Towards More Efficient Krylov and Multigrid Methods For PDE Based Systems

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Introduction

Modern applications often lead to large sparse linear systems arising from various PDE discretizations. Krylov subspace(KSP) methods are widely used in solving such systems.

Non-symmetric systems:
- Arise from PDE discretizations
- Boundary/jump conditions
- No KSP method is apparently optimal

Goals:
- Perform a systematic comparison
- Establish practical guidelines in choosing the best combinations of the pre-conditioned KSP solvers
- Develop a self-adapting framework to improve the productivity and efficiency of PDE based modeling

Multigrid Methods:
- Most sophisticated preconditioners
- Based on stationary iterative methods, accelerate the convergence by series of coarser representations
- Various parameters determine the performance

Comparison Setup

KSP methods:
- We consider four KSP methods, restarted GMRES(30), TFQMR, BiCGSTAB, QMRCGSTAB
- Perform detailed comparison based on Krylov subspaces, operation count, memory requirements

Preconditioners:
- We use right preconditioners considering the erratic behavior of the left preconditioners
- Focus on Gauss-Seidel, Incomplete LU (ILU), algebraic multigrid (AMG) preconditioners coupled with KSP methods

Benchmark Problems:
- We generate 2D and 3D benchmark problems using PDE discretizations (FEM, AES-FEM, GFD) at different resolutions
- DG and Mixed-FEM generated using FEniCS software

Hardware Used:
- High-performance LI-RED computing system at the Institute for Advanced Computational Science of Stony Brook University

Summary of test cases :

Matrix	Discretization	PDE	Size	nnz	Cond. No.
1	FEM 2D	Conv. Diff.	1,044,226	7,301,314	8.31e5
2	FEM 3D	Conv. Diff.	237,737	1.819,743	8.90e3
3	FEM 3D	Conv. Diff.	1,529,235	23,946,925	3.45e4
4	FEM 3D	Conv. Diff.	13,110,809	197,881,373	-
5	AES-FEM 2D	Conv. Diff.	1,044,226	13,484,418	9.77e5
6	AES-FEM 3D	Conv. Diff.	13,110,809	197,882,439	-
7	GFD 2D	Conv. Diff.	1,044,226	7,476,484	2.38e6
8	GFD 3D	Conv. Diff.	1,529,235	23,948,687	6.56e4
9	FDM 2D	Helmholtz	1,340,640	6,694,058	7.23e8
10	DG 2D	Advec. diff.	540,000	6,649,200	9.40e6
11	DG 2D	Advec. diff.	1,033,350	12,385,260	1.80e7
12	DG 3D	Advec. diff.	1,536,000	30,412,800	-
13	MIXED-POIS 2D	Mixed Pois.	1,156,720	12,421,400	8.86e4
14	MIXED-POIS 3D	Mixed Pois.	3,863,700	82,668,600	-

Example Numerical Results

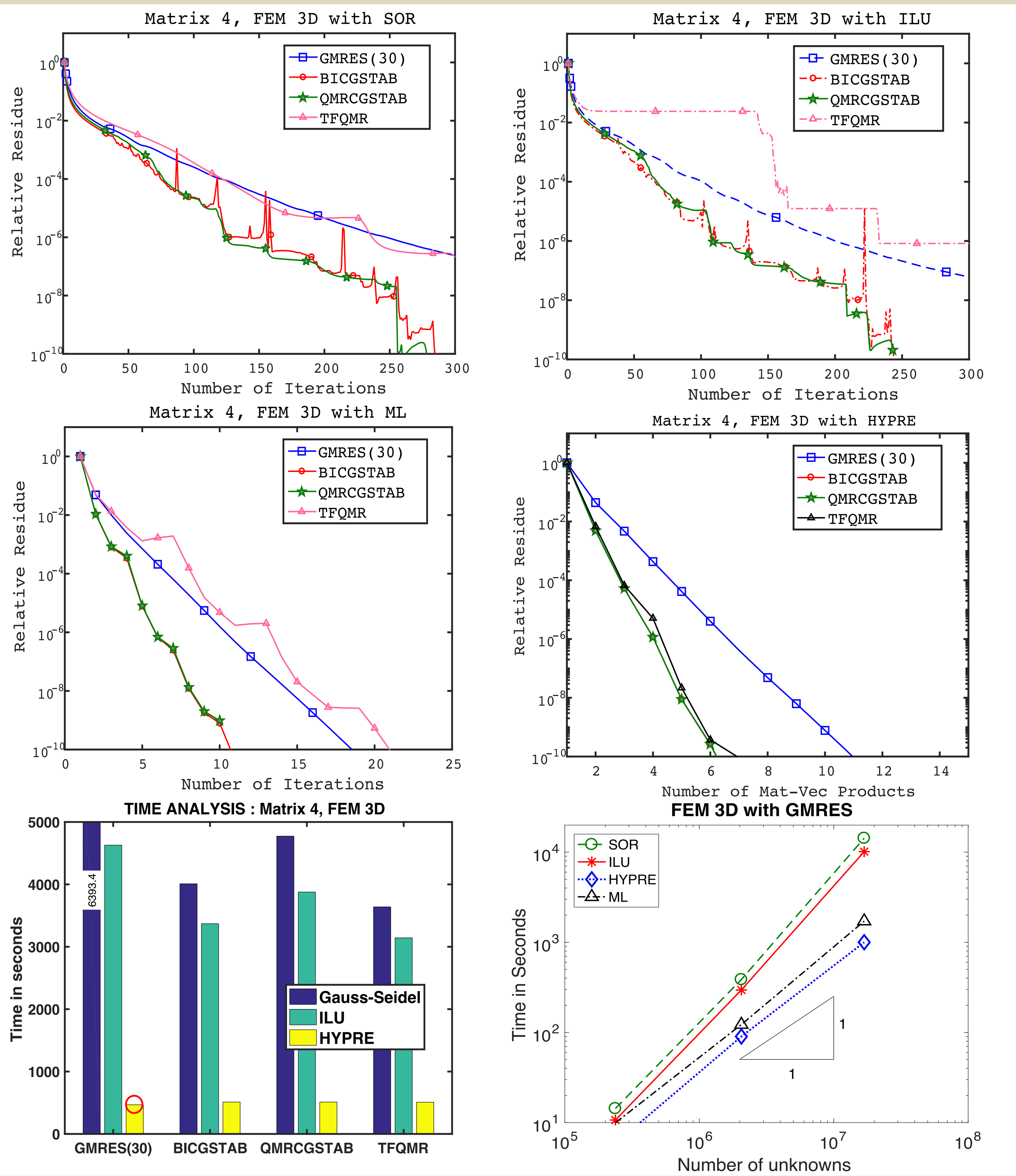


Figure 1: Convergence, timing and scalability results for FEM 3D

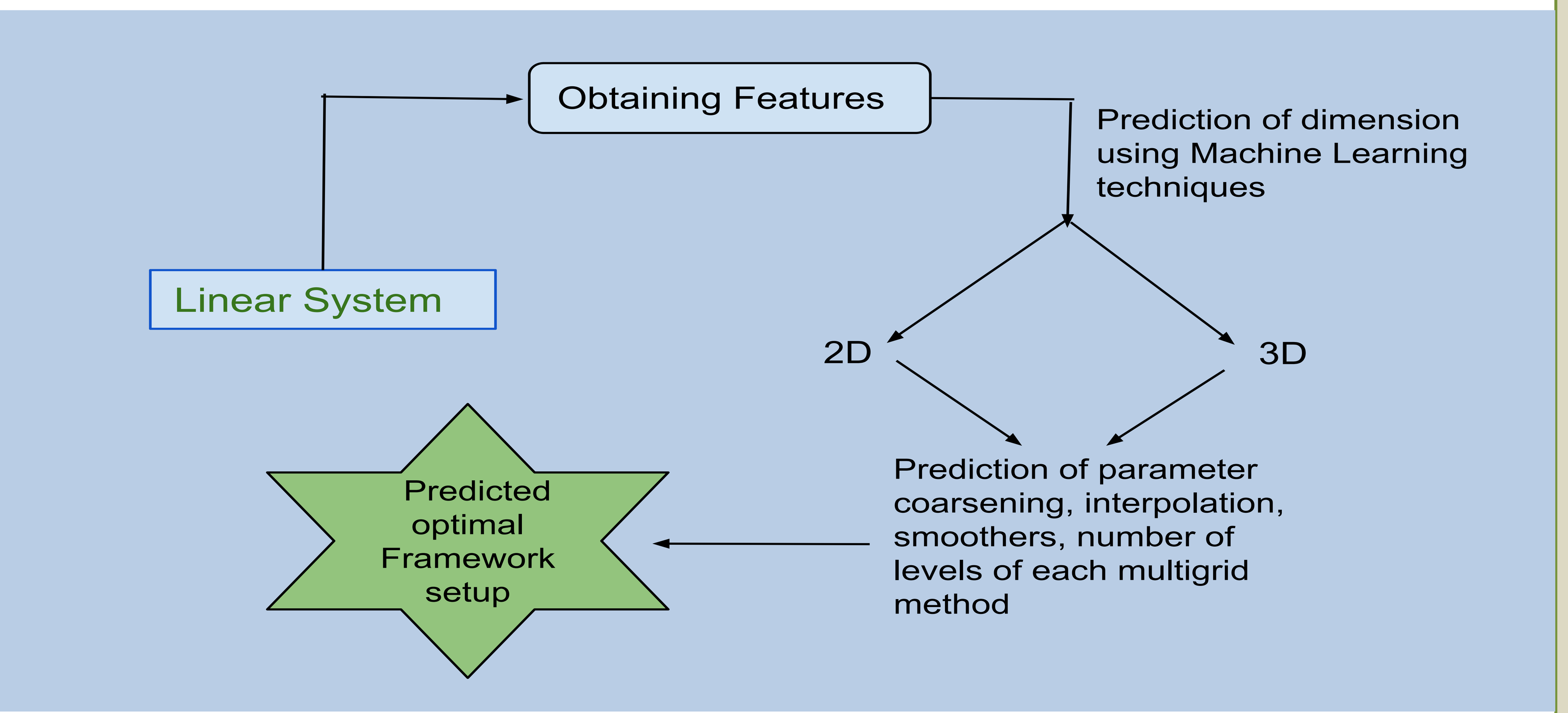
Recommendations:
- For a very large linear system
  - GMRES with classical AMG as right preconditioner
  - For HYPRE:
    - Strength threshold 0.25, truncating max elements per row for interpolation operator to 4, SOR/Jacobi smoother
    - 2D Parameters
      - Well conditioned system: PMIS coarsening, FF1 interpolation
      - Ill- conditioned : HMIS coarsening, FF1 interpolation
    - 3D Parameters: PMIS coarsening, FF1 interpolation
- If AMG is unavailable, and moderate problem size
  - BiCGSTAB with ILU as right preconditioner
- Zero-diagonal systems need to be addressed using ILUTP implementation (such as that in SuperLU)

Limitations:
- Parameter tuning can be problem dependent and tricky in some cases
- Most methods fail to converge or are inefficient for zero-diagonal problems
- Further development needed for better framework which overcomes the shortcomings and hence can be more efficient and robust

Further Improvements

The further improvements will cater two main ideas
- Prediction of the parameters
- Hybrid multigrid with more sophisticated smoothers (ILUTP)

Overall workflow towards the Adaptive Multigrid Framework selection process



Proposed Predictive Framework:
- Framework is adaptive, adjusts the parameters automatically using machine learning techniques, based on the type of the problem and its features (nnz, condition number, dimension, etc.)
- This self-adapting framework can make the parameter tuning much easier and effective

Proposed Hybrid Framework with ILUTP as smoother:
- Combining the ideas of algebraic multigrid with tuned parameters, geometric multigrid and p-multigrid
- Further development on ILUTP as a smoother for algebraic multigrid to increase the the robustness of multigrid especially for the zero-diagonal problems

Conclusions

- Classical AMG with fine-tuned parameters delivers better performance and exhibits better scalability than smoothed-aggregation AMG
- When other methods fail or stagnate, ILUTP may succeed
- By combining the above two ideas we propose an automated adaptive framework
- With capability of parameter prediction and efficiency of both multigrid methods and ILUTP, we can make PDE modeling more robust and effective

References

[Ghai A, Lu C, Jiao X. Comparison of Preconditioned Krylov Subspace Methods for Nonsymmetric Linear Systems. 2016 Preprint: http://arxiv.org/abs/1607.00351

Acknowledgements

Partially supported by DoD-ARO under contract #W911NF0910306 , in part by a subcontract to Stony Brook University from Argonne National Laboratory under Contract DE-AC02-06CH11357 for the SciDAC program of the U.S. DOE. Also supported by NSF under grant #ags1418309.