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Overview of Direct Sparse Linear Solvers for Power Grid Optimization Problems

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Oak Ridge Institute for Science and Education

ECP Exascale Computing Project

MSU Texas Midwestern State University

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Problem Statement

Solving large sparse linear systems of equations

$$\boldsymbol{Ax = b}$$

- $\boldsymbol{A}$ is a known coefficient matrix with dimension $n \times n$
- $\boldsymbol{b}$ is a known RHS vector with dimension $n \times 1$
- $\boldsymbol{x}$ is an unknown solution vector with dimension $n \times 1$

Factorize $\boldsymbol{A}$ into lower $\boldsymbol{L}$ and upper $\boldsymbol{U}$ triangulars, where

$$\boldsymbol{A = LU}$$

Solving $\boldsymbol{x = A^{-1}b}$ directly is too computationally expensive, so we solve by the substitutions,

1. $\boldsymbol{Ly = b}$ solve $\boldsymbol{y = L^{-1}b}$
2. $\boldsymbol{Ux = y}$ solve $\boxed{\boldsymbol{x = U^{-1}y}}$

Sparse Matrix

U

upper

$$\begin{bmatrix} 1.1 & 0 & 0 & 0 & 0 & 0 & 0.5 \\ 0 & 1.9 & 0 & 0 & 0 & 0 & 0.5 \\ 0 & 0 & 2.6 & 0 & 0 & 0 & 0.5 \\ 0 & 0 & 7.8 & 0.6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.5 & 2.7 & 0 & 0 \\ 1.6 & 0 & 0 & 0 & 0.4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.9 & 1.7 \end{bmatrix}$$

L

lower

Problem Statement

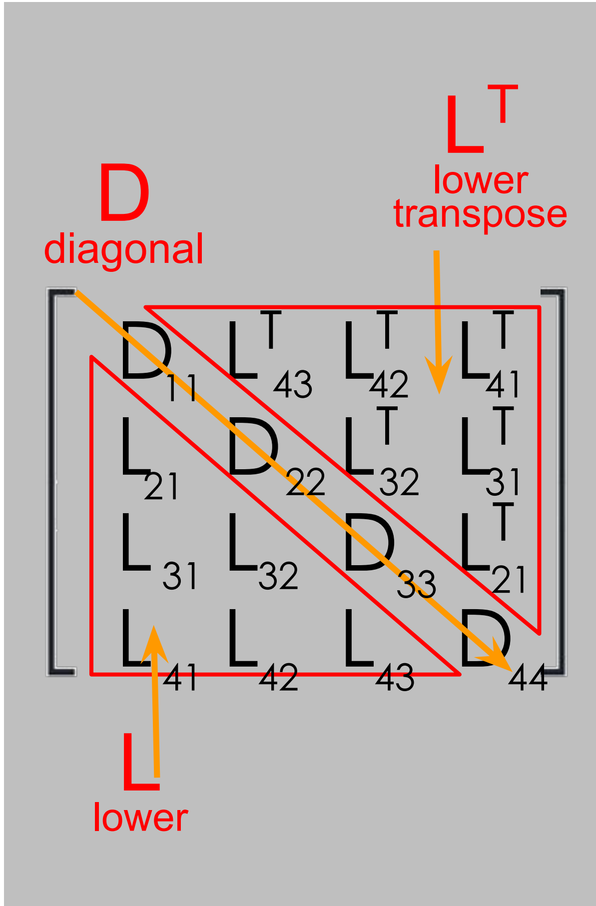
If we know we have a symmetric sparsity pattern, we can exploit matrix symmetry to further reduce computational cost by factoring ***A*** as,

$$A = LDL^T$$

- ***L*** is the lower triangular matrix
- ***D*** is a (1x1) or (2x2) the diagonal block
- L^T is the transpose of the lower triangular matrix

Solve $LDL^Tx = b$ with the substitutions,

1. $Ly = b$ solving $y = L^{-1}b$
2. $DL^Tx = y$ solving $x = (DL^T)^{-1}y$ which gives $\boxed{x = D^{-1}Ly}$ where only the lower triangular is needed for efficient solving.



Problem Statement

The residual vector ***r*** is calculated to determine the accuracy of our solution, the closer to zero the better.

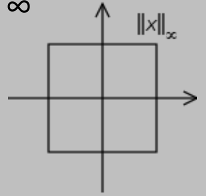
$$\boldsymbol{r = b - Ax}$$

We calculate the norm of the residual vector ***r*** and the norm of the RHS vector ***b***. The ratio of the norm of solution vector to the norm of the RHS vectors gives the relative residual. This is a measure of how well our solution converges.

$$||\boldsymbol{r}|| \;/\; ||\boldsymbol{b}||$$

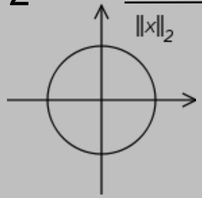
INF-norm

$$||x||_\infty = \max_i |x_i|$$



2-norm

$$||x||_2 = \sqrt{\sum |x_i|^2}$$

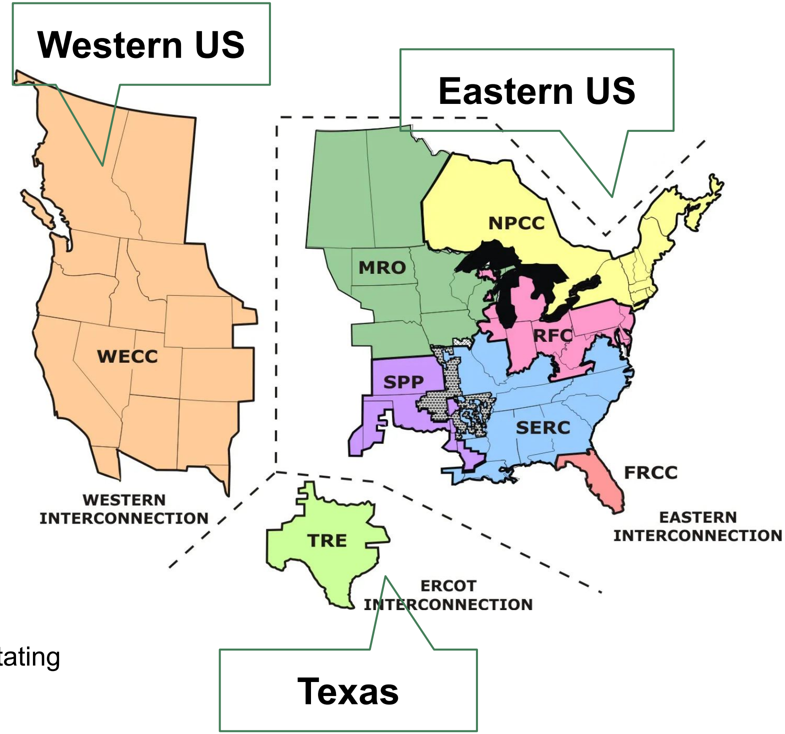


Note: The 2-norm may obscure errors compared to INF-norm, making the INF-norm preferable

Test Cases

Synthetic linear systems extracted from AC power flow analysis for power grids of Texas, Western US, and Eastern US.

Grid Model	rows	columns	NNZ	*Bus size
Texas 2000-bus	55667	55667	173710	2000
Western US 10k-bus	238072	238072	723720	10,000
Eastern US 70k-bus	1640411	1640411	4991820	70,000



* Buses serve as junction points within an electrical network, facilitating the connection of different elements of the electrical system.

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Testing Environments
Oak Ridge Leadership Computing Facility

- Summit

21 cores with each node consists of 2x IBM POWER9™ CPUs and 6 NVIDIA Volta v100 GPUs

- Frontier

64 cores with each node consists of 1x HPC and AI Optimized 3rd Gen AMD EPYC CPU and 4 Purpose Built AMD Instinct 250X GPUs

Sparse Linear Solver Packages

CPU

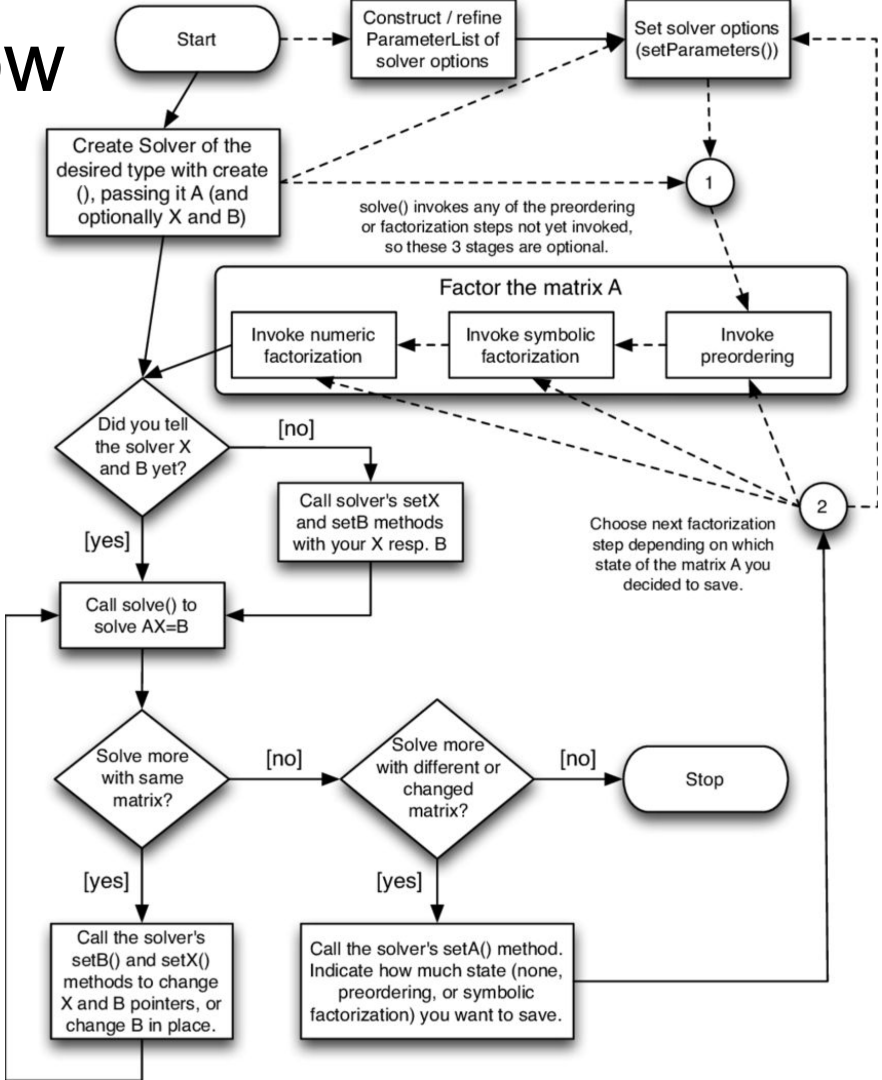
- HSL
  - MA57 (baseline)
- Trilinos Amesos2
  - KLU2
  - ShyLUBasker

GPU

- cuSolver
  - KLU-GLU
  - KLU-RFwFGMRES
- rocSOLVER
  - rocSolver-KLU-RF

Solver	MA 57	KLU2	ShyLU Basker	cuSolver KLU-GLU	cuSolver KLU-RF wGMRES	rocSolver KLU-RF
Exploits symmetry	Yes	No	No	No	No	No
Primary algorithm	LDL^T	LU	(I)LU	LU refact	LU refact	LU refact
Follows with IR	Yes	No	Yes	Yes	Yes	Yes
Norm eq used	INF-norm	2-norm	2-norm	INF-norm	INF-norm	INF-norm
GPU accelerated	No	No	No	Yes	Yes	Yes
compiler	gcc	gcc	gcc	nvcc	nvcc	hipcc
Open source	No	Yes	Yes	No	No	No

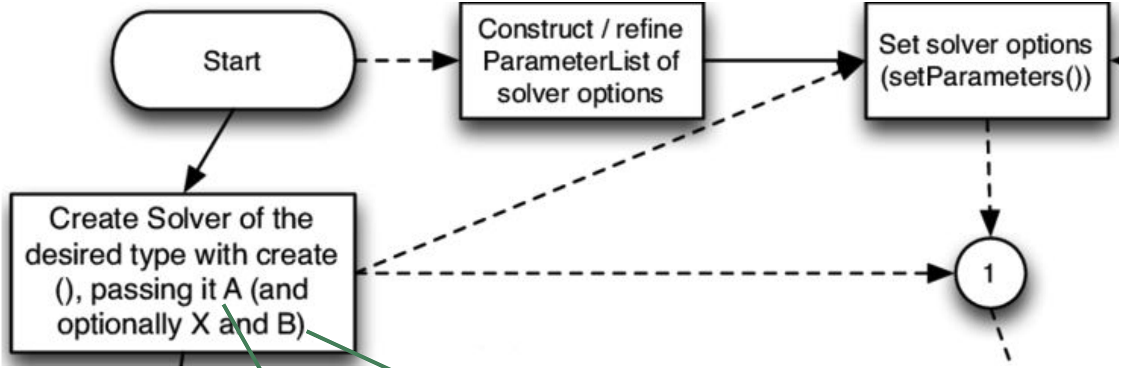
Workflow



AMESOS2

- Tasked with building a test bench for Amesos2 solvers in the ORNL Linear-Solver-Testing GitLab repository

Workflow

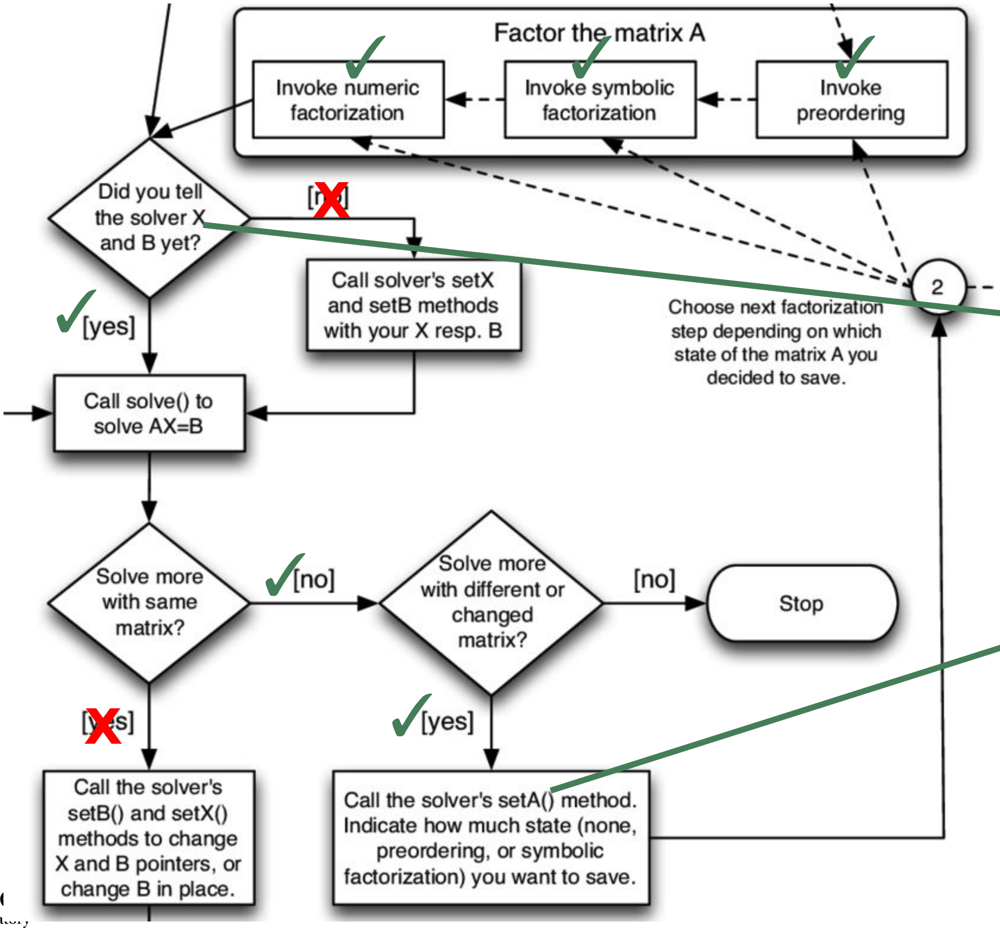


matrix A	vector B
reads in a series of given matrix market files	reads in a series of matching RHS matrix market files

Parameters

KLU2	**ShyLUBasker**
Equilibrate before solve	Set num threads (64)
Is contiguous	Use pivot
	Replace tiny pivot
	Use metis

Workflow

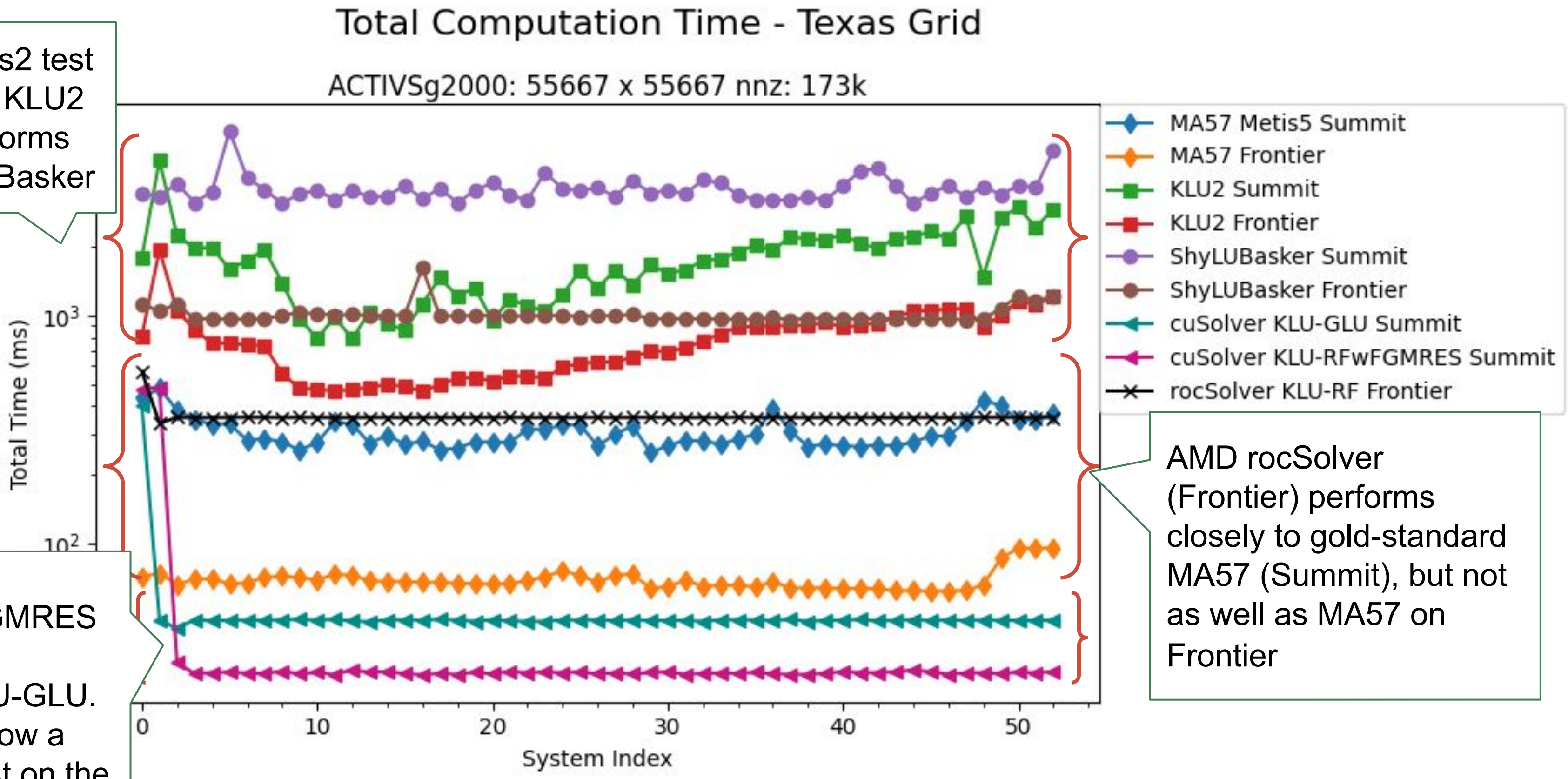


X is set to randomized values

setA(A, Amesos2::SYMBFACT)
reuse symbolic factorization

RESULTS

Amesos2 test bench: KLU2 outperforms ShyLUBasker

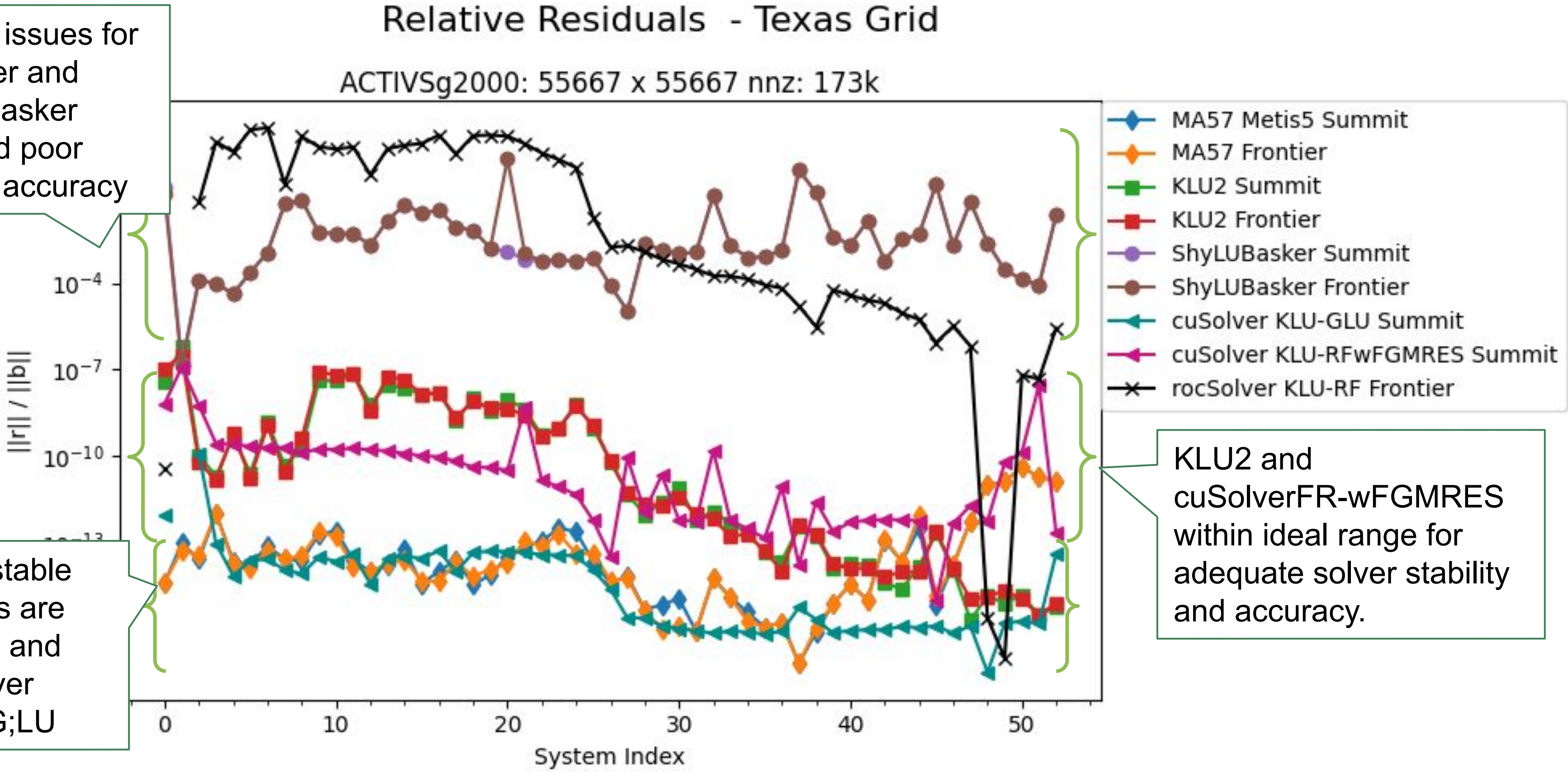


AMD rocSolver (Frontier) performs closely to gold-standard MA57 (Summit), but not as well as MA57 on Frontier

cuSolver KLU-RFwFGMRES outperforms cusolver KLU-GLU. Index 0-2 show a one time cost on the CPU before deployment on GPUs

Figure 1. Total runtimes for the Texas (2000-bus) grid model highlight performance disparities of linear solvers on different hardware architectures.

Stability issues for rocSolver and ShyLUBasker indicated poor solution accuracy

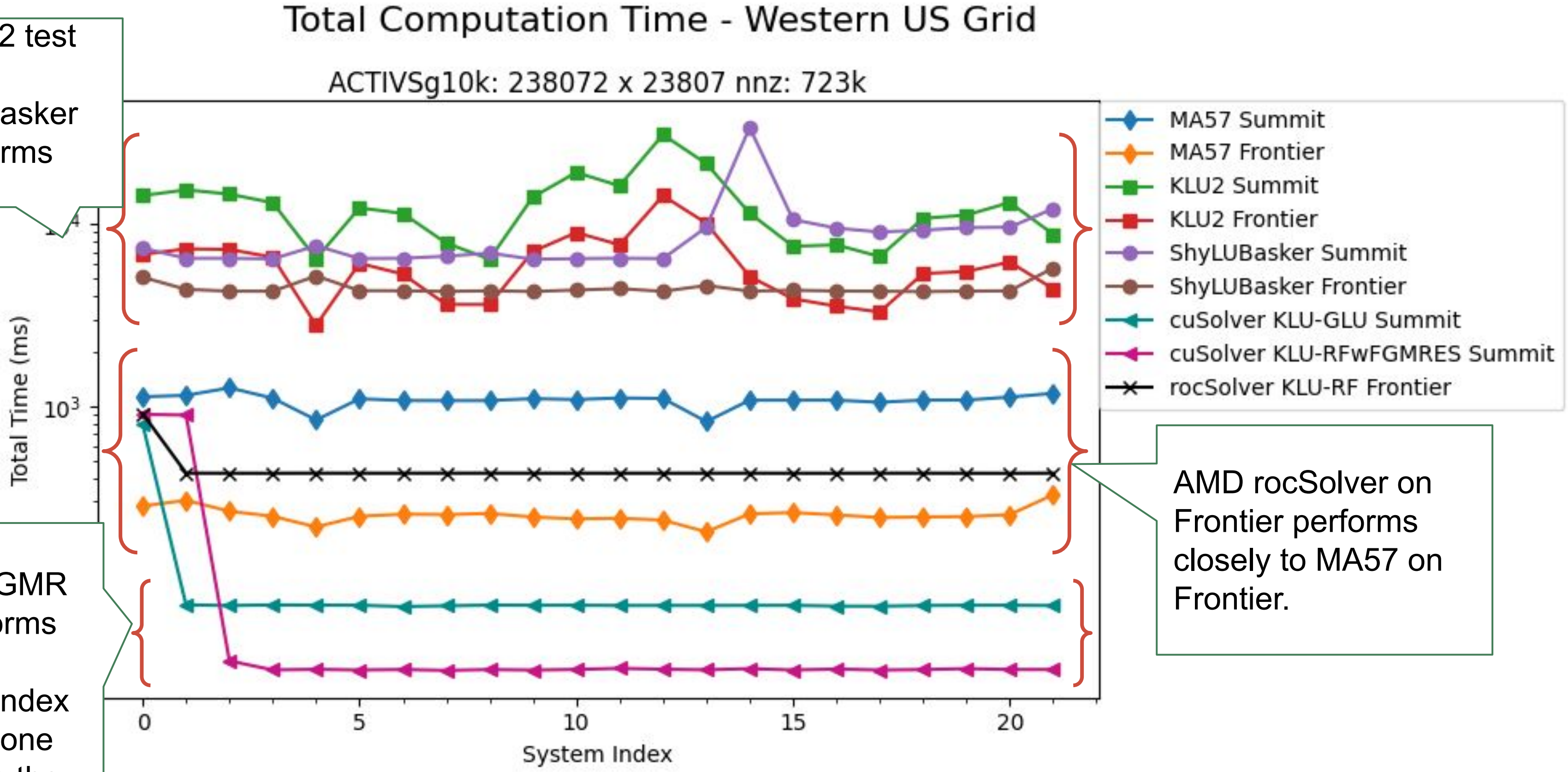


KLU2 and cuSolverFR-wFGMRES within ideal range for adequate solver stability and accuracy.

Most stable solvers are MA 57 and cuSolver KLU-G;LU

Figure 2. Relative residuals for the Texas (2000-bus) grid model accentuates the stability and accuracy of each solver. Note: A data point for rocSolver at index 1 is omitted due to convergence failure

Amesos2 test bench: ShyLUBasker outperforms KLU2

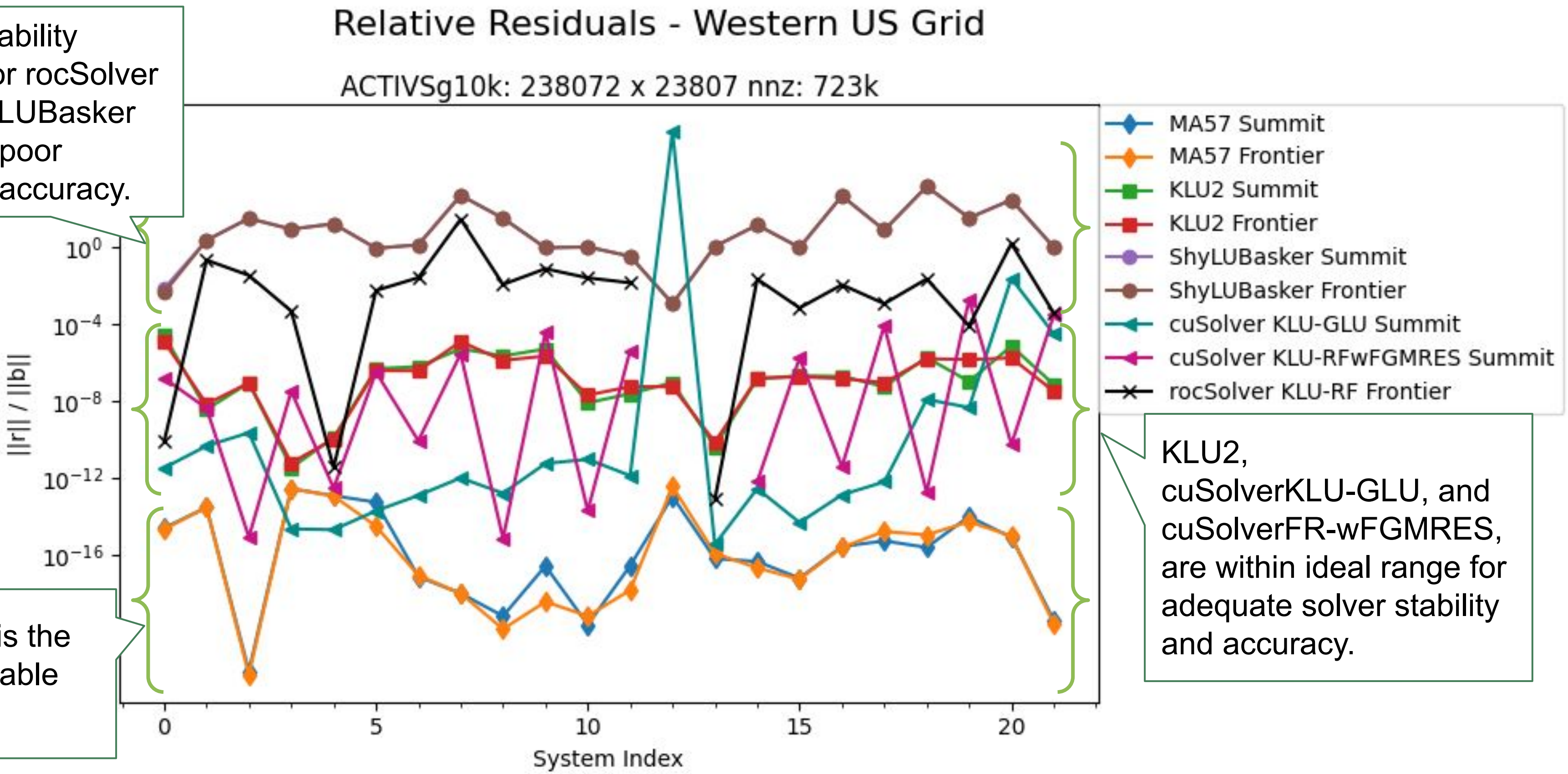


AMD rocSolver on Frontier performs closely to MA57 on Frontier.

cuSolver KLU-RFwFGMRES outperforms cusolver KLU-GLU. Index 0-2 show a one time cost on the CPU before deployment on GPUs

Figure 3. Total runtimes for the Western US (10k-bus) grid model highlights performance discrepancies of each solver

Some stability issues for rocSolver and ShyLUBasker indicate poor solution accuracy.



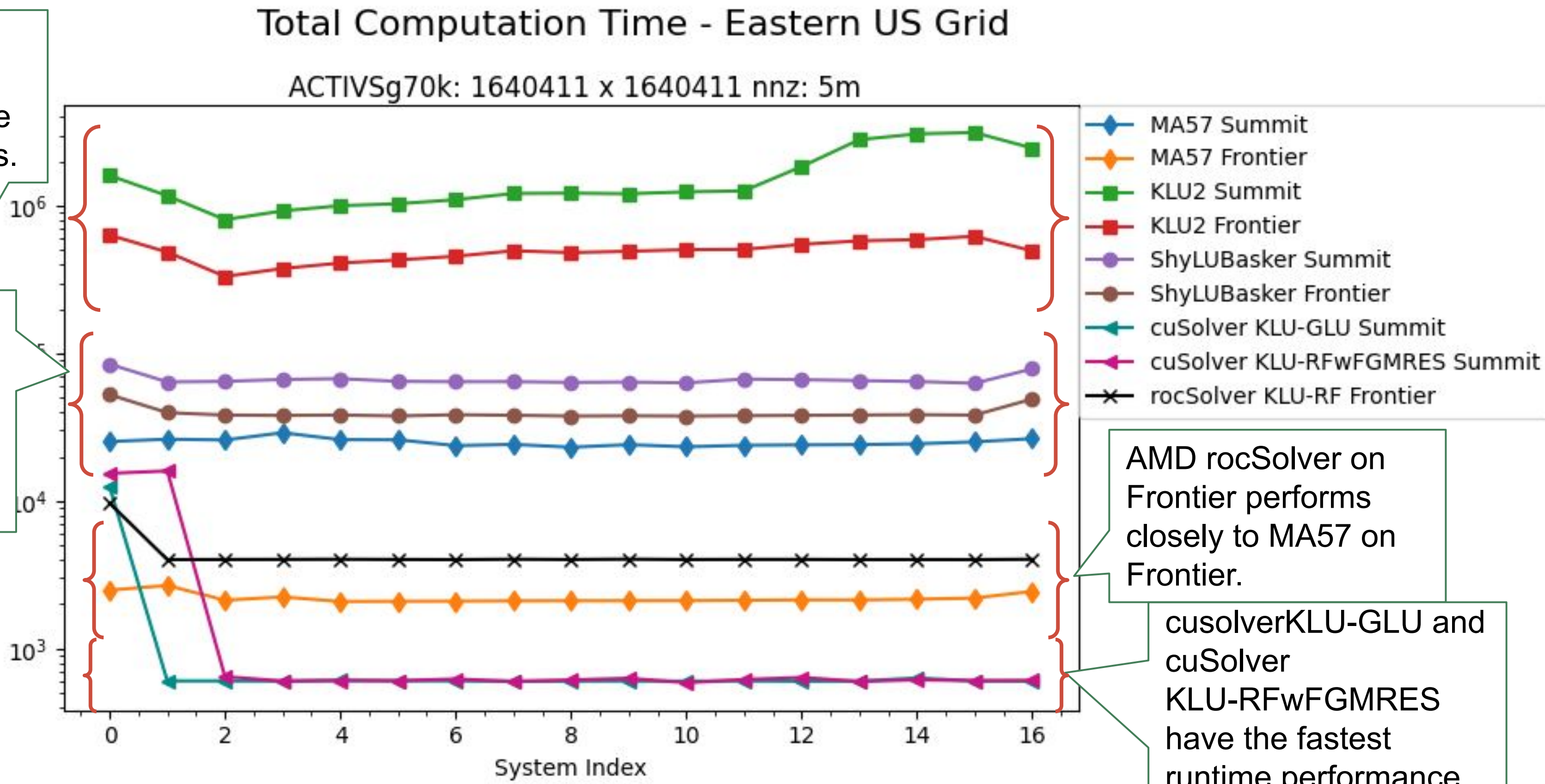
KLU2, cuSolverKLU-GLU, and cuSolverFR-wFGMRES, are within ideal range for adequate solver stability and accuracy.

MA 57 is the most stable solver.

Figure 4. Relative residuals for the Western US (10k-bus) grid model accentuates the stability and accuracy of each solver. Note: A data point for rocSolver at index 12 was omitted due to convergence failure.

KLU2 has the slowest performance of all solvers.

ShyLUBasker performs closely to gold-standard MA57 on Summit.



AMD rocSolver on Frontier performs closely to MA57 on Frontier.

cusolverKLU-GLU and cuSolver KLU-RFwFGMRES have the fastest runtime performance. Index 0-2 show a one time cost on the CPU before deployment on GPUs

Figure 5. Total runtimes for the Eastern US (70k-bus) grid model highlights performance discrepancies of each solver.

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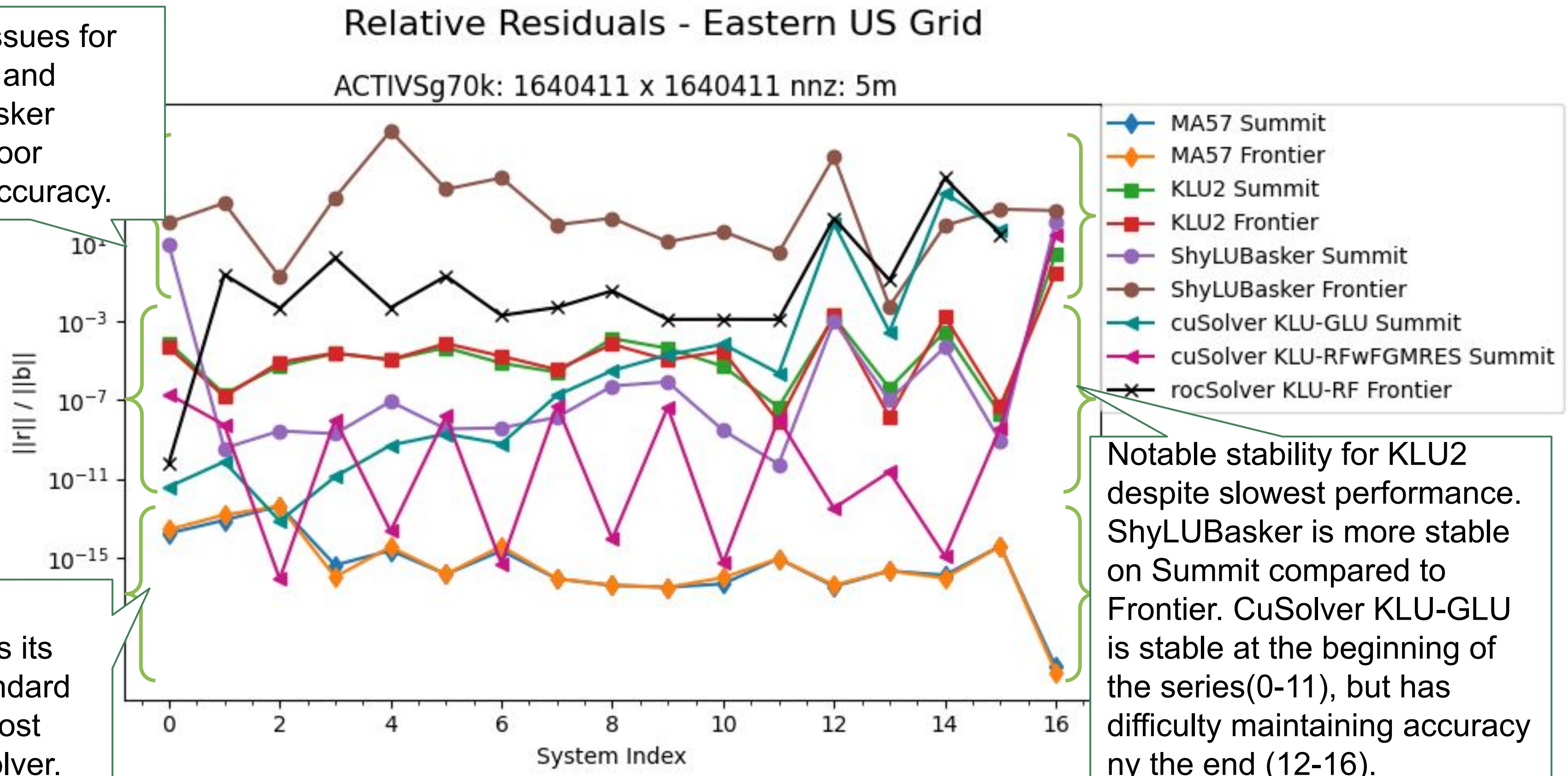
Stability issues for rocSolver and ShyLUBasker indicate poor solution accuracy.



MA 57 maintains its gold-standard as the most stable solver.

Figure 6. Relative residuals for the Eastern US (70k-bus) grid model accentuates the stability and accuracy of each solver. Note: Data points for rocSolver and cuSolverKLU-GLU at index 16 were omitted due to convergence failure.

Notable stability for KLU2 despite slowest performance. ShyLUBasker is more stable on Summit compared to Frontier. CuSolver KLU-GLU is stable at the beginning of the series(0-11), but has difficulty maintaining accuracy ny the end (12-16). CuSolverKLU-RF-wFGMRES maintains adequate stability throughout with exception at index 16

Results and Discussion

- CUDA GPU linear solvers significantly outperform CPU based solvers for all test cases provided.
- RocSolver performed closely to the MA57 “gold standard” CPU benchmark, some stability issues observed and worth further investigation.
- Amesos2 ShyLUBasker solver performance scales well with the number of threads, however, we observed serious stability issues for some test cases,
- Amesos2 KLU2 solver has limited parameters to adjust compared to vanilla KLU, e.g. it did not support COLAMD ordering, but proved to maintain a notable level of stability throughout despide longer runtimes.
- Amesos2 solvers highlight a trade off that can occur in runtime performance versus solver stability.

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Questions?

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References

Świrydowicz, K., Koukpaizan, N., Abhyankar, S., & Peleš, S. (2023). Towards efficient alternating current optimal power flow analysis on graphical processing units. 2023 XXIX International Conference on Information, Communication and Automation Technologies (ICAT). 10.1109/icat57854.2023.10171317

Świrydowicz, K., Darve, E., Jones, W., Maack, J., Regev, S., Saunders, M. A., Thomas, S. J., & Peleš, S. (2022). Linear solvers for power grid optimization problems: A review of GPU-accelerated linear solvers. Parallel Computing, 111, 102870. 10.1016/j.parco.2021.102870

Bavier, Eric & Hoemmen, Mark & Rajamanickam, Siva & Thornquist, Heidi. (2012). Amesos2 and Belos: Direct and Iterative Solvers for Large Sparse Linear Systems. Scientific Programming. 20.241-255. 10.1155/2012/243875.

Rajamanickam, Siva. KLU2 Direct Linear Solver Package. Computer software. https://www.osti.gov//servlets/purl/1253280. Vers. 00. USDOE. 4 Jan. 2012. Web.

[KLU2 header]