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Reproducible and Accurate Parallel Triangular Solver

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LabSTIC
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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.
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.

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

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

*ahttp://bebop.cs.berkeley.edu/reproblas/
Rounding Errors and Reproducibility

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

Philippe Langlois (UPVD) 
Reprod TRSV 
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Sequential computation

\[ x_1 = \frac{b_1}{t_{1,1}}. \]
\[ x_i = \left( b_i - \sum_{j=1}^{i-1} t_{i,j} \times x_j \right) / t_{i,i}. \]

Sources of non reproducibility

- Dot product accumulation
- SIMD lengths
- SIMD reduction schemes
Parallel Process

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

Parallel computation

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

Sources of non reproducibility

- Dot product: partial accumulations with respect to block size \( r \)
- Accumulation order with respect to \textit{gemv} scheduling
- \textit{gemv}: SIMD lengths, SIMD reduction schemes
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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
Rounding Errors and Reproducibility

Parallel Triangular Solver

Reproducible Triangular Solvers
- RTrsv
- BinnedTrsvIR

Accuracy and Performance

Conclusion and Future Works
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 \texttt{trsv}

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

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

\[
C
\]

result

error
Error-Free Transformation for \texttt{trsv}

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

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

\[ \text{result} \rightarrow \]

\[ \text{error} \rightarrow \]

\[ C \]

Philippe Langlois (UPVD)
Reprod TRSV
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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*}
Reproducible but a bit disappointing

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

\[ p_i = \sum_k v_k \]

\[ v_1 \]
\[ v_2 \]
\[ v_3 \]
\[ \vdots \]
\[ v_n \]
Fixed exponent range decomposition

\[ p_i = \sum_k v_k \]

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

De facto parallel sharing

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

Thread 0

Thread 1

Thread 2
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: $K = 1$

$p_i = \sum_{k} v_k$

\[ v_1 \quad v_2 \quad v_3 \quad \cdots \quad v_n \]

Thread 0

Thread 1

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

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

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

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

"Exact" thread accumulations

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

\( p_1 \)
\( p_2 \)
\( p_3 \)
\( \vdots \)
\( p_n \)

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

"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 & & \vdots \\
v_n & & \vdots 
\end{align*}
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.
   - \( \times \rightarrow \text{TwoProd} \)
   - 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
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**

- **Relative error:**
  - Log10 of the Forward Relative Error

- **Normalized residual:**
  - Log10 of the Normalized Residual

- **Graphs:**
  - Log10 of the Condition Number vs. Log10 of the Forward Relative Error
  - Log10 of the Condition Number vs. Log10 of the Normalized Residual

- **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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<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
Conclusion and Future Works

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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