Cray Scientific Libraries

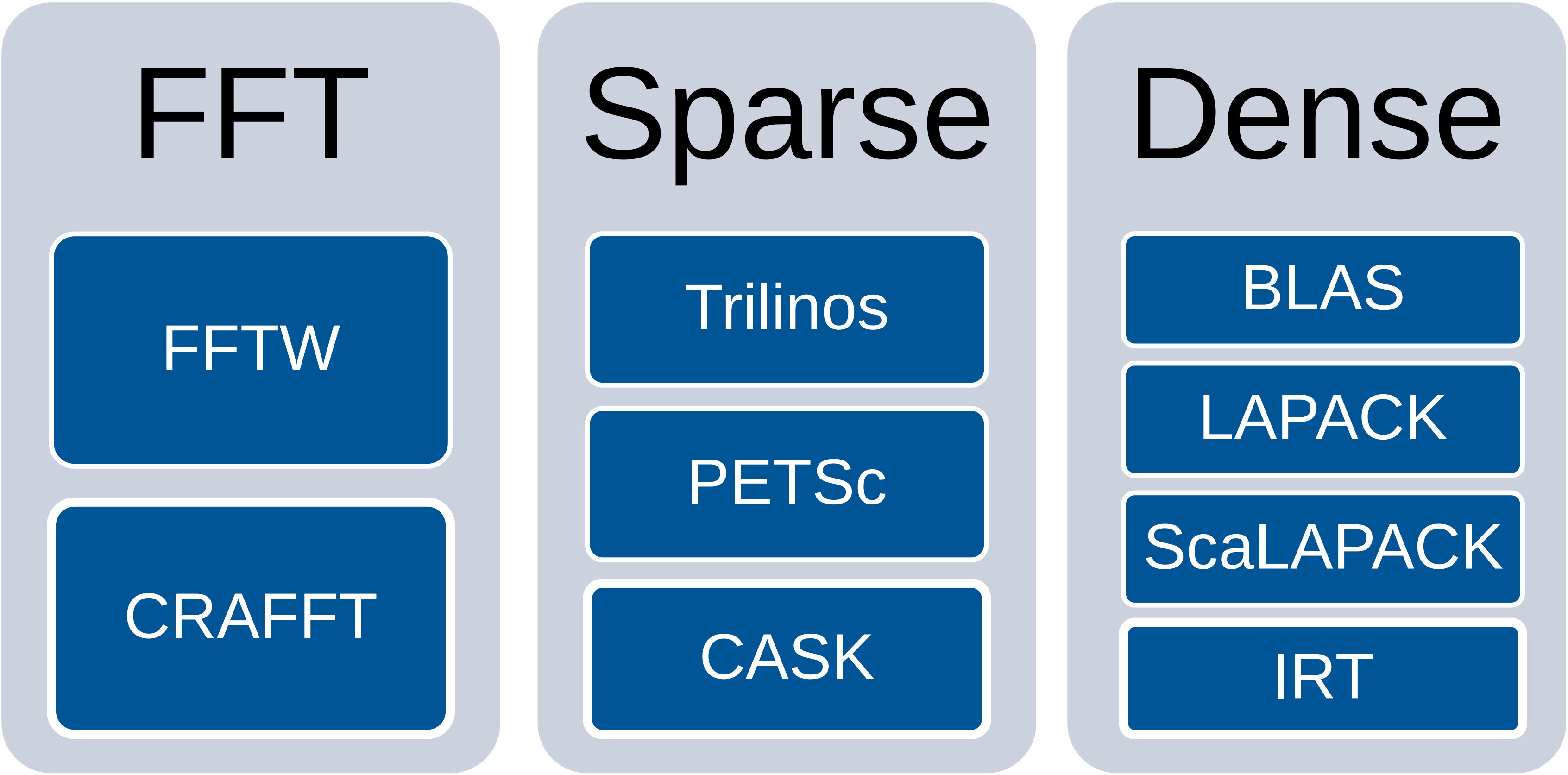
Overview

What are libraries for?

- **Building blocks for writing scientific applications**
- **Historically – allowed the first forms of code re-use**
- **Later – became ways of running optimized code**
- **Today the complexity of the hardware is very high**
- **The Cray PE insulates users from this complexity**
  - Cray module environment
  - CCE
  - Performance tools
  - Tuned MPI libraries (+PGAS)
  - Optimized Scientific libraries

Cray Scientific Libraries are designed to provide the maximum possible performance from Cray systems with minimum effort.

Scientific libraries on XC – functional view



FFT

FFTW

CRAFFT

Sparse

Trilinos

PETSc

CASK

Dense

BLAS

LAPACK

ScaLAPACK

IRT

What makes Cray libraries special

1. **Node performance**
   - Highly tuned routines at the low-level (ex. BLAS)
2. **Network performance**
   - Optimized for network performance
   - Overlap between communication and computation
   - Use the best available low-level mechanism
   - Use adaptive parallel algorithms
3. **Highly adaptive software**
   - Use auto-tuning and adaptation to give the user the known best (or very good) codes at runtime
4. **Productivity features**
   - Simple interfaces into complex software

LibSci usage

- **LibSci**
  - The drivers should do it all for you – no need to explicitly link
  - For threads, set OMP_NUM_THREADS
    - Threading is used within LibSci
    - If you call within a parallel region, single thread used
- **FFTW**
  - `module load fftw` (there are also wisdom files available)
- **PETSc**
  - `module load petsc` (or module load petsc-complex)
  - Use as you would your normal PETSc build
- **Trilinos**
  - `module load trilinos`
- **Cray Adaptive Sparse Kernels (CASK)**
  - You get optimizations for free

Your friends

- module command (module --help)
- PrgEnv modules:
- Component modules
- csmlversion (tool)
- Cray driver scripts ftn, cc, CC

```
TUNER/STUNER> module avail PrgEnv

PrgEnv-cray/3.1.35            PrgEnv-gnu/4.0.12A            PrgEnv-
pathscale/3.1.37G
PrgEnv-cray/3.1.37AA          PrgEnv-gnu/4.0.26A            PrgEnv-
pathscale/3.1.49A
PrgEnv-cray/3.1.37C           PrgEnv-gnu/4.0.36(default)    PrgEnv-
pathscale/3.1.61
PrgEnv-cray/3.1.37E           PrgEnv-intel/3.1.35           PrgEnv-
pathscale/4.0.12A
PrgEnv-cray/3.1.37G           PrgEnv-intel/3.1.37AA         PrgEnv-
pathscale/4.0.26A
PrgEnv-cray/3.1.49A           PrgEnv-intel/3.1.37C          PrgEnv-
pathscale/4.0.36(default)
PrgEnv-cray/3.1.61            PrgEnv-intel/3.1.37E          PrgEnv-pgi/3.1.35
PrgEnv-cray/4.0.12A           PrgEnv-intel/3.1.37G          PrgEnv-
pgi/3.1.37AA
PrgEnv-cray/4.0.26A           PrgEnv-intel/3.1.49A          PrgEnv-pgi/3.1.37C
PrgEnv-cray/4.0.36(default)   PrgEnv-intel/3.1.61           PrgEnv-
pgi/3.1.37E
PrgEnv-gnu/3.1.35             PrgEnv-intel/4.0.12A          PrgEnv-pgi/3.1.37G
PrgEnv-gnu/3.1.37AA           PrgEnv-intel/4.0.26A          PrgEnv-
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PrgEnv-gnu/3.1.37E            PrgEnv-pathscale/3.1.35       PrgEnv-
pgi/4.0.12A
PrgEnv-gnu/3.1.37G            PrgEnv-pathscale/3.1.37AA     PrgEnv-
pgi/4.0.26A
PrgEnv-gnu/3.1.49A            PrgEnv-pathscale/3.1.37C      PrgEnv-
pgi/4.0.36(default)
PrgEnv-gnu/3.1.61             PrgEnv-pathscale/3.1.37E
```

```
------------------------------------------------ /opt/cray/modulefiles ------------------------------------
-------

xt-libsci/10.5.02        xt-libsci/11.0.04        xt-libsci/11.0.05.1
xt-libsci/11.0.03        xt-libsci/11.0.04.8      xt-libsci/11.0.05.2(default)
```

Check you got the right library!

- Add options to the linker to make sure you have the correct library loaded.
- `-Wl` adds a command to the linker from the driver
- You can ask for the linker to tell you where an object was resolved from using the –y option.
  - E.g. `–Wl, -ydgemm_`

```
.//main.o: reference to dgemm_
/opt/xt-libsci/11.0.05.2/cray/73/mc12/lib/libsci_cray_mp.a(dgemm.o):
definition  of dgemm_
```

Note: do not explicitly link “-lsci”. This will not be found from libsci 11+ and means a single core library for 10.x.

Threading

- **LibSci is compatible with OpenMP**
  - Control the number of threads to be used in your program using **OMP_NUM_THREADS**
  - e.g., in job script `export OMP_NUM_THREADS=16`
  - Then run with `aprun -n1 -d16`
- **What behavior you get from the library depends on your code**
  1. No threading in code
     - The BLAS call will use OMP_NUM_THREADS threads
  2. Threaded code, outside parallel regions
     - The BLAS call will use OMP_NUM_THREADS threads
  3. Threaded code, inside parallel regions
     - The BLAS call will use a single thread

Threaded LAPACK

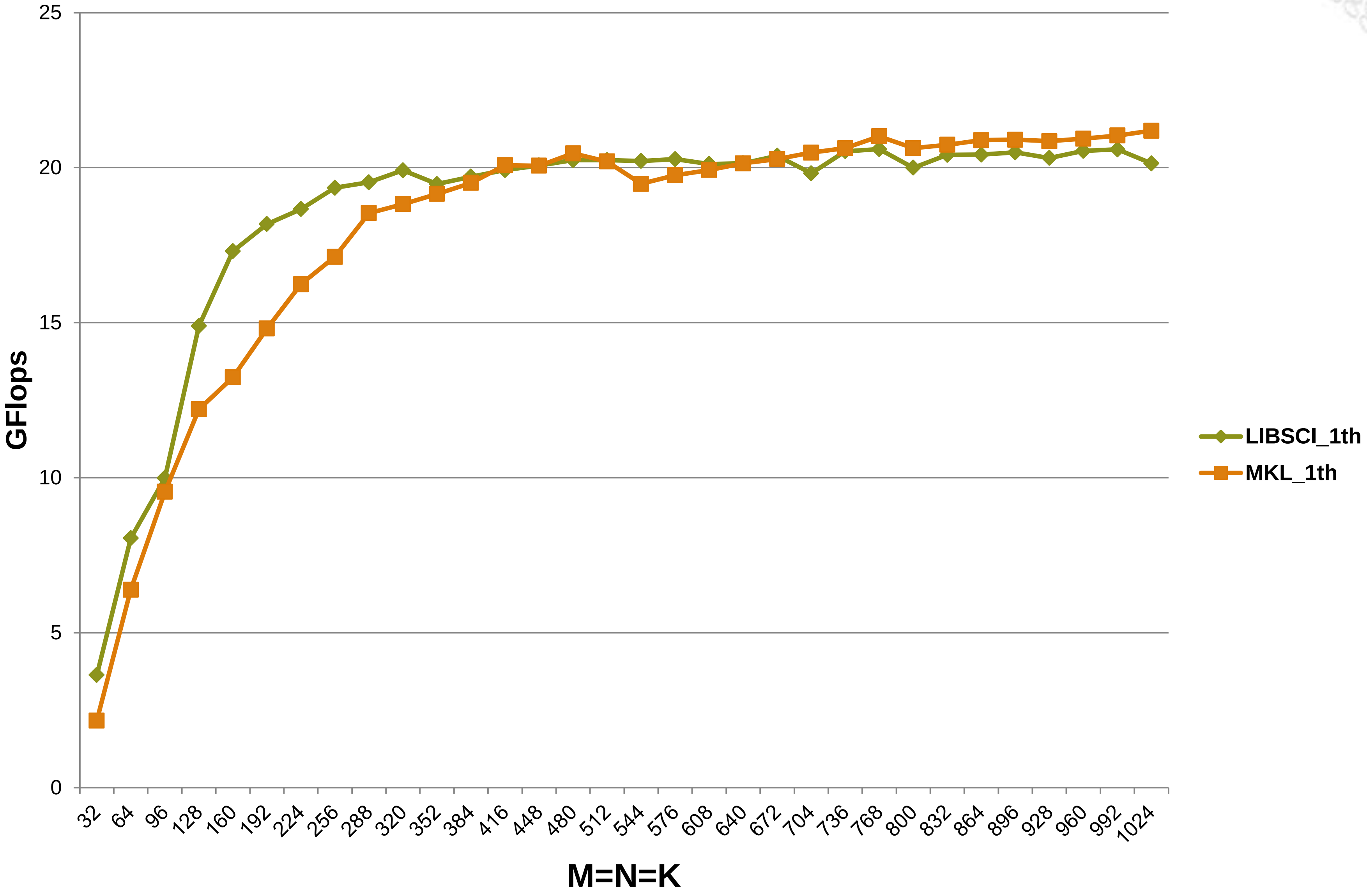
- Threaded LAPACK works exactly the same as threaded BLAS
- Anywhere LAPACK uses BLAS, those BLAS can be threaded
- Some LAPACK routines are threaded at the higher level
- No special instructions

Performance Focus and Autotuning

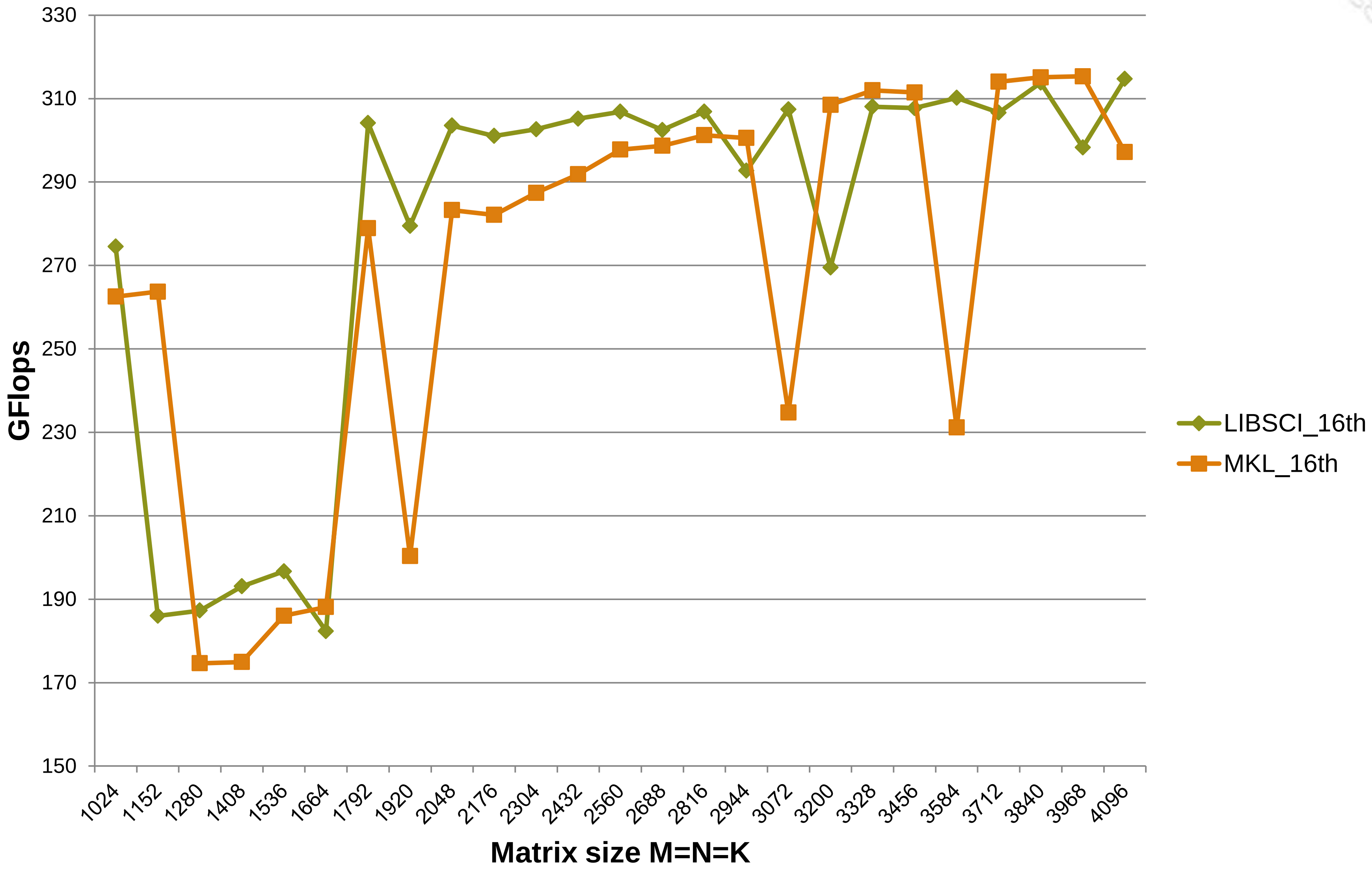
- **Some components of the library are performance critical**
  - For example BLAS and specifically GEMM
- **It is a significant challenge to get best performance across a range of architectures and problem sizes and thread counts**

- **Cray has an autotuning framework to address this:**
  - It uses a general GEMM framework
  - Offline tuning runs are done for a wide range of problem sizes
  - CPU and GPU targets
  - Knowledge gained from offline runs incorporated into the runtime library.

SANDYBRIDGE DGEMM - MEDIUM SQUARE
LIBSCI vs MKL (single thread)



SANDYBRIDGE DGEMM - LARGE SQUARE
LIBSCI vs MKL



Tuning requests

- **CrayBLAS is an auto-tuned library**
  - Generally, excellent performance is possible for all shapes and sizes
- **However, the adaptive CrayBLAS can be improved by tuning for exact sizes and shapes**
- **Send your specific tuning requirements to crayblas@cray.com**
  - Send the routine name and the list of calling sequences

ScaLAPACK and IRT

- **ScaLAPACK in LibSci is optimized for Gemini/Aries interconnect**
  - New collective communication procedures are added
  - Default topologies are changed to use the new optimizations
  - Much better strong scaling
- **It also benefits from the optimizations in CrayBLAS**
- **Iterative Refinement Toolkit (IRT) can provide further improvements**
  - Uses mixed precision
  - For some targets (CPU vector instructions and GPUs) single-precision can be much faster
  - Used for serial and parallel LU, Cholesky and QR
  - Either set IRT_USE_SOLVERS to 1
    or use the advanced API.

Cray Adaptive FFT (CRAFFT)

- **Serial version really just a productivity enhancer**
- **Supports plan/execute with wisdom or do both at once**
- **Load the module**
- **Fortran: use crafft**
- **Serial:**
  - Various simple-to-use interfaces with optional arguments
- **Parallel:**
  - Provides efficient network transposes but uses FFTW3 serial transforms
  - Various network optimizations including computation and communication overlap
  - Various 2d/3d real and complex transforms implemented

Summary

- **Do not re-invent the wheel but use scientific libraries wherever you can!**
- **All the most widely used library families and frameworks readily available as XE/XC optimized versions**
  - And if the cornerstone library of your application is still missing, let us know about it!
- **Make sure you use the optimized version provided by the system instead of a reference implementation**
- **... and give us feedback**