CAS 741 (Development of Scientific Computing Software)

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MPIR Verification and Validation Plan

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General Information

- MPIR is a sparse linear solver designed to solve large, sparse real matrices efficiently.
- It uses the General Minimal Residual (GMRES) method for internal matrix solves and iterative refinement techniques to improve both speed and accuracy.
- Intended for use in computational science, engineering, and numerical analysis applications.
- As a complete library suite, the software also includes example programs to demonstrate the solver interfaces and practical use cases of the solver.

Inputs

Variable	Description
Α	$n \times n$ matrix
b	<i>n</i> -vector
U_f	factorization precision
u_w	working precision
u_r	precision in which the residuals are computed

VnV Objectives

Primary Ensure the correctness, accuracy, and efficiency of MPIR in solving sparse linear systems.

Secondary Verify usability and maintainability of the software for integration with other numerical libraries.

Out of Scope Usability testing for non-expert users is not prioritized. External libraries used for matrix factorization, reading and writing sparse matrices in Matrix Market Exchange Format (*Matrix Market: File Formats* 2013), unit testing, and performance benchmarking are assumed to be correct.

VnV Team

Team Member	Role
Joe Ye	Lead developer and tester
Maris Chen	"Domain expert", provides feedbacks on
	documents per course guidelines and doc- ument templates
Dr. Nedialkov	Primary stakeholder, oversees project direction and validates all documents

Functional System Testing: Correctness and Accuracy

- Define acceptance criteria in terms of machine epsilon, the smallest difference in value that the computer can tell apart at a given precision.
- The condition number cond(A) is an important factor when choosing inputs.

Floating-Point Format	Machine Epsilon ($\epsilon_{ m mach}$)
bfloat16	3.91×10^{-3}
fp16 (IEEE 754 Half)	4.88×10^{-4}
fp32 (IEEE 754 Single)	1.19×10^{-7}
fp64 (IEEE 754 Double)	2.22×10^{-16}
fp128 (IEEE 754 Quad)	1.93×10^{-34}

The Known Solution Vector Approach

Test against manufactured solutions:

- 1. $\mathbf{x}_{ref} \leftarrow random \ vector$
- 2. $\mathbf{b} \leftarrow \mathbf{A} \mathbf{x}_{ref}$
- 3. Solve $\mathbf{A}\mathbf{x} = \mathbf{b}$
- 4. $e \leftarrow \frac{\|\mathbf{x} \mathbf{x}_{\text{ref}}\|_2}{\|\mathbf{x}_{\text{ref}}\|_2}$

Caveats:

- Large error does not necessarily mean the solver is incorrect. If cond(A) is large, the error is likely to be large as well.
- For well-conditioned matrices, e.g. $\operatorname{cond}(\mathbf{A}) < 10^4$, the relative error is expected to be $e \approx 10^{-12}$ in double precision $(\epsilon_{\mathrm{mach}} \approx 2.2 \times 10^{-16})$

The Trusted Solver Comparison Approach

- MATLAB® vpa
- Other readily available sparse solvers

The relative error, $e = \frac{\|\mathbf{x} - \mathbf{x}_{\mathrm{ref}}\|_2}{\|\mathbf{x}_{\mathrm{ref}}\|_2}$ should be within a reasonable multiple of ϵ_{mach} across a set of test problems.

Functional System Testing: the Plan

- Start with numerically stable inputs (well conditioned A) without mixed-precisions. Verify accuracy with both the "known solution vector" and "trusted solver comparison" approach.
- Hypothesize that the solver is able to solve systems with condition number up to COND_MAX. Test robustness by inputting ill-conditioned matrices with cond(A) at different magnitudes. (Non-functional?)
- 3. Hypothesize that the solver is able to maintain accuracy when mixed-precision technique is applied. Test accuracy by inputting different combinations of u_f , u_w , u_r .

Functional System Testing: an Example

test-id1 Control: Automatic

Initial State: matrix ${f A}$ is read from file and stored in memory. Expected exact solution ${f x}_{\rm ref}$ is prepared.

Input: matrix \boldsymbol{A} of size $10\,000\times10\,000$ with

$$\operatorname{cond}(\mathbf{A}) \approx 10^2$$
, **b** of size 10000, $u_f = u_w = u_r = \operatorname{double}$

Output: x of size 10 000 such that

$$e = \frac{\|\mathbf{x} - \mathbf{x}_{\text{ref}}\|_{2}}{\|\mathbf{x}_{\text{ref}}\|_{2}} < 10^{-12}$$

Test Case Derivation: $\mathbf{x}_{\mathrm{ref}}$ is randomly generated.

$$\mathbf{b} = \mathbf{A} \mathbf{x}_{\mathrm{ref}}$$

How test will be performed: Automatic

Non-Functional System Testing: Performance

Choice of performance metric?

- Convergence rate?
- Computation time/Wall-clock time

Potential Problems with Measuring Runtime

- CPU clock frequency, temperature; Caching
- OS scheduling, interrupts, context switching
- Hardware optimizations specifically for certain arithmetic/precision; CPU vs. GPU
- Inconsistency between runs, hard to reproduce results

Established Tools for Benchmarking

google/benchmark 2025

- Repeats benchmark cases until a statistically stable result is obtained
- Automatic CPU frequency scaling adjustments

Non-Functional System Testing: the Plan

1. Hypothesize that the use of mixed-precision technique brings consistent improvement in runtime. Given well-conditioned inputs, benchmark runtime by varying u_f , u_w , u_r .

References



google/benchmark (Feb. 14, 2025). original-date:

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https://github.com/google/benchmark (visited on 02/14/2025).



Matrix Market: File Formats (Aug. 14, 2013). The Matrix Market, URL:

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Questions