9th JLESC Workshop
April 15th-17th, 2019 | Knoxville, TN

ParILUT - A New Parallel Threshold ILU

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Joint Laboratory for Extreme-Scale Computing

Motivation

We are looking for a factorization-based preconditioner such that $A \approx L \cdot U$.
is a good approximation with moderate nonzero count (e.g. $nnz(L+U) = nnz(A)$).

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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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Incomplete LU Factorization (ILU)

- Focused on restricting fill-in to a specific sparsity pattern $\mathcal{S}$.

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- For **ILU(0)**, $\mathcal{S}$ is the sparsity pattern of A.
  - 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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Rethink the overall strategy!

- Use a parallel iterative process to generate factors.

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

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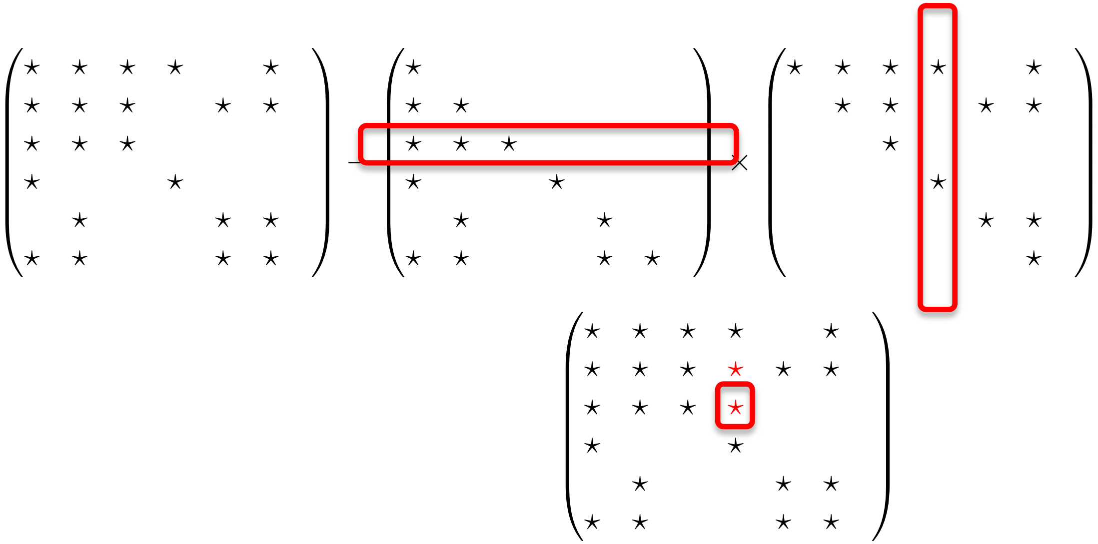

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- This is an optimization problem with $\color{red}{nnz(A - L \cdot U)}$ equations and $\color{blue}{nnz(L + U)}$ variables.

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- We may want to compute the values in L, U such that $R = A - L \cdot U = 0|_{\mathcal{S}}$, the approximation being exact in the locations included in $\mathcal{S}$, *but not outside!*

$nnz(L + U)$ equations
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- This is the underlying idea of Edmond Chow's parallel ILU algorithm[1]:

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

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

[1] Chow and Patel. **"Fine-grained Parallel Incomplete LU Factorization".** *In: SIAM J. on Sci. Comp. (2015).*

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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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- Comparing sparsity patterns extremely difficult.
- Maybe use the ILU residual as convergence check.

Compute ILU residual & check convergence.

Fixed-point sweep approximates incomplete factors.

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Compute ILU residual & check convergence.

- The sparsity pattern of A might be a good initial start for nonzero locations.

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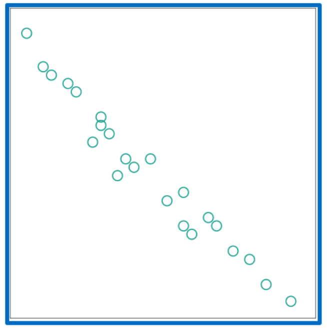
Identify locations with nonzero ILU residual.

Compute ILU residual & check convergence.



- The sparsity pattern of A might be a good initial start for nonzero locations.
- Then, the approximation will be exact for all locations $\mathcal{S}_0 = \mathcal{S}(L_0 + U_0)$ and nonzero in locations $\mathcal{S}_1 = (\mathcal{S}(A) \cup \mathcal{S}(L_0 \cdot U_0)) \setminus \mathcal{S}(L_0 + U_0)$[1].

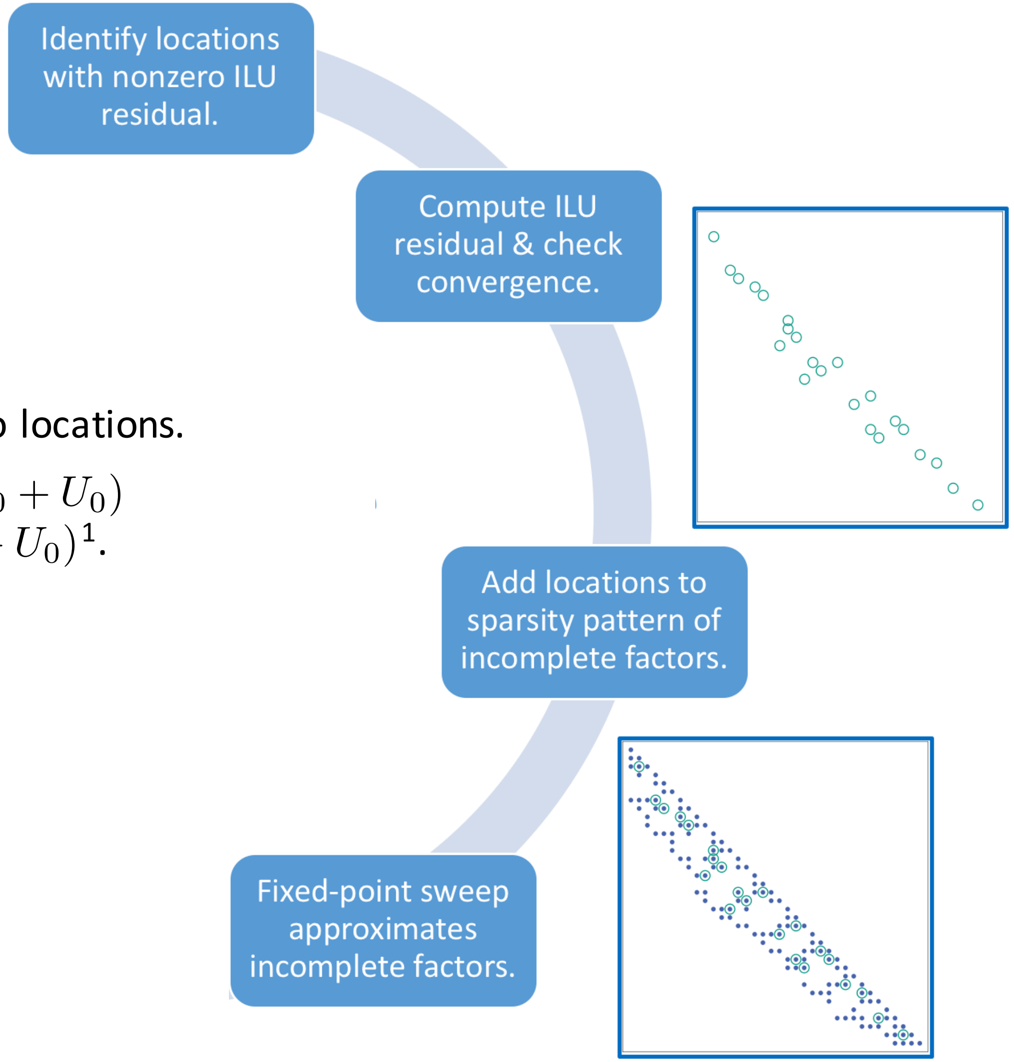
$$
\begin{pmatrix}
\star & \star & \star & \star & & \star \\
\star & \star & \star & & \star & \star \\
\star & \star & \star & & & \\
\star & & & \star & & \\
& \star & & & \star & \star \\
\star & \star & & & \star & \star
\end{pmatrix}
-
\begin{pmatrix}
\star & & & & & \\
{\color{blue}\star} & \star & & & & \\
{\color{blue}\star} & {\color{blue}\star} & \star & & & \\
{\color{blue}\star} & & & \star & & \\
& {\color{blue}\star} & & & \star & \\
{\color{blue}\star} & {\color{blue}\star} & & & {\color{blue}\star} & \star
\end{pmatrix}
\times
\begin{pmatrix}
{\color{blue}\star} & {\color{blue}\star} & {\color{blue}\star} & {\color{blue}\star} & & {\color{blue}\star} \\
& {\color{blue}\star} & {\color{blue}\star} & & {\color{blue}\star} & {\color{blue}\star} \\
& & {\color{blue}\star} & & & \\
& & & {\color{blue}\star} & & \\
& & & & {\color{blue}\star} & {\color{blue}\star} \\
& & & & & {\color{blue}\star}
\end{pmatrix}
=
\begin{pmatrix}
\star & \star & \star & \star & & \star \\
\star & \star & \star & {\color{red}\star} & \star & \star \\
\star & \star & \star & {\color{red}\star} & {\color{red}\star} & {\color{red}\star} \\
\star & {\color{red}\star} & {\color{red}\star} & \star & & {\color{red}\star} \\
& \star & {\color{red}\star} & & \star & \star \\
\star & \star & {\color{red}\star} & {\color{red}\star} & \star & \star
\end{pmatrix}
$$

Fixed-point sweep approximates incomplete factors.

[1]Saad. **"Iterative Methods for Sparse Linear Systems, 2nd Edition".** *(2003).*

Considerations

1. *Select a set of nonzero locations.*
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 stagnates.*



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- Adding all these locations (level-fill!) might be good idea…

$$\begin{pmatrix} \star & \star & \star & \star & & \star \\ \star & \star & \star & & \star & \star \\ \star & \star & \star & & & \\ \star & & & \star & & \\ & \star & & & \star & \star \\ \star & \star & & & \star & \star \end{pmatrix} - \begin{pmatrix} \star & & & & & \\ \star & \star & & & & \\ \star & \star & \star & & & \\ \star & \star & \star & \star & & \\ & \star & \star & & \star & \\ \star & \star & \star & \star & \star & \star \end{pmatrix} \times \begin{pmatrix} \star & \star & \star & \star & & \star \\ & \star & \star & \star & \star & \star \\ & & \star & \star & \star & \star \\ & & & \star & & \star \\ & & & & \star & \star \\ & & & & & \star \end{pmatrix}$$

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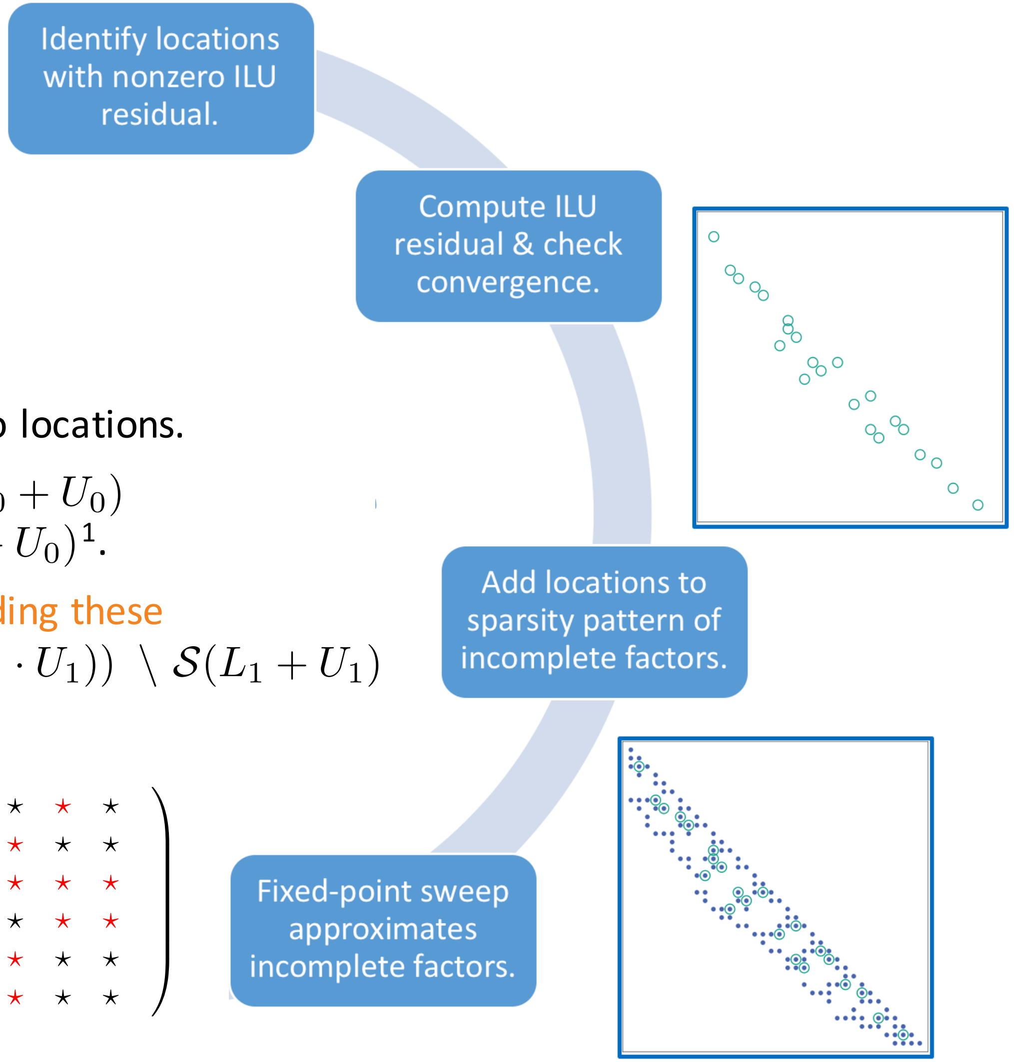

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- Adding all these locations (level-fill!) might be good idea, but adding these will again generate new nonzero residuals $\mathcal{S}_2 = (\mathcal{S}(A) \cup \mathcal{S}(L_1 \cdot U_1)) \setminus \mathcal{S}(L_1 + U_1)$

$$\begin{pmatrix} \star & \star & \star & \star & & \star \\ \star & \star & \star & & \star & \star \\ \star & \star & \star & & & \\ \star & & & \star & & \\ & \star & & & \star & \star \\ \star & \star & & & \star & \star \end{pmatrix} - \begin{pmatrix} \star & & & & & \\ \star & \star & & & & \\ \star & \star & \star & & & \\ \star & \star & \star & \star & & \\ & \star & \star & & \star & \\ \star & \star & \star & \star & \star & \star \end{pmatrix} \times \begin{pmatrix} \star & \star & \star & \star & & \star \\ & \star & \star & \star & \star & \star \\ & & \star & \star & \star & \star \\ & & & \star & & \star \\ & & & & \star & \star \\ & & & & & \star \end{pmatrix} = \begin{pmatrix} \star & \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star & \star \end{pmatrix}$$

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Considerations

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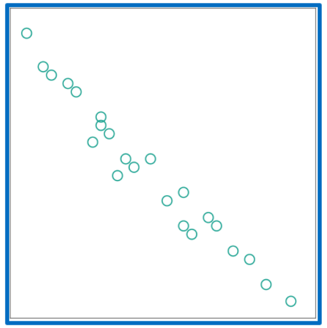
4. *Repeat until the preconditioner quality stagnates.*

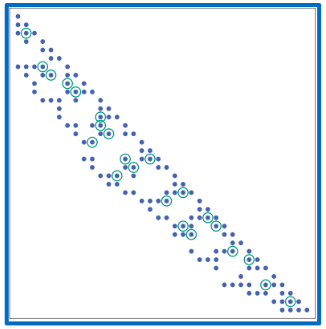
- At some point we should remove some locations again, e.g. the smallest elements, and start over looking at locations $R = A - L_k \cdot U_k$ …

Identify locations with nonzero ILU residual.

Compute ILU residual & check convergence.



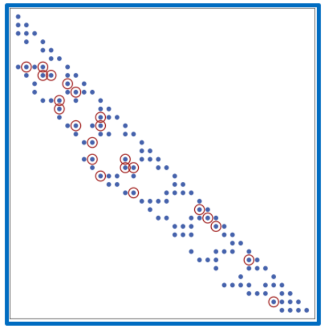
Add locations to sparsity pattern of incomplete factors.



Fixed-point sweep approximates incomplete factors.

Select a threshold separating smallest elements.

Remove smallest elements from incomplete factors.



Considerations

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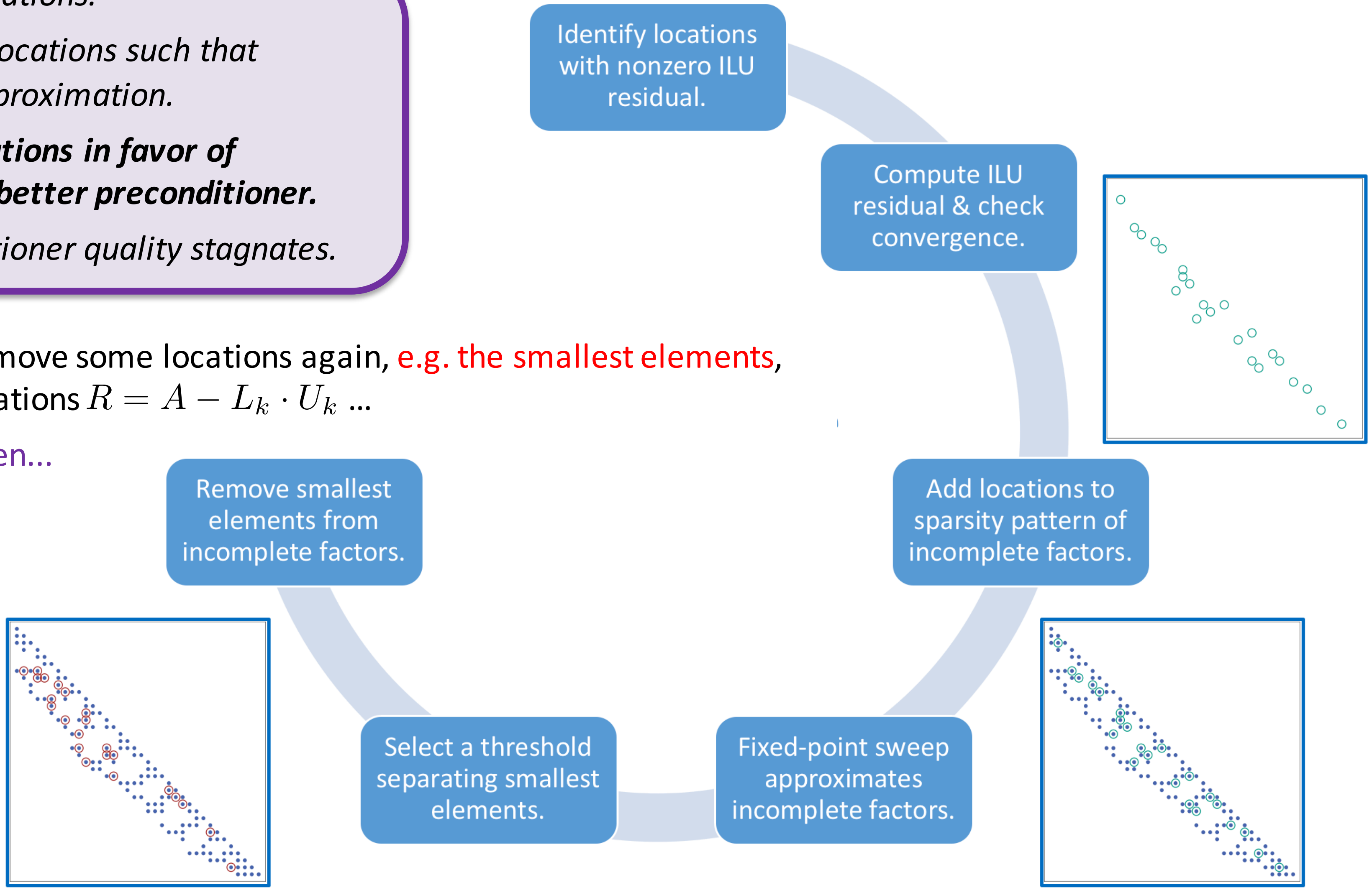
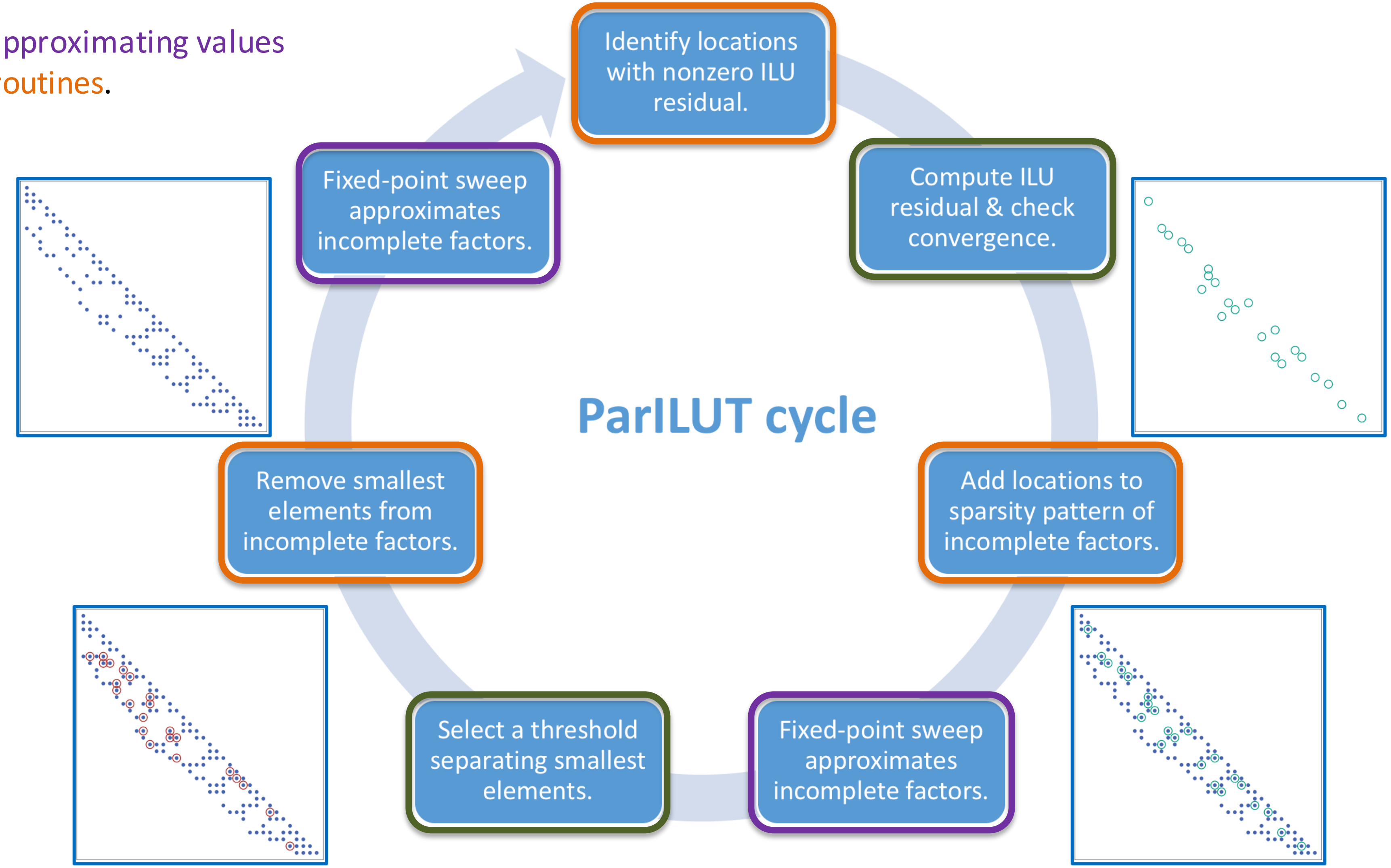
4. *Repeat until the preconditioner quality stagnates.*

- At some point we should remove some locations again, e.g. the smallest elements, and start over looking at locations $R = A - L_k \cdot U_k$ ...
- We need another sweep, then...



ParILUT

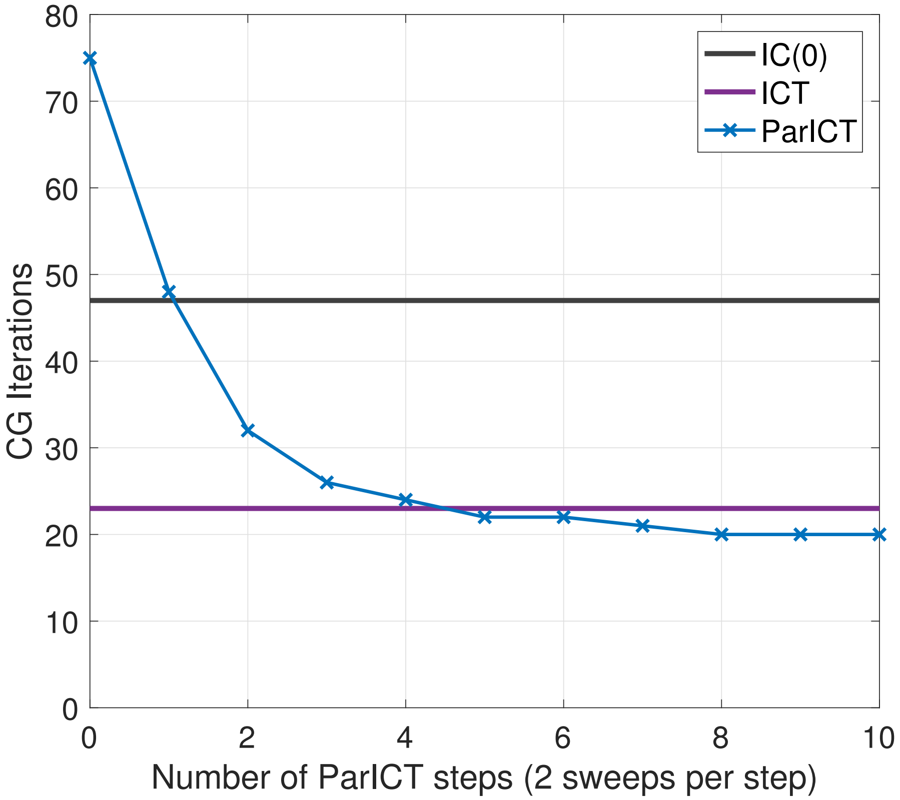
Interleaving fixed-point sweeps approximating values with pattern-changing symbolic routines.



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

ParILUT quality

Anisotropic fluid flow problem
n: 741, nz: 4,951



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

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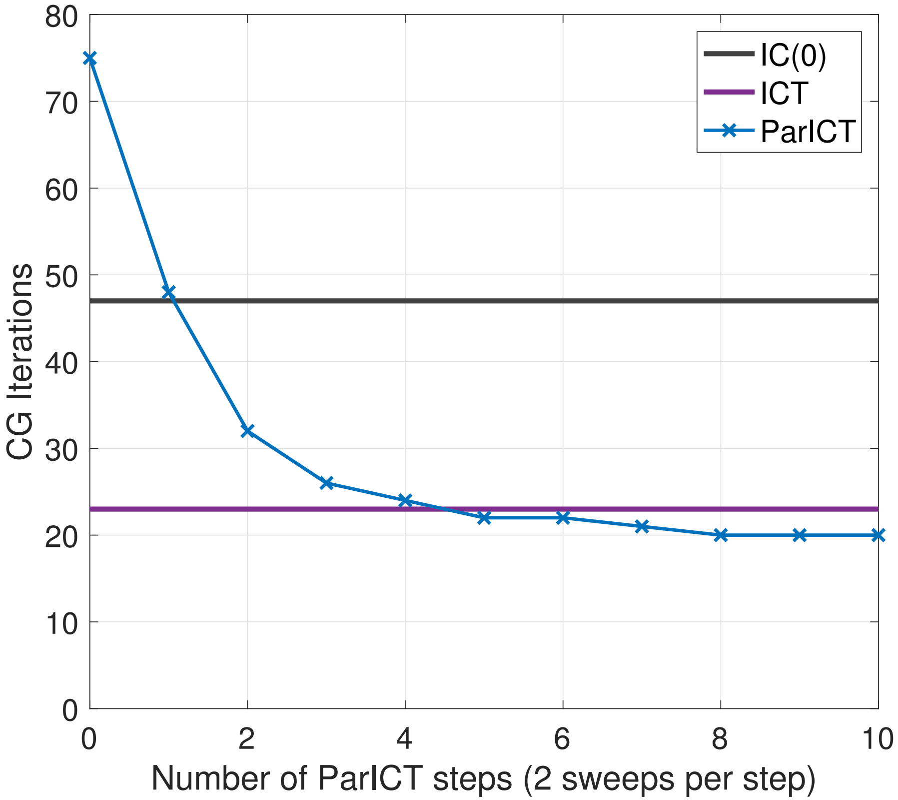

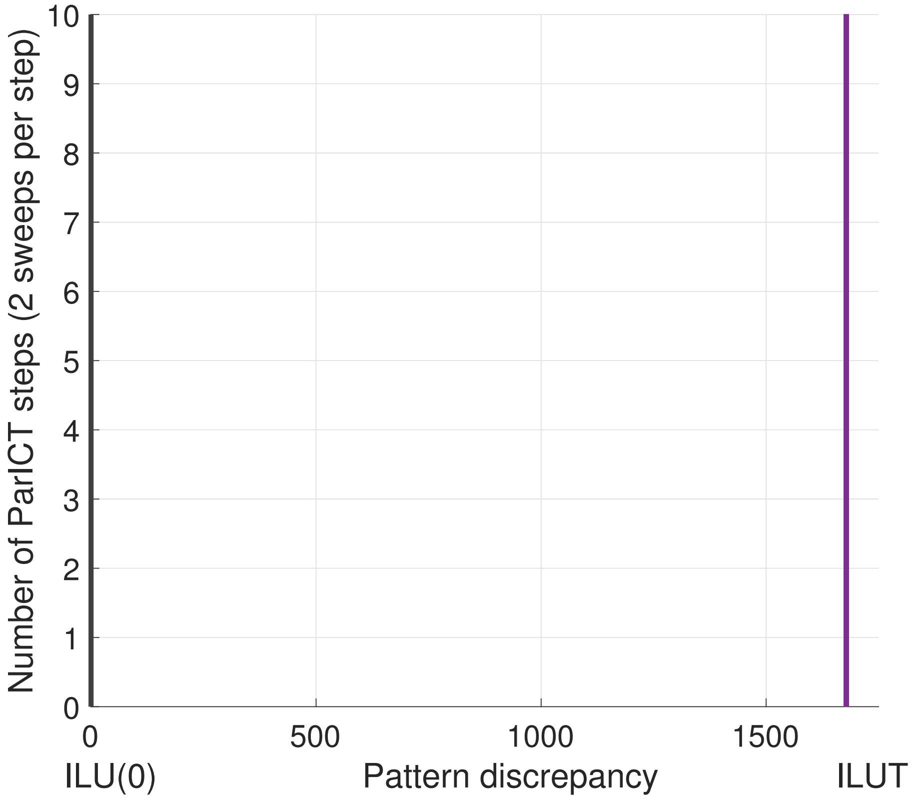

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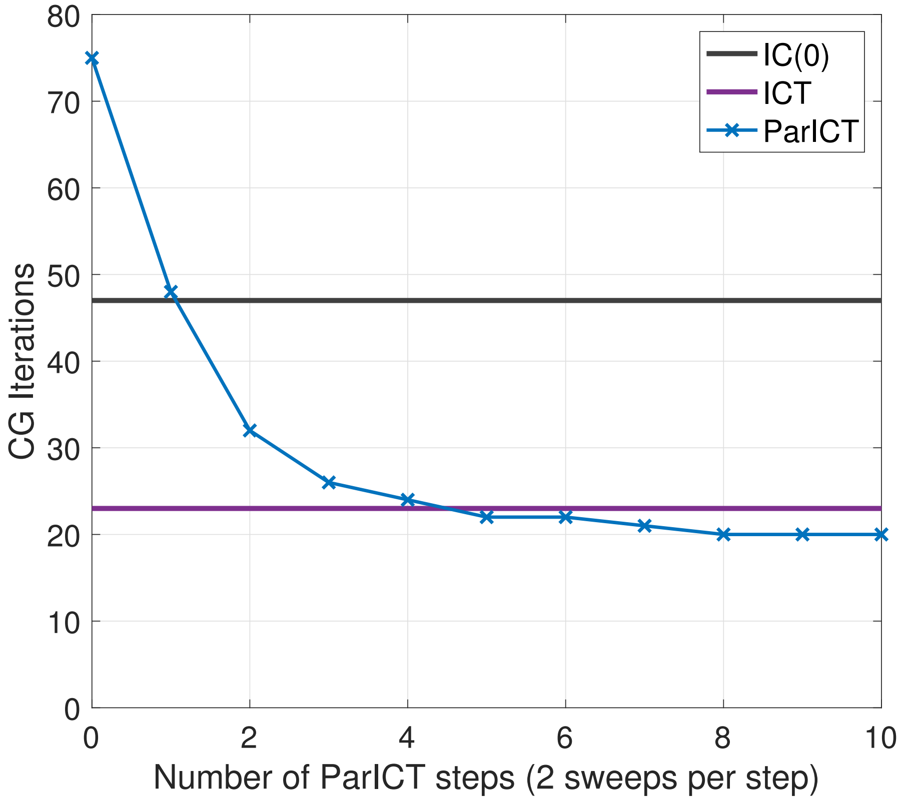

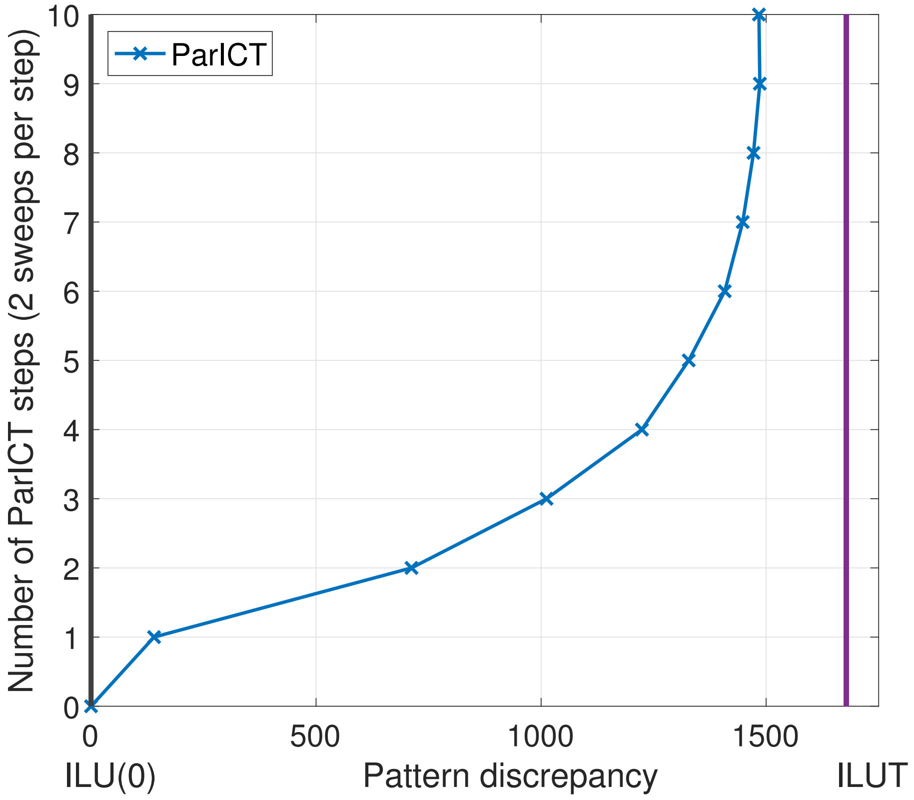

- Top-level solver iterations as quality metric.
- Few sweeps give a "better" preconditioner than ILU(0).
- Better than ILUT?

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

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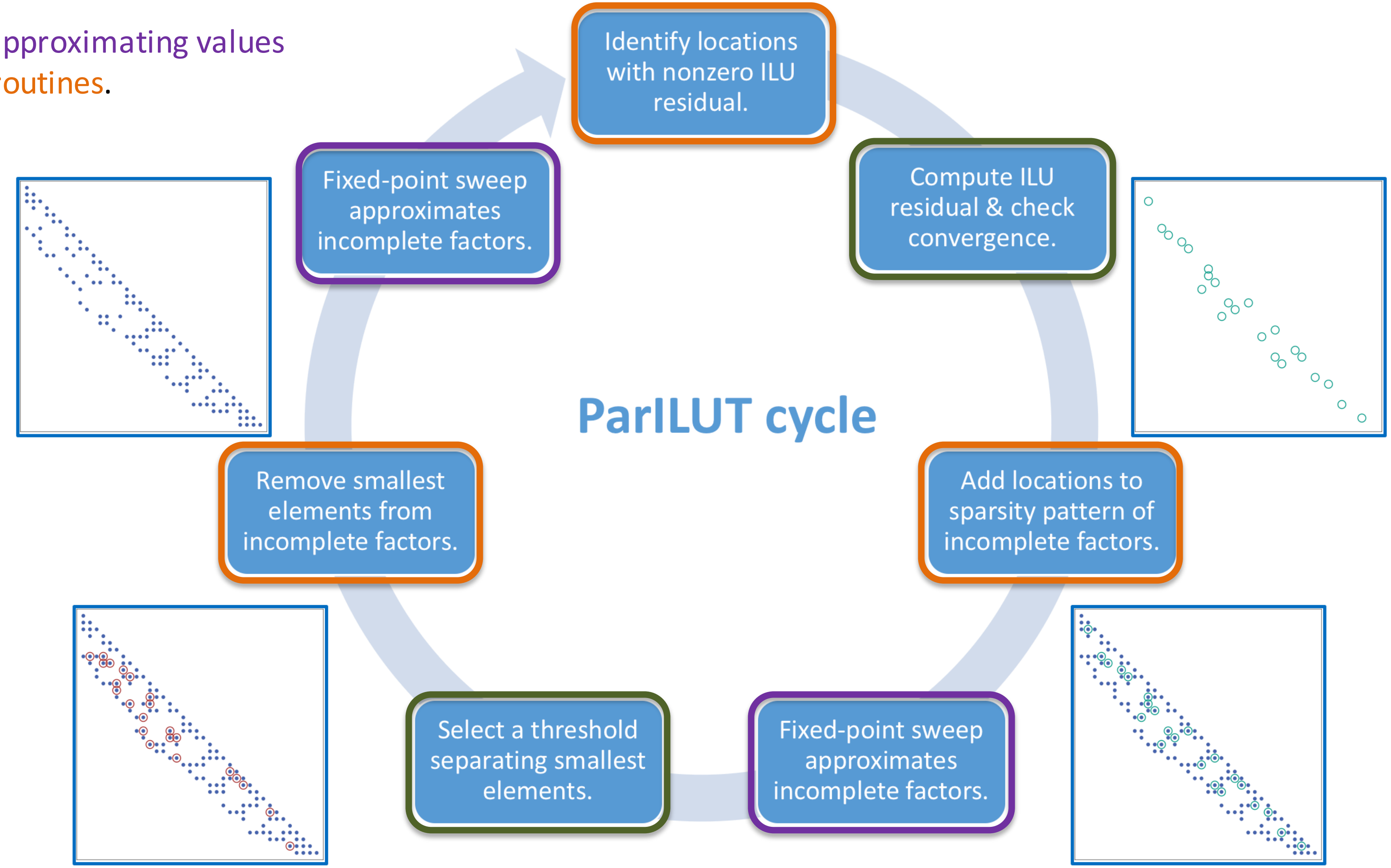
ParILUT

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



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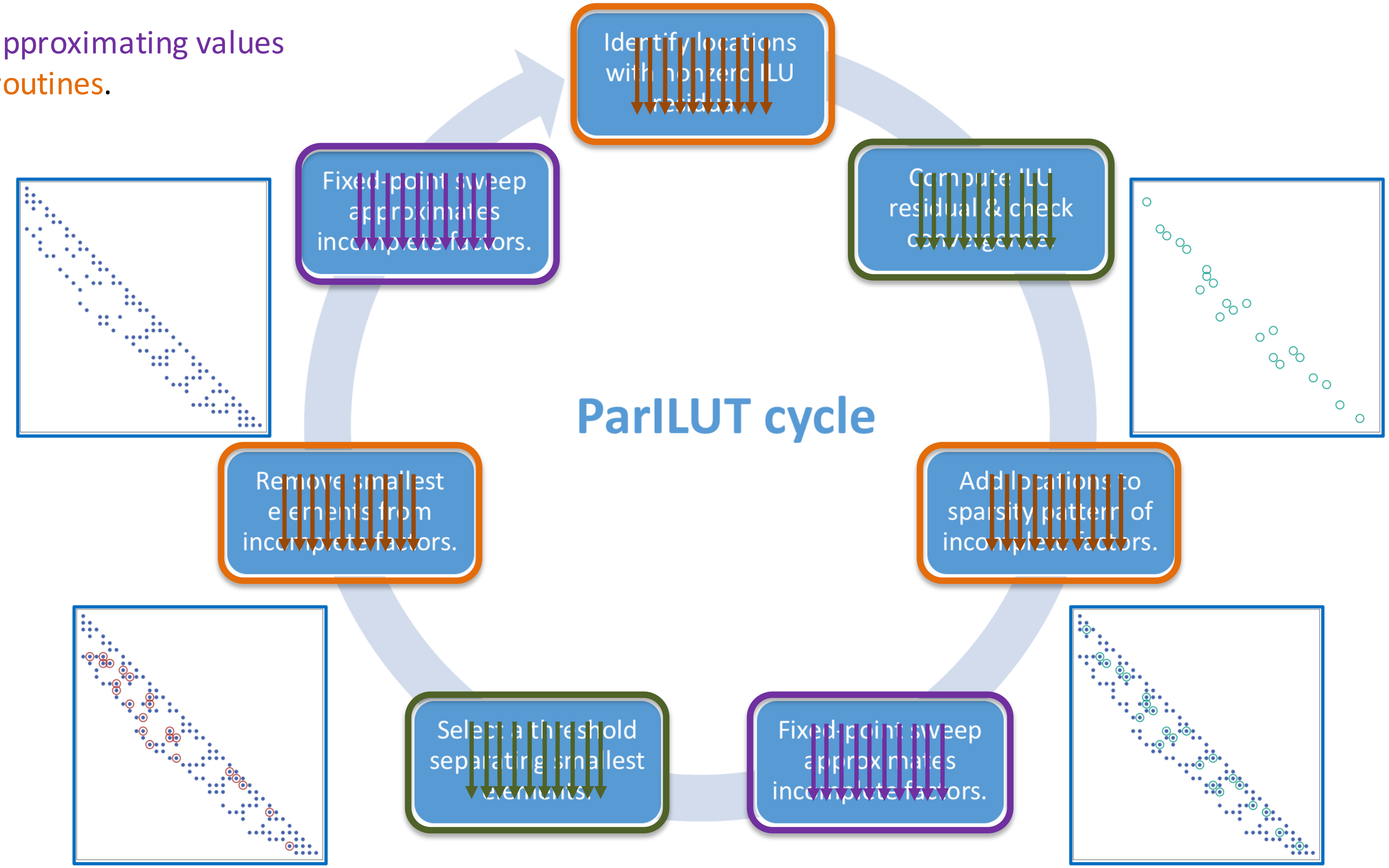
ParILUT – a parallel threshold ILU

Parallelism inside the building blocks.

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



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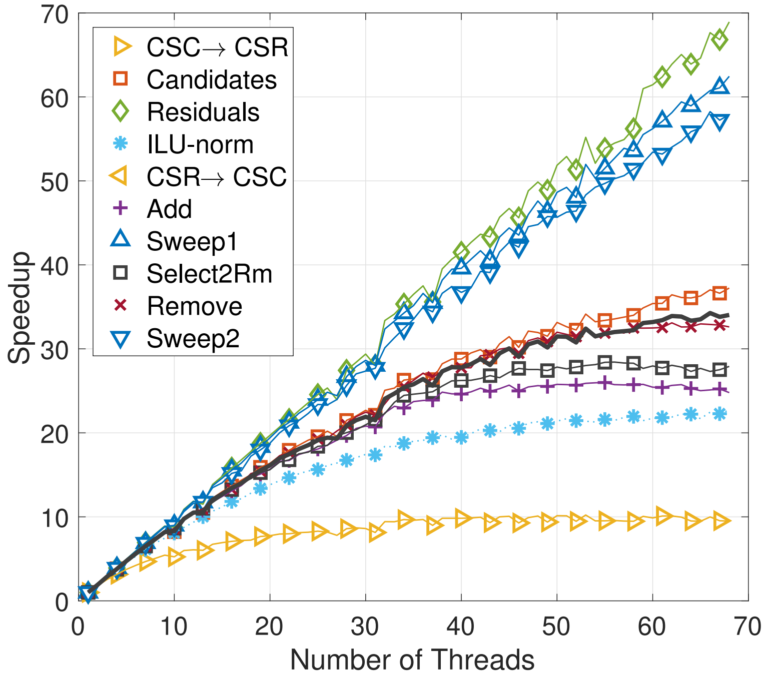
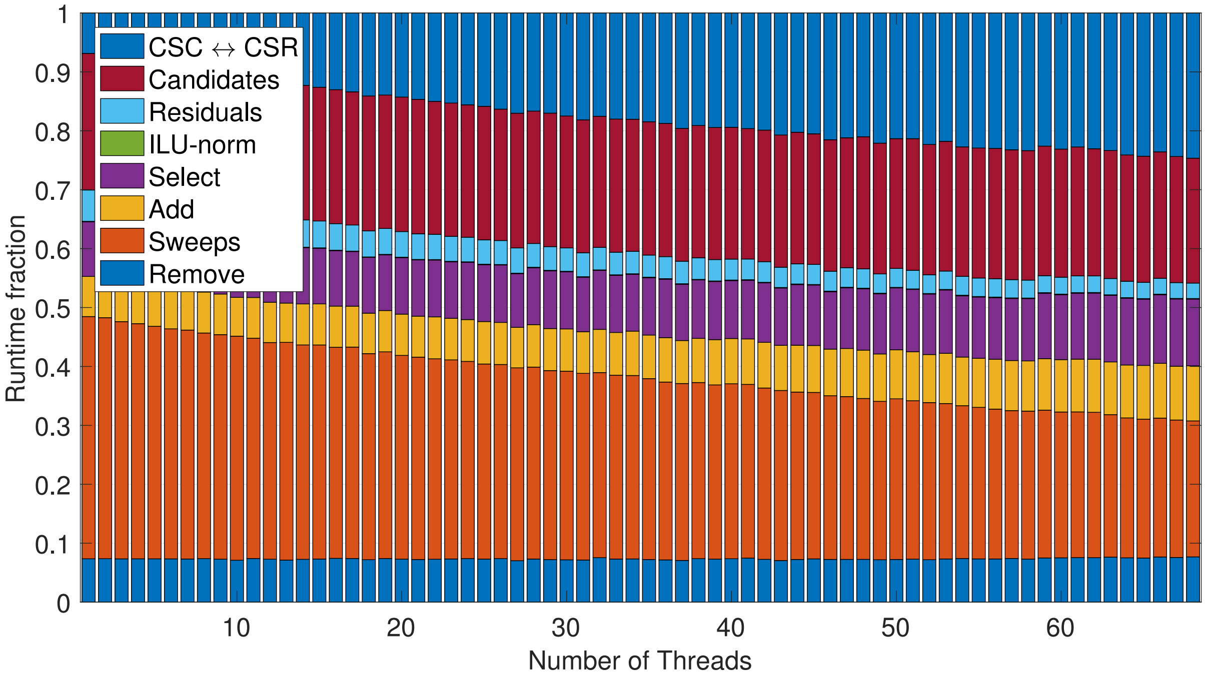
Scalability

Intel Xeon Phi 7250 "Knights Landing"
68 cores @1.40 GHz,
16GB MCDRAM @490 GB/s

`thermal2` matrix from SuiteSparse, RCM ordering, 8 el/row.





- Building blocks scale with 15% - 100% parallel efficiency.
- Transposition and sort are the bottlenecks.
- Overall speedup ~35x when using 68 KNL cores.

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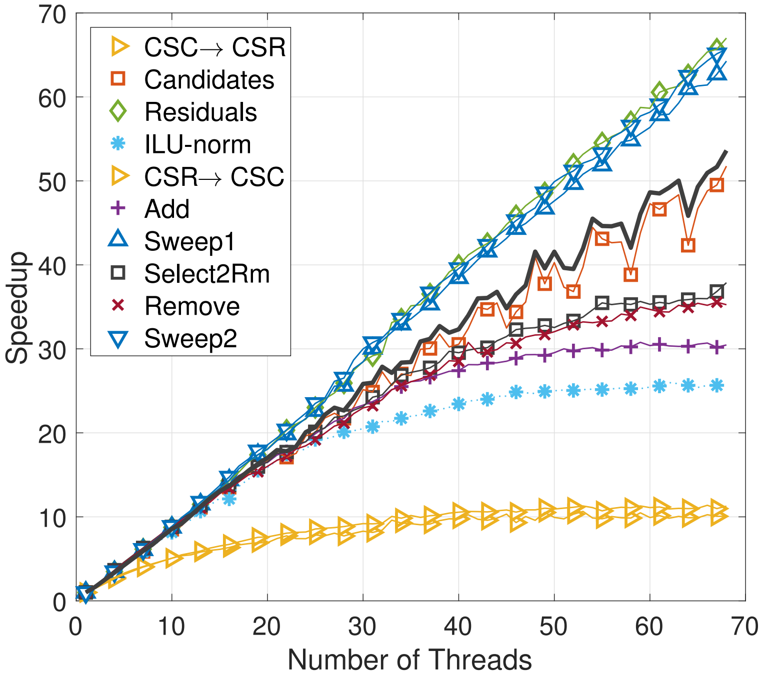
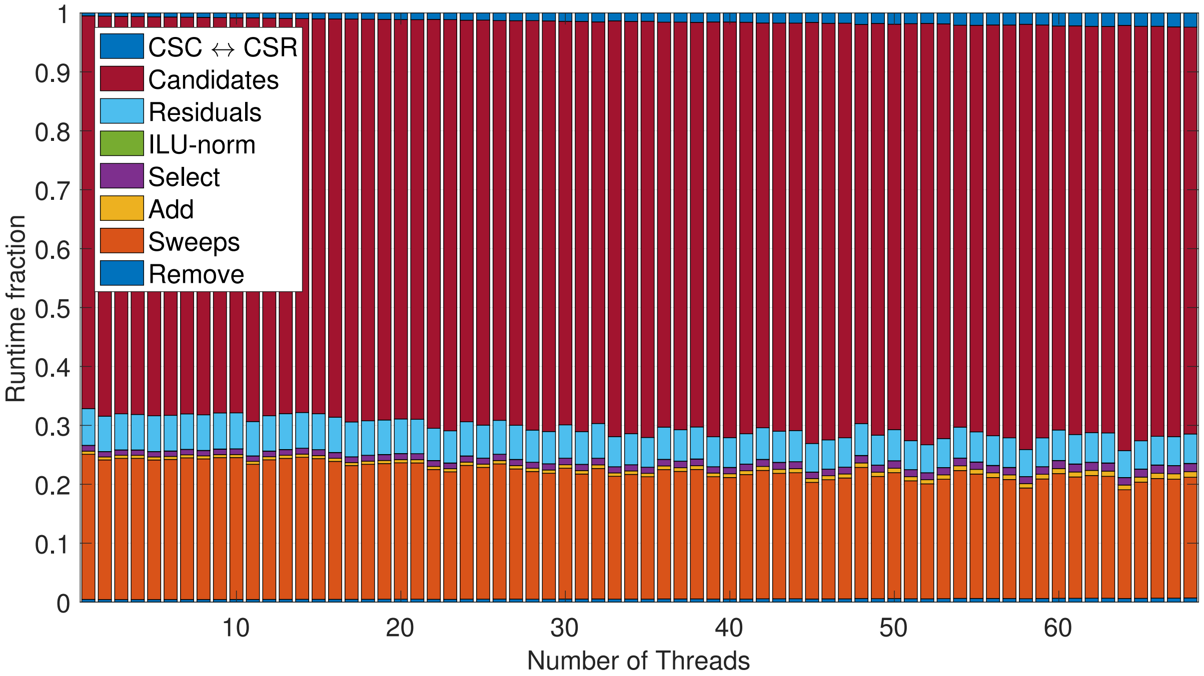
`topopt120` matrix from topology optimization, 67 el/row.





- Building blocks scale with 15% - 100% parallel efficiency.
- Dominated by candidate search.
- Overall speedup ~52x when using 68 KNL cores.

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Performance

Intel Xeon Phi 7250 "Knights Landing"
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Runtime of 5 ParILUT / ParICT steps and speedup over SuperLU ILUT*.

Matrix	Origin	Rows	Nonzeros	Ratio		SuperLU	ParILUT		ParICT	
ani7	2D Anisotropic Diffusion	203,841	1,407,811	6.91		10.48 s	0.45 s	23.34	0.30 s	35.16
apache2	Suite Sparse Matrix Collect.	715,176	4,817,870	6.74		62.27 s	1.24 s	50.22	0.65 s	95.37
cage11	Suite Sparse Matrix Collect.	39,082	559,722	14.32		60.89 s	0.54 s	112.56	--	
jacobianMat9	Fun3D Fluid Flow Problem	90,708	5,047,042	55.64		153.84 s	7.26 s	21.19	--	
thermal2	Thermal Problem (Suite Sp.)	1,228,045	8,580,313	6.99		91.83 s	1.23 s	74.66	0.68 s	134.25
tmt_sym	Suite Sparse Matrix Collect.	726,713	5,080,961	6.97		53.42 s	0.70 s	76.21	0.41 s	131.25
topopt120	Geometry Optimization	132,300	8,802,544	66.53		44.22 s	14.40 s	3.07	8.24 s	5.37
torso2	Suite Sparse Matrix Collect.	115,967	1,033,473	8.91		10.78 s	0.27 s	39.92	--	
venkat01	Suite Sparse Matrix Collect.	62,424	1,717,792	27.52		8.53 s	0.74 s	11.54	--	

We thank Sherry Li and Meiyue Shao for technical help in generating the performance numbers.

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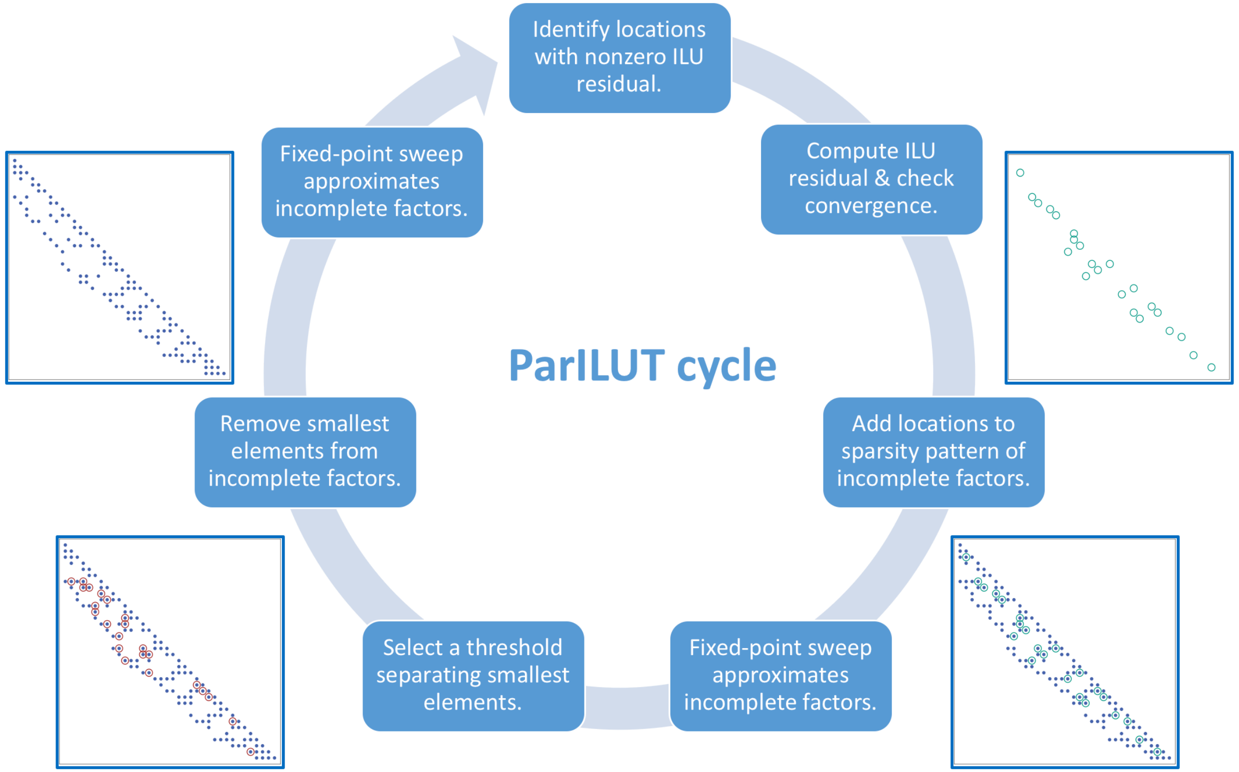
How about GPUs?

ParILUT - A Parallel Threshold ILU for GPUs

Hartwig Anzt*†, Tobias Ribizel*, Goran Flegar‡, Edmond Chow§, Jack Dongarra†¶‖
*Steinbuch Centre for Computing, Karlsruhe Institute of Technology, Germany
†Innovative Computing Lab (ICL), University of Tennessee, Knoxville, USA
‡Departamento de Ingeniería y Ciencia de Computadores, Universidad Jaume I Castellón, Spain
§School of Computational Science and Engineering, Georgia Institute of Technology, USA
¶University of Manchester, Manchester, UK
‖Oak Ridge National Lab (ORNL), Oak Ridge, USA
hartwig.anzt@kit.edu, tobias.ribizel@student.kit.edu, flegar@uji.es, echow@cc.gatech.edu, dongarra@icl.utk.edu

Accepted for IPDPS 2019



How about GPUs?

- Fine-grained parallelism
- High bandwidth for coalescent reads
- No deep cache hierarchy
- We need to oversubscribe cores for hiding latency

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Accepted for IPDPS 2019

Part of the ParILUT algorithm requires selecting the smallest k values for removal.

Selection and Sorting algorithms very inefficient on GPUs…

How about GPUs?

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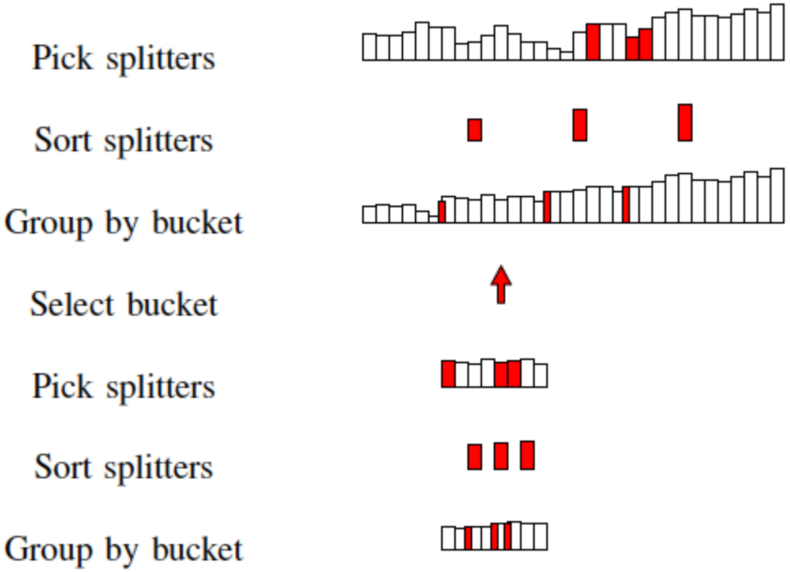
Accepted for IPDPS 2019

Part of the ParILUT algorithm requires selecting the smallest k values for removal.

SampleSelect:



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

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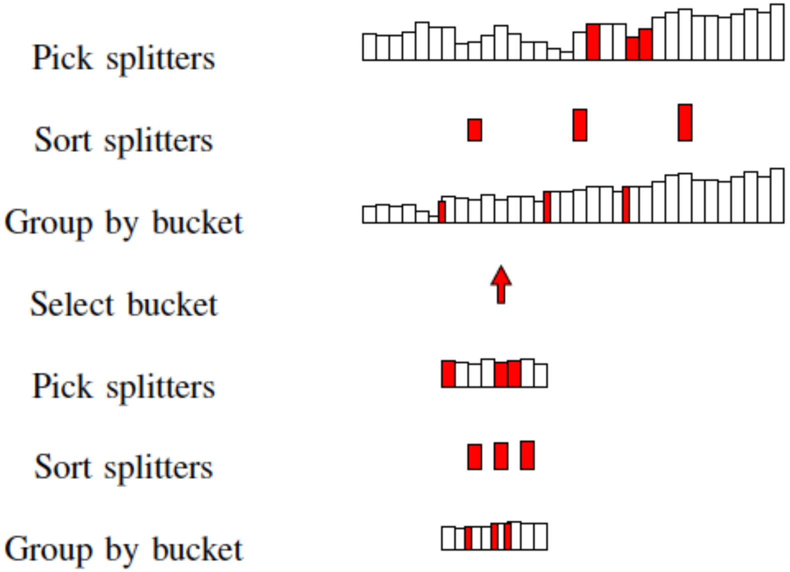

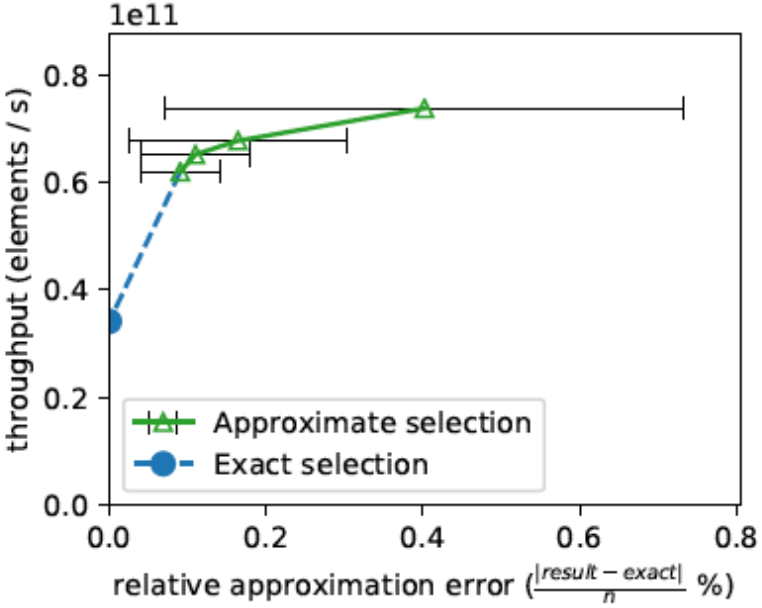

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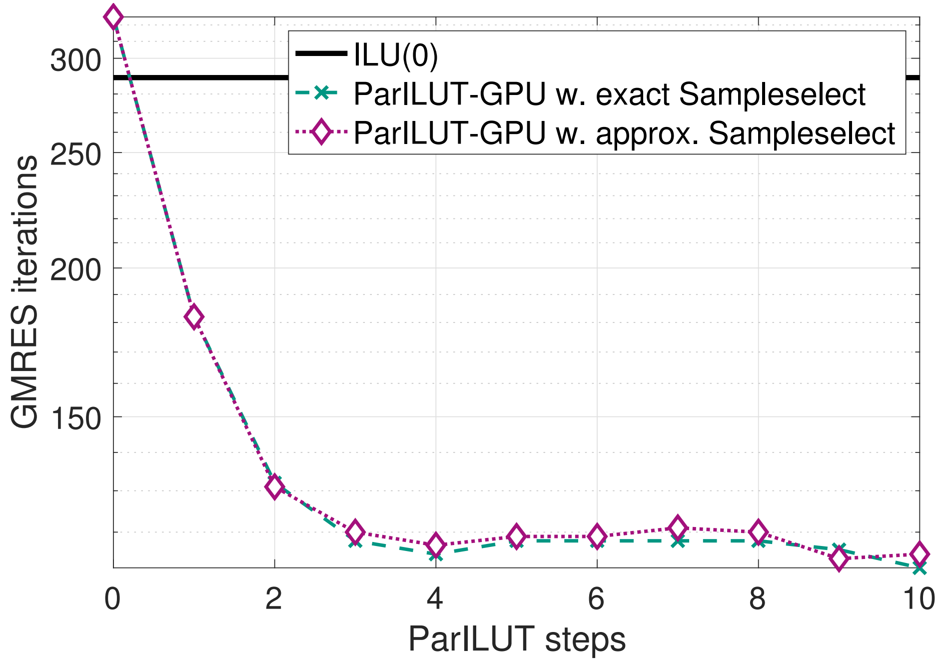
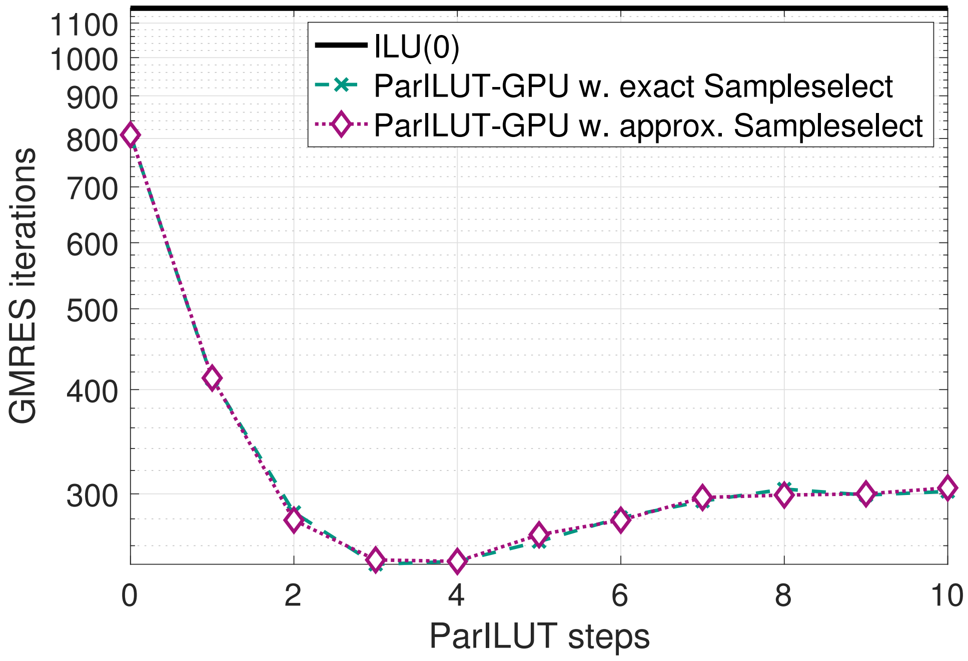
ParILUT - A Parallel Threshold ILU for GPUs

Impact of exact/approximate SampleSelect on ParILUT preconditioner quality

ANI5



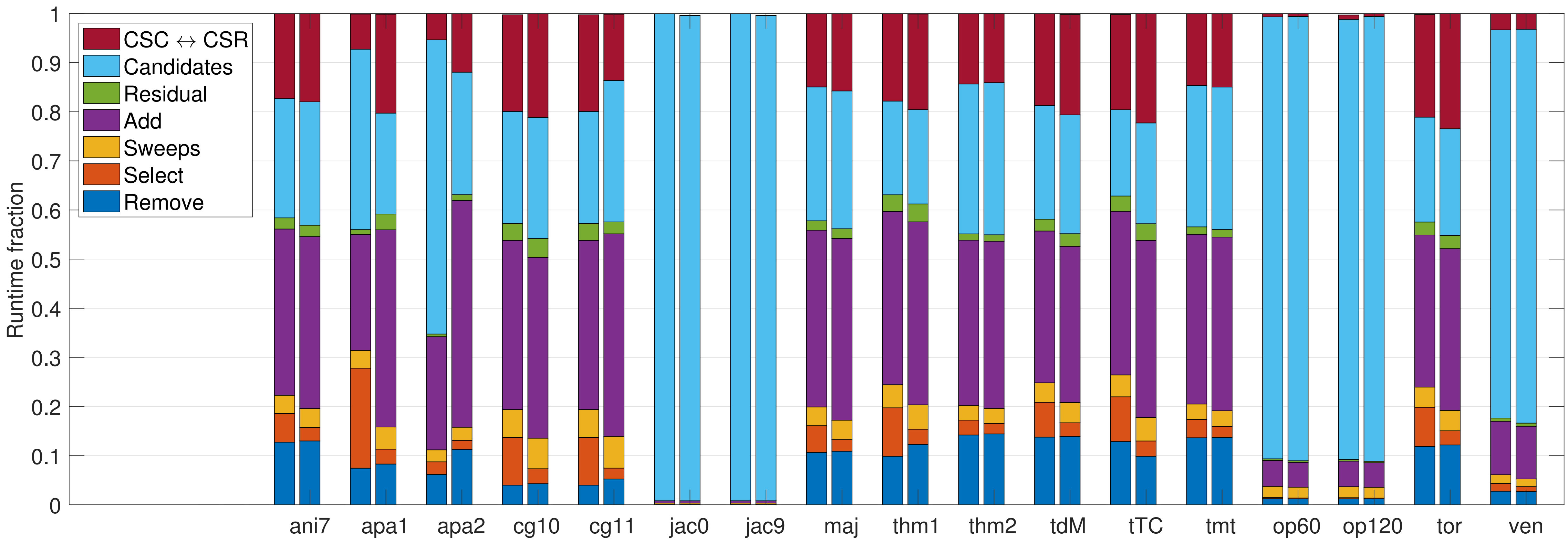
ANI6



[1]Anzt et al. **"ParILUT – A parallel threshold ILU for GPUs".** *In: IPDPS 2019, accepted.*

ParILUT - A Parallel Threshold ILU for GPUs

Impact of exact/approximate SampleSelect on ParILUT runtime breakdown



Matrices taken from Suite Sparse Matrix Collection.

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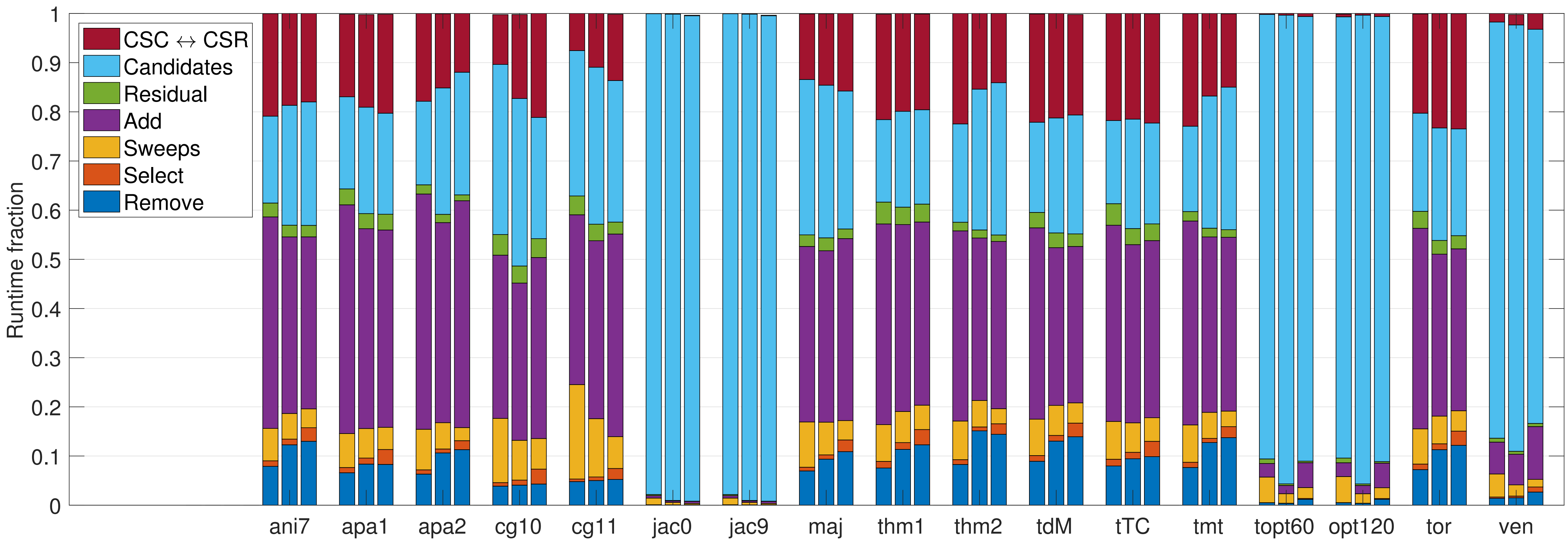
ParILUT - A Parallel Threshold ILU for GPUs

ParILUT performance across different GPU generations: 1st bar: NVIDIA K40
2nd bar: NVIDIA P100
3rd bar: NVIDIA V100



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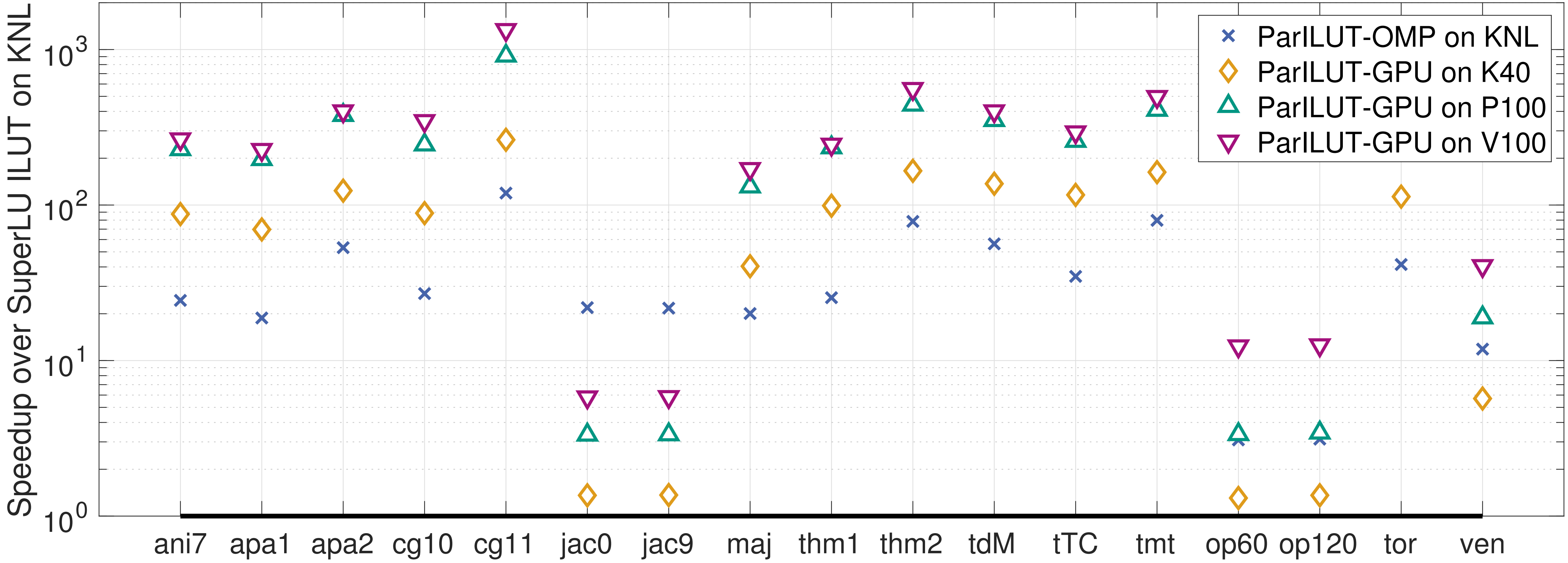
ParILUT Performance across architectures



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Is this a future-oriented algorithm?

- **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 – they will be in Ginkgo.

Karlsruher Institut für Technologie

The University of Tennessee Knoxville

Georgia Tech

MAGMA

Ginkgo

This research was sponsored by:

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

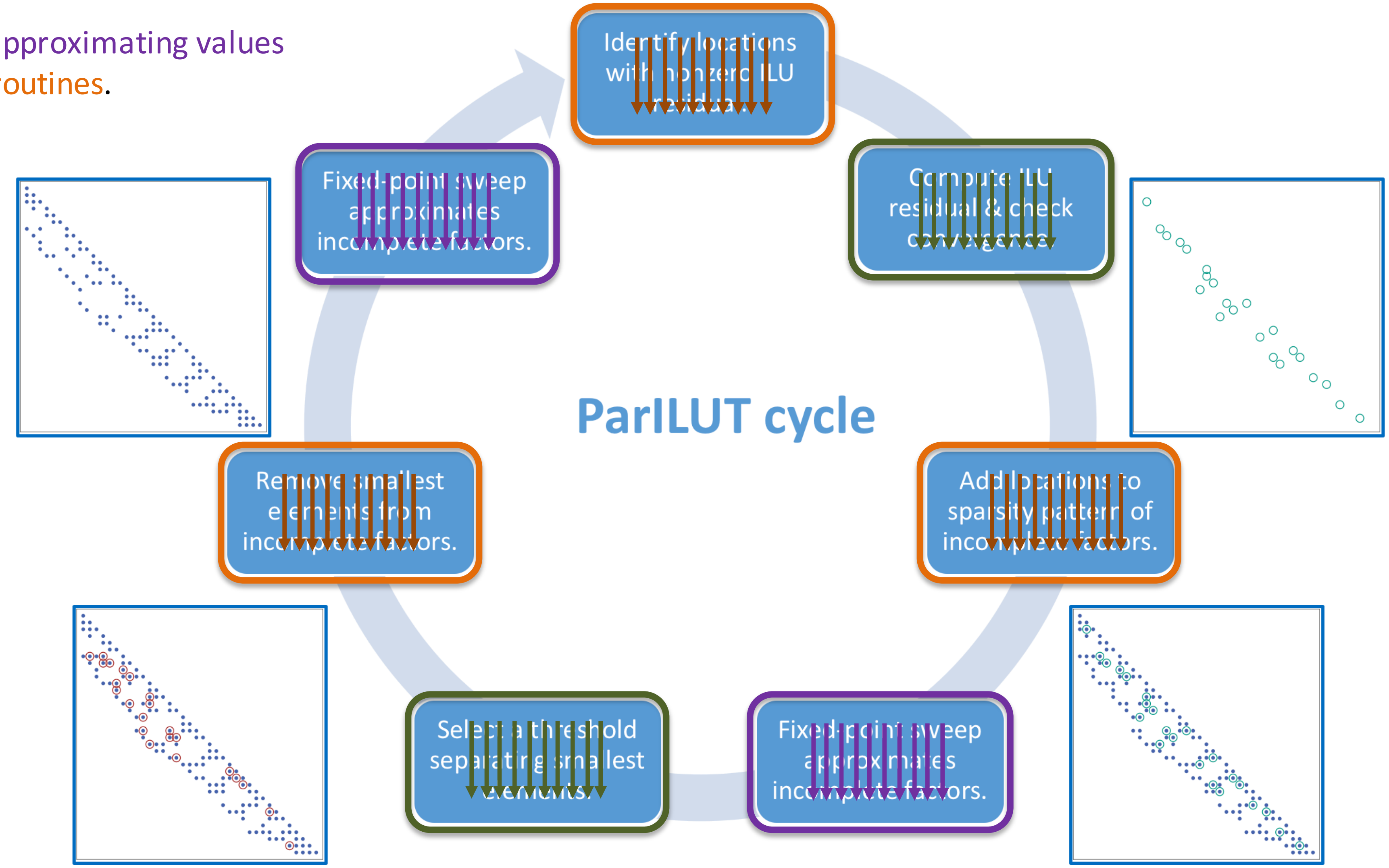
Convergence: CG iterations

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	–	–

Is this a future-oriented algorithm?

Parallelism inside the building blocks.

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



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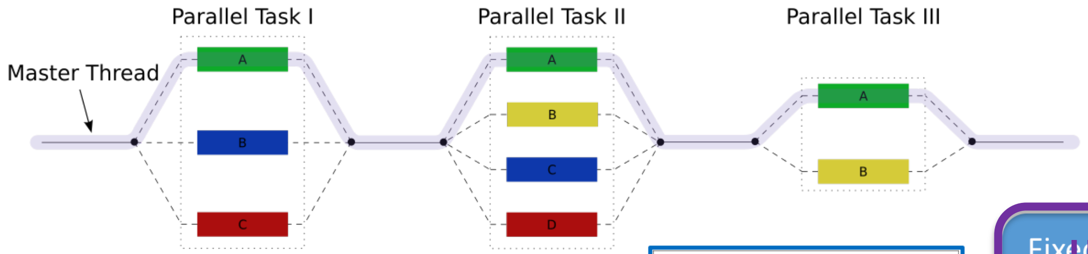
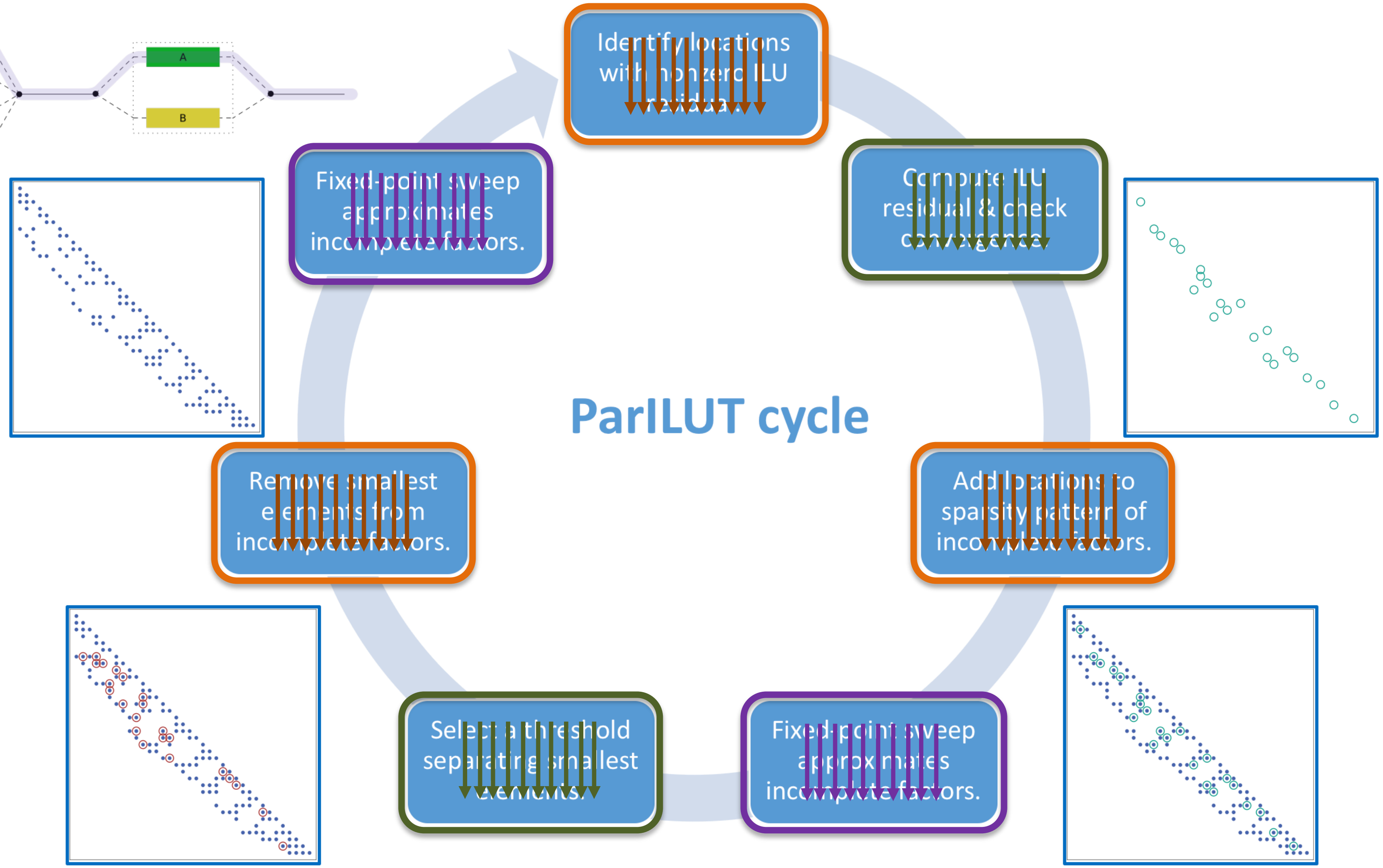


Bulk-Synchronous Algorithm!

…see John Shalf on Thursday…



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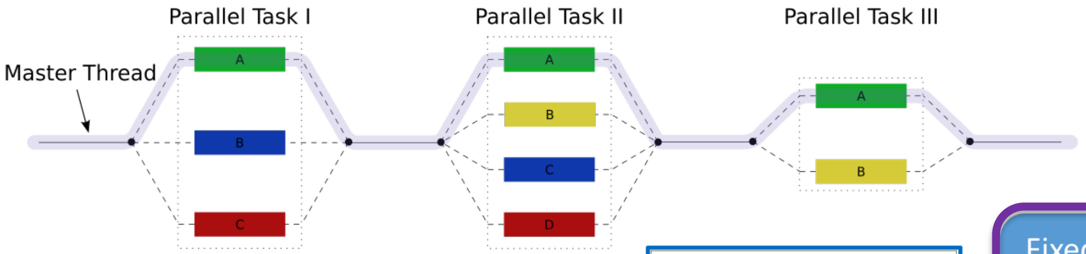
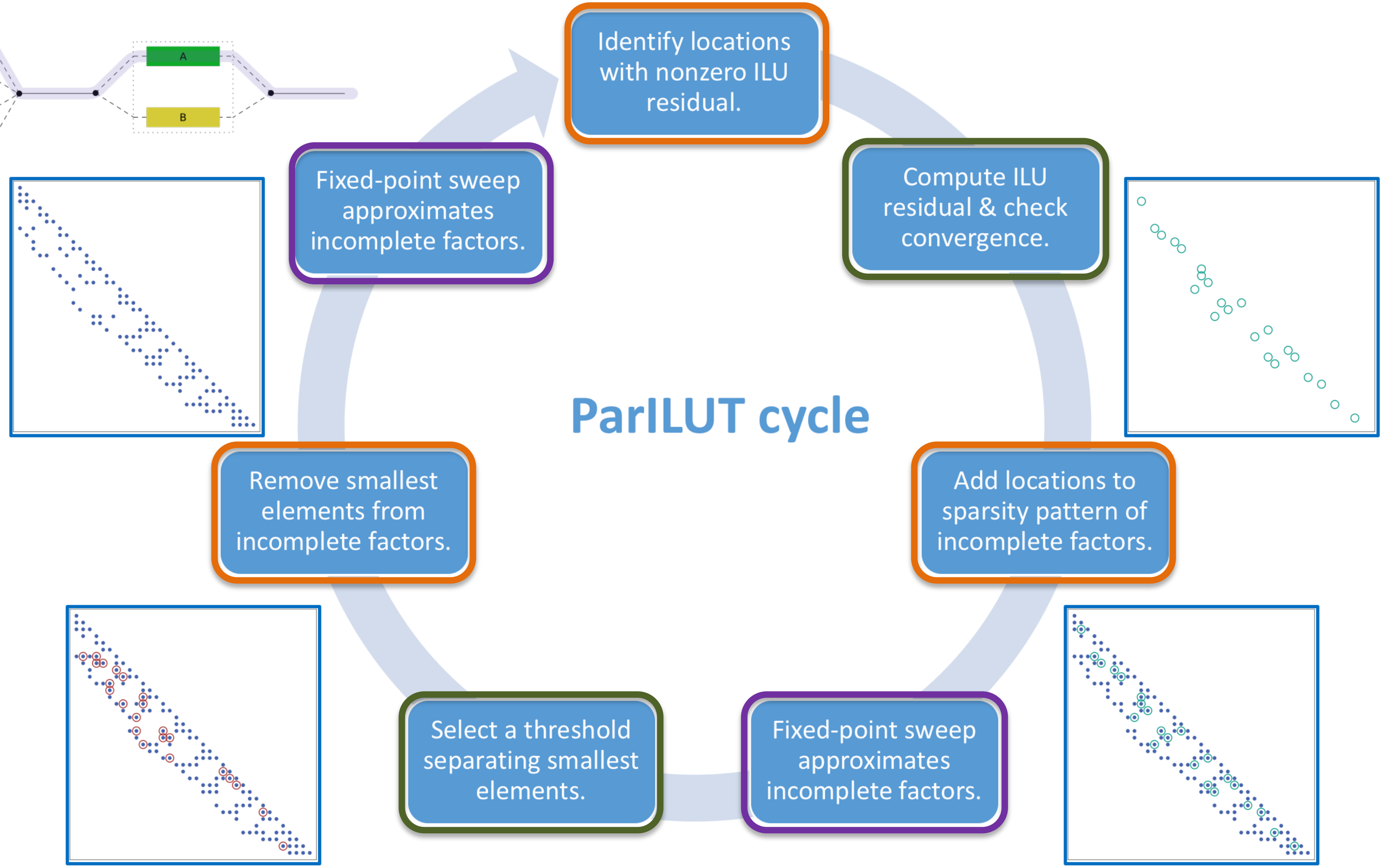


Bulk-Synchronous Algorithm!

Do we need that?



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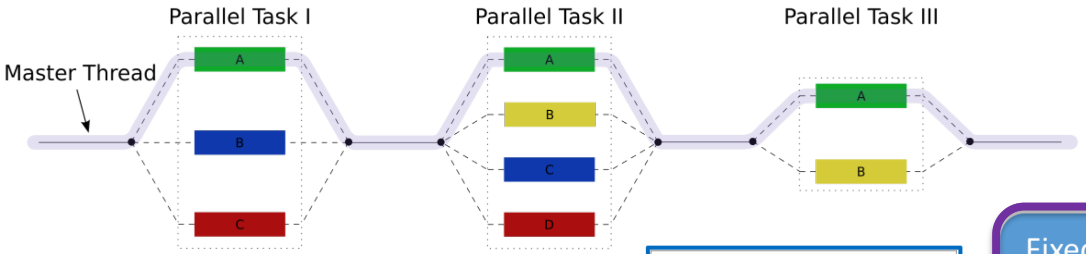

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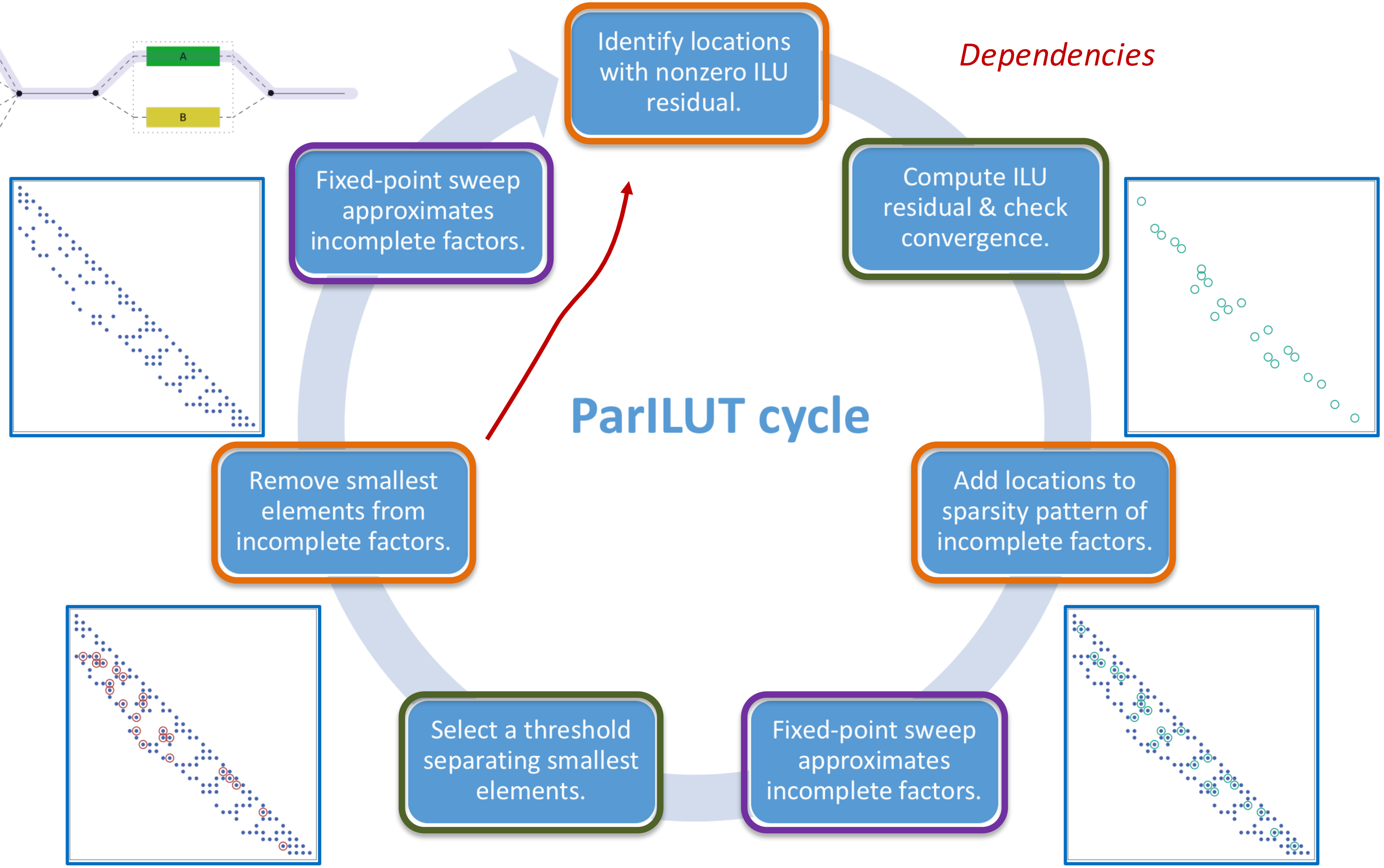

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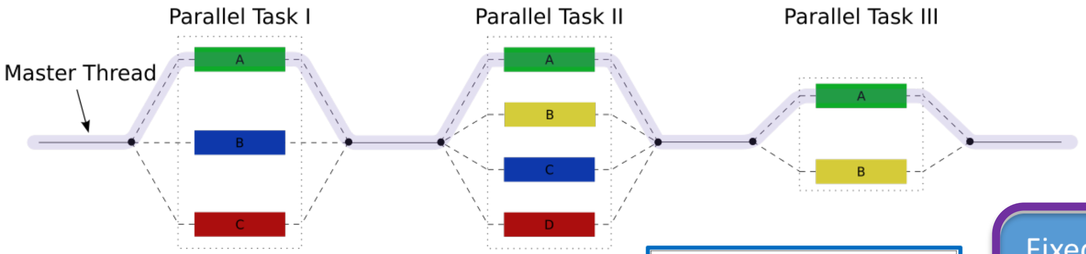

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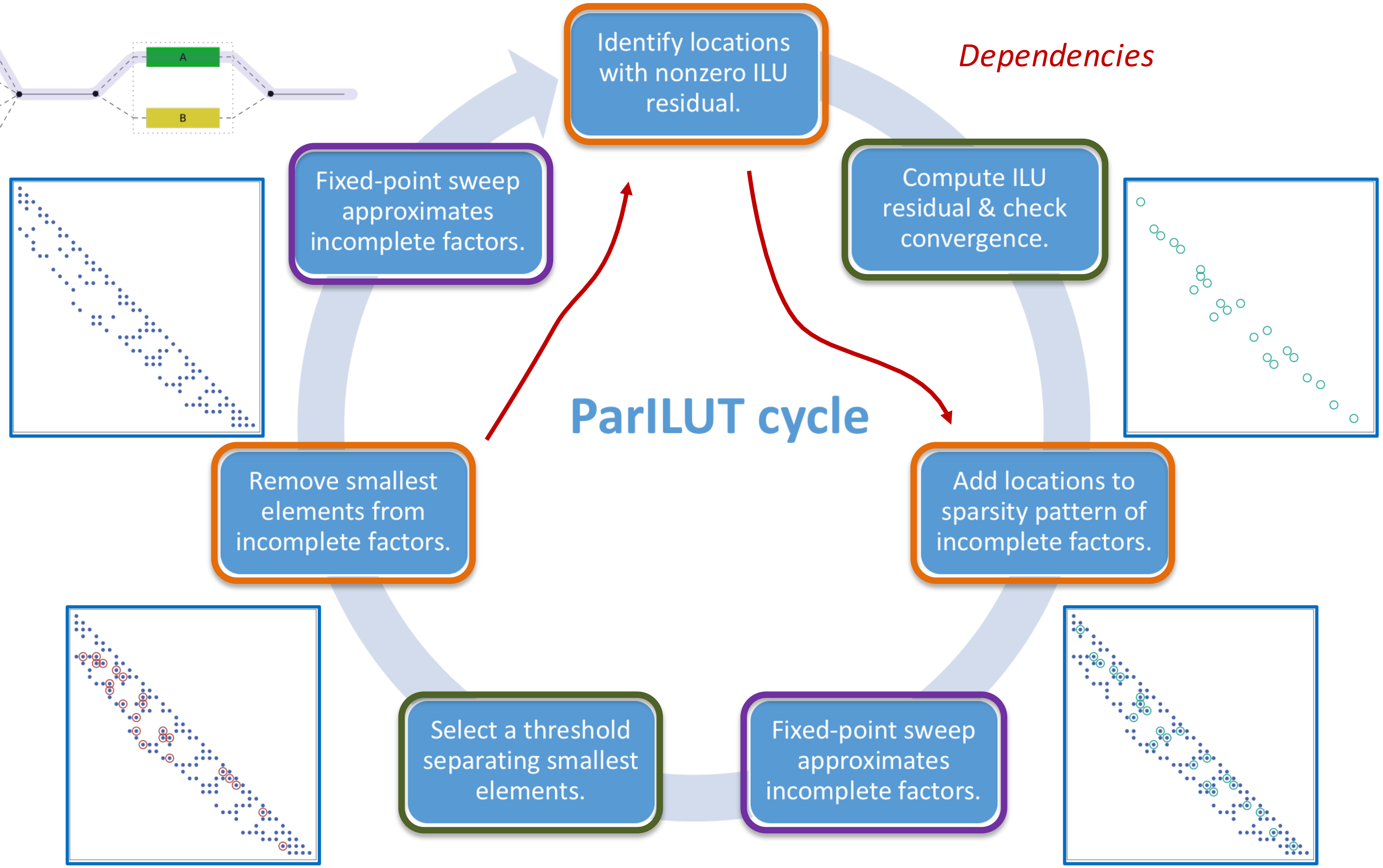

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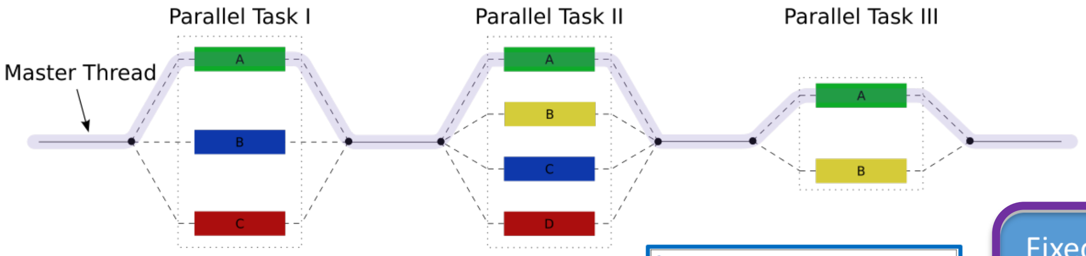

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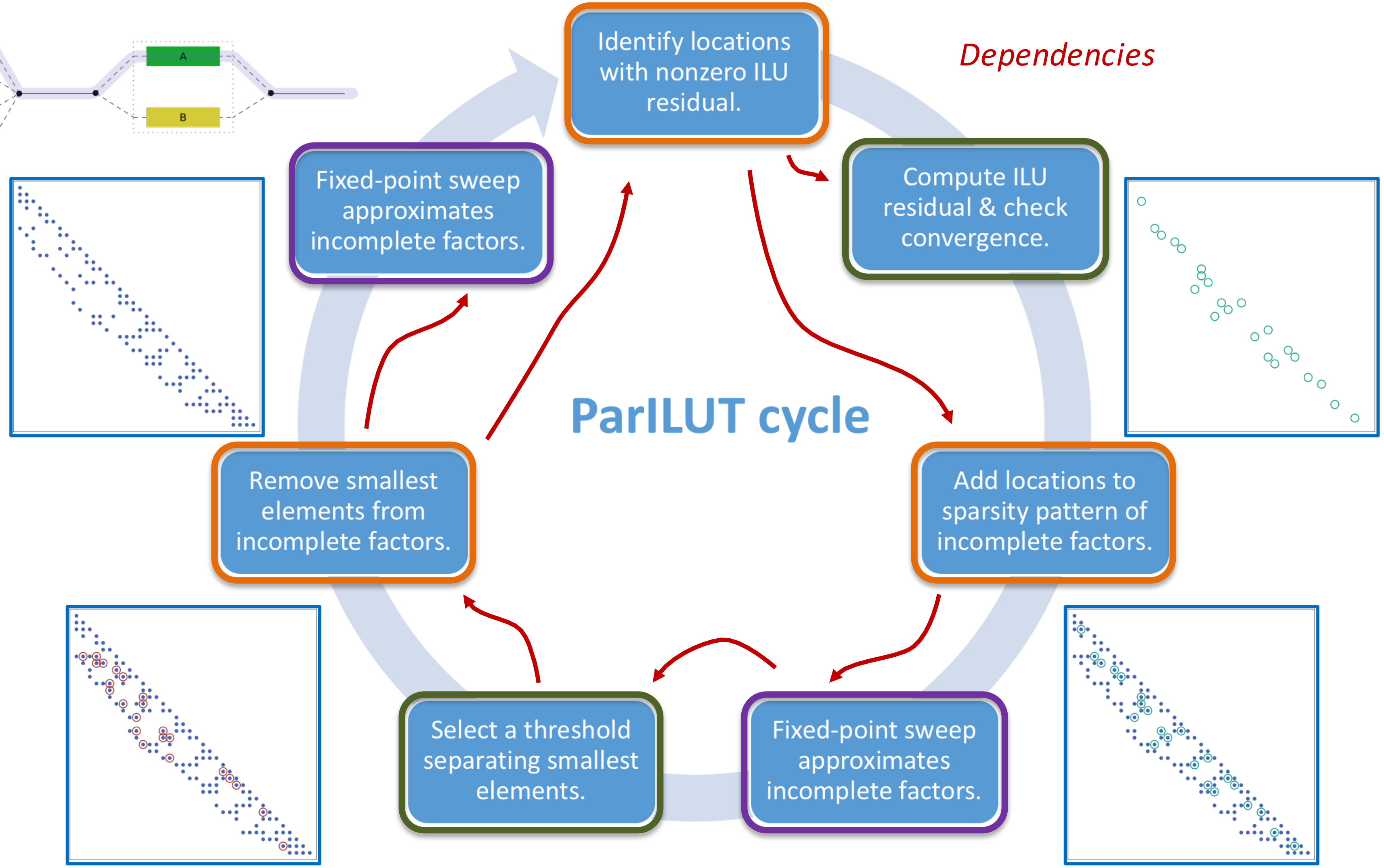

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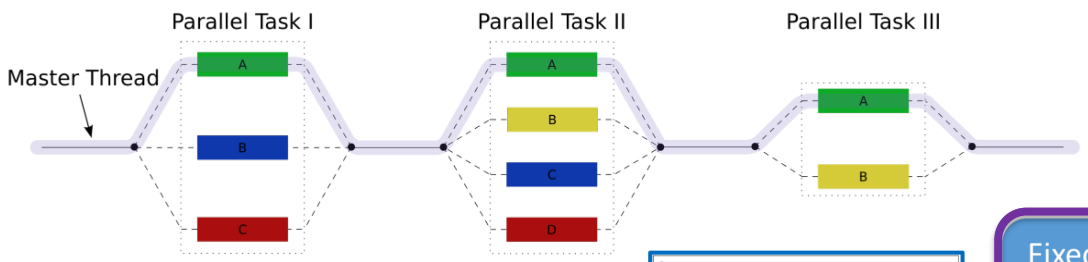

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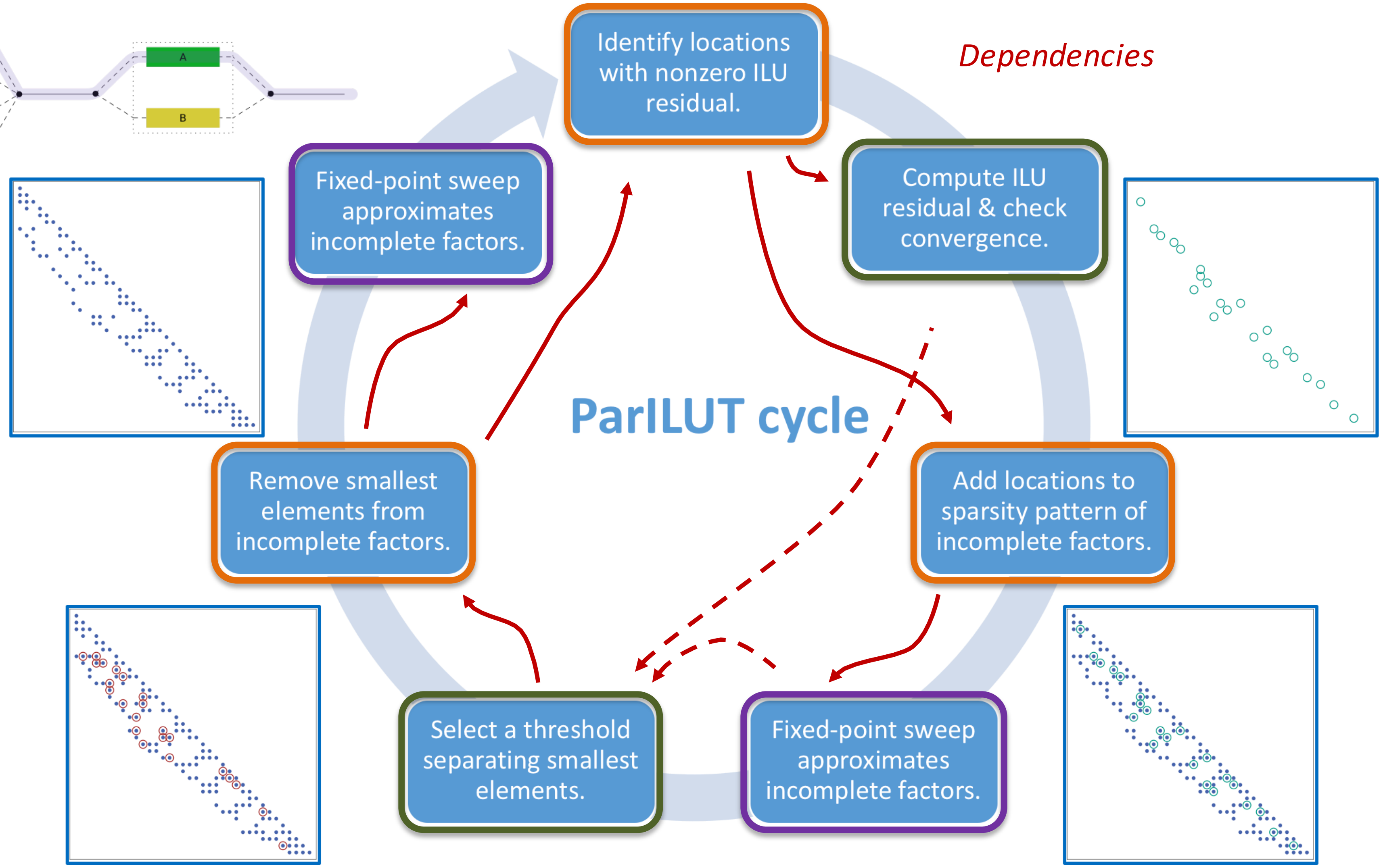

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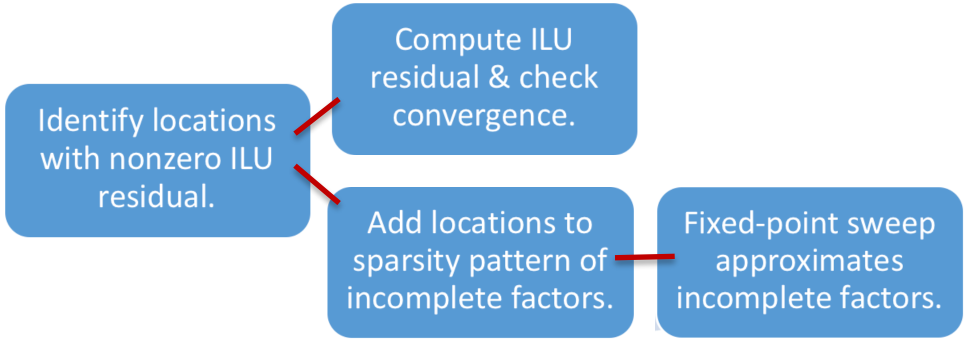

Strong dependency – *we can not start before finished.*
Weak dependency – *if we start before: +/- few nonzeros.*

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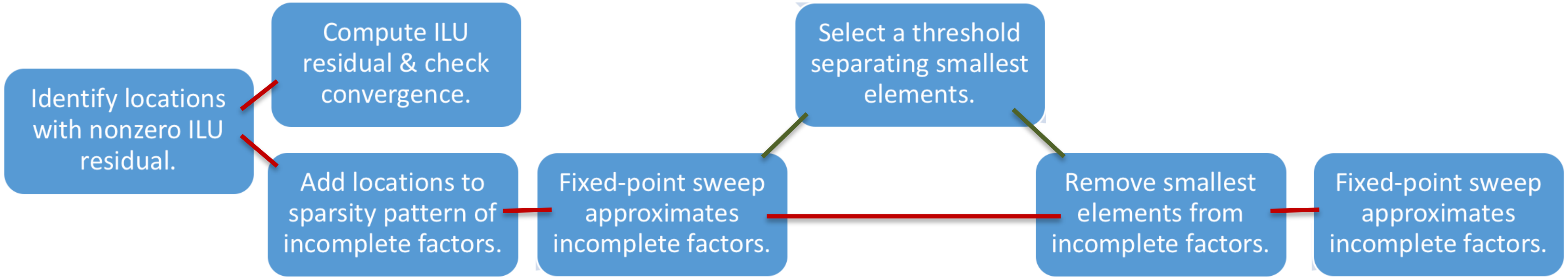

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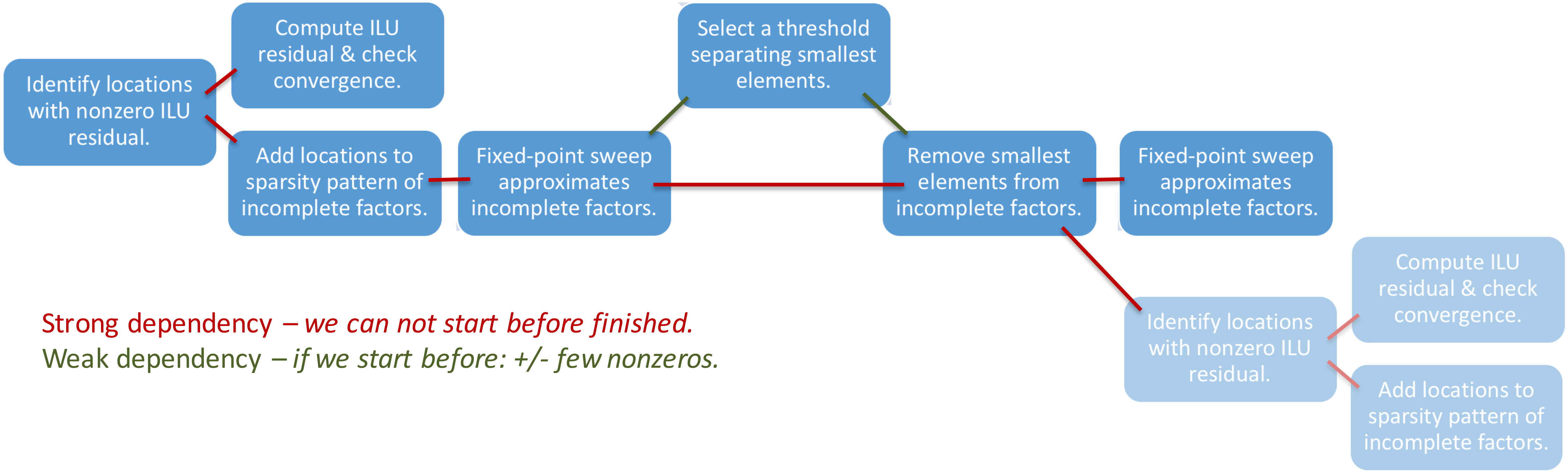

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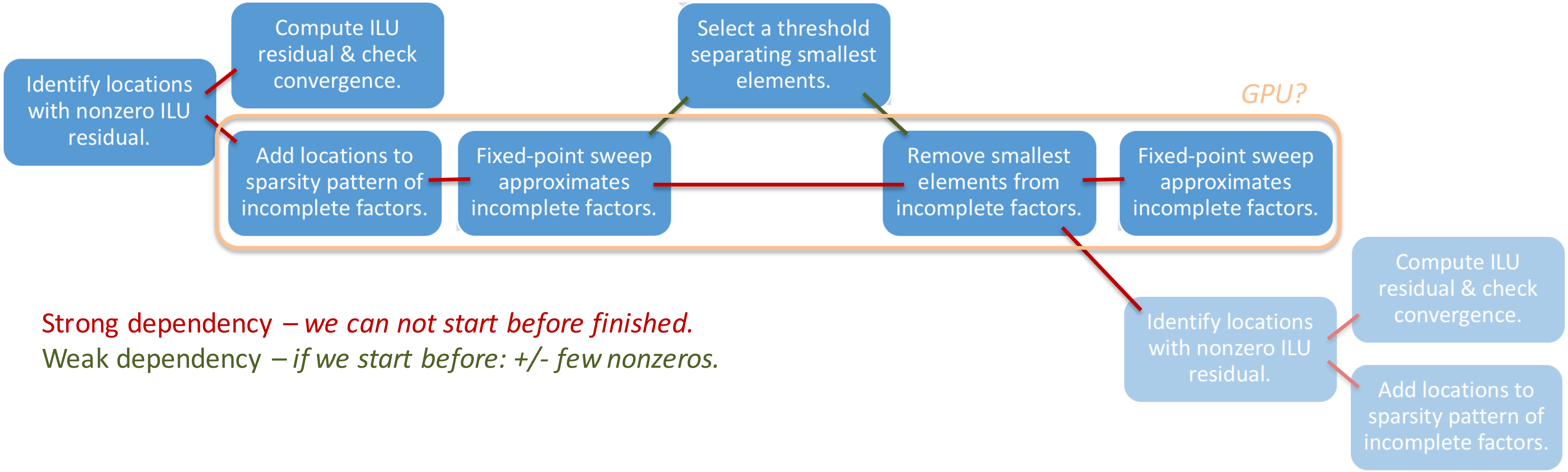

Strong dependency – *we can not start before finished.*

Weak dependency – *if we start before: +/- few nonzeros.*

Excellent candidate for hybrid hardware?

Asynchronous execution?