

# Overview of Direct Sparse Linear Solvers for Power Grid Optimization Problems

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EXASCALE COMPUTING PROJECT



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# Problem Statement

Solving large sparse linear systems of equations

$$\mathbf{Ax} = \mathbf{b}$$

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

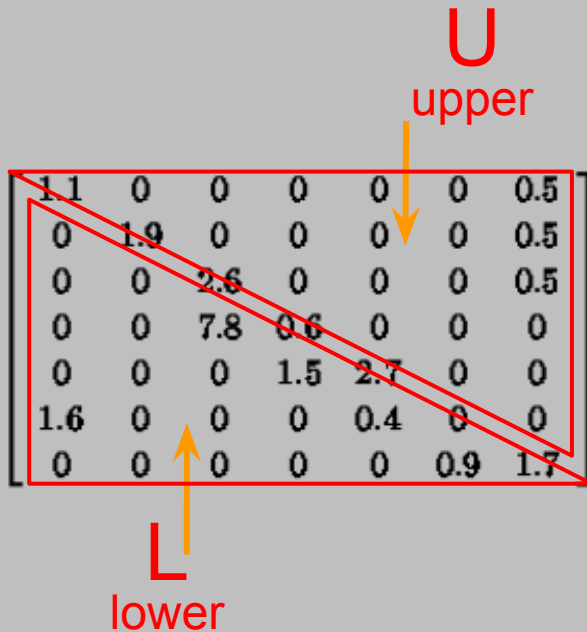
Factorize  $\mathbf{A}$  into lower  $\mathbf{L}$  and upper  $\mathbf{U}$  triangulars, where

$$\mathbf{A} = \mathbf{LU}$$

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

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

Sparse Matrix



# Problem Statement

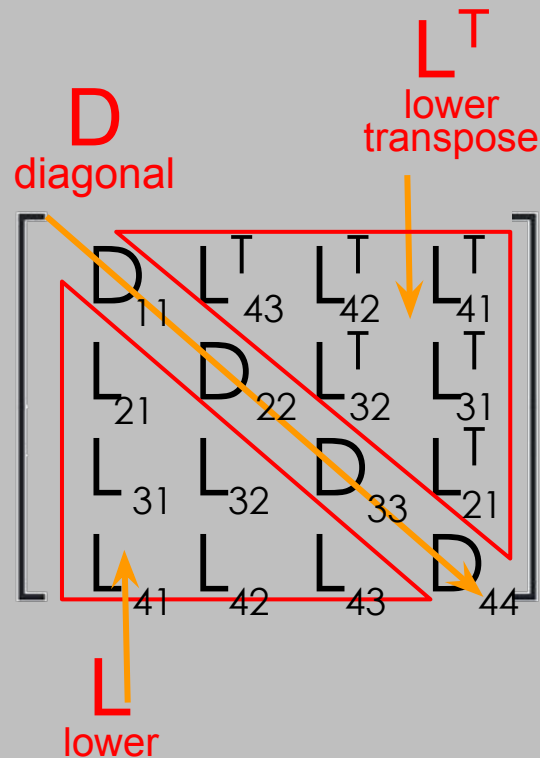
If we know we have a symmetric sparsity pattern, we can exploit matrix symmetry to further reduce computational cost by factoring  $\mathbf{A}$  as,

$$\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{L}^T$$

- $\mathbf{L}$  is the lower triangular
- $\mathbf{D}$  is the diagonal block
- $\mathbf{L}^T$  is the transpose of the lower triangular

Solve  $\mathbf{L}\mathbf{D}\mathbf{L}^T\mathbf{x} = \mathbf{b}$  with the substitutions,

1.  $\mathbf{L}\mathbf{y} = \mathbf{b}$  solve  $\mathbf{y} = \mathbf{L}^{-1}\mathbf{b}$
2.  $\mathbf{D}\mathbf{L}^T\mathbf{x} = \mathbf{y}$  solve  $\mathbf{x} = (\mathbf{D}\mathbf{L}^T)^{-1}\mathbf{y} = \mathbf{D}^{-1}\mathbf{L}\mathbf{y}$



# Problem Statement

The residual vector  $\mathbf{r}$  is calculated to determine the accuracy of our solution, the closer to zero the better.

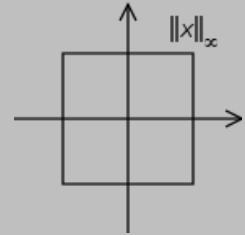
$$\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}$$

We then compute the norm of the residual vector  $\mathbf{r}$  and the norm of the RHS vector  $\mathbf{b}$  to obtain the relative residual  $\mathbf{R}_{rel}$  as a measure of how well our solution converges.

$$\mathbf{R}_{rel} = ||\mathbf{r}|| / ||\mathbf{b}||$$

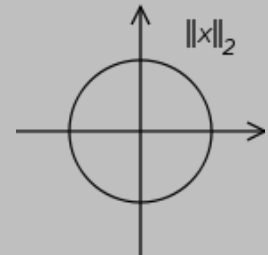
## INF-norm

$$||\mathbf{x}||_{\infty} = \max_i |x_i|$$



## 2-norm

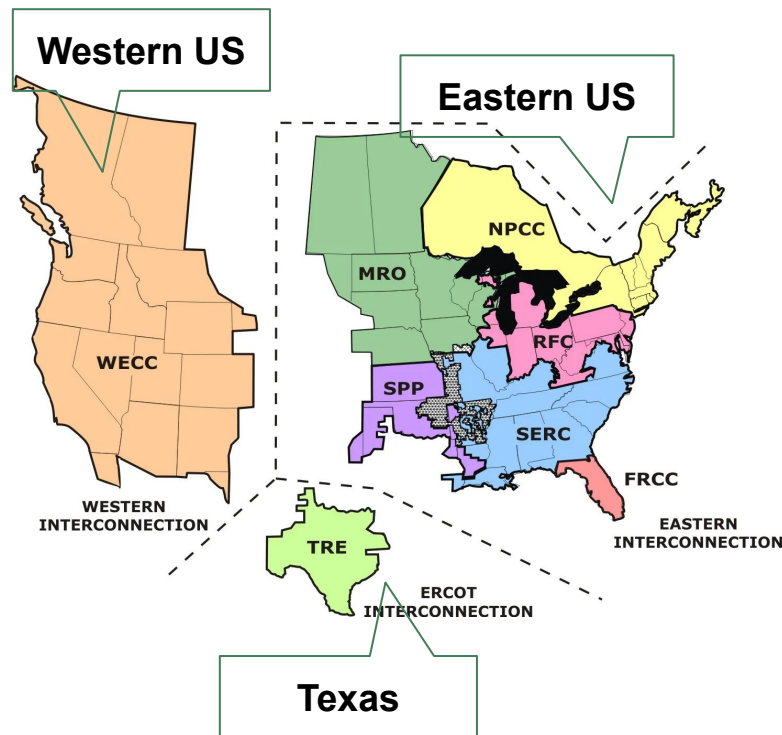
$$||\mathbf{x}||_2 = \sqrt{\sum |x_i|^2}$$



# Test Cases

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

Grid Model	rows	columns	NNZ	NNZ un
Texas 2000-bus	55667	55667	173710	291743
Western US 10k-bus	238072	238072	723720	1209368
Eastern US 70k-bus	1640411	1640411	4991820	8343229



# Testing Environments

## Oak Ridge Leadership Computing Facility

### - Summit

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

### - Frontier

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



# Sparse Linear Solver Packages

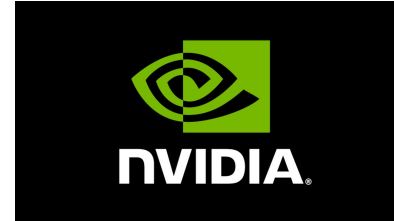
## CPU

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



## GPU

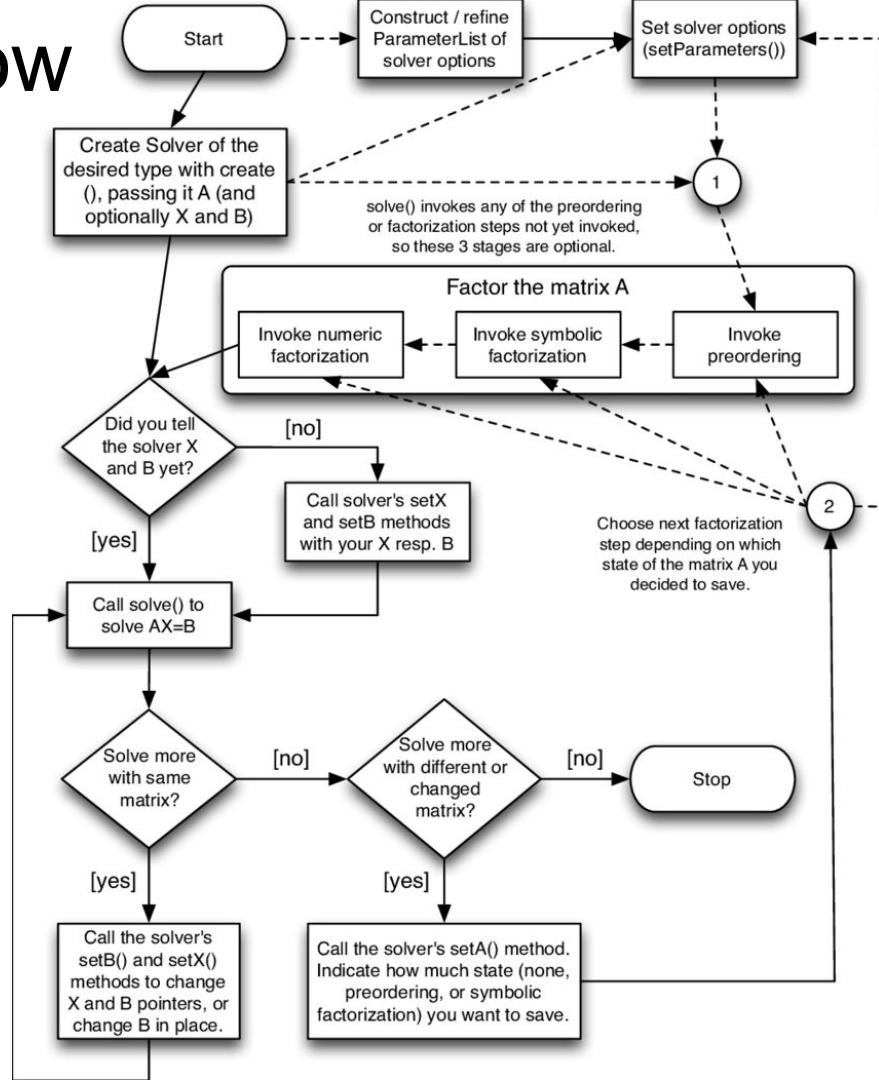
- cuSolver
  - KLU-GLU
  - KLU-RFwFGMRES
- rocSOLVER
  - rocSolver-KLU-RF



Solver	MA 57	KLU2	ShyLU Basker	cuSolver KLU-GLU	cuSolver KLU-RF wGMRES	rocSolver KLU
Exploits symmetry	Yes	No	No	No	No	No
Primary algorithm	LDL <sup>T</sup>	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

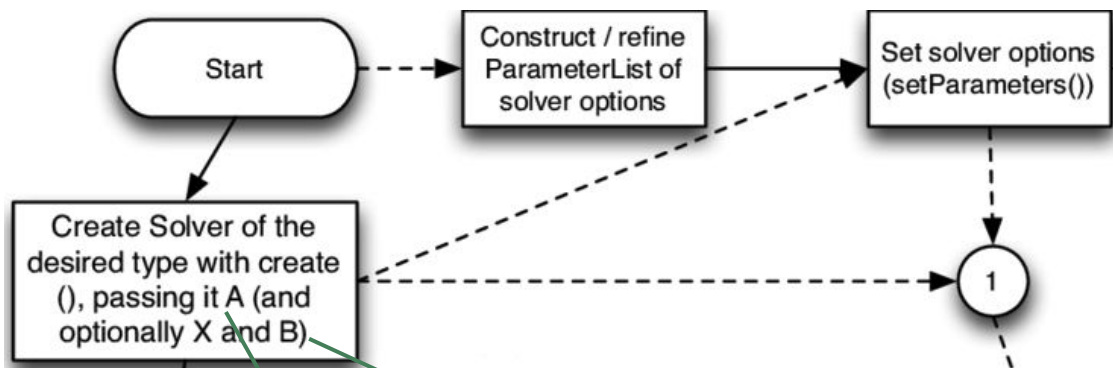


**AMESOS2**



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

# Workflow

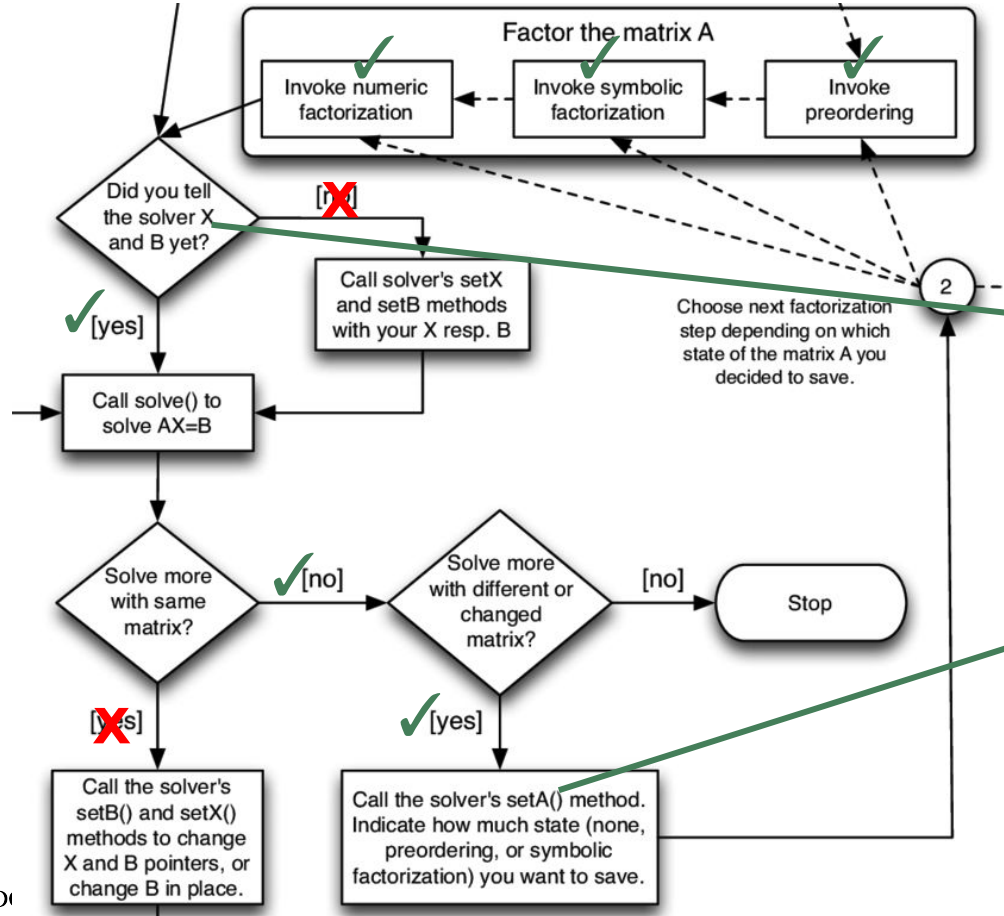


matrix A	vector B
reads in a series of given matrix market files	reads in a series of matching RHS matrix market files

## 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

The background of the slide is a vibrant teal and green gradient. It features a complex pattern of binary code (0s and 1s) that appears to be flowing or receding into the distance. Overlaid on this are several geometric and molecular motifs: a series of white hexagons arranged in a honeycomb-like pattern, some of which are filled with a lighter shade of green; and a network of small white dots connected by thin lines, resembling a molecular or data network. The overall aesthetic is high-tech and scientific.

# Total Computation Time - Texas Grid

ACTIVSg2000: 55667 x 55667 nnz: 173k

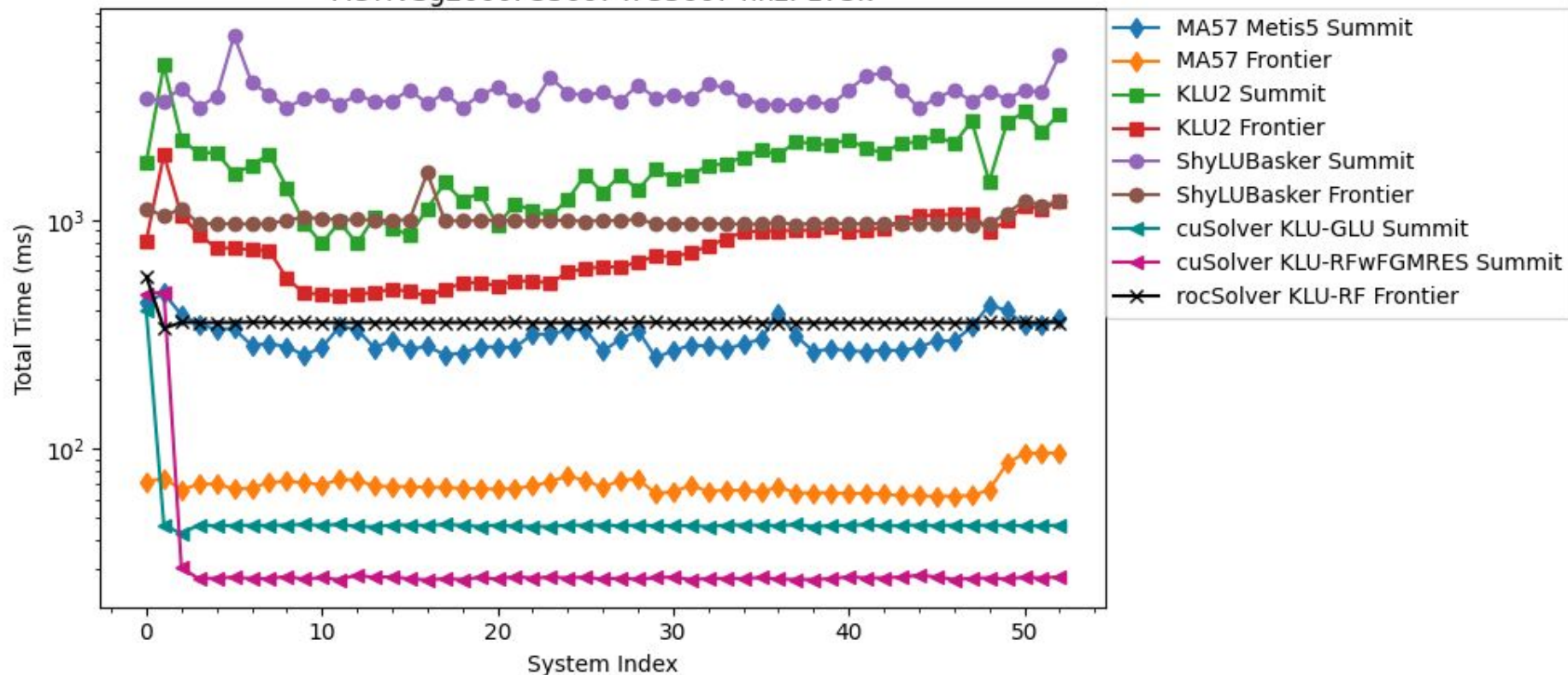


Figure 1. Total runtimes for the Texas (2000-bus) test case. ShyLUBasker performed significantly worse on Summit compared to Frontier and KLU2 performs better than ShyLUBasker. MA57 is much better on Frontier than Summit for the Texas grid test case. CUDA cuSolvers perform the best overall.



# Relative Residuals - Texas Grid

ACTIVSg2000: 55667 x 55667 nnz: 173k

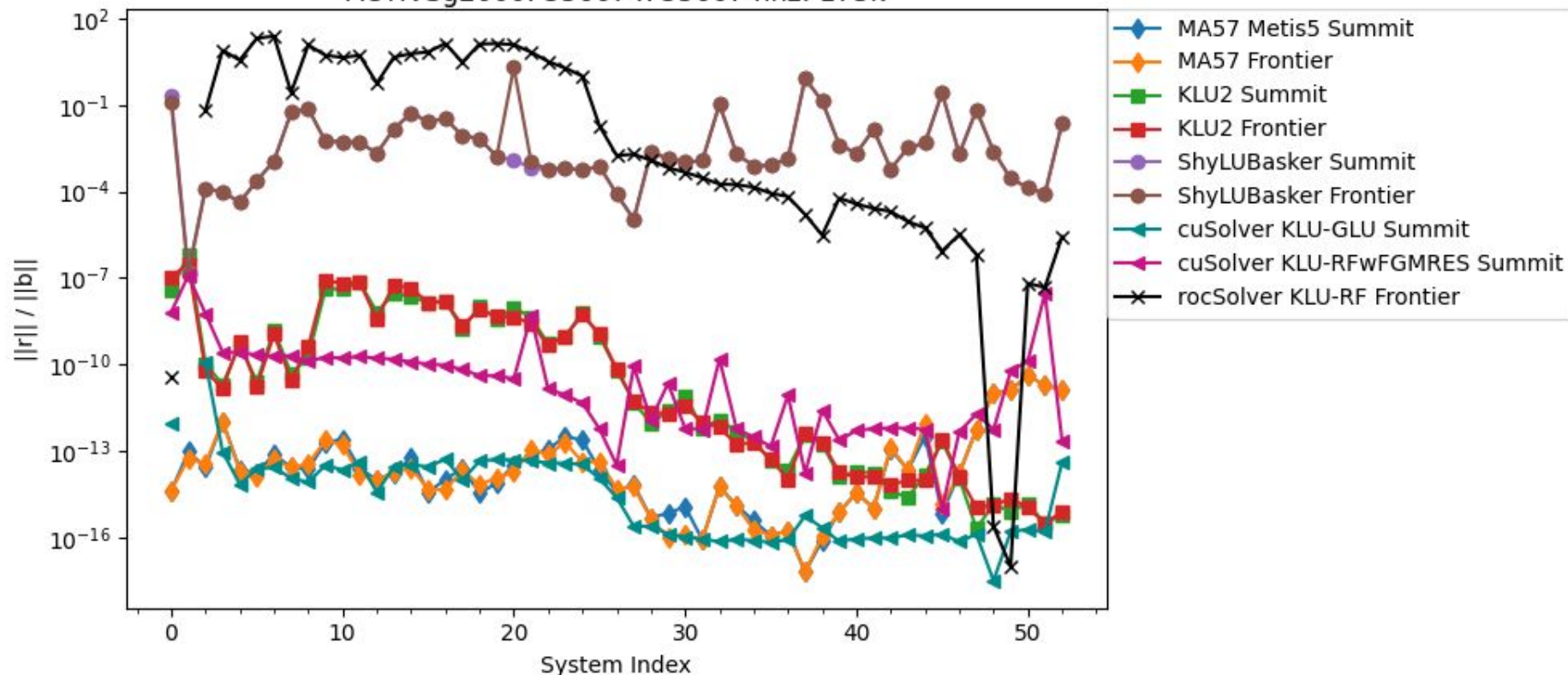


Figure 2. Relative residuals for the Texas (2000-bus) matrix market files. Data points for rocSolver and cuSolver KLU-GLU at index 2 were omitted where the solution failed to converge. ShyLUBasker and rocSolver have very poor accuracy, while MA57 and cuSolver KLU-GLU are the most stable for the Texas grid test case.

# Total Computation Time - Western US Grid

ACTIVSg10k: 238072 x 23807 nnz: 723k

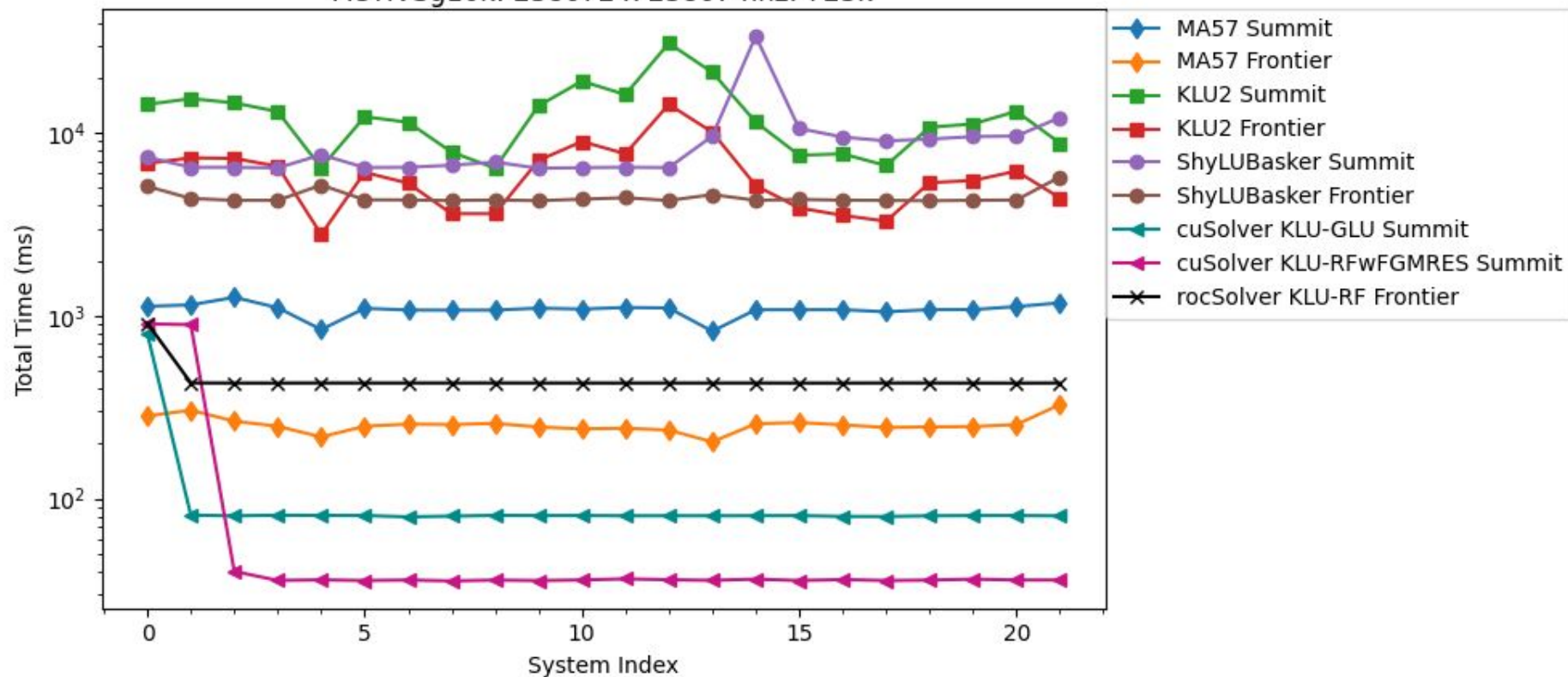


Figure 3. Total runtimes for the Western US (10k-bus) test cases. KLU2 and ShyLUBasker perform worse on Summit and slightly improve on Frontier. CUDA cuSolvers have the best runtimes that outperform the MA57 baseline.

## Relative Residuals - Western US Grid

ACTIVSg10k: 238072 x 23807 nnz: 723k

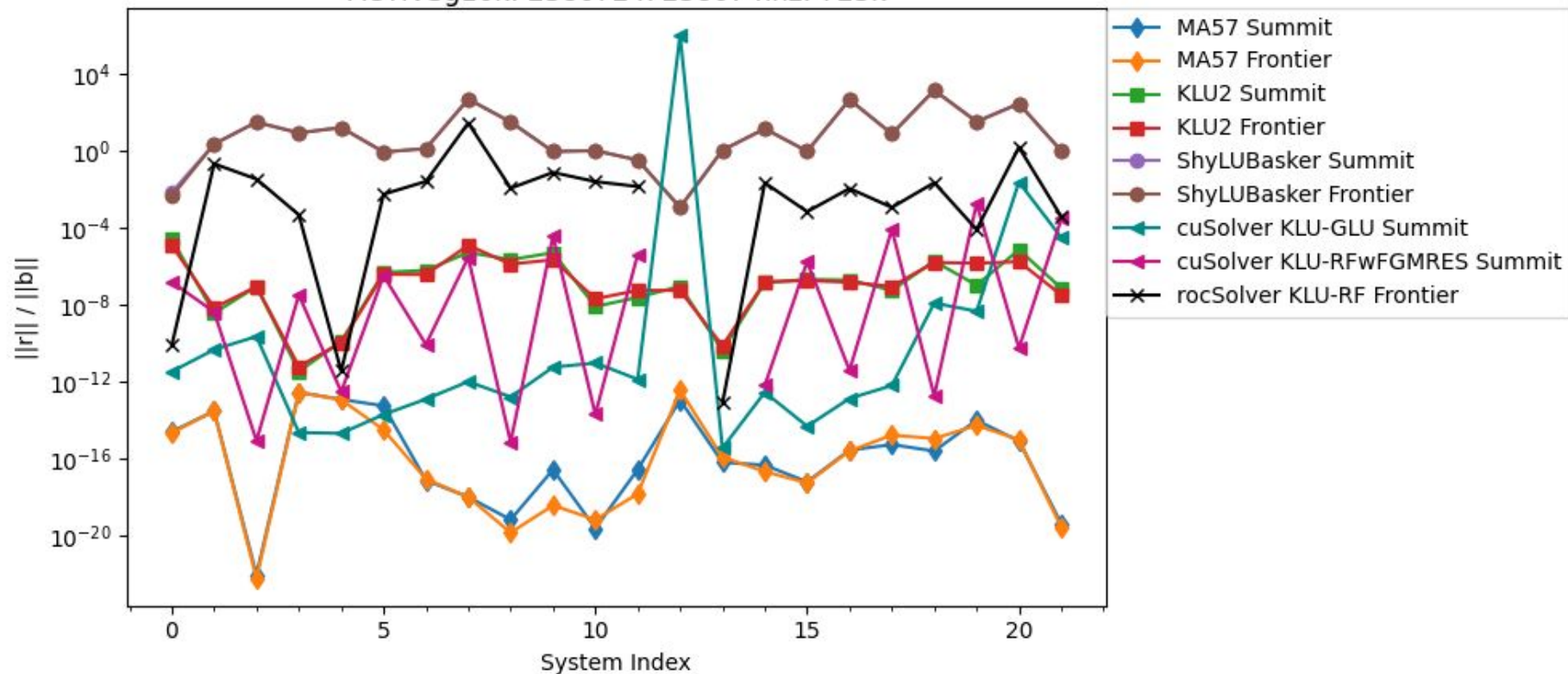


Figure 4. Relative residuals for the Western US (10k-bus) matrix market files. A data point for rocSolver at index 12 was omitted where the solution failed to converge. MA57 is the the most stable, while ShyLUBasker and rocSolver have very poor accuracy for the Western US grid.



## Total Computation Time - Eastern US Grid

ACTIVSg70k: 1640411 x 1640411 nnz: 5m

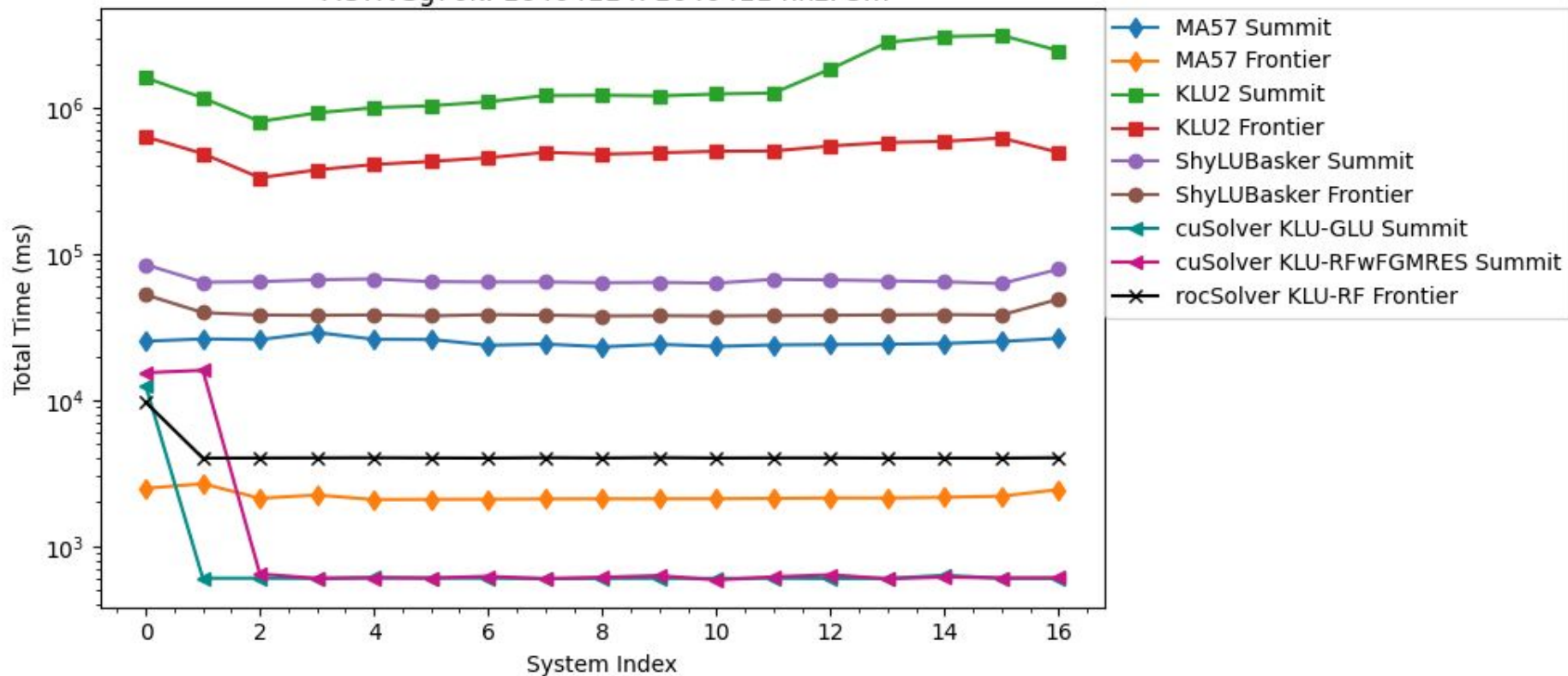


Figure 5. Total runtimes for the Eastern US (70k-bus) matrix market files. KLU2 performs significantly worse than all other solvers for the Eastern US test case and rocSolver performs better than MA57 on Summit.

# Relative Residuals - Eastern US Grid

ACTIVSg70k: 1640411 x 1640411 nnz: 5m

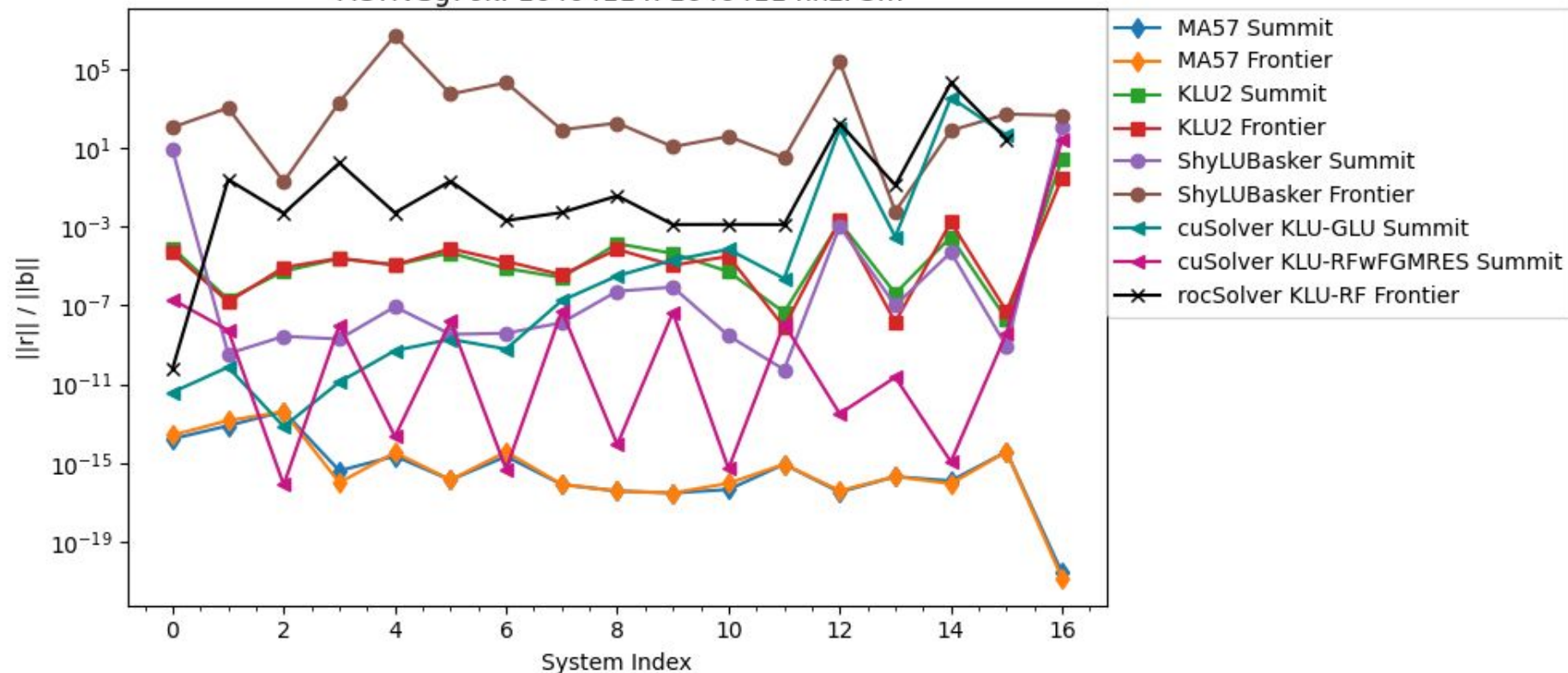


Figure 6. Relative residuals for the Eastern US (70k-bus) matrix market files. MA57 is the most stable, while ShyLUBasker and rocSolver is the least accurate overall for handling Eastern US test cases. Data points for rocSolver and cuSolver KLU-GLU at index 16 were omitted where the solution failed to converge.

# 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.
- 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.

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# Questions?

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[KLU2 header](#)