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Reproducible and Accurate Parallel Triangular Solver

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ICIAM 2019, Valencia, Spain.
Rounding Errors and Reproducibility

Parallel Triangular Solver

Reproducible Triangular Solvers
- RTrsv
- BinnedTrsvIR

Accuracy and Performance

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 $u = 2^{-53}$: $0 = -1 \oplus (1 \oplus u) \neq (-1 \oplus 1) \oplus u = u$. 
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)

<table>
<thead>
<tr>
<th>1 proc., $t = 0.2$ sec.</th>
<th>2 proc., 0.2 sec.</th>
<th>2 proc., 0.8 sec.</th>
<th>2 proc., 1.4 sec.</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Image 1" /></td>
<td><img src="image2.png" alt="Image 2" /></td>
<td><img src="image3.png" alt="Image 3" /></td>
<td><img src="image4.png" alt="Image 4" /></td>
</tr>
</tbody>
</table>
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).

*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 \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 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.
Table of Contents

1 Rounding Errors and Reproducibility

2 Parallel Triangular Solver

3 Reproducible Triangular Solvers
   - RTrsv
   - BinnedTrsvIR

4 Accuracy and Performance

5 Conclusion and Future Works
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. $x_j$, $j < i$. 
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
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
Reproducible Triangular Solvers

Table of Contents

1 Rounding Errors and Reproducibility

2 Parallel Triangular Solver

3 Reproducible Triangular Solvers
   - RTrsv
   - BinnedTrsvIR

4 Accuracy and Performance

5 Conclusion and Future Works
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
Table of Contents

1 Rounding Errors and Reproducibility

2 Parallel Triangular Solver

3 Reproducible Triangular Solvers
   - RTrsv
   - BinnedTrsvIR

4 Accuracy and Performance

5 Conclusion and Future Works
RTrsv: Relies on HybridSum (Zhu-Hayes, 2009)

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

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

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

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

\[ \text{error} \]

\[ \text{result} \]

\[ C \]

\[ \text{trsv} \]

\[ b_i - \sum_{m=1}^{t_i, j} x_j - \sum_{i=1}^{j=m+1} t_i, j \times x_j = \sum_{j=1}^{C} x_j \]
Error-Free Transformation for trsv

Parallel EFT

\[ \text{result} \]

\[ \text{error} \]

TwoProd\((t_{i,j}, x_j)\)

\[ t[i, :] \quad X[i] \]

\[ C \]

Philippe Langlois (UPVD)

Reprod TRSV

ICIAM 2019, Valencia, Spain
Error-Free Transformation for \texttt{trsv}

\begin{equation}
\begin{aligned}
    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{aligned}
\end{equation}
Reproducible but a bit disappointing

- Reproducible solver
- but correctly rounded accumulation $\vDash$ solution accuracy improvement
- with run-time overhead.
1. Rounding Errors and Reproducibility
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3. Reproducible Triangular Solvers
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   - BinnedTrsvIR
4. Accuracy and Performance
5. Conclusion and Future Works
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)

\[ p_i = \sum v_k \]

Fixed exponent range decomposition

\( E_{\text{max}} \)

\( \cdots \)

\( E_{\text{min}} \)

\( v_1 \)

\( v_2 \)

\( v_3 \)

\( \vdots \)

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

De facto parallel sharing

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

Thread 0

\( v_1 \)

\( v_2 \)

\( v_3 \)

\( \vdots \)

\( v_n \)

Thread 1

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

Independent first significant shrunk

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

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)

Reproducible Triangular Solvers

“Exact” thread accumulations

\[ p_i = \sum_k v_k \]

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

Thread 0
Thread 1
Thread 2
Indexed Floating-Point Numbers (Demmel-Nguyen, 2016)

\[ p_i = \sum_k v_k \]

"Exact" reduction and final rounding

\[ E_{\text{max}} \quad \rightarrow \quad E_{\text{min}} \]

\( p_i \) = sum\(_i\) \( v_k \)

Thread 0

Thread 1

Thread 2

Philippe Langlois (UPVD)
Reproducible Iterative Refinement

1. Solve the system with \textit{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 \textit{BinnedTrsv}

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

5. Repeat from 2 until $\hat{x}$ is accurate enough.
Table of Contents

1 Rounding Errors and Reproducibility

2 Parallel Triangular Solver

3 Reproducible Triangular Solvers
   - RTrsv
   - BinnedTrsvIR

4 Accuracy and Performance

5 Conclusion and Future Works
## 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: $n \in [10000, 15000]$
- \[ \text{Cond}(\mathbf{T}, \mathbf{x}) = \frac{||\mathbf{T}^{-1}|| \cdot ||\mathbf{T}|| \cdot ||\mathbf{x}||_{\infty}}{||\mathbf{x}||_{\infty}} \]
  - Accuracy: \( \text{Cond} \in [10^5, 10^{15}] \)
  - Run-time: \( \text{Cond} = 10^8 \)
- Reference solution: \( \tilde{\mathbf{x}} = \text{MPFR}(\mathbf{T}^{-1}\mathbf{b}) \)
- Relative error: \( \frac{||\tilde{\mathbf{x}} - \hat{\mathbf{x}}||_{\infty}}{||\tilde{\mathbf{x}}||_{\infty}} \)
- Normalized Residual: \( \frac{||\mathbf{b} - \mathbf{T}\hat{\mathbf{x}}||_{\infty}}{||\mathbf{b}||_{\infty}} \)

### Challenging solutions

- Accuracy: Intel MKL Trsv (b64)
- High accuracy: XBLAS double-doubled Trsv
- Performance: Intel MKL Trsv
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
<table>
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</tr>
</thead>
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<tr>
<td>1</td>
<td>Rounding Errors and Reproducibility</td>
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<td>Accuracy and Performance</td>
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<tr>
<td>5</td>
<td>Conclusion and Future Works</td>
</tr>
</tbody>
</table>
Conclusion and Future Works

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>
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<td>BinnedTrsvIR</td>
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<td>×8 − 10</td>
<td>×2</td>
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</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