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Intel MKL Usage

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High-Performance Computing Infrastructure
for South East Europe's Research Communities

The HP-SEE initiative is co-funded by the European Commission under the FP7 Research Infrastructures contract no. 261499

Agenda

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- Overview of MKL
- Things to know before starting
- Structure of MKL (Layered Model Concept)
- Linking with MKL
  - using -mkl compiler option
  - using single dynamic library
  - selecting libraries to link with
  - using the Link-line Advisor
  - using the Command-line link tool
- Example

Overview of MKL

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- Computing math library of highly optimized, extensively threaded routines for applications that require maximum performance.
- Works best with Intel CPUs where it exploits optimized instruction sets such as SSE2, SSE3, SSSE3 and others
- Threading enables it to utilize the growing number of cores per CPU

Overview of MKL

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- Major areas of computation supported:
  - BLAS (level 1, 2 and 3) and LAPACK linear algebra routines;
  - PARADISO direct sparse solver, an iterative sparse solver and supportin sparse BLAS (level 1, 2 and 3) routines for solving sparse systems of equations;
  - ScaLAPACK distributed processing linear algebra routines, BLACS and PBLAS;
  - FFT functions in one, two or three dimentions, and distributed versions;
  - Vector Math Library (VML)
  - Vector Statistics Library (VSL)
  - Data Fitting Library

Things to know before starting

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- Target platform
  - IA-32 or compatible
  - Intel® 64 or compatible
- Mathematical problem

BLAS, Sparse BLAS, LAPACK, PBLAS, ScaLAPACK, Sparse Solver routines, VML functions, FFT, Cluster FFT, Trigonometric Transform routines, Poisson, Laplace and Helmholtz Solver routines, Optimization (Trust-Region) Solver routines, Data Fitting Functions, GMP arithmetic functions

- Programming Language
  - C/C++ or Fortran
- Range of integer data
- Threading model and number of threads
- Linking model
- MPI used

Structure of MKL

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- Layered Model
  - Interface Layer
    - matches compiled application with the threading and computational parts of the library
  - Threading Layer
    - links the library with different threading compilers and enables threaded or sequential mode
  - Computational Layer
    - the core of the library
  - Compiler Run-time Libraries
    - support for threading with different compilers

Linking with MKL (1)

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- Ways of linking:
  - using the Intel® Composer XE compiler (using -mkl compiler option)
  - explicit dynamic linking
  - explicitly listing libraries on the link line
  - using an interactive interface (Link-line advisor)
  - using an internally provided tool (command line link tool)

note:

general compiler flags for linking are `-L<dir>` and `-l<name>` where `<dir>` is the directory where the library can be found and name is the name of the library without lib prefix and extension (i.e. libmkl_core.so goes to -lmkl_core)

Linking with MKL (2)

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- This is only available on Intel's compiler
- **`-mkl`** or **`-mkl=parallel`** links with standard threaded MKL
- **`-mkl=sequential`** links with sequential version of MKL
- **`-mkl=cluster`** links with cluster components (sequential) that use Intel MPI

Linking with MKL (3)

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- Explicit dynamic linking boils down to using a single dynamic library, abreviated SDL: libmkl_rt.so
- SDL allows selection of interface and threading library at runtime.
  - env variables:
    - $MKL_SET_INTERFACE_LAYER (values: LP64 or ILP64)
    - $MKL_SET_THREADING_LAYER (values: INTEL, SEQUENTIAL, GNU, PGI)
- By default it provides LP64 interface on Intel 64 bit architecture and Intel threading
- Example:

```
icc application.c -lmkl_rt
```

Linking with MKL (4)

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- Explicitly listing libraries to link with
  - choose one linbrary from the interface layer and one from threading layer
  - add the mkl core library and run-time libraries
- Interface layer:
  - **`libmkl_intel.a, libmkl_intel.so, libmkl_intel_lp64.a, libmkl_intel_lp64.so`**
- Threading layer:
  - **`libmkl_intel_thread.a, libmkl_intel_thread.so`**
- Computational layer
  - **`libmkl_core.a, libmkl_core.so`**
- Run-time layer
  - **`libiomp5.a, libiomp5.so`**

Linking with MKL (5)

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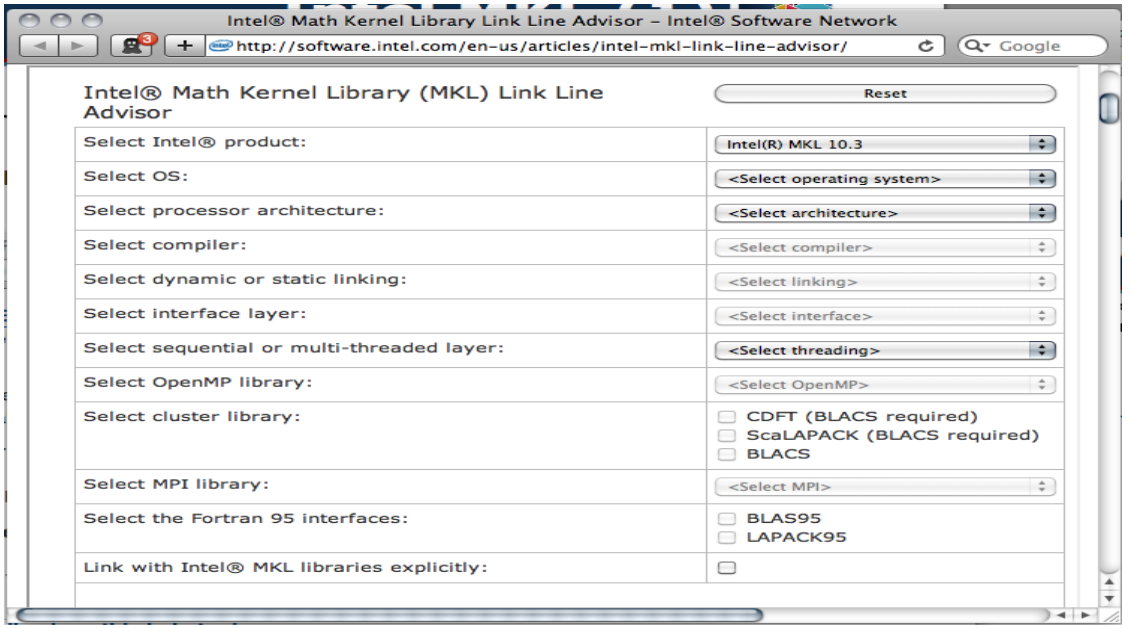
- Using the Link-line Advisor (Recommended)
- available at http://software.intel.com/en-us/articles/intel-mkl-link-line-advisor



Linking with MKL (6)

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- Using the Command line link Tool
  - mkl_link_tool can be found* in <mkl_directory>/tools directory
  - similar to Link line Advisor, but works offline.
  - modes:
    - inquiry `mkl_link_tool (-libs|-opts|-env) [Intel MKL Link Tool options]`
    - compilation `mkl_link_tool [options] <compiler> [options2] file1 [file2 ...]`
    - interactive `mkl_link_tool -interactive`

* actually not available in the installation on Paradox, and many others noted they couldn't find the tool in various versions of MKL (with and without Composer), more information can be found at: http://software.intel.com/en-us/articles/mkl-command-line-link-tool/

Example (1)

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- MKL versions on Paradox:
  - standalone at /opt/intel/mkl/10.2.3.029
  - with Composer XE at /opt/intel/composerxe/mkl
- activating MKL and Intel compiler:
  - **`source /opt/intel/composerxe/bin/compilervars.sh intel64`**
- activating specific MKL environment script (does not load Intel compiler)
  - **`source /opt/intel/mkl/10.2.3.029/tools/environment/mklvarsem64t.sh`**

Example (2)

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- Demo code is on ui.ipb.ac.rs at /tmp/mkl/matrix.c
- MKL environment setup:

```
source /opt/intel/composerxe/bin/compilervars.sh intel64
```

- Compile the code, linking with threaded and sequential versions of the library

Example (3)

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- Sequential:

```
icc -o matrix_sequential matrix.c -mkl=sequential -static-intel
```

or

```
icc -o matrix_sequential matrix.c -Wl,--start-group ${MKLROOT}/lib/
intel64/libmkl_intel_lp64.a ${MKLROOT}/lib/intel64/
libmkl_sequential.a ${MKLROOT}/lib/intel64/libmkl_core.a -Wl,--
endgroup -lpthread -static-intel
```

- Threaded:

```
icc -o matrix_threaded matrix.c -mkl -static-intel
```

or

```
icc -o matrix_threaded matrix.c -Wl,--start-group ${MKLROOT}/lib/
intel64/libmkl_intel_lp64.a ${MKLROOT}/lib/intel64/
libmkl_intel_thread.a ${MKLROOT}/lib/intel64/libmkl_core.a -Wl,--
end-group -openmp -lpthread -static-intel
```

Example (4)

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- Single Dynamic Library linking:

```
icc -o matrix_sdl matrix.c -lmkl_rt
```

- Set environment:

```
export MKL_INTERFACE_LAYER=LP64
export MKL_THREADING_LAYER=SEQUENTIAL
```

real 0m9.951s
user 0m6.324s
sys 0m0.271s

```
    export MKL_THREADING_LAYER=INTEL
```

real 0m3.571s
user 0m0.141s
sys 0m0.220s

References

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- Intel MKL: http://software.intel.com/en-us/articles/intel-mkl/
- MKL Documentation and User Guides: http://software.intel.com/en-us/articles/intel-math-kernel-library-documentation/
- Link-line Advisor: http://software.intel.com/en-us/articles/intel-mkl-link-line-advisor