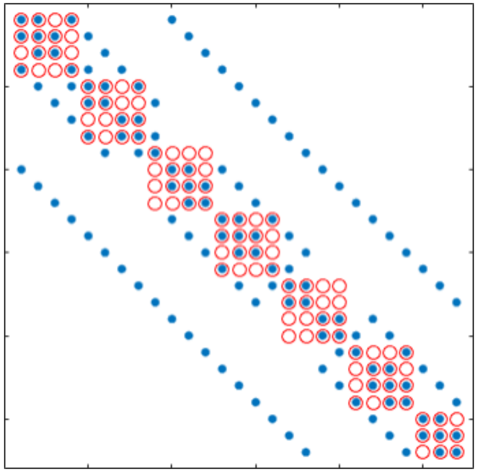
Generation via factory

Linear operator application

Ginkgo linear operator abstraction

Example: Block-Jacobi preconditioning

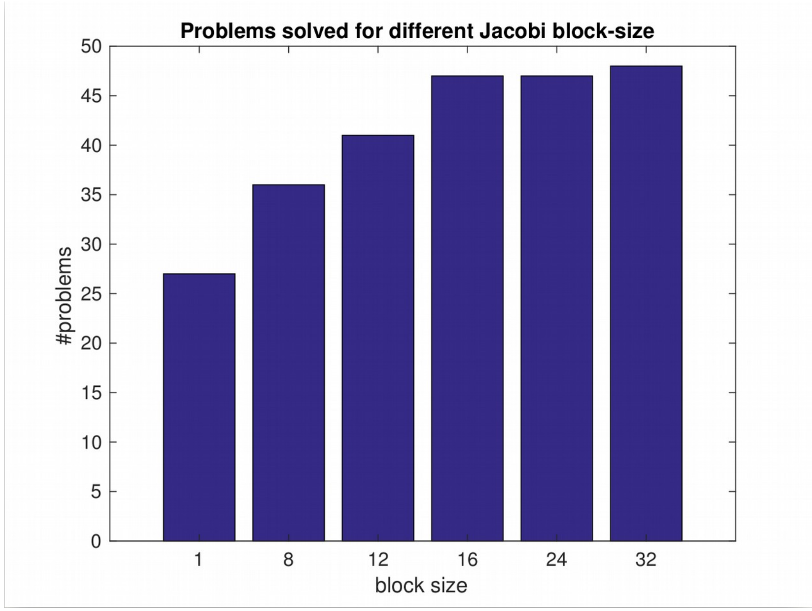


- Block-Jacobi preconditioning
  - Use only diagonal blocks for approximation

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

Benefits of block-Jacobi

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



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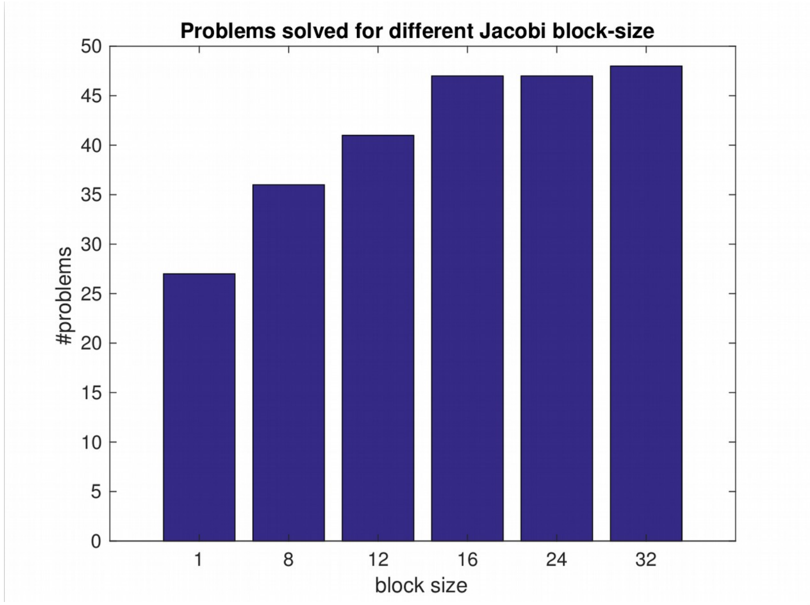
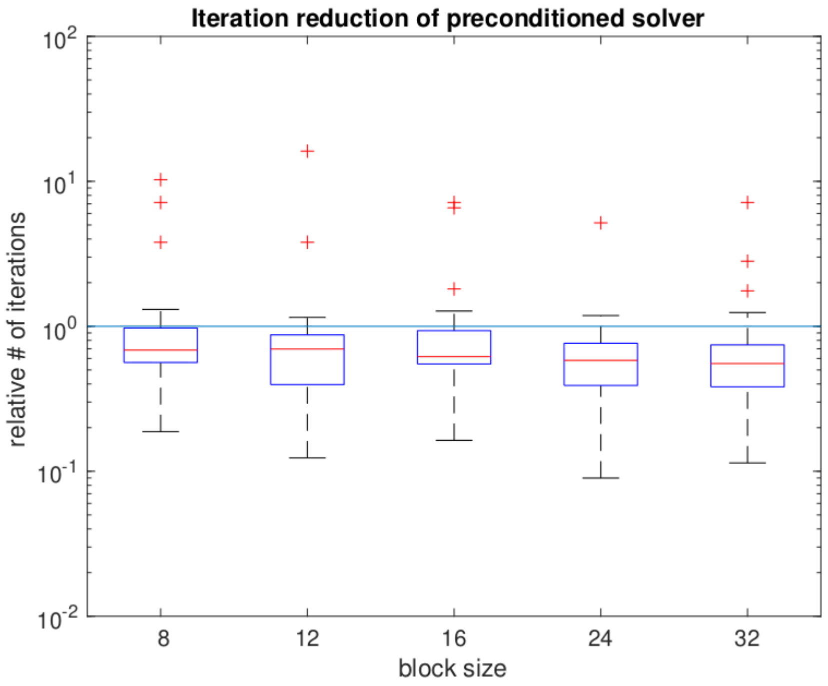
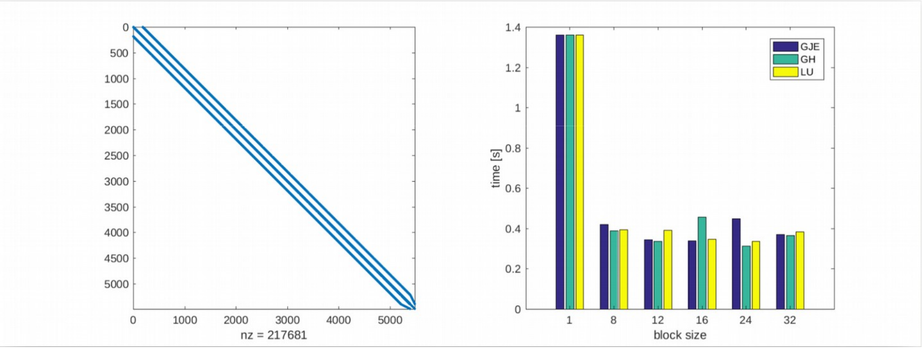


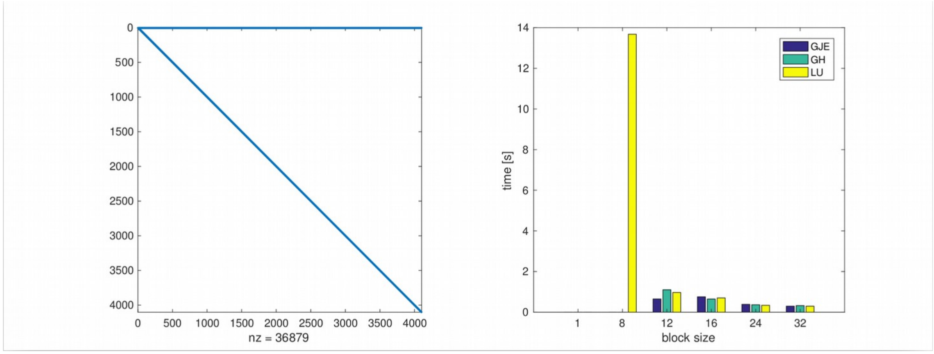


Complete solver runtime

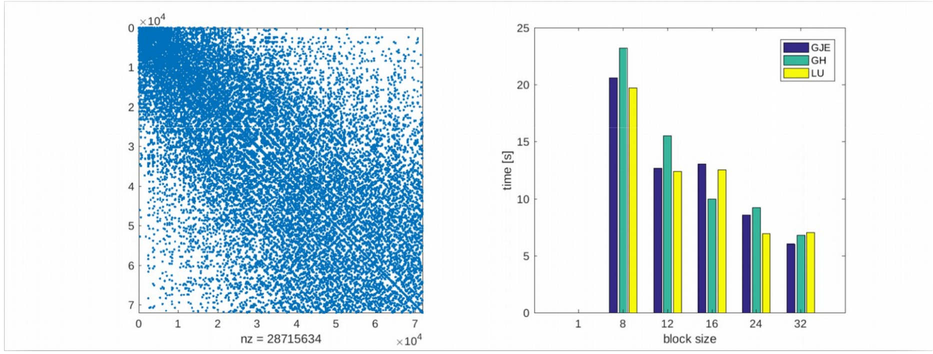
s2rmt3m1



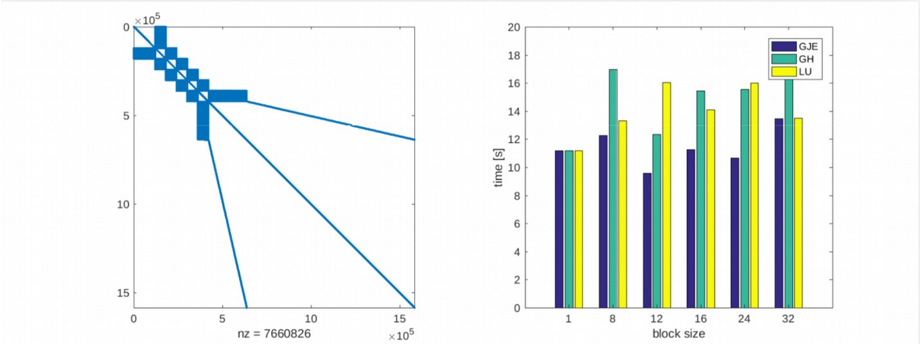
Chebyshev3



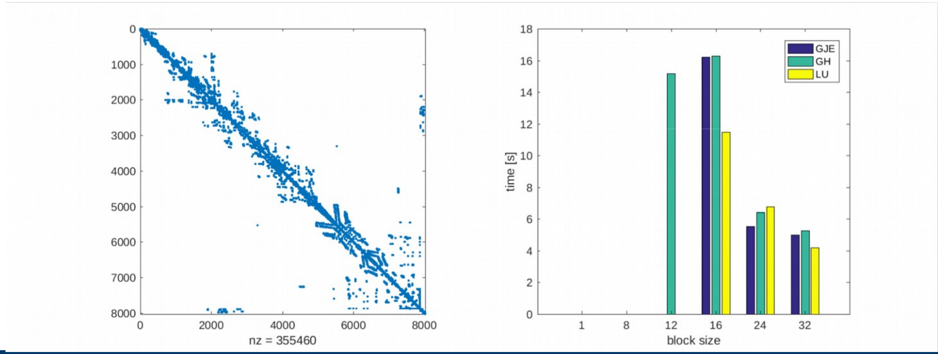
nd24k



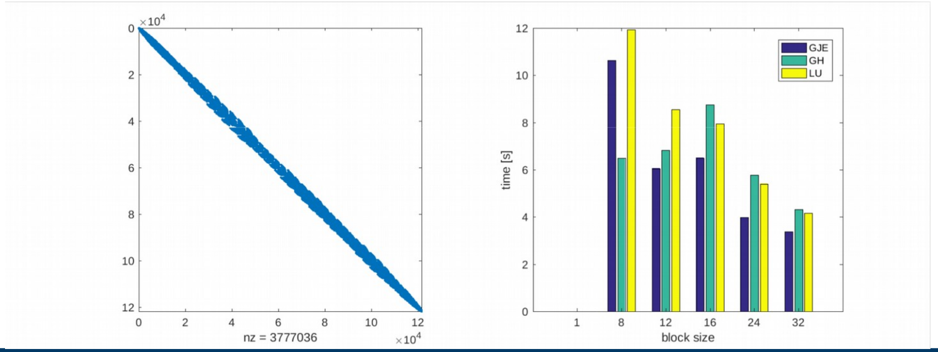
G3_circuit



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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Preconditioner application is memory bounded

- Most of the cost comes from reading the matrix from memory
- Idea: use lower precision to store the matrix

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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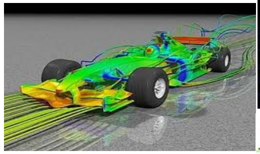

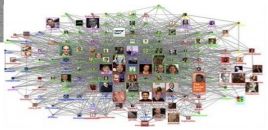

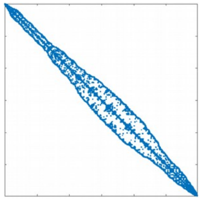

$$Ax = b$$

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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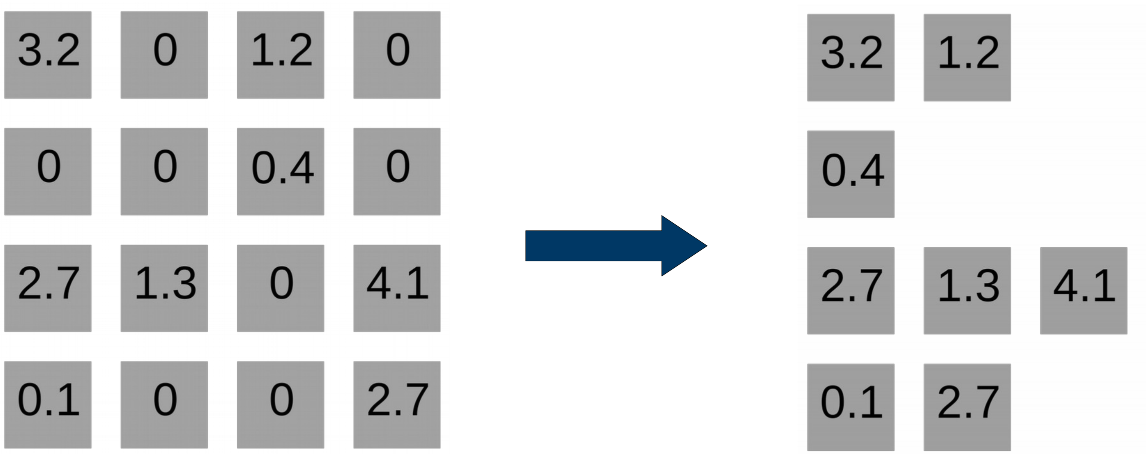
→

3.2	1.2	0.4	2.7	1.3	4.1	0.1	2.7	
0	0	1	2	2	2	3	3	row
0	2	2	0	1	3	0	3	column

COO

Sparse matrix formats



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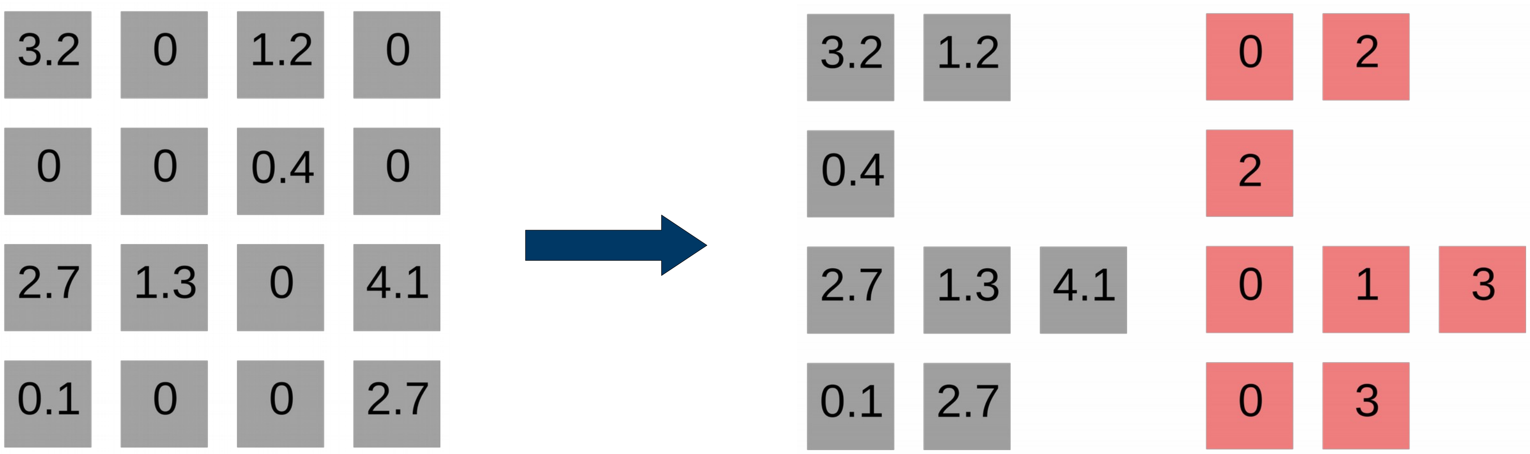

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0.4				2		
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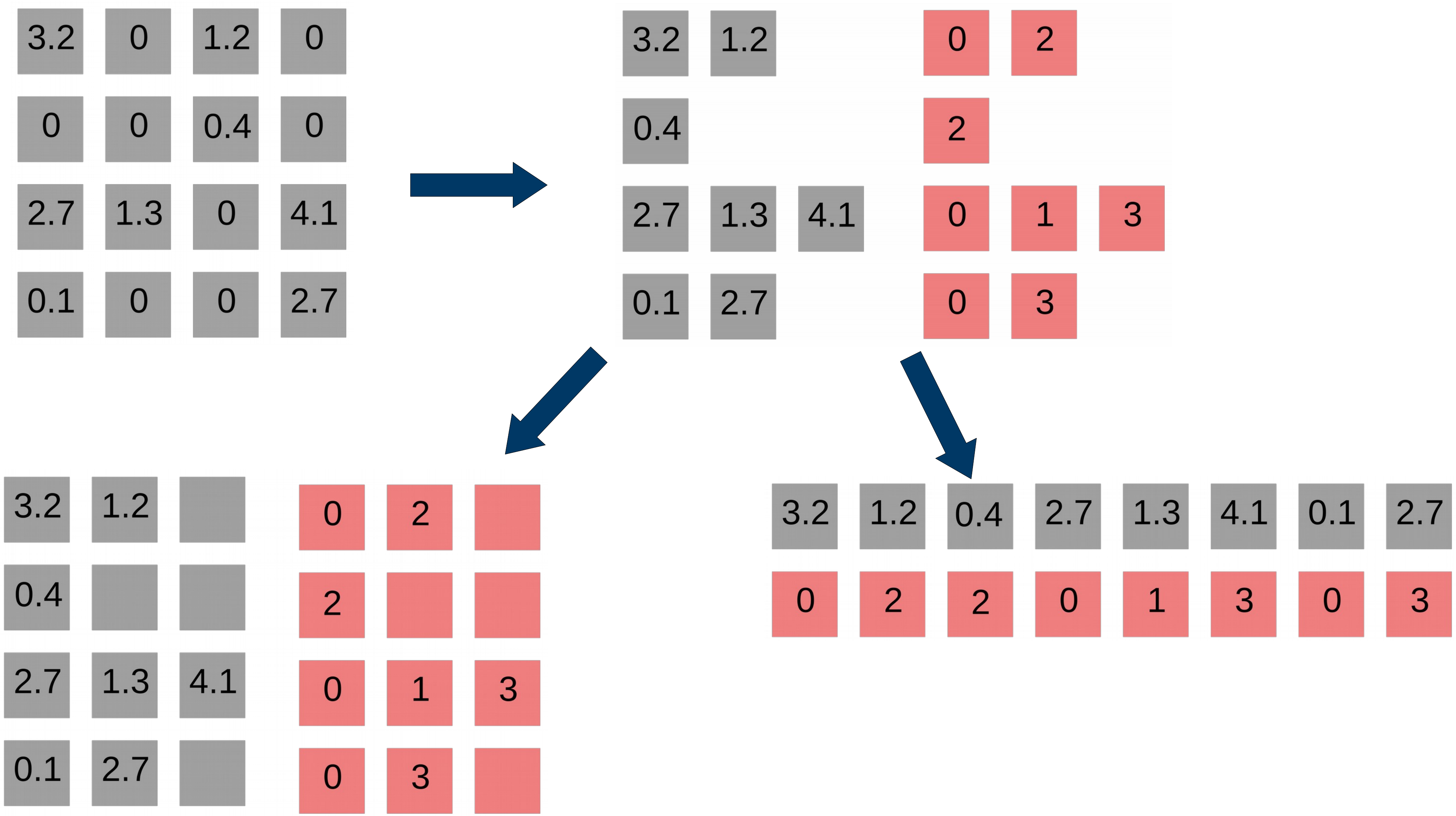
0.1	2.7			0	3	

ELL

Sparse matrix formats



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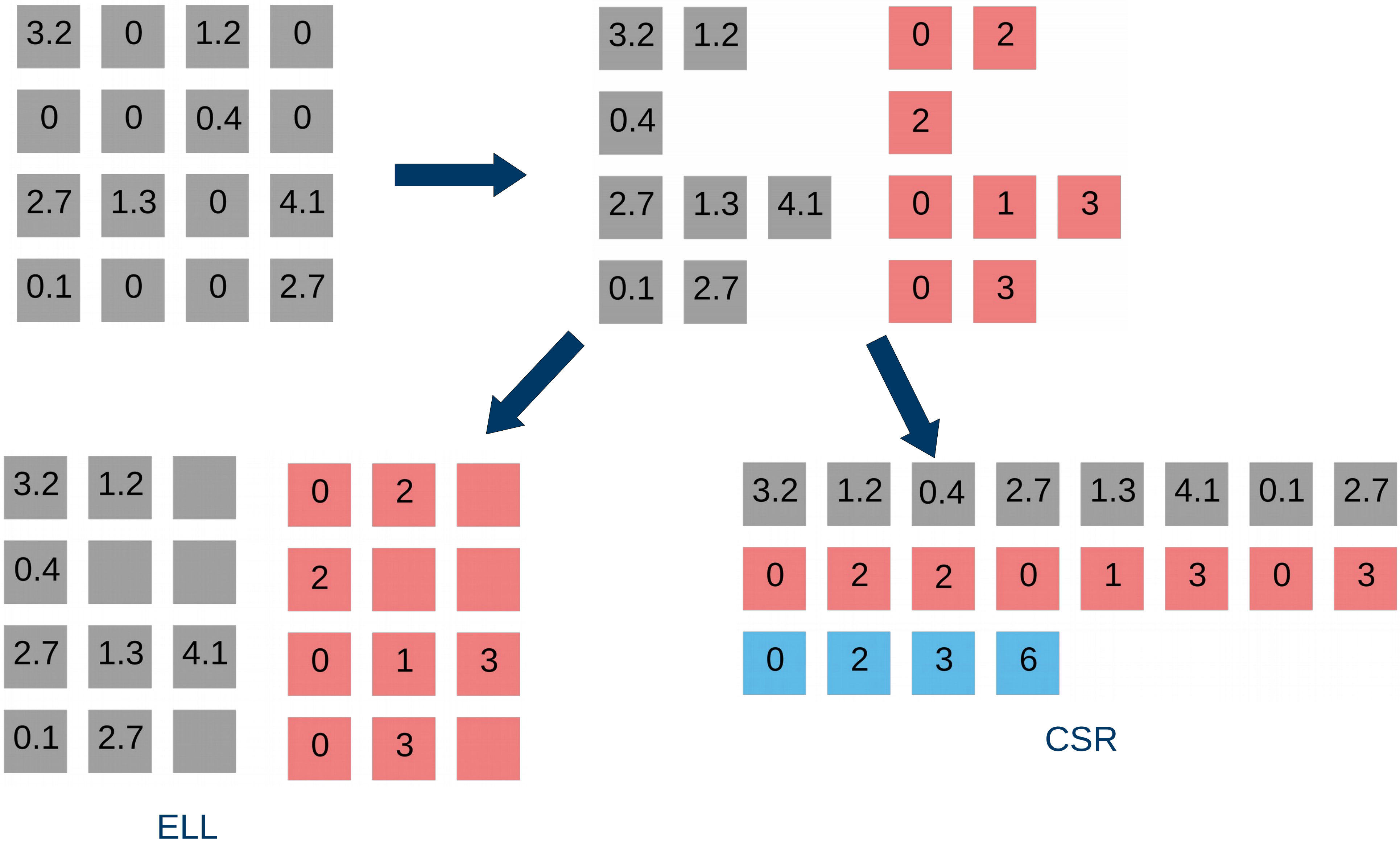

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0	2	0	2
2		1	3
3			

… leads to CSC

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… leads to CSC

3.2	1.2	0.4	2.7	1.3	4.1	0.1	2.7
0	2	2	0	1	3	0	3
0	2	3	6				

CSR

“Standard” approach

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)
0	2	3	6					Row pointers (rowptr)

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)
0	2	3	6					Row pointers (rowptr)

$$y := Ax$$

```
void SpMV_CSR(int m, int *rowptr, int *colidx, float *val, float *x, float *y) {
  for (int i = 0; i < m; ++i) {
    for (int j = rowptr[i]; j < rowptr[i+1]; ++j)
      y[i] +=  val[j] * x [ colidx[j] ];
  }
}
```

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)
0	2	3	6					Row pointers (rowptr)

$$y := Ax$$

```
void SpMV_CSR(int m, int *rowptr, int *colidx, float *val, float *x, float *y) {
  for (int i = 0; i < m; ++i) {
    for (int j = rowptr[i]; j < rowptr[i+1]; ++j)
      y[i] +=  val[j] * x [ colidx[j] ];
  }
}
```

Bell & Garland '08

- parallelize outer loop

~ cuSPARSE SpMV

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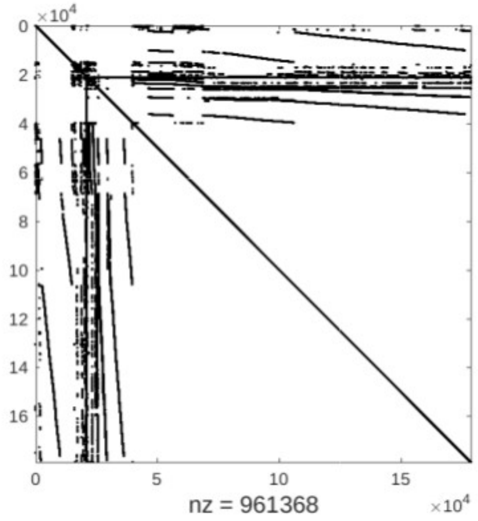
Load imbalance!

Example

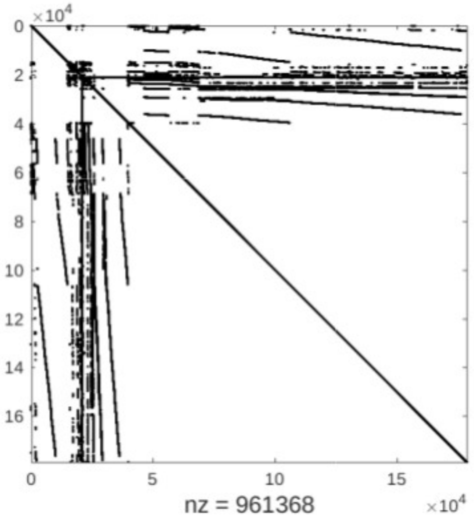
Freescale/transient

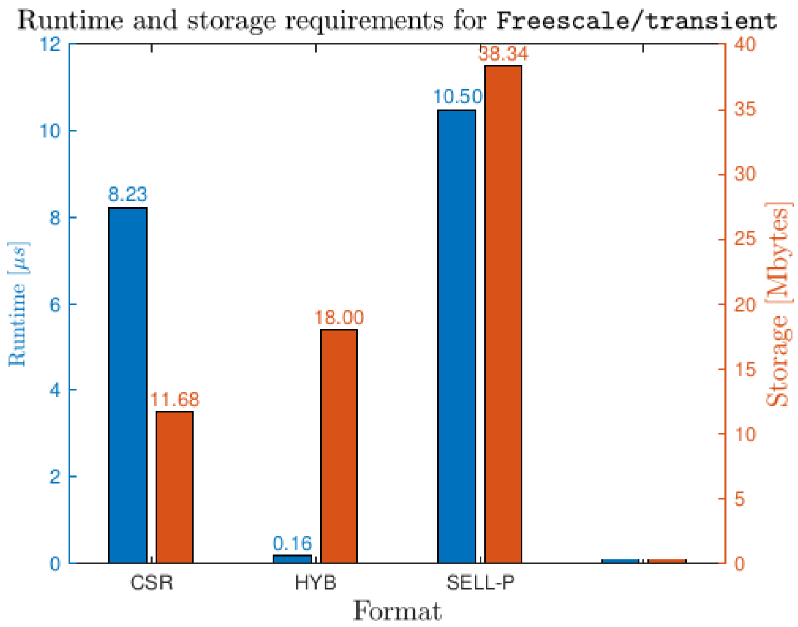


Example

* GTX 1080

Freescale/transient



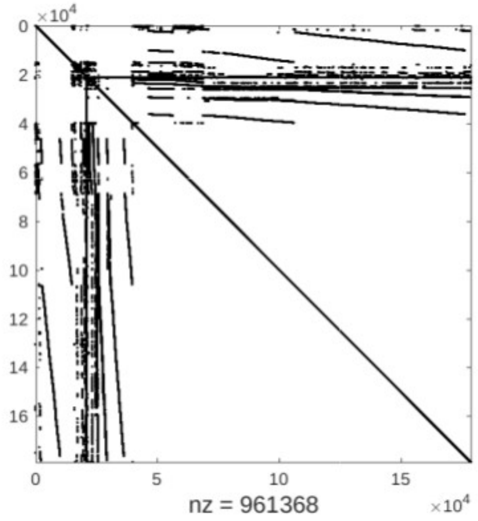


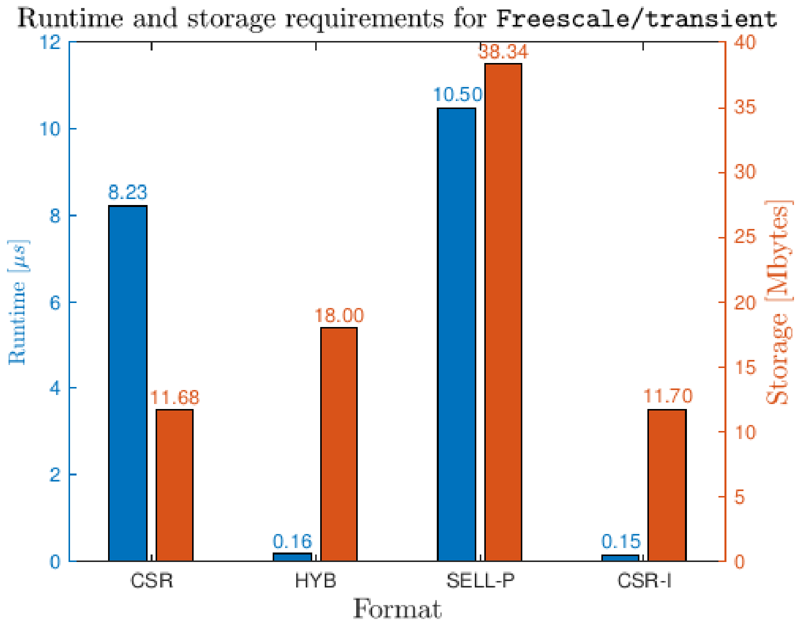
Can we do better than HYB using CSR?

Example

* GTX 1080

Freescale/transient





55x speedup

Can we do better than HYB using CSR?

YES!

Publish a paper about it?

You can…

How to publish an SpMV paper

<irony>

- Think of a “new” algorithm / format for sparse matrix-vector product.
  - Does not have to be great, can do stuff in software that the hardware will already do automatically, or not even give correct results (no one checks).

</irony>

Copyright notice: the “<irony>” tag was shamelessly stolen from Georg Hager’s “Thirteen modern ways to fool the masses with performance results on parallel computers” talk, see https://blogs.fau.de/hager/archives/category/fooling-the-masses

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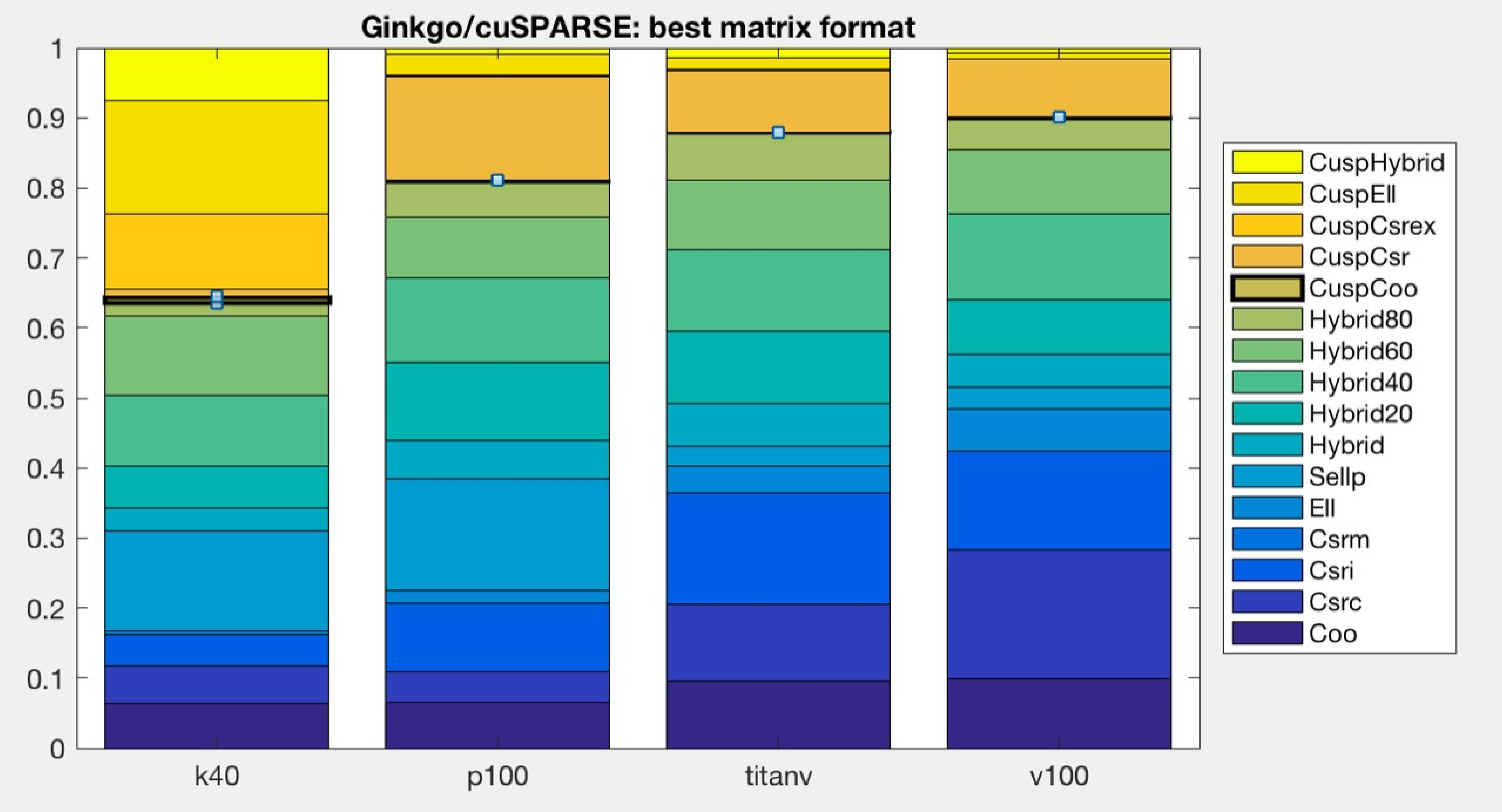
- **Victory!** Think of another format and repeat.

</irony>

In the real world...

THERE IS NO "BEST" SPARSE MATRIX FORMAT / SpMV ALGORITHM



Can we figure out which format is going to give best performance for a given problem?

Maybe...

Choosing the winner a priori

CSR-I designed for irregular patterns

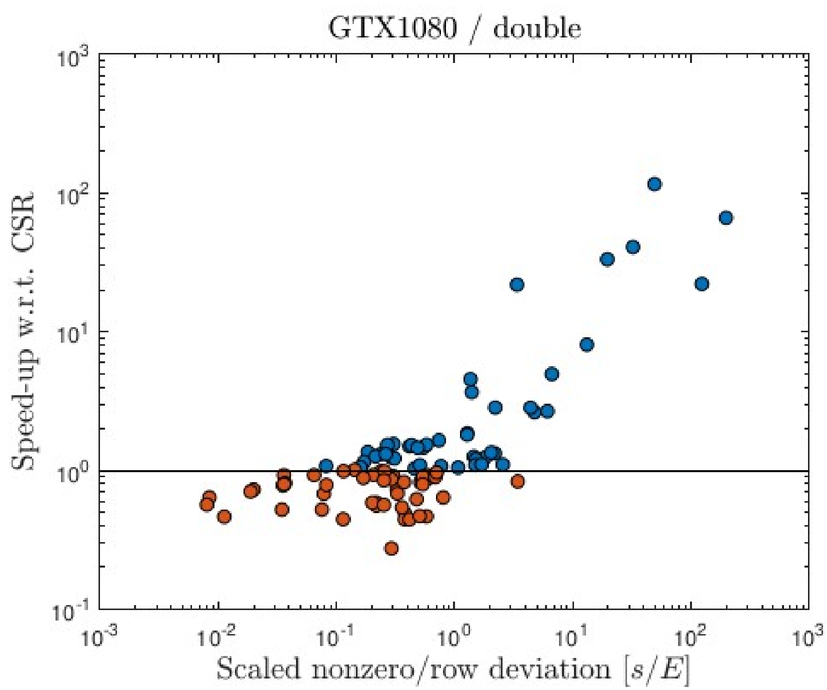
How to measure irregularity?

Deviation of row lengths from the mean.

Is “5” regular or irregular?

Depends on the density of the matrix (mean #rows)

Scatter plot of speedup vs normalized std. dev.



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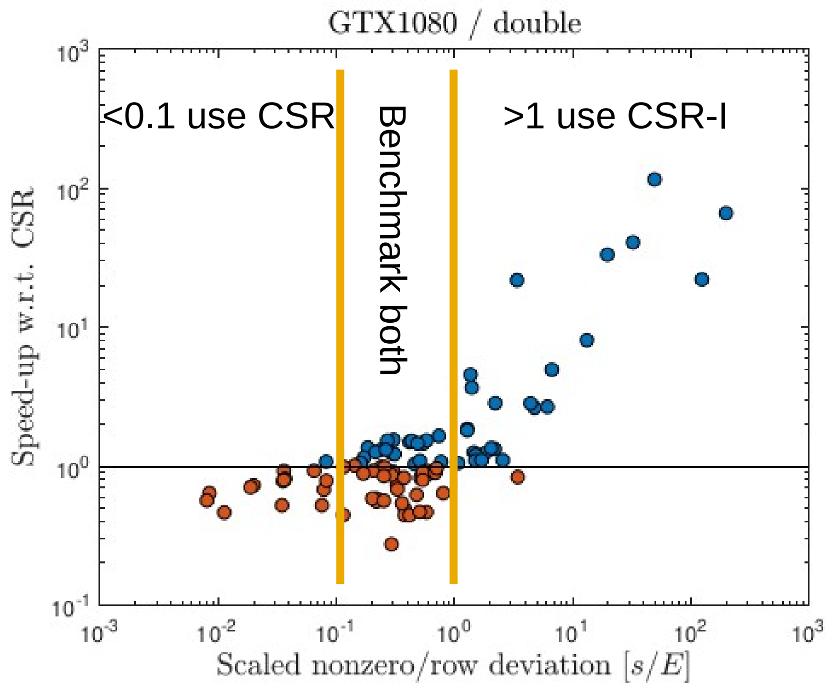
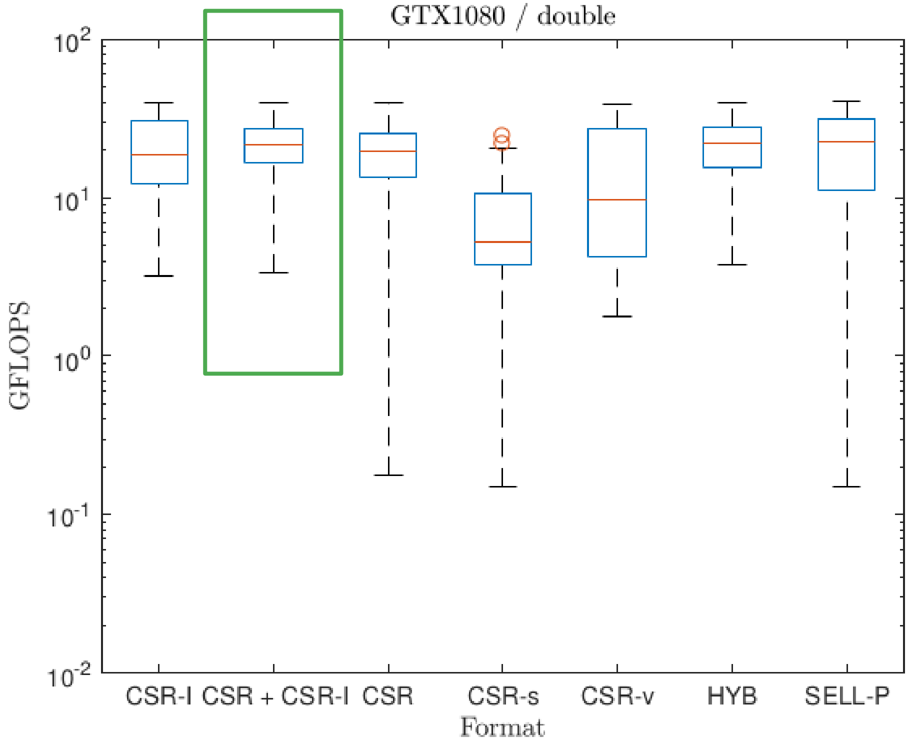
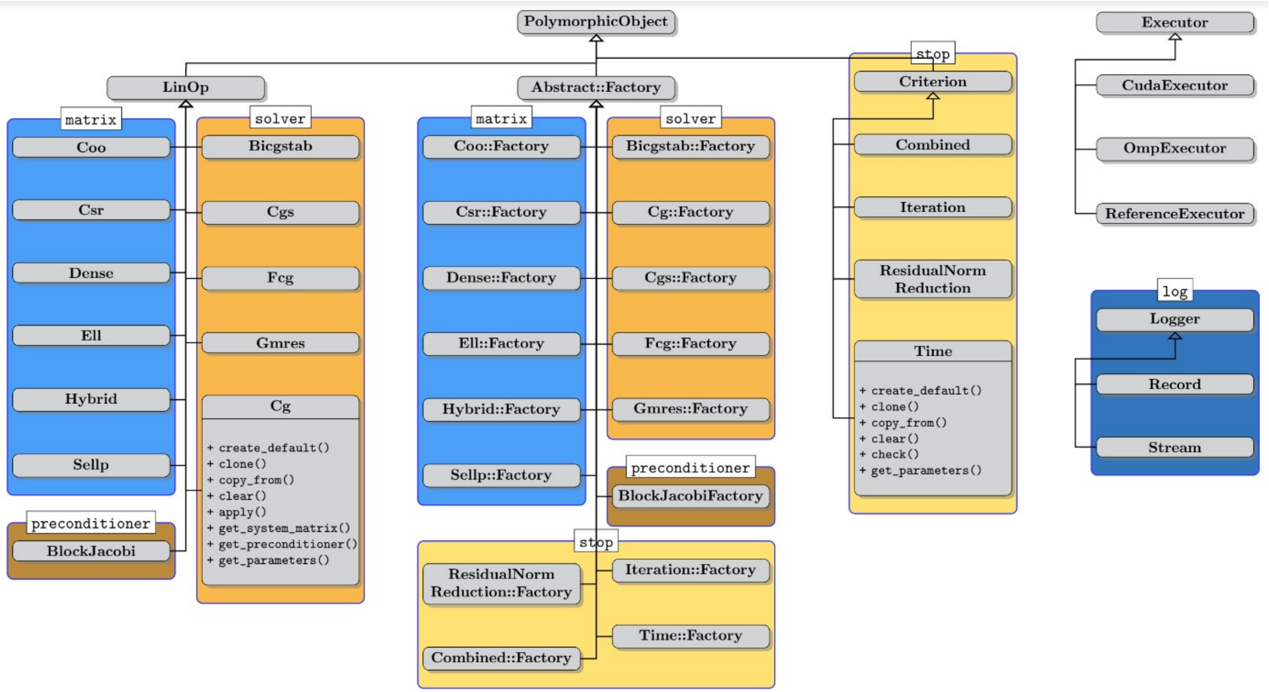


Combining both approaches



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?