The ELAPS Framework: Experimental Linear Algebra Performance Studies

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ABSTRACT
Optimal use of computing resources requires extensive coding, tuning and benchmarking. To boost developer productivity in these time-consuming tasks, we introduce the Experimental Linear Algebra Performance Studies framework (ELAPS), a multi-platform open source environment for fast yet powerful performance experimentation with dense linear algebra kernels, algorithms, and libraries. ELAPS allows users to construct experiments to investigate how performance and efficiency vary depending on factors such as caching, algorithmic parameters, problem size, and parallelism. Experiments are designed either through Python scripts or a specialized GUI, and run on the whole spectrum of architectures, ranging from laptops to clusters, accelerators, and supercomputers. The resulting experiment reports provide various metrics and statistics that can be analyzed both numerically and visually. We demonstrate the use of ELAPS in four concrete application scenarios and in as many computing environments, illustrating its practical value in supporting critical performance decisions.

1. INTRODUCTION
The field of high performance computing is largely concerned with the optimal usage of available resources. Since performance depends on the choice of algorithms, parameters, libraries and even computing environment, maximizing efficiency is a task that comes at the cost of extensive coding, tuning and benchmarking. To facilitate and support such time-consuming and repetitive activities within the development of dense linear algebra software, we propose a rich and flexible environment for rapid performance experimentation.
Many application-level tools for profiling and analyzing existing codes exist (examples include PAPI [5], Tau [20], Vampir [15], and Scalasca [11]); collectively, they offer support for the whole range of architectures, from single computing nodes to large distributed computers. In its current form, ELAPS targets shared-memory platforms, and early experimentation.

2. EXPERIMENTS

While performance experiments come in all kinds of shapes and sizes, many of them can be described by a few common features. Within the ELAPS framework, we combine and generalize such features to provide a versatile central concept of “experiment”. In this section, we discuss these basic features guided by deliberately simple examples. More complicated examples arising in actual applications are then presented in Sec. 4.

We begin with a most elementary experiment: Measuring the performance of the matrix-matrix product kernel \texttt{dgemm}.

\begin{verbatim}
E5-2670 OpenBLAS Experiment 1: \texttt{dgemm}  
# threads = 1  
dgemm:  
\begin{equation*}  
C := A \cdot B  
\end{equation*}  
A, B, C \in \mathbb{R}^{1000 \times 1000}  
\end{verbatim}

As shown schematically above, this experiment runs on one core of an Intel SandyBridge E5-2670 processor, using the OpenBLAS library [16], and executes the double precision kernel \texttt{dgemm} once on random square matrices of size 1000. Although simple, similar experiments are commonly used to determine the attainable peak performance of a given processor.

When combined with additional information on the hardware and the kernel’s complexity, the raw timing (in cycles) from this experiment leads to a number of metrics, which yield more insights into how efficiently the CPU is used.

| metric       | value          |
|--------------|----------------|
| cycles       | 272551028      |
| time [ms]    | 104.8          |
| GFlops/s     | 19.1           |
| flops/cycle  | 7.3            |
| efficiency [%] | 91.7          |

Furthermore, if available, the Performance Application Programming Interface (PAPI) [5] allows one to access useful hardware counters.

| metric                     | counter name | value       |
|----------------------------|--------------|-------------|
| Level 1 cache misses       | PAPI_L1_TCM  | 32933961    |
| Conditional branch         | PAPI_BR_MSP  | 3941        |
| instructions mispredicted  |               |             |

With ELAPS, all these metrics are readily available and easily extensible.

\begin{figure}[h]
\begin{center}
\includegraphics[width=\textwidth]{fig1.png}
\caption{Performance statistics from 10 repetitions of \texttt{dgemm}}
\end{center}
\end{figure}

2.1 Repetitions and Statistics

Multiple executions of a kernel often result in fluctuating timings; the reasons for such differences include library initialization overhead, cache locality, and system jitter. As customarily done, in ELAPS this issue is addressed by repeating each experiment several times, and by collecting statistics. As an example, let us consider an experiment that repeats the kernel execution from Experiment 1 ten times on the same input matrices (i.e., the same memory locations):

\begin{verbatim}
E5-2670 OpenBLAS Experiment 2: Repetitions  
# threads = 1  
repeat 10 times:  
dgemm:  
\begin{equation*}  
C := A \cdot B  
\end{equation*}  
A, B, C \in \mathbb{R}^{1000 \times 1000}  
\end{verbatim}

This second experiment produces ten measurements, from which we derive statistics as those presented in Fig. 1. It is worth pointing out that whenever multiple repetitions are executed and timed, the first one almost inevitably represents an outlier; for the most part, this phenomenon is connected to the initialization of the kernel library, but it is also due to the loading and caching of data and instructions. In general, a more accurate representation of the effective performance is obtained by dropping the first measurement of the lot. In Fig. 1 one can appreciate how significantly the first repetition affects the various statistics, and most noticeably, the minimum, the average and the standard deviation (std).

In order to avoid the impact of “first-execution” outliers, in all following examples and studies we always discard the measurement relative to the first repetition.

2.2 Data Placement: Varying Operands

In Experiment 2, the matrices \(A, B,\) and \(C\) were reused across repetitions, causing them to stay in cache; this scenario is also known as a “warm data”. Depending on the application, the assumption of warm data may or may not
be realistic; to reflect this in our experiments, we allow to “vary” the operands (i.e., use different memory locations) individually in each repetition. Furthermore, in ELAPS one can freely control the relative position of varying operands: They can be stacked horizontally or vertically, with or without an arbitrary offset.

In the following experiment, while $A$ and $B$ are fixed and quite small, $C$ varies in each repetition (hence the subscript in $C_{\text{rep}}$) and is therefore never cached (“cold data”).

In Fig. 2 we present the results of Experiment 3 and another experiment in which the matrices $A$, $B$, and $C$ are all fixed. The performance loss due to the enforced out-of-cache scenario for $C$ is clearly visible.

2.3 Sequences of Kernels

In addition to isolated kernels, ELAPS allows to experiment with sequences of calls. Let us use the solution of a linear system as an example: The problem

$$B := A^{-1}B$$

is typically solved by first LU-decomposing $A$ ($\text{dgetrf}$), and then by solving two triangular linear systems ($\text{dtrsm}$). The process—which is also implemented in LAPACK’s $\text{dgesv}$—is replicated in Experiment 4.\footnote{For simplicity, we don’t expose the pivoting vector and omit the row interchanging kernel $\text{dlaswp}$ that only contributes a lower order term to the execution time.}

For this experiment, Fig. 3 shows both the total execution time and the time spent in each individual kernel. It is easy to realize that for 200 right-hand sides, the LU decomposition $\text{dgetrf}$ is responsible for more than 60% of the total execution time, while each of the $\text{dtrsm}$’s only contribute less than 20%.

2.4 Parameter Range

So far we only considered experiments in which the sizes of the kernel operands where fixed. In many practical experiments however one wants to study the performance of a routine over a range of parameters. In the following example, we use the routine $\text{dgesv}$, which solves a linear system directly, to solve problems of size $n$ with 500 right hand sides, where $n$ ranges from 50 to 2000 in steps of 50.

For this experiment, Fig. 4 shows the increase in performance for increasing...
Figure 4: Solution of linear systems: performance.

Figure 5: Scalerability of LAPACK’s symmetric dense eigensolvers on random matrices

problem size, as typical for dense linear algebra kernels.

2.4.1 Threads Range

Scalability studies are extremely common examples of experiments that make use of ranges. In the following experiments, we compute the eigenvalue decomposition of a symmetric matrix (of fixed size) using from 1 up to 8 threads, and compare LAPACK’s solvers dasyev, dasyevx, dasyevr, and dasyevd (see [1] for details on these routines).

Figure 6: Influence of block-size on triangular inversion

As one can appreciate from Fig. 5, ELAPS makes it easy to set up, execute, and compare the results of multiple experiments with varying degrees of parallelism.

2.5 Sum- and OpenMP-Range

In loop-based algorithms, the total execution time is often more meaningful than an iteration-by-iteration breakdown. For this purpose, in addition to the “parameter range” described in the previous subsection, ELAPS also provides a “sum-range”, which yields the total contribution of the loop. For instance, the next experiment models the inversion of a lower triangular matrix of size 1000 via a blocked algorithm that traverses the matrix in steps of a fixed block-size nb.

2.5.1 OpenMP-Range

Fig. 6 reports the performance attained by this algorithm for different block-sizes nb; the maximum is observed for nb = 100. The choice of parameters represents an important step to tailor algorithms for a given architecture; for instance, the tuning of the block size is common to many of the algorithms included in LAPACK [1,22]. Notice that a simpler and finer-grained experiment to optimize the block-size is obtained by combining the sum-range with a parameter-range for nb.

Multi-threading can typically be exploited in two different ways.

2 LAPACK’s dtrtri computes the inverse of a triangular matrix using a similar algorithm.
3 dtrmm: Triangular matrix matrix multiplication.
4 dsyrk: Symmetric rank k update.
5 dtrti2: Unblocked triangular inversion.
Figure 7: Performance of threaded dtrsm vs. parallel dtrsv’s

ways, namely, either invoking a multi-threaded library (such as OpenBLAS), or through OpenMP. To investigate these alternatives, in the Experiments 8 and 9 we implement the solution of a triangular linear system with a tall and skinny right-hand side 1) with OpenBLAS’s threaded dtrsm kernel, and 2) as a series of parallel dtrsv’s using ELAPS’s OpenMP-range.

The results in Fig. 7 suggest that the parallel dtrsv’s are considerably faster than the threaded dtrsm’s, indicating that OpenBLAS is not optimally parallelized for such extremely skewed matrix sizes.

3. THE ELAPS FRAMEWORK

The ELAPS framework is built to support performance experiments combining the features and scenarios described in Sec. 2. In this section, we present the structure of the framework, focusing on the aspects that make it general and intuitive, yet powerful.

As shown in Fig. 8, ELAPS is structured in three layers.

- The first, “bottom” layer (Sec. 3.1) is written in C/C++ and contains the Sampler, a low-level command line tool responsible for executing and timing individual kernels. The Sampler has to be compiled for each specific combination of hardware and libraries (the only stage in which the user needs to configure the system); ELAPS can interface with any number of Samplers.

- The second, “middle” layer (Sec. 3.2) is the Python library elaps, which centers around the class Experiment that implements the previously introduced experiments. An Experiment can be executed on different Samplers, both locally or through job submission systems. The outcome is a Report, which provides not only structured access to the individual measurements, but also functionality to analyze different metrics and statistics.

This layer also includes the plot module, which is based on the matplotlib library, and is used to easily visualize Reports in graphical form.

- The third, “top” layer (Sec. 3.3) adds a graphical user interface, written in PyQt4, to both design Experiments in the PLAYMAT and study Reports and plots in the VIEWER.

The design of these three layers is discussed in the next subsections.

3.1 The Sampler

At the core of the ELAPS framework is a low-level performance measurement tool tailored to dense linear algebra operations: the Sampler. This tool, earlier versions of which were already utilized in [17] and [18], makes it possible to measure the performance of individual kernel executions, implementing this work-flow:

1. Read from stdin a list of calls, i.e., kernel names with corresponding lists of arguments;

2. execute the specified calls, thereby measuring their performance in terms of CPU cycles, and optionally through performance counters provided by the Performance Application Programming Interface (PAPI) [5];

3. All the plots in this paper were generated in this manner.
3. print the measured performance numbers to the standard output.

While reading the list of kernels from the standard input, the Sampler accepts several special commands: go executes, measures, and reports the results of all the calls previously read; {omp and } respectively start and end a list of calls to be executed as parallel OpenMP tasks; set_counters sets the PAPI counters for the next set of executions.

The Sampler accepts kernels and arguments in a format that agrees with the conventions used by standard libraries such as BLAS and LAPACK: Each argument is passed by reference, and is of type char *, int *, float *, or double *.

In a dense linear algebra kernel, these arguments are of one of two types:

- **Scalar arguments** point to scalar values, some of which may influence the kernel’s behavior and control flow. Examples include: flag arguments (e.g., side, transA), size arguments (e.g., m, n), scalars (e.g., alpha, beta), and leading dimensions (e.g., ldA, ldB).

  Within the Sampler, scalar argument values are stored consecutively in an array.

- **Data arguments** point to memory regions that hold the mathematical objects (such as vectors or matrices) involved in the kernel call. Generally, the actual contents of these arguments do not affect the control flow; nonetheless, these arguments may still have a significant impact on performance, depending on their location in the memory hierarchy.

The Sampler has two mechanisms to treat data arguments:

- **Named variables** are designated memory regions referenced by a variable names. A set of features to allocate (malloc), compute offsets (offsets) and free (free) such variables give users full control over where operands are stored in relation to each other.

- **Dynamic memory** offers a fast way to pass “unnamed” memory regions as data arguments. Within one call all such regions are guaranteed to be disjoint; across calls, however, the same memory regions may be reused arbitrarily.

To set up the contents of data arguments, the Sampler provides a set of simple utility-type kernels: memset fills every entry in a buffer with a single value, gerand fills it with random values (uniform in [0, 1]), and zporand generates a random symmetric (or Hermitian) positive definite matrix. Furthermore, zreadfile and zwritefile, read matrices from and write them to binary files, respectively.

3.2 The elaps Package

The middle layer of the ELAPS framework centers around the experimental features introduced in Sec. 2, encoded in the Python class Experiment. Instances of this class form the starting point for performance experiments; executing them using Samplers ultimately leads to Reports, which can be analyzed with respect to a variety of metrics and statistics.

3.2.1 Experiments

Experiment instances are both a static description of experiments, which are easily stored to and loaded from strings and files for portability, but also feature functionality to support their design and handling.

The kernel configurations at the center of each Experiment are its connection to libraries such as BLAS or LAPACK. While the interfaces of such libraries aim at being general by accommodating multiple functionalities, precisely because of their generality they are often unintuitive and hard to memorize. To counter this problem, elaps uses optional “Signatures” to annotate kernels, thereby providing possible value ranges and semantic connections between arguments. In the end, these Signatures allow Experiments to expose feasible values for arguments (such as trans or uplo) and automatically derive connected arguments such as operand sizes and leading dimensions, both within a single kernel and across multiple kernels.

The execution of an Experiment is initiated by the submit method. This method first generates the sequence of kernel calls for the Sampler and a shell script for its execution; it then either executes this script is locally or submits it to a batch job system.

3.2.2 Execution on Samplers

In this section, we describe how the Experiment features are translated into commands for the Sampler.

As input, the Sampler expects a raw list of kernel invocations. To produce this list, all ranges and repetitions in an Experiment are completely unrolled, thereby evaluating any symbolic (range-dependent) variable. The OpenMP-range is translated directly to the Sampler’s {omp and } commands. Using the parameter-range to vary the number of library threads requires to interface with said library; to avoid library-dependent kernels and Sampler features, we do so through environment variables (e.g., OPENBLAS_NUM_THREADS) and by starting the sampler separately for each thread count.

Data arguments in kernels are allocated as named variables in the Sampler at the beginning of the input. Arguments that vary with repetitions or the sum/OpenMP-range (i.e., they point to different locations) are first allocated as a single large block and then subdivided by calculating appropriate offsets, resulting in individual variables for each repetition and range iteration.

Finally, PAPI counters are also set at the beginning through the set_counters command.

3.2.3 Reports

\[8 \{i, x, d, c, z\} \text{identifies the data-type.}\]
Each Experiment execution results in a report file that, when read into elaps, turns into a Report instance. This object serves as a structured representation of the obtained measurements with respect to the underlying Experiment: Raw measurements are accessed through the hierarchy “parameter-range value → repetition → sum/OpenMP-range value → kernel” and yield the cycle count or PAPI counter measurements. Separately, a “reduced” view on the results accumulates the sum/OpenMP-range and the kernels according to the experiment semantic.

To turn these structured yet raw measurement results into more meaningful quantities, metrics combine them with the kernels’ flop counts and information on their execution environment. The easily extensible set of metrics ranges from “execution time in seconds” to “Gflops/s” and “efficiency”.

While a metric converts measurements values one-by-one, results from multiple repetitions are combined by statistics, such as “minimum”, “maximum”, “median” or “standard deviation”. As motivated in Sec. 2, the results from first repetitions are optionally discarded to hide overhead effects and make statistics more representative of in-application invocations.

3.2.4 Plotting
ELAPS’s plot module generates matplotlib figures from the structured data in Reports under consideration of both metrics and statistics. Depending on the type of experiment, it automatically generates appropriate bar- or line-plots that are easily exported to various file formats.

3.3 The Graphical User Interface
ELAPS’s Experiment and Report Python classes establish a flexible and powerful foundation for performance evaluations at a scripting level. In order to enable performance experimentation in an explorative fashion, and to facilitate more intuitive interaction, ELAPS features a graphical user interface. As shown in Fig. 8, this interface consists of components: While the PlayMat serves as a “playing mat” to develop Experiments, the Viewer interactively visualizes Reports.

The PlayMat, shown in Fig. 9, allows interactive access to the full functionality of an Experiment. To further guide the user, among other things, it visualizes the Experiment’s kernels based on their Signatures similar to how they are presented in this paper and automatically calculates matrix sizes and (if desired) deducible arguments, such as leading dimensions. It furthermore provides progress tracking of executing Experiments and can load completed Reports directly in the Viewer.

The Viewer, shown in Fig. 10, is an interactive means to analyze and compare Reports. It provides all metrics applicable to the selected Reports and its statistical plots are easily manipulated and exported.

4. APPLICATION EXAMPLES
In this section, we demonstrate the use of the ELAPS framework in several application examples. For this purpose, we deliberately chose a wide range of hardware systems and kernel libraries.

4.1 Algorithm Selection: Tensor Contractions
Let us consider the tensor contraction (in Einstein notation)

\[ C_{abc} := A_{ak} B_{kcb} \]  \hspace{1cm} \text{(2)}

with \( A \in \mathbb{R}^{1250 \times 750} \), \( B \in \mathbb{R}^{750 \times 500 \times n} \), and \( C \in \mathbb{R}^{1250 \times n \times 500} \), where \( n \) is between 100 and 10,000. Using an explicit index notation, \( C \) is computed as

\[ \forall a, \forall b, \forall c. \ C[a, b, c] := \sum_k A[a, k] \cdot B[k, c, b] \]  \hspace{1cm} \text{(3)}

and can be visualized as follows:

\[ \begin{array}{ccc}
A & B & C \\
\hline
\begin{array}{cc}
\vdots & \vdots \\
C[a, b, c] & \vdots \\
\end{array} & \begin{array}{cc}
\vdots & \vdots \\
A[k, a, c] & \vdots \\
\end{array} & \begin{array}{cc}
\vdots & \vdots \\
B[k, c, b] & \vdots \\
\end{array}
\end{array} \]

\((n = 100)\)  \hspace{1cm}  \((n = 1000)\)

A natural approach to efficiently compute such tensor contractions is to utilize the highly optimized dgemm kernel. For
Contraction (2), there are two ways of casting the computation as a series of \texttt{dgemm}'s:

\[
\forall b \in \{1, \ldots, n\} : \hspace{1cm} \begin{bmatrix} C \end{bmatrix} := \begin{bmatrix} A & B \end{bmatrix} \begin{bmatrix} b \end{bmatrix} \tag{4}
\]

\[
\forall c \in \{1, \ldots, 500\} : \hspace{1cm} \begin{bmatrix} C \end{bmatrix} := \begin{bmatrix} A & B \end{bmatrix} \begin{bmatrix} c \end{bmatrix} \tag{5}
\]

An inspection of these algorithms reveals that they both execute a \texttt{dgemm} of fixed size on varying data; in particular, the number of invocations in Algs. \(\forall b\) and \(\forall c\) are, respectively, \(n\) and 500. By virtue of this observation, Experiments 10 and 11 only perform 10 repetitions, thus reducing the experimentation time; while the results will not be meaningful estimates for the total execution time, they will expose the same computational efficiency (expressed in Gflops/s) as the full algorithms. Furthermore, since Alg. \(\forall b\) operates on matrices of fixed size and independent of \(n\), in Experiment 10 we also avoid the use of the parameter range.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
PowerPC A2 & ESSL & Experiment 10: Tensor algorithm \(\forall b\) \\
\hline
#threads = 64 & experiment 10: Tensor algorithm \(\forall b\) \\
\hline
\texttt{dgemm}: \(A_{\text{rep}}\) := \(A \times B_{\text{rep}}\) & & \\
\hline
\multicolumn{3}{|c|}{\(A \in \mathbb{R}^{1250 \times 1250}, B_{\text{rep}} \in \mathbb{R}^{750 \times 1250}, C_{\text{rep}} \in \mathbb{R}^{1250 \times 750}\)} \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
PowerPC A2 & ESSL & Experiment 11: Tensor algorithm \(\forall c\) \\
\hline
#threads = 64 & experiment 11: Tensor algorithm \(\forall c\) \\
\hline
\texttt{dgemm}: \(C_{\text{rep}}\) := \(A \times B_{\text{rep}}\) & & \\
\hline
\multicolumn{3}{|c|}{\(A \in \mathbb{R}^{1250 \times 1250}, B_{\text{rep}} \in \mathbb{R}^{750 \times 1250}, C_{\text{rep}} \in \mathbb{R}^{1250 \times 750}\)} \\
\hline
\end{tabular}
\end{table}

We perform Experiments 10 and 11 on a 16-core IBM POWERPC A2 node of the IBM BLUEGENE installation JUQUEEN at the JÜLICH SUPERCOMPUTING CENTER, linked to IBM’s optimized ESSL library. Only the \textsc{Sampler} is executed on this compute node, running the lightweight CNK operating system; it is accessed by \textsc{elaps} from a RED HAT ENTERPRISE LINUX 6.6 front-end node through the \textsc{LoadLeveler} batch job system.

Fig. 11 suggests that neither of the two algorithms is optimal for all cases: While for a small dimension \(n\), algorithm \(\forall b\) is better, algorithm \(\forall c\) dominates for large \(n\). Interestingly, the crossover point is not at \(n = 500\), where both algorithms work with matrices of equal size, but already around \(n = 300\).

### 4.2 Library Selection: Sylvester Equation

Choosing the right library can be a crucial step in attaining high performance. In this section, we demonstrate its importance by considering the triangular Sylvester equation

\[
\begin{bmatrix} A \end{bmatrix} X + \begin{bmatrix} X \end{bmatrix} \begin{bmatrix} B \end{bmatrix} = \begin{bmatrix} C \end{bmatrix},
\]

\text{(6)}

to be solved for \(X\), which is central to problems in control theory. In addition to LAPACK’s \textsc{dtrsyl}, several other libraries offer this kernel with the same interface. In our tests, we consider

- LAPACK 3.5 [1] linked to OPENBLAS 0.2.14 [16],
- RECSY 0.01 [14] linked to OPENBLAS,
- libFLAME\textsuperscript{10} 5.1.0-18 [21] linked to OPENBLAS, and
- \textsc{Intel}’s commercial MKL 11.0 [13].

To compare these libraries, we launch Experiment 12 on a 10-core \textsc{Intel} \textsc{IvyBridge} E5-2680 v2 processor with \textsc{Samplers} linked to the above libraries. This machine, which is part of a compute cluster is accessed through the \textsc{Platform LSF} 9.1.2 batch job system with both the front-end (\textsc{elaps}) and back-end (the \textsc{Samplers}) running \textsc{Scientific Linux} 6.6.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
E5-2680 \textsc{v2} & see above & Experiment 12: Sylvester solver \\
\hline
#threads = 10 for \(i = 100:100:6000\); & & \\
\multicolumn{3}{|c|}{\texttt{dtrsyl}: \(C := \text{Sylv} \begin{bmatrix} A \end{bmatrix}, \begin{bmatrix} B \end{bmatrix}, \begin{bmatrix} C \end{bmatrix}\)} \\
\hline
\multicolumn{3}{|c|}{\(A \in \mathbb{R}^{8 \times 8}, B \in \mathbb{R}^{128 \times 128}, C \in \mathbb{R}^{128 \times 128}\)} \\
\hline
\end{tabular}
\end{table}

Fig. 12 shows the performance attained by the different libraries. LAPACK, which only provides an unblocked algorithm for \textsc{dtrsyl}, reaches 2Gflops/s for small problems but\textsuperscript{10}\textsc{libFLAME}’s LAPACK interface does by default not call its optimized Sylvester solver, it is easily exposed.
eventually falls below 1 Gflops/s. The specialized RECSY library on the other hand attains the best performance of up to 24.5 Gflops/s. libFLAME is initially competitive with RECSY but eventually tops at 20.5 Gflops/s. Surprisingly, the otherwise very efficient MKL seems poorly optimized for this problem and is as fast as LAPACK.

### 4.3 Multithreading: Sequence of LUs

In a certain type of electronic structure calculations [2], one has to solve a series of fairly small linear systems. As already mentioned, a possible approach involves the LU factorization (dgetrf) and two triangular linear systems (dtrsm) for each matrix; since each system only involves two right-hand sides, the cost for the dtrsm’s is entirely negligible.

On multi-core machines, the sequence of LUs can be parallelized at the granularity of one matrix, via a multi-threaded dgetrf kernel, or by assigning different matrices to different threads, via OpenMP (hybrid solutions are also possible). Performance-wise, there are arguments both in favor and against each of these two alternatives: Using BLAS’s internal parallelism ensures that only one kernel uses the CPU’s caches at a time; on the other hand, OpenMP’s parallelism increases the amount of work that the CPU’s cores can perform simultaneously.

The next three experiments use ELAPS’s sum-range and OpenMP-range constructs to model the scenarios in which 1) a multi-threaded kernel is used, 2) OpenMP runs sequential kernels in parallel, and 3) OpenMP runs multi-threaded kernels in parallel. Each of them measures the time it takes to LU decompose an increasing number of square matrices of size 800.

These three experiments are executed on a MacBook Pro running OS X 10.9.4 with a quad-core Intel Haswell i7-4850HQ CPU (Turbo Boost disabled) using Apple’s Accelerate framework; both the Sampler and elaps run on the same platform.

Fig. 13 indicates that of the two “pure” approaches, if more than 8 LU’s are performed (i.e., more than the CPU has hardware threads), OpenMP with single-threaded kernels outperforms Accelerate’s parallel kernel. However, the mixed approach, in which Accelerate uses up to 8 threads, while OpenMP is allowed to schedule the LU decomposition tasks, is even more efficient, reaching up to 75 Gflops/s.

### 4.4 Algorithmic Optimization: GWAS

Genome Wide Association Studies (GWAS) investigate how human traits (e.g. eye color or genetic deceases) are related to certain locations in the human genome [4, 24]. Computationally, GWAS can be cast as a sequence of Generalized Least Squares (GLS) problems

\[
b_k := \left( X^T M^{-1} X \right)^{-1} X^T y.
\]  

Even though the Turbo Boost was disabled and no other application was running, noticeable performance fluctuations were observed. This is to be expected on laptop-systems.

---

11 This third experiment is not displayed: It is obtained from Experiment 14, changing #threads to 8.
Experiment 16: Combining $X$

where $M \in \mathbb{R}^{n \times n}$ is symmetric positive definite, $X_i \in \mathbb{R}^{n \times p}$, $y \in \mathbb{R}^n$, and $b_i \in \mathbb{R}^p$ with $1000 \leq n \leq 5000$, $p \leq 20$ and $i \in \{1, \ldots m\}$, where $m$ can be in the millions.

A straightforward implementation of this equation (e.g., using R or Matlab) might compute each $b_i$ individually by solving Equation 7 from right to left, as modeled in this experiment (with $n = 1000$ and $p = 4$):

For Experiments 15 and 16, we choose a 60-core Intel Xeon Phi co-processor using Intel MKL. ELAPS’s python library and the PLAYMAT are run on this system’s Host processor (Scientific Linux 6.6); only the SAMPLER is executed natively on the co-processor.

Fig. 14 shows both the execution time of Experiment 14, as well as a breakdown thereof. The runtime is clearly dominated by the dpotrs and dposv kernels involving $M$.

From a first analysis of these two kernels, one realizes that the dposv ($y := M^{-1}y$) is independent of $i$, and can thus be taken out of the loop and computed just once. This modification reduces dposv’s contribution to the total runtime by a factor of $m$, effectively shifting the bottleneck onto dpotrs.

A further analysis reveals that all the dpotrs linear systems involve the same matrix $M$; this observation suggests to combine the right-hand sides $X_i \in \mathbb{R}^{m \times 4}$ for all $i$ into a single large matrix $X \in \mathbb{R}^{1000 \times 4m}$. The following experiment solves a linear system with this matrix as the right-hand side with a single invocation of dpotrs:

For the selected range of $m$, the runtime of this experiment is below 200 ms, i.e., already more than 1 order of magnitude less than the previous experiment. Furthermore, for larger problems, the dpotrs kernel can make good use of the co-processor’s many cores and reaches over 550 Gflops/s. For an in depth study of performance optimizations for GWAS we refer the reader to [7] and [9].

5. CONCLUSION

We introduced the Experimental Linear Algebra Performance Studies framework (ELAPS), a set of tools and features to design, execute, measure and analyze dense linear algebra performance experiments. With its intuitive interface, ELAPS assists users in investigating performance behaviors and in making informed decisions. Throughout this paper, we applied ELAPS to a wide range of scenarios, including parameter optimization (Sec. 2.5), algorithm selection (Sec. 2.4.1, Sec. 4.1), library comparison (Sec. 4.2), and parallelism and library threading (Sec. 2.5.1, Sec. 4.3). We demonstrated the framework’s flexibility by linking it with seven kernel-libraries, and by executing experiments on five different platforms, including the Xeon Phi co-processor and two different batch-job systems. In summary, ELAPS covers many aspects of shared-memory optimizations, a critical step towards achieving large-scale performance.

Having established the foundations of a framework for rapid experimentation, we foresee many opportunities for extensions. In particular, we envision 1) coverage of a broader range of architectures, including GPUs and ARM-based CPUs, 2) support for metrics related to data movement and energy consumption, and 3) interfaces for distributed memory libraries such as SCALAPACK.

Software

ELAPS is open source (BSD license) and available on GitHub: http://github.com/elmar-peise/ELAPS

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