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Reproducible and Accurate Parallel Triangular Solver

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ICIAM 2019, Valencia, Spain.
1 Rounding Errors and Reproducibility

2 Parallel Triangular Solver

3 Reproducible Triangular Solvers
   - RTrsv
   - BinnedTrsvIR

4 Accuracy and Performance

5 Conclusion and Future Works
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 $u = 2^{-53}$:
  - $0 = -1 \oplus (1 \oplus u) \neq (-1 \oplus 1) \oplus u = u$. 
**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.
- Higher precision (Villa et al., 2009, Iakymchuk et al., 2015).
- **Correctly rounded** (Chohra et al., 2016).

[^1]: `http://bebop.cs.berkeley.edu/reproblas/`
Our Aim

RARE-BLAS (2017-)

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

\textsuperscript{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.
1 Rounding Errors and Reproducibility

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**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. $x_j$, $j < i$. 

---

Parallel Triangular Solver

From Classic Forward Substitution to Parallel trsv
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
# Reproducible Triangular Solvers

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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.
- \( trsv \) 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

\[ V \]

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

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

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

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

\[ T[i, :] \times X[:], \text{result} \]

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

\[ \text{error} \]

\[ \sum_{m}^{i-1} t_{i,j} \times x_j - \sum_{i}^{m+1} t_{i,j} \times x_j = \sum_{j}^{2048} C_j \]
Error-Free Transformation for \texttt{trsv}

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

\[
\text{Parallel EFT}
\]

\[
\text{error}
\]

\[
\text{result}
\]

\[
C
\]

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

\[
\text{result}
\]

\[
\text{error}
\]

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

\[
T[i, :] X[j] = \sum_{j=1}^{m} t_{i,j} \times x_j - \sum_{j=m+1}^{i-1} t_{i,j} \times x_j = \sum_{j=1}^{2048} C_j
\]
First Results (detail later)

Reproducible but a bit disappointing

- Reproducible solver
- but correctly rounded accumulation $\implies$ 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)

\[ p_i = \sum_k v_k \]

\begin{align*}
  v_1 & \quad \quad \quad \quad \\
  v_2 & \quad \quad \quad \quad \\
  v_3 & \quad \quad \quad \quad \\
  \vdots & \quad \quad \quad \quad \\
  \vdots & \quad \quad \quad \quad \\
  v_n & \quad \quad \quad \quad 
\end{align*}
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

Fixed exponent range decomposition

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

$v_1$

$v_2$

$v_3$

...$

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

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

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

\[ v_1 \]
\[ v_2 \]
\[ v_3 \]
\[ \vdots \]
\[ v_n \]

Thread 0
Thread 1
Thread 2
Operand splitting: \( K = 1 \)

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

Thread 0

\( v_1 \)

\( v_2 \)

\( v_3 \)

\( \ldots \)

\( v_n \)

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
"Exact" thread accumulations

\[ p_i = \sum_k v_k \]

\begin{align*}
v_1 & \\
v_2 & \\
v_3 & \\
\vdots & \\
v_n & \\
\end{align*}

Thread 0

Thread 1

Thread 2
"Exact" reduction and final rounding

\[ p_i = \sum_k v_k \]

\begin{align*}
  v_1 & \quad \text{Thread 0} \\
  v_2 & \quad \text{Thread 1} \\
  v_3 & \quad \text{Thread 2} \\
  \vdots & \\
  v_n &
\end{align*}
Reproducible Triangular Solvers

BinnedTrsvIR: BinnedTrsv + Iterative Refinement

Reproducible Iterative Refinement

1. Solve the system with $\text{BinnedTrsv}$ and $K = 2$.
   - Reproducibility
   - Tradeoff efficiency vs. initial accuracy

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

3. Solve the system $Ad^{(i)} = r^{(i)}$ with reproducible $\text{BinnedTrsv}$

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: $n \in [10000, 15000]$

- $\text{Cond}(T, x) = \frac{||T^{-1}|| \cdot |T| \cdot |x|}{||x||^\infty}$
  - 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
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.

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<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>
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<td>BinnedTrsvIR</td>
<td>×15 – 20</td>
<td>×8 – 10</td>
<td>×2</td>
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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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Future Works

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