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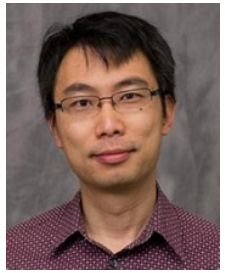
ParILUT - A Parallel Threshold ILU for multicore and GPUs

Hartwig Anzt, Edmond Chow, Goran Flegar, Tobias Ribizel, Jack Dongarra



The Exascale Computing Project

A Collaborative effort of the U.S. Department of Energy Office of Science And the National Nuclear Security Administration

U.S. Department of Energy
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Helmholtz Impuls und Vernetzungsfond
VH-NG-1241

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We are looking for a factorization-based preconditioner such that $A \approx L \cdot U$
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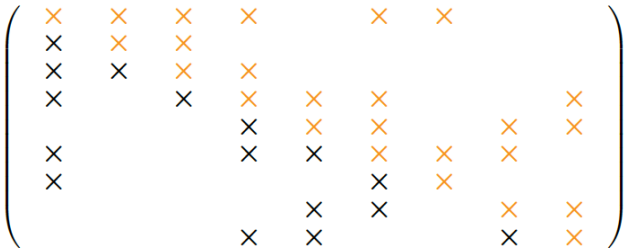
Exact LU Factorization

- Decompose system matrix into product $A = L \cdot U$.
- Based on Gaussian elimination.
- Triangular solves to solve a system $Ax = b$:

$$Ly = b \Rightarrow y \qquad \Rightarrow \qquad Ly = b \Rightarrow x$$

- De-Facto standard for solving dense problems.
- *What about sparse? Often significant fill-in...*



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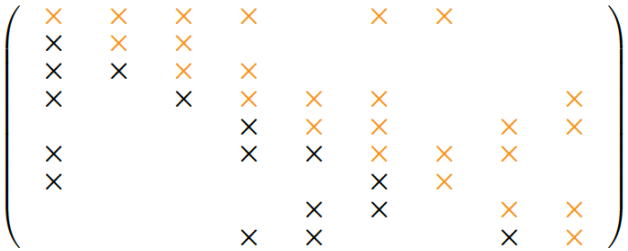

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  - Works well for many problems.
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- Fill-in in threshold ILU (**ILUT**) bases $\mathcal{S}$ on the significance of elements (e.g. magnitude).
  - Often better preconditioners than level-based ILU.
  - Difficult to parallelize.

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2. *Compute values in those locations such that $A \approx L \cdot U$ is a "good" approximation.*
3. *Maybe change some locations in favor of locations that result in a better preconditioner.*
4. *Repeat until the preconditioner quality does no longer improve for the nonzero count.*

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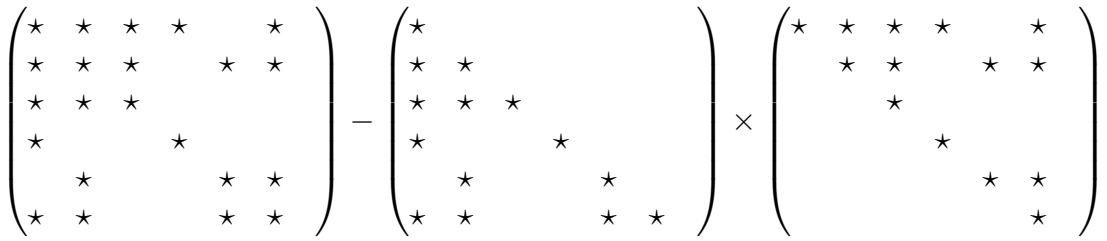

ILU residual $R = A - L \times U$

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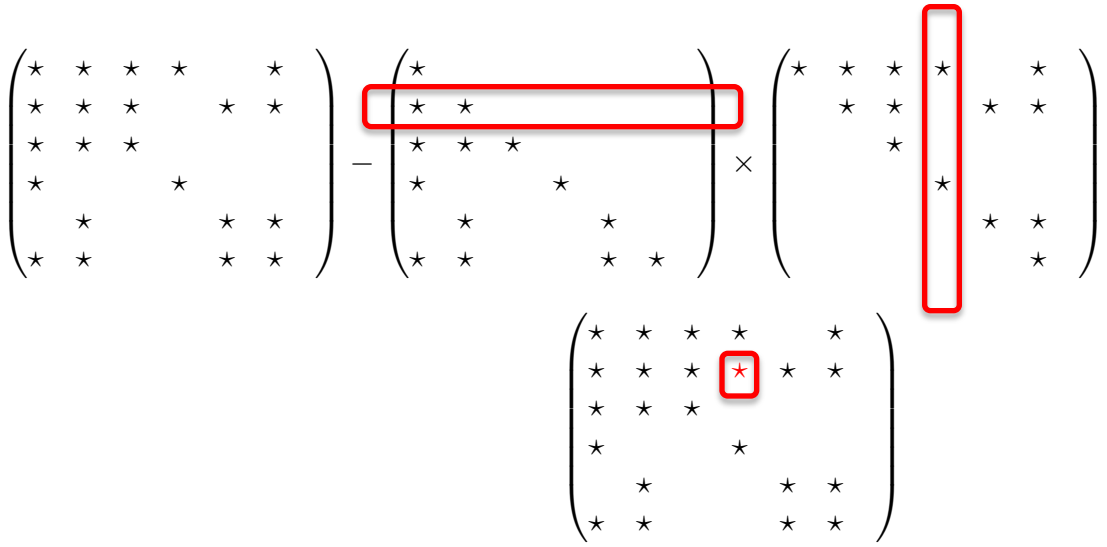

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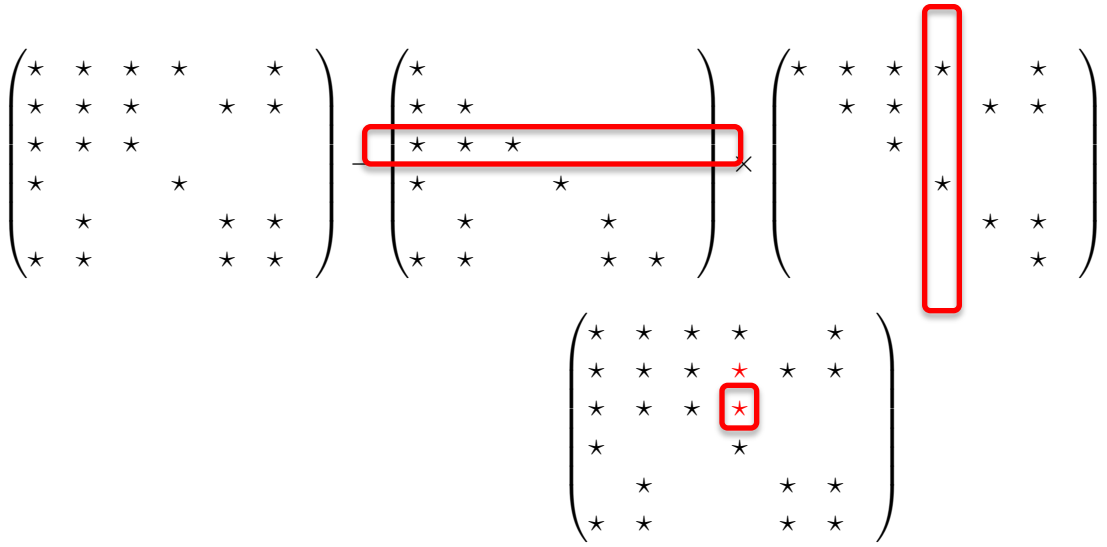

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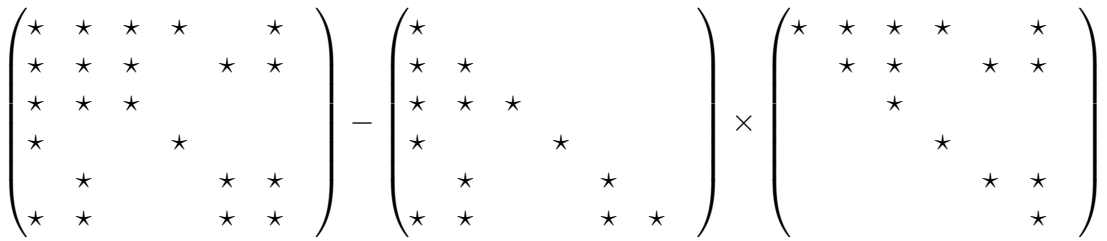

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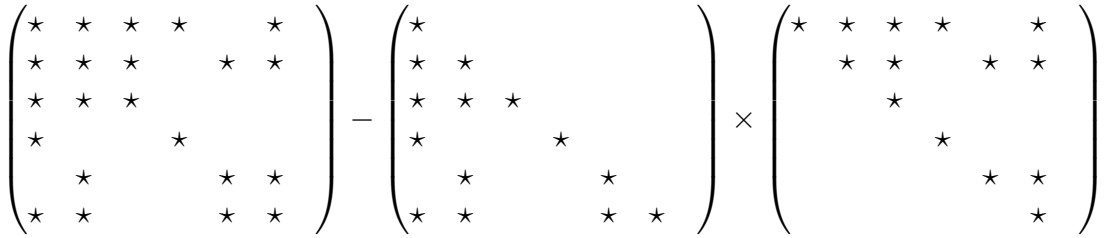

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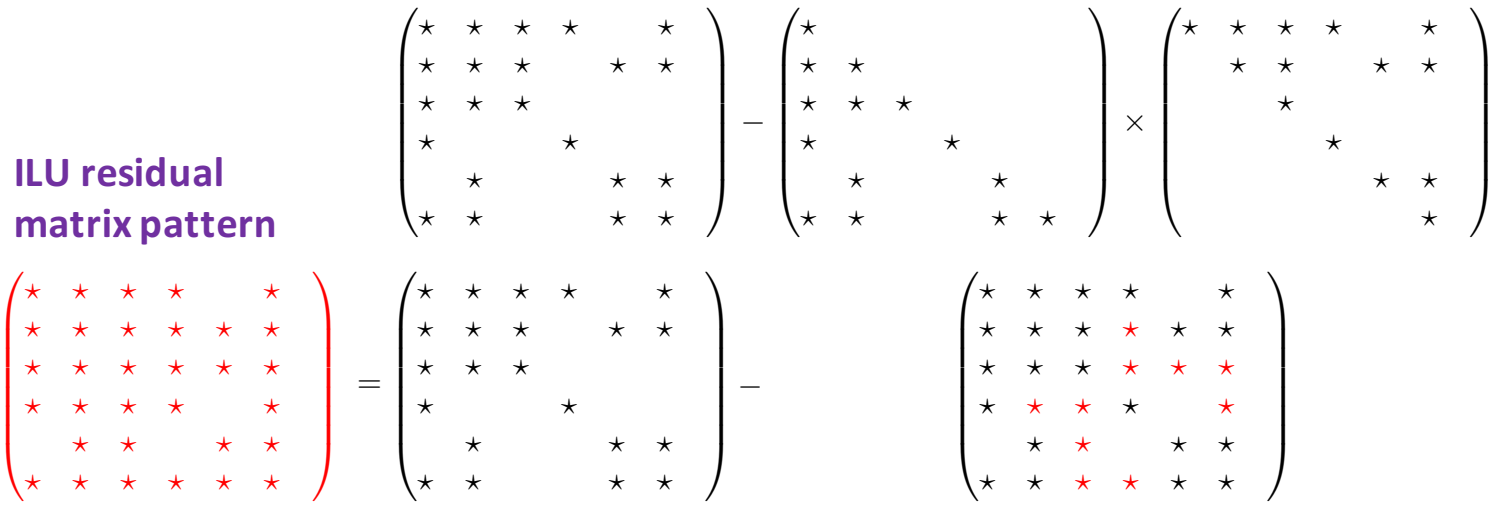
ILU residual matrix pattern



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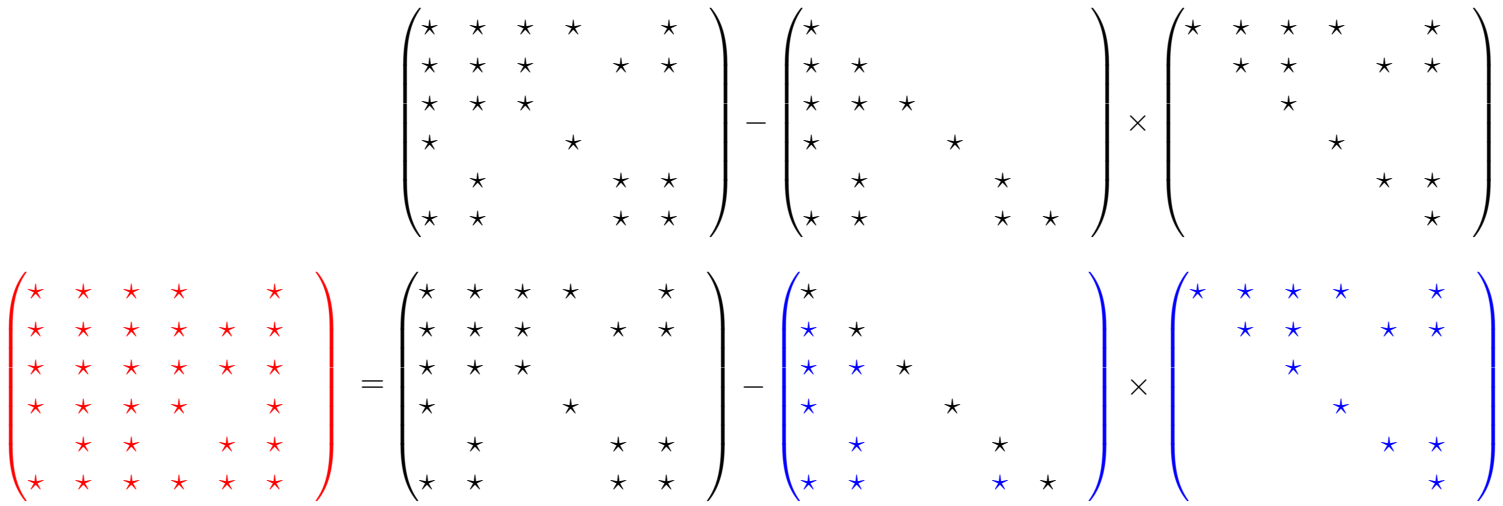

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$nnz(L + U)$ equations
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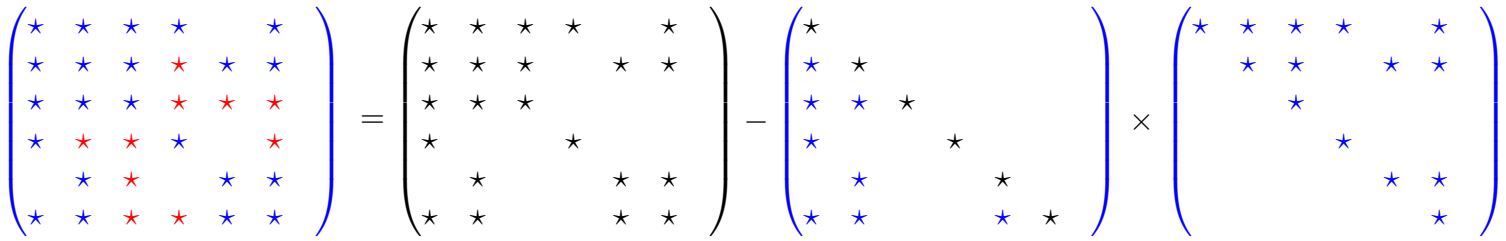

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- This is the underlying idea of Edmond Chow's parallel ILU algorithm[1]:

$$F(L,U) = \begin{cases} \frac{1}{u_{jj}} \left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \right), & i > j \\ a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}, & i \leq j \end{cases}$$

- Converges in the asymptotic sense towards incomplete factors L, U such that $R = A - L \cdot U = 0|_{\mathcal{S}}$

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- We may not need high accuracy here, because we may change the pattern again… One single fixed-point sweep.

Fixed-point sweep approximates incomplete factors.

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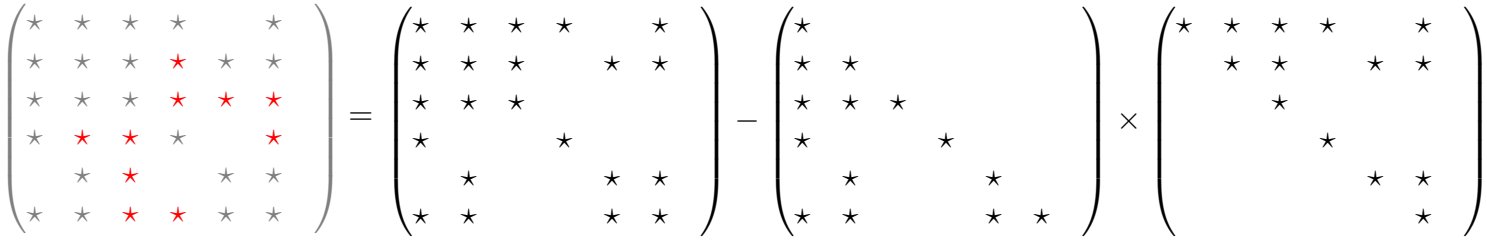
- Maybe use the ILU residual as quality metric.



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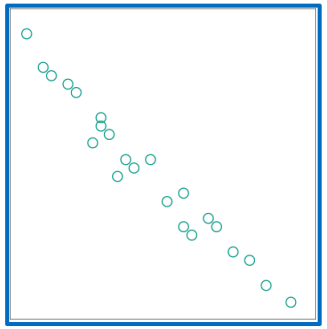

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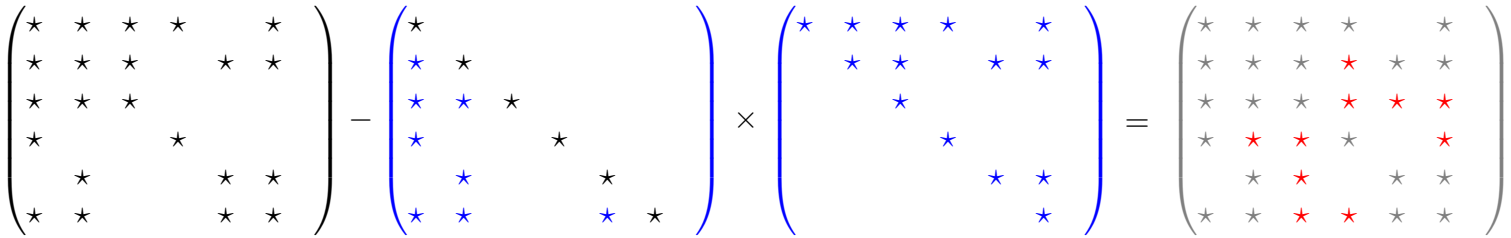

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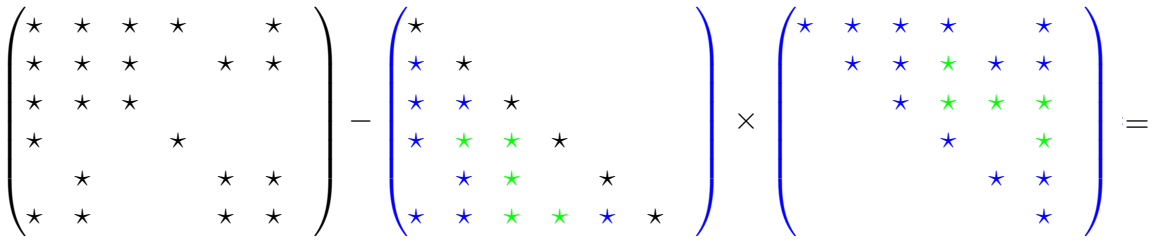

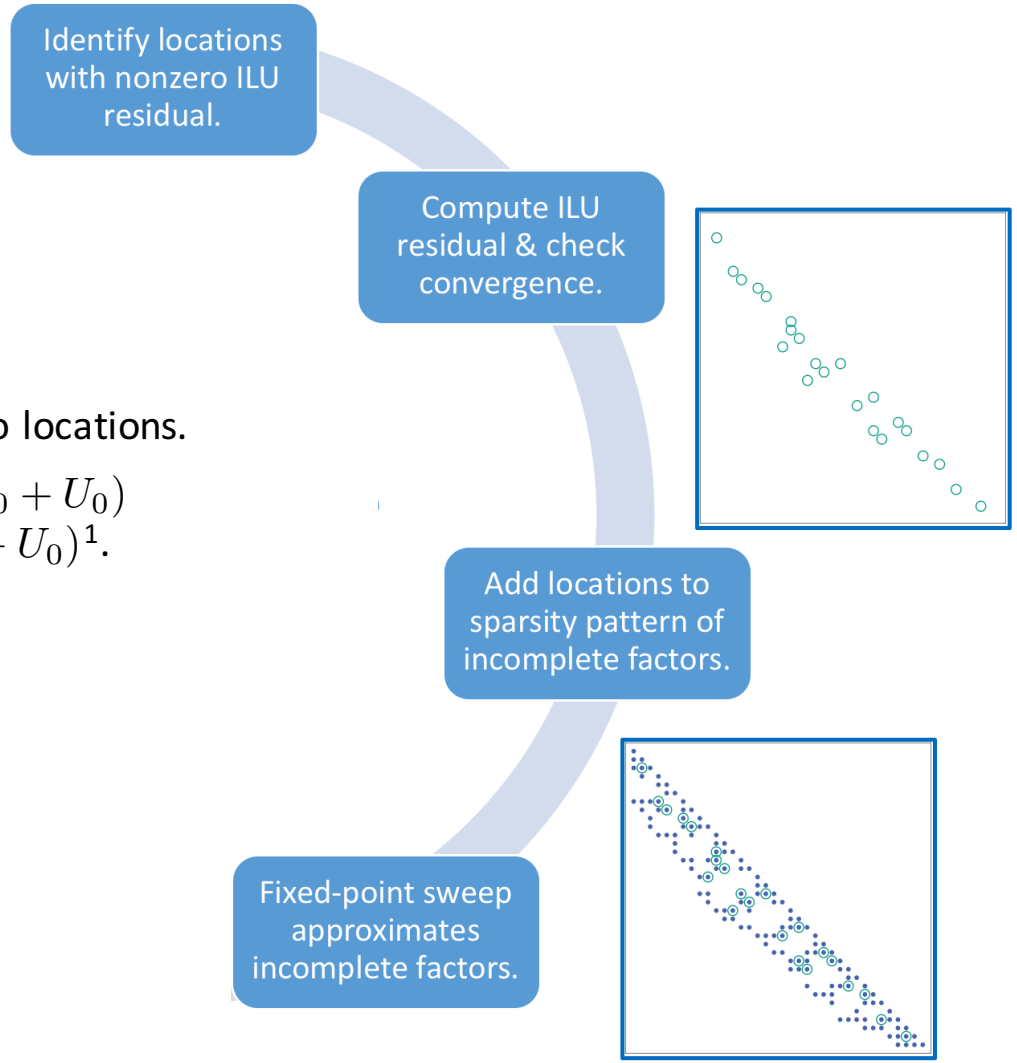

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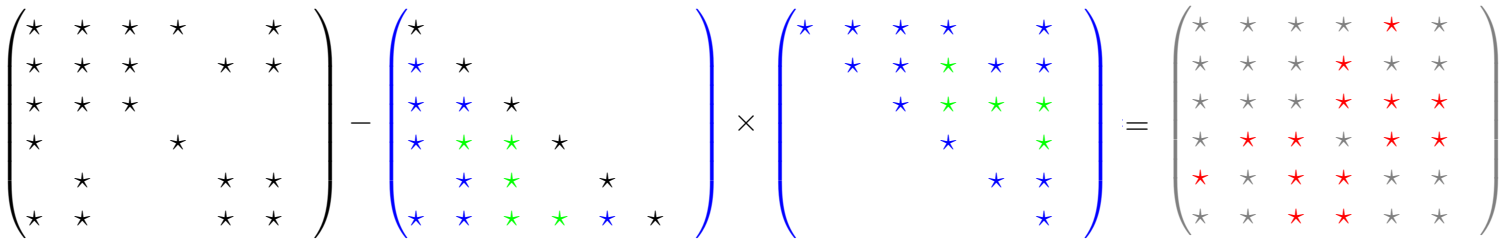
- Adding all these locations (level-fill!) might be good idea, but adding these will again generate new nonzero residuals $\mathcal{S}_2 = (\mathcal{S}(A) \cup \mathcal{S}(L_1 \cdot U_1)) \setminus \mathcal{S}(L_1 + U_1)$



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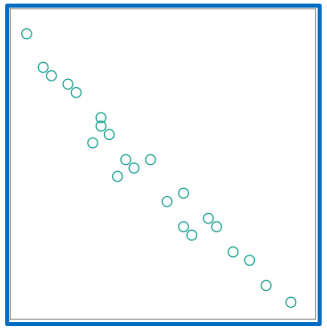
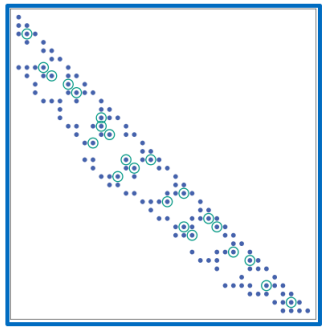


Add locations to sparsity pattern of incomplete factors.

Fixed-point sweep approximates incomplete factors.



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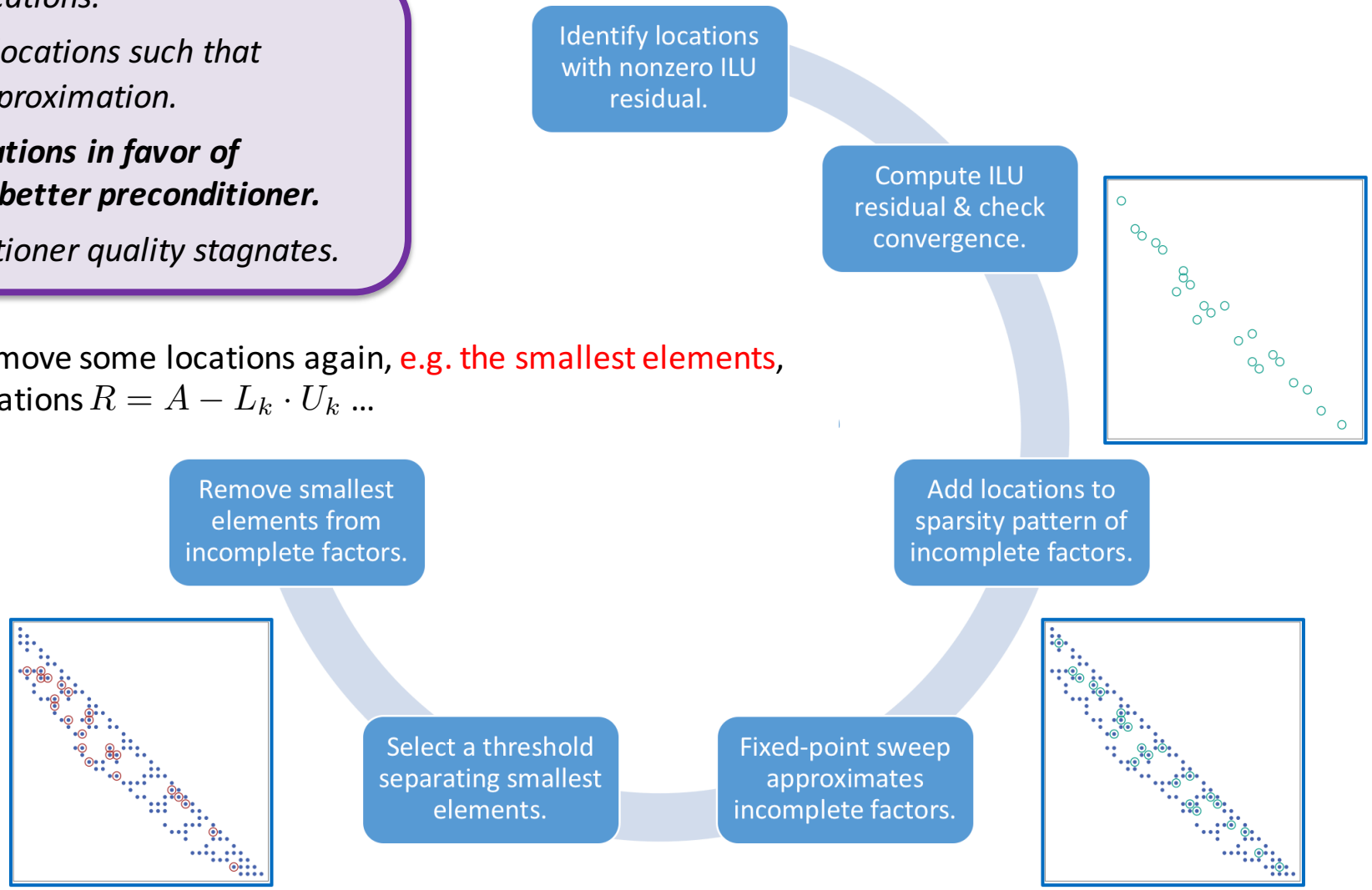

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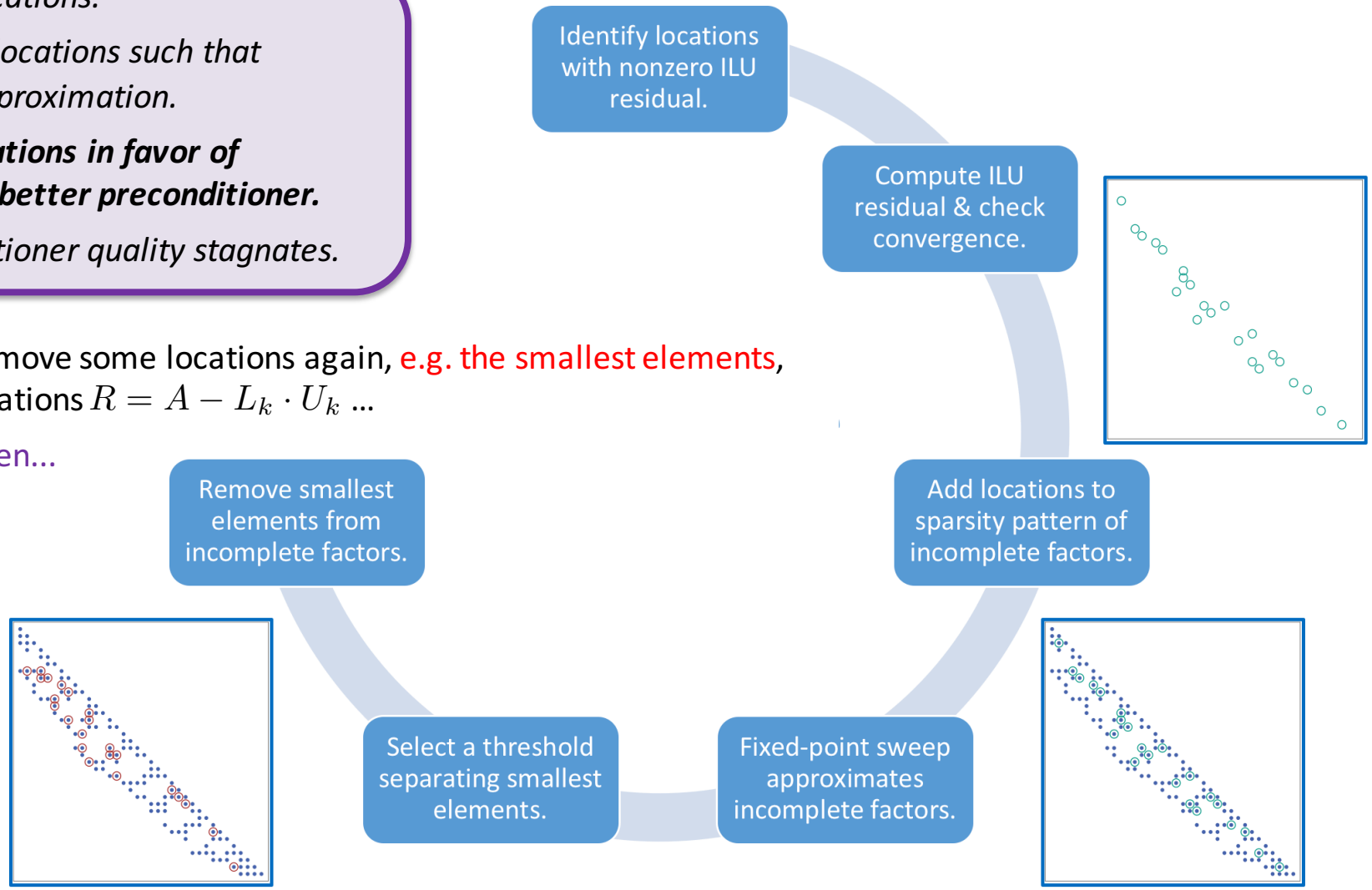
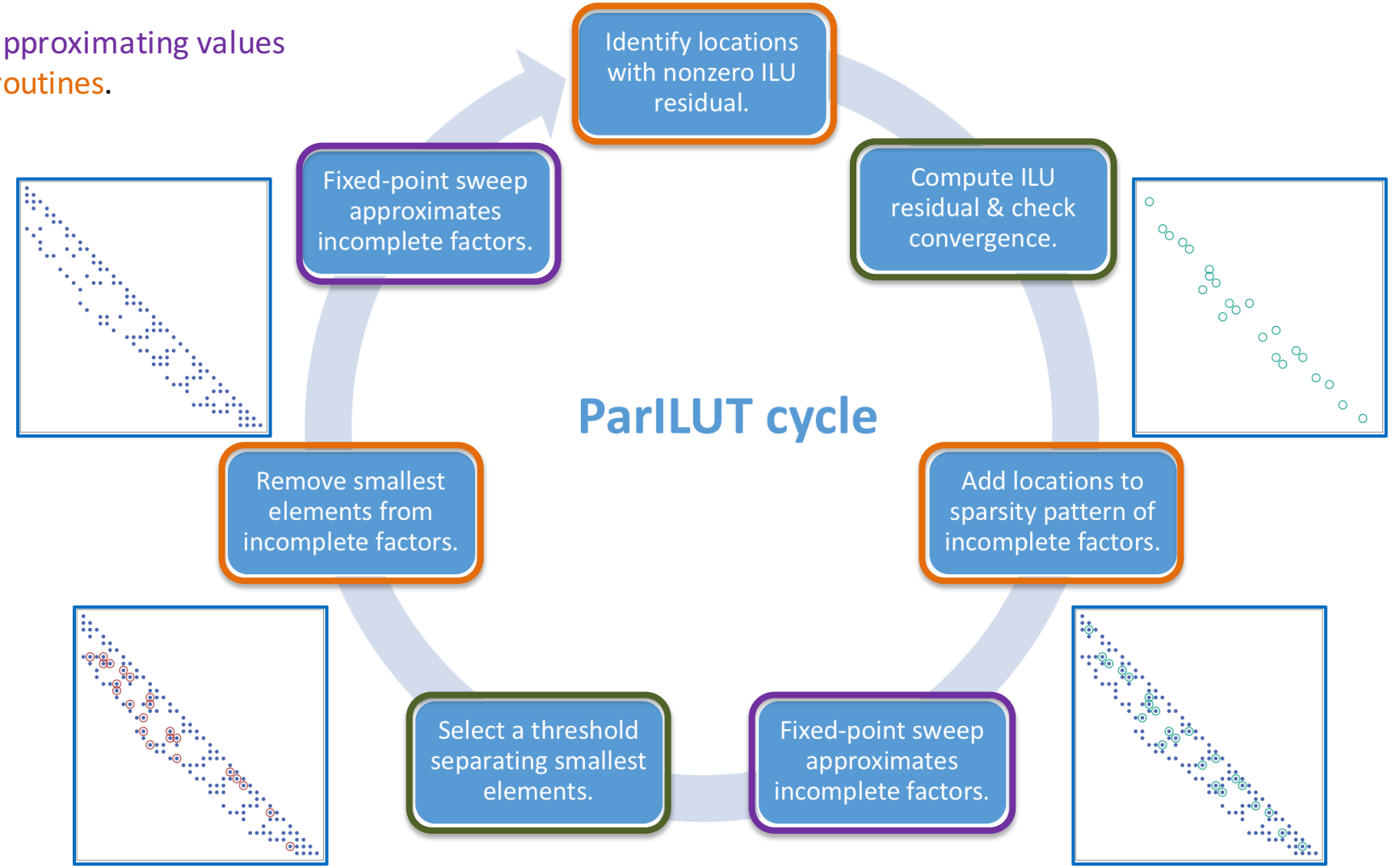
- We need another sweep, then...



ParILUT

Interleaving fixed-point sweeps approximating values with pattern-changing symbolic routines.



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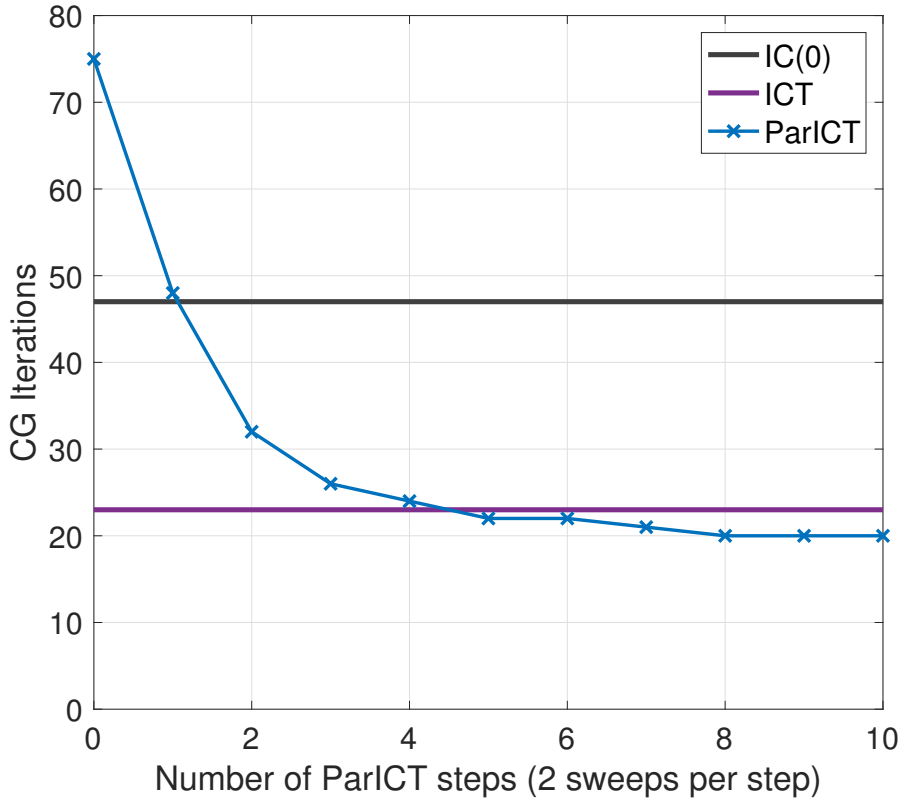
ParILUT quality

Anisotropic diffusion problem
n: 741, nz: 4,951

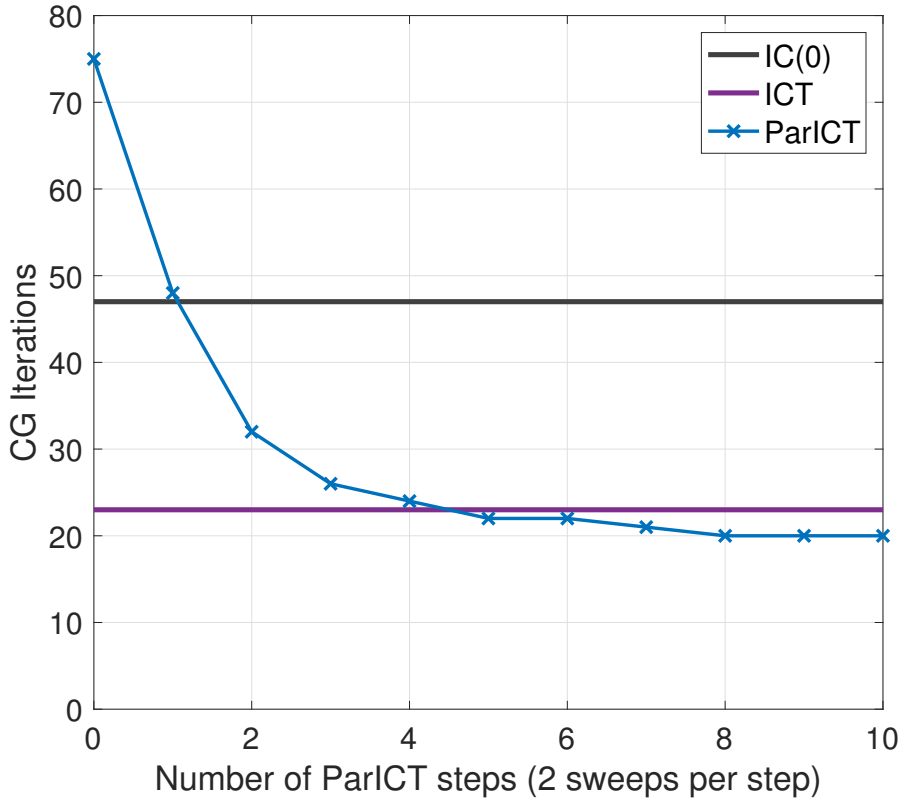


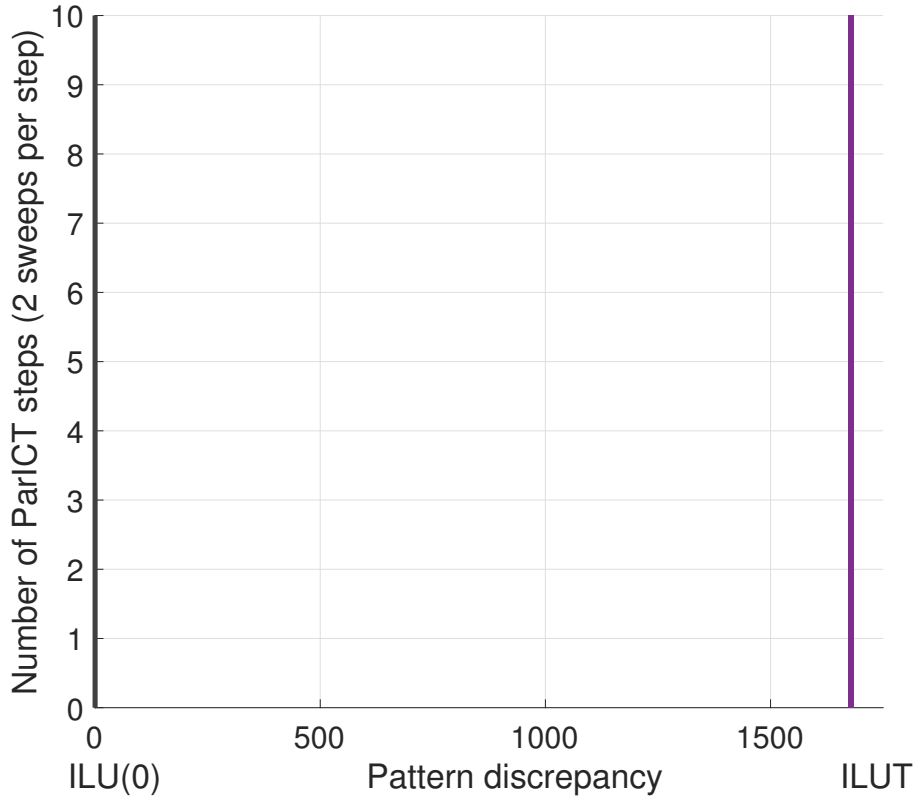
- Top-level solver iterations as quality metric.
- Few sweeps give a "better" preconditioner than ILU(0).
- Better than conventional ILUT?

[1]Anzt et al. **"ParILUT – A new parallel threshold ILU".** *In: SIAM J. on Sci. Comp. (2018).*

ParILUT quality

Anisotropic diffusion problem
n: 741, nz: 4,951





- Top-level solver iterations as quality metric.
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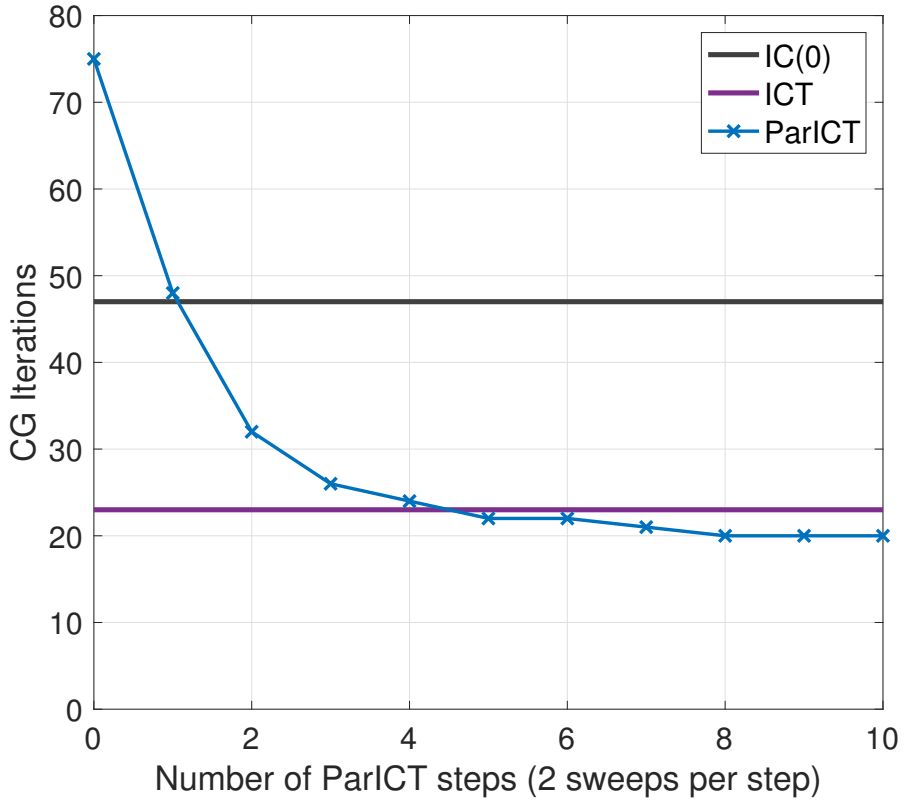
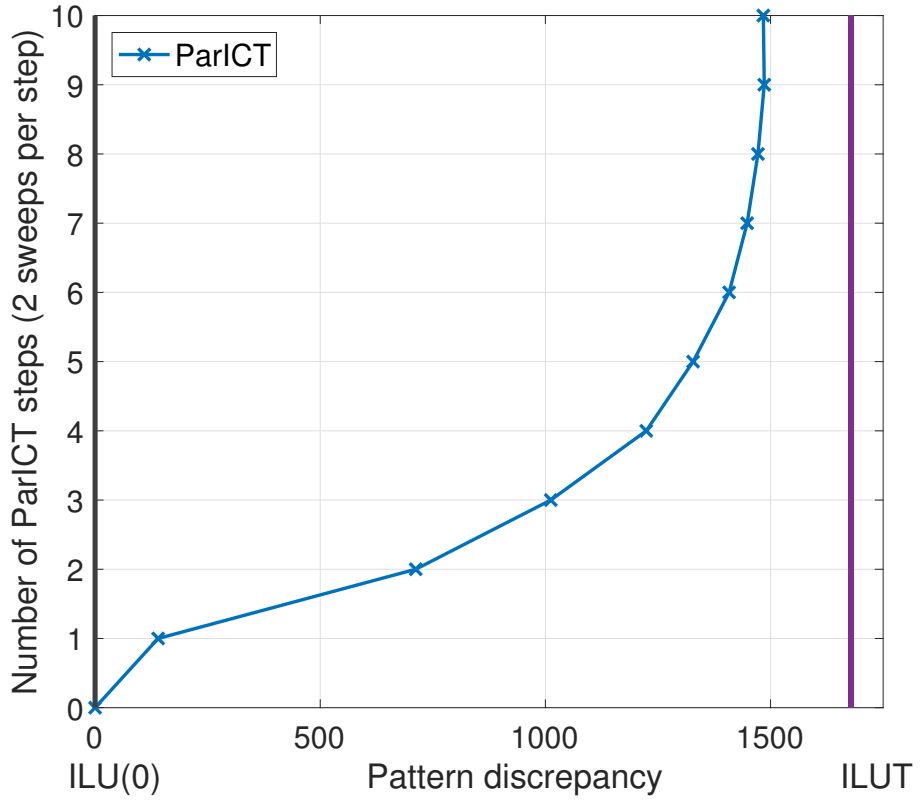




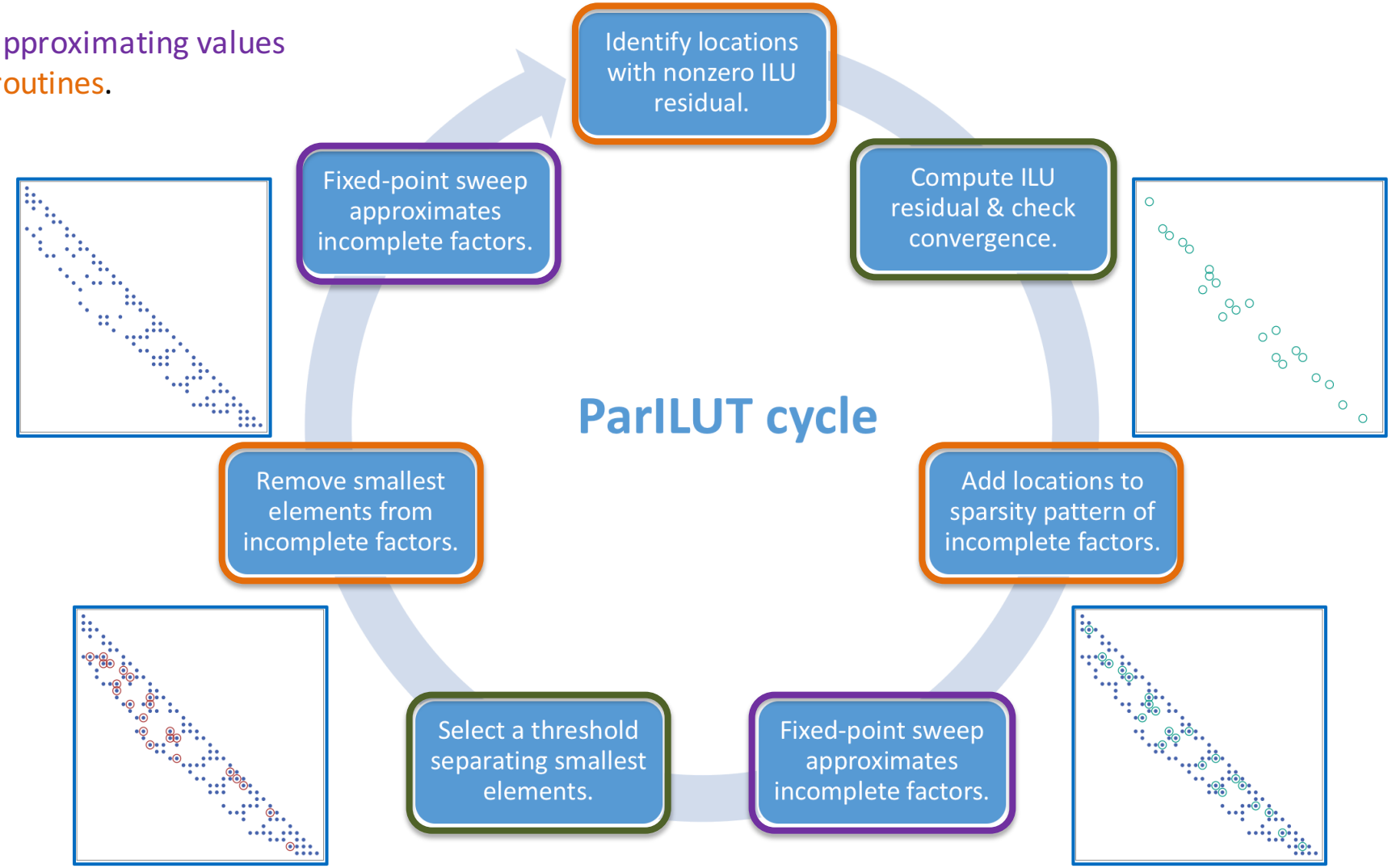
- Top-level solver iterations as quality metric.
- Few sweeps give a "better" preconditioner than ILU(0).
- Better than ILUT?

- Pattern converges after few sweeps.
- Pattern "more like" ILUT than ILU(0).

[1]Anzt et al. **"ParILUT – A new parallel threshold ILU".** *In: SIAM J. on Sci. Comp. (2018).*

ParILUT – A Parallel Threshold ILU for GPUs

Interleaving fixed-point sweeps approximating values with pattern-changing symbolic routines.



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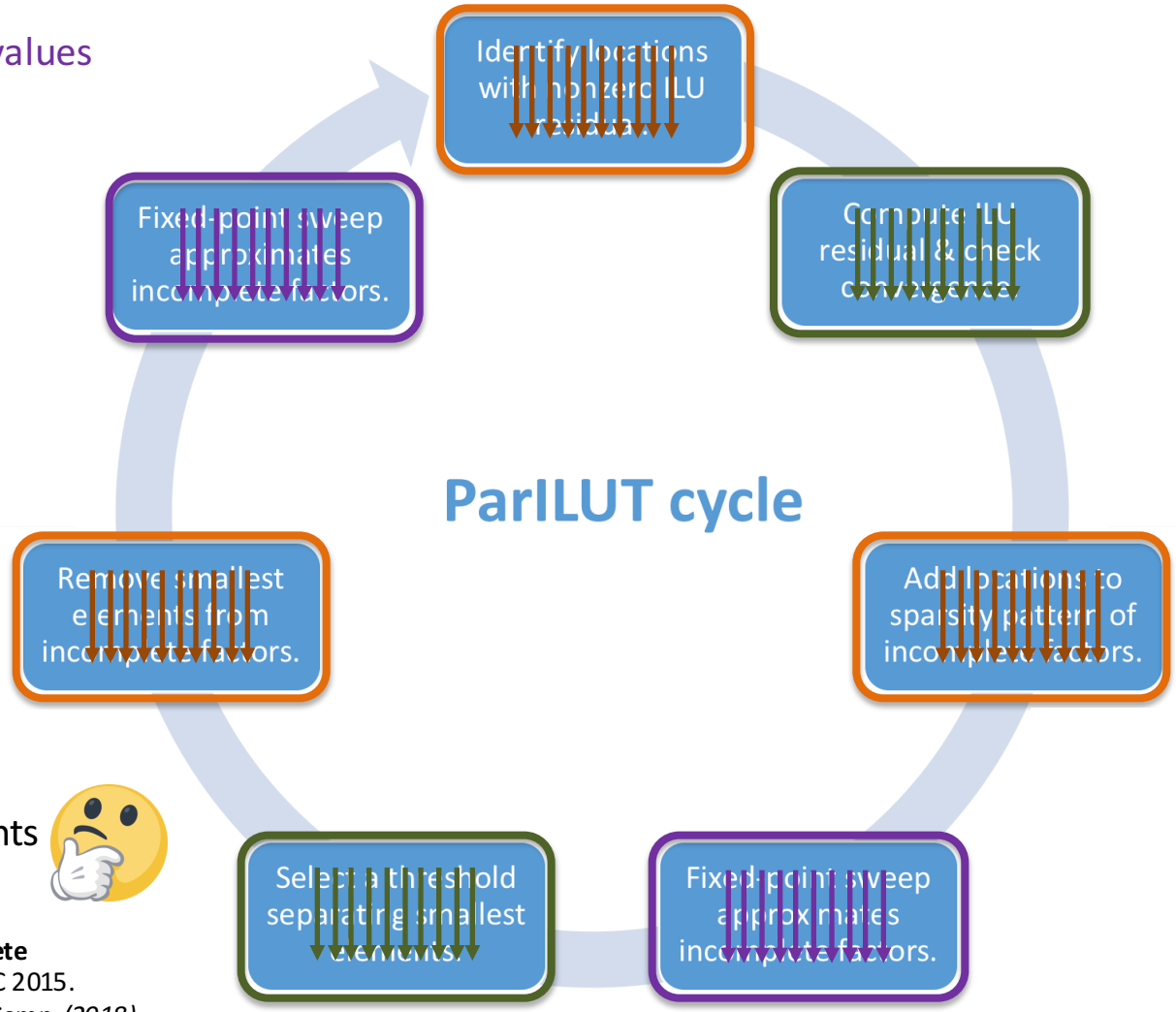

Parallelism inside the building blocks:

- Fixed-Point Sweeps[1] ✓
- Residuals[1] ✓
- Identify Fill-In Locations[2] ✓
- Add Locations[2] ✓
- Remove Locations[2] ✓
- Select Threshold Separating Smallest Elements

[1]Chow et al. **"Asynchronous Iterative Algorithm for Computing Incomplete Factorizations on GPUs"**. In ISC 2015.

[2]Anzt et al. **"ParILUT – A new parallel threshold ILU".** *In: SIAM J. on Sci. Comp. (2018).*

Threshold Selection on GPUs

This is equivalent to the Selection Problem!

Given an unsorted sequence of real numbers $x_0, x_1, x_2, x_3, \ldots x_{n-1}$, we want to find the element x_{i_k} such that in the sorted sequence

$$x_{i_0} \leq x_{i_1} \leq x_{i_2} \leq x_{i_3} \leq \cdots \leq x_{i_k} \leq \ldots x_{i_{n-1}}$$

k

the element x_{i_k} is located in position k.

We do not necessarily need to sort the complete sequence!

Approximate and Exact Selection on GPUs

Tobias Ribizel*, Hartwig Anzt*†
*Steinbuch Centre for Computing, Karlsruhe Institute of Technology, Germany
†Innovative Computing Lab (ICL), University of Tennessee, Knoxville, USA
tobias.ribizel@student.kit.edu, hartwig.anzt@kit.edu

http://bit.ly/SampleSelectGPU

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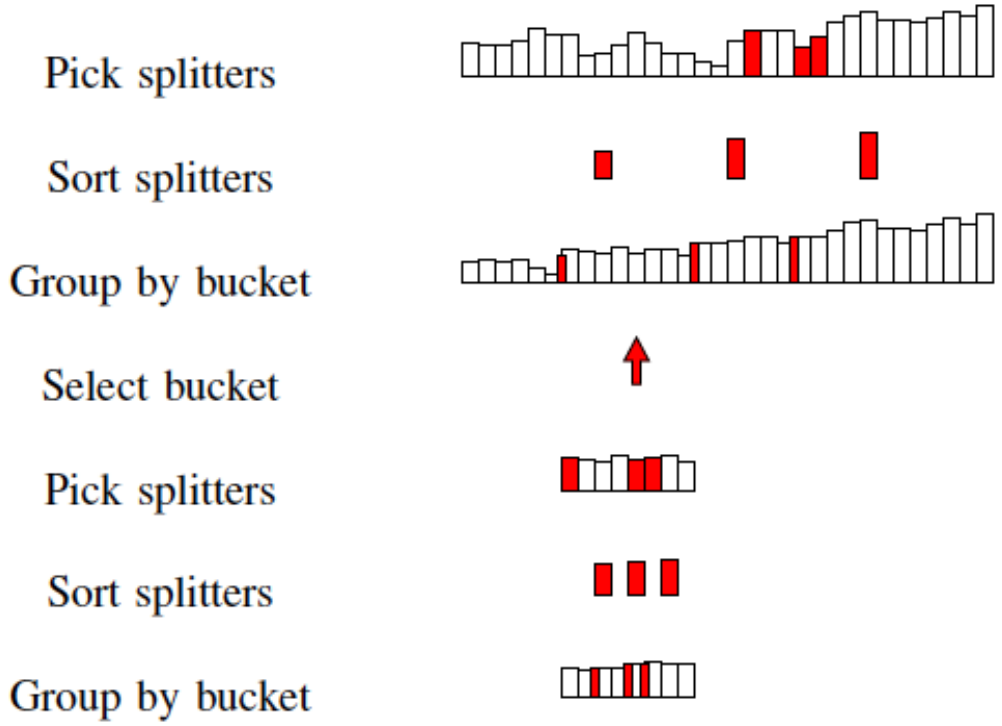
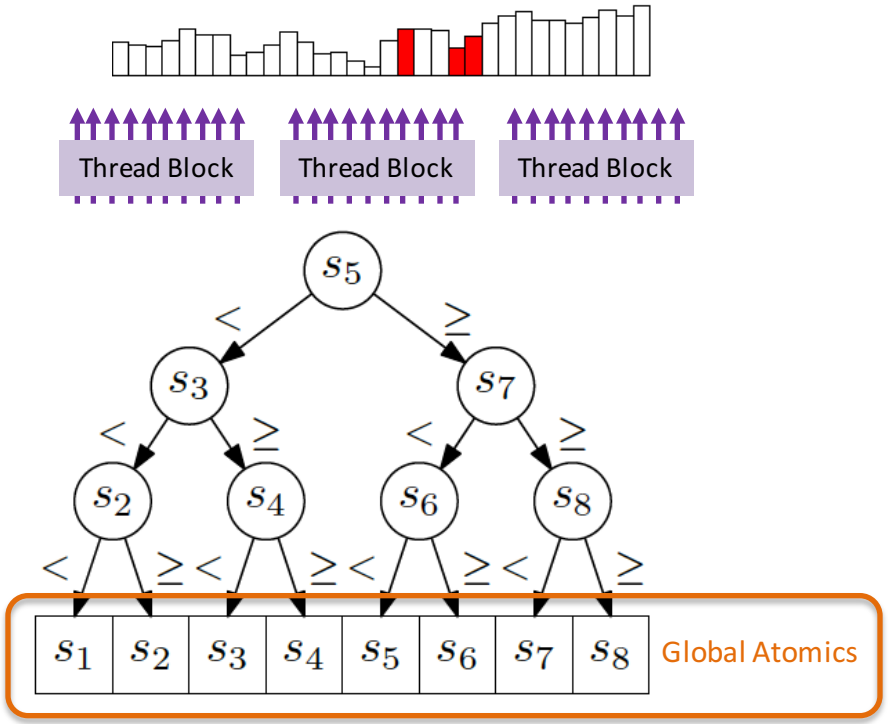
SampleSelect Algorithm



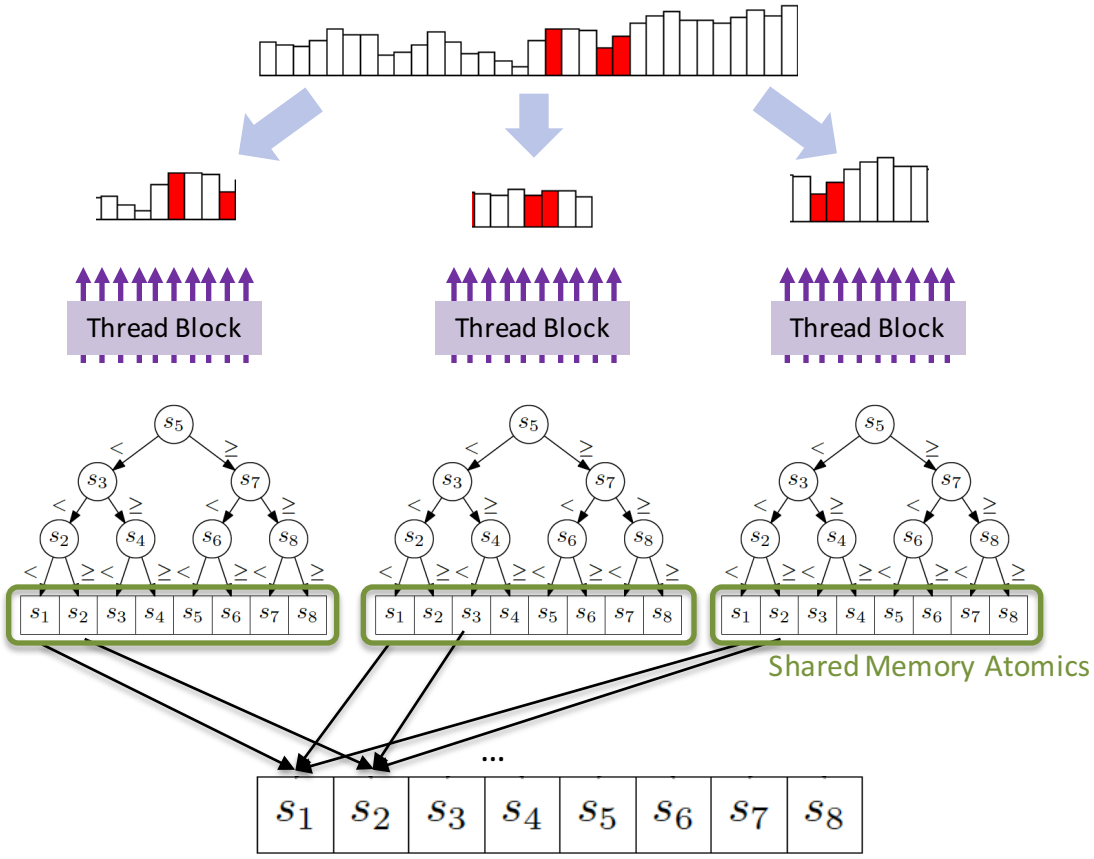
Parallelization & Communication of SampleSelect on GPUs

Global Memory Atomics



- Run SampleSelect using all resources on complete data set;
- Use global atomics to generate bucket counts;

Shared Memory Atomics

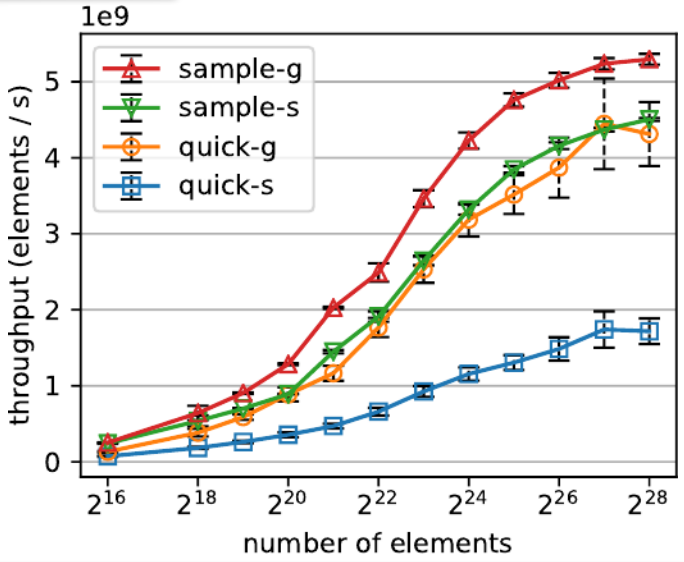


- Split data set into chunks, assign to thread blocks;
- Each thread block runs bucket count on its data;
- Use a global reduction to get global bucket counts;

Global vs. Local Memory Atomics

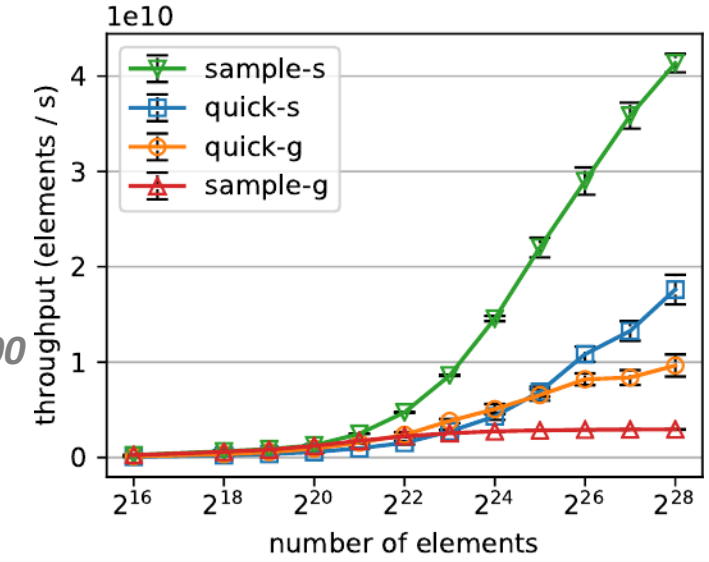
-g : global memory atomics
-s: shared memory atomics

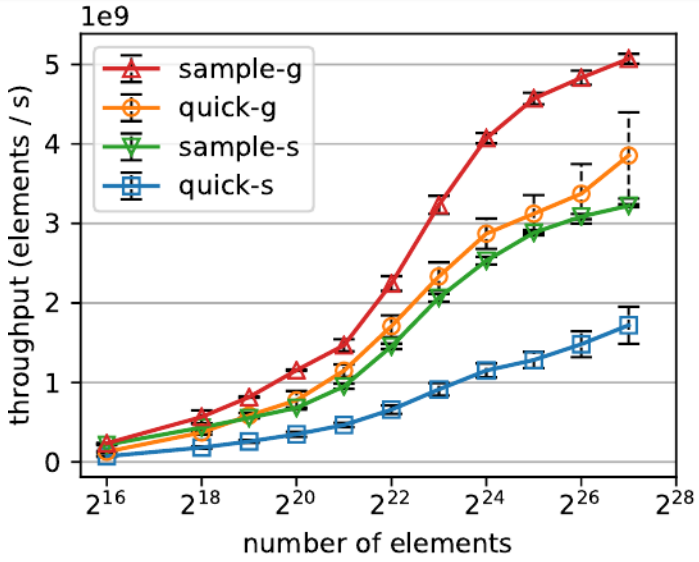
NVIDIA K40



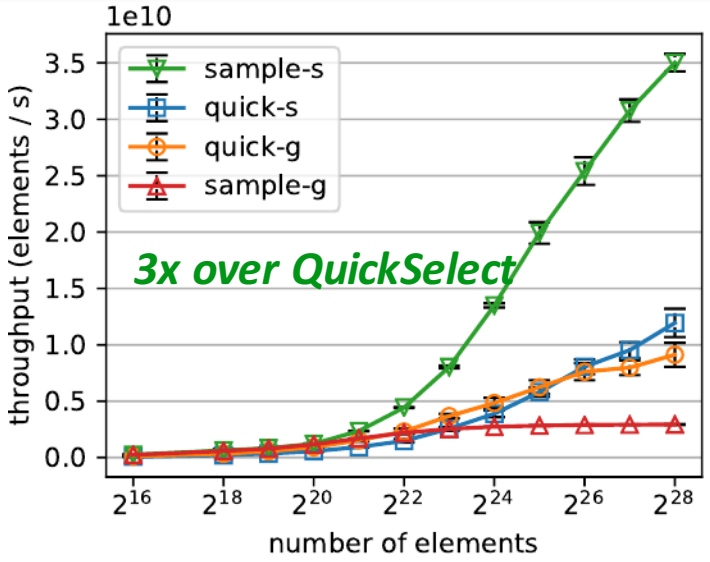
single precision

NVIDIA V100



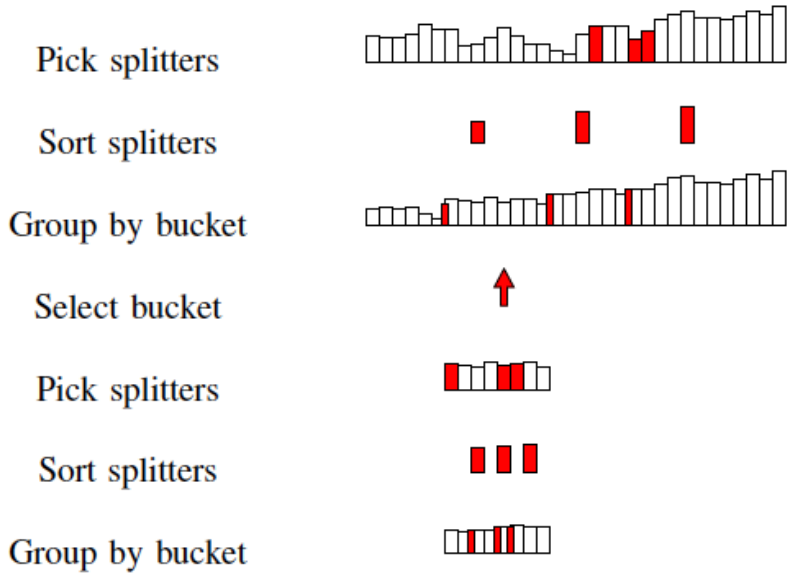


double precision



Approximate and Exact Selection on GPUs[1]

SampleSelect Algorithm



Approximate and Exact Selection on GPUs

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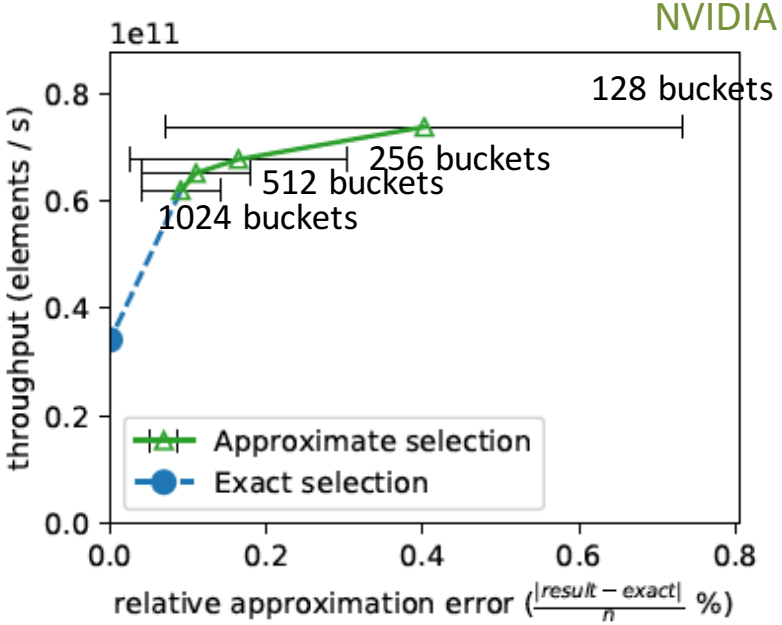
http://bit.ly/SampleSelectGPU

We do not descent to the lowest level of the recursion tree if we accept an approximate threshold.

- Accuracy depends on the ratio splitters vs. dataset size;
- Independent of value distribution (works on ranks, only);

NVIDIA V100 GPU



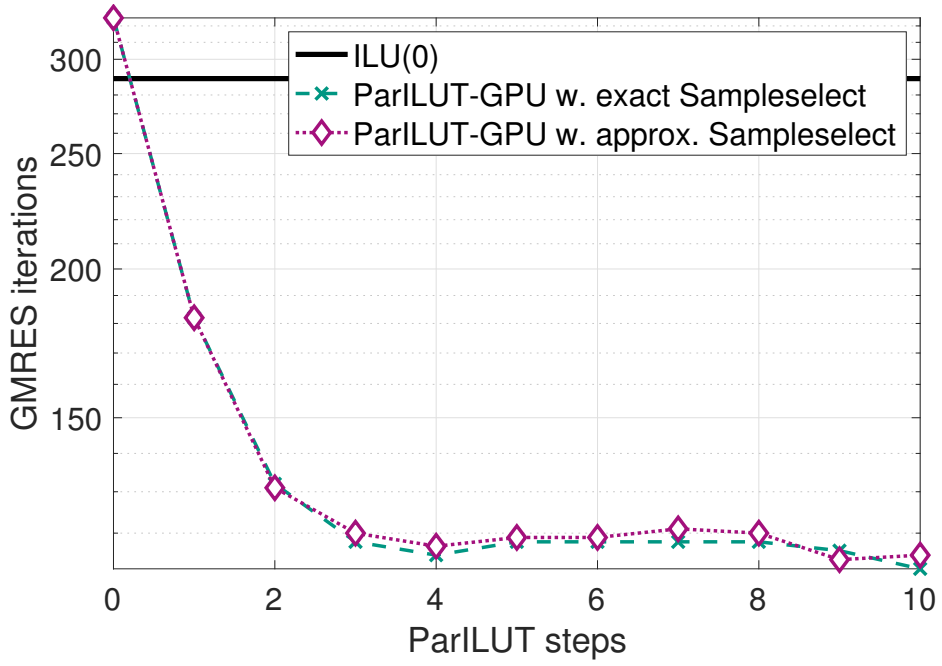
Approximate selection on 2^{28} uniformly distributed single precision values using 1 recursion level, only.

[1]Ribizel and Anzt. **"Approximate and Exact Selection on GPUs".** *In: ASHES workshop 2019.*

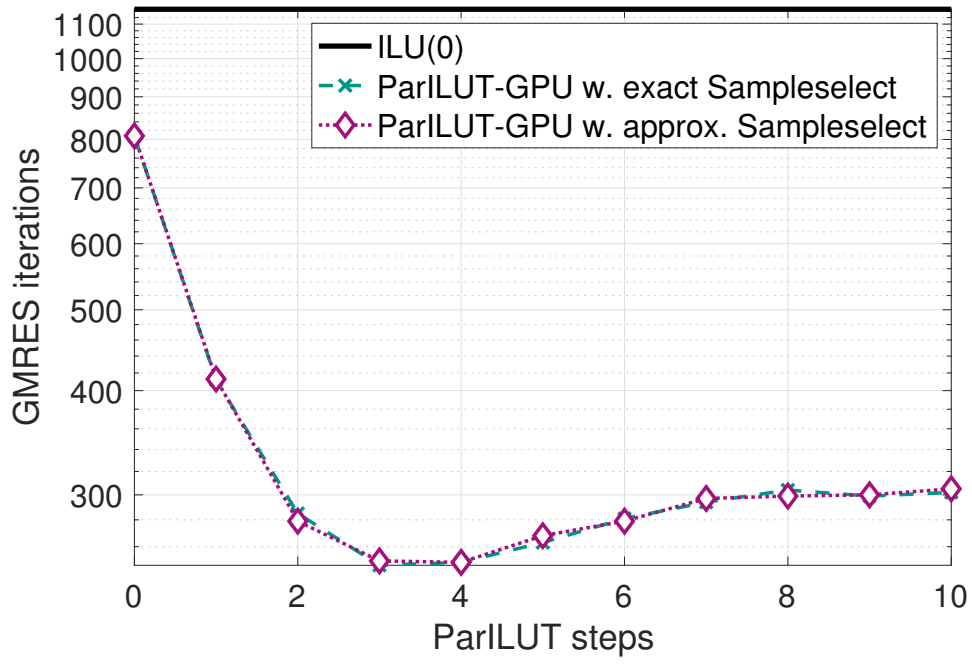
ParILUT - A Parallel Threshold ILU for GPUs

Impact of exact/approximate SampleSelect on ParILUT preconditioner quality

ANI5



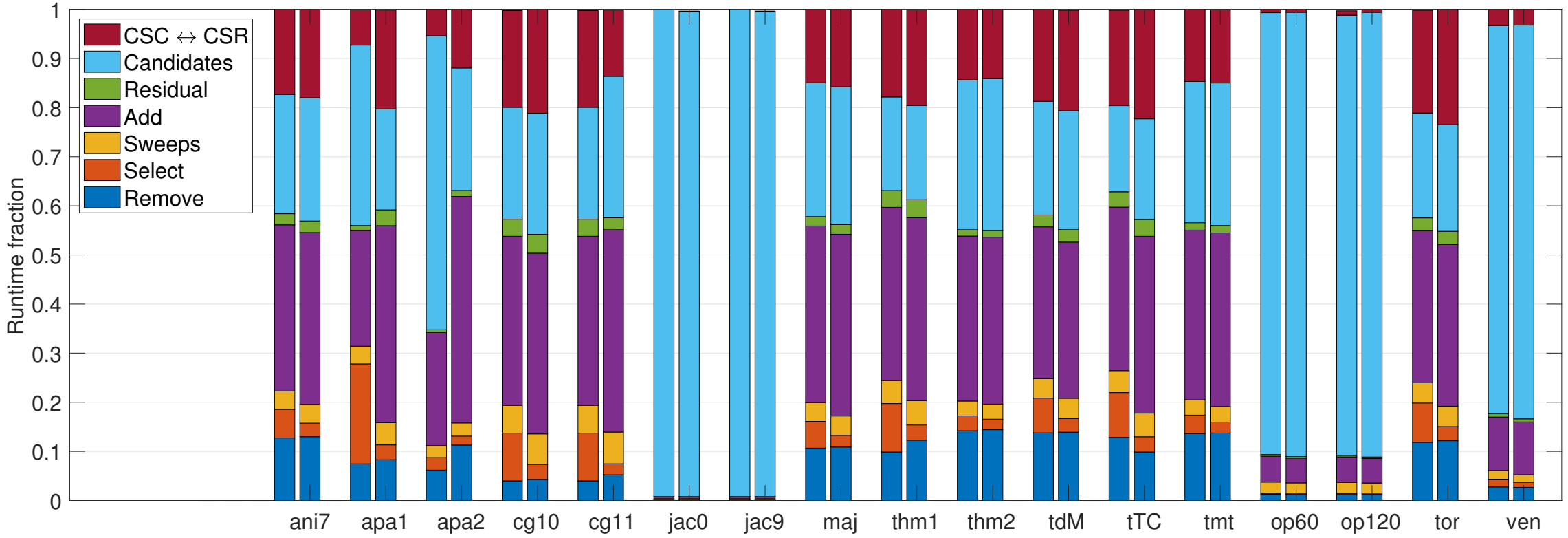
ANI6



ParILUT - A Parallel Threshold ILU for GPUs

Impact of exact/approximate SampleSelect on ParILUT runtime breakdown

NVIDIA V100 GPU



Anzt, Ribizel, Flegar, Chow, Dongarra. "**ParILUT - a parallel threshold ILU for GPUs**", IPDPS (2019)

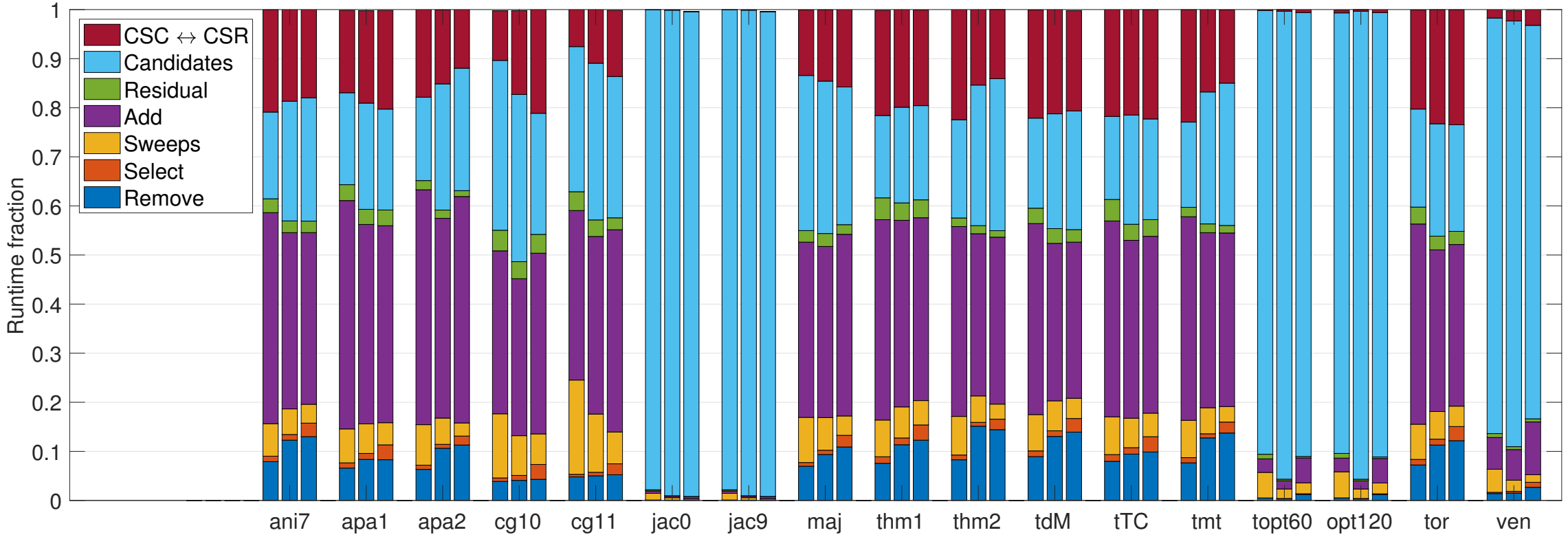
https://bit.ly/ParILUTGPU

Matrices taken from Suite Sparse Matrix Collection.

ParILUT - A Parallel Threshold ILU for GPUs

ParILUT performance across different GPU generations:

1st bar: NVIDIA K40
2nd bar: NVIDIA P100
3rd bar: NVIDIA V100



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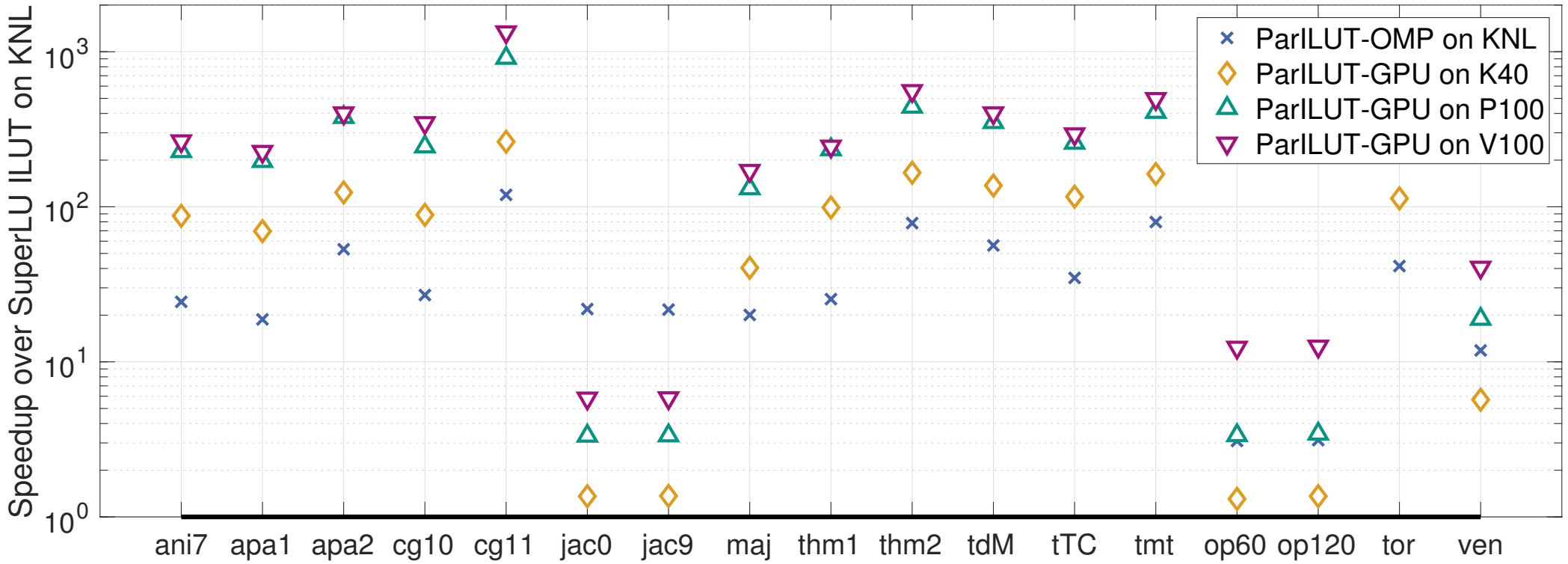
ParILUT Performance across architectures



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Next Steps …

- **Hybrid ParILUT** version utilizing GPU and CPU, overlapping communication & computation.
- **Asynchronous** version relaxing dependencies.
- Use a **different sparsity-pattern generator**:
  - Randomized?
  - Machine learning techniques?
- **Increasing fill-in** towards “full” factorization.
- **ParILUT routines available in MAGMA-sparse and Ginkgo.**

http://bit.ly/ParILUTGPU

Karlsruher Institut für Technologie

THE UNIVERSITY OF TENNESSEE KNOXVILLE

MAGMA

Ginkgo

Georgia Tech

The Exascale Computing Project

A Collaborative effort of the U.S. Department of Energy Office of Science And the National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY
Office of Science

U.S. Department of Energy
ASCR Award Number DE-SC0016513

HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

Helmholtz Impuls und Vernetzungsfond
VH-NG-1241

Test matrices

Matrix	Origin	SPD	Num. Rows	Nz	Nz/Row
ANI5	2D anisotropic diffusion	yes	12,561	86,227	6.86
ANI6	2D anisotropic diffusion	yes	50,721	349,603	6.89
ANI7	2D anisotropic diffusion	yes	203,841	1,407,811	6.91
APACHE1	Suite Sparse [10]	yes	80,800	542,184	6.71
APACHE2	Suite Sparse	yes	715,176	4,817,870	6.74
CAGE10	Suite Sparse	no	11,397	150,645	13.22
CAGE11	Suite Sparse	no	39,082	559,722	14.32
JACOBIANMAT0	Fun3D fluid flow [20]	no	90,708	5,047,017	55.64
JACOBIANMAT9	Fun3D fluid flow	no	90,708	5,047,042	55.64
MAJORBASIS	Suite Sparse	no	160,000	1,750,416	10.94
TOPOPT010	Geometry optimization [24]	yes	132,300	8,802,544	66.53
TOPOPT060	Geometry optimization	yes	132,300	7,824,817	59.14
TOPOPT120	Geometry optimization	yes	132,300	7,834,644	59.22
THERMAL1	Suite Sparse	yes	82,654	574,458	6.95
THERMAL2	Suite Sparse	yes	1,228,045	8,580,313	6.99
THERMOMECH_TC	Suite Sparse	yes	102,158	711,558	6.97
THERMOMECH_DM	Suite Sparse	yes	204,316	1,423,116	6.97
TMT_SYM	Suite Sparse	yes	726,713	5,080,961	6.99
TORSO2	Suite Sparse	no	115,967	1,033,473	8.91
VENKAT01	Suite Sparse	no	62,424	1,717,792	27.52

Convergence: GMRES iterations

Matrix	no prec.	ILU(0)	ILUT	ParILUT 0	1	2	3	4	5
ANI5	882	172	78	278	161	105	84	74	66
ANI6	1,751	391	127	547	315	211	168	143	131
ANI7	3,499	828	290	1,083	641	459	370	318	289
CAGE10	20	8	8	9	7	8	8	8	8
CAGE11	21	9	8	9	7	7	7	7	7
JACOBIANMAT0	315	40	34	63	36	33	33	33	33
JACOBIANMAT9	539	66	65	110	60	55	54	53	53
MAJORBASIS	95	15	9	26	12	11	11	11	11
TOPOPT010	2,399	565	303	835	492	375	348	340	339
TOPOPT060	2,852	666	397	963	584	445	417	412	410
TOPOPT120	2,765	668	396	959	584	445	416	408	408
TORSO2	46	10	7	18	8	6	7	7	7
VENKAT01	195	22	17	42	18	17	17	17	17

Convergence: CG iterations

Matrix	no prec.	IC(0)	ICT	ParICT 0	1	2	3	4	5
ANI5	951	226	–	297	184	136	108	93	86
ANI6	1,926	621	–	595	374	275	219	181	172
ANI7	3,895	1,469	–	1,199	753	559	455	405	377
APACHE1	3,727	368	331	1,480	933	517	321	323	323
APACHE2	4,574	1,150	785	1,890	1,197	799	766	760	754
THERMAL1	1,640	453	412	626	447	409	389	385	383
THERMAL2	6,253	1,729	1,604	2,372	1,674	1,503	1,457	1,472	1,433
THERMOMECH_DM	21	8	8	8	7	7	7	7	7
THERMOMECH_TC	21	8	7	8	7	7	7	7	7
TMT_SYM	5,481	1,453	1,185	1,963	1,234	1,071	1,012	992	1,004
TOPOPT010	2,613	692	331	845	551	402	342	316	313
TOPOPT060	3,123	871	–	988	749	693	1,116	–	–
TOPOPT120	3,062	886	–	991	837	784	2,185	–	–