LIBHSL: THE ULTIMATE COLLECTION FOR LARGE-SCALE SCIENTIFIC COMPUTATION

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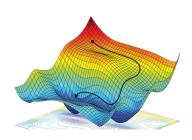


Introduction

The HSL Mathematical Software Library $^{\rm 1}$ is a key resource for **numerical computations**, offering robust and efficient routines for **sparse linear systems** and **eigenvalue problems**.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \qquad \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \lambda \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

These routines are **essential tools** to address complex problems, including those arising in **continuous optimization** and **partial differential equations**.



^{1.} Harwell Subroutine Library - https://www.hsl.rl.ac.uk

What is libHSL?

■ LibHSL is a collection of more than 160 HSL packages.



It aims to facilitate the use of HSL in Julia as well as Fortran, C, C++, and Python such as Ipopt, GALAHAD and CasADi.



 LibHSL provides the source code of the included HSL packages, pre-built binaries with shared libraries, and a Julia package named HSL_jll.jl.

How to use HSL_jll.jl in the Julia ecosystem

To install the package $HSL_jII.jI$, you only need the following commands in the Julia REPL:

```
julia> ]
pkg> dev path_to_hsl_jll
```

HSL_ill.jl is a **registered Julia package** and can be added as a **dependency** of any Julia package.

How to use HSL_jll.jl in Julia packages

ullet A version of HSL_jll.jl based on a dummy LibHSL was precompiled with Yggdrasil 1 .

```
using HSL_jll

function LIBHSL_isfunctional()
    @ccall libhsl.LIBHSL_isfunctional()::Bool
end

bool = LIBHSL_isfunctional()
```

• In the dummy version, LIBHSL_isfunctional returns the boolean false. In the full-featured version provided by LibHSL, this C function returns the boolean true.

```
if LIBHSL_isfunctional()
   ... # solve a symmetric linear system with HSL_MA57
else
   ... # solve a symmetric linear system with SuiteSparse
end
```

^{1.} https://github.com/JuliaPackaging/Yggdrasil

HSL.jl

- The package **HSL.jl** ¹ provides wrappers for all HSL packages with a C interface or those written in Fortran 77.
- Wrappers are Julia functions that call C and Fortran routines with the macro @ccall.
- The combination of HSL.jl and HSL_jll.jl enables users to abstract away from low-level C and Fortran languages, allowing them to utilize most HSL packages as if they were native Julia packages.



^{1.} https://github.com/JuliaSmoothOptimizers/HSL.jl

How to use HSL_jll.jl in lpopt.jl

For the Julia interface Ipopt.jl 1, HSL_jll.jl must be used directly.

```
using JuMP, Ipopt, HSL ill
# An optimization problem
model = Model(Ipopt.Optimizer)
@variable(model, x)
Cobjective (model, Min, (x - 2)^2)
# Use the linear solver MA57
set_attribute(model, "linear_solver", "ma57")
optimize! (model)
# Use the linear solver MA97
set attribute (model, "linear solver", "ma97")
optimize! (model)
```

The available HSL linear solvers are "ma27", "ma57", "ma77", "ma86" and "ma97".

^{1.} https://github.com/jump-dev/Ipopt.jl

BLAS and LAPACK demuxing

 ${\sf HSL_jll.jl}$ is compiled with ${\sf libblastrampoline}^1$ (LBT) and offers the possibility to switch between ${\it BLAS}$ and ${\it LAPACK}$ backends in Julia.



```
# Load OpenBLAS
using OpenBLAS32_jll
BLAS.lbt_forward(libopenblas)

# Load MKL
using MKL

# Load AppleAccelerate
using AppleAccelerate
# BLAS and LAPACK backends loaded
BLAS.lbt_get_config()
```

HSL vs MUMPS

```
This is Ipopt version 3.14.14, running with linear solver X.
Number of nonzeros in equality constraint Jacobian ...:
                                                    3194444
Number of nonzeros in inequality constraint Jacobian .:
                                                   756090
Number of nonzeros in Lagrangian Hessian....:
                                                    5708220
Total number of variables....:
                                                     674143
                   variables with only lower bounds:
               variables with lower and upper bounds:
                                                     595665
                   variables with only upper bounds:
Total number of equality constraints....:
                                                     661017
Total number of inequality constraints....:
                                                     378045
       inequality constraints with only lower bounds:
  inequality constraints with lower and upper bounds:
                                                     126015
       inequality constraints with only upper bounds:
                                                     252030
```

Linear solver	Elapsed time (in seconds)
MUMPS	1445.870
MA27	302.216
MA57	319.198

^{1.} https://github.com/JuliaLinearAlgebra/libblastrampoline

Future improvements

Support for 64-bit integers: A planned enhancement is to add support for 64-bit integers in HSL packages. This upgrade would enable the solution of even larger-scale problems.

<u>GPU-accelerated linear solvers</u>: We anticipate integrating **GPU support** for BLAS libraries, such as CUBLAS for NVIDIA GPUs, rocBLAS for <u>AMD GPUs</u>, or oneMKL for <u>Intel GPUs</u>. This integration could significantly <u>enhance</u> <u>performance</u> in linear solvers.

Conclusion

- \star $\mbox{\bf LibHSL}$ provides $\mbox{\bf everything}$ that you could need in $\mbox{\bf HSL}$ $\mbox{\bf packages}$;
- HSL_jll.jl is a pre-built version of LibHSL to be readily used in the Julia ecosystem;
- * HSL_jll.jl is precompiled for various operating systems (Windows, Mac, Linux, FreeBSD) and architectures (x64, arm64, ppc64);
- * The combination of HSL.jl and HSL_jll.jl allows one to abstract away from the low-level C and Fortran languages;
- * LibHSL is free if you can request an academic licence!



https://licences.stfc.ac.uk/product/libhsl