MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

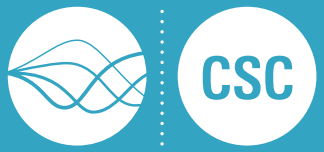
FlexiBLAS

A BLAS and LAPACK wrapper library with runtime exchangable backends

Martin Köhler

March 29, 2020

EasyBuild tech talks III: FlexiBLAS



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."[1]

[1] From: `http://www.netlib.org/blas/faq.html` – What and where are the BLAS?

What is BLAS?

BLAS routine organization

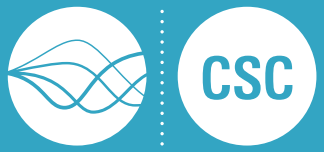
Let α, β be scalars, x, y be vectors, A, B, C be matrices.

level	included operations	data	flops
1	αx, $\alpha x + y$, $x^* y$, $\|\|x\|\|_2$, $\|\|x\|\|_1$, $\|\|x\|\|_\infty$	$\mathcal{O}(n)$	$\mathcal{O}(n)$
2	$\alpha Ax + \beta y$, $\alpha A^* x + \beta y$, $A + \alpha xy^*$, $A + \alpha xx^*$, $A + \alpha xy^* + \beta yx^*$	$\mathcal{O}(n^2)$	$\mathcal{O}(n^2)$
3	$\alpha AB + \beta C$, $\alpha AB^* + \beta C$, $\alpha A^* B^* + \beta C$, $\alpha AA^* + \beta C$, $\alpha A^* A + \beta C$ rank k updates $\alpha A^* B + \beta C$, $\alpha B^* A + \beta C$ rank $2k$ updates	$\mathcal{O}(n^2)$	$\mathcal{O}(n^3)$

What is BLAS?
Some important BLAS implementations

Open Source

- NetLib BLAS: `http://www.netlib.org/blas/`
- OpenBLAS: `http://www.openblas.net/`
- Automatically Tuned Linear Algebra Software (ATLAS): `http://math-atlas.sourceforge.net/`
- BLIS (BLAS-like Library Instantiation Software Framework): `https://github.com/flame/blis`



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Hardware Vendor Implementations

- Intel® Math kernel library (MKL): `http://software.intel.com/en-us/intel-mkl/`
- AMD Core Math Library (ACML): . . . discontinued
- Apple Accelerate, IBM ESSL, ARM Perfromance Libraries . . .

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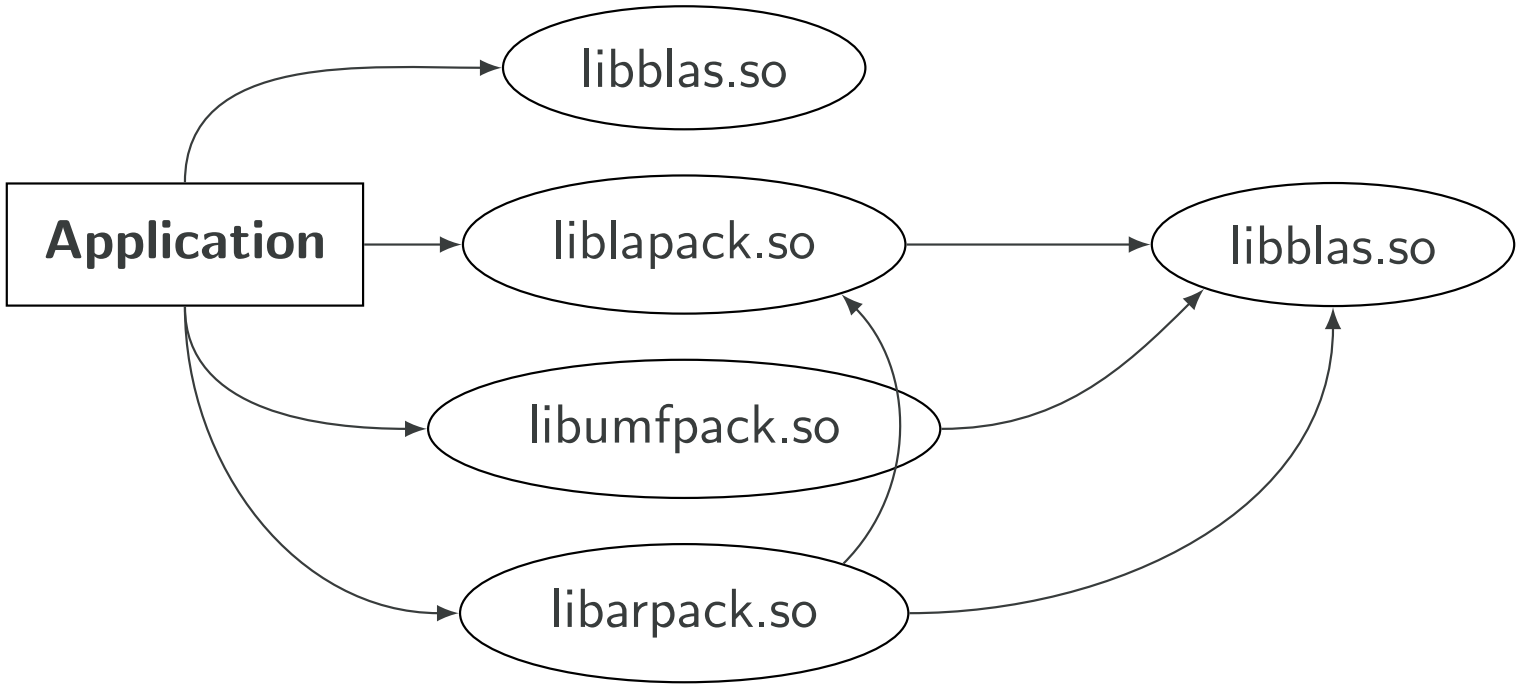
Linker Problems

Example application:



Compiled with:

```
$ gcc -o application app.o -larpack -lumfpack ↩
    -llapack -lblas
```

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```
$ ldd ./application
linux-vdso.so.1 => (0x00007ffc2d1de000)
libarpack.so.2.1.0 => /.../libarpack.so.2.1.0
libumfpack.so.5.7.1 => /.../libumfpack.so.5.7.1
liblapack.so.3 => /.../liblapack.so.3
libblas.so.3 => /.../libblas.so.3
libc.so.6 => /.../libc.so.6
...
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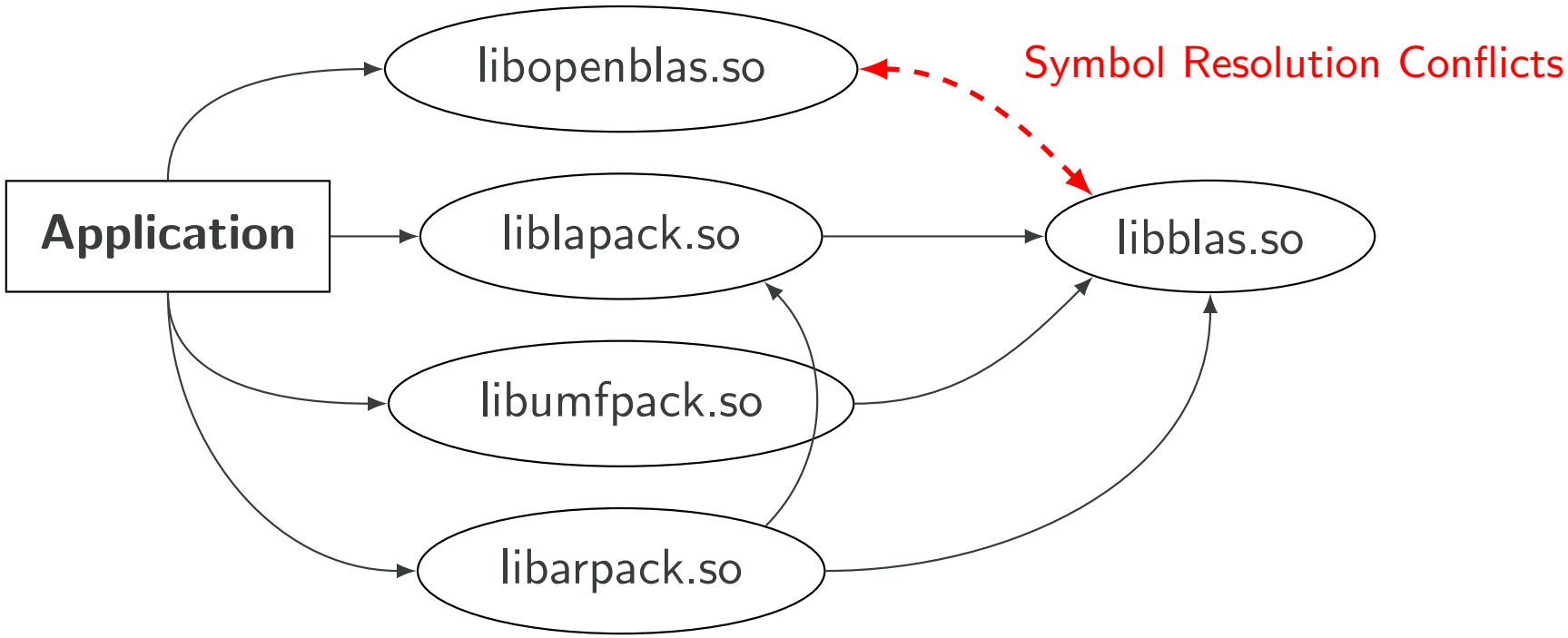

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libopenblas.so.0 => /.../libopenblas.so.0
libc.so.6 => /.../libc.so.6
libm.so.6 => /.../libm.so.6
libblas.so.3 => /.../libblas.so.3
...
```

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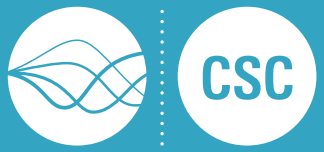
Why do we need yet another BLAS library?

Linker Problems: Existing Solutions

- `LD_LIBRARY_PATH` / `LD_PRELOAD`
  only applicable for single file implementations
  (i.e. NOT Intel® MKL, or ATLAS)
- static libraries
  drastically increased binary sizes, often complicated linking, painful in large projects
- `update-alternatives` (Debian/Ubuntu/Suse)
  requires super-user privileges and has similar restrictions as `LD_LIBRARY_PATH` / `LD_PRELOAD`
- `eselect` / `pkg-config` (Gentoo)
  requires super-user privileges and switches at build-time only
- *BSD ports/pkgsrc/dports
  Links agains libblas.so if already installed otherwise installs some BLAS implementation depending on the maintainer.

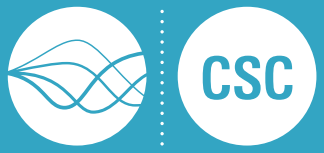


Why do we need yet another BLAS library?

Compatibility Issues

`gfortran` vs `g77/intel` interface style

- **different calling sequences:**
  `gfortran` and `g77/f2c/intel` return complex numbers as additional function parameters.
- **affected routines:** `zdotc`, `zdotu`, `cdotc`, `cdotu` (level 1)



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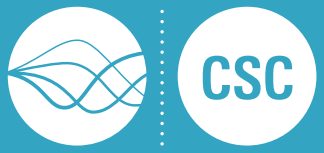
- Routines `sc/dzabs1` are missing in ATLAS and derived implementations, such as Apple Accelerate / AMD ACML.
- IBM ESSL make only a few LAPACK symbols available.



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auxiliary routines

- Intel® MKL and OpenBLAS extend the BLAS routine set by:
  `xAXPBY`, `xOMATCOPY`, ...

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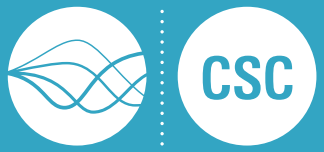
Compatibility Issues

dependency detection problems

Correct/reliable detection of alternative BLAS implementations not guaranteed for many software packages:

- faulty `autotools` scripts,
- old CMake versions,
- hard-coded library names,
- non-standard library locations.



Our Solution – FlexiBLAS

- Initial idea: Summer 2013 after struggling with the linking issue
- First release: December 2013 (BLAS and CBLAS only)
- 2017: Version 2.x wraps LAPACK, switching the BLAS library from the inside of an application
- 2020: Version 3.0.x hooks can be installed around BLAS calls
- October 2020: default BLAS in Fedora 33+ (thanks to Iñaki Ucar)
- Provides interfaces for BLAS, CBLAS, and LAPACK.
- Automatic code generation for the wrappers
- API interface for GNU Octave
- API interface for R (thanks to Iñaki Ucar[2])
- **Latest version: 3.0.4 – October 22nd, 2020**
- **License:** GPLv3+ with linking exception

[2] Twitter/Github: @Enchufa2

How does it work?
General Approach

Long Story Short

We employ a plugin-like framework on top of the POSIX features for dynamic loading of shared libraries at runtime.

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We employ a plugin-like framework on top of the POSIX features for dynamic loading of shared libraries at runtime.

POSIX.1 2001 `dl*`-family

`dlopen` add a shared library and its dynamic dependencies to the current address space.

`dlsym` search for symbols in the current address space beginning in the handle retrieved by `dlopen`.

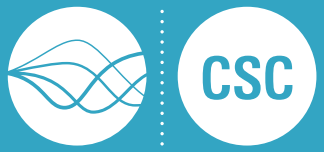
`dlclose` close a previously opened shared library if no other references to the library exist.

`dlerror` provide human readable error messages.

How does it work?
General Approach

`dlopen` based issues to solve

1. `dlopen` only integrates selected parts of the library:
   Each required BLAS call needs to be initialized separately.
2. Dynamically (runtime) loaded symbols can not be resolved while linking a program.
3. `dlopen` only loads a single file:
   Multi-file implementations require additional treatment.



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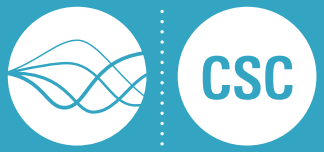
Initialization

`__attribute__((constructor))`

- automatically executed before the program starts.
- replaces deprecated `_init()`.
- Here used to read configuration and explicitly resolve all BLAS-routines to make sure they get loaded by `dlopen` as an initialization stage.



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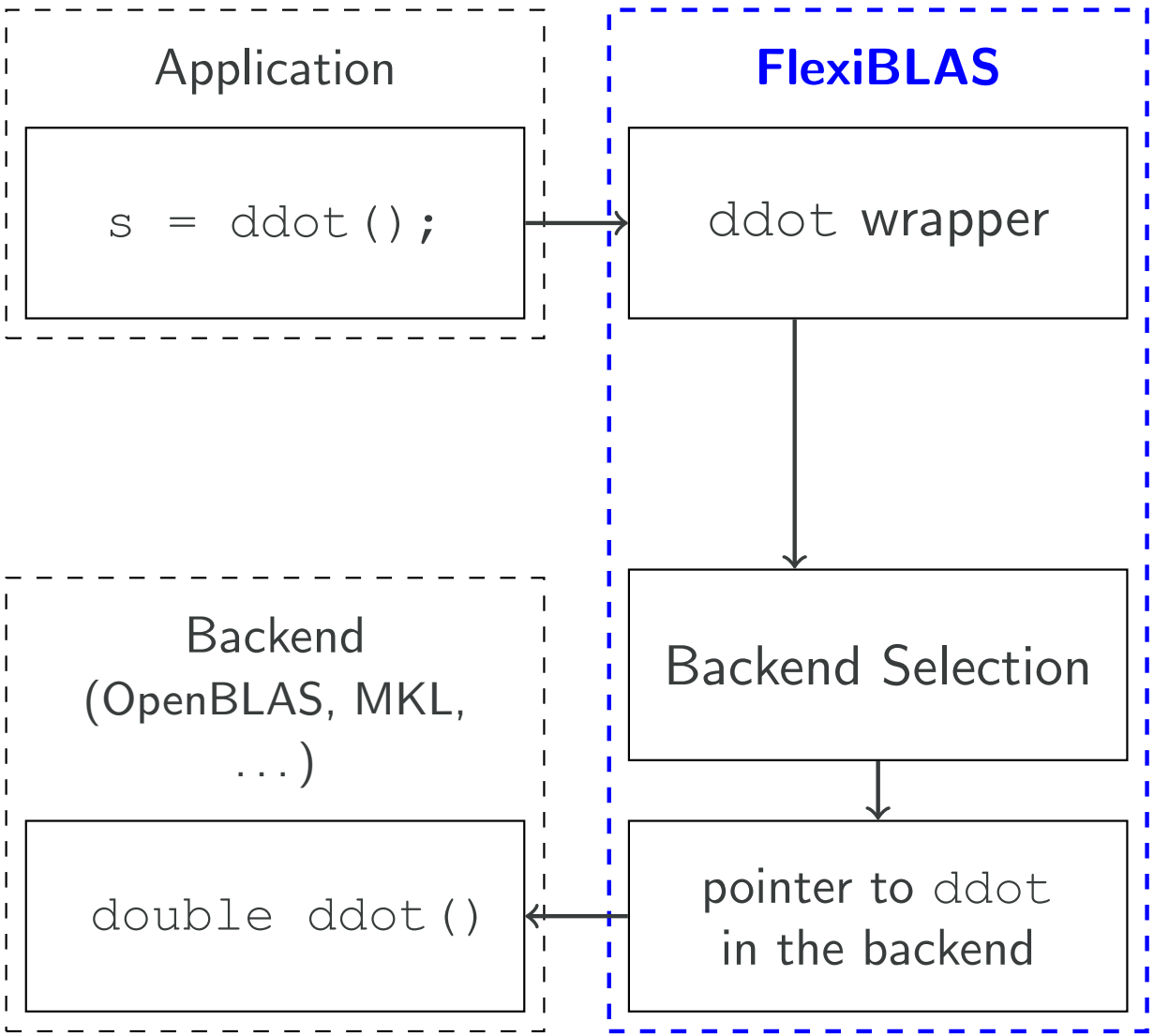
`__attribute__((destructor))`

- automatically executed after the main program exits.
- replaces deprecated `_fini()`.
- Here used to cleanly close the loaded shared library and potentially print profiling data.

How does it work?
Wrapper Functions



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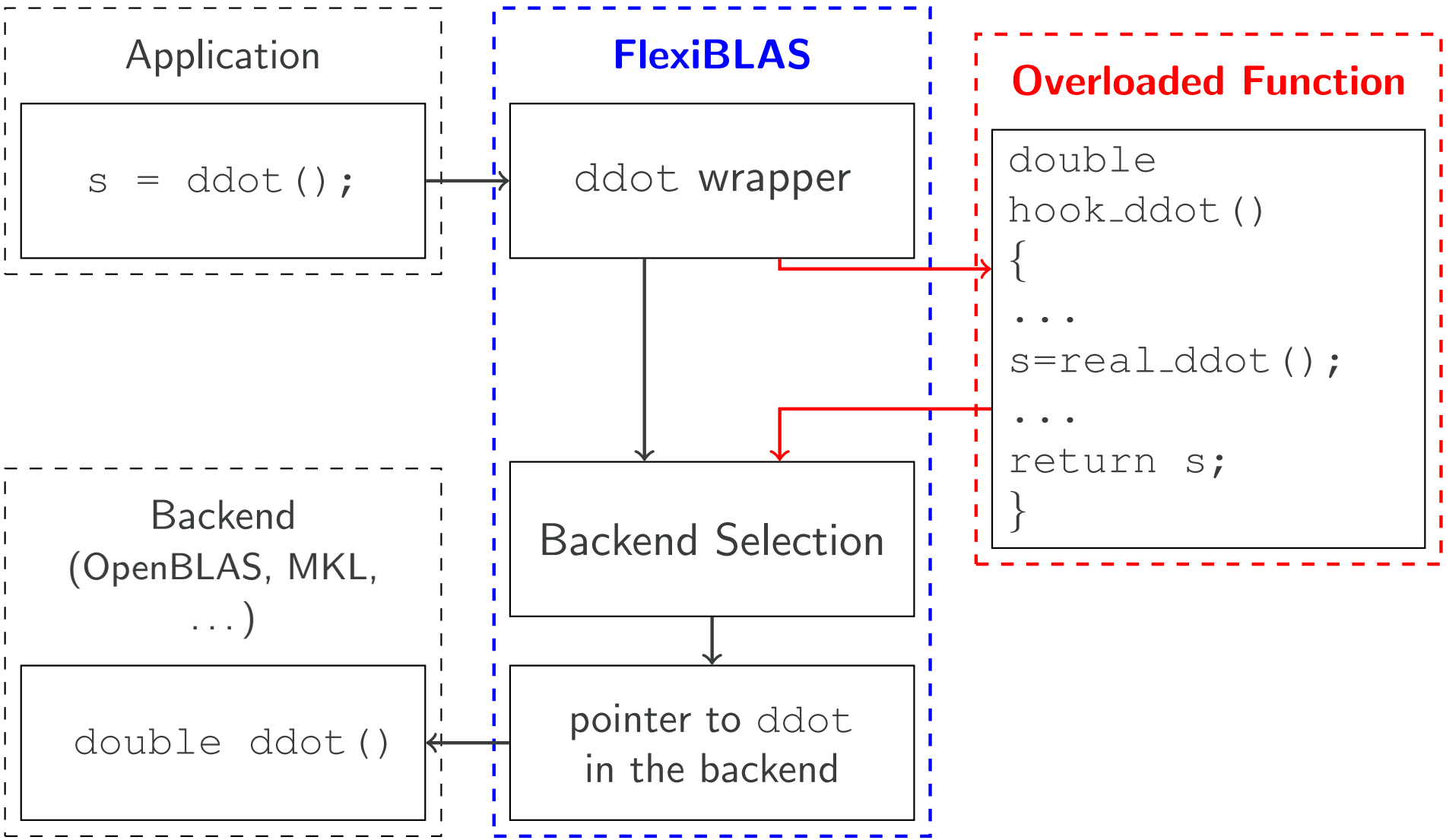

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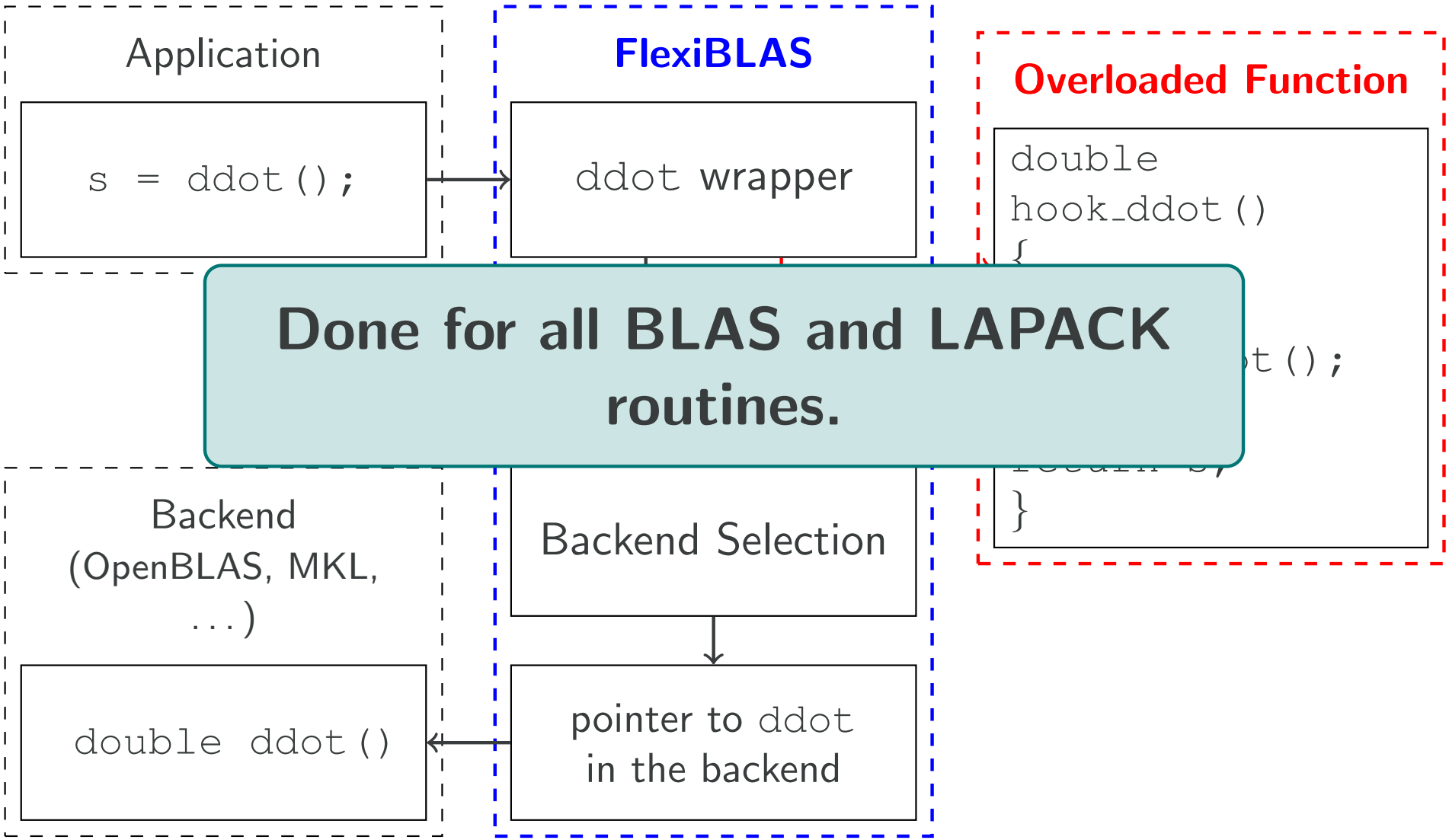

Python based code-gen

- NumPy's `f2py` module allows to parse f77/f90 function headers.
- Extracted function headers are translated into Fortran-ABI compatible C functions containing the wrapper.

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From

```
SUBROUTINE DAXPY(N, ALPHA, X, INCX, Y, INCY)
```

we obtain

```
void daxpy_(Int *N, double *ALPHA, double *X,
 Int *INCX,double *Y, Int * INCY) {
  ...
  fncall_daxypy = backend->daxpy.ffunction;
  fncall_daxpy(N,ALPHA,X,INCX,Y,INCY);
  ... }
```

How does it work?
Multi-file BLAS treatment

Remaining Question

How do we treat BLAS libraries consisting of multiple files (e.g. MKL and some versions of ATLAS), when the `dl*`-family can only use single file shared object libraries?

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Simple trick

Place an additional surrogate library between FlexiBLAS and, e.g., MKL that references all necessary symbols in MKL and behaves like a Netlib-BLAS interface from the view of the dynamic linker.

Intel MKL provides the *mkl-builder* makefile to create such dummy libraries containing arbitrary BLAS symbols.

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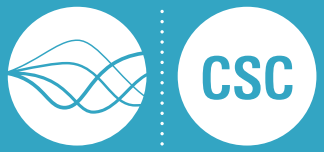
Never use the libmkl_rt.so library!



How is it used?

We provide a tool that closely follows Gentoo's `eselect` syntax.
To check for backends, do

```
flexiblas list
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To select the active backend, use

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flexiblas default BLAS_BACKEND_NAME
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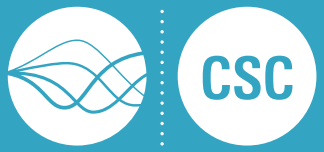

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Alternatively we use an environment variable as in:

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export FLEXIBLAS=/usr/lib/libopenblas.so
```

or

```
export FLEXIBLAS=ATLAS
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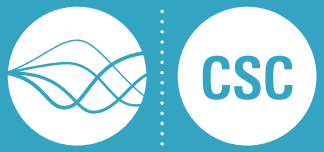

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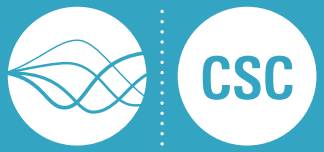
config files: `/etc/flexiblasrc`, `~/.flexiblasrc`, and `~/.flexiblasrc.$(hostname)`



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Other environment variables to control the behavior:

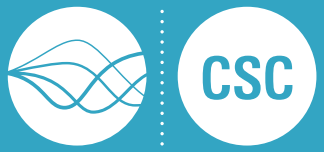
`FLEXIBLAS_VERBOSE` Turn on additional debug outputs.

`FLEXIBLAS_NOLAPACK` Do not load LAPACK from the backend. Only the internal NETLIB version is used.

`FLEXIBLAS_COLOR_OUTPUT` Switch the color output in verbose mode.

`FLEXIBLAS_CONFIG` specify a different `flexiblasrc` file

`FLEXIBLAS_LIBRARY_PATH` specify addtional library search paths



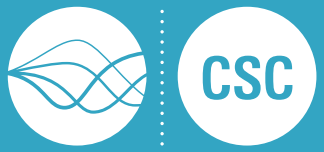
What is the Overhead?

Test Setup

- Ubuntu 20.04, gcc 9.3, Intel Core i5-8500, OpenBLAS/OpenMP
- Measure the shortest successful return path of a BLAS routine, i.e. size zero inputs, with `rdtsc`:

```
__asm__ __volatile__ ("rdtsc" : "=a"(los),"=d"(his));
daxpy(&(int){0}, &(double){1.0}, NULL,&(int){1},
      NULL, &(int){1});
__asm__ __volatile__ ("rdtsc" : "=a"(loe),"=d"(hie));
```

- average over 100 000 000 runs



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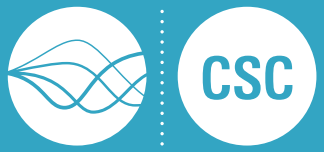
`RDTSC` ticks until return	Linked with		Difference
	OpenBLAS/OpenMP	FlexiBLAS	
`DAXPY`	19.03	24.19	5.16
`DGEMV`	22.92	37.03	14.11
`DGEMM`	28.40	44.47	16.07



Overloading Functions

All BLAS and LAPACK routines can be overloaded:

- build profiling frameworks,
- dynamically offload them to accelerators, (first experiments done)
- introduce faulty behavior for debugging purpose,
- several hooks can be chained,
- original BLAS implementation is callable by a separate pointer.

Example - `DASUM` with perturbed output

```
double hook_dasum(Int *N, double *X, Int *INCX) {
 double res = flexiblas_chain_dasum(N,X,INCX);
 return res + ((*N)*2.2e-16);
}
```

Overloading Functions
Profiling Hook

Functionality:

- measures cumulative the runtime of each BLAS call
- counts the number of calls to each BLAS routine

Usage:

```
FLEXIBLAS_HOOK=libflexiblas_hook_profile.so ./yourapp
```

or

```
FLEXIBLAS_HOOK=PROFILE ./yourapp
```

Overloading Functions

BLAS and GNU Octave 4.2.1

```
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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    p = r + (rsnew / rsold) * p;
    rsold = rsnew;
  end
end

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

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?

Overloading Functions

BLAS and GNU Octave 4.2.1

```
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  p = r;
  rsold = r' * r;
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    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
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A = full(sprandsym(1000,1.0));
b = A*ones(1000,1);
x = conjgrad(A,b,zeros(1000,1));
norm(A*x-b)/norm(b)
```

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 $\beta = 0$

Overloading Functions

BLAS and GNU Octave 4.2.1

```
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

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$\rightarrow$ Misuse of `DSYRK` to compute the squared 2-norm of a vector.

Overloading Functions

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.

In an application we store T with leading dimension 64 and increase n from 1 to 64 during an iterative process:

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

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Hook for DTRSV – Compute with OpenBLAS + Netlib and compare:

```
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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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.
- Affects also a other race condition on the OpenPOWER 8 platform.
- The `DAXPY` operation seems to be involved as well.

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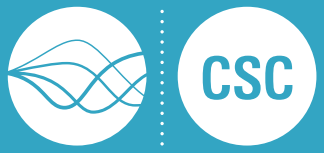
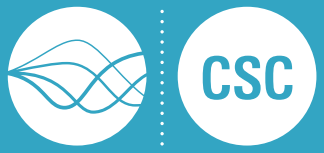
Finding such errors is easier with FlexiBLAS.



That's it!

Outlook:

- meta-data logging hook ready, but no cool analysis tools yet
  - planned: replay tool for correctness and accuracy checking
  - planned: replay tool for application-driven performance optimization
- MacOS X support in testing
- planned: suffixed symbols (in a consistent way)
- planned: per application BLAS selection
- planned: per routine BLAS selection
- planned: LAPACKE support
- planned: proper way to handle `XERBLA` and `cblas_xerbla`
- New release: autumn 2021



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Thank you very much for your attention!

for the software package visit:

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

`https://github.com/mpimd-csc/flexiblas/`

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