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Reproducible and Accurate Parallel Triangular Solver

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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?

Rounding Errors and Reproducibility

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.

Philippe Langlois (UPVD)
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/
Rounding Errors and Reproducibility

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: $\times 1 \rightarrow \times 10$

*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.
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Parallel Triangular Solver

From Classic Forward Substitution to Parallel trsv

Trifangular 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. $x_j$, $j < i$. 
Triangular Solver: Sequential but SIMD-zed

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 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 \( (v_j, H, L) \)

\[ C_{exp}(L) \leftarrow L \]

\[ C_{exp}(H) \leftarrow H \]

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

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

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

\[ \text{result} \]

\[ \text{error} \]

\[ C \]

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

\[ T[i, :] \times X[:], \text{ TwoProd}(t_{i,j}, x_j) \rightarrow \text{ error} \rightarrow \text{ result} \]

Parallel EFT

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

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

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

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

Reproducible but a bit disappointing

- Reproducible solver
- but correctly rounded accumulation $\not\Rightarrow$ 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)

$p_i = \sum_k v_k$

$E_{\text{max}}$  $E_{\text{min}}$

$v_1$

$v_2$

$v_3$

$\vdots$

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

Fixed exponent range decomposition

\[ p_i = \sum v_k \]

\[ v_1 \]

\[ v_2 \]

\[ v_3 \]

\[ \vdots \]

\[ v_n \]
\[ p_i = \sum_{k=1}^{n} v_k \]

*De facto* parallel sharing

\[ \begin{array}{c|c|c}
\text{E}_{\text{max}} & & \text{E}_{\text{min}} \\
\hline
p_1 & & \\
\hline
\vdots & & \\
\hline
p_i & & \\
\hline
\vdots & & \\
\hline
p_n & & \\
\end{array} \]

Thread 0

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: $K = 1$

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

Thread 0

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

"Exact" thread accumulations

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

Thread 0

Thread 1

Thread 2
“Exact” reduction and final rounding

\[ p_i = \sum_k v_k \]

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

Thread 0

Thread 1

Thread 2
Reproducible Triangular Solvers

BinnedTrsvIR: BinnedTrsv + Iterative Refinement

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.
   - $\times \rightarrow \text{TwoProd}$
   - 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.
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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

**Experiments**

- **System size**
  - Accuracy: $n = 1000$
  - Run-time: $n \in [10000, 15000]$
  
- Cond($T, x$) = $\|\| T^{-1} \| T \| x \| \|/\| x \|\|$
  - Accuracy: Cond $\in [10^5, 10^{15}]$
  - Run-time: Cond $= 10^8$
  
- Reference solution: $\hat{x} = \text{MPFR}(T^{-1}b)$
  - Relative error = $\|\| \hat{x} - \tilde{x} \| \|/\| \tilde{x} \|\|$
  - Normalized Residual = $\|\| b - T\hat{x} \| \|/\| b \|\|$

**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**
- **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 = $10^8$.

<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):

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<td>×5 − 10</td>
</tr>
<tr>
<td>BinnedTrsvIR</td>
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<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