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To cite this version:
Chemseddine Chohra, Philippe Langlois, David Parello. Reproducible and Accurate Parallel Triangular Solver. 9th International Congress on Industrial and Applied Mathematics (ICIAM), Jul 2019, Valencia, Spain. lirmm-02427986

HAL Id: lirmm-02427986
https://hal-lirmm.ccsd.cnrs.fr/lirmm-02427986
Submitted on 4 Jan 2020

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Reproducible and Accurate Parallel Triangular Solver

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July, 17\textsuperscript{th} 2019

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.
- *binary64* and RTN in this talk.

Floating-Point Operations

- For \( x, y \in \mathbb{IF} \) and \( x + y \notin \mathbb{IF} \), \( x + y \neq x \oplus y = \text{round}(x + y). \)
- 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 *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., $t = 0.2$ 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/
Our Aim

RARE-BLAS (2017-)

- Reproducible, Accurately Rounded and Efficient BLAS
- 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: $\times 1 \rightarrow \times 10$

*ahttps://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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Parallel Triangular Solver

From Classic Forward Substitution to Parallel trsv

Triangular solver

- 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. $x_j$, $j < i$. 
Sequential computation:

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

Sources of non reproducibility:

- Dot product accumulation
- SIMD lengths
- SIMD reduction schemes
Parallel Triangular Solver

Triangular Solver: Parallel Case

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

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

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
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Reproducible Triangular Solvers

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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RTrsv: Relies on HybridSum (Zhu-Hayes, 2009)

Parallel Process

- EFT blocks use HybridSum to transform several rows in parallel.
- 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

\[ V \]

Split \((v_j, H, L)\)

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

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

\[ \sum_{j=1}^{2048} v_j = \sum_{j=1}^{2048} c_j \]
Error-Free Transformation for \texttt{trsv}

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

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

\[ \text{result} \]

\[ X[:] \]

\[ C \]

\[ b_i - \sum_{m} t_{i,j} \times x_j - \sum_{i}^{m+1} t_{i,j} \times x_j = \sum_{j=1}^{C} x_j \]

Philippe Langlois (UPVD)
Error-Free Transformation for \texttt{trsv}

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

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

\[
\text{result}
\]

\[
\text{Parallel EFT}
\]

\[
C
\]
Error-Free Transformation for trsv

\[ C_i = \sum_{j=1}^{2048} C_j \]

\[ b_i - \sum_{j=1}^{m} t_{i,j} \times x_j - \sum_{j=m+1}^{i-1} t_{i,j} \times x_j = \sum_{j=1}^{2048} C_j \]
Reproducible but a bit disappointing

- Reproducible solver
- but correctly rounded accumulation $\Rightarrow$ solution accuracy improvement
- with run-time overhead.
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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

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

Thread 0
Thread 1
Thread 2
De facto parallel sharing

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

Thread 0

Thread 1

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

Independent first significant shrunk

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

$$v_1$$

$$v_2$$

$$v_3$$

\ldots

$$v_n$$

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
Operand splitting: $K = 2$

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

<table>
<thead>
<tr>
<th>$v_1$</th>
<th>$v_2$</th>
<th>$v_3$</th>
<th>...</th>
<th>$v_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Thread 0

Thread 1

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

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

“Exact” thread accumulations

\[
\begin{align*}
&v_1 & \quad & \text{Thread 0} \\
&v_2 & \quad & \text{Thread 1} \\
&v_3 & \quad & \text{Thread 2} \\
&\vdots & \quad & \\
&v_n & \quad & \\
\end{align*}
\]
“Exact” reduction and final rounding

\[ p_i = \sum k v_k \]

Thread 0
Thread 1
Thread 2

\( v_1 \)
\( v_2 \)
\( v_3 \)
\( \vdots \)
\( v_n \)
Reproducible Triangular Solvers

BinnedTrsvIR: BinnedTrsv + Iterative Refinement

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 $Ad^{(i)} = r^{(i)}$ 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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### 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
## Accuracy and Performance Experiments

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

### Cond (\( T, x \))
\[
\text{Cond}(T, x) = \frac{\| |T^{-1}| |T||x|\|_{\infty}}{\|x\|_{\infty}}
\]
- **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
Reproducible Solvers: Accuracy Results

- 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):

<table>
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<th>Parallel Accelerator</th>
</tr>
</thead>
<tbody>
<tr>
<td>RTrsv</td>
<td>×10</td>
<td>×5</td>
<td>×5 − 10</td>
</tr>
<tr>
<td>BinnedTrsvIR</td>
<td>×15 − 20</td>
<td>×8 − 10</td>
<td>×2</td>
</tr>
</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