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Reproducible and Accurate Parallel Triangular Solver

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ICIAM 2019, Valencia, Spain.
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IEEE-754 Floating-Point Numbers

- Approximate real numbers on computer.
- \( f = \pm \text{mantissa} \cdot 2^{\text{exponent}} \).
- IEEE-754 standard defines formats and rounding modes.
- \textit{binary64} and RTN in this talk.

Floating-Point Operations

- For \( x, y \in \mathbb{F} \) and \( x + y \notin \mathbb{F} \), \( x + y \neq x \oplus y = \text{round}(x + y) \).
- The same applies for \( \ominus \), \( \otimes \) and \( \oslash \).

Operation Order Matters: FP Addition is not Associative

- \( a \oplus (b \oplus c) \neq (a \oplus b) \oplus c \).
- For \textit{binary64}'s round-off unit \( u = 2^{-53} \):
  \[ 0 = -1 \oplus (1 \oplus u) \neq (-1 \oplus 1) \oplus u = u. \]
Does Numerical Reproducibility Matter?

Numerical Reproducibility and HPC

- Reproducibility: bitwise *identical* results for every \( p \)-parallel run, \( p \geq 1 \)
- Reproducibility \( \neq \) Accuracy
- How to **debug**? to **test**? to **validate**? to receive legal agreements?
  - Debug: rounding errors vs. bugs? reproduce errors?
  - Validate: reproduce *the* reference result? the same results from one run to another?

In Practice?


Telemac2D simulation: a white plot displays a non reproducible result (Nheili *et al.*, 2016)

1 proc., \( t = 0.2 \text{sec.} \) | 2 proc., 0.2 sec. | 2 proc., 0.8 sec. | 2 proc., 1.4 sec.
Strategies for Reproducibility

- Static order of operations
  - Static scheduling.
  - Deterministic Reduction.
  - Intel MKL Conditional Numerical Reproducibility (CNR).

- Pre-rounding Techniques.
  - ReprodSum and FastReprodSum (Demmel et al., 2013).
  - **Indexed (Binned) floating-point format** (Demmel et al., 2016).
    - Used in ReproBLAS library\(^a\).

- Higher precision (Villa et al., 2009, Iakymchuk et al., 2015).

**Correctly rounded** (Chohra et al., 2016).

\(^a\)http://bebop.cs.berkeley.edu/reproblas/
Rounding Errors and Reproducibility

Our Aim

RARE-BLAS (2017-)

- Reproducible, Accurately Rounded and Efficient BLAS\(^a\)
- Parallel BLAS 1: correctly rounded `dot` and `asum`, reproducible and faithfully rounded `nrm2`
- Parallel BLAS 2: correctly rounded `gemv`
- Accuracy vs. efficiency
  - Chose and tune summation algorithms wrt. architecture and problem constraints.
  - SIMD (AVX2-512), openMP, MPI
  - Run-time overhead ratio: \(\times 1 \rightarrow \times 10\)

\(^a\)https://gite.lirmm.fr/rare-blas-group/rare-blas

Today: Reproducible Parallel `trsv`

- Provide a reproducible, accurate and efficient triangular solver.
- Two different approaches are presented and compared.
- Performance evaluation on CPU and Intel Xeon Phi accelerator.
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Given a lower triangular \( n \times n \)-matrix \( T \) and \( n \)-vector \( b \).

Find \( x \) such that \( Tx = b \).

Forward substitution: \( x_i = \left( b_i - \sum_{j=1}^{i-1} t_{i,j} \times x_j \right) / t_{i,i} \).

Dependency of \( x_i \) wrt. \( x_j \), \( j < i \).
Parallel Triangular Solver

Triangular Solver: Sequential but SIMD-zed

Sequential computation
- $x_1 = b_1 / t_{1,1}$.
- $x_i = (b_i - \sum_{j=1}^{i-1} t_{i,j} \times x_j) / t_{i,i}$.

Sources of non reproducibility
- Dot product accumulation
- SIMD lengths
- SIMD reduction schemes

Philippe Langlois (UPVD)
Reprod TRSV
ICIAM 2019, Valencia, Spain
Parallel Triangular Solver

Triangular Solver: Parallel Case

Parallel Process
- \textit{trsv}: sequential.
- \textit{gemv}: parallel.

Parallel computation
- \[ x_i = \left( b_i - \sum_{j=1}^{r} t_{i,j} \times x_j \right. \]
- \[ \left. - \sum_{j=r+1}^{2r} t_{i,j} \times x_j \right) - \sum_{j=2r+1}^{i-1} t_{i,j} \times x_j \right) / t_{i,i}. \]

Sources of non reproducibility
- Dot product: partial accumulations wrt. block size \( r \)
- Accumulation order wrt. \textit{gemv} scheduling
- \textit{gemv}: SIMD lengths, SIMD reduction schemes
Rounding Errors and Reproducibility

Parallel Triangular Solver

Reproducible Triangular Solvers
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Accuracy and Performance

Conclusion and Future Works
Trade-off

Efficiency vs. Accuracy vs. Reproducibility

**RTrsv**
- Correctly rounded $b_i - \sum_{j=1}^{i-1} t_{i,j} \times x_j$
- EFT: TwoProd, HybridSum (Zhu-Hayes, 2009)

**BinnedTrsvIR**
- Reproducibility: BinnedTrsv
  - Binned accumulation à la Demmel-Nguyen’s ReproBLAS.
  - Efficiency: “only” target reproducibility
- Accuracy: Iterative refinement
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Parallel Process

- EFT blocks use HybridSum to transform several rows in parallel.
- \textit{trsv} blocks build on previous transformation to ensure correctly rounded \( b_i - \sum_{j=1}^{i-1} t_{i,j} \times x_j \) and then divide it by \( t_{i,i} \).
Error-Free Transformation for summation

\[ V \]

\[ \text{Split}(v_j, H, L) \]

\[ C_{\exp}(L) + = L \]

\[ C_{\exp}(H) + = H \]

\[ \sum_{j=1}^{n} v_j = \sum_{j=1}^{2048} c_j \]
Reproducible Triangular Solvers

Error-Free Transformation for t_\text{rsv}

\[ T[i, :] X[\cdot] \]

\[ C \]

\[ \text{TwoProd}(t_{i, j}, x_j) \]

\[ \text{result} \]

\[ \text{error} \]
Error-Free Transformation for \texttt{trsv}

\[ T[i, :] X[j] \]

\[ \text{TwoProd}(t_{i,j}, x_j) \]

\[ \text{error} \]

\[ \text{result} \]

\[ C \]
Error-Free Transformation for \texttt{trsv}

\[
\begin{align*}
    b_i - \sum_{j=1}^{m} t_{i,j} \times x_j - \sum_{j=m+1}^{i-1} t_{i,j} \times x_j &= \sum_{j=1}^{2048} C_j
\end{align*}
\]
First Results (detail later)

Reproducible but a bit disappointing

- Reproducible solver
- but correctly rounded accumulation $\not\Rightarrow$ solution accuracy improvement
- with run-time overhead.
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Reproducible Triangular Solvers BinnedTrsvIR

BinnedTrsv: Relies on Indexed Floating-Point Format

Parallel Process
- The input matrix is recursively decomposed into:
  - Square GEMV blocks.
  - Triangular TRSV blocks.
- Sequential small TRSV blocks
- Parallel GEMV blocks.

Reproducibility
- FP multiplications and divisions
- All accumulations are performed into a $n$-vector of Indexed FP numbers: one for every $x_i$
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

\[ p_i = \sum_k v_k \]

\[ v_1 \]
\[ v_2 \]
\[ v_3 \]
\[ \vdots \]
\[ v_n \]
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

Fixed exponent range decomposition

\[ p_i = \sum_{k} v_k \]

\[ v_1, v_2, v_3, \ldots, v_n \]
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

De facto parallel sharing

\[ p_i = \sum_{k=1}^{n} v_k \]

\[ \text{Thread 0} \]
\[ \text{Thread 1} \]
\[ \text{Thread 2} \]
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

Independent first significant shrunk

\[ p_i = \sum_{k=1}^{n} v_k \]

Thread 0

Thread 1

Thread 2
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

Operand splitting: $K = 1$

$p_i = \sum_{k=1}^{K} v_k$

Thread 0

Thread 1

Thread 2
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

Operand splitting: $K = 2$

$$p_i = \sum_{k} v_k$$

Thread 0

Thread 1

Thread 2
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

“Exact” thread accumulations

$p_i = \sum_k v_k$

Thread 0

Thread 1

Thread 2
"Exact" reduction and final rounding

\[ p_i = \sum_k v_k \]

\( v_1 \)
\( v_2 \)
\( v_3 \)
\( \vdots \)
\( v_n \)

Thread 0
Thread 1
Thread 2
### Reproducible Iterative Refinement

1. Solve the system with *BinnedTrsv* and $K = 2$.
   - Reproducibility
   - Tradeoff efficiency vs. initial accuracy

2. Compute $r^{(i)} = b - T\hat{x}$ using higher precision.
   - $\times \rightarrow$ TwoProd
   - Higher precision indexed FP numbers: $K = 3$
   - Parallel and reproducible

3. Solve the system $A d^{(i)} = r^{(i)}$ with reproducible *BinnedTrsv*

4. Update $\hat{x} = \hat{x} + d^{(i)}$.

5. Repeat from 2 until $\hat{x}$ is accurate enough.
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Accuracy and Performance

Experimental Framework: Hardware and Software Configurations

CPU Configuration
- Dual Intel Xeon E5-2650 v2 16 cores (8 per socket).
- Memory bandwidth 59.7 GB/s.

Many-core Accelerator
- Intel Xeon Phi 7120 accelerator, 60 cores.
- Memory bandwidth 352 GB/s.

Compiler and Options
- Intel compiler (17.0.1)
- Intel OpenMP 5.0
- `-O3 -fp-model double -fp-model strict -funroll-all-loops`
  - `-fp-model double`: rounds intermediate results to 53-bit precision
  - `-fp-model strict`: disable contractions
### Experiments

- **System size**
  - **Accuracy:** \( n = 1000 \)
  - **Run-time:** \( n \in [10000, 15000] \)

- **\( \text{Cond}(T, x) = \| T^{-1} \| T \| x \| \infty / \| x \| \infty \)**
  - **Accuracy:** \( \text{Cond} \in [10^5, 10^{15}] \)
  - **Run-time:** \( \text{Cond} = 10^8 \)

- **Reference solution:** \( \tilde{x} = \text{MPFR}(T^{-1}b) \)

- **Relative error:** \( \| \tilde{x} - \hat{x} \| \infty / \| \tilde{x} \| \infty \)

- **Normalized Residual:** \( \| b - T\hat{x} \| \infty / \| b \| \infty \)

### Challenging solutions

- **Accuracy:** Intel MKL Trsv (b64)
- **High accuracy:** XBLAS double-doubled Trsv
- **Performance:** Intel MKL Trsv
**Accuracy and Performance**

**Reproducible Solvers: Accuracy Results**

- **Relative error**
  - Log10 of the Forward Relative Error
  - Log10 of the Condition Number
  - MKLTrsv, Rtrsv, BinnedTrsv, BinnedTrsvIR, XBLASTrsv

- **Normalized residual**
  - Log10 of the Normalized Residual
  - Log10 of the Condition Number
  - MKLTrsv, Rtrsv, BinnedTrsv, BinnedTrsvIR, XBLASTrsv

- **Accuracy:** correctly rounded (RTrsv) vs. reproducible (BinnedTrsv) dot prods → slightly but not significantly better
- **More accuracy:** similar and classic iterative refinement effect
- **Residual:** no condition effect, nor solution accuracy significance, slight effect of the correctly rounded version (RTrsv)
Reproducible Solvers: Performance Results

Run-time overhead ratio vs. MKL Trsv, Cond = 10^8.

<table>
<thead>
<tr>
<th></th>
<th>Sequential</th>
<th>Parallel CPU</th>
<th>Parallel Accelerator</th>
</tr>
</thead>
<tbody>
<tr>
<td>RTrsv</td>
<td>×10</td>
<td>×5</td>
<td>×5 – 10</td>
</tr>
<tr>
<td>BinnedTrsv</td>
<td>×2</td>
<td>×1</td>
<td>×0.7 – 1.2</td>
</tr>
<tr>
<td>BinnedTrsvIR</td>
<td>×15 – 20</td>
<td>×8 – 10</td>
<td>×2</td>
</tr>
</tbody>
</table>

Note: no accelerator benefit (trsv dependencies – as it)

- Parallel solutions scale well
- Reproducibility: from no over-cost to very reasonable cost with BinnedTrsv
- Accuracy cost: not free (iterative refinement) but interesting for accelerator
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Conclusion

- Numerical reproducibility for SIMD, multi-core, many-core architectures
- Accuracy: similar to XBLAS
- Run-time performance (vs. MKLTrsv):

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</tbody>
</table>

Future Works

- Higher level BLAS: compute bound algorithms ⇒ need for other strategies
- Auto tuning to easy optimization
- Build a reproducible LAPACK upon RARE-BLAS