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HAL Id: lirmm-02427986
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Submitted on 4 Jan 2020

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Reproducible and Accurate Parallel Triangular Solver

Chemseddine Chohra\textsuperscript{1}, Philippe Langlois\textsuperscript{2} and David Parello\textsuperscript{2}

\textsuperscript{1}University 8 Mai 1945 Guelma, LabSTIC, Algeria
\textsuperscript{2}DALI-LIRMM, U. Perpignan Via Domitia, U. Montpellier, CNRS, France

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 \( u = 2^{-53} \):
  \( 0 = -1 \oplus (1 \oplus u) \neq (-1 \oplus 1) \oplus u = u \).
Rounding Errors and Reproducibility

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.
How to Solve Numerical Reproducibility Problems?

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\(^a\)
- Parallel BLAS 1: correctly rounded \texttt{dot} and \texttt{asum}, reproducible and faithfully rounded \texttt{nrm2}
- Parallel BLAS 2: correctly rounded \texttt{gemv}
- Accuracy vs. efficiency
  - Chose and tune summation algorithms \textit{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 \texttt{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.
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

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

Sources of non reproducibility

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

Triangular Solver: Parallel Case

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

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

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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Reprod TRSV
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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
# Reproducible Triangular Solvers

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

- 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 $t_{i,i}$. 

Parallel Process
Error-Free Transformation for summation

\[ V \]

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

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

\[ \sum_{j=1}^{n} v_j = \sum_{j=1}^{2048} c_j \]
Error-Free Transformation for \( \text{trsv} \)

\[
T[i, \cdot] X[\cdot] \quad \text{TwoProd}(t_i, j, x_j) \quad \text{result} \quad \text{error}
\]

\[
\begin{align*}
&b_i - \sum_{m=j+1}^{t_i, j} x_j - \sum_{i=2048}^{j} C_j \quad \text{error} \quad \text{result}
\end{align*}
\]
Error-Free Transformation for \texttt{trsv}

\[ \begin{align*}
T[i,:,:] X[\cdot] & \rightarrow \text{TwoProd}(t_{i,j}, x_j) \\
\text{result} & \rightarrow \text{error} \\
C & \rightarrow \text{Parallel EFT}
\end{align*} \]
Error-Free Transformation for trsv

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

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

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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

\[ p_i = \sum_k v_k \]

\( p_i \) = \sum_k v_k

\( v_1 \)

\( v_2 \)

\( v_3 \)

\( \vdots \)

\( v_n \)
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

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

*De facto* parallel sharing

\[ E_{\text{max}} \quad \text{Thread 0} \]

\[ \text{Thread 1} \]

\[ \text{Thread 2} \]

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

Independent first significant shrunk

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

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: $K = 2$

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

Thread 0

Thread 1

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

"Exact" thread accumulations

\[ p_i = \sum_k v_k \]

- \( v_1 \) Thread 0
- \( v_2 \) Thread 0
- \( v_3 \) Thread 1
- \( \vdots \)
- \( v_n \) Thread 2
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

"Exact" reduction and final rounding

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

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

Thread 0  Thread 1  Thread 2
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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### 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: \( n \in [10000, 15000] \)
- \( \text{Cond}(T, x) = \frac{\| T^{-1} \| T \| x \|_\infty}{\| x \|_\infty} \)
  - 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 = \( \frac{\| \tilde{x} - \hat{x} \|_\infty}{\| \tilde{x} \|_\infty} \)
- Normalized Residual = \( \frac{\| b - T \hat{x} \|_\infty}{\| b \|_\infty} \)

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)
### Accuracy and Performance

## 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>$\times 10$</td>
<td>$\times 5$</td>
<td>$\times 5 - 10$</td>
</tr>
<tr>
<td>BinnedTrsv</td>
<td>$\times 2$</td>
<td>$\times 1$</td>
<td>$\times 0.7 - 1.2$</td>
</tr>
<tr>
<td>BinnedTrsvIR</td>
<td>$\times 15 - 20$</td>
<td>$\times 8 - 10$</td>
<td>$\times 2$</td>
</tr>
</tbody>
</table>

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

### Graphs

- **Sequential**
- **Parallel: CPU**
- **Parallel: Xeon Phi**

- 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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<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