Profiling and Inspecting Linear Algebra Applications using FlexiBLAS

Martin Köhler

joint work with Jens Saak, Christian Himpe, and Jörn Papenbroock

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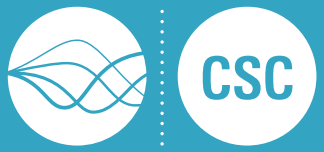

What is BLAS?

Basic Linear Algebra Subprograms (BLAS)

"The BLAS (Basic Linear Algebra Subprograms) are routines that provide standard building blocks for performing basic vector and matrix operations. . . . Because the BLAS are efficient, portable, and widely available, they are commonly used in the development of high quality linear algebra software, LAPACK for example."[4]

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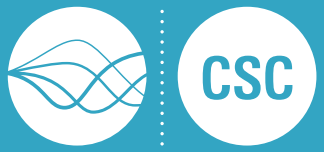

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Used in many software packages:

- MATLAB, GNU Octave
- NumPy, SciPy
- Julia
- FEM Packages like FEniCS, DEAL.II, . . .
- Libraries like PetSC, Trillinos, Eigen, SuiteSparse, . . .

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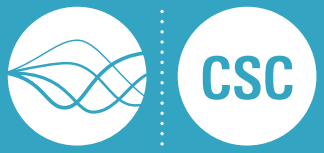

What is BLAS?

Some important BLAS implementations:

- NetLib BLAS: `http://www.netlib.org/blas/` (the reference)
- OpenBLAS: `http://www.openblas.net/` (uses assembler level optimization)
- Automatically Tuned Linear Algebra Software (ATLAS):
  `http://math-atlas.sourceforge.net/` (automatic compile-time tuning)
- BLIS (BLAS-like Library Instantiation Software Framework):
  `https://github.com/flame/blis` (alternative approach to BLAS)
- Intel® Math kernel library (MKL):
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FlexiBLAS

- Lightweight wrapper library around all BLAS and LAPACK subroutines using a plugin framework.
- Ability to overload all BLAS and LAPACK subroutines.
- Developed since 2013.

Why do we develop FlexiBLAS?

Main Reason: Linker Problems

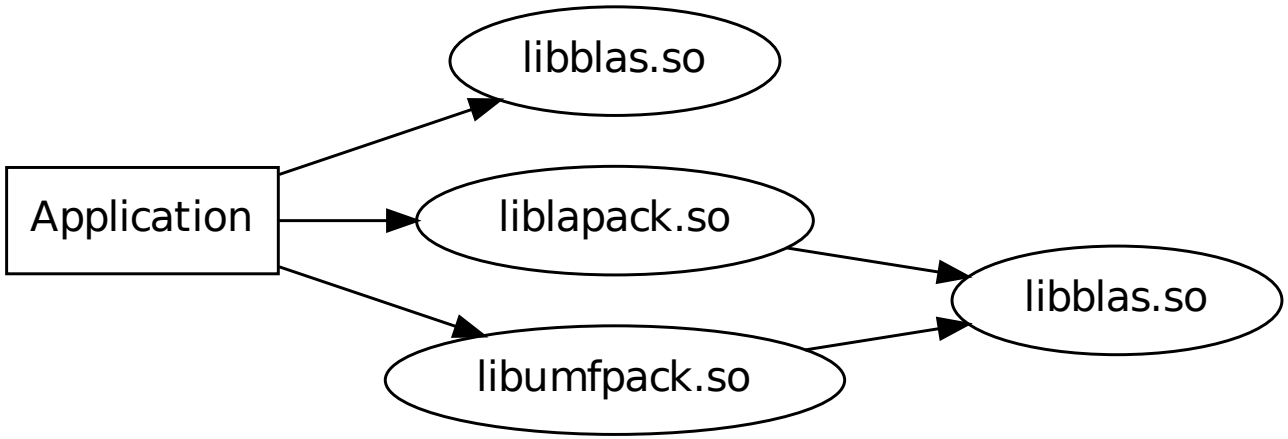

Figure: A sample application using BLAS

```
gcc -o application app.o -lumfpack -llapack -lblas
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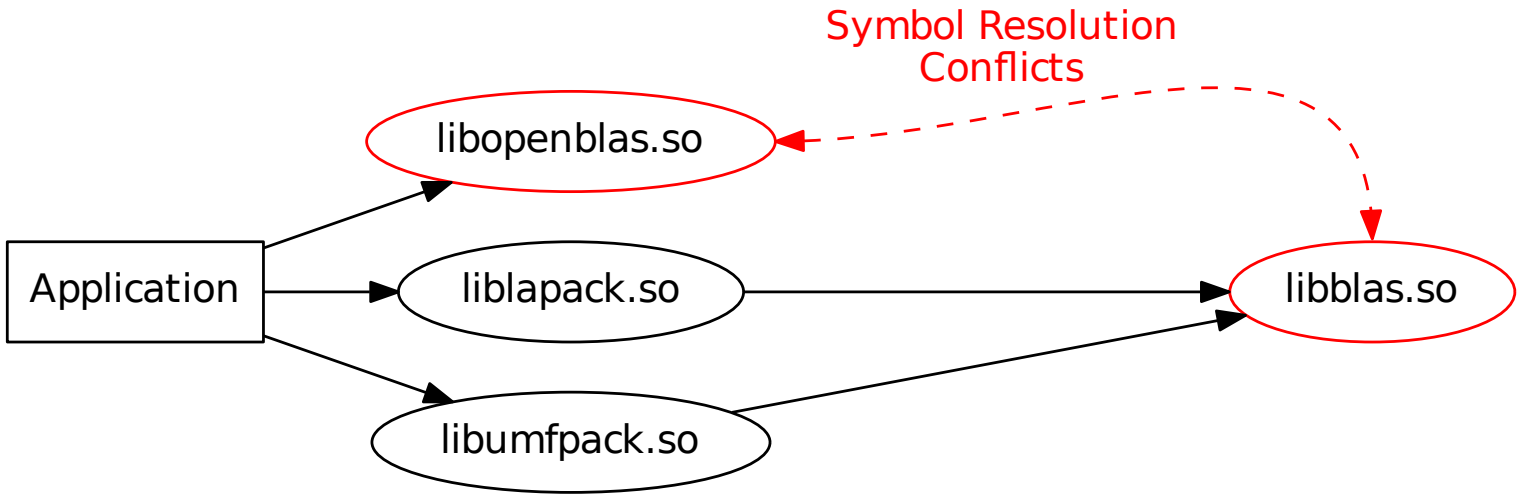

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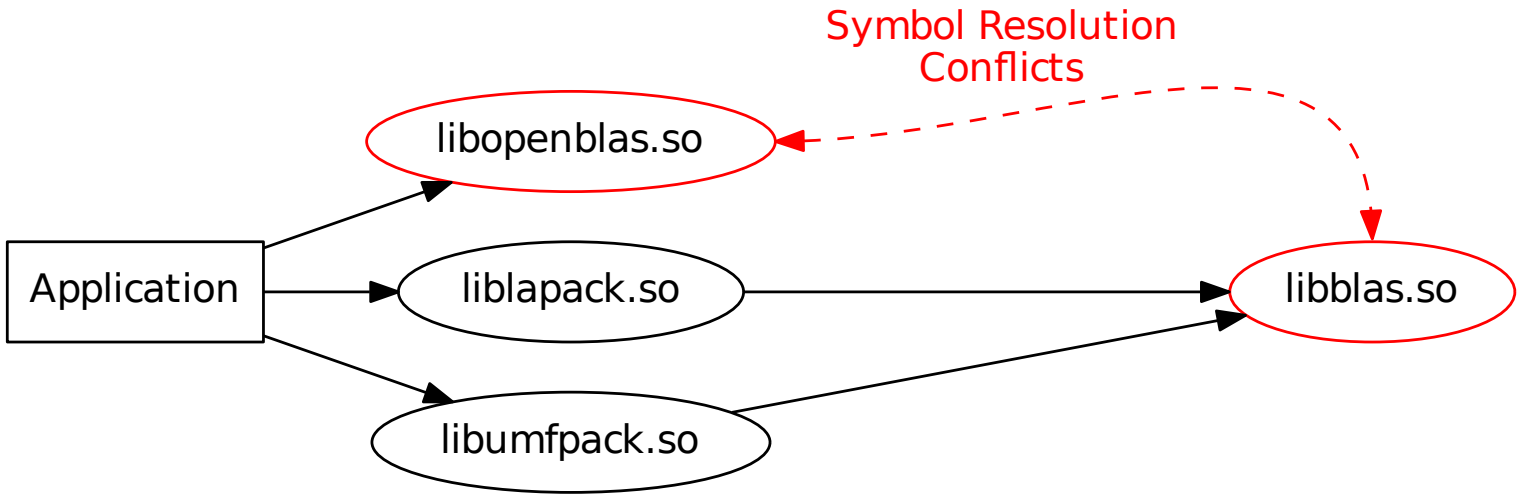

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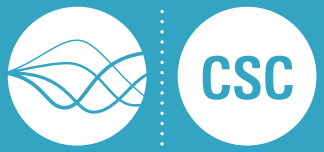
With FlexiBLAS one switches the BLAS library without relinking and producing such conflicts.



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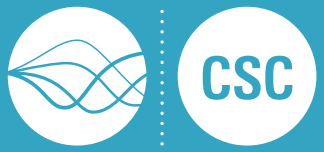
Further Reasons

- **Compatibility:** Different interface styles of GNU Fortran, Intel Fortran,...
- **Vendor-added Routines:** `xAXPBY`, `xOMATCOPY`, ...
- **Bad Linking Behavior:** e.g. longish linker setups for MKL or ATLAS.
- **Time consuming rebuilding:** Switching BLAS and LAPACK may require rebuilding a whole project.
- **Super User Privileges:** Most solutions provided by OS vendors require administrator rights for this.



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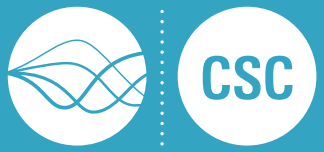
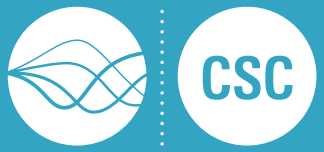
FlexiBLAS provides easy to use solutions for these problems.



Profiling

- Profiling usually requires additional compiler settings.
- Profiling data requires additional (sometimes confusing) tools for evaluation.
- Profiling often induce considerable overhead influencing the runtime behavior of the profiled application.
- **Hardly possible if only precompiled binaries are available.**



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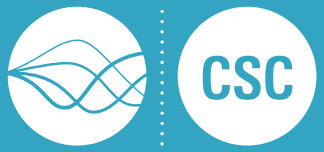

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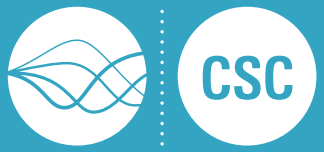
To get an idea of what is going on in the application, we need to collect some basic statistics.



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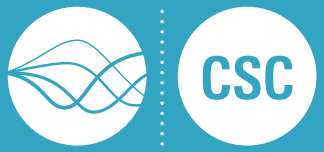
Basic profiling should:

- **count the number of calls** for each BLAS subroutine
- and **measure the runtime** taken by the BLAS library

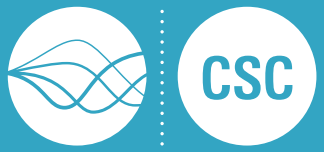
without recompiling/patching/modifying the application.



Inspecting

Similar to profiling but:

- works **for each function/subroutine call** individually
- and gathers runtime, function/subroutine arguments, threads-ids, ...



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- code compiled with debug information or annotations,
- tools for dynamic insertion of code into binaries, (e.g.: Dyninst, Score-P)
- OS support for various tracing tools, (e.g.: DTrace, FTrace)
- modified (wrapper) libraries, (e.g.: eztrace)
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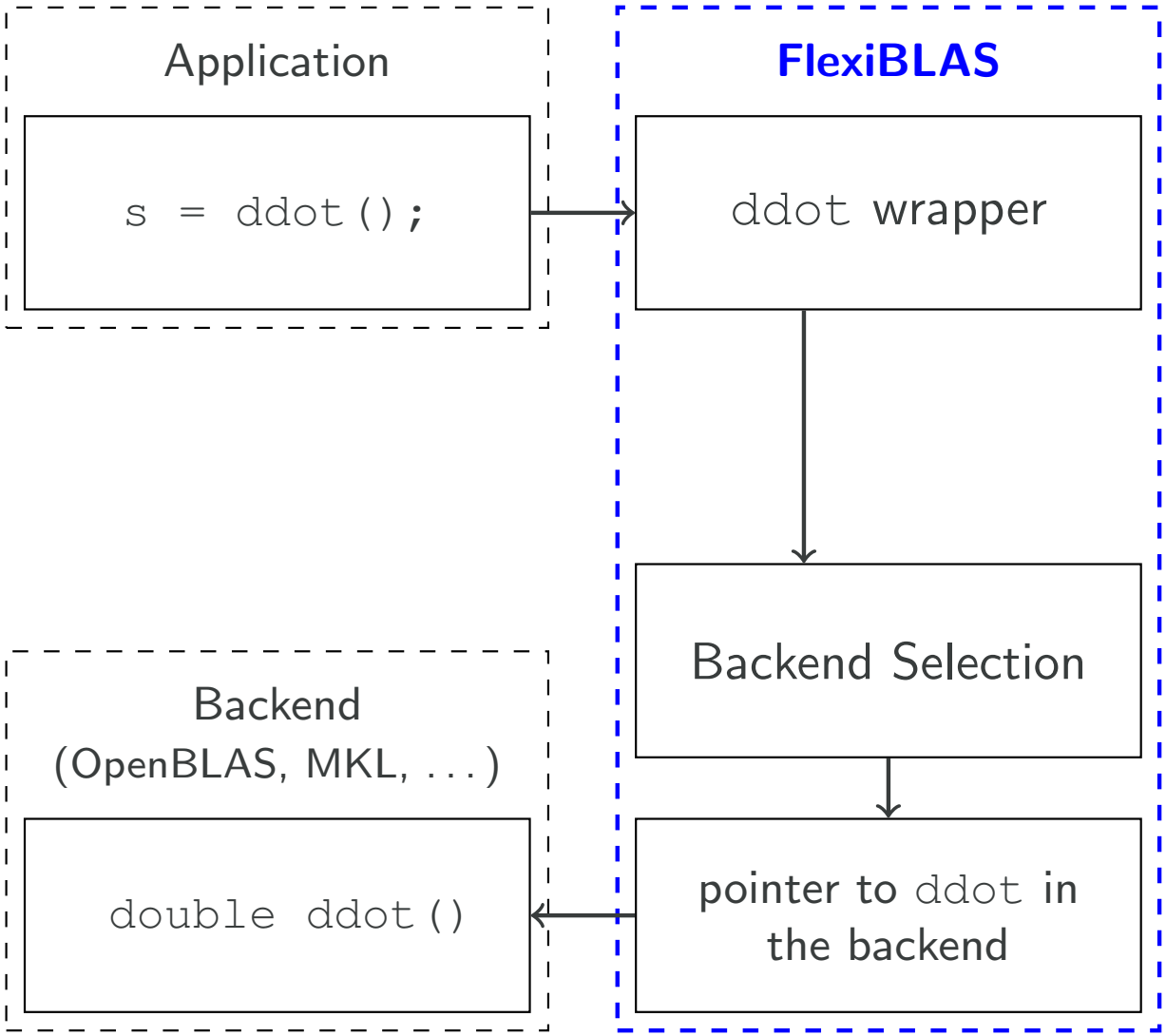
Our Goal

Collect the meta information of all BLAS calls including scalar function arguments, starting and finishing times, and the id of the executing thread.

How is it Implemented?



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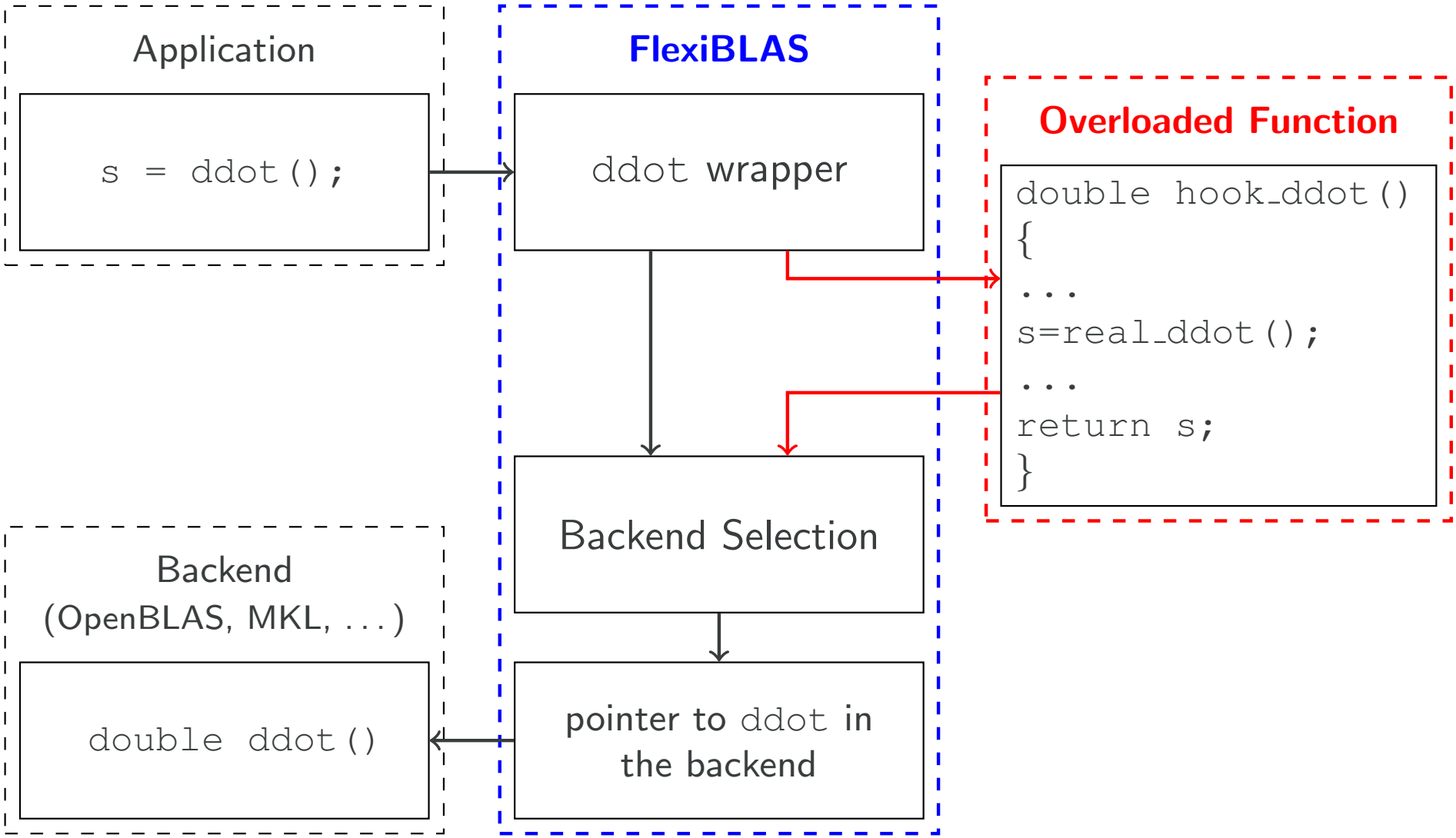

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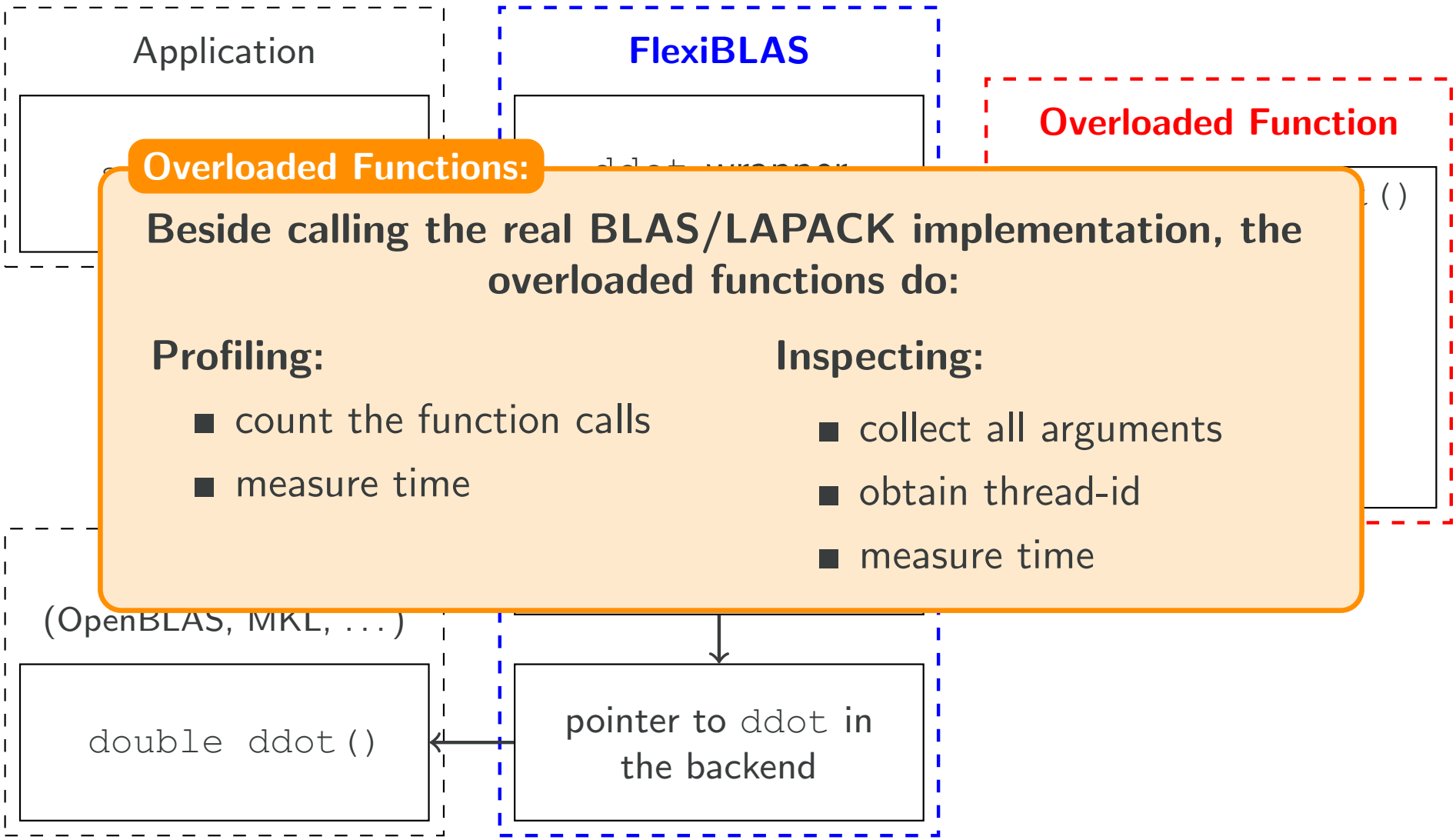
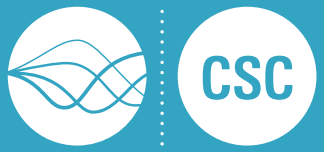
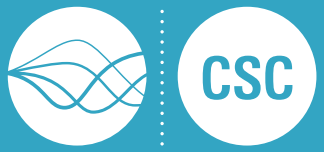




How is it Implemented?

We have $\approx$ 140 BLAS and more than 1 500 LAPACK subroutines.



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- NumPy's `f2py` module allows f77/f90 function headers to be parsed:
  - Extracts all subroutine/function headers.
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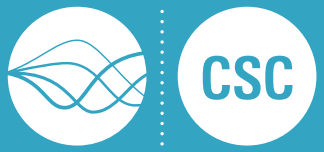
- FlexiBLAS uses the Python template engines to create Fortran-ABI compatible C functions for all extracted subroutines/functions.



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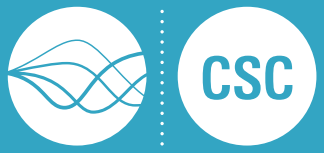
Storing Inspection Data

- Everything is stored in a fixed size buffer. (50 000 entries by default)
- The buffer is secured using atomic variables or mutexes.
- If the buffer is full or the program ends, the buffer is flushed to an SQLite database.
  → Fast and structured access to the collected data.



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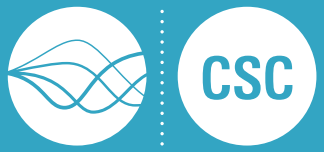

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Execute each BLAS/LAPACK call again with random data

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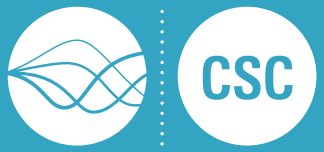

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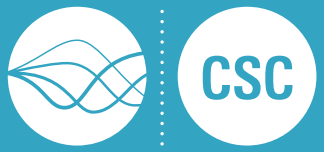

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Alternative Usage of Overloading Capabilities – Automatic Offload

The collected data can help determine if there is a benefit to offloading certain operations to accelerator devices (GPUs, Xeon Phis, FPGAs). FlexiBLAS allows this to be done automatically per BLAS/LAPACK function.

Example Usage
BLAS and GNU Octave 4.2.1

How does GNU Octave use the BLAS library?

```
function [x] = conjgrad(A, b, x)
  r = b - A * x;
  p = r;
  rsold = r' * r;
  for i = 1:length(b)
    Ap = A * p;
    alpha = rsold / (p' * Ap);
    x = x + alpha * p;
    r = r - alpha * Ap;
    rsnew = r' * r;
    if sqrt(rsnew) < 1e-10
       break;
    end;
    p = r + (rsnew / rsold) * p;
    rsold = rsnew;
 end
end

A = full(sprandsym(1000,1.0));
b = A*ones(1000,1);
x = conjgrad(A,b,zeros(1000,1));
norm(A*x-b)/norm(b)
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Profiling:

Subroutine	# Calls	acc. Time
ddot	1000	1.11e-03s
dgemv	1003	4.04e-01s
dsyrk	**1001**	**5.61e-03s**
dlamch	5	2.69e-05s

Observations

- Vector addition/scaling/norms not mapped to BLAS.
- Where does the symmetric rank-k update come from?

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Inspecting:

`DSYRK` computes

$$C := \alpha A \cdot A^T + \beta C \quad \text{if } \texttt{trans='N'}$$

or

$$C := \alpha A^T A + \beta C, \quad \text{if } \texttt{trans='T'}$$

with $A \in \mathbb{R}^{n \times k}$ or $A \in \mathbb{R}^{k \times n}$ and $C \in \mathbb{R}^{n \times n}$.

All 1001 DSYRK calls use:

- `trans = 'T'`
- $n = 1$, $k = 1000$,
- $\alpha = 1.0$, and $\beta = 0$

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→ **Misuse of `DSYRK` to compute the squared 2-norm of a vector.**

Example Usage

OpenBLAS – Issue #1332

Bug Description: **(OpenBLAS up to version 0.2.20)**

The `DTRMV` routine computes

$$x := \alpha T x$$

with $\alpha \in \mathbb{R}$, $x \in \mathbb{R}^n$, and $T \in \mathbb{R}^{n \times n}$ upper or lower triangular.

For example we had production code, where T was stored with leading dimension 64 and n increased from 1 to 64 during an iterative process:

- if $n > 16$, the result x gets perturbed,
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Detection through replaying and comparison to Netlib BLAS:

```
...
Cor.  RESULT: DTRMV(U,N,N, 16, A, 64, X, 1) MAXERR = 0.00D+00
Pert. RESULT: DTRMV(U,N,N, 17, A, 64, X, 1) MAXERR = 0.56D-13
...
Pert. RESULT: DTRMV(U,N,N, 32, A, 64, X, 1) MAXERR = 0.58D-10
Wrong RESULT: DTRMV(U,N,N, 33, A, 64, X, 1) MAXERR = 0.59D+06
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```
...
Corr. RESULT: DTRMV(U,N,N, 16, A, 64, X, 1) MAXERR = 0.00D+00
Pert. RESULT: DTRMV(U,N,N, 17, A, 64, X, 1) MAXERR = 0.56D-13
...
Pert. RESULT: DTRMV(U,N,N, 32, A, 64, X, 1) MAXERR = 0.58D-10
Wrong RESULT: DTRMV(U,N,N, 33, A, 64, X, 1) MAXERR = 0.59D+06
...
```

Race-Condition: The error only appears if OpenBLAS uses multi-threading on highly optimized platforms.

First Workaround: Threading for `xTRMV` is deactivated.

Current Situation:

- Seems to exist more than 10 years.
- Longish discussion (more than 60 comments).
- Still not clear where the race condition comes from.
- Also affects another race condition on the OpenPOWER 8 platform.
- The `DAXPY` operation seems to be involved as well.

Example Usage
OpenBLAS – Issue #1332

Bug Description: **(OpenBLAS up to version 0.2.20)**

The DTRMV routine computes

$$x := \alpha Tx$$

with $\alpha \in \mathbb{R}^n$ and $T \in \mathbb{R}^{n \times n}$ upper triangular.

For example, in the reduction code, where T was stored with leading dimension 64 and n increased from 1 to 64 during an iterative process:

- if $n > 16$ the result x gets perturbed
- if $n > 32$ the result x is completely wrong

Race-Condition: The error only appears if OpenBLAS uses multi-threading on highly optimized platforms.

First Workaround: Threading for `xTRMV` is deactivated.

Current Situation:

- Seems to exist more than 10 years.
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- Still not clear where the race condition comes from.
- Also affects another race condition on the OpenPOWER 8 platform.
- The `DAXPY` operation seems to be involved as well.

FlexiBLAS helps to accelerate the testing of different OpenBLAS configurations.

Detection through replaying and comparison to Netlib BLAS:

```
...
Cor. RESULT: DTRMV(U,N,N, 16, A, 64, X, 1) MAXERR = 0.00D+00
Per. RESULT: DTRMV(U,N,N, 32, A, 64, X, 1) MAXERR = 0.58D-13
...
Per. RESULT: DTRMV(U,N,N, 32, A, 64, X, 1) MAXERR = 0.58D-13
Wrong RESULT: DTRMV(U,N,N, 33, A, 64, X, 1) MAXERR = 0.59D+06
...
```

TileQR [Buttari et. al. '09 – '15]

Reformulation of the Storage Compact QR decomposition parallelized using Direct-Acylic-Graph(DAG) on top of OpenMP 4.

```
do k=1, min(mb,nb)
  !$omp task depend(inout:a(k,k))
  call dgeqrt(a(k,k))
  !$omp end task
  do j=k+1,nb
    !$omp task depend(in:a(k,k)) depend(inout:a(k,j))
     call dgemqrt(a(k,k), a(k,j))
    !$omp end task
  end do
  do i=k+1, mb
    !$omp task depend(inout:a(k,k), a(i,k))
    call dtpqrt(a(k,k), a(i,k))
    !$omp end task
    do j=k+1, nb
      !$omp task depend(in:a(k,k),a(i,k)) &
      ! & depend(inout:a(k,j),a(i,j))
      call dtpmqrt(a(k,k), a(i,k), a(k,j), a(i,j))
      !$omp end task
    end do
  end do
end do
```

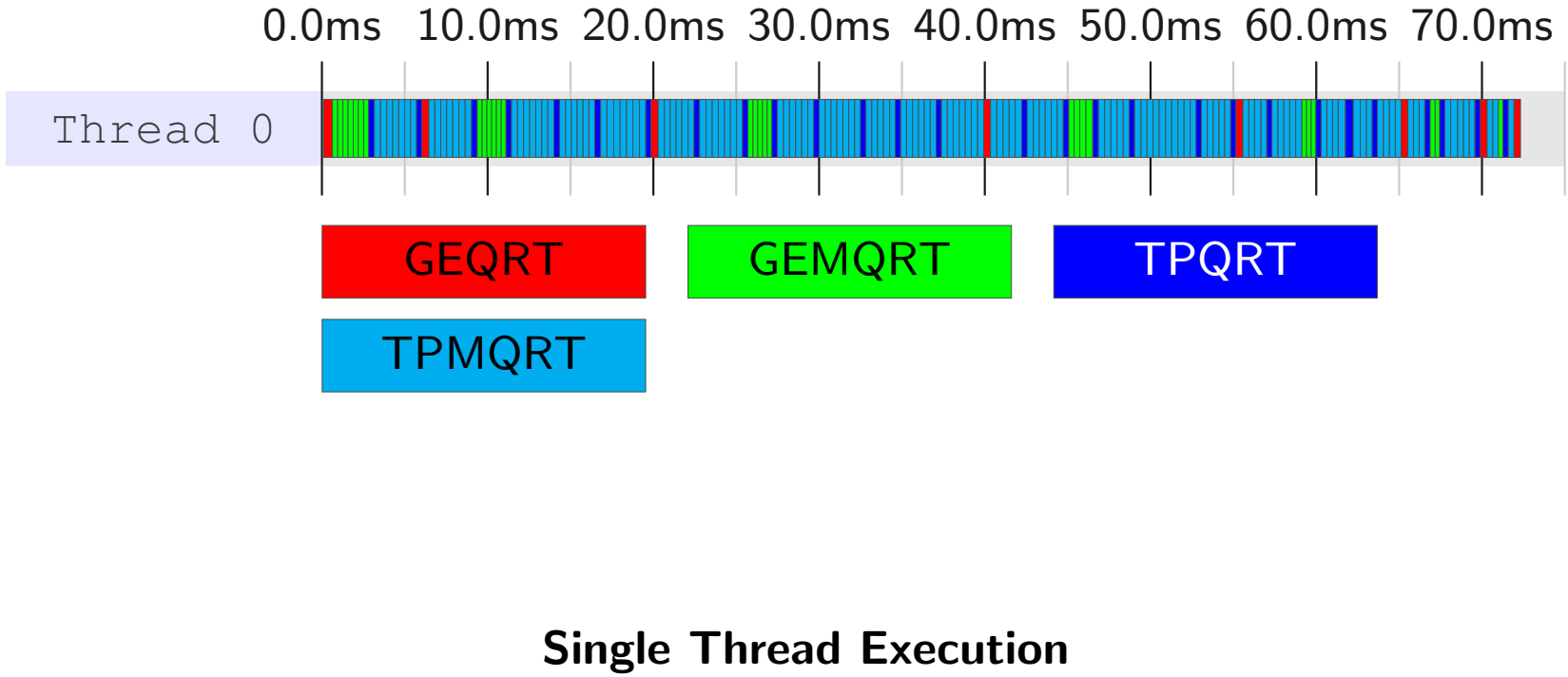
Scales well on Multi-Core CPU.

No threading support in BLAS required.

But how are the single LAPACK calls executed in parallel?

Visualization:

Use start-time, end-time, and thread-id from the SQLite database to visualize the program flow directly as TikZ/LaTeX:

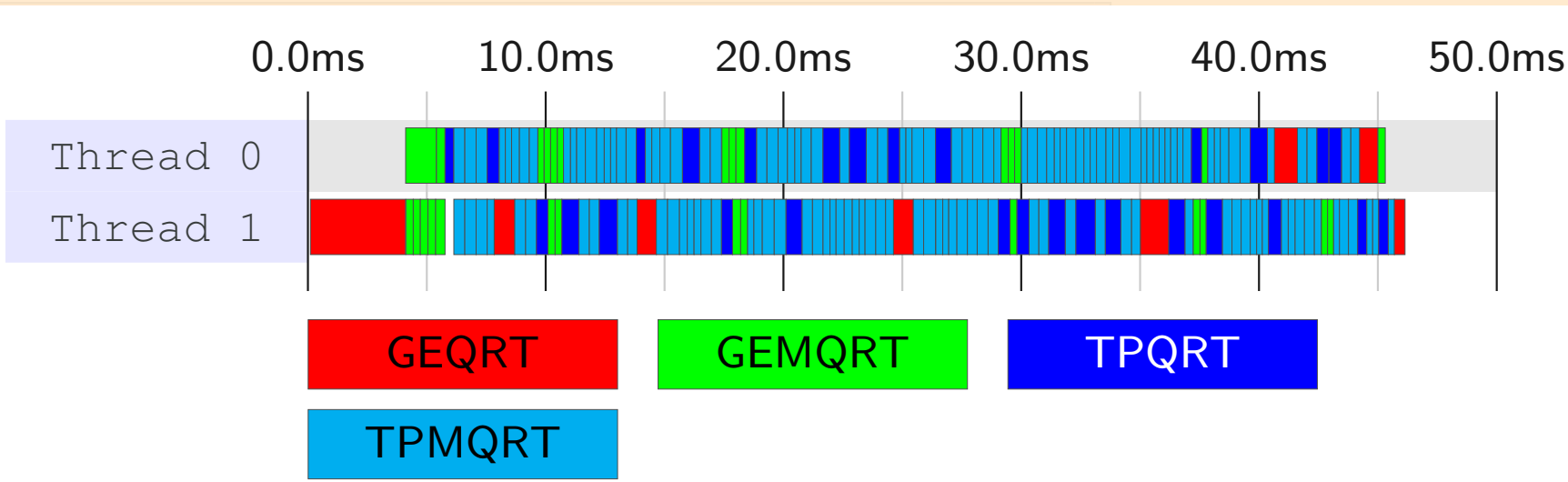


Single Thread Execution

```
    end do
  end do
end do
```

Visualization:

Use start-time, end-time, and thread-id from the SQLite database to visualize the program flow directly as TikZ/LaTeX:

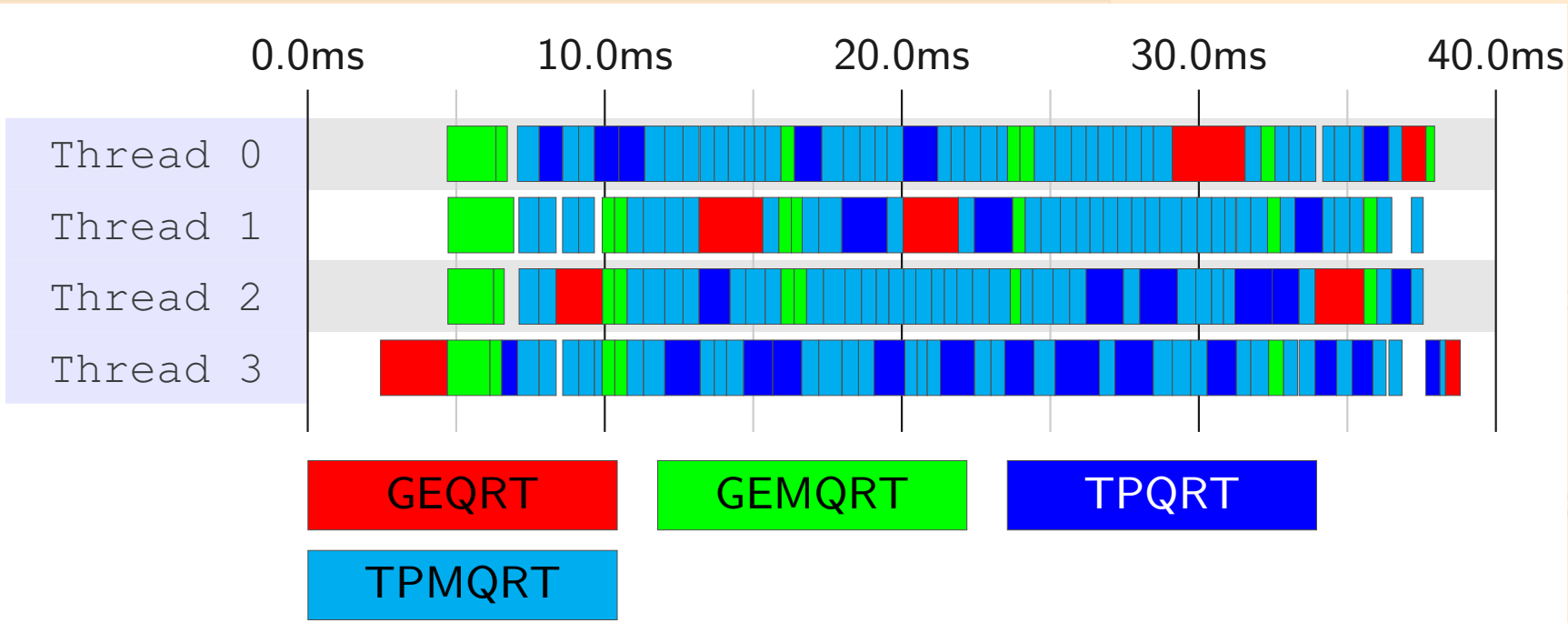


Two Thread Execution

```
    end do
  end do
end do
```

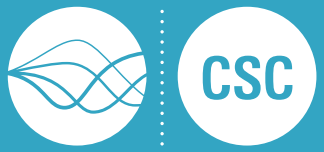
Visualization:

Use start-time, end-time, and thread-id from the SQLite database to visualize the program flow directly as TikZ/LaTeX:



Four Thread Execution

```
    end do
  end do
end do
```



Conclusions and Outlook

Conclusions

- Used FlexiBLAS's overloaded functions for debugging.
- Implemented a profiling/inspection using SQLite as a data store.
- Developed analysis tools to assist debugging and performance analysis.
- Found some interesting bugs in software packages (ours and others).

Outlook

- Develop more analysis tools and continue improving existing ones.
- Integrate automatic offloading as overloaded functions.

Details:

M. Köhler and J. Saak, *FlexiBLAS - A flexible BLAS library with runtime exchangeable backends*, Tech. Rep. 284, LAPACK Working Note, Jan. 2014.

Conclusions and Outlook

Conclusions

- Used FlexiBLAS's overloaded functions for debugging

Thank you very much for your attention!

for the software package visit:

http://www.mpi-magdeburg.mpg.de/projects/flexiblas

https://doi.org/10.5281/zenodo.569102

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M. Köhler and J. Saak, *FlexiBLAS - A flexible BLAS library with runtime exchangeable backends*, Tech. Rep. 284, LAPACK Working Note, Jan. 2014.