

# Intel® Math Kernel Library for Linux\* OS

**User's Guide** 

Intel® MKL 11.2 - Linux\* OS

Revision: 048

Legal Information

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# Getting Help and Support

Intel provides a support web site that contains a rich repository of self help information, including getting started tips, known product issues, product errata, license information, user forums, and more. Visit the Intel MKL support website at http://www.intel.com/software/products/support/.

# Introducing the Intel® Math Kernel Library

Intel® Math Kernel Library (Intel® MKL) is a computing math library of highly optimized, extensively threaded routines for applications that require maximum performance. The library provides Fortran and C programming language interfaces. Intel MKL C language interfaces can be called from applications written in either C or C++, as well as in any other language that can reference a C interface.

Intel MKL provides comprehensive functionality support in these major areas of computation:

- BLAS (level 1, 2, and 3) and LAPACK linear algebra routines, offering vector, vector-matrix, and matrix-matrix operations.
- ScaLAPACK distributed processing linear algebra routines for Linux\* and Windows\* operating systems, as
  well as the Basic Linear Algebra Communications Subprograms (BLACS) and the Parallel Basic Linear
  Algebra Subprograms (PBLAS).
- The PARDISO direct sparse solver, an iterative sparse solver, and supporting sparse BLAS (level 1, 2, and 3) routines for solving sparse systems of equations, as well as a distributed version of PARDISO solver provided for use on clusters of the Linux\* and Windows\* operating systems.
- Fast Fourier transform (FFT) functions in one, two, or three dimensions with support for mixed radices (not limited to sizes that are powers of 2), as well as distributed versions of these functions provided for use on clusters of the Linux\* and Windows\* operating systems.
- Vector Math Library (VML) routines for optimized mathematical operations on vectors.
- Vector Statistical Library (VSL) routines, which offer high-performance vectorized random number generators (RNG) for several probability distributions, convolution and correlation routines, and summary statistics functions.
- Data Fitting Library, which provides capabilities for spline-based approximation of functions, derivatives and integrals of functions, and search.
- Extended Eigensolver, a shared memory programming (SMP) version of an eigensolver based on the Feast Eigenvalue Solver.

For details see the Intel® MKL Reference Manual.

Intel MKL is optimized for the latest Intel processors, including processors with multiple cores (see the *Intel MKL Release Notes* for the full list of supported processors). Intel MKL also performs well on non-Intel processors.

For Windows\* and Linux\* systems based on Intel® 64 Architecture, Intel MKL also includes support for the Intel® Many Integrated Core (Intel® MIC) Architecture and provides libraries to help you port your applications to Intel MIC Architecture.

#### **NOTE**

It is your responsibility when using Intel MKL to ensure that input data has the required format and does not contain invalid characters. These can cause unexpected behavior of the library.

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### **Optimization Notice**

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# What's New

This User's Guide documents Intel® Math Kernel Library (Intel® MKL) 11.2 update 4.

The document has been updated to reflect changes to the product and to improve usability and clarity:

- An environment variable has been added to specify matrix size thresholds for ?GEMM computations in the Automatic Offload mode (for details, see Automatic Offload Controls).
- Interaction with the Intel® MPI Library has been described, as well as related recommendations (for details, see Interaction with Message-Passing Interface).

Additionally, minor updates have been made to fix inaccuracies in the document.

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# Notational Conventions

The following term is used in reference to the operating system.

Linux\*OS This term refers to information that is valid on all supported Linux\* operating

systems.

The following notations are used to refer to Intel MKL directories.

<parent product
directory>

The installation directory for the larger product that includes Intel MKL; for example,

Intel® Parallel Studio XE Composer Edition.

<mkl directory>

The main directory where Intel MKL is installed:

<mkl directory>=<parent product directory>/mkl.

Replace this placeholder with the specific pathname in the configuring, linking, and

building instructions.

The following font conventions are used in this document.

Italic Italic Italic is used for emphasis and also indicates document names in body text, for

example:

see Intel MKL Reference Manual.

Monospace lowercase

Indicates filenames, directory names, and pathnames, for example: ./benchmarks/

linpack

Monospace

lowercase mixed with uppercase

Indicates:

· Commands and command-line options, for example,

icc myprog.c -L\$MKLPATH -I\$MKLINCLUDE -lmkl -liomp5 -lpthread

· Filenames, directory names, and pathnames, for example,

C/C++ code fragments, for example,
 a = new double [SIZE\*SIZE];

UPPERCASE

Indicates system variables, for example, \$MKLPATH.

MONOSPACE

Monospace italic

Indicates a parameter in discussions, for example, 1da.

When enclosed in angle brackets, indicates a placeholder for an identifier, an expression, a string, a symbol, or a value, for example, <mkl directory>.

Substitute one of these items for the placeholder.

[ items ] Square brackets indicate that the items enclosed in brackets are optional.

{ item | item } Braces indicate that only one of the items listed between braces should be selected.

A vertical bar ( | ) separates the items.

# Related Information

To reference how to use the library in your application, use this guide in conjunction with the following documents:

- The *Intel*® *Math Kernel Library Reference Manual*, which provides *reference* information on routine functionalities, parameter descriptions, interfaces, calling syntaxes, and return values.
- The Intel® Math Kernel Library for Linux\* OS Release Notes.

# **Getting Started**



#### **Optimization Notice**

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# **Checking Your Installation**

After installing the Intel® Math Kernel Library (Intel® MKL), verify that the library is properly installed and configured:

- **1.** Intel MKL installs in the cparent product directory directory.
  - Check that the subdirectory of <parent product directory> referred to as <mkl directory> was created.
- 2. If you want to keep multiple versions of Intel MKL installed on your system, update your build scripts to point to the correct Intel MKL version.
- **3.** Check that the following files appear in the <mkl directory>/bin directory and its subdirectories:

```
mklvars.sh
mklvars.csh
ia32/mklvars_ia32.sh
ia32/mklvars_ia32.csh
intel64/mklvars_intel64.sh
intel64/mklvars_intel64.csh
```

Use these files to assign Intel MKL-specific values to several environment variables, as explained in Setting Environment Variables

- **4.** To understand how the Intel MKL directories are structured, see Structure of the Intel® Math Kernel Library.
- **5.** To make sure that Intel MKL runs on your system, launch an Intel MKL example, as explained in Using Code Examples.

#### See Also

**Notational Conventions** 

## **Setting Environment Variables**

#### See Also

Setting the Number of Threads Using an OpenMP\* Environment Variable

#### **Scripts to Set Environment Variables**

When the installation of Intel MKL for Linux\* OS is complete, set the INCLUDE, MKLROOT, LD\_LIBRARY\_PATH, MIC\_LD\_LIBRARY\_PATH, LIBRARY\_PATH, CPATH, and NLSPATH environment variables in the command shell using one of the script files in the bin subdirectory of the Intel MKL installation directory. The environment variable MIC\_LD\_LIBRARY\_PATH specifies locations of shared objects for Intel® Many Integrated Core (Intel® MIC) Architecture.

Choose the script corresponding to your system architecture and command shell as explained in the following table:

Architecture	Shell	Script File
IA-32	С	ia32/mklvars_ia32.csh
IA-32	Bash and Bourne (sh)	ia32/mklvars_ia32.sh
Intel® 64	С	intel64/mklvars_intel64.csh
Intel 64	Bash and Bourne (sh)	intel64/mklvars_intel64.sh
All supported architectures	С	mklvars.csh
All supported architectures	Bash and Bourne (sh)	mklvars.sh

#### **Running the Scripts**

The parameters of the scripts specify the following:

- Architecture.
- Use of Intel MKL Fortran modules precompiled with the Intel® Fortran compiler. Supply this parameter only if you are using this compiler.
- Programming interface (LP64 or ILP64).

Usage and values of these parameters depend on the name of the script (regardless of the extension). The following table lists values of the script parameters.

Script	Architecture (required, when applicable)	Use of Fortran Modules (optional)	Interface (optional)
mklvars_ia32	n/a <sup>†</sup>	mod	n/a
mklvars_intel64	n/a	mod	lp64 <b>, default</b> ilp64
mklvars	ia32 intel64 mic	mod	lp64 <b>, default</b> ilp64

<sup>†</sup> Not applicable.

#### For example:

· The command

mklvars.sh ia32

sets the environment for Intel MKL to use the IA-32 architecture.

The command

mklvars.sh intel64 mod ilp64

sets the environment for Intel MKL to use the Intel 64 architecture, ILP64 programming interface, and Fortran modules.

The command

mklvars.sh intel64 mod

sets the environment for Intel MKL to use the Intel 64 architecture, LP64 interface, and Fortran modules.

The command

mklvars.sh mic 1p64

sets the environment for Intel MKL to use the Intel MIC Architecture and LP64 programming interface.

#### **NOTE**

Supply the parameter specifying the architecture first, if it is needed. Values of the other two parameters can be listed in any order.

#### See Also

High-level Directory Structure
Interface Libraries and Modules
Fortran 95 Interfaces to LAPACK and BLAS
Setting the Number of Threads Using an OpenMP\* Environment Variable

#### **Automating the Process of Setting Environment Variables**

To automate setting of the INCLUDE, MKLROOT, LD\_LIBRARY\_PATH, MANPATH, LIBRARY\_PATH, CPATH, and NLSPATH environment variables, add mklvars\*.\*sh to your shell profile so that each time you login, the script automatically executes and sets the paths to the appropriate Intel MKL directories. To do this, with a local user account, edit the following files by adding the appropriate script to the path manipulation section right before exporting variables:

Shell	Files	Commands
bash	~/.bash_profile,	# setting up MKL environment for bash
~/.bash_login or ~/.profile		<pre>. <absolute_path_to_installed_mkl>/bin [/<arch>]/mklvars[<arch>].sh [<arch>] [mod] [lp64 ilp64]</arch></arch></arch></absolute_path_to_installed_mkl></pre>
sh	~/.profile	# setting up MKL environment for sh
		<pre>. <absolute_path_to_installed_mkl>/bin [/<arch>]/mklvars[<arch>].sh [<arch>] [mod] [lp64 ilp64]</arch></arch></arch></absolute_path_to_installed_mkl></pre>
csh	~/.login	# setting up MKL environment for sh
		<pre>. <absolute_path_to_installed_mkl>/bin [/<arch>]/mklvars[<arch>].csh [<arch>] [mod] [lp64 ilp64]</arch></arch></arch></absolute_path_to_installed_mkl></pre>

In the above commands, replace <arch> with ia32 or intel64.

If you have super user permissions, add the same commands to a general-systemfile in/etc/profile(for bash and sh) or in/etc/csh.login(for csh).

#### **CAUTION**

Before uninstalling Intel MKL, remove the above commands from all profile files where the script execution was added. Otherwise you may experience problems logging in.

#### See Also

Scripts to Set Environment Variables

# **Compiler Support**

Intel® MKL supports compilers identified in the *Release Notes*. However, the library has been successfully used with other compilers as well.

When building Intel MKL code examples for either C or Fortran, you can select a compiler: Intel®, GNU\*, or PGI\*.

Intel MKL provides a set of include files to simplify program development by specifying enumerated values and prototypes for the respective functions. Calling Intel MKL functions from your application without an appropriate include file may lead to incorrect behavior of the functions.

#### See Also

Include Files

## **Using Code Examples**

The Intel MKL package includes code examples, located in the <code>examples</code> subdirectory of the installation directory. Use the examples to determine:

- Whether Intel MKL is working on your system
- How you should call the library
- How to link the library

If an Intel MKL component that you selected during installation includes code examples, these examples are provided in a separate archive. Extract the examples from the archives before use.

For each component, the examples are grouped in subdirectories mainly by Intel MKL function domains and programming languages. For instance, the blas subdirectory (extracted from the <code>examples\_core</code> archive) contains a makefile to build the BLAS examples and the <code>vmlc</code> subdirectory contains the makefile to build the C VML examples. You can find examples of Automatic Offload in the  $mic_ao$  subdirectory (extracted from the <code>examples\_mic</code> archive) and examples of Compiler Assisted Offload in the  $mic_offload$  subdirectory. Source code for the examples is in the next-level <code>sources</code> subdirectory.

#### See Also

High-level Directory Structure
Using Intel® Math Kernel Library on Intel® Xeon Phi™ Coprocessors

# What You Need to Know Before You Begin Using the Intel® Math Kernel Library

#### Target platform

Identify the architecture of your target machine:

- IA-32 or compatible
- Intel® 64 or compatible

**Reason:** Because Intel MKL libraries are located in directories corresponding to your particular architecture (seeArchitecture Support), you should provide proper paths on your link lines (see Linking Examples). To configure your development environment for the use with Intel MKL, set your environment variables using the script corresponding to your architecture (see Scripts to Set Environment Variables Setting Environment Variables for details).

# Mathematical problem

Identify all Intel MKL function domains that you require:

- BLAS
- Sparse BLAS
- LAPACK

- PBLAS
- ScaLAPACK
- Sparse Solver routines
- Parallel Direct Sparse Solvers for Clusters
- Vector Mathematical Library functions (VML)
- Vector Statistical Library functions
- Fourier Transform functions (FFT)
- Cluster FFT
- Trigonometric Transform routines
- Poisson, Laplace, and Helmholtz Solver routines
- · Optimization (Trust-Region) Solver routines
- Data Fitting Functions
- Extended Eigensolver Functions

**Reason:** The function domain you intend to use narrows the search in the *Reference Manual* for specific routines you need. Additionally, if you are using the Intel MKL cluster software, your link line is function-domain specific (see Working with the Intel® Math Kernel Library Cluster Software). Coding tips may also depend on the function domain (see Other Tips and Techniques to Improve Performance).

# Programming language

Intel MKL provides support for both Fortran and C/C++ programming. Identify the language interfaces that your function domains support (see Appendix A: Intel® Math Kernel Library Language Interfaces Support).

**Reason:** Intel MKL provides language-specific include files for each function domain to simplify program development (see Language Interfaces Support\_ by Function Domain).

For a list of language-specific interface libraries and modules and an example how to generate them, see also Using Language-Specific Interfaces with Intel® Math Kernel Library.

# Range of integer data

If your system is based on the Intel 64 architecture, identify whether your application performs calculations with large data arrays (of more than  $2^{31}$ -1 elements).

**Reason:** To operate on large data arrays, you need to select the ILP64 interface, where integers are 64-bit; otherwise, use the default, LP64, interface, where integers are 32-bit (see Using the ILP64 Interface vs. LP64 Interface).

#### Threading model

Identify whether and how your application is threaded:

- · Threaded with the Intel compiler
- · Threaded with a third-party compiler
- · Not threaded

**Reason:** The compiler you use to thread your application determines which threading library you should link with your application. For applications threaded with a third-party compiler you may need to use Intel MKL in the sequential mode (for more information, see Linking with Threading Libraries).

#### Number of threads

Determine the number of threads you want Intel MKL to use.

**Reason:** Intel MKL is based on the OpenMP\* threading. By default, the OpenMP\* run-time library sets the number of threads for Intel MKL. If you need a different number, you have to set it yourself using one of the available mechanisms. For more information, see Improving Performance with Threading.

#### Linking model

Decide which linking model is appropriate for linking your application with Intel MKL libraries:

- Static
- Dynamic

**Reason:** The link line syntax and libraries for static and dynamic linking are different. For the list of link libraries for static and dynamic models, linking examples, and other relevant topics, like how to save disk space by creating a custom dynamic library, see Linking Your Application with the Intel® Math Kernel Library.

MPI used

Decide what MPI you will use with the Intel MKL cluster software. You are strongly encouraged to use the latest available version of Intel® MPI.

**Reason:** To link your application with ScaLAPACK and/or Cluster FFT, the libraries corresponding to your particular MPI should be listed on the link line (see Working with the Intel® Math Kernel Library Cluster Software).

# Structure of the Intel® Math Kernel Library

#### **Optimization Notice**

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Notice revision #20110804

## **Architecture Support**

Intel® Math Kernel Library (Intel® MKL) for Linux\* OS provides architecture-specific implementations for supported platforms. The following table lists the supported architectures and directories where each architecture-specific implementation is located.

Architecture	Location
IA-32 or compatible	<mkl directory="">/lib/ia32</mkl>
Intel® 64 or compatible	<mkl directory="">/lib/intel64</mkl>
Intel® Many Integrated Core (Intel® MIC)	<mkl directory="">/lib/mic</mkl>

#### See Also

High-level Directory Structure
Notational Conventions
Detailed Structure of the IA-32 Architecture Directories
Detailed Structure of the Intel® 64 Architecture Directories

# **High-level Directory Structure**

Directory	Contents
<mkl directory=""></mkl>	Installation directory of the Intel® Math Kernel Library (Intel® MKL)
Subdirectories of <mkl dire<="" th=""><th>ectory&gt;</th></mkl>	ectory>
bin	Scripts to set environmental variables in the user shell
bin/ia32	Shell scripts for the IA-32 architecture
bin/intel64	Shell scripts for the Intel® 64 architecture
benchmarks/linpack	Shared-memory (SMP) version of the LINPACK benchmark
benchmarks/mp_linpack	Message-passing interface (MPI) version of the LINPACK benchmark

Directory	Contents
examples	Source and data files for Intel MKL examples. Provided in archives corresponding to Intel MKL components selected during installation.
include	Include files for the library routines, as well as for tests and examples
include/ia32	Fortran 95 .mod files for the IA-32 architecture and Intel $\ensuremath{^{9}}$ Fortran compiler
include/intel64/lp64	Fortran 95 .mod files for the Intel® 64 architecture, Intel Fortran compiler, and LP64 interface
include/intel64/ilp64	Fortran 95 .mod files for the Intel $^{\tiny \odot}$ 64 architecture, Intel Fortran compiler, and ILP64 interface
include/mic/lp64	Fortran 95 .mod files for the Intel $^{\tiny \odot}$ MIC architecture, Intel Fortran compiler, and LP64 interface
include/mic/ilp64	Fortran 95 .mod files for the Intel $^{\tiny \odot}$ MIC architecture, Intel Fortran compiler, and ILP64 interface
include/fftw	Header files for the FFTW2 and FFTW3 interfaces
interfaces/blas95	Fortran 95 interfaces to BLAS and a makefile to build the library
interfaces/fftw2x_cdft	MPI FFTW 2.x interfaces to the Intel MKL Cluster FFT
interfaces/fftw3x_cdft	MPI FFTW 3.x interfaces to the Intel MKL Cluster FFT
interfaces/fftw2xc	FFTW 2.x interfaces to the Intel MKL FFT (C interface)
interfaces/fftw2xf	FFTW 2.x interfaces to the Intel MKL FFT (Fortran interface)
interfaces/fftw3xc	FFTW 3.x interfaces to the Intel MKL FFT (C interface)
interfaces/fftw3xf	FFTW 3.x interfaces to the Intel MKL FFT (Fortran interface)
interfaces/lapack95	Fortran 95 interfaces to LAPACK and a makefile to build the library
lib/ia32	Static libraries and shared objects for the IA-32 architecture
lib/intel64	Static libraries and shared objects for the Intel® 64 architecture
lib/mic	Static libraries and shared objects for the Intel® MIC architecture
tests	Source and data files for tests. Provided in archives corresponding to Intel MKL components selected during installation.
tools	Tools and plug-ins
tools/builder	Tools for creating custom dynamically linkable libraries
Subdirectories of <parent p<="" td=""><td>product directory&gt;</td></parent>	product directory>
Documentation/en_US/mkl	Intel MKL documentation.

#### **See Also**

**Notational Conventions** Using Code Examples

# **Layered Model Concept**

Intel MKL is structured to support multiple compilers and interfaces, both serial and multi-threaded modes, different implementations of threading run-time libraries, and a wide range of processors. Conceptually Intel MKL can be divided into distinct parts to support different interfaces, threading models, and core computations:

- 1. Interface Layer
- 2. Threading Layer
- 3. Computational Layer

You can combine Intel MKL libraries to meet your needs by linking with one library in each part layer-bylayer.

To support threading with different compilers, you also need to use an appropriate threading run-time library (RTL). These libraries are provided by compilers and are not included in Intel MKL.

The following table provides more details of each layer.

Layer	Description
Interface Layer	This layer matches compiled code of your application with the threading and/or computational parts of the library. This layer provides:
	<ul> <li>LP64 and ILP64 interfaces.</li> <li>Compatibility with compilers that return function values differently.</li> <li>A mapping between single-precision names and double-precision names for applications using Cray*-style naming (SP2DP interface).</li> </ul>
Threading Layer	This layer:
	<ul><li>Provides a way to link threaded Intel MKL with supported compilers.</li><li>Enables you to link with a threaded or sequential mode of the library.</li></ul>
	This layer is compiled for different environments (threaded or sequential) and compilers (from Intel, $GNU^*$ , and $PGI^*$ ).
Computational Layer	This layer accommodates multiple architectures through identification of architecture features and chooses the appropriate binary code at run time.

#### See Also

Using the ILP64 Interface vs. LP64 Interface Using the SP2DP Interface Linking Your Application with the Intel® Math Kernel Library Linking with Threading Libraries

### **Contents of the Documentation Directories**

File name	Comment	
Files in <pre><pre>parent product directory&gt;/Documentation</pre></pre>		
<pre><locale>/clicense or <locale>/flicense</locale></locale></pre>	Common end user license for the larger product that includes Intel $\ensuremath{MKL}.$	
mklsupport.txt	Information on package number for customer support reference	

File name	Comment	
Contents of <pre><pre>contents of <pre>contents of <pre>c</pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre></pre>		
redist.txt	List of redistributable files	
mkl_documentation.htm	Overview and links for the Intel MKL documentation	
get_started.html	Brief introduction to Intel MKL	
<pre>tutorials/mkl_mmx_c/ index.htm</pre>	Getting Started Tutorials "Using Intel® Math Kernel Library for Matrix Multiplication (C Language)"	
<pre>tutorials/mkl_mmx_f/ index.htm</pre>	Getting Started Tutorials "Using Intel® Math Kernel Library for Matrix Multiplication (Fortran Language)"	
mklman90.pdf <sup>†</sup>	Intel MKL 9.0 Reference Manual in Japanese	
Release_Notes.htm	Intel MKL Release Notes	
mkl_userguide/index.htm	Intel MKL User's Guide in an uncompressed HTML format, this document	
mkl_link_line_advisor.htm	Intel MKL Link-line Advisor	

 $<sup>^{\</sup>scriptscriptstyle \dagger}$  Included only in a localized Japanese version of the Intel $^{\scriptscriptstyle \circledcirc}$  MKL. Please see the Release Notes for information on Intel MKL localization.

For more documents, search Intel MKL documentation at http://software.intel.com/en-us/articles/intel-math-kernel-library-documentation/.

#### See Also

**Notational Conventions** 

# Linking Your Application with the Intel® Math Kernel Library



#### **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

Notice revision #20110804

# **Linking Quick Start**

Intel® Math Kernel Library (Intel® MKL) provides several options for quick linking of your application, which depend on the way you link:

Using the Intel® Parallel Studio XE Composer Edition compiler see Using the -mkl Compiler Option.

Explicit dynamic linking see Using the Single Dynamic Library for how to simplify your link line.

Explicitly listing libraries on your link line see Selecting Libraries to Link with for a summary of the libraries.

Using an interactive interface see Using the Link-line Advisor to determine libraries and options to specify

on your link or compilation line.

Using an internally provided tool

see Using the Command-line Link Tool to
determine libraries, options, and
environment variables or even compile and

build your application.

#### **Using the -mkl Compiler Option**

The Intel®Parallel Studio XE Composer Edition compiler supports the following variants of the -mkl compiler option:

-mkl or to link with standard threaded Intel MKL.

-mkl=parallel

-mkl=sequential to link with sequential version of Intel MKL.

-mkl=cluster to link with Intel MKL cluster components (sequential) that use

Intel MPI.

For more information on the -mkl compiler option, see the Intel Compiler User and Reference Guides.

On Intel® 64 architecture systems, for each variant of the -mkl option, the compiler links your application using the LP64 interface.

If you specify any variant of the -mkl compiler option, the compiler automatically includes the Intel MKL libraries. In cases not covered by the option, use the Link-line Advisor or see Linking in Detail.

#### See Also

Listing Libraries on a Link Line Using the ILP64 Interface vs. LP64 Interface Using the Link-line Advisor

Intel® Software Documentation Library for Intel® compiler documentation

#### **Using the Single Dynamic Library**

You can simplify your link line through the use of the Intel MKL Single Dynamic Library (SDL).

To use SDL, place libmkl rt.so on your link line. For example:

icc application.c -lmkl\_rt

SDL enables you to select the interface and threading library for Intel MKL at run time. By default, linking with SDL provides:

- Intel LP64 interface on systems based on the Intel® 64 architecture
- Intel interface on systems based on the IA-32 architecture
- Intel threading

To use other interfaces or change threading preferences, including use of the sequential version of Intel MKL, you need to specify your choices using functions or environment variables as explained in section Dynamically Selecting the Interface and Threading Layer.

#### **Selecting Libraries to Link with**

To link with Intel MKL:

- Choose one library from the Interface layer and one library from the Threading layer
- Add the only library from the Computational layer and run-time libraries (RTL)

The following table lists Intel MKL libraries to link with your application.

	Interface layer	Threading layer	Computational layer	RTL
IA-32 architecture, static linking	libmkl_intel.a	libmkl_intel_ thread.a	libmkl_core.a	libiomp5.so
IA-32 architecture, dynamic linking	libmkl_intel.	libmkl_intel_ thread.so	libmkl_core.	libiomp5.so
Intel® 64 architecture, static linking	libmkl_intel_ lp64.a	libmkl_intel_ thread.a	libmkl_core.a	libiomp5.so
Intel® 64 architecture, dynamic linking	libmkl_intel_ lp64.so	libmkl_intel_ thread.so	libmkl_core.	libiomp5.so
Intel® Many Integrated Core (Intel® MIC) Architecture,	<pre>libmkl_intel_ lp64.a</pre>	<pre>libmkl_intel_ thread.a</pre>	libmkl_core.a	libiomp5.so

	Interface layer	Threading layer	Computational layer	RTL
static linking				
Intel MIC Architecture, dynamic linking	libmkl_intel_ lp64.so	libmkl_intel_ thread.so	libmkl_core.so	libiomp5.so

The Single Dynamic Library (SDL) automatically links interface, threading, and computational libraries and thus simplifies linking. The following table lists Intel MKL libraries for dynamic linking using SDL. See Dynamically Selecting the Interface and Threading Layer for how to set the interface and threading layers at run time through function calls or environment settings.

	SDL	RTL
IA-32 and Intel® 64 architectures	libmkl_rt.so	libiomp5.so <sup>††</sup>

<sup>&</sup>lt;sup>††</sup>Use the Link-line Advisor to check whether you need to explicitly link the libiomp5.so RTL.

For exceptions and alternatives to the libraries listed above, see Linking in Detail.

#### See Also

Layered Model Concept

Using the Link-line Advisor

Using the -mkl Compiler Option

Working with the Intel® Math Kernel Library Cluster Software

Linking for Compiler Assisted Offload For special linking needed for Compiler Assisted Offload

#### **Using the Link-line Advisor**

Use the Intel MKL Link-line Advisor to determine the libraries and options to specify on your link or compilation line.

The latest version of the tool is available at http://software.intel.com/en-us/articles/intel-mkl-link-line-advisor. The tool is also available in the documentation directory of the product.

The Advisor requests information about your system and on how you intend to use Intel MKL (link dynamically or statically, use threaded or sequential mode, and so on). The tool automatically generates the appropriate link line for your application.

#### See Also

High-level Directory Structure

#### **Using the Command-line Link Tool**

Use the command-line Link tool provided by Intel MKL to simplify building your application with Intel MKL.

The tool not only provides the options, libraries, and environment variables to use, but also performs compilation and building of your application.

The tool mkl link tool is installed in the <mkl directory>/tools directory.

See the knowledge base article at http://software.intel.com/en-us/articles/mkl-command-line-link-tool for more information.

## **Linking Examples**

#### See Also

Using the Link-line Advisor Examples of Linking for Clusters

#### **Linking on IA-32 Architecture Systems**

The following examples illustrate linking that uses Intel(R) compilers.

The examples use the .f Fortran source file. C/C++ users should instead specify a .cpp (C++) or .c (C) file and replace ifort with icc.

#### In these examples,

MKLPATH=\$MKLROOT/lib/ia32, MKLINCLUDE=\$MKLROOT/include.

#### **NOTE**

If you successfully completed the Scripts to Set Environment Variables Setting Environment Variables step of the Getting Started process, you can omit  $-\protect\operatorname{ISMKLINCLUDE}$  in all the examples and omit  $-\protect\operatorname{LSMKLIPATH}$  in the examples for dynamic linking.

• Static linking of myprog.f and parallel Intel MKL:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-Wl,--start-group $MKLPATH/libmkl_intel.a $MKLPATH/libmkl_intel_thread.a $MKLPATH/
libmkl_core.a
-Wl,--end-group -liomp5 -lpthread -lm
```

• Dynamic linking of myprog.f and parallel Intel MKL:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-lmkl intel -lmkl intel thread -lmkl core -liomp5 -lpthread -lm
```

• Static linking of myprog.f and sequential version of Intel MKL:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-Wl,--start-group $MKLPATH/libmkl_intel.a $MKLPATH/libmkl_sequential.a $MKLPATH/
libmkl_core.a
-Wl,--end-group -lpthread -lm
```

Dynamic linking of myprog.f and sequential version of Intel MKL:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-lmkl_intel -lmkl_sequential -lmkl_core -lpthread -lm
```

• Dynamic linking of myprog.f and parallel or sequential Intel MKL (Call the mkl\_set\_threading\_layer function or set value of the MKL\_THREADING\_LAYER environment variable to choose threaded or sequential mode):

```
ifort myprog.f -lmkl_rt
```

Static linking of myprog.f, Fortran 95 LAPACK interface, and parallel Intel MKL:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE -I$MKLINCLUDE/ia32
-lmkl_lapack95
-Wl,--start-group $MKLPATH/libmkl_intel.a $MKLPATH/libmkl_intel_thread.a $MKLPATH/libmkl_core.a
-Wl,--end-group
-liomp5 -lpthread -lm
```

Static linking of myprog.f, Fortran 95 BLAS interface, and parallel Intel MKL:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE -I$MKLINCLUDE/ia32
-lmkl_blas95
```

```
-Wl,--start-group $MKLPATH/libmkl_intel.a $MKLPATH/libmkl_intel_thread.a $MKLPATH/libmkl_core.a -Wl,--end-group -liomp5 -lpthread -lm
```

#### See Also

Fortran 95 Interfaces to LAPACK and BLAS

Examples for Linking a C Application

Examples for Linking a Fortran Application

Using the Single Dynamic Library

Linking with System Libraries for specifics of linking with a GNU or PGI compiler

#### Linking on Intel(R) 64 Architecture Systems

The following examples illustrate linking that uses Intel(R) compilers.

The examples use the .f Fortran source file. C/C++ users should instead specify a .cpp (C++) or .c (C) file and replace ifort with icc.

#### In these examples,

```
MKLPATH=$MKLROOT/lib/intel64, MKLINCLUDE=$MKLROOT/include.
```

#### **NOTE**

If you successfully completed the Scripts to Set Environment Variables Setting Environment Variables step of the Getting Started process, you can omit -I\$MKLINCLUDE in all the examples and omit -L\$MKLPATH in the examples for dynamic linking.

• Static linking of myprog.f and parallel Intel MKL supporting the LP64 interface:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-Wl,--start-group $MKLPATH/libmkl_intel_lp64.a $MKLPATH/libmkl_intel_thread.a
$MKLPATH/libmkl core.a -Wl,--end-group -liomp5 -lpthread -lm
```

• Dynamic linking of myprog.f and parallel Intel MKL supporting the LP64 interface:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core
-liomp5 -lpthread -lm
```

• Static linking of myprog.f and sequential version of Intel MKL supporting the LP64 interface:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-Wl,--start-group $MKLPATH/libmkl_intel_lp64.a $MKLPATH/libmkl_sequential.a
$MKLPATH/libmkl core.a -Wl,--end-group -lpthread -lm
```

• Dynamic linking of myprog.f and sequential version of Intel MKL supporting the LP64 interface:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-lmkl_intel lp64 -lmkl sequential -lmkl_core -lpthread -lm
```

• Static linking of myprog.f and parallel Intel MKL supporting the ILP64 interface:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-Wl,--start-group $MKLPATH/libmkl_intel_ilp64.a $MKLPATH/libmkl_intel_thread.a
$MKLPATH/libmkl core.a -Wl,--end-group -liomp5 -lpthread -lm
```

• Dynamic linking of myprog.f and parallel Intel MKL supporting the ILP64 interface:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-lmkl_intel_ilp64 -lmkl_intel_thread -lmkl_core -liomp5 -lpthread -lm
```

• Dynamic linking of user code myprog.f and parallel or sequential Intel MKL (Call appropriate functions or set environment variables to choose threaded or sequential mode and to set the interface):

```
ifort myprog.f -lmkl rt
```

Static linking of myprog.f, Fortran 95 LAPACK interface, and parallel Intel MKL supporting the LP64 interface:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE -I$MKLINCLUDE/intel64/lp64
-lmkl_lapack95_lp64 -Wl,--start-group $MKLPATH/libmkl_intel_lp64.a $MKLPATH/
libmkl_intel_thread.a
$MKLPATH/libmkl core.a -Wl,--end-group -liomp5 -lpthread -lm
```

Static linking of myprog.f, Fortran 95 BLAS interface, and parallel Intel MKL supporting the LP64 interface:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE -I$MKLINCLUDE/intel64/lp64
-lmkl_blas95_lp64 -Wl,--start-group $MKLPATH/libmkl_intel_lp64.a $MKLPATH/
libmkl_intel_thread.a
$MKLPATH/libmkl_core.a -Wl,--end-group -liomp5 -lpthread -lm
```

#### See Also

Fortran 95 Interfaces to LAPACK and BLAS Examples for Linking a C Application Examples for Linking a Fortran Application Using the Single Dynamic Library

Linking with System Libraries for specifics of linking with a GNU or PGI compiler

## **Linking in Detail**

This section recommends which libraries to link with depending on your Intel MKL usage scenario and provides details of the linking.

#### **Listing Libraries on a Link Line**

To link with Intel MKL, specify paths and libraries on the link line as shown below.

#### **NOTE**

The syntax below is for dynamic linking. For static linking, replace each library name preceded with "1" with the path to the library file. For example, replace -lmkl\_core with \$MKLPATH/libmkl\_core.a,
where \$MKLPATH is the appropriate user-defined environment variable.

```
<files to link>
-L<MKL path>-I<MKL include>
[-I<MKL include>/{ia32|intel64|{ilp64|lp64}}]

[-lmkl_blas{95|95_ilp64|95_lp64}]

[-lmkl_lapack{95|95_ilp64|95_lp64}]

[<cluster components>]
-lmkl_{intel|intel_ilp64|intel_lp64|intel_sp2dp|gf|gf_ilp64|gf_lp64}}
-lmkl_{intel_thread|gnu_thread|pgi_thread|sequential}}
-lmkl_core

[-liomp5] [-lpthread] [-lm] [-ld1]
```

In case of static linking, enclose the cluster components, interface, threading, and computational libraries in grouping symbols (for example, -Wl,--start-group \$MKLPATH/libmkl\_cdft\_core.a \$MKLPATH/libmkl\_blacs\_intelmpi\_ilp64.a \$MKLPATH/libmkl\_intel\_ilp64.a \$MKLPATH/libmkl intel thread.a \$MKLPATH/libmkl core.a -Wl,--end-group).

The order of listing libraries on the link line is essential, except for the libraries enclosed in the grouping symbols above.

#### See Also

Using the Link-line Advisor Linking Examples

Working with the Intel® Math Kernel Library Cluster Software

#### Dynamically Selecting the Interface and Threading Layer

The Single Dynamic Library (SDL) enables you to dynamically select the interface and threading layer for Intel MKL.

#### **Setting the Interface Layer**

To set the interface layer at run time, use the mkl\_set\_interface\_layer function or the MKL INTERFACE LAYER environment variable.

Available interface layers depend on the architecture of your system.

The following table lists available interface layers for Intel® 64 architecture along with the values to be used to set each layer.

#### Specifying the Interface Layer for Intel® 64 Architecture

Interface Layer	Value of MKL_INTERFACE_LAYER	Value of the Parameter of mkl_set_interface_layer
Intel LP64, default	LP64	MKL_INTERFACE_LP64
Intel ILP64	ILP64	MKL_INTERFACE_ILP64
GNU* LP64	GNU, LP64	MKL_INTERFACE_LP64+MKL_INTERFACE_GNU
GNU ILP64	GNU, ILP64	MKL_INTERFACE_ILP64+MKL_INTERFACE_GNU

If the mkl\_set\_interface\_layer function is called, the environment variable MKL\_INTERFACE\_LAYER is ignored.

See the Intel MKL Reference Manual for details of the mkl set interface layer function.

The following table lists available interface layers for IA-32 architecture along with the values to be used to set each layer.

#### **Specifying the Interface Layer for IA-32 Architecture**

Interface Layer	Value of MKL_INTERFACE_LAYER	Value of the Parameter of mkl_set_interface_layer
Intel, default	LP64	MKL_INTERFACE_LP64
GNU	GNU, LP64	MKL_INTERFACE_LP64+MKL_INTERFACE_GNU
	or	or
	GNU	MKL_INTERFACE_GNU

#### **Setting the Threading Layer**

To set the threading layer at run time, use the <code>mkl\_set\_threading\_layer</code> function or the <code>MKL\_THREADING\_LAYER</code> environment variable. The following table lists available threading layers along with the values to be used to set each layer.

#### **Specifying the Threading Layer**

Threading Layer	Value of MKL_THREADING_LAYER	Value of the Parameter of mkl_set_threading_layer
Intel threading, default	INTEL	MKL_THREADING_INTEL
Sequential mode of Intel MKL	SEQUENTIAL	MKL_THREADING_SEQUENTIAL
GNU threading <sup>†</sup>	GNU	MKL_THREADING_GNU
PGI threading <sup>†</sup>	PGI	MKL_THREADING_PGI

<sup>&</sup>lt;sup>†</sup> Not supported by the SDL for Intel® Many Integrated Core Architecture.

If the mkl\_set\_threading\_layer function is called, the environment variable MKL\_THREADING\_LAYER is ignored.

See the Intel MKL Reference Manual for details of the mkl set threading layer function.

#### See Also

Using the Single Dynamic Library Layered Model Concept Directory Structure in Detail

#### **Linking with Interface Libraries**

#### Using the ILP64 Interface vs. LP64 Interface

The Intel MKL ILP64 libraries use the 64-bit integer type (necessary for indexing large arrays, with more than  $2^{31}$ -1 elements), whereas the LP64 libraries index arrays with the 32-bit integer type.

The LP64 and ILP64 interfaces are implemented in the Interface layer. Link with the following interface libraries for the LP64 or ILP64 interface, respectively:

- libmkl intel lp64.a or libmkl intel ilp64.a for static linking
- libmkl intel lp64.so or libmkl intel ilp64.so for dynamic linking

The ILP64 interface provides for the following:

- Support large data arrays (with more than 2<sup>31</sup>-1 elements)
- $\bullet$   $\,$  Enable compiling your Fortran code with the -i8 compiler option

The LP64 interface provides compatibility with the previous Intel MKL versions because "LP64" is just a new name for the only interface that the Intel MKL versions lower than 9.1 provided. Choose the ILP64 interface if your application uses Intel MKL for calculations with large data arrays or the library may be used so in future.

Intel MKL provides the same include directory for the ILP64 and LP64 interfaces.

#### Compiling for LP64/ILP64

The table below shows how to compile for the ILP64 and LP64 interfaces:

Fortran	
Compiling for ILP64	ifort -i8 -I <mkl directory="">/include</mkl>
Compiling for LP64	ifort -I <mkl directory="">/include</mkl>

C or C++	
Compiling for ILP64	icc -DMKL_ILP64 -I <mkl directory="">/include</mkl>
Compiling for LP64	icc -I <mkl directory="">/include</mkl>

# **CAUTION**

Linking of an application compiled with the -i8 or  $-DMKL\_ILP64$  option to the LP64 libraries may result in unpredictable consequences and erroneous output.

# **Coding for ILP64**

You do not need to change existing code if you are not using the ILP64 interface.

To migrate to ILP64 or write new code for ILP64, use appropriate types for parameters of the Intel MKL functions and subroutines:

Integer Types	Fortran	C or C++
32-bit integers	INTEGER*4 or INTEGER(KIND=4)	int
Universal integers for ILP64/ LP64:	INTEGER without specifying KIND	MKL_INT
<ul><li>64-bit for ILP64</li><li>32-bit otherwise</li></ul>		
Universal integers for ILP64/ LP64:	INTEGER*8 or INTEGER(KIND=8)	MKL_INT64
• 64-bit integers		
FFT interface integers for ILP64/ LP64	INTEGER without specifying KIND	MKL_LONG

To determine the type of an integer parameter of a function, use appropriate include files. For functions that support only a Fortran interface, use the C/C++ include files \*.h.

The above table explains which integer parameters of functions become 64-bit and which remain 32-bit for ILP64. The table applies to most Intel MKL functions except some VML and VSL functions, which require integer parameters to be 64-bit or 32-bit regardless of the interface:

- **VML:** The mode parameter of VML functions is 64-bit.
- Random Number Generators (RNG):

All discrete RNG except viRngUniformBits64 are 32-bit.

The viRngUniformBits64 generator function and vslSkipAheadStream service function are 64-bit.

• **Summary Statistics:** The *estimate* parameter of the vslsSSCompute/vsldSSCompute function is 64-bit.

Refer to the Intel MKL Reference Manual for more information.

To better understand ILP64 interface details, see also examples and tests.

#### Limitations

All Intel MKL function domains support ILP64 programming but FFTW interfaces to Intel MKL:

- FFTW 2.x wrappers do not support ILP64.
- FFTW 3.x wrappers support ILP64 by a dedicated set of functions plan guru64.

#### See Also

High-level Directory Structure
Include Files
Language Interfaces Support, by Function Domain
Layered Model Concept
Directory Structure in Detail

# **Using the SP2DP Interface**

If your application is targeted to the Intel 64 architecture and uses Cray\*-style naming and ILP64 interface, SP2DP interface enables you to call Intel MKL BLAS and/or LAPACK functions from your application with minimal changes to the code.

SP2DP interface maps single-precision names (for both real and complex types) in the application to double-precision names in Intel MKL BLAS and LAPACK. Function names are mapped as shown in the following example for BLAS functions ?GEMM:

```
SGEMM -> DGEMM
DGEMM -> DGEMM
CGEMM -> ZGEMM
ZGEMM -> ZGEMM
```

#### **NOTE**

No changes are made to double-precision names.

The SP2DP interface is implemented in the Interface layer. To use the SP2DP interface, link your application with the following interface library:

- libmkl intel sp2dp.a for static linking
- libmkl intel sp2dp.so for dynamic linking

For example, use the following link line to statically link your Fortran application with the threaded version of Intel MKL using the SP2DP interface:

```
ifort myprog.f -L$MKLPATH -I$MKLINCLUDE
-Wl,--start-group $MKLPATH/libmkl_intel_sp2dp.a $MKLPATH/libmkl_intel_thread.a
$MKLPATH/libmkl core.a -Wl,--end-group -liomp5 -lpthread -lm
```

# See Also

High-level Directory Structure Layered Model Concept Directory Structure in Detail

# **Linking with Fortran 95 Interface Libraries**

The <code>libmkl\_blas95\*.a</code> and <code>libmkl\_lapack95\*.a</code> libraries contain Fortran 95 interfaces for BLAS and LAPACK, respectively, which are compiler-dependent. In the Intel MKL package, they are prebuilt for the Intel® Fortran compiler. If you are using a different compiler, build these libraries before using the interface.

#### See Also

Fortran 95 Interfaces to LAPACK and BLAS Compiler-dependent Functions and Fortran 90 Modules

# **Linking with Threading Libraries**

Intel MKL threading layer defines how Intel MKL functions utilize multiple computing cores of the system that the application runs on. You must link your application with one appropriate Intel MKL library in this layer, as explained below. Depending on whether this is a threading or a sequential library, Intel MKL runs in a parallel or sequential mode, respectively.

In the *parallel mode*, Intel MKL utilizes multiple processor cores available on your system, uses the OpenMP\* threading technology, and requires a proper OpenMP\* run-time library (RTL) to be linked with your application. Independently of use of Intel MKL, the application may also require a threading RTL. You should link not more than one OpenMP RTL to your application. This OpenMP RTL is provided by your compiler. Intel MKL provides several threading libraries, each dependent on the OpenMP RTL of a certain compiler, and your choice of the Intel MKL threading library must be consistent with the OpenMP RTL that you use in your application.

The OpenMP RTL of the Intel® compiler is the libiomp5.so library, located under caparent product
directory>/compiler/lib. This RTL is compatible with the GNU\* compilers (gcc and gfortran). You can
find additional information about the Intel OpenMP RTL at https://www.openmprtl.org.

In the *sequential mode*, Intel MKL runs unthreaded code, does not require an OpenMP RTL, and does not respond to environment variables and functions controlling the number of threads. Avoid using the library in the sequential mode unless you have a particular reason for that, such as the following:

- Your application needs an OpenMP RTL that none of Intel MKL threading libraries is compatible with
- Your application is already threaded at a top level, and using parallel Intel MKL only degrades the
  application performance by interfering with that threading
- Your application is intended to be run on a single thread, like a message-passing Interface (MPI)
  application

It is critical to link the application with the proper RTL. The table below explains what library in the Intel MKL threading layer and what OpenMP RTL you should choose under different scenarios:

Application		Intel MKL		RTL Required
Uses OpenMP	Compiled with	Execution Mode	Threading Layer	
no	any compiler	parallel	Static linking:	libiomp5.so
			<pre>libmkl_intel_ thread.a</pre>	
			Dynamic linking:	
			<pre>libmkl_intel_ thread.so</pre>	
no	any compiler	sequential	Static linking:	none <sup>†</sup>
			libmkl_ sequential.a	
			Dynamic linking:	
			libmkl_ sequential.so	
yes	Intel compiler	parallel	Static linking:	libiomp5.so
			<pre>libmkl_intel_ thread.a</pre>	
			Dynamic linking:	
			<pre>libmkl_intel_ thread.so</pre>	
yes	GNU compiler	parallel		Recommended!

Application		Intel MKL		RTL Required
Uses OpenMP	Compiled with	Execution Mode	Threading Layer	-
			Static linking:	libiomp5.so
			<pre>libmkl_intel_ thread.a</pre>	
			Dynamic linking:	
			<pre>libmkl_intel_ thread.so</pre>	
yes	GNU compiler	parallel	Static linking:	GNU OpenMP RTL
			libmkl_gnu_ thread.a	
			Dynamic linking:	
			libmkl_gnu_ thread.so	
yes PGI* compiler	parallel	Static linking:	PGI OpenMP RTL	
		libmkl_pgi_ thread.a		
			Dynamic linking:	
			<pre>libmkl_pgi_ thread.so</pre>	
yes	any other compiler	parallel	Not supported. Use Intel MKL in the sequential mode.	

<sup>&</sup>lt;sup>†</sup> For the sequential mode, add the POSIX threads library (libpthread) to your link line because the libmkl sequential.a and libmkl sequential.so libraries depend on libpthread.

# See Also

Layered Model Concept Notational Conventions

# **Linking with Computational Libraries**

If you are not using the Intel MKL ScaLAPACK and Cluster Fast Fourier Transforms (FFT), you need to link your application with only one computational library, depending on the linking method:

Static Linking	Dynamic Linking
libmkl_core.a	libmkl_core.so

# Computational Libraries for Applications that Use ScaLAPACK or Cluster FFT

ScaLAPACK and Cluster FFT require more computational libraries, which may depend on your architecture.

The following table lists computational libraries for IA -32 architecture applications that use ScaLAPACK or Cluster FFT.

# **Computational Libraries for IA-32 Architecture**

Function domain	Static Linking	Dynamic Linking
ScaLAPACK †	libmkl_scalapack_core.a	libmkl_scalapack_core.so
	libmkl_core.a	libmkl_core.so
Cluster Fourier Transform	libmkl_cdft_core.a	libmkl_cdft_core.so
Functions <sup>†</sup>	libmkl_core.a	libmkl_core.so

<sup>&</sup>lt;sup>†</sup> Also add the library with BLACS routines corresponding to the MPI used.

The following table lists computational libraries for Intel® 64 or Intel® Many Integrated Core Architecture applications that use ScaLAPACK or Cluster FFT.

# Computational Libraries for the Intel® 64 or Intel® Many Integrated Core Architecture

Function domain	Static Linking	Dynamic Linking
ScaLAPACK, LP64	libmkl_scalapack_lp64.a	libmkl_scalapack_lp64.so
interface <sup>‡</sup>	libmkl_core.a	libmkl_core.so
ScaLAPACK, ILP64	libmkl_scalapack_ilp64.a	libmkl_scalapack_ilp64.so
interface <sup>‡</sup>	libmkl_core.a	libmkl_core.so
Cluster Fourier	libmkl_cdft_core.a	libmkl_cdft_core.so
Transform Functions <sup>‡</sup>	libmkl_core.a	libmkl_core.so

<sup>&</sup>lt;sup>‡</sup> Also add the library with BLACS routines corresponding to the MPI used.

# See Also

Linking with Intel MKL Cluster Software Using the Link-line Advisor Using the ILP64 Interface vs. LP64 Interface

# **Linking with Compiler Run-time Libraries**

Dynamically link libiomp5 library even if you link other libraries statically.

Linking to the libiomp5 statically can be problematic because the more complex your operating environment or application, the more likely redundant copies of the library are included. This may result in performance issues (oversubscription of threads) and even incorrect results.

To link libiomp5 dynamically, be sure the LD\_LIBRARY\_PATH environment variable is defined correctly.

# See Also

Scripts to Set Environment Variables Layered Model Concept

# **Linking with System Libraries**

To use the Intel MKL FFT, Trigonometric Transform, or Poisson, Laplace, and HelmholtzSolver routines, link also the math support system library by adding "-lm" to the link line.

The libiomp5 library relies on the native pthread library for multi-threading. Any time libiomp5 is required, add -lpthreadto your link line afterwards (the order of listing libraries is important).

#### **NOTE**

To link with Intel MKL statically using a GNU or PGI compiler, link also the system library libdl by adding -ldl to your link line. The Intel compiler always passes -ldl to the linker.

# See Also

Linking Examples

# **Building Custom Shared Objects**

Custom shared objects reduce the collection of functions available in Intel MKL libraries to those required to solve your particular problems, which helps to save disk space and build your own dynamic libraries for distribution.

The Intel MKL custom shared object builder enables you to create a dynamic library (shared object) containing the selected functions and located in the tools/builder directory. The builder contains a makefile and a definition file with the list of functions.

#### **NOTE**

The objects in Intel MKL static libraries are position-independent code (PIC), which is not typical for static libraries. Therefore, the custom shared object builder can create a shared object from a subset of Intel MKL functions by picking the respective object files from the static libraries.

# **Using the Custom Shared Object Builder**

To build a custom shared object, use the following command:

make target [<options>]

The following table lists possible values of target and explains what the command does for each value:

Value	Comment
libia32	The builder uses static Intel MKL interface, threading, and core libraries to build a custom shared object for the IA-32 architecture.
libintel64	The builder uses static Intel MKL interface, threading, and core libraries to build a custom shared object for the Intel $^{\odot}$ 64 architecture.
soia32	The builder uses the single dynamic library $libmkl\_rt.so$ to build a custom shared object for the IA-32 architecture.
sointel64	The builder uses the single dynamic library <code>libmkl_rt.so</code> to build a custom shared object for the Intel® 64 architecture.
help	The command prints Help on the custom shared object builder

The <options> placeholder stands for the list of parameters that define macros to be used by the makefile. The following table describes these parameters:

Parameter [Values]	Description
<pre>interface = {lp64 ilp64}</pre>	Defines whether to use LP64 or ILP64 programming interfacefor the Intel 64architecture. The default value is $1p64$ .

Parameter [Values]	Description
threading = {parallel  sequential}	Defines whether to use the Intel MKL in the threaded or sequential mode. The default value is parallel.
<pre>export = <file name=""></file></pre>	Specifies the full name of the file that contains the list of entry-point functions to be included in the shared object. The default name is <code>user_example_list</code> (no extension).
name = <so name=""></so>	Specifies the name of the library to be created. By default, the names of the created library is mkl_custom.so.
<pre>xerbla = <error handler=""></error></pre>	Specifies the name of the object file $< user\_xerbla>.o$ that contains the user's error handler. The makefile adds this error handler to the library for use instead of the default Intel MKL error handler $xerbla$ . If you omit this parameter, the native Intel MKL $xerbla$ is used. See the description of the $xerbla$ function in the Intel MKL Reference Manual on how to develop your own error handler.
<pre>MKLROOT = <mkl directory=""></mkl></pre>	Specifies the location of Intel MKL libraries used to build the custom shared object. By default, the builder uses the Intel MKL installation directory.

All the above parameters are optional.

In the simplest case, the command line is make ia32, and the missing options have default values. This command creates the  $mkl\_custom.so$  library for processors using the IA-32 architecture. The command takes the list of functions from the user list file and uses the native Intel MKL error handler xerbla.

An example of a more complex case follows:

```
make ia32 export=my func list.txt name=mkl small xerbla=my xerbla.o
```

In this case, the command creates the  $mkl\_small.so$  library for processors using the IA-32 architecture. The command takes the list of functions from  $my\_func\_list.txt$  file and uses the user's error handler  $my\_xerbla.o.$ 

The process is similar for processors using the Intel® 64 architecture.

# See Also

Using the Single Dynamic Library

# **Composing a List of Functions**

To compose a list of functions for a minimal custom shared object needed for your application, you can use the following procedure:

- 1. Link your application with installed Intel MKL libraries to make sure the application builds.
- 2. Remove all Intel MKL libraries from the link line and start linking.

  Unresolved symbols indicate Intel MKL functions that your application uses.
- **3.** Include these functions in the list.

# **Important**

Each time your application starts using more Intel MKL functions, update the list to include the new functions

# See Also

Specifying Function Names

# **Specifying Function Names**

In the file with the list of functions for your custom shared object, adjust function names to the required interface. For example, for Fortran functions append an underscore character "\_" to the names as a suffix:

dgemm\_ ddot\_ dgetrf

For more examples, see domain-specific lists of functions in the <mkl directory>/tools/builder folder.

#### **NOTE**

The lists of functions are provided in the <mkl directory>/tools/builder folder merely as examples. See Composing a List of Functions for how to compose lists of functions for your custom shared object.

#### **TIP**

Names of Fortran-style routines (BLAS, LAPACK, etc.) can be both upper-case or lower-case, with or without the trailing underscore. For example, these names are equivalent:

BLAS: dgemm, DGEMM, dgemm , DGEMM

LAPACK: dgetrf, DGETRF, dgetrf\_, DGETRF\_.

Properly capitalize names of C support functions in the function list. To do this, follow the guidelines below:

- 1. In the mkl\_service.h include file, look up a #define directive for your function (mkl service.h is included in the mkl.h header file).
- **2.** Take the function name from the replacement part of that directive.

For example, the #define directive for the mkl\_disable\_fast\_mm function is #define mkl\_disable\_fast\_mm MKL\_Disable\_Fast\_MM.

Capitalize the name of this function in the list like this: MKL Disable Fast MM.

For the names of the Fortran support functions, see the tip.

# **NOTE**

If selected functions have several processor-specific versions, the builder automatically includes them all in the custom library and the dispatcher manages them.

# **Distributing Your Custom Shared Object**

To enable use of your custom shared object in a threaded mode, distribute <code>libiomp5.so</code> along with the custom shared object.

# Managing Performance and Memory

# **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

Notice revision #20110804

# Improving Performance with Threading

Intel® Math Kernel Library (Intel® MKL) is extensively parallelized. See Threaded Functions and Problems for lists of threaded functions and problems that can be threaded.

Intel MKL is thread-safe, which means that all Intel MKL functions (except the LAPACK deprecated routine ? lacon) work correctly during simultaneous execution by multiple threads. In particular, any chunk of threaded Intel MKL code provides access for multiple threads to the same shared data, while permitting only one thread at any given time to access a shared piece of data. Therefore, you can call Intel MKL from multiple threads and not worry about the function instances interfering with each other.

The library uses OpenMP\* threading technology, so you can use the environment variable <code>OMP\_NUM\_THREADS</code> to specify the number of threads or the equivalent OpenMP run-time function calls. Intel MKL also offers variables that are independent of OpenMP, such as <code>MKL\_NUM\_THREADS</code>, and equivalent Intel MKL functions for thread management. The Intel MKL variables are always inspected first, then the OpenMP variables are examined, and if neither is used, the OpenMP software chooses the default number of threads.

By default, Intel MKL uses the number of threads equal to the number of physical cores on the system.

To achieve higher performance, set the number of threads to the number of processors or physical cores, as summarized in Techniques to Set the Number of Threads.

# See Also

Managing Multi-core Performance

# Threaded Functions and Problems

The following Intel MKL function domains are threaded:

- Direct sparse solver.
- LAPACK.

For a list of threaded routines, see LAPACK Routines.

Level1 and Level2 BLAS.

For a list of threaded routines, see BLAS Level1 and Level2 Routines.

- All Level 3 BLAS and all Sparse BLAS routines except Level 2 Sparse Triangular solvers.
- All mathematical VML functions.
- FFT

For a list of FFT transforms that can be threaded, see Threaded FFT Problems.



#### **LAPACK Routines**

In this section, ? stands for a precision prefix of *each* flavor of the respective routine and may have the value of s, d, c, or z.

The following LAPACK routines are threaded:

- Linear equations, computational routines:
  - Factorization: ?getrf, ?getrfnpi, ?gbtrf, ?potrf, ?pptrf, ?sytrf, ?hetrf, ?sptrf, ?hptrf
  - Solving: ?dttrsb, ?gbtrs, ?gttrs, ?pptrs, ?pbtrs, ?pttrs, ?sytrs, ?sptrs, ?hptrs, ?tptrs, ?tbtrs
- Orthogonal factorization, computational routines:

```
?geqrf, ?ormqr, ?unmqr, ?ormlq, ?unmlq, ?ormql, ?unmql, ?ormrq, ?unmrq
```

• Singular Value Decomposition, computational routines:

```
?gebrd, ?bdsqr
```

• Symmetric Eigenvalue Problems, computational routines:

```
?sytrd, ?hetrd, ?sptrd, ?hptrd, ?steqr, ?stedc.
```

• Generalized Nonsymmetric Eigenvalue Problems, computational routines: chgeqz/zhgeqz.

A number of other LAPACK routines, which are based on threaded LAPACK or BLAS routines, make effective use of parallelism:

```
?gesv, ?posv, ?gels, ?gesvd, ?syev, ?heev, cgegs/zgegs, cgegv/zgegv, cgges/zgges, cggesx/zggesx, cggev/zggev, cggevx/zggevx, and so on.
```

#### Threaded BLAS Level1 and Level2 Routines

In the following list, ? stands for a precision prefix of *each* flavor of the respective routine and may have the value of s, d, c, or z.

The following routines are threaded for Intel® Core™2 Duo and Intel® Core™ i7 processors:

• Level1 BLAS:

```
?axpy, ?copy, ?swap, ddot/sdot, cdotc, drot/srot
```

Level2 BLAS:

```
?gemv, ?trmv, dsyr/ssyr, dsyr2/ssyr2, dsymv/ssymv
```

#### **Threaded FFT Problems**

The following characteristics of a specific problem determine whether your FFT computation may be threaded:

- rank
- domain
- size/length
- precision (single or double)
- placement (in-place or out-of-place)
- strides
- number of transforms
- layout (for example, interleaved or split layout of complex data)

Most FFT problems are threaded. In particular, computation of multiple transforms in one call (number of transforms > 1) is threaded. Details of which transforms are threaded follow.

# One-dimensional (1D) transforms

1D transforms are threaded in many cases.

1D complex-to-complex (c2c) transforms of size N using interleaved complex data layout are threaded under the following conditions depending on the architecture:

Architecture	Conditions
Intel® 64	$N$ is a power of 2, $log_2(N) > 9$ , the transform is double-precision out-of-place, and input/output strides equal 1.
IA-32	$N$ is a power of 2, $log_2(N) > 13$ , and the transform is single-precision.
	$N$ is a power of 2, $log_2(N) > 14$ , and the transform is double-precision.
Any	$N$ is composite, $log_2(N) > 16$ , and input/output strides equal 1.

1D complex-to-complex transforms using split-complex layout are not threaded.

#### **Multidimensional transforms**

All multidimensional transforms on large-volume data are threaded.

# **Avoiding Conflicts in the Execution Environment**

Certain situations can cause conflicts in the execution environment that make the use of threads in Intel MKL problematic. This section briefly discusses why these problems exist and how to avoid them.

If you thread the program using OpenMP directives and compile the program with Intel compilers, Intel MKL and the program will both use the same threading library. Intel MKL tries to determine if it is in a parallel region in the program, and if it is, it does not spread its operations over multiple threads unless you specifically request Intel MKL to do so via the MKL\_DYNAMIC functionality. However, Intel MKL can be aware that it is in a parallel region only if the threaded program and Intel MKL are using the same threading library. If your program is threaded by some other means, Intel MKL may operate in multithreaded mode, and the performance may suffer due to overuse of the resources.

The following table considers several cases where the conflicts may arise and provides recommendations depending on your threading model:

Threading model	Discussion
You parallelize the program using OS threads (for example: pthreads on Linux* OS).	If more than one thread calls Intel MKL, and the function being called is threaded, it may be important that you turn off Intel MKL threading. Set the number of threads to one by any of the available means (see Techniques to Set the Number of Threads).
You parallelize the program using OpenMP directives and/or pragmas and compile the program using a non-Intel compiler.	This is more problematic because setting of the <code>OMP_NUM_THREADS</code> environment variable affects both the compiler's threading library and <code>libiomp5</code> . In this case, choose the threading library that matches the layered Intel MKL with the OpenMP compiler you employ (see Linking Examples on how to do this). If this is not possible, use Intel MKL in the sequential mode. To do this, you should link with the appropriate threading library: <code>libmkl_sequential.aorlibmkl_sequential.so</code> (see <code>Directory Structure in Detail</code> ).
There are multiple programs running on a multiple-cpu system, for example, a parallelized program that runs using MPI for communication in which each processor is treated as a node.	The threading software will see multiple processors on the system even though each processor has a separate MPI process running on it. In this case, one of the solutions is to set the number of threads to one by any of the available means (see Techniques to Set the Number of Threads). Section Intel® Optimized MP LINPACK Benchmark for Clusters discusses another solution for a Hybrid (OpenMP* + MPI) mode.

Using the  $mkl\_set\_num\_threads$  and  $mkl\_domain\_set\_num\_threads$  functions to control parallelism of Intel MKL from parallel user threads may result in a race condition that impacts the performance of the application because these functions operate on internal control variables that are global, that is, apply to all threads. For example, if parallel user threads call these functions to set different numbers of threads for the

same function domain, the number of threads actually set is unpredictable. To avoid this kind of data races, use the mkl\_set\_num\_threads\_local function (see the "Support Functions" chapter in the *Intel MKL Reference Manual* for the function description).

#### See Also

Using Additional Threading Control Linking with Compiler Run-time Libraries

# **Techniques to Set the Number of Threads**

Use the following techniques to specify the number of OpenMP threads to use in Intel MKL:

- Set one of the OpenMP or Intel MKL environment variables:
  - OMP NUM THREADS
  - MKL NUM THREADS
  - MKL DOMAIN NUM THREADS
- Call one of the OpenMP or Intel MKL functions:
  - omp set num threads()
  - mkl set num threads()
  - mkl\_domain\_set\_num\_threads()
  - mkl set num threads local()

When choosing the appropriate technique, take into account the following rules:

- The Intel MKL threading controls take precedence over the OpenMP controls because they are inspected first.
- A function call takes precedence over any environment settings. The exception, which is a consequence of
  the previous rule, is that a call to the OpenMP subroutine omp\_set\_num\_threads() does not have
  precedence over the settings of Intel MKL environment variables such as MKL\_NUM\_THREADS. See Using
  Additional Threading Control for more details.
- You cannot change run-time behavior in the course of the run using the environment variables because they are read only once at the first call to Intel MKL.

# Setting the Number of Threads Using an OpenMP\* Environment Variable

You can set the number of threads using the environment variable <code>OMP\_NUM\_THREADS</code>. To change the number of OpenMP threads, use the appropriate command in the command shell in which the program is going to run, for example:

- For the bash shell, enter:
  - export OMP NUM THREADS=<number of threads to use>
- For the csh or tcsh shell, enter:

```
setenv OMP_NUM_THREADS <number of threads to use>
```

#### See Also

Using Additional Threading Control

# Changing the Number of OpenMP\* Threads at Run Time

You cannot change the number of OpenMP threads at run time using environment variables. However, you can call OpenMP routines to do this. Specifically, the following sample code shows how to change the number of threads during run time using the <code>omp\_set\_num\_threads()</code> routine. For more options, see also Techniques to Set the Number of Threads.

The example is provided for both C and Fortran languages. To run the example in C, use the <code>omp.h</code> header file from the Intel(R) compiler package. If you do not have the Intel compiler but wish to explore the functionality in the example, use Fortran API for <code>omp\_set\_num\_threads()</code> rather than the C version. For example, <code>omp set num threads()</code> is one of the following set of the composition of the example of t

```
// ****** C language ******
#include "omp.h"
#include "mkl.h"
#include <stdio.h>
#define SIZE 1000
int main(int args, char *argv[]) {
double *a, *b, *c;
a = (double*)malloc(sizeof(double)*SIZE*SIZE);
b = (double*)malloc(sizeof(double)*SIZE*SIZE);
c = (double*)malloc(sizeof(double)*SIZE*SIZE);
double alpha=1, beta=1;
int m=SIZE, n=SIZE, k=SIZE, lda=SIZE, ldb=SIZE, ldc=SIZE, i=0, j=0;
char transa='n', transb='n';
for( i=0; i<SIZE; i++) {
for( j=0; j<SIZE; j++) {
a[i*SIZE+j]= (double)(i+j);
b[i*SIZE+j]= (double)(i*j);
c[i*SIZE+j]= (double)0;
cblas dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
m, n, k, alpha, a, lda, b, ldb, beta, c, ldc);
printf("row\ta\tc\n");
for (i=0;i<10;i++) {
printf("%d:\t%f\t%f\n", i, a[i*SIZE], c[i*SIZE]);
omp set num threads(1);
for( i=0; i<SIZE; i++) {
for( j=0; j<SIZE; j++){
a[i*SIZE+j] = (double)(i+j);
b[i*SIZE+j] = (double)(i*j);
c[i*SIZE+j]= (double)0;
cblas dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
m, n, k, alpha, a, lda, b, ldb, beta, c, ldc);
printf("row\ta\tc\n");
for (i=0;i<10;i++){
printf("%d:\t%f\t%f\n", i, a[i*SIZE], c[i*SIZE]);
omp set num threads(2);
for( i=0; i<SIZE; i++) {
for( j=0; j<SIZE; j++){
a[i*SIZE+j] = (double)(i+j);
b[i*SIZE+j]= (double)(i*j);
c[i*SIZE+j]= (double)0;
cblas dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
m, n, k, alpha, a, lda, b, ldb, beta, c, ldc);
printf("row\ta\tc\n");
for (i=0;i<10;i++){
printf("%d:\t%f\t%f\n", i, a[i*SIZE],
c[i*SIZE]);
```

```
free (a);
free (b);
free (c);
return 0;
}
```

```
// ****** Fortran language ******
PROGRAM DGEMM DIFF THREADS
INTEGER N, I, J
PARAMETER (N=100)
REAL*8 A(N,N), B(N,N), C(N,N)
REAL*8 ALPHA, BETA
ALPHA = 1.1
BETA = -1.2
DO I=1, N
DO J=1, N
A(I,J) = I+J
B(I,J) = I*j
C(I,J) = 0.0
END DO
CALL DGEMM('N', 'N', N, N, N, ALPHA, A, N, B, N, BETA, C, N)
print *, 'Row A C'
DO i=1,10
write (*, '(I4, F20.8, F20.8)') I, A(1,I), C(1,I)
END DO
CALL OMP SET NUM THREADS (1);
DO I=1, N
DO J=1,N
A(I,J) = I+J
B(I,J) = I*j
C(I,J) = 0.0
END DO
END DO
CALL DGEMM('N', 'N', N, N, N, ALPHA, A, N, B, N, BETA, C, N)
print *, 'Row A C'
DO i=1,10
write(*,'(I4,F20.8,F20.8)') I, A(1,I),C(1,I)
END DO
CALL OMP SET NUM THREADS (2);
DO I=1, N
DO J=1, N
A(I,J) = I+J
B(I,J) = I*j
C(I,J) = 0.0
END DO
CALL DGEMM('N', 'N', N, N, N, ALPHA, A, N, B, N, BETA, C, N)
print *, 'Row A C'
DO i=1,10
write(*,'(I4,F20.8,F20.8)') I, A(1,I),C(1,I)
END DO
STOP
END
```

# **Using Additional Threading Control**

# **Intel MKL-specific Environment Variables for Threading Control**

Intel MKL provides environment variables and support functions to control Intel MKL threading independently of OpenMP. The Intel MKL-specific threading controls take precedence over their OpenMP equivalents. Use the Intel MKL-specific threading controls to distribute OpenMP threads between Intel MKL and the rest of your program.

#### NOTE

Some Intel MKL routines may use fewer OpenMP threads than suggested by the threading controls if either the underlying algorithms do not support the suggested number of OpenMP threads or the routines perform better with fewer OpenMP threads because of lower OpenMP overhead and/or better data locality. Set the MKL\_DYNAMIC environment variable to FALSE or call mkl\_set\_dynamic(0) to use the suggested number of OpenMP threads whenever the algorithms permit and regardless of OpenMP overhead and data locality.

Section "Number of User Threads" in the "Fourier Transform Functions" chapter of the *Intel MKL Reference Manual* shows how the Intel MKL threading controls help to set the number of threads for the FFT computation.

The table below lists the Intel MKL environment variables for threading control, their equivalent functions, and OMP counterparts:

Environment Variable	Support Function	Comment	Equivalent OpenMP* Environment Variable
MKL_NUM_THREADS	<pre>mkl_set_num_threads mkl_set_num_threads _local</pre>	Suggests the number of OpenMP threads to use.	OMP_NUM_THREADS
MKL_DOMAIN_NUM_ THREADS	<pre>mkl_domain_set_num_ threads</pre>	Suggests the number of OpenMP threads for a particular function domain.	
MKL_DYNAMIC	mkl_set_dynamic	Enables Intel MKL to dynamically change the number of OpenMP threads.	OMP_DYNAMIC

# NOTE

Call mkl\_set\_num\_threads() to force Intel MKL to use a given number of OpenMP threads and prevent it from reacting to the environment variables MKL\_NUM\_THREADS, MKL\_DOMAIN\_NUM\_THREADS, and OMP NUM THREADS.

The example below shows how to force Intel MKL to use one thread:

```
// ****** C language ******
#include <mkl.h>
```

```
...
mkl_set_num_threads ( 1 );

// ****** Fortran language ******
...
call mkl_set_num_threads( 1 )
```

See the *Intel MKL Reference Manual* for the detailed description of the threading control functions, their parameters, calling syntax, and more code examples.

# **MKL DYNAMIC**

The MKL DYNAMIC environment variable enables Intel MKL to dynamically change the number of threads.

The default value of MKL DYNAMIC is TRUE, regardless of OMP DYNAMIC, whose default value may be FALSE.

When MKL\_DYNAMIC is TRUE, Intel MKL may use fewer OpenMP threads than the maximum number you specify.

For example, MKL\_DYNAMIC set to TRUE enables optimal choice of the number of threads in the following cases:

- If the requested number of threads exceeds the number of physical cores (perhaps because of using the Intel® Hyper-Threading Technology), Intel MKL scales down the number of OpenMP threads to the number of physical cores.
- If you are able to detect the presence of a message-passing interface (MPI), but cannot determine whether it has been called in a thread-safe mode (it is impossible to detect this with MPICH 1.2.x, for instance), Intel MKL runs one OpenMP thread.

When MKL\_DYNAMIC is FALSE, Intel MKL uses the suggested number of OpenMP threads whenever the underlying algorithms permit. For example, if you attempt to do a size one matrix-matrix multiply across eight threads, the library may instead choose to use only one thread because it is impractical to use eight threads in this event.

If Intel MKL is called from an OpenMP parallel region in your program, Intel MKL uses only one thread by default. If you want Intel MKL to go parallel in such a call, link your program against an OpenMP threading RTL supported by Intel MKL and set the environment variables:

- OMP NESTED to TRUE
- OMP DYNAMIC and MKL DYNAMIC to FALSE
- MKL NUM THREADS to some reasonable value

With these settings, Intel MKL uses  $\texttt{MKL\_NUM\_THREADS}$  threads when it is called from the OpenMP parallel region in your program.

In general, set MKL\_DYNAMIC to FALSE only under circumstances that Intel MKL is unable to detect, for example, to use nested parallelism where the library is already called from a parallel section.

# MKL DOMAIN NUM THREADS

The MKL\_DOMAIN\_NUM\_THREADS environment variable suggests the number of OpenMP threads for a particular function domain.

MKL\_DOMAIN\_NUM\_THREADS accepts a string value <MKL-env-string>, which must have the following format:

```
<MKL-domain-env-name> ::= MKL_DOMAIN_ALL | MKL_DOMAIN_BLAS | MKL_DOMAIN_FFT |
MKL_DOMAIN_VML | MKL_DOMAIN_PARDISO

<uses> ::= [ <space-symbol>* ] ( <space-symbol> | <equality-sign> | <comma-symbol>)
[ <space-symbol>* ]
<number-of-threads> ::= <positive-number>
<positive-number> ::= <decimal-positive-number> | <octal-number> | <hexadecimal-number>
In the syntax above, values of <MKL-domain-env-name> indicate function domains as follows:
```

```
MKL_DOMAIN_BLAS

MKL_DOMAIN_FFT

MKL_DOMAIN_FFT

MKL_DOMAIN_VML

MKL_DOMAIN_VML

MKL_DOMAIN_PARDISO

All function domains

BLAS Routines

non-cluster Fourier Transform Functions

Vector Mathematical Functions

PARDISO
```

#### For example,

```
MKL_DOMAIN_ALL 2 : MKL_DOMAIN_BLAS 1 : MKL_DOMAIN_FFT 4

MKL_DOMAIN_ALL=2 : MKL_DOMAIN_BLAS=1 : MKL_DOMAIN_FFT=4

MKL_DOMAIN_ALL=2, MKL_DOMAIN_BLAS=1, MKL_DOMAIN_FFT=4

MKL_DOMAIN_ALL=2; MKL_DOMAIN_BLAS=1; MKL_DOMAIN_FFT=4

MKL_DOMAIN_ALL = 2 MKL_DOMAIN_BLAS 1 , MKL_DOMAIN_FFT 4

MKL_DOMAIN_ALL, 2: MKL_DOMAIN_BLAS 1, MKL_DOMAIN_FFT, 4 .
```

The global variables MKL\_DOMAIN\_ALL, MKL\_DOMAIN\_BLAS, MKL\_DOMAIN\_FFT, MKL\_DOMAIN\_VML, and MKL\_DOMAIN\_PARDISO, as well as the interface for the Intel MKL threading control functions, can be found in the mkl.h header file.

The table below illustrates how values of MKL DOMAIN NUM THREADS are interpreted.

Value of MKL_DOMAIN_NUM_ THREADS	Interpretation
MKL_DOMAIN_ALL=	All parts of Intel MKL should try four OpenMP threads. The actual number of threads may be still different because of the MKL_DYNAMIC setting or system resource issues. The setting is equivalent to MKL_NUM_THREADS = $4$ .
MKL_DOMAIN_ALL= 1, MKL_DOMAIN_BLAS =4	All parts of Intel MKL should try one OpenMP thread, except for BLAS, which is suggested to try four threads.
MKL_DOMAIN_VML=	VML should try two OpenMP threads. The setting affects no other part of Intel MKL.

Be aware that the domain-specific settings take precedence over the overall ones. For example, the "MKL\_DOMAIN\_BLAS=4" value of MKL\_DOMAIN\_NUM\_THREADS suggests trying four OpenMP threads for BLAS, regardless of later setting MKL\_NUM\_THREADS, and a function call "mkl\_domain\_set\_num\_threads (4, MKL\_DOMAIN\_BLAS);" suggests the same, regardless of later calls to mkl\_set\_num\_threads(). However, a function call with input "MKL\_DOMAIN\_ALL", such as "mkl\_domain\_set\_num\_threads (4, MKL\_DOMAIN\_ALL); " is equivalent to "mkl\_set\_num\_threads(4)", and thus it will be overwritten by later calls to mkl\_set\_num\_threads. Similarly, the environment setting of MKL\_DOMAIN\_NUM\_THREADS with "MKL\_DOMAIN\_ALL=4" will be overwritten with MKL\_NUM\_THREADS = 2.

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Whereas the MKL\_DOMAIN\_NUM\_THREADS environment variable enables you set several variables at once, for example, "MKL\_DOMAIN\_BLAS=4, MKL\_DOMAIN\_FFT=2", the corresponding function does not take string syntax. So, to do the same with the function calls, you may need to make several calls, which in this example are as follows:

```
mkl_domain_set_num_threads ( 4, MKL_DOMAIN_BLAS );
mkl domain set num threads ( 2, MKL DOMAIN FFT );
```

# **Setting the Environment Variables for Threading Control**

To set the environment variables used for threading control, in the command shell in which the program is going to run, enter the export or setenv commands, depending on the shell you use.

For a bash shell, use the export commands:

```
export <VARIABLE NAME>=<value>
For example:
export MKL_NUM_THREADS=4
export MKL_DOMAIN_NUM_THREADS="MKL_DOMAIN_ALL=1, MKL_DOMAIN_BLAS=4"
export MKL_DYNAMIC=FALSE
For the csh or tcsh shell, use the setenv commands:
setenv <VARIABLE NAME><value>.
For example:
setenv MKL_NUM_THREADS 4
setenv MKL_DOMAIN_NUM_THREADS "MKL_DOMAIN_ALL=1, MKL_DOMAIN_BLAS=4"
setenv MKL_DYNAMIC FALSE
```

# Calling Intel MKL Functions from Multi-threaded Applications

This section summarizes typical usage models and available options for calling Intel MKL functions from multi-threaded applications. These recommendations apply to any multi-threading environments: OpenMP\*, Intel® Threading Building Blocks, POSIX\* threads, and others.

# Usage model: disable Intel MKL internal threading for the whole application

**When used:** Intel MKL internal threading interferes with application's own threading or may slow down the application.

**Example:** the application is threaded at top level, or the application runs concurrently with other applications.

# **Options:**

- Link statically or dynamically with the sequential library
- Link with the Single Dynamic Library mkl\_rt.so and select the sequential library using an environment variable or a function call:
  - Set MKL\_THREADING\_LAYER=sequential
  - Call mkl set threading layer (MKL THREADING SEQUENTIAL) \*
- Link with a threading library, but disable Intel MKL threading using an environment variable or a function call:
  - set MKL NUM THREADS=1
  - call mkl set num threads(1).

In particular, use to temporarily disable Intel MKL threading at run time.

- Link with the Single Dynamic Library mkl\_rt.so and select a threading library using an environment variable or a function call below, but disable threading as in the case above:
  - set MKL THREADING LAYER=intel
  - call mkl set threading layer (MKL THREADING INTEL)

# Usage model: partition system resources among application threads

When used: application threads are specialized for a particular computation.

**Example:** one thread solves equations on all cores but one, while another thread running on a single core updates a database.

# **Linking Options:**

- Link statically or dynamically with a threading library
- Link with the Single Dynamic Library mkl\_rt.so and select a threading library using an environment variable or a function call:
  - set MKL THREADING LAYER=intel
  - call mkl set threading layer (MKL THREADING INTEL)

# Other Options:

- Set the MKL NUM THREADS environment variable to a desired number of OpenMP threads for Intel MKL.
- Set the MKL\_DOMAIN\_NUM\_THREADS environment variable to a desired number of OpenMP threads for Intel MKL for a particular function domain.

Use if the application threads work with different Intel MKL function domains.

• Call mkl set num threads()

Use to globally set a desired number of OpenMP threads for Intel MKL at run time.

• Call mkl\_domain\_set\_num\_threads().

Use if at some point application threads start working with different Intel MKL function domains.

Call mkl set num threads local().

Use to set the number of OpenMP threads for Intel MKL called from a particular thread.

# **NOTE**

If your application uses OpenMP\* threading, you may need to provide additional settings:

- Set the environment variable <code>OMP\_NESTED=TRUE</code>, or alternatively call <code>omp\_set\_nested(1)</code>, to enable <code>OpenMP</code> nested parallelism.
- Set the environment variable MKL\_DYNAMIC=FALSE, or alternatively call mkl\_set\_dynamic(0), to prevent Intel MKL from dynamically reducing the number of OpenMP threads in nested parallel regions.

# **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessordependent optimizations in this product are intended for use with Intel microprocessors. Certain

<sup>&</sup>lt;sup>‡</sup> For details of the mentioned functions, see the Support Functions section of the *Intel MKL Reference Manual*, available in the Intel Software Documentation Library.



# **Optimization Notice**

optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

Notice revision #20110804

#### See Also

Linking with Threading Libraries

Dynamically Selecting the Interface and Threading Layer

Intel MKL-specific Environment Variables for Threading Control

MKL\_DOMAIN\_NUM\_THREADS

Avoiding Conflicts in the Execution Environment

Intel Software Documentation Library

# **Using Intel® Hyper-Threading Technology**

Intel® Hyper-Threading Technology (Intel® HT Technology) is especially effective when each thread performs different types of operations and when there are under-utilized resources on the processor. However, Intel MKL fits neither of these criteria because the threaded portions of the library execute at high efficiencies using most of the available resources and perform identical operations on each thread. You may obtain higher performance by disabling Intel HT Technology.

If you run with Intel HT Technology enabled, performance may be especially impacted if you run on fewer threads than physical cores. Moreover, if, for example, there are two threads to every physical core, the thread scheduler may assign two threads to some cores and ignore the other cores altogether. If you are using the OpenMP\* library of the Intel Compiler, read the respective User Guide on how to best set the thread affinity interface to avoid this situation. For Intel MKL, apply the following setting:

set KMP AFFINITY=granularity=fine,compact,1,0

# **Managing Multi-core Performance**

You can obtain best performance on systems with multi-core processors by requiring thatthreads do not migrate from core to core. To do this, bind threads to the CPU cores bysetting an affinity mask to threads. Use one of the following options:

- OpenMP facilities (recommended, if available), for example, the KMP\_AFFINITY environment variable using the Intel OpenMP library
- A system function, as explained below

Consider the following performance issue:

- The system has two sockets with two cores each, for a total of four cores (CPUs).
- The application sets the number of OpenMP threads to two and calls Intel MKL to perform a Fourier transform. This call takes considerably different amounts of time from run to run.

To resolve this issue, before calling Intel MKL, set an affinity mask for each OpenMP thread using the KMP\_AFFINITY environment variable or the sched\_setaffinity system function. The following code example shows how to resolve the issue by setting an affinity mask by operating system means using the Intel compiler. The code calls the functionsched\_setaffinityto bind the threads tothecoreson different sockets. Then the Intel MKLFFT function called:

```
#define _GNU_SOURCE //for using the GNU CPU affinity
// (works with the appropriate kernel and glibc)
// Set affinity mask
#include <sched.h>
#include <stdio.h>
#include <unistd.h>
```

```
#include <omp.h>
int main(void) {
    int NCPUs = sysconf( SC NPROCESSORS CONF);
    printf("Using thread affinity on %i NCPUs\n", NCPUs);
#pragma omp parallel default(shared)
        cpu set t new mask;
        cpu set t was mask;
        int tid = omp get thread num();
        CPU ZERO(&new mask);
        // 2 packages x 2 cores/pkg x 1 threads/core (4 total cores)
        CPU SET(tid==0 ? 0 : 2, &new mask);
        if (sched getaffinity(0, sizeof(was mask), &was mask) == -1) {
            printf("Error: sched getaffinity(%d, sizeof(was mask), &was mask)\n", tid);
        if (sched setaffinity(0, sizeof(new mask), &new mask) == -1) {
           printf("Error: sched setaffinity(%d, sizeof(new mask), &new mask)\n", tid);
        printf("tid=%d new mask=%08X was mask=%08X\n", tid,
                        *(unsigned int*)(&new_mask), *(unsigned int*)(&was_mask));
    // Call Intel MKL FFT function
    return 0;
```

Compile the application with the Intel compiler using the following command:

```
icc test application.c -openmp
```

where test application.cis the filename for the application.

Build the application. Run it intwothreads, for example, by using the environment variable to set the number of threads:

```
env OMP NUM THREADS=2 ./a.out
```

SeetheLinux Programmer's Manual(in man pages format)forparticulars of the sched\_setaffinity function used in the above example.

# **Improving Performance for Small Size Problems**

The overhead of calling an Intel MKL function for small problem sizes can be significant when the function has a large number of parameters or internally checks parameter errors. To reduce the performance overhead for these small size problems, the Intel MKL *direct call* feature works in conjunction with the compiler to preprocess the calling parameters to <code>?gemm</code> functions and directly call or inline special optimized small-matrix kernels that bypass error checking.

To activate the feature, do the following:

• Compile your C or Fortran code with the preprocessor macro depending on whether a threaded or sequential mode of Intel MKL is required by supplying the compiler option as explained below:

Intel MKL Mode	Macro	Compiler Option
Threaded	MKL_DIRECT_CALL	-DMKL_DIRECT_CALL
Sequential	MKL_DIRECT_CALL_SEQ	-DMKL_DIRECT_CALL_SEQ

- For Fortran applications:
  - Enable preprocessor by using the -fpp option for Intel® Fortran Compiler and -Mpreprocess option for PGI\* compilers.
  - Include the Intel MKL Fortran include file mkl direct call.fi.

Intel MKL skips error checking and intermediate function calls if the problem size is small enough (for example, a dgemm function call with matrix ranks smaller than 50).

# **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

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# Using MKL\_DIRECT\_CALL in C Applications

The following examples of code and link lines show how to activate direct calls to Intel MKL kernels in C applications:

Include the mkl.h header file:

```
#include "mkl.h"
int main(void) {

// Call Intel MKL DGEMM

return 0;
}
```

For multi-threaded Intel MKL, compile with MKL DIRECT CALL preprocessor macro:

```
icc -DMKL_DIRECT_CALL -std=c99 your_application.c -Wl,--start-group $(MKLROOT)/lib/intel64/
libmkl_intel_lp64.a
$(MKLROOT)/lib/intel64/libmkl_core.a
$(MKLROOT)/lib/intel64/libmkl_intel_thread.a -Wl,--end-group -lpthread -lm -openmp -I$(MKLROOT)/
include
```

• To use Intel MKL in the sequential mode, compile with MKL DIRECT CALL SEQ preprocessor macro:

```
icc -DMKL_DIRECT_CALL_SEQ -std=c99 your_application.c -Wl,--start-group $(MKLROOT)/lib/intel64/
libmkl_intel_lp64.a
$(MKLROOT)/lib/intel64/libmkl_core.a
$(MKLROOT)/lib/intel64/libmkl sequential.a -Wl,--end-group -lpthread -lm -I$(MKLROOT)/include
```

# Using MKL\_DIRECT\_CALL in Fortran Applications

The following examples of code and link lines show how to activate direct calls to Intel MKL kernels in Fortran applications:

• Include mkl\_direct\_call.fi, to be preprocessed by the Fortran compiler preprocessor

```
# include "mkl_direct_call.fi"
    program    DGEMM_MAIN
....
* Call Intel MKL DGEMM
....
call sub1()
```

```
stop 1
end

* A subroutine that calls DGEMM
subroutine sub1
* Call Intel MKL DGEMM
end
```

• For multi-threaded Intel MKL, compile with -fpp option for Intel Fortran compiler (or with -Mpreprocess for PGI compilers) and with MKL DIRECT CALL preprocessor macro:

```
ifort -DMKL_DIRECT_CALL -fpp your_application.f -Wl,--start-group
$(MKLROOT)/lib/intel64/libmkl_intel_lp64.a
$(MKLROOT)/lib/intel64/libmkl_core.a $(MKLROOT)/lib/intel64/libmkl_intel_thread.a -Wl,--end-group
-lpthread -lm -openmp -I$(MKLROOT)/include
```

• To use Intel MKL in the sequential mode, compile with -fpp option for Intel Fortran compiler (or with - Mpreprocess for PGI compilers) and with MKL DIRECT CALL SEQ preprocessor macro:

```
ifort -DMKL_DIRECT_CALL_SEQ -fpp your_application.f -Wl,--start-group
$(MKLROOT)/lib/intel64/libmkl_intel_lp64.a
$(MKLROOT)/lib/intel64/libmkl_core.a $(MKLROOT)/lib/intel64/libmkl_sequential.a -Wl,--end-group
-lpthread -lm -I$(MKLROOT)/include
```

# Limitations of the Direct Call

Directly calling the Intel MKL kernels has the following limitations:

• If the MKL\_DIRECT\_CALL or MKL\_DIRECT\_CALL\_SEQ macro is used, Intel MKL may skip error checking.

# **Important**

With a limited error checking, you are responsible for checking the correctness of function parameters to avoid unsafe and incorrect code execution.

- The feature is only available for <code>?gemm, ?gemm3m, ?syrk, ?trsm, ?axpy, and ?dot functions.</code>
- Intel MKL Verbose mode, Conditional Numerical Reproducibility, and BLAS95 interfaces are not supported.
- GNU\* Fortran compilers are not supported.
- For C applications, you must enable mixing declarations and user code by providing the -std=c99 option for Intel® compilers.
- In a fixed format Fortran (FORTRAN77) source code compiled with PGI compilers, the lines containing Intel MKL functions must end at least seven columns before the line ending column, usually, in a column with the index not greater than 72 7 = 65.

#### NOTE

The direct call feature substitutes the names of Intel MKL functions with longer counterparts, which can cause the lines to exceed the column limit for a fixed format Fortran source code compiled with PGI compilers. Because the compilers ignore any part of the line that exceeds the limit, the behavior of the program can be unpredictable.

# Other Tips and Techniques to Improve Performance

# See Also

Managing Performance of the Cluster Fourier Transform Functions
Improving Performance on Intel Xeon Phi Coprocessors Tips for Intel® Many Integrated Core
Architecture

# **Coding Techniques**

To improve performance, properly align arrays in your code. Additional conditions can improve performance for specific function domains.

# **Data Alignment**

To improve performance of your application that calls Intel MKL, align your arrays on 64-byte boundaries and ensure that the leading dimensions of the arrays are divisible by 64.

#### **LAPACK Packed Routines**

The routines with the names that contain the letters HP, OP, PP, SP, TP, UP in the matrix type and storage position (the second and third letters respectively) operate on the matrices in the packed format (see LAPACK "Routine Naming Conventions" sections in the Intel MKL Reference Manual). Their functionality is strictly equivalent to the functionality of the unpacked routines with the names containing the letters HE, OR, PO, SY, TR, UN in the same positions, but the performance is significantly lower.

If the memory restriction is not too tight, use an unpacked routine for better performance. In this case, you need to allocate  $N^2/2$  more memory than the memory required by a respective packed routine, where N is the problem size (the number of equations).

For example, to speed up solving a symmetric eigenproblem with an expert driver, use the unpacked routine:

```
call dsyevx(jobz, range, uplo, n, a, lda, vl, vu, il, iu, abstol, m, w, z, ldz, work, lwork, iwork, ifail, info)
```

where a is the dimension 1 da-by-n, which is at least  $N^2$  elements, instead of the packed routine:

```
call dspevx(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol, m, w, z, ldz, work, iwork, ifail, info)
```

where ap is the dimension  $N^*(N+1)/2$ .

#### See Also

Example of Data Alignment
Improving Performance on Intel Xeon Phi Coprocessors
Managing Performance of the Cluster Fourier Transform Functions

# Improving Intel(R) MKL Performance on Specific Processors

#### Dual-Core Intel® Xeon® Processor 5100 Series

To get the best performance with Intel MKL on Dual-Core Intel® Xeon® processor 5100 series systems, enable the Hardware DPL (streaming data) Prefetcher functionality of this processor. To configure this functionality, use the appropriate BIOS settings, as described in your BIOS documentation.

# **Operating on Denormals**

The IEEE 754-2008 standard, "An IEEE Standard for Binary Floating-Point Arithmetic", defines *denormal* (or *subnormal*) numbers as non-zero numbers smaller than the smallest possible normalized numbers for a specific floating-point format. Floating-point operations on denormals are slower than on normalized operands because denormal operands and results are usually handled through a software assist mechanism rather than directly in hardware. This software processing causes Intel MKL functions that consume denormals to run slower than with normalized floating-point numbers.

You can mitigate this performance issue by setting the appropriate bit fields in the MXCSR floating-point control register to flush denormals to zero (FTZ) or to replace any denormals loaded from memory with zero (DAZ). Check your compiler documentation to determine whether it has options to control FTZ and DAZ. Note that these compiler options may slightly affect accuracy.

# **Fast Fourier Transform Optimized Radices**

You can improve the performance of Intel MKL Fourier Transform Functions if the length of your data vector permits factorization into powers of optimized radices.

In Intel MKL, the optimized radices are 2, 3, 5, 7, 11, and 13.

# **Using Memory Functions**

# **Avoiding Memory Leaks in Intel MKL**

When running, Intel MKL allocates and deallocates internal buffers to facilitate better performance. However, in some cases this behavior may result in memory leaks.

To avoid memory leaks, you can do either of the following:

- Set the MKL\_DISABLE\_FAST\_MM environment variable to 1 or call the mkl\_disable\_fast\_mm() function. Be aware that this change may negatively impact performance of some Intel MKL functions, especially for small problem sizes.
- Call the mkl\_free\_buffers() function or the mkl\_thread\_free\_buffers() function in the current thread.

For the descriptions of the memory functions, see the Intel MKL Reference Manual, available in the Intel Software Documentation Library.

# See Also

Intel Software Documentation Library

# **Redefining Memory Functions**

In C/C++ programs, you can replace Intel MKL memory functions that the library uses by default with your own functions. To do this, use the *memory renaming* feature.

# **Memory Renaming**

Intel MKL memory management by default uses standard C run-time memory functions to allocate or free memory. These functions can be replaced using memory renaming.

Intel MKL accesses the memory functions by pointers  $i_{malloc}$ ,  $i_{free}$ ,  $i_{calloc}$ , and  $i_{realloc}$ , which are visible at the application level. These pointers initially hold addresses of the standard C run-time memory functions malloc, free, calloc, and realloc, respectively. You can programmatically redefine values of these pointers to the addresses of your application's memory management functions.

Redirecting the pointers is the only correct way to use your own set of memory management functions. If you call your own memory functions without redirecting the pointers, the memory will get managed by two independent memory management packages, which may cause unexpected memory issues.

# **How to Redefine Memory Functions**

To redefine memory functions, use the following procedure:

- 1. Include the i\_malloc.h header file in your code.

  This header file contains all declarations required for replacing the memory allocation functions. The header file also describes how memory allocation can be replaced in those Intel libraries that support this feature.
- **2.** Redefine values of pointers i\_malloc, i\_free, i\_calloc, and i\_realloc prior to the first call to MKL functions, as shown in the following example:

```
#include "i_malloc.h"
...
i_malloc = my_malloc;
i_calloc = my_calloc;
i_realloc = my_realloc;
i_free = my_free;
...
// Now you may call Intel MKL functions
```

# Language-specific Usage Options



The Intel® Math Kernel Library (Intel® MKL) provides broad support for Fortran and C/C++ programming. However, not all functions support both Fortran and C interfaces. For example, some LAPACK functions have no C interface. You can call such functions from C using mixed-language programming.

If you want to use LAPACK or BLAS functions that support Fortran 77 in the Fortran 95 environment, additional effort may be initially required to build compiler-specific interface libraries and modules from the source code provided with Intel MKL.

# **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

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# Using Language-Specific Interfaces with Intel® Math Kernel Library

This section discusses mixed-language programming and the use of language-specific interfaces with Intel MKL.

See also the "FFTW Interface to Intel® Math Kernel Library" Appendix in the Intel MKL Reference Manual for details of the FFTW interfaces to Intel MKL.

# **Interface Libraries and Modules**

You can create the following interface libraries and modules using the respective makefiles located in the interfaces directory.

File name	Contains	
Libraries, in Intel MKL architecture-specific directories		
libmkl_blas95.a <sup>1</sup>	Fortran 95 wrappers for BLAS (BLAS95) for IA-32 architecture.	
libmkl_blas95_ilp64.a <sup>1</sup>	Fortran 95 wrappers for BLAS (BLAS95) supporting LP64 interface.	
libmkl_blas95_lp64.a <sup>1</sup>	Fortran 95 wrappers for BLAS (BLAS95) supporting ILP64 interface.	
libmkl_lapack95.a <sup>1</sup>	Fortran 95 wrappers for LAPACK (LAPACK95) for IA-32 architecture.	
libmkl_lapack95_lp64.a <sup>1</sup>	Fortran 95 wrappers for LAPACK (LAPACK95) supporting LP64 interface.	

File name	Contains
libmkl_lapack95_ilp64.a <sup>1</sup>	Fortran 95 wrappers for LAPACK (LAPACK95) supporting ILP64 interface.
libfftw2xc_intel.a <sup>1</sup>	Interfaces for FFTW version 2.x (C interface for Intel compilers) to call Intel MKL FFT.
libfftw2xc_gnu.a	Interfaces for FFTW version $2.x$ (C interface for GNU compilers) to call Intel MKL FFT.
libfftw2xf_intel.a	Interfaces for FFTW version 2.x (Fortran interface for Intel compilers) to call Intel MKL FFT.
libfftw2xf_gnu.a	Interfaces for FFTW version 2.x (Fortran interface for GNU compiler) to call Intel MKL FFT.
libfftw3xc_intel.a <sup>2</sup>	Interfaces for FFTW version $3.x$ (C interface for Intel compiler) to call Intel MKL FFT.
libfftw3xc_gnu.a	Interfaces for FFTW version $3.x$ (C interface for GNU compilers) to call Intel MKL FFT.
libfftw3xf_intel.a <sup>2</sup>	Interfaces for FFTW version 3.x (Fortran interface for Intel compilers) to call Intel MKL FFT.
libfftw3xf_gnu.a	Interfaces for FFTW version 3.x (Fortran interface for GNU compilers) to call Intel MKL FFT.
libfftw2x_cdft_SINGLE.a	Single-precision interfaces for MPI FFTW version 2.x (C interface) to call Intel MKL cluster FFT.
libfftw2x_cdft_DOUBLE.a	Double-precision interfaces for MPI FFTW version 2.x (C interface) to call Intel MKL cluster FFT.
libfftw3x_cdft.a	Interfaces for MPI FFTW version 3.x (C interface) to call Intel MKL cluster FFT.
libfftw3x_cdft_ilp64.a	Interfaces for MPI FFTW version 3.x (C interface) to call Intel MKL cluster FFT supporting the ILP64 interface.
Modules, in architecture- and int directory	terface-specific subdirectories of the Intel MKL include
$blas95.mod^1$	Fortran 95 interface module for BLAS (BLAS95).
lapack95.mod <sup>1</sup>	Fortran 95 interface module for LAPACK (LAPACK95).
1	E

$blas95.mod^1$	Fortran 95 interface module for BLAS (BLAS95).
${\tt lapack95.mod}^{1}$	Fortran 95 interface module for LAPACK (LAPACK95).
f95_precision.mod <sup>1</sup>	Fortran 95 definition of precision parameters for BLAS95 and LAPACK95.
mkl service.mod <sup>1</sup>	Fortran 95 interface module for Intel MKL support functions.

<sup>&</sup>lt;sup>1</sup> Prebuilt for the Intel® Fortran compiler

# See Also

Fortran 95 Interfaces to LAPACK and BLAS

 $<sup>^2</sup>$  FFTW3 interfaces are integrated with Intel MKL. Look into <mkl directory>/interfaces/fftw3x\*/makefile for options defining how to build and where to place the standalone library with the wrappers.

# Fortran 95 Interfaces to LAPACK and BLAS

Fortran 95 interfaces are compiler-dependent. Intel MKL provides the interface libraries and modules precompiled with the Intel® Fortran compiler. Additionally, the Fortran 95 interfaces and wrappers are delivered as sources. (For more information, see Compiler-dependent Functions and Fortran 90 Modules). If you are using a different compiler, build the appropriate library and modules with your compiler and link the library as a user's library:

- 1. Go to the respective directory <mk1 directory>/interfaces/blas95 or <mk1 directory>/interfaces/lapack95
- **2.** Type one of the following commands depending on your architecture:
  - For the IA-32 architecture,

```
make libia32 INSTALL DIR=<user dir>
```

For the Intel® 64 architecture,

make libintel64 [interface=lp64|ilp64] INSTALL DIR=<user dir>

#### **Important**

The parameter INSTALL DIR is required.

As a result, the required library is built and installed in the  $<user\ dir>/lib\ directory$ , and the .mod files are built and installed in the  $<user\ dir>/include/<arch>[/{lp64|ilp64}]\ directory$ , where <arch> is one of {ia32, intel64}.

By default, the ifort compiler is assumed. You may change the compiler with an additional parameter of <code>make:</code>

FC=<compiler>.

For example, the command

```
make libintel64 FC=pgf95 INSTALL DIR=<userpgf95 dir> interface=lp64
```

builds the required library and .mod files and installs them in subdirectories of <userpqf95 dir>.

To delete the library from the building directory, use one of the following commands:

• For the IA-32 architecture,

```
make cleania32 INSTALL DIR=<user dir>
```

For the Intel® 64 architecture,

```
make cleanintel64 [interface=lp64|ilp64] INSTALL_DIR=<user dir>
```

For all the architectures,

```
make clean INSTALL DIR=<user dir>
```

#### **CAUTION**

Even if you have administrative rights, avoid setting INSTALL\_DIR=../.. or INSTALL\_DIR=< mk1 directory> in a build or clean command above because these settings replace or delete the Intel MKL prebuilt Fortran 95 library and modules.

# **Compiler-dependent Functions and Fortran 90 Modules**

Compiler-dependent functions occur whenever the compiler inserts into the object code function calls that are resolved in its run-time library (RTL). Linking of such code without the appropriate RTL will result in undefined symbols. Intel MKL has been designed to minimize RTL dependencies.



In cases where RTL dependencies might arise, the functions are delivered as source code and you need to compile the code with whatever compiler you are using for your application.

In particular, Fortran 90 modules result in the compiler-specific code generation requiring RTL support. Therefore, Intel MKL delivers these modules compiled with the Intel compiler, along with source code, to be used with different compilers.

# Mixed-language Programming with the Intel Math Kernel Library

Appendix A Intel® Math Kernel Library Language Interfaces Support lists the programming languages supported for each Intel MKL function domain. However, you can call Intel MKL routines from different language environments.

See also these Knowledge Base articles:

- http://software.intel.com/en-us/articles/performance-tools-for-software-developers-how-do-i-use-intel-mkl-with-java for how to call Intel MKL from Java\* applications.
- http://software.intel.com/en-us/articles/how-to-use-boost-ublas-with-intel-mkl for how to perform BLAS matrix-matrix multiplication in C++ using Intel MKL substitution of Boost\* uBLAS functions.
- http://software.intel.com/en-us/articles/intel-mkl-and-third-party-applications-how-to-use-them-together for a list of articles describing how to use Intel MKL with third-party libraries and applications.

# Calling LAPACK, BLAS, and CBLAS Routines from C/C++ Language Environments

Not all Intel MKL function domains support both C and Fortran environments. To use Intel MKL Fortran-style functions in C/C++ environments, you should observe certain conventions, which are discussed for LAPACK and BLAS in the subsections below.

#### **CAUTION**

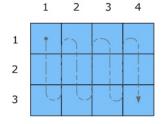
Avoid calling BLAS 95/LAPACK 95 from C/C++. Such calls require skills in manipulating the descriptor of a deferred-shape array, which is the Fortran 90 type. Moreover, BLAS95/LAPACK95 routines contain links to a Fortran RTL.

# **LAPACK and BLAS**

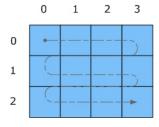
Because LAPACK and BLAS routines are Fortran-style, when calling them from C-language programs, follow the Fortran-style calling conventions:

- Pass variables by address, not by value.
   Function calls in Example "Calling a Complex BLAS Level 1 Function from C++" and Example "Using CBLAS Interface Instead of Calling BLAS Directly from C" illustrate this.
- Store your data in Fortran style, that is, column-major rather than row-major order.

With row-major order, adopted in C, the last array index changes most quickly and the first one changes most slowly when traversing the memory segment where the array is stored. With Fortran-style column-major order, the last index changes most slowly whereas the first index changes most quickly (as illustrated by the figure below for a two-dimensional array).



A: Column-major order (Fortran-style)



B: Row-major order (C-style)

For example, if a two-dimensional matrix A of size mxn is stored densely in a one-dimensional array B, you can access a matrix element like this:

```
A[i][j] = B[i*n+j] in C ( i=0, \ldots, m-1, j=0, \ldots, -1)

A(i,j) = B((j-1)*m+i) in Fortran ( i=1, \ldots, m, j=1, \ldots, n).
```

When calling LAPACK or BLAS routines from C, be aware that because the Fortran language is case-insensitive, the routine names can be both upper-case or lower-case, with or without the trailing underscore. For example, the following names are equivalent:

- LAPACK: dgetrf, DGETRF, dgetrf, and DGETRF
- BLAS: dgemm, DGEMM, dgemm, and DGEMM

See Example "Calling a Complex BLAS Level 1 Function from C++" on how to call BLAS routines from C. See also the Intel(R) MKL Reference Manual for a description of the C interface to LAPACK functions.

#### **CBLAS**

Instead of calling BLAS routines from a C-language program, you can use the CBLAS interface.

CBLAS is a C-style interface to the BLAS routines. You can call CBLAS routines using regular C-style calls. Use the mkl.h header file with the CBLAS interface. The header file specifies enumerated values and prototypes of all the functions. It also determines whether the program is being compiled with a C++ compiler, and if it is, the included file will be correct for use with C++ compilation. Example "Using CBLAS Interface Instead of Calling BLAS Directly from C" illustrates the use of the CBLAS interface.

#### C Interface to LAPACK

Instead of calling LAPACK routines from a C-language program, you can use the C interface to LAPACK provided by Intel MKL.

The C interface to LAPACK is a C-style interface to the LAPACK routines. This interface supports matrices in row-major and column-major order, which you can define in the first function argument  $matrix\_order$ . Use the mkl.h header file with the C interface to LAPACK. mkl.h includes the  $mkl\_lapacke.h$  header file, which specifies constants and prototypes of all the functions. It also determines whether the program is being compiled with a C++ compiler, and if it is, the included file will be correct for use with C++ compilation. You can find examples of the C interface to LAPACK in the examples/lapacke subdirectory in the Intel MKL installation directory.

# Using Complex Types in C/C++

As described in the documentation for the Intel® Fortran Compiler, C/C++ does not directly implement the Fortran types COMPLEX(4) and COMPLEX(8). However, you can write equivalent structures. The type COMPLEX(4) consists of two 4-byte floating-point numbers. The first of them is the real-number component, and the second one is the imaginary-number component. The type COMPLEX(8) is similar to COMPLEX(4) except that it contains two 8-byte floating-point numbers.

Intel MKL provides complex types  $MKL\_Complex8$  and  $MKL\_Complex16$ , which are structures equivalent to the Fortran complex types COMPLEX(4) and COMPLEX(8), respectively. The  $MKL\_Complex8$  and  $MKL\_Complex16$  types are defined in the  $mkl\_types.h$  header file. You can use these types to define complex data. You can also redefine the types with your own types before including the  $mkl\_types.h$  header file. The only requirement is that the types must be compatible with the Fortran complex layout, that is, the complex type must be a pair of real numbers for the values of real and imaginary parts.

For example, you can use the following definitions in your C++ code:

#define MKL Complex8 std::complex<float>

and

#define MKL Complex16 std::complex<double>



See Example "Calling a Complex BLAS Level 1 Function from C++" for details. You can also define these types in the command line:

```
-DMKL_Complex8="std::complex<float>"
-DMKL_Complex16="std::complex<double>"
```

# See Also

Intel® Software Documentation Library for the Intel® Fortran Compiler documentation

# Calling BLAS Functions that Return the Complex Values in C/C++ Code

Complex values that functions return are handled differently in C and Fortran. Because BLAS is Fortran-style, you need to be careful when handling a call from C to a BLAS function that returns complex values. However, in addition to normal function calls, Fortran enables calling functions as though they were subroutines, which provides a mechanism for returning the complex value correctly when the function is called from a C program. When a Fortran function is called as a subroutine, the return value is the first parameter in the calling sequence. You can use this feature to call a BLAS function from C.

The following example shows how a call to a Fortran function as a subroutine converts to a call from C and the hidden parameter result gets exposed:

```
Normal Fortran function call: result = cdotc(n, x, 1, y, 1)
A call to the function as a subroutine: call cdotc(result, n, x, 1, y, 1)
A call to the function from C: cdotc(\&result, \&n, x, \&one, y, \&one)
```

#### NOTE

Intel MKL has both upper-case and lower-case entry points in the Fortran-style (case-insensitive) BLAS, with or without the trailing underscore. So, all these names are equivalent and acceptable: cdotc, CDOTC, cdotc, and CDOTC\_.

The above example shows one of the ways to call several level 1 BLAS functions that return complex values from your C and C++ applications. An easier way is to use the CBLAS interface. For instance, you can call the same function using the CBLAS interface as follows:

```
cblas cdotc( n, x, 1, y, 1, &result )
```

#### **NOTE**

The complex value comes last on the argument list in this case.

The following examples show use of the Fortran-style BLAS interface from C and C++, as well as the CBLAS (C language) interface:

- Example "Calling a Complex BLAS Level 1 Function from C"
- Example "Calling a Complex BLAS Level 1 Function from C++"
- Example "Using CBLAS Interface Instead of Calling BLAS Directly from C"

# Example "Calling a Complex BLAS Level 1 Function from C"

The example below illustrates a call from a C program to the complex BLAS Level 1 function zdotc(). This function computes the dot product of two double-precision complex vectors.

In this example, the complex dot product is returned in the structure c.

```
#include "mkl.h"
#define N 5
int main()
```

```
{
int n = N, inca = 1, incb = 1, i;
MKL_Complex16 a[N], b[N], c;
for( i = 0; i < n; i++ ){
    a[i].real = (double)i; a[i].imag = (double)i * 2.0;
    b[i].real = (double) (n - i); b[i].imag = (double)i * 2.0;
}
zdotc( &c, &n, a, &inca, b, &incb );
printf( "The complex dot product is: ( %6.2f, %6.2f) \n", c.real, c.imag );
return 0;
}</pre>
```

# Example "Calling a Complex BLAS Level 1 Function from C++"

Below is the C++ implementation:

```
#include <complex>
#include <iostream>
#define MKL_Complex16 std::complex<double>
#include "mkl.h"

#define N 5

int main()
{
    int n, inca = 1, incb = 1, i;
    std::complex<double> a[N], b[N], c;
    n = N;

    for( i = 0; i < n; i++) {
        a[i] = std::complex<double>(i,i*2.0);
        b[i] = std::complex<double>(n-i,i*2.0);
}
zdotc(&c, &n, a, &inca, b, &incb);
std::cout << "The complex dot product is: " << c << std::endl;
    return 0;
}</pre>
```

# Example "Using CBLAS Interface Instead of Calling BLAS Directly from C"

This example uses CBLAS:

```
#include <stdio.h>
#include "mkl.h"

typedef struct{ double re; double im; } complex16;
#define N 5
int main()
{
  int n, inca = 1, incb = 1, i;
  complex16 a[N], b[N], c;
  n = N;
  for( i = 0; i < n; i++ ){
  a[i].re = (double)i; a[i].im = (double)i * 2.0;
  b[i].re = (double) (n - i); b[i].im = (double)i * 2.0;
}
cblas_zdotc_sub(n, a, inca, b, incb, &c );
printf( "The complex dot product is: ( %6.2f, %6.2f)\n", c.re, c.im );</pre>
```

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return 0;
}

# Obtaining Numerically Reproducible Results

Intel® Math Kernel Library (Intel® MKL) offers functions and environment variables that help you obtain Conditional Numerical Reproducibility (CNR) of floating-point results when calling the library functions from your application. These new controls enable Intel MKL to run in a special mode, when functions return bitwise reproducible floating-point results from run to run under the following conditions:

- Calls to Intel MKL occur in a single executable
- The number of computational threads used by the library does not change in the run

It is well known that for general single and double precision IEEE floating-point numbers, the associative property does not always hold, meaning (a+b)+c may not equal a +(b+c). Let's consider a specific example. In infinite precision arithmetic  $2^{-63} + 1 + -1 = 2^{-63}$ . If this same computation is done on a computer using double precision floating-point numbers, a rounding error is introduced, and the order of operations becomes important:

$$(2^{-63} + 1) + (-1) \simeq 1 + (-1) = 0$$

versus

$$2^{-63} + (1 + (-1)) \simeq 2^{-63} + 0 = 2^{-63}$$

This inconsistency in results due to order of operations is precisely what the new functionality addresses.

The application related factors that affect the order of floating-point operations within a single executable program include selection of a code path based on run-time processor dispatching, alignment of data arrays, variation in number of threads, threaded algorithms and internal floating-point control settings. You can control most of these factors by controlling the number of threads and floating-point settings and by taking steps to align memory when it is allocated (see the Getting Reproducible Results with Intel® MKL knowledge base article for details). However, run-time dispatching and certain threaded algorithms do not allow users to make changes that can ensure the same order of operations from run to run.

Intel MKL does run-time processor dispatching in order to identify the appropriate internal code paths to traverse for the Intel MKL functions called by the application. The code paths chosen may differ across a wide range of Intel processors and Intel architecture compatible processors and may provide differing levels of performance. For example, an Intel MKL function running on an Intel® Pentium® 4 processor may run one code path, while on the latest Intel® Xeon® processor it will run another code path. This happens because each unique code path has been optimized to match the features available on the underlying processor. One key way that the new features of a processor are exposed to the programmer is through the instruction set architecture (ISA). Because of this, code branches in Intel MKL are designated by the latest ISA they use for optimizations: from the Intel® Streaming SIMD Extensions 2 (Intel® SSE2) to the Intel® Advanced Vector Extensions 2 (Intel® AVX2). The feature-based approach introduces a challenge: if any of the internal floating-point operations are done in a different order or are re-associated, the computed results may differ.

Dispatching optimized code paths based on the capabilities of the processor on which the code is running is central to the optimization approach used by Intel MKL. So it is natural that consistent results require some performance trade-offs. If limited to a particular code path, performance of Intel MKL can in some circumstances degrade by more than a half. To understand this, note that matrix-multiply performance nearly doubled with the introduction of new processors supporting Intel AVX2 instructions. Even if the code branch is not restricted, performance can degrade by 10-20% because the new functionality restricts algorithms to maintain the order of operations.

# **Optimization Notice**

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# **Optimization Notice**

dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

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# **Getting Started with Conditional Numerical Reproducibility**

Intel MKL offers functions and environment variables to help you get reproducible results. You can configure Intel MKL using functions or environment variables, but the functions provide more flexibility.

The following specific examples introduce you to the conditional numerical reproducibility.

While these examples recommend aligning input and output data, you can supply unaligned data to Intel MKL functions running in the CNR mode, but refer to Reproducibility Conditions for details related to data alignment.

# **Intel CPUs supporting Intel AVX2**

To ensure Intel MKL calls return the same results on every Intel CPU supporting Intel AVX2 instructions:

- **1.** Make sure that your application uses a fixed number of threads
- 2. (Recommended) Properly align input and output arrays in Intel MKL function calls
- **3.** Do either of the following:
  - Call

```
mkl cbwr set(MKL CBWR AVX2)
```

Set the environment variable:

```
export MKL CBWR = "AVX2"
```

#### **NOTE**

On non-Intel CPUs and on Intel CPUs that do not support Intel AVX2, this environment setting may cause results to differ because the AUTO branch is used instead, while the above function call returns an error and does not enable the CNR mode.

# **Intel CPUs supporting Intel SSE2**

To ensure Intel MKL calls return the same results on every Intel CPU supporting Intel SSE2 instructions:

- **1.** Make sure that your application uses a fixed number of threads
- 2. (Recommended) Properly align input and output arrays in Intel MKL function calls
- **3.** Do either of the following:
  - Call

```
mkl_cbwr_set(MKL_CBWR_SSE2)
```

Set the environment variable:

```
export MKL CBWR = "SSE2"
```

#### **NOTE**

On non-Intel CPUs, this environment setting may cause results to differ because the AUTO branch is used instead, while the above function call returns an error and does not enable the CNR mode.

#### Intel or Intel compatible CPUs supporting Intel SSE2

On non-Intel CPUs, only the MKL\_CBWR\_AUTO and MKL\_CBWR\_COMPATIBLE options are supported for function calls and only AUTO and COMPATIBLE options for environment settings.

To ensure Intel MKL calls return the same results on all Intel or Intel compatible CPUs supporting Intel SSE2 instructions:

- 1. Make sure that your application uses a fixed number of threads
- 2. (Recommended) Properly align input and output arrays in Intel MKL function calls
- **3.** Do either of the following:
  - Call

```
mkl cbwr set (MKL CBWR COMPATIBLE)
```

• Set the environment variable:

```
export MKL CBWR = "COMPATIBLE"
```

#### **NOTE**

The special MKL\_CBWR\_COMPATIBLE/COMPATIBLE option is provided because Intel and Intel compatible CPUs have a few instructions, such as approximation instructions rcpps/rsqrtps, that may return different results. This option ensures that Intel MKL does not use these instructions and forces a single Intel SSE2 only code path to be executed.

#### **Next steps**

•	
See Specifying the Code Branches	for details of specifying the branch using environment variables.
See the following sections in the Intel MKL Reference Manual:	
Support Functions for Conditional Numerical Reproducibility	for how to configure the CNR mode of Intel MKL using functions.
PARDISO - Parallel Direct Sparse Solver Interface	for how to configure the CNR mode for PARDISO.

#### See Also

Code Examples

## **Specifying the Code Branches**

Intel MKL provides conditional numerically reproducible results for a code branch determined by the supported instruction set architecture (ISA). The values you can specify for the  $\texttt{MKL\_CBWR}$  environment variable may have one of the following equivalent formats:

- MKL CBWR="<branch>"
- MKL\_CBWR="BRANCH=<branch>"

The <br/>placeholder specifies the CNR branch with one of the following values:

Value	Description
AUTO	CNR mode uses the standard ISA-based dispatching model while ensuring fixed cache sizes, deterministic reductions, and static scheduling

$\mathbf{n}$	
$\mathbf{\circ}$	

Value	Description
	CNR mode uses the branch for the following ISA:
COMPATIBLE	Intel® Streaming SIMD Extensions 2 (Intel® SSE2) without rcpps/rsqrtps instructions
SSE2	Intel SSE2
SSE3	DEPRECATED. Intel® Streaming SIMD Extensions 3 (Intel® SSE3). This setting is kept for backward compatibility and is equivalent to SSE2.
SSSE3	Supplemental Streaming SIMD Extensions 3 (SSSE3)
SSE4_1	Intel® Streaming SIMD Extensions 4-1 (Intel® SSE4-1)
SSE4_2	Intel® Streaming SIMD Extensions 4-2 (Intel® SSE4-2)
AVX	Intel® Advanced Vector Extensions (Intel® AVX)
AVX2	Intel® Advanced Vector Extensions 2 (Intel® AVX2)

When specifying the CNR branch, be aware of the following:

- Reproducible results are provided under Reproducibility Conditions.
- Settings other than AUTO or COMPATIBLE are available only for Intel processors.
- To get the CNR branch optimized for the processor where your program is currently running, choose the value of AUTO or call the mkl cbwr get auto branch function.

Setting the MKL\_CBWR environment variable or a call to an equivalent  $mkl_set_cbwr_branch$  function fixes the code branch and sets the reproducibility mode.

- If the value of the branch is incorrect or your processor or operating system does not support the specified ISA, CNR ignores this value and uses the AUTO branch without providing any warning messages.
- Calls to functions that define the behavior of CNR must precede any of the math library functions that they control.
- Settings specified by the functions take precedence over the settings specified by the environment variable.

See the Intel MKL Reference Manual for how to specify the branches using functions.

#### See Also

Getting Started with Conditional Numerical Reproducibility

## **Reproducibility Conditions**

To get reproducible results from run to run, ensure that the number of threads is fixed and constant. Specifically:

- If you are running your program on different processors, explicitly specify the number of threads.
- To ensure that your application has deterministic behavior with OpenMP\* parallelization and does not adjust the number of threads dynamically at run time, set MKL\_DYNAMIC and OMP\_DYNAMIC to FALSE. This is especially needed if you are running your program on different systems.
  - As usual, you should align your data, even in CNR mode, to obtain the best possible performance. While CNR mode also fully supports unaligned input and output data, the use of it might reduce the performance of some Intel MKL functions on earlier Intel processors. Refer to coding techniques that improve performance for more details.

- Conditional Numerical Reproducibility does not ensure that bitwise-identical NaN values are generated when the input data contains NaN values.
- If dynamic memory allocation fails on one run but succeeds on another run, you may fail to get reproducible results between these two runs.

#### See Also

MKL\_DYNAMIC
Coding Techniques

# Setting the Environment Variable for Conditional Numerical Reproducibility

The following examples illustrate the use of the  $\texttt{MKL\_CBWR}$  environment variable. The first command in each list sets Intel MKL to run in the CNR mode based on the default dispatching for your platform. The other two commands in each list are equivalent and set the CNR branch to Intel AVX.

#### For the bash shell:

```
export MKL_CBWR="AUTO"
export MKL_CBWR="AVX"
export MKL_CBWR="BRANCH=AVX"

For the C shell (csh or tcsh):
```

```
setenv MKL_CBWR "AUTO"setenv MKL_CBWR "AVX"setenv MKL CBWR "BRANCH=AVX"
```

#### See Also

Specifying the Code Branches

### **Code Examples**

The following simple programs show how to obtain reproducible results from run to run of Intel MKL functions. See the *Intel MKL Reference Manual* for more examples.

#### **C Example of CNR**

```
#include <mkl.h>
int main(void) {
   int my_cbwr_branch;
   /* Align all input/output data on 64-byte boundaries */
   /* "for best performance of Intel MKL */
   void *darray;
   int darray size=1000;
   /* Set alignment value in bytes */
   int alignment=64;
   /* Allocate aligned array */
   darray = mkl malloc (sizeof(double)*darray size, alignment);
   /* Find the available MKL CBWR BRANCH automatically */
   my cbwr branch = mkl cbwr get auto branch();
   /* User code without Intel MKL calls */
   /* Piece of the code where CNR of Intel MKL is needed */
   ^{\prime\star} The performance of Intel MKL functions might be reduced for CNR mode ^{\star\prime}
   /* If the "IF" statement below is commented out, Intel MKL will run in a regular mode, */
   /* and data alignment will allow you to get best performance */
   if (mkl cbwr set(my cbwr branch)) {
```

```
printf("Error in setting MKL_CBWR_BRANCH! Aborting...\n");
    return;
}
/* CNR calls to Intel MKL + any other code */
/* Free the allocated aligned array */
    mkl_free(darray);
}
```

#### **Fortran Example of CNR**

```
PROGRAM MAIN
   INCLUDE 'mkl.fi'
   INTEGER*4 MY CBWR BRANCH
! Align all input/output data on 64-byte boundaries
! "for best performance of Intel MKL
! Declare Intel MKL memory allocation routine
#ifdef IA32
   INTEGER MKL MALLOC
#else
   INTEGER*8 MKL MALLOC
#endif
   EXTERNAL MKL MALLOC, MKL FREE
   DOUBLE PRECISION DARRAY
   POINTER (P DARRAY, DARRAY(1))
   INTEGER DARRAY SIZE
   PARAMETER (DARRAY SIZE=1000)
! Set alignment value in bytes
   INTEGER ALIGNMENT
   PARAMETER (ALIGNMENT=64)
! Allocate aligned array
    P DARRAY = MKL MALLOC (%VAL(8*DARRAY SIZE), %VAL(ALIGNMENT));
! Find the available MKL CBWR BRANCH automatically
   MY CBWR BRANCH = MKL CBWR GET AUTO BRANCH()
! User code without Intel MKL calls
! Piece of the code where CNR of Intel MKL is needed
! The performance of Intel MKL functions may be reduced for CNR mode
! If the "IF" statement below is commented out, Intel MKL will run in a regular mode,
! and data alignment will allow you to get best performance
    IF (MKL CBWR SET (MY CBWR BRANCH) .NE. MKL CBWR SUCCESS) THEN
        PRINT *, 'Error in setting MKL CBWR BRANCH! Aborting...'
        RETURN
   ENDIF
! CNR calls to Intel MKL + any other code
! Free the allocated aligned array
   CALL MKL FREE (P DARRAY)
    END
```

#### Use of CNR with Unaligned Data in C

```
#include <mkl.h>
int main(void) {
    int my_cbwr_branch;
    /* If it is not possible to align all input/output data on 64-byte boundaries */
    /* to achieve performance, use unaligned IO data with possible performance */
    /* penalty */
    /* Using unaligned IO data */
    double *darray;
    int darray_size=1000;
    /* Allocate array, malloc aligns data on 8/16-byte boundary only */
    darray = (double *)malloc (sizeof(double)*darray_size);
    /* Find the available MKL_CBWR_BRANCH automatically */
```

```
my_cbwr_branch = mkl_cbwr_get_auto_branch();
    /* User code without Intel MKL calls */
    /* Piece of the code where CNR of Intel MKL is needed */
    /* The performance of Intel MKL functions might be reduced for CNR mode */
    /* If the "IF" statement below is commented out, Intel MKL will run in a regular mode, */
    /* and you will NOT get best performance without data alignment */
    if (mkl_cbwr_set(my_cbwr_branch)) {
        printf("Error in setting MKL_CBWR_BRANCH! Aborting...\n");
        return;
}

/* CNR calls to Intel MKL + any other code */
    /* Free the allocated array */
    free(darray);
```

#### Use of CNR with Unaligned Data in Fortran

```
PROGRAM MAIN
    INCLUDE 'mkl.fi'
    INTEGER*4 MY CBWR BRANCH
! If it is not possible to align all input/output data on 64-byte boundaries
! to achieve performance, use unaligned IO data with possible performance
! penalty
    DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: DARRAY
    INTEGER DARRAY SIZE, STATUS
    PARAMETER (DARRAY SIZE=1000)
! Allocate array with undefined alignment
    ALLOCATE (DARRAY (DARRAY SIZE));
! Find the available MKL CBWR BRANCH automatically
    MY CBWR BRANCH = MKL CBWR GET AUTO BRANCH()
! User code without Intel MKL calls
! Piece of the code where CNR of Intel MKL is needed
! The performance of Intel MKL functions might be reduced for CNR mode
! If the "IF" statement below is commented out, Intel MKL will run in a regular mode,
! and you will NOT get best performance without data alignment
    IF (MKL CBWR SET(MY CBWR BRANCH) .NE. MKL CBWR SUCCESS) THEN
          PRINT *, 'Error in setting MKL CBWR BRANCH! Aborting...'
         RETURN
    ENDIF
! CNR calls to Intel MKL + any other code
! Free the allocated array
    DEALLOCATE (DARRAY)
    END
```

## **Coding Tips**

This section provides coding tips for managing data alignment and version-specific compilation.

## **Example of Data Alignment**

Needs for best performance with Intel MKL or for reproducible results from run to run of Intel MKL functions require alignment of data arrays. The following example shows how to align an array on 64-byte boundaries. To do this, use  $mkl_malloc()$  in place of system provided memory allocators, as shown in the code example below.

#### **Aligning Addresses on 64-byte Boundaries**

```
// ****** C language ******
...
#include <stdlib.h>
#include <mkl.h>
...
void *darray;
int workspace;
// Set value of alignment
int alignment=64;
...
// Allocate aligned workspace
darray = mkl_malloc( sizeof(double) *workspace, alignment );
...
// call the program using MKL
mkl_app( darray );
...
// Free workspace
mkl_free( darray );
```

```
! ******* Fortran language ******
...
! Set value of alignment
integer alignment
parameter (alignment=64)
...
! Declare Intel MKL routines
#ifdef _IA32
integer mkl_malloc
#else
integer*8 mkl_malloc
#endif
external mkl_malloc, mkl_free, mkl_app
...
double precision darray
pointer (p_wrk,darray(1))
integer workspace
...
! Allocate aligned workspace
```

```
p_wrk = mkl_malloc( %val(8*workspace), %val(alignment) )
...
! call the program using Intel MKL
call mkl_app( darray )
...
! Free workspace
call mkl_free(p_wrk)
```

# Using Predefined Preprocessor Symbols for Intel® MKL Version-Dependent Compilation

Preprocessor symbols (macros) substitute values in a program before it is compiled. The substitution is performed in the preprocessing phase.

The following preprocessor symbols are available:

Predefined Preprocessor Symbol	Description
INTEL_MKL	Intel MKL major version
INTEL_MKL_MINOR	Intel MKL minor version
INTEL_MKL_UPDATE	Intel MKL update number
INTEL_MKL_VERSION	Intel MKL full version in the following format:
	<pre>INTEL_MKL_VERSION = (_ INTEL_MKL_ *100+_ INTEL_MKL_MINOR_)*100+_ I NTEL_MKL_UPDATE</pre>

These symbols enable conditional compilation of code that uses new features introduced in a particular version of the library.

To perform conditional compilation:

- 1. Include in your code the file where the macros are defined:
  - mkl.h for C/C++
  - mkl.fi for Fortran
- 2. [Optionally] Use the following preprocessor directives to check whether the macro is defined:
  - #ifdef, #endif for C/C++
  - !DEC\$IF DEFINED, !DEC\$ENDIF for Fortran
- **3.** Use preprocessor directives for conditional inclusion of code:
  - #if, #endif for C/C++
  - !DEC\$IF, !DEC\$ENDIF for Fortran

#### Example

This example shows how to compile a code segment conditionally for a specific version of Intel MKL. In this case, the version is 10.3 Update 4:

#### C/C++:

```
#include "mkl.h"
#ifdef INTEL_MKL_VERSION
#if INTEL_MKL_VERSION == 100304
// Code to be conditionally compiled
#endif
#endif
```

#### Fortran:

include "mkl.fi"
!DEC\$IF DEFINED INTEL\_MKL\_VERSION
!DEC\$IF INTEL\_MKL\_VERSION .EQ. 100304
\* Code to be conditionally compiled
!DEC\$ENDIF
!DEC\$ENDIF

## **Managing Output**

## **Using Intel MKL Verbose Mode**

If your application calls Intel MKL functions, you may want to know what computational functions are called, what parameters are passed to them, and how much time is spent to execute the functions. Your application can print this information to a standard output device if Intel MKL Verbose mode is enabled. Functions that can print this information are referred to as *verbose-enabled* functions. While not all Intel MKL functions are verbose-enabled, see *Intel MKL Release Notes* for the Intel MKL function domains that support the Verbose mode.

In the Verbose mode, every call of a verbose-enabled function finishes with printing a human readable line describing the call. If the application is terminated during the function call, no information for that function is printed. The first call to a verbose-enabled function also prints a version information line.

To enable the Intel MKL Verbose mode for an application, do one of the following:

- Set the environment variable MKL VERBOSE to 1.
- Call the support function mkl verbose(1).

The function call mkl\_verbose(0) disables the Verbose mode. Enabling or disabling the Verbose mode using the function call takes precedence over the environment setting. For a full description of the mkl\_verbose function, see the *Intel MKL Reference Manual*, available in the Intel® Software Documentation Library.

Intel MKL Verbose mode is not a thread-local but a global state. It means that if an application changes the mode from multiple threads, the result is undefined.

#### **WARNING**

The performance of an application may degrade with the Verbose mode enabled, especially when the number of calls to verbose-enabled functions is large, because every call to a verbose-enabled function requires an output operation.

#### See Also

Intel Software Documentation Library

#### **Version Information Line**

In the Intel MKL Verbose mode, the first call to a verbose-enabled function prints a version information line. The line begins with the MKL\_VERBOSE character string and uses spaces as delimiters. The format of the rest of the line may change in a future release.

The following table lists information contained in a version information line and provides available links for more information:

Information	Description	Related Links
Intel MKL version.	This information is separated by a comma from the rest of the line.	
Operating system.	Possible values:	
	<ul><li>Lnx for Linux* OS</li><li>Win for Windows* OS</li></ul>	

Information	Description	Related Links
	OSX for OS X*	
The host CPU frequency.		
Intel MKL interface layer used by the application.	<ul> <li>No value on systems based on the IA-32 architecture.</li> <li>1p64 or ilp64 on systems based on the Intel® 64 architecture.</li> </ul>	Using the ILP64 Interface vs. LP64 Interface
Intel MKL threading layer used by the application.	Possible values: intel_thread, gnu_thread, pgi_thread, or sequential.	Linking with Threading Libraries
The number of Intel® Xeon Phi™ coprocessors detected.	Nothing is printed if no coprocessors are detected.  The number printed is prefixed with NMICDev: .  Intel MKL attempts to detect the coprocessors unless it runs in the sequential mode because Automatic Offload functionality is only provided by threaded Intel MKL.	Automatic Offload

#### The following is an example of a version information line:

MKL\_VERBOSE Intel(R) MKL 11.2 Beta build 20131126 for Intel(R) 64 architecture Intel(R) Advanced Vector Extensions (Intel(R) AVX) Enabled Processor, Lnx 3.10GHz lp64 intel\_thread NMICDev:2

#### **Call Description Line**

In Intel MKL Verbose mode, each verbose-enabled function called from your application prints a call description line. The line begins with the  $\texttt{MKL\_VERBOSE}$  character string and uses spaces as delimiters. The format of the rest of the line may change in a future release.

The following table lists information contained in a call description line and provides available links for more information:

Information	Description	Related Links
The name of the function.	Although the name printed may differ from the name used in the source code of the application (for example, the cblas_ prefix of CBLAS functions is not printed), you can easily recognize the function by the printed name.	
Values of the arguments.	<ul> <li>The values are listed in the order of the formal argument list. The list directly follows the function name, it is parenthesized and comma-separated.</li> <li>Arrays are printed as addresses (to see the alignment of the data).</li> <li>Integer scalar parameters passed by reference are printed by value. Zero values are printed for NULL references.</li> <li>Character values are printed without quotes.</li> <li>For all parameters passed by reference, the values printed are the values returned by the function. For example, the printed value of the info parameter of a LAPACK function is its value after the function execution.</li> </ul>	

Information	Description	Related Links
Time taken by the function.	<ul> <li>The time is printed in convenient units (seconds, milliseconds, and so on), which are explicitly indicated.</li> <li>The time may fluctuate from run to run.</li> <li>The time printed may occasionally be larger than the time actually taken by the function call, especially for small problem sizes and multi-socket machines. To reduce this effect, bind threads that call Intel MKL to CPU cores by setting an affinity mask.</li> </ul>	Managing Multi- core Performance for options to set an affinity mask.
Value of the MKL_CBWR environment variable.	The value printed is prefixed with $\ensuremath{\mathtt{CNR}}$ :	Getting Started with Conditional Numerical Reproducibility
Value of the MKL_DYNAMIC environment variable.	The value printed is prefixed with Dyn:	MKL_DYNAMIC
Status of the Intel MKL memory manager.	The value printed is prefixed with FastMM:	Avoiding Memory Leaks in Intel MKL for a description of the Intel MKL memory manager
OpenMP* thread number of the calling thread.	The value printed is prefixed with TID:	
Values of Intel MKL environment variables defining the general and domain-specific numbers of threads, separated by a comma.	The first value printed is prefixed with NThr:	Intel MKL-specific Environment Variables for Threading Control
Value of the MKL_HOST_ WORKDIVISION environment variable.	The value printed is prefixed with WDiv:HOST:	Automatic Offload Controls
Values of the MKL_MIC_ <number> _WORKDIVISION environment variables for each Intel® Xeon Phi™ coprocessor available on the system, where <number> is the number of the coprocessor.</number></number>	The first value printed is prefixed with WDiv: <number>:</number>	Automatic Offload Controls

The following is an example of a call description line:

MKL\_VERBOSE DGEMM(n,n, 1000,1000,240,0x7ffff708bb30,0x7ff2aea4c000,1000,0x7ff28e92b000,240,0x7ffff708bb38,0x7f f28e08d000,1000) 1.66ms CNR:OFF Dyn:1 FastMM:1 TID:0 NThr:16,FFT:2 WDiv:HOST:-1.000 WDiv:0:-1.000 WDiv:1:-1.000

The following information is not printed because of limitations of Intel MKL Verbose mode:

- Input values of parameters passed by reference if the values were changed by the function.

  For example, if a LAPACK function is called with a workspace query, that is, the value of the <code>lwork</code> parameter equals -1 on input, the call description line prints the result of the query and not -1.
- Return values of functions.

For example, the value returned by the function <code>ilaenv</code> is not printed.

• Floating-point scalars passed by reference.

## Working with the Intel® Math Kernel Library Cluster Software

Intel® Math Kernel Library (Intel® MKL) includes distributed memory function domains for use on clusters of the Linux\* and Windows\* operating systems:

- ScaLAPACK
- Cluster Fourier Transform Functions (Cluster FFT)
- Parallel Direct Sparse Solvers for Clusters (Cluster Sparse Solver)

While ScaLAPACK and Cluster FFT support both IA-32 and Intel® 64 architectures, Cluster Sparse Solver is only provided for the Intel® 64 architecture.

#### **Important**

ScaLAPACK, Cluster FFT, and Cluster Sparse Solver function domains are not installed by default. To use them, explicitly select the appropriate component during installation.

#### **NOTE**

Support of the IA-32 architecture by the cluster components is deprecated and will be removed in a future release.

#### **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

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## **Linking with Intel MKL Cluster Software**

The Intel MKL ScaLAPACK, Cluster FFT, and Cluster Sparse Solver support MPI implementations identified in the *Intel MKL Release Notes*.

To link a program that calls ScaLAPACK, Cluster FFT, or Cluster Sparse Solver, you need to know how to link a message-passing interface (MPI) application first.

Use mpi scripts to do this. For example, mpicc or mpif77 are C or FORTRAN 77 scripts, respectively, that use the correct MPI header files. The location of these scripts and the MPI library depends on your MPI implementation. For example, for the default installation of MPICH, /opt/mpich/bin/mpicc and /opt/mpich/bin/mpif77 are the compiler scripts and /opt/mpich/lib/libmpich.a is the MPI library.

Check the documentation that comes with your MPI implementation for implementation-specific details of linking.

To link with ScaLAPACK, Cluster FFT, and/or Cluster Sparse Solver, use the following general form:

```
<MPI linker script> <files to link>
-L <MKL path> [-Wl,--start-group] [<MKL cluster library>] \
```

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<BLACS> <MKL core libraries> [-Wl,--end-group]

where the placeholders stand for paths and libraries as explained in the following table:

One of libraries for ScaLAPACK or Cluster FFT and appropriate <MKL cluster library> architecture and programming interface (LP64 or ILP64). Available libraries are listed in Appendix C: Directory Structure in Detail. For example, for the Intel® 64 architecture and LP64 interface, it is -lmkl scalapack lp64 or -lmkl cdft core. Cluster Sparse Solver does not require an additional computation library. <BLACS> The BLACS library corresponding to your architecture, programming interface (LP64 or ILP64), and MPI used. Available BLACS libraries are listed in Appendix C: Directory Structure in Detail. For example, for the Intel® 64 architecture, choose one of -lmkl blacs intelmpi 1p64 or lmkl blacs intelmpi ilp64. <MKL core libraries> Processor optimized kernels, threading library, and system library for threading support, linked as described in Listing Libraries on a Link Line. A linker script that corresponds to the MPI version. <MPI linker script>

For example, if you are using Intel MPI, want to statically link with ScaLAPACK using the LP64 interface, and have only one MPI process per core (and thus do not use threading), specify the following linker options:

-L\$MKLPATH -I\$MKLINCLUDE -W1,--start-group \$MKLPATH/libmkl\_scalapack\_lp64.a \$MKLPATH/libmkl\_blacs\_intelmpi\_lp64.a \$MKLPATH/libmkl\_intel\_lp64.a \$MKLPATH/libmkl\_sequential.a \$MKLPATH/libmkl core.a -static mpi -W1,--end-group -lpthread -lm

#### NOTE

Grouping symbols -W1, --start-group and -W1, --end-group are required for static linking.

#### TIP

Use the Using the Link-line Advisor to quickly choose the appropriate set of <MKL cluster Library>, <BLACS>, and <MKL core libraries>.

#### See Also

Linking Your Application with the Intel® Math Kernel Library Examples of Linking for Clusters

## Setting the Number of Threads

The OpenMP\* run-time library responds to the environment variable <code>OMP\_NUM\_THREADS</code>. Intel MKL also has other mechanisms to set the number of OpenMP threads, such as the <code>MKL\_NUM\_THREADS</code> or <code>MKL\_DOMAIN\_NUM\_THREADS</code> environment variables (see Using Additional Threading Control).

Make sure that the relevant environment variables have the same and correct values on all the nodes. Intel MKL does not set the default number of OpenMP threads to one, but depends on the OpenMP libraries used with the compiler to set the default number. For the threading layer based on the Intel compiler (libmkl intel thread.a), this value is the number of CPUs according to the OS.

#### **CAUTION**

Avoid over-prescribing the number of OpenMP threads, which may occur, for instance, when the number of MPI ranks per node and the number of OpenMP threads per node are both greater than one. The number of MPI ranks per node multiplied by the number of OpenMP threads per node should not exceed the number of hardware threads per node.

If you are using your login environment to set an environment variable, such as <code>OMP\_NUM\_THREADS</code>, remember that changing the value on the head node and then doing your run, as you do on a shared-memory (SMP) system, does not change the variable on all the nodes because <code>mpirun</code> starts a fresh default shell on all the nodes. To change the number of OpenMP threads on all the nodes, in <code>.bashrc</code>, add a line at the top, as follows:

```
OMP NUM THREADS=1; export OMP NUM THREADS
```

You can run multiple CPUs per node using MPICH. To do this, build MPICH to enable multiple CPUs per node. Be aware that certain MPICH applications may fail to work perfectly in a threaded environment (see the Known Limitations section in the *Release Notes*. If you encounter problems with MPICH and setting of the number of OpenMP threads is greater than one, first try setting the number of threads to one and see whether the problem persists.

#### **Important**

For Cluster Sparse Solver, set the number of OpenMP threads to a number greater than one because the implementation of the solver only supports a multithreaded algorithm.

#### See Also

Techniques to Set the Number of Threads

## **Using Shared Libraries**

All needed shared libraries must be visible on all nodes at run time. To achieve this, set the  $LD\_LIBRARY\_PATH$  environment variable accordingly.

If Intel MKL is installed only on one node, link statically when building your Intel MKL applications rather than use shared libraries.

The Intel® compilers or GNU compilers can be used to compile a program that uses Intel MKL. However, make sure that the MPI implementation and compiler match up correctly.

## Interaction with the Message-passing Interface

To improve performance of cluster applications, it is critical for Intel MKL to use the optimal number of threads, as well as the correct thread affinity. Usually, the optimal number is the number of available cores per node divided by the number of MPI processes per node. You can set the number of threads using one of the available methods, described in Techniques to Set the Number of Threads.

If the number of threads is not set, Intel MKL checks whether it runs under MPI provided by the Intel® MPI Library. If this is true, the following environment variables define Intel MKL threading behavior:

- I MPI THREAD LEVEL
- MKL MPI PPN
- I MPI NUMBER OF MPI PROCESSES PER NODE
- I MPI PIN MAPPING
- OMPI COMM WORLD LOCAL SIZE
- MPI LOCALNRANKS

The threading behavior depends on the value of I MPI THREAD LEVEL as follows:

• 0 or undefined.

Intel MKL considers that thread support level of Intel MPI Library is MPI\_THREAD\_SINGLE and defaults to sequential execution.

• 1, 2, or 3.

This value determines Intel MKL conclusion of the thread support level:

- 1 MPI THREAD FUNNELED
- 2 MPI THREAD SERIALIZED
- 3 MPI THREAD MULTIPLE

In all these cases, Intel MKL determines the number of MPI processes per node using the other environment variables listed and defaults to the number of threads equal to the number of available cores per node divided by the number of MPI processes per node.

#### **Important**

Instead of relying on the discussed implicit settings, explicitly set the number of threads for Intel MKL.

#### **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

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#### See Also

Managing Multi-core Performance

Intel® Software Documentation Library for more information on Intel MPI Library

### **Building ScaLAPACK Tests**

When building ScaLAPACK tests:

- For the IA-32 architecture, add libmkl\_scalapack\_core.a to your link command.
- For the Intel® 64 or Intel® Many Integrated Core architecture, add libmkl\_scalapack\_lp64.a or libmkl scalapack ilp64.a, depending on the desired interface.

## **Examples of Linking for Clusters**

This section provides examples of linking with ScaLAPACK, Cluster FFT, and Cluster Sparse Solver.

Note that a binary linked with the Intel MKL cluster function domains runs the same way as any other MPI application (refer to the documentation that comes with your MPI implementation). For instance, the script mpirun is used in the case of MPICH2 and OpenMPI, and a number of MPI processes is set by -np. In the case of MPICH2 and all Intel MPIs, start the daemon before running your application; the execution is driven by the script mpiexec.

For further linking examples, see the support website for Intel products at http://www.intel.com/software/products/support/.

#### See Also

Directory Structure in Detail

#### **Examples for Linking a C Application**

These examples illustrate linking of an application under the following conditions:

- Main module is in C.
- You are using the Intel® C++ Compiler.
- You are using MPICH2.
- Intel MKL functions use LP64 interfaces.
- The PATH environment variable contains a directory with the MPI linker scripts.
- \$MKLPATH is a user-defined variable containing <mkl directory>/lib/intel64.

To link dynamically with ScaLAPACK for a cluster of systems based on the Intel® 64 architecture, use the following link line:

```
mpicc <user files to link>
    -L$MKLPATH
    -lmkl_scalapack_lp64
    -lmkl_blacs_intelmpi_lp64
    -lmkl_intel_lp64
    -lmkl_intel_thread -lmkl_core
    -liomp5 -lpthread
```

To link statically with Cluster FFT for a cluster of systems based on the Intel® 64 architecture, use the following link line:

```
mpicc <user files to link>
   -Wl,--start-group
   $MKLPATH/libmkl_cdft_core.a
   $MKLPATH/libmkl_blacs_intelmpi_lp64.a
   $MKLPATH/libmkl_intel_lp64.a
   $MKLPATH/libmkl_intel_thread.a
   $MKLPATH/libmkl_core.a
   -Wl,--end-group
   -liomp5 -lpthread
```

To link dynamically with Cluster Sparse Solver for a cluster of systems based on the Intel® 64 architecture, use the following link line:

```
mpicc <user files to link>
    -L$MKLPATH
    -lmkl_blacs_intelmpi_lp64
    -lmkl_intel_lp64
    -lmkl_intel_thread -lmkl_core
    -liomp5 -lpthread
```

#### See Also

Linking with Intel MKL Cluster Software Using the Link-line Advisor

#### **Examples for Linking a Fortran Application**

These examples illustrate linking of an application under the following conditions:

- Main module is in Fortran.
- You are using the Intel® Fortran Compiler.
- You are using the Intel MPI library.



- Intel MKL functions use LP64 interfaces.
- The PATH environment variable contains a directory with the MPI linker scripts.
- \$MKLPATH is a user-defined variable containing <mk1 directory>/lib/intel64.

To link dynamically with ScaLAPACK for a cluster of systems based on the Intel® 64 architecture, use the following link line:

```
mpiifort <user files to link>
    -L$MKLPATH
    -lmkl_scalapack_lp64
    -lmkl_blacs_intelmpi_lp64
    -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core
    -liomp5 -lpthread
```

To link statically with Cluster FFT for a cluster of systems based on the Intel® 64 architecture, use the following link line:

```
mpiifort <user files to link>
    -Wl,--start-group
    $MKLPATH/libmkl_cdft_core.a
    $MKLPATH/libmkl_blacs_intelmpi_lp64.a
    $MKLPATH/libmkl_intel_lp64.a
    $MKLPATH/libmkl_intel_thread.a
    $MKLPATH/libmkl_core.a
    -Wl,--end-group
    -liomp5 -lpthread
```

To link statically with Cluster Sparse Solver for a cluster of systems based on the Intel® 64 architecture, use the following link line:

```
mpiifort <user files to link>
    -Wl,--start-group
    $MKLPATH/libmkl_blacs_intelmpi_lp64.a
    $MKLPATH/libmkl_intel_lp64.a
    $MKLPATH/libmkl_intel_thread.a
    $MKLPATH/libmkl_core.a
    -Wl,--end-group
    -liomp5 -lpthread
```

#### See Also

Linking with Intel MKL Cluster Software Using the Link-line Advisor

## Using Intel® Math Kernel Library on Intel® Xeon Phi™ Coprocessors



Intel® Math Kernel Library (Intel® MKL) offers two sets of libraries to support Intel® Many Integrated Core (Intel® MIC) Architecture:

- For the host computer based on Intel® 64 or compatible architecture and running a Linux\* operating system
- For Intel® Xeon Phi<sup>™</sup> coprocessors

You can control how Intel MKL offloads computations to Intel® Xeon Phi<sup>™</sup> coprocessors. Either you can offload computations automatically or use Compiler Assisted Offload:

- Automatic Offload.
  - On Linux\* OS running on Intel® 64 or compatible architecture systems, Automatic Offload automatically detects the presence of coprocessors based on Intel MIC Architecture and automatically offloads computations that may benefit from additional computational resources available. This usage model enables you to call Intel MKL routines as you would normally do with minimal changes to your program. The only change needed to enable Automatic Offload is either the setting of an environment variable or a single function call. For details see Automatic Offload.
- · Compiler Assisted Offload.

This usage model enables you to use the Intel compiler and its offload pragma support to manage the functions and data offloaded to a coprocessor. Within an offload region, you should specify both the input and output data for the Intel MKL functions to be offloaded. After linking with the Intel MKL libraries for Intel MIC Architecture, the compiler provided run-time libraries transfer the functions along with their data to a coprocessor to carry out the computations. For details see Compiler Assisted Offload.

In addition to offloading computations to coprocessors, you can call Intel MKL functions from an application that runs natively on a coprocessor. Native execution occurs when an application runs entirely on Intel MIC Architecture. Native mode is a fast way to make an existing application run on Intel MIC Architecture with minimal changes to the source code. For more information, see Running Intel MKL on an Intel Xeon Phi Coprocessor in Native Mode.

Intel MKL ScaLAPACK and Cluster FFT can benefit from yet another usage model offered by the Intel® MPI Library. The Intel MPI Library treats each Intel Xeon Phi coprocessor as a regular node in a cluster of Intel® Xeon® processors and Intel Xeon Phi coprocessors. To run your application on a coprocessor, you can specify an MPI rank on the coprocessor, build the application for Intel MIC Architecture, and launch the built executable from the host computer or the coprocessor. For usage details of the MPI on coprocessors, see documentation for the Intel MPI Library, available in the Intel Software Documentation Library. For details of building MPI applications that use Intel MKL, see Using ScaLAPACK and Cluster FFT on Intel Xeon Phi Coprocessors.

Intel MKL functionality offers different levels of support for Intel MIC Architecture:

- Optimized
- Supported

Please see the Intel MKL Release Notes for details.

#### **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or

#### **Optimization Notice**

effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

Notice revision #20110804

### **Automatic Offload**

Automatic Offload provides performance improvements with fewer changes to the code than Compiler Assisted Offload. If you are executing a function on the host CPU, Intel MKL running in the Automatic Offload mode may offload part of the computations to one or multiple Intel Xeon Phi coprocessors without you explicitly offloading computations. By default, Intel MKL determines the best division of the work between the host CPU and coprocessors. However, you can specify a custom work division.

To enable Automatic Offload and control the division of work, use environment variables or support functions. See the *Intel MKL Reference Manual* for detailed descriptions of the support functions.

#### **Important**

Use of Automatic Offload does not require changes in your link line.

#### **Automatic Offload Controls**

The table below lists the environment variables for Automatic Offload and the functions that cause *similar* results. See the *Intel MKL Reference Manual* for detailed descriptions of the functions. To control the division of work between the host CPU and Intel Xeon Phi coprocessors, the environment variables use a fractional measure ranging from zero to one.

Environment Variable	Support Function	Description	Value	
MKL_MIC_ENABLE	mkl_mic_enable	Enables Automatic Offload (AO).	1	
OFFLOAD_DEVICES	None	OFFLOAD_DEVICES is a common setting for Intel MKL and Intel® Compilers. It specifies a list of coprocessors to be used for any offload, including Intel MKL AO.	A comma-separated list of integers, each ranging from 0 to the largest number of an Intel Xeon Phi coprocessor on the system, with the maximum of 31. Values out of this range are ignored. Moreover, if the list contains any non-integer data, the list is ignored completely as if the environment variable were not set at all.	integers, each ranging from 0 to the largest number of an Intel Xeon Phi coprocessor on the system, with the maximum of 31. Values out of this range are ignored. Moreover, if the list
		In particular, this setting may help you to configure the environment for an MPI		
		application to run Intel MKL in the AO mode.	For example, if your system has 4 Intel Xeon Phi coprocessors and	
	all the coprocessors available on the system are used for AO.  MKL used for AO.  MKL used for AO.  MKL used for AO.  A purple is not set, and 3 for an in the system of the system and 3 for an in the system and 3 for an in the system are used for AO.		the value of the list is 1,3, Intel MKL uses only coprocessors 1 and 3 for AO, and Intel MKL support functions and environment variables refer to these coprocessors as coprocessors 0 and 1.	

Environment Variable	Support Function	Description	Value
		You can set this environment variable if AO is enabled by the environment setting or function call.	
		Setting this variable to an empty value is equivalent to completely disabling AO regardless of the value of MKL_MIC_ENABLE.	
		After setting this environment variable, Intel MKL support functions and environment variables refer to the specified coprocessors by their indexes in the list, starting with zero.	
		For more information, refer to the <i>Intel® Compiler User and Reference Guides</i> .	
OFFLOAD_ENABLE_ ORSL	None	Enables the mode in which Intel MKL and Intel Compilers synchronize their accesses to coprocessors. Set this variable if your application uses both Compiler Assisted and AO but does not implement its own synchronization.	1
MKL_HOST_ WORKDIVISION	mkl_mic_set_ workdivision	Specifies the fraction of work for the host CPU to do.	A floating-point number ranging from 0.0 to 1.0. For example, the value could be 0.2 or 0.33. Intel MKL ignores negative values and treats values greater than 1 as 1.0.
MKL_MIC_ WORKDIVISION	mkl_mic_set_ workdivision	Specifies the fraction of work to do on all the Intel Xeon Phi coprocessors on the system.	See MKL_HOST_WORKDIVISION
MKL_MIC_ <number>_ WORKDIVISION</number>	mkl_mic_set_ workdivision	Specifies the fraction of work to do on a specific Intel Xeon Phi coprocessor. Here <number> is an integer ranging from 0 to the largest number of an Intel Xeon Phi coprocessor on the</number>	See MKL_HOST_WORKDIVISION

Environment Variable	Support Function	Description	Value
		system, with the maximum of 31. For example, if the system has two Intel Xeon Phi coprocessors, <number> can be 0 or 1.</number>	
MKL_MIC_ MAX_MEMORY	mkl_mic_set_ max_memory	Specifies the maximum coprocessor memory reserved for AO computations on all of the Intel Xeon Phi coprocessors on the system. Each process that performs AO computations uses additional coprocessor memory specified by the environment variable.	Memory size in Kilobytes (K), megabytes (M), gigabytes (G), or terabytes (T). For example, MKL_MIC_MAX_MEMORY = 4096M limits the coprocessor memory reserved for AO computations to 4096 megabytes or 4 gigabytes. Setting MKL_MIC_MAX_MEMORY = 4G specifies the same amount of memory in gigabytes.
MKL_MIC_ <number>_ MAX_MEMORY</number>	mkl_mic_set_ max_memory	Specifies the maximum coprocessor memory reserved for AO computations on a specific Intel Xeon Phi coprocessor on the system.  Here <number> is an integer ranging from 0 to the largest number of an Intel Xeon Phi coprocessor on the system, with the maximum of 31. For example, if the system has two Intel Xeon Phi coprocessors, <number> can be 0 or 1.</number></number>	Memory size in Kilobytes (K), megabytes (M), gigabytes (G), or terabytes (T). For example,  MKL_MIC_MAX_MEMORY = 4096M limits the coprocessor memory reserved for AO computations to 4096 megabytes or 4 gigabytes.  Setting MKL_MIC_MAX_MEMORY = 4G specifies the same amount of memory in gigabytes.
MKL_MIC_ REGISTER_ MEMORY	mkl_mic_ register_ memory	Enables/disables the mkl_malloc function running in AO mode to register allocated memory.  If AO is disabled, this	Desired behavior of mkl_malloc:  0 - not register allocated memory  1 - register allocated memory
		setting has no effect.	
		Setting this environment variable to 1 may improve performance if the same memory region allocated by mkl_malloc is passed multiple times to Intel MKL functions enabled for AO (for a list of AO enabled functions, see <i>Intel MKL Release Notes</i> ).	

Using Intel® Math Kernel Library on Intel® Xeon Phi™ Coprocessors <b>L</b> U				
Environment Variable	Support Function	Description	Value	
MKL_MIC_RESOURCE_LIMIT	mkl_mic_set_ resource_ limit	Specifies how much of the computational resources of Intel Xeon Phi coprocessors can be used by the calling process. Use this environment variable if you need to share Intel Xeon Phi coprocessor cores automatically across multiple processes that call Intel MKL in the AO mode. For example, this might be useful in MPI applications.  Actual reservation is made during a call to an Intel MKL AO function.	A floating-point number ranging from 0.0 to 1.0.  Special values:  • 0.0 - do not share Intel Xeon Phi coprocessors across multiple processes. Default.  • MKL_MPI_PPN - enable special fully automated mode for MPI applications. In this mode Intel MKL tries to read the number of MPI processes per node (ppn) from the environment variables passed to the process by MPI. If this attempt is successful, Intel MKL sets the actual resource limit to 1.0/ppn.  NOTE  For Intel® MPI Library, Open MPI, and IBM Platform MPI, Intel MKL automatically detects ppn. For other MPI implementations, use the MKL_MPI_PPN environment variable to set ppn.  Examples:  1. Two 61-core Intel Xeon Phi coprocessors are available on the system. Three processes simultaneously set MKL_MIC_RESOURCE_LIMIT= 0.34 and then call dpotrf in AO mode. As a result, one process receives 40 cores from coprocessor 1, another process receives 40 cores from coprocessor 2, and the remaining process receives 40 cores from coprocessor 3 are available on the system. The user makes these settings  MKL_MIC_1_WORKDIVISION= 0.0  MKL_MIC_1_WORKDIVISION= 0.0  MKL_MIC_PPN=4  MKL_MIC_RESOURCE_LIMIT=	
			MKL_MPI_PPN	

Environment Variable	Support Function	Description	Value
			and then runs an MPI application with Intel MKL AO calls. As a result, each MPI process receives 14 cores on Intel Xeon Phi coprocessor 0 because the user excluded coprocessor 1 from computations by setting zero workdivision for it.
MIC_OMP_ NUM_THREADS	mkl_mic_set_ device_num_ threads	Specifies the maximum number of OpenMP* threads to use for AO computations on all the Intel Xeon Phi coprocessors on the system.	An integer greater than 0.
MIC_ <number>_ OMP_NUM_ THREADS</number>	mkl_mic_set_ device_num_ threads	Specifies the maximum number of OpenMP threads to use for AO computations on a specific Intel Xeon Phi coprocessor on the system.	An integer greater than 0.
		Here <number> is an integer ranging from 0 to the largest number of an Intel Xeon Phi coprocessor on the system, with the maximum of 31. For example, if the system has two Intel Xeon Phi coprocessors, <number> can be 0 or 1.</number></number>	
OFFLOAD_ REPORT	mkl_mic_set_ offload_report	OFFLOAD_REPORT is a common setting for Intel MKL and Intel® Compilers. It specifies the profiling report level for any offload, including Intel MKL AO.  For more information, refer to the Intel® Compiler User and Reference Guides.  Note that the mkl_mic_set_offload _report function enables you to turn profile reporting on/off at run time but does not change the reporting level.	An integer ranging from 0 to 2:  0 - No reporting, default.  1 - The report includes:  • The name of the function called in the AO mode.  • Effective work division. The value of -1 indicates that the hint, that is, the work division specified by the mkl_mic_set_workdivison function or the appropriate MKL_*_WORKDIVISION environment variable was ignored in this function call.  • The time spent on the host CPU during the call.  • The time spent on each available Intel Xeon Phi coprocessor during the call.

Environment Variable	Support Function	Description	Value
			2 - In addition to the above information, the report includes:
			<ul> <li>The amounts of data transferred to and from each available coprocessor during the call.</li> </ul>
LD_LIBRARY_PATH	None	Specifies the search path for host-side dynamic libraries.	Must contain the path to host- side Intel MIC Platform Software Stack libraries used by Intel MKL. The default path is /opt/ intel/mic/coi/host-linux- release/lib.
MIC_LD_LIBRARY_	None	Specifies the search path	Must contain:
PATH		for coprocessor-side dynamic libraries.	<ul> <li>The path to coprocessor-side Intel MIC Platform Software Stack libraries used by Intel MKL. The default path is /opt/intel/mic/coi/device-linux-release/lib.</li> <li>The path to Intel MKL coprocessor-side libraries. The default path is <mkl directory="">/lib/mic.</mkl></li> </ul>
MKL_MIC_ THRESHOLDS_ ?GEMM	None	Specifies matrix size thresholds for ?GEMM computations in the AO mode.	Three comma-separated integers: $M$ , $N$ , $K$ . If this environment variable is set, any call to a ?GEMM function with problem sizes $M_1$ , $N_1$ , and $K_1$ tries to offload computations only if $M_1 > M$ , $N_1 > N$ , and $K_1 > K$ . This setting is only a hint, and Intel MKL may decide to not offload computations depending on the problem size and environment.  Example: To set the thresholds to $M = 2000$ , $N = 1000$ , $K = 500$ for DGEMM, set
			MKL_MIC_THRESHOLDS_DGEMM=20 00,1000,500.

- Settings specified by the functions take precedence over the settings specified by the respective environment variables.
- Intel MKL interprets the values of MKL\_HOST\_WORKDIVISION, MKL\_MIC\_WORKDIVISION, and MKL\_MIC\_<number>\_WORKDIVISION as guidance toward dividing work between coprocessors, but the library may choose a different work division if necessary.
- For LAPACK routines, setting the fraction of work to any value other than 0.0 enables the specified processor for AO mode. However Intel MKL LAPACK does not use the value specified to divide the workload. For example, setting the fraction to 0.5 has the same effect as setting the fraction to 1.0.

#### See Also

Setting Environment Variables for Automatic Offload

Intel® Software Documentation Library for Intel® Compiler User and Reference Guides

#### **Setting Environment Variables for Automatic Offload**

#### **Important**

To use Automatic Offload:

- If you completed the Scripts to Set Environment Variables Setting Environment Variables step of
  the Getting Started process, MKL\_MIC\_ENABLE is the only environment variable that you need to
  set.
- Otherwise, you must also set the LD\_LIBRARY\_PATH and MIC\_LD\_LIBRARY\_PATH environment variables.

To set the environment variables for Automatic Offload mode, described in Automatic Offload Controls, use the appropriate commands in your command shell:

• For the bash shell, set the appropriate environment variable(s) as follows:

```
export MKL_MIC_ENABLE=1
export OFFLOAD DEVICES=<list>
For example: export OFFLOAD DEVICES=1,3
export OFFLOAD ENABLE ORSL=1
export MKL HOST WORKDIVISION=<value>
For example: export MKL HOST WORKDIVISION=0.2
export MKL MIC WORKDIVISION=<value>
export MKL MIC <number> WORKDIVISION=<value>
For example: export MKL MIC 2 WORKDIVISION=0.33
export MKL MIC MAX MEMORY=<value>
export MKL MIC <number> MAX MEMORY=<value>
For example: export MKL MIC 0 MAX MEMORY=2G
export MKL MIC REGISTER MEMORY=1
export MKL MIC RESOURCE LIMIT=<value>
For example: export MKL MIC RESOURCE LIMIT=0.34
export MIC OMP NUM THREADS=<value>
export MIC <number> OMP NUM THREADS=<value>
For example: export MIC 0 OMP NUM THREADS=240
export OFFLOAD REPORT=<level>
For example: export OFFLOAD REPORT=2
export LD LIBRARY PATH="/opt/intel/mic/coi/host-linux-release/lib:$
{LD LIBRARY PATH}"
export MIC_LD_LIBRARY_PATH="/opt/intel/mic/coi/device-linux-release/lib:$
{MKLROOT}/lib/mic:${MIC LD LIBRARY PATH}"
export MKL MIC THRESHOLDS ?GEMM="<N>, <M>, <K>"
For example: export MKL MIC THRESHOLDS ?GEMM="2000,1000,500"
```

• For a C shell (csh or tcsh), set the appropriate environment variable(s) as follows:

```
setenv MKL MIC ENABLE 1
setenv OFFLOAD DEVICES <list>
For example: setenv OFFLOAD DEVICES 1,3
setenv OFFLOAD ENABLE ORSL 1
setenv MKL HOST WORKDIVISION <value>
For example: setenv MKL HOST WORKDIVISION 0.2
setenv MKL MIC WORKDIVISION <value>
setenv MKL MIC <number> WORKDIVISION<value>
For example: setenv MKL_MIC_2_WORKDIVISION 0.33
setenv MKL MIC MAX MEMORY <value>
setenv MKL MIC <number> MAX MEMORY <value>
For example: setenv MKL MIC 0 MAX MEMORY 2G
setenv MKL MIC REGISTER MEMORY 1
setenv MKL MIC RESOURCE LIMIT <value>
For example: setenv MKL MIC RESOURCE LIMIT 0.34
setenv MIC OMP NUM THREADS <value>
setenv MIC <number> OMP NUM THREADS <value>
For example: setenv MIC 0 OMP NUM THREADS 240
setenv OFFLOAD REPORT < level>
For example: setenv OFFLOAD REPORT 2
setenv LD LIBRARY PATH "/opt/intel/mic/coi/host-linux-release/lib:$
{LD LIBRARY PATH}"
setenv MIC LD LIBRARY PATH "/opt/intel/mic/coi/device-linux-release/lib:$
{MKLROOT}/lib/mic:${MIC LD LIBRARY PATH}"
setenv MKL MIC THRESHOLDS ?GEMM "<N>, <M>, <K>"
For example: setenv MKL MIC THRESHOLDS ?GEMM "2000,1000,500"
```

#### See Also

Automatic Offload Controls

Detailed Directory Structure of the lib/mic Directory

## **Compiler Assisted Offload**

Compiler Assisted Offload is a method to offload computations to Intel Xeon Phi coprocessors that uses the Intel® compiler and its offload pragma support to manage the functions and data offloaded. See *Intel® Compiler User and Reference Guides* for more details.

#### Important

The Intel compilers support Intel MIC Architecture starting with version 13.

#### See Also

**Automatic Offload** 

Running Intel MKL on an Intel Xeon Phi Coprocessor in Native Mode

#### **Examples of Compiler Assisted Offload**

The following are examples of Compiler Assisted Offload. Please see *Intel® Compiler User and Reference Guide* for more details.

These examples show how to call Intel MKL from offload regions that are executed on coprocessors based on Intel MIC Architecture and how to reuse data that already exists in the memory of the coprocessor and thus minimize data transfer.

#### **Fortran**

```
Upload A and B to the card, and do not deallocate them after the
C
     pragma. C is uploaded and downloaded back, but the allocated memory
     is retained
     !DEC$ ATTRIBUTES OFFLOAD : MIC :: SGEMM
      !DEC$ OFFLOAD TARGET ( MIC:0 ) IN ( N ), &
      !DEC$ IN( A: LENGTH( N * N ) ALLOC IF(.TRUE.) FREE IF(.FALSE.)), &
      !DEC$ IN( B: LENGTH( N * N ) ALLOC IF(.TRUE.) FREE IF(.FALSE.)), &
      !DEC$ INOUT( C: LENGTH( N * N ) ALLOC IF(.TRUE.) FREE IF(.FALSE.))
     CALL SGEMM( 'N', 'N', N, N, N, 1.0, A, N, B, N, 1.0, C, N)
С
     Change C here
     Reuse A and B on the card, and upload the new C. Free all the
С
C
     memory on the card
     !DEC$ ATTRIBUTES OFFLOAD : MIC :: SGEMM
      !DEC$ OFFLOAD TARGET( MIC:0 ) IN( N ), &
      !DEC$ NOCOPY( A: LENGTH( N * N ) ALLOC IF(.FALSE.) FREE IF(.TRUE.)), &
      !DEC$ NOCOPY( B: LENGTH( N * N ) ALLOC_IF(.FALSE.) FREE IF(.TRUE.)), &
      !DEC$ INOUT( C: LENGTH( N * N ) ALLOC IF(.FALSE.) FREE IF(.TRUE.))
     CALL SGEMM( 'N', 'N', N, N, N, 1.0, A, N, B, N, -1.0, C, N)
```

#### C

```
/* Upload A and B to the card, and do not deallocate them after the pragma.
    * C is uploaded and downloaded back, but the allocated memory is retained. */
#pragma offload target(mic:0) \
   in(A: length(matrix elements) alloc if(1) free if(0)) \
   in (B: length (matrix elements) alloc if (1) free if (0)) \
   in(transa, transb, N, alpha, beta) \
   inout(C:length(matrix elements) alloc if(1) free if(0))
   {
        sgemm(&transa, &transb, &N, &N, &N, &alpha, A, &N, B, &N,
               &beta, C, &N);
   /* Change C here */
   /* Reuse A and B on the card, and upload the new C. Free all the memory on
    * the card. */
#pragma offload target(mic:0) \
   nocopy(A: length(matrix elements) alloc if(0) free if(1)) \
   nocopy(B: length(matrix elements) alloc if(0) free if(1)) \
   in(transa, transb, N, alpha, beta) \
   inout(C:length(matrix elements) alloc if(0) free if(1))
       sgemm(&transa, &transb, &N, &N, &Alpha, A, &N, B, &N,
                &beta, C, &N);
```

#### See Also

Intel® Software Documentation Library for Intel® Compiler User and Reference Guides

#### **Linking for Compiler Assisted Offload**

Intel MKL provides both static and dynamic libraries for coprocessors based on Intel MIC Architecture, but the Single Dynamic Library is unavailable for the coprocessors.

See Selecting Libraries to Link with for libraries to list on your link line in the simplest case.

See Detailed Directory Structure for a full list of libraries provided in the <mk1 directory>/lib/mic directory.

You can link either static or dynamic host-side libraries and either static or dynamic coprocessor-side libraries independently.

To run applications linked dynamically with the host-side and coprocessor-side libraries, perform the Scripts to Set Environment Variables Setting Environment Variables step of the Getting Started process. In addition to other environment variables, it sets:

- LD LIBRARY PATH to contain <mkl directory>/lib/intel64
- MIC LD LIBRARY PATH to contain <mkl directory>/lib/mic

To make Intel MKL functions available on the coprocessor side, provide the -offload-attribute-target=mic option on your link line.

#### **Important**

Because Intel MKL provides both LP64 and ILP64 interfaces, ensure that the host and coprocessor-side executables use the same interface or cast all 64-bit integers to 32-bit integers (or vice-versa) before calling coprocessor-side functions in your application.

The following examples illustrate linking for compiler assisted offload to Intel Xeon Phi coprocessors.

The examples use a .f (Fortran) source file and Intel® Fortran Compiler. C/C++ users should instead specify a .cpp (C++) or .c (C) file and replace ifort with icc.

If you successfully completed the Scripts to Set Environment Variables Setting Environment Variables step of the Getting Started process, you can omit the -I\$MKLROOT/include parameter in these examples:

 Static linking of myprog.f, host-side and coprocessor-side libraries for parallel Intel MKL using LP64 interface:

```
ifort myprog.f -I$MKLROOT/include -offload-attribute-target=mic
-W1,--start-group $MKLROOT/lib/intel64/libmkl_intel_lp64.a
$MKLROOT/lib/intel64/libmkl_intel_thread.a
$MKLROOT/lib/intel64/libmkl_core.a -W1,--end-group
-openmp -lpthread -lm
-offload-option,mic,compiler,"-W1,--start-group $MKLROOT/lib/mic/libmkl_intel_lp64.a
$MKLROOT/lib/mic/libmkl_intel_thread.a
$MKLROOT/lib/mic/libmkl_core.a -W1,--end-group"
or
```

ifort myprog.f -offload-attribute-target=mic -static-intel -mkl

Dynamic linking of myprog.f, host-side and coprocessor-side libraries for parallel Intel MKL using LP64 interface:

```
ifort myprog.f -I$MKLROOT/include -offload-attribute-target=mic
-L$MKLROOT/lib/intel64
-lmkl_intel_lp64 -lmkl_intel_thread
-lmkl_core -openmp -lpthread -lm
-offload-option,mic,compiler,"-L$MKLROOT/lib/mic
```

```
-lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core"

or

ifort myprog.f -offload-attribute-target=mic -mkl
```

• Static linking of myprog.f, host-side and coprocessor-side libraries for parallel Intel MKL using ILP64 interface:

```
ifort myprog.f -I$MKLROOT/include -offload-attribute-target=mic
-Wl,--start-group $MKLROOT/lib/intel64/libmkl_intel_ilp64.a
$MKLROOT/lib/intel64/libmkl_intel_thread.a
$MKLROOT/lib/intel64/libmkl_core.a -Wl,--end-group
-openmp -lpthread -lm
-offload-option,mic,compiler,"-Wl,--start-group
$MKLROOT/lib/mic/libmkl_intel_ilp64.a $MKLROOT/lib/mic/libmkl_intel_thread.a
$MKLROOT/lib/mic/libmkl core.a -Wl,--end-group"
```

Dynamic linking of myprog.f, host-side and coprocessor-side libraries for parallel Intel MKL using ILP64 interface:

```
ifort myprog.f -I$MKLROOT/include -offload-attribute-target=mic
-L$MKLROOT/lib/intel64
-lmkl_intel_ilp64 -lmkl_intel_thread
-lmkl_core -openmp -lpthread -lm
-offload-option,mic,compiler,"-L$MKLROOT/lib/mic -lmkl_intel_ilp64
-lmkl_intel_thread -lmkl_core"
```

• Static linking of myprog.f, host-side and coprocessor-side libraries for sequential version of Intel MKL using LP64 interface:

```
ifort myprog.f -I$MKLROOT/include -offload-attribute-target=mic
-Wl,--start-group $MKLROOT/lib/intel64/libmkl_intel_lp64.a
$MKLROOT/lib/intel64/libmkl_sequential.a
$MKLROOT/lib/intel64/libmkl_core.a -Wl,--end-group -lm
-offload-option,mic,compiler,"-Wl,--start-group $MKLROOT/lib/mic/libmkl_intel_lp64.a
$MKLROOT/lib/mic/libmkl sequential.a $MKLROOT/lib/mic/libmkl_core.a -Wl,--end-group"
```

Dynamic linking of myprog.f, host-side and coprocessor-side libraries for sequential version of Intel MKL using LP64 interface:

```
ifort myprog.f -I$MKLROOT/include -offload-attribute-target=mic
-L$MKLROOT/lib/intel64
-lmkl_intel_lp64 -lmkl_sequential -lmkl_core -lm
-offload-option,mic,compiler,"-L$MKLROOT/lib/mic
-lmkl_intel_lp64 -lmkl_sequential -lmkl_core"
```

#### See Also

Linking Your Application with the Intel® Math Kernel Library Linking with System Libraries Using the Link-line Advisor

# Using Automatic Offload and Compiler Assisted Offload in One Application

You can use Automatic Offload and Compiler Assisted Offload in the same application. However, to avoid oversubscription of computational resources of the coprocessors, synchronize Intel MKL and Intel Compiler accesses to coprocessors using either of the these techniques:

- In your code, manually synchronize #pragma offload regions and calls of Intel MKL functions that support Automatic Offload.
- Set the OFFLOAD ENABLE ORSL environment variable to 1 to enable automatic synchronization.

#### See Also

Automatic Offload Compiler Assisted Offload

# Running Intel MKL on an Intel Xeon Phi Coprocessor in Native Mode

Some applications can benefit from running on Intel Xeon Phi coprocessors in native mode. In this mode, the application runs directly on a coprocessor and its Linux\* operating system without being offloaded from a host system. To run on Intel MIC Architecture in the native mode, an application requires minimal changes to the source code.

Because in the native mode the code runs exclusively on a coprocessor, binaries built for native runs contain only the code to be run on a coprocessor. Intel compilers provide a specialized option to support building applications to be run in the native mode.

To build an application that calls Intel MKL and natively run it on a coprocessor, you need to perform these high-level steps:

- 1. On the host system, compile and build the application using the -mmic option.
- 2. Transfer the executable and all the dynamic libraries it requires to the coprocessor:
  - The Intel MKL libraries in the <mkl directory>/lib/mic directory.
  - libiomp5.so in the cparent product directory>/compiler/lib/mic directory.
- **3.** Use the Secure Shell (SSH) or Telnet protocol to execute on the coprocessor and add the paths to the dynamic libraries transferred to the coprocessor in step 2 and to the value of the LD\_LIBRARY\_PATH environment variable.
- **4.** Set OpenMP\* thread affinity and the OMP NUM THREADS environment variable.
- **5.** Execute just as you would on a standard Linux\* system.

For more information, see *Intel® Compiler User and Reference Guides*, available in the Intel Software Documentation Library.

#### See Also

Detailed Directory Structure of the lib/mic Directory Improving Performance on Intel Xeon Phi Coprocessors Intel Software Documentation Library

#### Using ScaLAPACK and Cluster FFT on Intel Xeon Phi Coprocessors

Intel MKL ScaLAPACK and Cluster FFT support only Intel MPI Library on Intel Xeon Phi coprocessors.

The Intel MPI library can treat each Intel Xeon Phi coprocessor as a regular node in a cluster of processors based on Intel 64 architecture and Intel Xeon Phi coprocessors and enables a straightforward way to run an MPI application on clusters that contain both processors and coprocessors as compute nodes.

The documentation for the Intel MPI library recommends the following steps to run an MPI application on the specific Intel Xeon Phi coprocessor and the host node if the nodes are properly specified on the cluster and the network protocols and environment are properly set up:

- **1.** Build the application for the Intel 64 architecture.
- 2. Build the application for the Intel MIC Architecture.
- **3.** Launch the application from the host computer.

#### **NOTE**

If you need to run the application on the coprocessor only, you can alternatively launch it from the coprocessor.

For more details, check the Intel MPI Library documentation, available in the Intel Software Documentation Library.

To run a dynamically linked application natively, perform the Scripts to Set Environment Variables Setting Environment Variables step of the Getting Started process. In addition to other environment variables, it sets:

- LD LIBRARY PATH to contain <mkl directory>/lib/intel64
- MIC LD LIBRARY PATH to contain <mkl directory>/lib/mic

When building your application that uses Intel MKL ScaLAPACK or Cluster FFT, follow the linking guidelines in the Linking with Intel MKL Cluster Software, but be aware that only Intel compiler and Intel MPI are supported, and only Intel threading layer is provided for Intel MKL.

You can find a full list of Intel MKL libraries for Intel MIC architecture in Detailed Directory Structure. Be aware that coprocessors run a Unix\* operating system.

#### **TIP**

Use the Using the Link-line Advisor to quickly choose the appropriate set of libraries and linker options.

#### See Also

Linking Your Application with the Intel® Math Kernel Library Intel Software Documentation Library

## Examples of Linking with ScaLAPACK and Cluster FFT for Intel(R) Many Integrated Core Architecture

#### **Examples of Linking a C Application**

These examples illustrate linking of an application for Intel MIC Architecture under the following conditions:

- The application uses Intel MKL ScaLAPACK or Cluster FFT.
- Main module is in C.
- You are using the Intel® C++ Compiler.
- Your programming interface is LP64.
- <path to mpi binaries> is the path to Intel MPI binaries for Intel MIC Architecture.
- \$MKLPATH is a user-defined variable that contains \$MKLROOT/lib/mic

See the *Intel MKL Release Notes* for details of system requirements.

To link with ScaLAPACK for native runs on a cluster of systems based on the Intel MIC architecture, use the following link line:

```
<path to mpi binaries>/mpicc -mmic <files to link> \
-L$MKLPATH \
-lmkl_scalapack_lp64 \
-lmkl_blacs_intelmpi_lp64 \
-lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core \
-liomp5 -lpthread -lm
```

To link with Cluster FFT for native runs on a cluster of systems based on the Intel MIC architecture, use the following link line:

```
<path to mpi binaries>/mpicc -mmic <files to link> \
-Wl,--start-group \
```

```
$MKLPATH/libmkl_cdft_core.a \
$MKLPATH/libmkl_blacs_intelmpi_lp64.a \
$MKLPATH/libmkl_intel_lp64.a \
$MKLPATH/libmkl_intel_thread.a \
$MKLPATH/libmkl_core.a \
-Wl,--end-group \
-liomp5 -lpthread -lm
```

#### See Also

Working with the Intel® Math Kernel Library Cluster Software Using the Link-line Advisor

#### **Examples of Linking a Fortran Application**

These examples illustrate linking of an application for Intel MIC Architecture under the following conditions:

- The application uses Intel MKL ScaLAPACK or Cluster FFT.
- Main module is in Fortran.
- You are using the Intel® Fortran Compiler.
- Your programming interface is LP64.
- <path to mpi binaries> is the path to Intel MPI binaries for Intel MIC Architecture.
- \$MKLPATH is a user-defined variable that contains \$MKLROOT/lib/mic.

See the Intel MKL Release Notes for details of system requirements.

To link with ScaLAPACK for native runs on a cluster of systems based on the Intel MIC architecture, use the following link line:

```
<path to mpi binaries>/mpiifort -mmic <files to link> \
-L$MKLPATH \
-lmkl_scalapack_lp64 \
-lmkl_blacs_intelmpi_lp64 \
-lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core \
-liomp5 -lpthread -lm
```

To link with Cluster FFT for native runs on a cluster of systems based on the Intel MIC architecture, use the following link line:

```
<path to mpi binaries>/mpiifort -mmic <files to link> \
-Wl,--start-group \
$MKLPATH/libmkl_cdft_core.a \
$MKLPATH/libmkl_blacs_intelmpi_lp64.a \
$MKLPATH/libmkl_intel_lp64.a \
$MKLPATH/libmkl_intel_thread.a \
$MKLPATH/libmkl_core.a \
-Wl,--end-group \
-liomp5 -lpthread -lm
```

#### See Also

Working with the Intel® Math Kernel Library Cluster Software Using the Link-line Advisor

## Threading Behavior of Intel MKL on Intel MIC Architecture

To avoid performance drops caused by oversubscribing Intel Xeon Phi coprocessors, Intel MKL limits the number of OpenMP threads it uses to parallelize computations:

• For native runs on coprocessors, Intel MKL uses 4\*Number-of-Phi-Cores threads by default and scales down the number of threads back to this value if you request more threads and MKL DYNAMIC is true.

- For runs that offload computations, Intel MKL uses 4\*(Number-of-Phi-Cores-1) threads by default and scales down the number of threads back to this value if you request more threads and MKL\_DYNAMIC is true
- If you request fewer threads than the default number, Intel MKL will use the requested number.

Here Number-of-Phi-Cores is the number of cores per coprocessor.

#### See Also

MKL\_DYNAMIC Automatic Offload Controls Techniques to Set the Number of Threads

## **Improving Performance on Intel Xeon Phi Coprocessors**

To improve performance of Intel MKL on Intel Xeon Phi coprocessors, use the following tips, which are specific to Intel MIC Architecture. General performance improvement recommendations provided in Coding Techniques also apply.

#### **Memory Allocation**

Performance of many Intel MKL routines improves when input and output data reside in memory allocated with 2MB pages because this enables you to address more memory with less pages and thus reduce the overhead of translating between virtual and physical memory addresses compared to memory allocated with the default page size of 4K. For more information, refer to Intel® 64 and IA-32 Architectures Optimization Reference Manual and Intel® 64 and IA-32 Architectures Software Developer's Manual (connect to http://www.intel.com/ and enter the name of each document in the **Find Content** text box).

To allocate memory with 2MB pages, you can use the mmap system call with the MAP\_HUGETLB flag. You can alternatively use the libhugetlbfs library. See the white paper at http://software.intel.com/sites/default/files/Large\_pages\_mic\_0.pdf for more information.

To enable allocation of memory with 2MB pages for data of size exceeding 2MB and transferred with offload pragmas, set the MIC\_USE\_2MB\_BUFFERS environment variable to an appropriate value. This setting ensures that all pointer-based variables whose run-time length exceeds this value will be allocated in 2MB pages. For example, with MIC\_USE\_2MB\_BUFFERS=64K, variables with run-time length exceeding 64 KB will be allocated in 2MB pages. For more details, see *Intel® Compiler User and Reference Guides*, available in the Intel Software Documentation Library.

Specifying the maximum amount of memory on a coprocessor that can be used for Automatic Offload computations typically enhances the performance by enabling Intel MKL to reserve and keep the memory on the coprocessor during Automatic Offload computations. You can specify the maximum memory by setting the MKL MIC MAX MEMORY environment variable to a value such as 2 GB.

#### **Data Alignment and Leading Dimensions**

To improve performance of Intel MKL FFT functions, follow these recommendations:

- Align the first element of the input data on 64-byte boundaries
- For two- or higher-dimensional single-precision transforms, use leading dimensions (strides) divisible by 8 but not divisible by 16
- For two- or higher-dimensional double-precision transforms, use leading dimensions divisible by 4 but not divisible by 8

For other Intel MKL function domains, use general recommendations for data alignment.

#### **OpenMP and Threading Settings**

To improve performance of Intel MKL routines, use the following OpenMP and threading settings:

• For all function domains:

Set KMP AFFINITY=balanced

• For FFT:

Also use a number of threads depending on the total size of the input and output data for the transform:

- A power of two, if the total size is less than Number-of-Phi-Cores/2 MB
- 4\*Number-of-Phi-Cores, if the total size is not less than Number-of-Phi-Cores/2 MB

Here Number-of-Phi-Cores is the number of Intel Xeon Phi coprocessors on the system.

For more information, see the Knowledge Base article at http://software.intel.com/en-us/articles/performance-tips-of-using-intel-mkl-on-intel-xeon-phi-coprocessor.

### See Also

Examples of Compiler Assisted Offload Intel Software Documentation Library

## Managing Behavior of the Intel(R) Math Kernel Library with Environment Variables



### **Managing Behavior of Function Domains**

### Setting the Default Mode of the Vector Mathematical Library with an Environment Variable

Intel® Math Kernel Library (Intel® MKL) enables overriding the default setting of the Vector Mathematical Library (VML) global mode using the MKL VML MODE environment variable.

Because the mode is set or can be changed in different ways, their precedence determines the actual mode used. The settings and function calls that set or change the VML mode are listed below, with the precedence growing from lowest to highest:

- 1. The default setting
- 2. The MKL VML MODE environment variable
- **3.** A call vmlSetMode function
- 4. A call to any VML function other than a service function

For more details, see the Vector Mathematical Functions section in the *Intel MKL Reference Manual* and the description of the <code>vmlSetMode</code> function in particular.

To set the MKL VML MODE environment variable, use the following command in your command shell:

• For the bash shell:

```
export MKL_VML_MODE=<mode-string>For a C shell (csh or tcsh):setenv MKL VML MODE <mode-string>
```

In these commands, <mode-string> controls error handling behavior and computation accuracy, consists of one or several comma-separated values of the mode parameter listed in the table below, and meets these requirements:

- Not more than one accuracy control value is permitted
- Any combination of error control values except VML ERRMODE DEFAULT is permitted
- No denormalized numbers control values are permitted

### Values of the mode Parameter

Value of <i>mode</i>	Description			
Accuracy Control				
VML_HA	high accuracy versions of VML functions			
VML_LA	low accuracy versions of VML functions			
VML EP	enhanced performance accuracy versions of VML functions			
Denormalized Numbers Handling Control				
VML_FTZDAZ_ON	Faster processing of denormalized inputs is enabled.			
VML_FTZDAZ_OFF	Faster processing of denormalized inputs is disabled.			
Error Mode Control				

Value of <i>mode</i>	Description
VML_ERRMODE_IGNORE	No action is set for computation errors.
VML_ERRMODE_STDERR	On error, the error text information is written to stderr.
VML_ERRMODE_EXCEPT	On error, an exception is raised.
VML_ERRMODE_CALLBACK	On error, an additional error handler function is called.
VML_ERRMODE_DEFAULT	On error, an exception is raised and an additional error handler function is called.

These commands provide an example of valid settings for the  $\texttt{MKL\_VML\_MODE}$  environment variable in your command shell:

- For the bash shell:
  - export MKL VML MODE=VML LA, VML ERRMODE ERRNO, VML ERRMODE STDERR
- For a C shell (csh or tcsh):

setenv MKL VML MODE VML LA, VML ERRMODE ERRNO, VML ERRMODE STDERR

### **NOTE**

VML ignores the  $\texttt{MKL\_VML\_MODE}$  environment variable in the case of incorrect or misspelled settings of mode.

### Managing Performance of the Cluster Fourier Transform Functions

Performance of Intel MKL Cluster FFT (CFFT) in different applications mainly depends on the cluster configuration, performance of message-passing interface (MPI) communications, and configuration of the run. Note that MPI communications usually take approximately 70% of the overall CFFT compute time. For more flexibility of control over time-consuming aspects of CFFT algorithms, Intel MKL provides the MKL\_CDFT environment variable to set special values that affect CFFT performance. To improve performance of your application that intensively calls CFFT, you can use the environment variable to set optimal values for you cluster, application, MPI, and so on.

The MKL CDFT environment variable has the following syntax, explained in the table below:

MKL CDFT=option1[=value1], option2[=value2], ..., optionN[=valueN]

### **Important**

While this table explains the settings that usually improve performance under certain conditions, the actual performance highly depends on the configuration of your cluster. Therefore, experiment with the listed values to speed up your computations.

Option	Possible Values	Description
alltoallv	0 (default)	Configures CFFT to use the standard MPI_Alltoallv function to perform global transpositions.
	1	Configures CFFT to use a series of calls to MPI_Isend and MPI_Irecv instead of the MPI_Alltoallv function.
	4	Configures CFFT to merge global transposition with data movements in the local memory. CFFT performs global transpositions by calling MPI_Isend and MPI_Irecv in this case.
		Use this value in a hybrid case (MPI $\pm$ OpenMP), especially when the number of processes per node equals one.
wo_omatcopy	0	Configures CFFT to perform local FFT and local transpositions separately.

Option	Possible Values	Description
		CFFT usually performs faster with this value than with wo_omatcopy = 1 if the configuration parameter DFTI_TRANSPOSE has the value of DFTI_ALLOW. See the <i>Intel MKL Reference Manual</i> for details.
	1	Configures CFFT to merge local FFT calls with local transpositions.
		<pre>CFFT usually performs faster with this value than with wo_omatcopy = 0 if DFTI_TRANSPOSE has the value of DFTI_NONE.</pre>
	-1 (default)	Enables CFFT to decide which of the two above values to use depending on the value of DFTI_TRANSPOSE.
enable_soi	Not applicable	A flag that enables low-communication Segment Of Interest FFT (SOI FFT) algorithm for one-dimensional complex-to-complex CFFT, which requires fewer MPI communications than the standard nine-step (or six-step) algorithm.
		<b>CAUTION</b> While using fewer MPI communications, the SOI FFT algorithm incurs a minor loss of precision (about one decimal digit).

The following example illustrates usage of the environment variable assuming the bash shell:

export MKL\_CDFT=wo\_omatcopy=1,alltoallv=4,enable\_soi
mpirun -ppn 2 -n 16 ./mkl\_cdft app

### **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

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### **Enabling Intel® MKL to Dispatch New Intel® Architectures**

Intel® MKL provides support for Intel® Advanced Vector Extensions 512 (Intel® AVX-512) instruction-set architecture (ISA) ahead of hardware availability, but the CPU does not automatically dispatch this ISA by default. To turn on automatic CPU-based dispatching for a hardware or in a simulated environment that supports this ISA, follow the instructions below that depend on the processor family of your system:

### Systems Based on Intel® Xeon® Processors

Do either of the following:

Call

mkl enable instructions (MKL ENABLE AVX512)

- Set the environment variable:
  - For the bash shell:

```
export MKL ENABLE INSTRUCTIONS="AVX512"
```

• For a C shell (csh or tcsh):

```
setenv MKL ENABLE INSTRUCTIONS "AVX512"
```

### Systems Based on Intel® Xeon Phi™ Processors and Coprocessors

Do either of the following:

Call

```
mkl enable instructions (MKL ENABLE AVX512 MIC)
```

- Set the environment variable:
  - For the bash shell:

```
export MKL ENABLE INSTRUCTIONS="AVX512 MIC"
```

• For a C shell (csh or tcsh):

```
setenv MKL ENABLE INSTRUCTIONS "AVX512 MIC"
```

For more details of the mkl\_enable\_instructions function, see the Intel MKL Reference Manual.

### **NOTE**

Settings specified by the  $mkl\_enable\_instructions$  function take precedence over the settings specified by the  $mkl\_enable\_instructions$  environment variable.

### **Optimization Notice**

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Notice revision #20110804

# Configuring Your Integrated Development Environment to Link with Intel(R) Math Kernel Library



### Configuring the Eclipse\* IDE CDT to Link with Intel MKL

This section explains how to configure the Eclipse\* Integrated Development Environment (IDE) C/C++ Development Tools (CDT) to link with Intel® Math Kernel Library (Intel® MKL).

### TIP

After configuring your CDT, you can benefit from the Eclipse-provided <code>code assist</code> feature. See Code/Context Assist description in the CDT Help for details.

To configure your Eclipse IDE CDT to link with Intel MKL, you need to perform the steps explained below. The specific instructions for performing these steps depend on your version of the CDT and on the tool-chain/compiler integration. Refer to the CDT Help for more details.

To configure your Eclipse IDE CDT, do the following:

- 1. Open **Project Properties** for your project.
- **2.** Add the Intel MKL include path, that is, <mkl directory>/include, to the project's include paths.
- **3.** Add the Intel MKL library path for the target architecture to the project's library paths. For example, for the Intel® 64 architecture, add <mkl directory>/lib/intel64.
- **4.** Specify the names of the Intel MKL libraries to link with your application. For example, you may need the following libraries: mkl\_intel\_lp64, mkl\_intel\_thread, mkl\_core, and iomp5.

### **NOTE**

Because compilers typically require library names rather than file names, omit the "lib" prefix and "a" or "so" extension.

### See Also

Selecting Libraries to Link with Linking in Detail

### LINPACK and MP LINPACK Benchmarks



### **Optimization Notice**

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### Intel® Optimized LINPACK Benchmark for Linux\* OS

Intel® Optimized LINPACK Benchmark is a generalization of the LINPACK 1000 benchmark. It solves a dense (real\*8) system of linear equations (Ax=b), measures the amount of time it takes to factor and solve the system, converts that time into a performance rate, and tests the results for accuracy. The generalization is in the number of equations (N) it can solve, which is not limited to 1000. It uses partial pivoting to assure the accuracy of the results.

Do not use this benchmark to report LINPACK 100 performance because that is a compiled-code only benchmark. This is a shared-memory (SMP) implementation which runs on a single platform. Do not confuse this benchmark with:

- MP LINPACK, which is a distributed memory version of the same benchmark.
- LINPACK, the library, which has been expanded upon by the LAPACK library.

Intel provides optimized versions of the LINPACK benchmarks to help you obtain high LINPACK benchmark results on your genuine Intel processor systems more easily than with the High Performance Linpack (HPL) benchmark.

Additional information on this software, as well as on other Intel® software performance products, is available at http://www.intel.com/software/products/.

### **Contents of the Intel® Optimized LINPACK Benchmark**

The Intel Optimized LINPACK Benchmark for Linux\* OS contains the following files, located in the ./ benchmarks/linpack/ subdirectory of the Intel® Math Kernel Library (Intel® MKL) directory:

File in ./benchmarks/linpack/	Description
xlinpack_xeon32	The 32-bit program executable for a system based on Intel® Xeon® processor or Intel® Xeon® processor MP with or without Streaming SIMD Extensions 3 (SSE3).
xlinpack_xeon64	The 64-bit program executable for a system with Intel Xeon processor using Intel® 64 architecture. This program may accelerate execution by using Intel® Xeon Phi™ coprocessors if they are available on the system.

File in ./benchmarks/	Description
xlinpack_mic	The 64-bit program executable for a native run on an Intel Xeon Phi coprocessor.
runme_xeon32	A sample shell script for executing a pre-determined problem set for $xlinpack\_xeon32$ .
runme_xeon64	A sample shell script for executing a pre-determined problem set for ${\tt xlinpack\_xeon64}.$
runme_xeon64_ao	A sample shell script for executing a pre-determined problem set for $xlinpack\_xeon64$ . The script enables acceleration by offloading computations to Intel Xeon Phi coprocessors available on the system.
runme_mic	A sample shell script for executing a pre-determined problem set for ${\tt xlinpack\_mic.}$
lininput_xeon32	Input file for a pre-determined problem for the <pre>runme_xeon32</pre> script.
lininput_xeon64	Input file for a pre-determined problem for the runme_xeon64 script.
lininput_xeon64_ao	Input file for a pre-determined problem for the runme_xeon64_ao script.
lininput_mic	Input file for a pre-determined problem for the runme_mic script.
help.lpk	Simple help file.
xhelp.lpk	Extended help file.
These files are not available appropriate runme script.	ple immediately after installation and appear as a result of execution of an
lin_xeon32.txt	Result of the runme_xeon32 script execution.
lin_xeon64.txt	Result of the runme_xeon64 script execution.
lin_xeon64_ao.txt	Result of the runme_xeon64_ao script execution.
lin_mic.txt	Result of the runme_mic script execution.

### See Also

High-level Directory Structure

### **Running the Software**

To obtain results for the pre-determined sample problem sizes on a given system, type one of the following, as appropriate:

```
./runme_xeon32
./runme_xeon64
./runme_xeon64_ao
./runme_mic
```

To run the software for other problem sizes, see the extended help included with the program. Extended help can be viewed by running the program executable with the -e option:

```
./xlinpack_xeon32 -e
./xlinpack_xeon64 -e
```

./xlinpack mic -e

The pre-defined data input fileslininput\_xeon32, lininput\_xeon64, lininput\_xeon64\_ao, and lininput\_mic are examples. Different systems have different numbers of processors or amounts of memory and therefore require new input files. The extended help can give insight into proper ways to change the sample input files.

Each input file requires at least the following amount of memory:

lininput_xeon32	2 GB
lininput_xeon64	16 GB
lininput_xeon64_ao	8 GB
lininput_mic	8 GB

If the system has less memory than the above sample data input requires, you may need to edit or create your own data input files, as explained in the extended help.

The Intel Optimized LINPACK Benchmark determines the optimal number of OpenMP threads to use. To run a different number, you can set the <code>OMP\_NUM\_THREADS</code> or <code>MKL\_NUM\_THREADS</code> environment variable inside a sample script. If you run the Intel Optimized LINPACK Benchmark without setting the number of threads, it defaults to the number of physical cores.

### **Optimization Notice**

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Notice revision #20110804

### **Known Limitations of the Intel® Optimized LINPACK Benchmark**

The following limitations are known for the Intel Optimized LINPACK Benchmark for Linux\* OS:

- Intel Optimized LINPACK Benchmark is threaded to effectively use multiple processors. So, in multiprocessor systems, best performance will be obtained with the Intel® Hyper-Threading Technology turned off, which ensures that the operating system assigns threads to physical processors only.
- If an incomplete data input file is given, the binaries may either hang or fault. See the sample data input files and/or the extended help for insight into creating a correct data input file.

### **Intel® Optimized MP LINPACK Benchmark for Clusters**

### Overview of the Intel Optimized MP LINPACK Benchmark

The Intel® Optimized MP LINPACK Benchmark for Clusters (Intel® Optimized MP LINPACK Benchmark) is based on modifications and additions to High-Performance LINPACK (HPL) 2.1 (http://www.netlib.org/benchmark/hpl) from Innovative Computing Laboratories (ICL) at the University of Tennessee, Knoxville. The Intel Optimized MP LINPACK Benchmark can be used for TOP500 runs (see http://www.top500.org). To use the benchmark you need be familiar with HPL usage. The Intel Optimized MP LINPACK Benchmark provides some additional enhancements designed to make the HPL usage more convenient and to use Intel® Message-Passing Interface (MPI) settings that may enhance performance. The ./benchmarks/mp\_linpack directory adds techniques to minimize search times frequently associated with long runs.

The Intel® Optimized MP LINPACK Benchmark implements the Massively Parallel (MP) LINPACK benchmark using HPL code. It solves a random dense system of linear equations (Ax=b) in real\*8 precision, measures the amount of time it takes to factor and solve the system, converts that time into a performance rate, and tests the results for accuracy. You are not limited to solving a number of equations N equal to 1000 because the implementation can be generalized to solve any size system of equations that meets the restrictions imposed by the MPI implementation chosen. The benchmark uses proper random number generation technique and full row pivoting to ensure the accuracy of the results.

Do not use this benchmark to report LINPACK 100 performance. Do not confuse this benchmark with:

- LINPACK, the library, which has been expanded upon by the LAPACK library.
- Intel Optimized LINPACK Benchmark, which is a shared memory (SMP) version of the same benchmark. While the Intel Optimized MP LINPACK Benchmark can be run on both a single node and a cluster, the Intel Optimized LINPACK Benchmark can only be run on a single node.

Intel provides optimized versions of the LINPACK benchmarks to help you obtain high LINPACK benchmark results on your systems based on genuine Intel processors more easily than with the standard HPL benchmark. Use the Intel Optimized MP LINPACK Benchmark to benchmark your cluster. The prebuilt binaries require Intel® MPI library be installed on the cluster.

### **NOTE**

Intel Optimized MP LINPACK Benchmark prebuilt binaries cannot run with the symmetric model of the Intel MPI library. For details, see the article at https://software.intel.com/en-us/articles/using-the-intel-mpi-library-on-intel-xeon-phi-coprocessor-systems.

The run-time version of Intel MPI library is free and can be downloaded from http://www.intel.com/software/products/.

### NOTE

If you are unsure which prebuilt binary to use, start with the hybrid offload binaries, even when the system does not have any Intel<sup>®</sup> Xeon Phi<sup>™</sup> coprocessors.

The Intel package includes software developed at the University of Tennessee, Knoxville, ICL, and neither the University nor ICL endorse or promote this product. Although HPL 2.1 is redistributable under certain conditions, this particular package is subject to the Intel MKL license.

Intel MKL has introduced a new *hybrid* build functionality into MP LINPACK, while continuing to support the previous, non-hybrid build. The term *hybrid* refers to special optimizations added to take advantage of mixed OpenMP\*/MPI parallelism.

If you want to use one MPI process per node and to achieve further parallelism by means of OpenMP, use the hybrid build. In general, the hybrid build is useful when the number of MPI processes per core is less than one. If you want to rely exclusively on MPI for cross-node parallelism and use one MPI process per core, use the non-hybrid build.

In addition to supplying certain hybrid prebuilt binaries, Intel MKL supplies some hybrid prebuilt libraries for Intel® MPI to take advantage of the additional OpenMP optimizations.

To enable you to offload computations from recent Intel® Xeon® processors to between zero and eight Intel Xeon Phi coprocessors, Intel MKL supplies a hybrid offload binary. The hybrid offload binary contains the latest optimizations for the Previous Generation Intel® Core™ and higher processors, and you are encouraged to use this binary even when the system does not have any Intel Xeon Phi coprocessors. The hybrid offload binary uses system-specific threading APIs to exploit mixed parallelism.

If you want to use an MPI version other than Intel MPI, you can do so by using the MP LINPACK source code provided. You can use the source code to build a non-hybrid version that may be used in a hybrid mode, but it would be missing some of the optimizations added to the hybrid version.

Non-hybrid builds are the default of the source code makefiles provided. In some cases, the use of the hybrid mode is required for external reasons. If you have a choice, the non-hybrid code may be faster. To use the non-hybrid code in a hybrid mode, use the threaded version of Intel MKL BLAS, link with a thread-safe MPI (for example: use the  $-mt_mpi$  option with Intel MPI library), and call function  $MPI_init_thread()$  so that MPI is thread-safe.

Intel MKL provides prebuilt binaries that are linked against Intel MPI libraries either statically or dynamically.

### **NOTE**

Performance of statically and dynamically linked prebuilt binaries may be different. The performance of both depends on the version of Intel MPI you are using.

You can build binaries statically linked against a particular version of Intel MPI by yourself.

### **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

Notice revision #20110804

### Usage Modes of Intel Optimized MP LINPACK Benchmark for Intel® Xeon Phi™ Coprocessors

Intel MKL supports Intel<sup>®</sup> Xeon Phi<sup>™</sup> coprocessors in these modes:

- Native
- Hybrid Offload

For details of the Native mode, see Using Intel® Math Kernel Library on Intel® Xeon Phi™ Coprocessors.

The Hybrid Offload mode combines use of different parallelization methods and offloading computations to coprocessors. In this mode, the host processor uses fewer cores for MPI than the total number of physical cores, also uses OpenMP\* or POSIX threads, and offloads chunks of the problem to the Intel Xeon Phi coprocessor.

Native mode is required to run MPI processes directly on the Intel Xeon Phi coprocessors. If the MPI processes run solely on the Intel® Xeon® processors, the coprocessors are used in an offload mode.

In many cases, the host Intel Xeon processor has more memory than the Intel Xeon Phi coprocessor. Therefore, the MPI processes have access to more memory when run on the host processors than on the coprocessors.

HPL code is homogeneous by nature: it requires that each MPI process runs in an environment with similar CPU and memory constraints. If for some reason, one node is twice as powerful as another node, in the past you could balance this only by running two MPI processes on the faster node.

Intel MKL now supports heterogeneous Intel Optimized MP LINPACK Benchmark. Heterogeneity means that Intel MKL supports a data distribution that can be balanced to the performance requirements of each node if there is enough memory on that node to support any additional work. The Intel Optimized MP LINPACK Benchmark supports:

- Intra-node heterogeneity,
  - where a node includes different processing units with different compute capabilities. To use intra-node heterogeneity, where work is shared between the Intel Xeon processors and Intel Xeon Phi coprocessors, use the hybrid offload techniques.
- Inter-node heterogeneity,

where the nodes themselves can differ. For information on how to configure Intel MKL to use the internode heterogeneity, see Heterogeneous Intel Optimized MP LINPACK Benchmark.

To maximize performance, increase the memory on the host processor or processors (64 GB per coprocessor is ideal) and run a large problem and large block-size. Such runs offload pieces of work to the coprocessors. Although this method increases the PCIe bus traffic, it is worthwhile for solving a problem that is large enough.

If the amount of memory on the host processor is small, you might get the best performance by running natively instead of offloading.

### **Contents of the Intel Optimized MP LINPACK Benchmark**

The Intel Optimized MP LINPACK Benchmark includes the entire HPL 2.1 distribution, but with modifications to several files, and files specific to the Intel Optimized MP LINPACK Benchmark. All the files are located in the ./benchmarks/mp\_linpack/ subdirectory of the Intel MKL directory. Files specific to the Intel Optimized MP LINPACK Benchmark are listed below.

<pre>Directory/File in <mkl directory="">/ benchmarks/mp_linpack/</mkl></pre>	Contents
Make.ia32	Sample architecture makefile for processors using the IA-32 architecture.
Make.intel64	Sample architecture makefile for processors using the Intel® 64 architecture and Linux OS.
Make.mic	Sample architecture makefile for native runs on Intel® Xeon $Phi^{TM}$ coprocessors.
HPL.dat	A duplicate of ${\tt testing/ptest/HPL.dat}$ in the top-level directory.
Prebuilt executables for simple performan	ce testing
bin_intel/ia32/xhpl_ia32	Prebuilt binary for the IA-32 architecture statically linked against Intel $^{\circ}$ MPI library $^{\dagger}$ .
bin_intel/ia32/xhpl_ia32_dynamic	Prebuilt binary for the IA-32 architecture dynamically linked against Intel MPI library.
<pre>bin_intel/ia32/xhpl_hybrid_ia32</pre>	Prebuilt hybrid binary for the IA-32 architecture statically linked against Intel MPI library.
<pre>bin_intel/ia32/ xhpl_hybrid_ia32_dynamic</pre>	Prebuilt hybrid binary for the IA-32 architecture dynamically linked against Intel MPI library.
bin_intel/intel64/xhpl_intel64	Prebuilt binary for the Intel $^{\scriptsize \odot}$ 64 architecture statically linked against Intel MPI library.
<pre>bin_intel/intel64/ xhpl_intel64_dynamic</pre>	Prebuilt binary for the Intel® 64 architecture dynamically linked against Intel MPI library.
<pre>bin_intel/intel64/ xhpl_hybrid_intel64</pre>	Prebuilt hybrid binary for the Intel® 64 architecture statically linked against Intel MPI library.
<pre>bin_intel/intel64/ xhpl_hybrid_intel64_dynamic</pre>	Prebuilt hybrid binary for the Intel® 64 architecture dynamically linked against Intel MPI library.
bin_intel/intel64/ xhpl_offload_intel64	Prebuilt static binary for Previous Generation Intel® Core™ and higher processors, offload mode, and Intel MPI library. The binary accelerates execution by offloading computations to Intel Xeon Phi coprocessors if they are available on the system and is optimized for hybrid offloads.

<pre>Directory/File in <mkl directory="">/ benchmarks/mp_linpack/</mkl></pre>	Contents
bin_intel/intel64/ xhpl_offload_intel64_dynamic	Prebuilt dynamic binary for Previous Generation Intel® Core™ and higher processors, offload mode, and Intel MPI library. The binary accelerates execution by offloading computations to Intel Xeon Phi coprocessors if they are available on the system and is optimized for hybrid offloads.
bin_intel/mic/xhpl_mic	Prebuilt binary for native runs on Intel Xeon Phi coprocessors. Statically linked against Intel MPI library.
bin_intel/mic/xhpl_mic_dynamic	Prebuilt binary for native runs on Intel Xeon Phi coprocessors. Dynamically linked against Intel MPI library.
bin_intel/mic/xhpl_hybrid_mic	Prebuilt hybrid binary for native runs on Intel Xeon Phi coprocessors. Statically linked against Intel MPI library.
<pre>bin_intel/mic/ xhpl_hybrid_mic_dynamic</pre>	Prebuilt hybrid binary for native runs on Intel Xeon Phi coprocessors. Dynamically linked against Intel MPI library.
Prebuilt libraries	
lib_hybrid/ia32/libhpl_hybrid.a	Prebuilt library with the hybrid version of the Intel Optimized MP LINPACK Benchmark for the IA-32 architecture and Intel MPI library.
<pre>lib_hybrid/intel64/ libhpl_hybrid.a</pre>	Prebuilt library with the hybrid version of the Intel Optimized MP LINPACK Benchmark for the Intel® 64 architecture and Intel MPI library.
<pre>lib_hybrid/intel64/ libhpl_offload.a</pre>	Prebuilt library with the offload version of the Intel Optimized MP LINPACK Benchmark for the Intel® 64 architecture and Intel MPI library.
lib_hybrid/mic/libhpl_hybrid.a	Prebuilt library with the hybrid version of the Intel Optimized MP LINPACK Benchmark for native runs on Intel Xeon Phi coprocessors.
Run scripts and examples of input files	
bin_intel/ia32/runme_ia32	Sample run script for the IA-32 architecture and pure MPI binary statically linked against Intel MPI library.
<pre>bin_intel/ia32/ runme_ia32_dynamic</pre>	Sample run script for the IA-32 architecture and pure MPI binary dynamically linked against Intel MPI library.
bin_intel/ia32/HPL_serial.dat	Example of an input file for the IA-32 architecture and a pure MPI binary.
bin_intel/ia32/runme_hybrid_ia32	Sample run script for the IA-32 architecture and hybrid binary statically linked against Intel MPI library.
<pre>bin_intel/ia32/ runme_hybrid_ia32_dynamic</pre>	Sample run script for the IA-32 architecture and hybrid binary dynamically linked against Intel MPI library.
bin_intel/ia32/HPL_hybrid.dat	Example of an input file for the IA-32 architecture and a hybrid binary.
bin_intel/intel64/runme_intel64	Sample run script for the Intel® 64 architecture and pure MPI binary statically linked against Intel MPI library.
<pre>bin_intel/intel64/ runme_intel64_dynamic</pre>	Sample run script for the Intel® 64 architecture and pure MPI binary dynamically linked against Intel MPI library.

<pre>Directory/File in <mkl directory="">/ benchmarks/mp_linpack/</mkl></pre>	Contents
bin_intel/intel64/HPL_serial.dat	Example of an input file for the Intel® 64 architecture and a pure MPI binary.
<pre>bin_intel/intel64/ runme_hybrid_intel64</pre>	Sample run script for the Intel® 64 architecture and hybrid binary statically linked against Intel MPI library.
<pre>bin_intel/intel64/ runme_hybrid_intel64_dynamic</pre>	Sample run script for the Intel® 64 architecture and hybrid binary dynamically linked against Intel MPI library.
bin_intel/intel64/HPL_hybrid.dat	Example of an input file for the Intel $\!^{\tiny{\textcircled{\tiny{0}}}}$ 64 architecture and a hybrid binary.
<pre>bin_intel/intel64/ runme_offload_intel64</pre>	Sample run script for the Intel $^{\mbox{\scriptsize 0}}$ 64 architecture and offload static binary.
<pre>bin_intel/intel64/ runme_offload_intel64_dynamic</pre>	Sample run script for the Intel® 64 architecture and offload dynamic binary.
<pre>bin_intel/intel64/ runme_offload_intel64_ prv</pre>	A script that sets HPL environment variables based on the number of Intel Xeon Phi coprocessors per MPI core. The script is called by runme_offload_intel64 and runme_offload_intel64_dynamic.
bin_intel/intel64/ HPL_offload.dat	Example of an input file for the Intel $\!^{\tiny{\textcircled{\tiny{0}}}}$ 64 architecture and an offload binary.
bin_intel/mic/runme_hybrid_mic	Sample run script for native runs on Intel Xeon Phi coprocessors and the hybrid binary statically linked against Intel MPI library.
<pre>bin_intel/mic/ runme_hybrid_mic_dynamic</pre>	Sample run script for native runs on Intel Xeon Phi coprocessors and the hybrid binary dynamically linked against Intel MPI library.
bin_intel/mic/HPL_hybrid.dat	Example of an input file for native runs on Intel Xeon Phi coprocessors and a hybrid binary.
nodeperf.c	Sample utility that tests the DGEMM speed across the cluster.

<sup>&</sup>lt;sup>‡</sup> For a list of supported versions of the Intel MPI Library, see system requirements in the Intel MKL Release Notes.

### **See Also**

High-level Directory Structure

### **Compile Options Specific to the Intel Optimized MP LINPACK Benchmark**

The Intel Optimized MP LINPACK Benchmark has some additional compile options available over the standard HPL 2.1 distribution. These new options are:

**ASYOUGO:** Provides non-impacting performance information while runs proceed. There are only a few outputs and this information does not impact performance. This can be useful for runs that otherwise can execute for hours without providing any information.

**ASYOUGO2:** Provides additional performance information at a modest performance cost by intercepting every DGEMM call.

 $\textbf{ASYOUGO2\_DISPLAY:} \ \ \textbf{Displays} \ \ \textbf{the performance of all the significant DGEMM calls in the run.}$ 

**ENDEARLY:** Displays performance hints and then terminates the run early.

**FASTSWAP:** Inserts the LAPACK-optimized DLASWP into the HPL code. You can experiment with this to determine best results.

**HYBRID:** Establishes the Hybrid OpenMP/MPI mode of MP LINPACK, enabling the use of threaded Intel MKL and prebuilt MP LINPACK hybrid libraries.

### **CAUTION**

Use this option only with an Intel® compiler and the Intel® MPI library version 3.1 or higher.

### **Building the Intel Optimized MP LINPACK Benchmark**

The Intel Optimized MP LINPACK Benchmark contains a few sample architecture makefiles, which you can edit to fit your configuration. Specifically:

- Set TOPdir to the directory where the Intel Optimized MP LINPACK Benchmark is being built.
- (Optional) Set MPI variables: MPdir, MPinc, and MPlib.
- Specify the location of Intel MKL and of files to be used (LAdir, LAinc, LAlib).
- Adjust compiler and compiler/linker options.
- Specify the architecture by setting the architecture parameter arch for the make command:
  - ia32 for MPI processes to run on a 32-bit host processor.
  - intel64 for MPI processes to run on a 64-bit host processor and use the Intel MKL hybrid offload methodology if Intel Xeon Phi coprocessors are available on the cluster.
  - mic for MPI processes to run only on the Intel Xeon Phi coprocessors.

In this case, the makefile creates pure native mode binaries. Note that this option is limited by the size of memory on the coprocessors. For more details, see Usage Modes of Intel Optimized MP LINPACK Benchmark for Intel<sup>®</sup> Xeon Phi™ Coprocessors.

• By default, the non-hybrid version of MP LINPACK is built. To build a different version, set the version parameter for the make command to hybrid or offload, as appropriate.

For example:

```
make arch=intel64 version=offload install
```

The makefile creates the binary in the bin/<arch> subdirectory of your mp\_linpack directory (for example, bin/intel64).

The makefiles contain common values for some sample cases, such as Linux systems based on the Intel® 64 architecture. To change these values, you must be familiar with building an HPL and picking appropriate values for the variables in the makefiles.

### **Ease-of-use Command-line Parameters**

The Intel Optimized MP LINPACK Benchmark supports command-line parameters for HPL that help you to avoid making small changes in the HPL.dat input files every time you do a new run.

Placeholders in this command line illustrate these parameters:

./xhpl -n cproblem size> -m <memory size in Mbytes> -b <block size> -p <grid row dimn> -q <grid column dimn>

You can also use command-line parameters to run prebuilt binaries and runme scripts. For example:

- ./runme\_offload\_intel64 -n <problem size> -m <memory size in Mbytes> -b <block size> -p <qrid row dimn> -q <qrid column dimn>

For more command-line parameters, see Heterogeneous Intel Optimized MP LINPACK Benchmark.

If you want to run for N=10000 on a 1x3 grid, execute this command, provided that the other parameters in HPL.dat are correct:

```
./xhpl -n 10000 -p 1 -q 3
```

By using the m parameter you can scale by the memory size instead of the problem size. The m parameter only refers to the size of the matrix storage and not to the coprocessor memory size or other buffers. So if you want to use matrices that fit in 50000 Mbytes with NB=1024 on 16 nodes, 32 nodes, and 128 nodes, execute these commands:

```
./xhpl -m 50000 -b 1024 -p 4 -q 4
./xhpl -m 50000 -b 1024 -p 4 -q 8
./xhpl -m 50000 -b 1024 -p 8 -q 16
```

### **Heterogeneous Intel Optimized MP LINPACK Benchmark**

The Intel Optimized MP LINPACK Benchmark supports both inter-node and intra-node heterogeneity. Only the hybrid offload version of the prebuilt binaries supports node-to-node heterogeneity.

Intel MKL achieves heterogeneous support by distributing the matrix data unequally between the nodes. You do not need to run a different number of MPI processes on the faster nodes. Heterogeneous support can work by running only one MPI process per node (although you can run more MPI processes) and assigning more work to the more powerful nodes. The heterogeneous factor command-line parameter  ${\tt f}$  controls the amount of work to be assigned to the more powerful nodes:

```
./xhpl -n 100000 -b 1024 -p 8 -q 16 -f <heterogeneous factor>
```

The heterogeneous factor does not need to be integer. If the heterogeneous factor is 2.5, roughly 2.5 times the work will be put on the more powerful nodes. The heterogeneous factor is an important tuning parameter. The more work you put on the more powerful nodes, the more memory you might be wasting on the other nodes. Intel MKL achieves load balance by distributing the work unevenly. You can balance for speed or balance for memory, but not both. If your cluster includes many different types of nodes, you may need multiple heterogeneous factors.

Suppose you have a cluster with 32 GB per node, but some of the nodes are twice as fast, so you put twice as much work on them. Because they only have 32 GB per node as well, all the other nodes must be treated as 16 GB nodes, and effectively waste half the memory. Note that wasting memory might require a smaller problem size, which lowers the overall performance.

Let P be the number of rows and Q the number of columns in your processor grid (PxQ). The work must be homogeneous within each processor column because vertical operations, such as pivoting, are synchronizing operations.

When there are two different types of nodes, use MPI to process all the faster nodes first, and make sure the "PMAP process mapping" (line 9) of HPL.dat is set to 1, for Column-major mapping. Because all the nodes must be the same within a process column, the number of faster nodes must always be a multiple of P, and you can specify the faster nodes by setting the number of process columns C for the faster nodes with the c command-line parameter:

```
./xhpl -n 100000 -b 1024 -p 8 -q 16 -f <heterogeneous factor> -c <number of faster processor columns>
```

Use both f and c command-line parameters together. The -f 1.0 -c 0 setting returns you to the default homogeneous behavior.

To understand how to choose the problem size N for a heterogeneous run, first consider a homogeneous system, where you might choose N as follows:

```
N \sim = sqrt(Memory\ Utilization\ *\ P\ *\ Q\ *\ Memory\ Size\ in\ GBytes\ /\ 8)
```

Memory Utilization is usually around 0.8 for homogeneous Intel Xeon processor systems. With Intel Xeon Phi coprocessors involved, Memory Utilization is probably around 0.7 due to extra buffers needed for communication.

On a heterogeneous system, you might apply a different formula for N for each "cluster" of nodes that are the same and take the minimum N involved. Suppose you have a cluster with only one heterogeneous factor F and the number of processor columns (out of the total Q) in the group with that heterogeneous factor equal to C. That group contains  $P^*C$  nodes. First compute the sum of the parts:  $S = F^*P^*C + P^*(Q-C)$ . Note that  $S = P^*Q, F = 1$ , and C = Q on a homogeneous system. So take N as

 $N \sim = sqrt(Memory\ Utilization\ *\ P\ *\ Q\ *\ ((F*P*C)/S)\ *\ Memory\ Size\ in\ GBytes\ /\ 8)$ 

or simply scale down the value of N for the homogeneous system by sqrt(F\*P\*C/S).

### Example

Suppose the cluster has 100 nodes each having 64 GB of memory, and 20 of the nodes are 2.7 times as powerful as the other 80. Run *one* MPI process per node for a total of 100 MPI processes. Assume a square processor grid P=Q=10, which conveniently divides up the faster nodes evenly. Normally, the HPL documentation recommends choosing a matrix size that consumes 80 percent of available memory. If N is the size of the matrix, the matrix consumes  $8N^2/(P*Q)$ . So a homogeneous run might look like:

```
./xhpl -n 820000 -b 256 -p 10 -q 10
```

Unfortunately, the HPL from Netlib runs this problem as slow as the slowest node, and all the extra performance potential from the faster nodes is lost. However, if you redistribute the matrix and run the heterogeneous Intel Optimized MP LINPACK Benchmark, you can take advantage of the faster nodes. But because some of the nodes will contain 2.7 times as much data as the other nodes, you must shrink the problem size (unless the faster nodes also happen to have 2.7 times as much memory). Instead of 0.8\*64GB\*100 total memory size, we have only 0.8\*64GB\*20 + 0.8\*64GB/2.7\*80 total memory, which is less than half the original space. So the problem size in this case would be 526000. If the faster nodes are faster because of the presence of Intel Xeon Phi coprocessors (intra-node heterogeneity), you might need to choose a larger block size as well (which reduces scalability to some extent). Because P=10 and there are 20 faster nodes, two processor columns are faster. If you arrange MPI to send these nodes first to the application, the command line looks like:

```
./xhpl -n 526000 -b 1024 -p 10 -q 10 -f 2.7 -c 2
```

The m parameter may be misleading for heterogeneous calculations, because it calculates the problem size assuming all the nodes have the same amount of data.

### WARNING

The number of faster nodes must be  $C^*P$ . If the number of faster nodes is not divisible by P, you might not be able to take advantage of the extra performance potential by giving the faster nodes extra work.

While it suffices to provide f and c command-line parameters if you need one heterogeneous factor, to support multiple heterogeneous factors, you must add lines to the HPL.dat input as explained below.

For example, if there are three different types of nodes in a cluster and you need at least two heterogeneous factors:

1. Add these lines to the end of the HPL.dat:

```
number of heterogeneous factors
1 3 2.7 [start column, stop column, heterogeneous factor for that range]
```

### **NOTE**

Numbering of processor columns starts at 0. The start and stopping numbers must be between 0 and Q-1 (inclusive).

You can also perform this step instead of providing the command-line parameters if you need only one heterogeneous factor.

**2.** For two heterogeneous factors, change the number in the first row above from 1 to 2 and follow that line with two lines specifying the start column, stopping column, and heterogeneous factor.

When choosing parameters for heterogeneous support in HPL.dat, primarily focus on the most powerful nodes. However, the larger the heterogeneous factor, the more balanced the cluster may be from a performance viewpoint, but the more imbalanced from a memory viewpoint. At some point, further performance balancing might affect the memory too much. If this is the case, try to reduce any changes done for the faster nodes (such as in block sizes). Experiment with values in HPL.dat carefully because wrong values may greatly hinder performance.

When tuning on a heterogeneous cluster, do not immediately attempt a heterogeneous run, but do the following:

- 1. Break the cluster down into multiple homogeneous clusters.
- **2.** Make heterogeneous adjustments for performance balancing. For instance, if you have two different sets of nodes where one is three times as powerful as the other, it must do three times the work.
- 3. Figure out the approximate size of the problem (per node) that you can run on each piece.
- **4.** Do some homogeneous runs with those problem sizes per node and the final block size needed for the heterogeneous run and find the best parameters.
- **5.** Use these parameters for an initial heterogeneous run.

### **Running the Intel Optimized MP LINPACK Benchmark**

### See Also

Building the Intel Optimized MP LINPACK Benchmark

### **Running the Benchmark on One Node**

To run the Intel Optimized MP LINPACK Benchmark binary on a cluster node, follow the steps below.

### **NOTE**

While these instructions assume the Intel® 64 architecture, they are more widely applicable. The instructions directly apply to Previous Generation Intel® Core $^{\text{TM}}$  or higher Intel® processors. For IA-32 architecture processors and for earlier Intel® 64 architecture processors, omit the version parameter of the make command. For IA-32 architecture processors, also adjust directory names and the value of the arch parameter.

1. Load the necessary environment variables for Intel MKL, Intel MPI, and the Intel® compiler and build the binary:

```
<parent product directory>/bin/compilervars.sh intel64
<mpi directory>/bin64/mpivars.sh
<mkl directory>/bin/mklvars.sh intel64
make arch=intel64 version=offload
```

2. Change directory to bin/intel64:

```
cd <mkl directory>/benchmarks/mp linpack/bin/intel64
```

This directory contains files:

- xhpl the Intel® 64 architecture binary.
- HPL.dat the HPL input data set.
- 3. Execute the binary for a small test run:

```
./xhpl
```

**4.** Modify the HPL.dat file to match the memory on the host processor by increasing the value in line 6 before Ns:

```
    For 16 GB: 12000 Ns
    For 32 GB: 56000 Ns
```

• For 64 GB: 83000 Ns

In general, you can compute the memory required to store the matrix (which does not count numerous buffers) as 8 \* N \* N / (P \* Q) bytes, where N is the problem size, and P and Q are the process grids in HPL.dat. HPL documentation generally recommends choosing a problem size that fills 80% of memory, but you can sometimes use more.

**5.** Execute the binary again and take note of the new result.

```
./xhpl
```

For specifics of running hybrid offload binaries, see Running Hybrid Offload Binaries.

### See Also

Notational Conventions
Building the Intel Optimized MP LINPACK Benchmark
Expanding the Benchmark to Two or More Nodes

### **Expanding the Benchmark to Two or More Nodes**

To run the Intel Optimized MP LINPACK Benchmark on multiple nodes, you need to use MPI and either modify the HPL.dat or use Ease-of-use Command-line Parameters as explained in this section.

### NOTE

While these instructions assume the Intel® 64 architecture, they are more widely applicable. The instructions directly apply to Previous Generation Intel® Core $^{\text{TM}}$  or higher Intel® processors. For IA-32 architecture processors and for earlier Intel® 64 architecture processors, omit the version parameter of the make command. For IA-32 architecture processors, also adjust directory names and the value of the arch parameter.

To expand runs of the Intel Optimized MP LINPACK Benchmark to more nodes, perform these steps:

**1.** Load the necessary environment variables for Intel MKL, Intel MPI, and the Intel® compiler and build the binary:

```
<parent product directory>/bin/compilervars.sh intel64
<mpi directory>/bin64/mpivars.sh
<mkl directory>/bin/mklvars.sh intel64
make arch=intel64 version=offload
```

2. Change directory to bin/intel64:

```
cd <mkl directory>/benchmarks/mp_linpack/bin/intel64
```

This directory contains files:

- xhpl the Intel® 64 architecture binary.
- HPL.dat the HPL input data set.
- 3. In the HPL.dat file, set the problem size N to 10000. Because this setting is for a test run, the problem size should be small.
- **4.** In the HPL.dat file, set the parameters Ps and Qs so that Ps \* Qs equals the number of nodes. For example, for 2 nodes, set Ps to 1 and Qs to 2. It is easier to achieve optimal result if Ps = Qs, so choose them as close to each other as possible so that Ps  $\leq$  Qs.

The resulting HPL.dat file for 2 nodes is as follows:

```
HPLinpack benchmark input file
Innovative Computing Laboratory, University of Tennessee
HPL.out output file name (if any)
6 device out (6=stdout,7=stderr,file)
1 # of problems sizes (N)
10000 Ns
1 # of NBs
```

```
1280
             NBs
             PMAP process mapping (0=Row-,1=Column-major)
1
1
             # of process grids (P x Q)
1
2
             0s
16.0
            threshold
1
             # of panel fact
2
            PFACTs (0=left, 1=Crout, 2=Right)
1
            # of recursive stopping criterium
4
            NBMINs (>= 1)
1
            # of panels in recursion
            NDIVs
1
            # of recursive panel fact.
1
            RFACTs (0=left, 1=Crout, 2=Right)
1
            # of broadcast
           BCASTs (0=1rg,1=1rM,2=2rg,3=2rM,4=Lng,5=LnM)
1
            # of lookahead depth
1
             DEPTHs (>=0)
0
             SWAP (0=bin-exch, 1=long, 2=mix)
1
             swapping threshold
1
             L1 in (0=transposed,1=no-transposed) form
             U in (0=transposed,1=no-transposed) form
1
0
             Equilibration (0=no,1=yes)
             memory alignment in double (> 0)
```

Alternatively, launch with -n, -p, and -q parameters and leave the HPL.dat file as is.

### The resulting HPL.dat file for 4 nodes is as follows:

```
HPLinpack benchmark input file
Innovative Computing Laboratory, University of Tennessee
            output file name (if any)
            device out (6=stdout,7=stderr,file)
             # of problems sizes (N)
10000
            Ns
             # of NBs
1280
            NBs
            PMAP process mapping (0=Row-,1=Column-major)
1
1
             # of process grids (P x Q)
2
            Ps
2
            0s
16.0
            threshold
             # of panel fact
1
2
            PFACTs (0=left, 1=Crout, 2=Right)
1
            # of recursive stopping criterium
4
            NBMINs (>= 1)
1
            # of panels in recursion
2
           NDIVs
            # of recursive panel fact.
            RFACTs (0=left, 1=Crout, 2=Right)
1
1
             # of broadcast
0
            BCASTs (0=1rg, 1=1rM, 2=2rg, 3=2rM, 4=Lng, 5=LnM)
1
             # of lookahead depth
1
             DEPTHs (>=0)
            SWAP (0=bin-exch, 1=long, 2=mix)
0
1
             swapping threshold
1
             L1 in (0=transposed, 1=no-transposed) form
1
             U in (0=transposed,1=no-transposed) form
0
             Equilibration (0=no,1=yes)
```

```
8 memory alignment in double (> 0)
```

Alternatively, launch with -n, -p, -q parameters and leave the HPL.dat file as is.

**5.** Run the xhpl binary under MPI control on two nodes:

```
mpirun --perhost 1 -n 2 -hosts Node1,Node2 \
-genv MIC_LD_LIBRARY_PATH $MIC_LD_LIBRARY_PATH \
-genv LD LIBRARY PATH $LD LIBRARY PATH ./xhp1
```

**6.** Rerun the HPL test increasing the size of the problem until the matrix size uses about 80% of the available memory. To do this, either modify Ns in HPL.dat or use the -m command-line parameter.

For specifics of running hybrid offload binaries, see Running Hybrid Offload Binaries.

### See Also

Notational Conventions
Building the Intel Optimized MP LINPACK Benchmark
Running the Benchmark on One Node
Improving Performance of Your Cluster
Ease-of-use Command-line Parameters

### **Running Hybrid Offload Binaries**

Hybrid offload binaries of the Intel Optimized MP LINPACK Benchmark inform you how many Intel Xeon Phi coprocessors are detected during the run. Top of the output has a line like this:

Number of Intel Xeon Phi coprocessors: 1

### **NOTE**

This number counts only one Intel Xeon Phi coprocessor per MPI process.

If Intel Xeon Phi coprocessors are available on your cluster and you expect offloading to occur, but the number printed is zero, it is likely that the correct compiler environment was not loaded. Specifically, check whether the LD\_LIBRARY\_PATH environment variable contains shared libraries libcoi\_host.so.0 and libscif.so.0, which are installed by the Intel® Manycore Platform Software Stack (Intel® MPSS).

You can use environment variables specific to hybrid offload binaries to adjust the behavior of your runs. For a list of supported environment variables, see <a href="Environment Variables for the Hybrid Offload">Environment Variables for the Hybrid Offload</a>. Hybrid offload binaries also react to <a href="MKL\_MIC\_ENABLE">MKL\_MIC\_ENABLE</a> and <a href="OFFLOAD\_DEVICES">OFFLOAD\_DEVICES</a> environment variables for automatic offload to Intel Xeon Phi coprocessors.

The scripts runme\_offload\_intel64 or runme\_offload\_intel64\_dynamic can set the HPL environment variables (such as HPL\_MIC\_DEVICE and HPL\_MIC\_SHAREMODE) for a given numbers of MPI ranks per node and Intel Xeon Phi coprocessors per node so that MPI ranks share the Intel Xeon Phi coprocessors optimally. Set the following variables at the top of these scripts according to your cluster configuration:

MPI\_PROC\_NUM The total number of MPI processes.

MPI PER NODE The number of MPI processes per each cluster node.

### **TIP**

To get best performance of HPL, enable non-uniform memory access (NUMA) and set MPI\_PER\_NODE equal to the number of NUMA sockets.

NUMMIC The number of Intel Xeon Phi coprocessors per each cluster node.

The scripts launch the hybrid offload HPL binary for a given number of MPI processes and write the results to the output file.

### **Optimization Notice**

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### See Also

Usage Modes of Intel Optimized MP LINPACK Benchmark for Intel® Xeon Phi™ Coprocessors Running the Benchmark on One Node Expanding the Benchmark to Two or More Nodes Automatic Offload Controls

### **Improving Performance of Your Cluster**

While it is relatively easy to get high performance of the HPL test on a single node, it is more complicated in a cluster. To achieve high performance of the test in a cluster, follow these steps, provided all the needed installations are done on each node:

- 1. Reboot all nodes.
- **2.** Ensure all nodes are in identical conditions and no zombie processes are left running from prior HPL runs.

To do this, run single-node Stream and HPL LINPACK or the Intel MKL program nodeperf on every node. For more details, see also Optimizing the Result on a Cluster. Ensure results are within 2% of each other (problem size must be large enough depending on memory size and CPU speed). Investigate nodes with low performance for hardware/software problems.

- **3.** Check that your cluster interconnects are working. Run a test over the complete cluster using an MPI test for bandwidth and latency. The IMB and Microway\* Linkchecker tests of Intel MPI are two of many benchmarking methods that can be useful for this step.
- **4.** Run an HPL benchmark on pairs of two or four nodes and ensure results are within 4% of each other. The problem size must be large enough depending on the memory size and CPU speed (for example, refer here).
- **5.** Run a small HPL workload over the complete cluster to ensure correctness.
- **6.** Increase the problem size and run the real test load. Rerun at the real size at least three times.
- 7. In case of problems go back to step 2.

### WARNING

Each step is important, so skipping a step like 4, you can waste a lot of time.

Before making a heterogeneous inter-node run, always run its homogeneous equivalent first. If you are using Intel Xeon Phi coprocessors in an offload mode for intra-node heterogeneity, first run on the Intel Xeon processors alone.

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### **Optimization Notice**

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### See Also

Expanding the Benchmark to Two or More Nodes Heterogeneous Intel Optimized MP LINPACK Benchmark

### More Details of the Intel Optimized MP LINPACK Benchmark

The Intel Optimized MP LINPACK Benchmark does Gaussian elimination with row pivoting to compute an LU decomposition of the matrix. If P is a permutation matrix representing row pivots, then PA = LU where L is a lower unit triangular matrix and U is an upper triangular matrix. The algorithm is blocked to increase cache reuse of the data. The sequential algorithm closest to the Intel Optimized MP LINPACK Benchmark is DGETRF from LAPACK or PDGETRF from Scalapack, referred to by the generic name \*GETRF. However, \*GETRF retains L, which is not necessary in the Intel Optimized MP LINPACK Benchmark. A system of equations Ax = b can be solved with \*GETRF by performing these steps:

- **1.** Compute PA = LU
- **2.** Solve Ly=Pb for y
- **3.** Solve Ux = y for x

L to the left can be discarded if b is replaced with y above while going through the problem. This saves a forward solve at the end (which is not so critical), and it means that as long as you do an LU decomposition on the column-augmented system [A|b], when doing pivots you can skip pivoting to the left while using a right-looking algorithm.

### **NOTE**

While it is acceptable in the Intel Optimized MP LINPACK Benchmark to skip pivoting to the left, the LAPACK and ScaLAPACK  $\star$  GETRF algorithms must add pivoting to the left if step 2 might be used later.

\*GETRF makes several BLAS calls. Assuming N is the problem size and NB is the column block size used in the blocking above, then as long as N is sufficiently greater than NB, most of the floating-point operations (FLOPs) are found in \*GEMM. Some FLOPs may also be present in \*TRSM. Although other BLAS calls may be necessary, these are the performance critical functions. \*GETRF does computation in one of three spots: \*GEMM, \*TRSM, and a local LU factorization.

- \*GEMM overwrites C with
- \* op(A) \* op(B) +  $\beta$ \* C.

and  $\beta$  are both scalars, and A, B, and C are matrices. op(A) denotes A or the transpose of A and similarly for op(B). op(A) is an  $m \times k$  matrix, op(B) is a  $k \times n$  matrix, and C is an  $m \times n$  matrix.

Assuming that N is the global problem size and that the matrix is distributed on a 2-dimensional (2D) block cyclic mapping on a P by Q processor grid with the block size NB, initial values of m, n, and k for the first few \*GEMM calls are  $m \approx N/P$ ,  $n \approx N/Q$ , and k = NB.

The number of FLOPs executed in \*GEMM for each block iteration starts off at approximately 2\*N\*N\*NB/(P\*Q). The size of each \*GEMM may decrease, depending on whether the node in question owns the previous block row or block column.

\*TRSM solves a triangular system of equations of size NB by NB, with typically N/Q solution vectors to compute. It has roughly NB\*NB\*(N/Q) FLOPs. So, as long as N >> P\*NB, there is more work in \*GEMM than in \*TRSM.

Additionally, each iteration does a local LU-factorization that starts at the size N/P by NB. Although the row pivoting along the entire column has to be done, the computation is the same as factoring an  $NB \times NB$  matrix, which is approximately 2\*NB\*NB\*NB/3 FLOPs. If N >> P\*NB, there are fewer FLOPs in this computation than in \*TRSM.

HPL requires row pivoting, which, while it does not involve FLOPs, can still be time consuming. It is not acceptable to replace the random matrix generator of HPL with a matrix that requires less pivoting (for example, a diagonally dominant matrix).

It is also necessary to get the data around the 2D PxQ grid since each node needs this data to do the work for row pivoting. Each node in the PxQ grid can be represented as the pair (i, j) where  $0 \le i < P$ , and  $0 \le j < Q$ .

The algorithm involves a horizontal broadcast and a vertical broadcast across the grid.

The horizontal broadcast (which contains pivot information and the A matrix of the above \*GEMM) is usually ring broadcast along Q nodes. For example, node (2,3) has to get data to every other node in the block row given by (2, j). The reason for using a ring broadcast, as opposed to a tree broadcast, is that horizontal motion in the grid can often be overlapped with other operations. The broadcast itself consumes time, but some of this effect can be hidden, depending on the input parameters.

The vertical broadcast (which contains the B matrix of the above \*GEMM) is usually a tree broadcast along P nodes because processor columns must be synchronized. In many HPL configurations,  $P \le 2Q$  is chosen.

For details of broadcasting in HPL, see www.netlib.org/benchmark/hpl/algorithm.html#bcast.

The other communication is the pivoting itself.

The offload portion of the code is typically some piece of the \*GEMM or \*TRSM because they have the highest ratio of FLOPs to data and data must move across the PCIe bus.

The fastest way to offload DGEMM is to send some portion of A and B to the coprocessor and have the coprocessor return C (assuming that  $\beta$  was zero) in an Intel Xeon Phi coprocessor native DGEMM call.

*NB* must be larger than is required for Intel® Xeon® processors alone. Choosing 400 for *NB* offers no acceleration through offloading. However, choosing a value larger than 960 for *NB* has proven to offer considerable acceleration.

Large values of NB require extra memory on the host processor and coprocessor. If this memory is low, the problem size N does not satisfy the inequality N >> NB. In that event, it is better not to use the offload version of the Intel Optimized MP LINPACK Benchmark.

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### Configuring the Hybrid Offload Version of the Intel Optimized MP LINPACK Benchmark

The most significant parameters in HPL.dat are N, NB, P and Q. Specify them as follows, as well as some other parameters:

ullet P and Q - the number of rows and columns in the process grid, respectively.

P\*Q must be the number of MPI processes that HPL is using.

For the hybrid offload version of the Intel Optimized MP LINPACK Benchmark, keep P and Q roughly the same size.

### **NOTE**

This setting is different from settings recommended for most HPL implementations, which usually recommend to choose P < Q and possibly with the 1:4 ratio.

• NB - block size of the data distribution.

The table below shows recommended values of NB for  $2^{nd}$  and  $3^{rd}$  generation Intel® Core<sup>TM</sup> processors and for different numbers of Intel Xeon Phi coprocessors. The values may vary and depend on the PCI Express settings and performance of main memory.

No coprocessors	1 coprocessor	2 coprocessors	3 coprocessors
256	960	1024	1200

- N the problem size:
  - For homogeneous runs, choose N divisible by NB\*LCM(P,Q), where LCM is the least common multiple
    of the two numbers.
  - For heterogeneous runs, refer to Heterogeneous Intel Optimized MP LINPACK Benchmark.

Note that increasing *N* usually increases performance, but the size of *N* is bounded by memory.

Other parameters.

To use Intel MKL BPUSH algorithm for horizontal broadcast, in line 23 of HPL.dat, set the BCASTs parameter to 6.

Enabling NUMA on your system and running an MPI process for each NUMA socket usually improves the hybrid offload performance. Refer to your BIOS settings for enabling NUMA on your system. You can use HPL\_MIC\_DEVICE and HPL\_MIC\_SHAREMODE environment variables to share the Intel Xeon Phi coprocessors among MPI processes (see Environment Variables for the Hybrid Offload for details). The scripts runme\_offload\_intel64 and runme\_offload\_intel64\_dynamic set these environment variables for you for a given number of MPI ranks per node.

### **Environment Variables for the Hybrid Offload**

The table below lists Intel MKL environment variables to control runs of the Intel Optimized MP LINPACK Benchmark in the hybrid offload mode. Each of these environment variables has a default value. Use them with hybrid builds of the benchmark.

### NOTE

While these environment variables impact performance of the hybrid offload binaries, they do not impact performance of other binaries. Environment variables for automatic offload, listed in Automatic Offload Controls, do not impact performance or behavior of the hybrid offload binaries.

Environment Variable	Description	Value
HPL_LARGEPAGE	Defines the memory mapping to be used for both the Intel Xeon processor and Intel Xeon Phi coprocessors.	<ul> <li>0 or 1:</li> <li>0 - normal memory mapping, default.</li> <li>1 - memory mapping with</li> </ul>
		large pages (2 MB per page mapping). It may increase performance.
HPL_LOG	Controls the level of detail for the HPL output.	An integer ranging from 0 to 2:
		<ul> <li>0 - no log is displayed (printed).</li> <li>1 - only one root node displays a log, exactly the same as the ASYOUGO option provides.</li> </ul>

Environment Variable	Description	Value
		• 2 - the most detailed log is displayed. All <i>P</i> root nodes in the processor column that owns the current column block display a log.
HPL_HOST_CORE, HPL_HOST_NODE	Specifies cores or Non-Uniform Memory Access (NUMA) nodes to be used.	A list of integers ranging from 0 to the largest number of a core or NUMA node in the
	HPL_HOST_NODE requires NUMA mode to be enabled. You can check whether it is enabled by the numactlhardware command.	cluster and separated as explained in example 3.
	The default behavior is autodetection of the core or NUMA node.	
HPL_SWAPWIDTH	Specifies width for each swap operation.	16 or 24. The default is 24.
HPL_MIC_DEVICE	Specifies Intel Xeon Phi coprocessor(s) to be used. All available Intel Xeon Phi coprocessors are used by default.	A comma-separated list of integers, each ranging from 0 to the largest number of an Intel Xeon Phi coprocessor on the node.
	NOTE To avoid oversubscription of resources that might occur if you use multiple MPI processes per node, set this environment variable to specify which coprocessors each MPI process should use.	
HPL_PNUMMICS	Specifies the number of Intel Xeon Phi coprocessors to be used. The HPL_MIC_DEVICE environment variable takes precedence over HPL_PNUMMICS, and the value of HPL_PNUMMICS is ignored if you set HPL_MIC_DEVICE.	An integer ranging from 0 to the number of Intel Xeon Phi coprocessors in the node. If the value is 0, the core ignores all Intel Xeon Phi coprocessors.
	The default behavior is autodetection of the number of coprocessors.	
HPL_MIC_CORE, HPL_MIC_NODE	Specifies which CPU core will be used for an Intel Xeon Phi coprocessor. Each Intel Xeon Phi coprocessor needs a dedicated CPU	An integer ranging from 0 to the largest number of a core or NUMA node for the coprocessor.
	core. By setting these variables for an Intel Xeon Phi coprocessor, you reserve:	Can be provided in a comma- separated list, each integer corresponding to one
	<ul> <li>HPL_MIC_CORE - a specific core.</li> <li>HPL_MIC_NODE - one of the cores on the specified NUMA node</li> </ul>	coprocessor.

node.

Environment Variable	Description	Value
	While the default for HPL_MIC_CORE is some core, the default for HPL_MIC_NODE is a core that the coprocessor shares with the same NUMA node.	
HPL_MIC_NUMCORES	Number of cores to be used for an Intel Xeon Phi coprocessor. All the coprocessor cores are used by default, which produces best performance.	An integer ranging from 1 to the number of cores of the coprocessor.
HPL_MIC_SHAREMODE	Specifies whether and how an Intel Xeon Phi coprocessor is shared among two MPI processes.  See example 5 for details.	<ul> <li>An integer ranging from 0 to 2:</li> <li>0 - no sharing, default</li> <li>1 - the lower half of the cores will be used for the MPI process.</li> <li>2 - the upper half of the cores will be used for the MPI process.</li> </ul>
HPL_MIC_EXQUEUES	Specifies the queue size on an Intel Xeon Phi coprocessor. Using a larger number is typically better while it increases the memory consumption for the Intel Xeon Phi coprocessor. If out of memory errors are encountered, try a lower number.	An integer ranging from 0 to 512. The default is 128.
HPL_MIC_WIDTH	Computation width for Intel Xeon Phi DGEMM/DTRSM. If the Intel Xeon Phi coprocessor memory is insufficient, change the settings as follows:  1. Reduce HPL_MIC_WIDTH to 16.	16 or 24. The default is 24.
	This might reduce performance of the node.  2. If Intel Xeon Phi coprocessor still reports a memory allocation error:  • Reduce the value of the HPL_MIC_EXQUEUES environment variable.  • If the node has more than two Intel Xeon Phi coprocessors, use twice larger P, the number of rows in the processor grid.	

<b>Environment Variable</b>	Description	Value
	<b>3.</b> If memory allocation er still reported, keep reduthe problem size <i>N</i> untierrors are no longer rep	ucing I the

You can set HPL environment variables using the PMI\_RANK and PMI\_SIZE environment variables of the Intel MPI library, and you can create a shell script to automate the process.

### **Examples of Environment Settings for Hybrid Offload**

#	Settings	Behavior of the Intel Optimized MP Linpack Benchmark
1	Nothing specified	xhpl uses all Intel Xeon processors and all Intel Xeon Phi coprocessors in the cluster.
2	HPL_PNUMMICS=0	xhpl ignores Intel Xeon Phi coprocessors and works as a regular HPL.
3	HPL_MIC_DEVICE=0,2	Only Intel Xeon Phi coprocessors 0 and 2 and Intel Xeon
	HPL_HOST_CORE=1-3,8-10	processor cores 1,2,3,8,9, and 10 are used.
4	HPL_HOST_NODE=1	Only cores on NUMA node 1 are used.
5	HPL_MIC_DEVICE=0,1	Only Intel Xeon Phi coprocessors 0 and 1 are used:
	HPL_MIC_SHAREMODE=0,2	<ul><li>On the coprocessor 0, all cores are used.</li><li>On the coprocessor 1, the upper half of the cores is used.</li></ul>
		For a 61-core Intel Xeon Phi coprocessor, the upper half includes cores 31-61.
		This setting is useful to share an Intel Xeon Phi coprocessor among two MPI processes for an odd number of Intel Xeon Phi coprocessors.

### See Also

Compile Options Specific to the Intel Optimized MP LINPACK Benchmark

### Optimizing the Result on a Cluster

To benchmark a cluster, follow the sequence of steps below (some of them are optional). Pay special attention to the iterative steps 3 and 4. They make a loop that searches for HPL parameters (specified in HPL.dat) that enable you to maximize the performance of your cluster.

- 1. Install HPL and make sure HPL is functional on all the nodes.
- 2. (Optional) Run nodeperf.c (included in the distribution) to see the performance of DGEMM on all the nodes.

Compile nodeperf.c with your MPI and Intel MKL. For example:

```
mpiicc -03 nodeperf.c -openmp -Wl,--start-group \
$MKLPATH/libmkl_intel_lp64.a $MKLPATH/libmkl_intel_thread.a \
$MKLPATH/libmkl_core.a -Wl,--end-group -lpthread -o nodeperf
```

Launching nodeperf on all the nodes is especially helpful in a very large cluster.nodeperf enables quick identification of a potential problem spot without numerous small runs of the Intel Optimized MP LINPACK Benchmark around the cluster in search of a bad node. It goes through all the nodes, one at a time, and reports the performance of DGEMM followed by the host identifier. Therefore, the higher the DGEMM performance, the faster that node was performing.

- **3.** Edit HPL.dat to fit your cluster needs.
  - See the HPL documentation for more information. Note, however, that you should use at least 4 nodes.
- **4.** Make an HPL run, using compile options such as ASYOUGO, ASYOUGO2, or ENDEARLY to aid in your search. These options enable you to gain insight into the performance sooner than HPL would normally give this insight.

When doing so, follow these recommendations:

• Use the Intel Optimized MP LINPACK Benchmark, which is a patched version of HPL, to save time in the search.

All the features impacting performance are optional in the Intel Optimized MP LINPACK Benchmark. That is, if you do not use the new options to reduce search time, these features are disabled. The primary purpose of the additions is to assist you in finding solutions.

While HPL requires a long time to search for many different parameters, in the Intel Optimized MP LINPACK Benchmark, the goal is to get the best possible number.

Given that the input is not fixed, there is a large parameter space you must search over. An exhaustive search of all possible inputs is improbably large even for a powerful cluster. The Intel Optimized MP LINPACK Benchmark optionally prints information on performance as it proceeds. You can also terminate early.

- Save time by compiling with -DENDEARLY-DASYOUGO2 and using a negative threshold (do not use a negative threshold on the final run that you intend to submit as a TOP500 entry). Set the threshold in line 13 of the HPL 2.1 input file HPL.dat.
- If you are going to run a problem to completion, do it with -DASYOUGO.
- **5.** Using the quick performance feedback, return to step 3 and iterate until you are sure that the performance is as good as possible.

### See Also

Options to Reduce Search Time

### **Options to Reduce Search Time**

Running large problems to completion on large numbers of nodes can take many hours. The search space for the Intel Optimized LINPACK Benchmark is also large: you can vary several parameters to improve performance, such as problem size, block size, grid layout, lookahead steps, factorization methods, and so on. You might not want to run a large problem to completion only to discover that it ran 0.01% slower than your previous best problem.

Use the following options to reduce the search time:

- DASYOUGO
- DENDEARLY,
- -DASYOUGO2,

Use <code>-DASYOUGO2</code> cautiously because it has a marginal performance impact. To see <code>DGEMM</code> internal performance, compile with <code>-DASYOUGO2</code> and <code>-DASYOUGO2\_DISPLAY</code>. These options provide useful <code>DGEMM</code> performance information at the cost of around 0.2% performance loss.

If you want to use the original HPL, simply omit these options and recompile from scratch. To do this, try "make  $arch=\langle arch \rangle$  clean\_arch\_all".

### -DASYOUGO

-DASYOUGO gives performance data as the run proceeds. The performance always starts off higher and then drops because the LU decomposition slows down as it goes. So the ASYOUGO performance estimate is usually an overestimate, but it gets more accurate as the problem proceeds. The greater the lookahead step, the less accurate the first number may be. ASYOUGO tries to estimate where execution is in the LU decomposition that Intel Optimized LINPACK Benchmark performs, and this is always an overestimate as compared to ASYOUGO2, which measures actually achieved DGEMM performance. Note that the ASYOUGO output is a subset of the information that ASYOUGO2 provides. Refer to the description of the DASYOUGO2 option below for the details of the output.

### -DENDEARLY

-DENDEARLY terminates the problem after a few steps, so that you can set up 10 or 20 HPL runs without monitoring them, see how they all do, and then only run the fastest ones to completion. -DENDEARLY assumes -DASYOUGO. You can define both, but it is not necessary. To avoid the residual check for a problem that terminates early, set the threshold parameter in HPL.dat to a negative number when testing ENDEARLY. It also sometimes gives more information to compile with -DASYOUGO2 when using -DENDEARLY.

Usage notes on -DENDEARLY follow:

- -DENDEARLY stops the problem after a few iterations of DGEMM on the block size (the bigger the blocksize, the further it gets). It prints only five or six updates, whereas -DASYOUGO prints about 46 or so output elements before the problem completes.
- Performance for -DASYOUGO and -DENDEARLY always starts off at one speed, slowly increases, and then slows down toward the end (reflecting the progress of the LU decomposition). -DENDEARLY is likely to terminate before it starts to slow down.
- DENDEARLY terminates the problem early with an HPL Error exit. It means that you need to ignore the
  missing residual results, which are wrong because the problem never completed. However, you can get an
  idea what the initial performance was, and if it is acceptable, run the problem to completion without –
  DENDEARLY. To avoid the error check, you can set the threshold parameter in HPL.dat to a negative
  number
- Though -DENDEARLY terminates early, HPL treats the problem as completed and computes GFLOP rating as though the problem ran to completion. Ignore this erroneously high rating.
- The bigger the problem, the more accurately the last update that <code>-DENDEARLY</code> returns is close to what happens when the problem runs to completion. <code>-DENDEARLY</code> is a poor approximation for small problems. It is for this reason that you should use <code>ENDEARLY</code> in conjunction with <code>ASYOUGO2</code>, because <code>ASYOUGO2</code> reports actual <code>DGEMM</code> performance, which can be a closer approximation to problems just starting.

### -DASYOUGO2

-DASYOUGO2 gives detailed single-node DGEMM performance information. It captures all DGEMM calls (if you use Fortran BLAS) and records their data. Because of this, the routine has a marginal performance overhead. Unlike -DASYOUGO, which does not impact performance, -DASYOUGO2 interrupts every DGEMM call to monitor its performance. You should be aware of this overhead, although for big problems, it is less than 0.2%.

A sample ASYOUGO2 output appears as follows:

Col=001280 Fract=0.050 Mflops=42454.99 (DT=9.5 DF=34.1 DMF=38322.78).

### **NOTE**

The values of Col, Fract, and Mflops are also produced for ASYOUGO and ENDEARLY.

In this example, the problem size is 16000 and a block size is 128. After processing 10 blocks, or 1280 columns (Col), an output was sent to the screen. Here, the fraction of columns completed (Fract) is 1280/16000 = 0.08. Only up to 111 outputs are printed, at various places through the matrix decomposition:

```
0.005 0.010 0.015 0.020 0.025 0.030 0.035 0.040 0.045 0.050 0.055 0.060 0.065 0.070 0.075 0.080 0.085 0.090 0.095 0.100 0.105 0.110 0.115 0.120 0.125 0.130 0.135 0.140 0.145 0.150 0.155 0.160 0.165 0.170 0.175 0.180 0.185 0.190 0.195 0.200 0.205 0.210 0.215 0.220 0.225 0.230 0.235 0.240 0.245 0.250 0.255 0.260 0.265 0.270 0.275 0.280 0.285 0.290 0.295 0.300 0.305 0.310 0.315 0.320 0.325 0.330 0.335 0.340 0.345 0.350 0.355 0.360 0.365 0.370 0.375 0.380 0.385 0.390 0.395 0.400 0.405 0.410 0.415 0.420 0.425 0.430 0.435 0.440 0.445 0.450 0.455 0.460 0.465 0.470 0.475 0.480 0.485 0.490 0.495 0.515 0.535 0.555 0.575 0.595 0.615 0.635 0.655 0.675 0.695 0.795 0.895.
```

However, this problem size is so small and the block size so big by comparison that as soon as it prints the value for 0.045, it was already through 0.08 fraction of the columns. On a really big problem, the fractional number is more accurate.

-DASYOUGO2 never prints more than the 112 numbers above. So, smaller problems have fewer than 112 updates, and the biggest problems have precisely 112 updates.

Mflops is an estimate based on the number of columns of the LU decomposition being completed. However, with lookahead steps, sometimes that work is not actually completed when the output is made. Nevertheless, this is a good estimate for comparing identical runs.

The three parenthesized numbers are ASYOUGO2 add-ins that impact performance. DT is the total time that processor 0 has spent in DGEMM. DF is the number of billion operations that have been performed in DGEMM by one processor. Therefore, the performance of processor 0 (in GFLOPs) in DGEMM is always DF/DT. Using the number of DGEMM FLOPs as a basis instead of the number of LU FLOPs, you get a lower bound on performance of the run by looking at DMF, which can be compared to Mflops above.

Note that when using the performance monitoring tools described in this section to compare different  ${\tt HPL.dat}$  input data sets, you should be aware that the pattern of performance drop-off that LU experiences is sensitive to sizes of input data. For instance, when you try very small problems, the performance drop-off from the initial values to end values is very rapid. The larger the problem, the less the drop-off, and it is probably safe to use the first few performance values to estimate the difference between a problem size 700000 and 701000, for instance. Another factor that influences the performance drop-off is the relationship of the grid dimensions (P and Q). For big problems, the performance tends to fall off less from the first few steps when P and Q are roughly equal. You can make use of a large number of parameters, such as broadcast types, and change them so that the final performance is determined very closely by the first few steps.

Use of these tools can increase the amount of data you can test.

### See Also

Optimizing the Result on a Cluster

## Intel® Math Kernel Library Language Interfaces Support



### Language Interfaces Support, by Function Domain

The following table shows language interfaces that Intel® Math Kernel Library (Intel® MKL) provides for each function domain. However, Intel MKL routines can be called from other languages using mixed-language programming. See Mixed-language Programming with the Intel Math Kernel Library for an example of how to call Fortran routines from C/C++.

Function Domain	Fortran int erface	C/C++ interface
Basic Linear Algebra Subprograms (BLAS)	Yes	via CBLAS
BLAS-like extension transposition routines	Yes	Yes
Sparse BLAS Level 1	Yes	via CBLAS
Sparse BLAS Level 2 and 3	Yes	Yes
LAPACK routines for solving systems of linear equations	Yes	Yes
LAPACK routines for solving least-squares problems, eigenvalue and singular value problems, and Sylvester's equations	Yes	Yes
Auxiliary and utility LAPACK routines	Yes	Yes
Parallel Basic Linear Algebra Subprograms (PBLAS)	Yes	
ScaLAPACK routines	Yes	†
Direct Sparse Solvers/PARDISO - Parallel Direct Sparse Solver	Yes	Yes
Parallel Direct Sparse Solvers for Clusters	Yes	Yes
Other Direct and Iterative Sparse Solver routines	Yes	Yes
Vector Mathematical Library (VML) functions	Yes	Yes
Vector Statistical Library (VSL) functions	Yes	Yes
Fourier Transform functions (FFT)	Yes	Yes
Cluster FFT functions	Yes	Yes
Trigonometric Transform routines	Yes	Yes
Fast Poisson, Laplace, and Helmholtz Solver (Poisson Library) routines	Yes	Yes
Optimization (Trust-Region) Solver routines	Yes	Yes
Data Fitting functions	Yes	Yes
Extended Eigensolver functions	Yes	Yes
Support functions (including memory allocation)	Yes	Yes

<sup>&</sup>lt;sup>†</sup> Supported using a mixed language programming call. See Include Files for the respective header file.



### **Include Files**

The table below lists Intel MKL include files.

### **NOTE**

The  $\star.f90$  include files supersede the  $\star.f77$  include files and can be used for FORTRAN 77 as well as for later versions of Fortran. However, the  $\star$  . £77 files are kept for backward compatibility.

Function domain	Fortran Include Files	C/C++ Include Files
All function domains	mkl.fi	mkl.h
BLACS Routines		mkl_blacs.h <sup>‡‡</sup>
BLAS Routines	blas.f90 mkl_blas.fi <sup>†</sup>	mkl_blas.h <sup>‡</sup>
BLAS-like Extension Transposition Routines	mkl_trans.fi <sup>†</sup>	mkl_trans.h <sup>‡</sup>
CBLAS Interface to BLAS		mkl_cblas.h <sup>‡</sup>
Sparse BLAS Routines	mkl_spblas.fi <sup>†</sup>	mkl_spblas.h <sup>‡</sup>
LAPACK Routines	<pre>lapack.f90 mkl_lapack.fi<sup>†</sup></pre>	mkl_lapack.h <sup>‡</sup>
C Interface to LAPACK		mkl_lapacke.h <sup>‡</sup>
PBLAS Routines		mkl_pblas.h <sup>‡‡</sup>
ScaLAPACK Routines		mkl_scalapack.h <sup>##</sup>
All Sparse Solver Routines	mkl_solver.f90 mkl_solver.fi <sup>†</sup>	mkl_solver.h <sup>‡</sup>
PARDISO - Parallel Direct Sparse Solver	mkl_pardiso.f90 mkl_pardiso.fi <sup>†</sup>	mkl_pardiso.h <sup>‡</sup>
Parallel Direct Sparse Solvers for Clusters	mkl_cluster_ sparse_solver.f90	mkl_cluster_ sparse_solver.h <sup>‡</sup>
Direct Sparse Solver (DSS)	mkl_dss.f90 mkl_dss.fi <sup>†</sup>	mkl_dss.h <sup>‡</sup>
RCI Iterative Solvers ILU Factorization	mkl_rci.f90 mkl_rci.fi <sup>†</sup>	mkl_rci.h <sup>‡</sup>
Optimization Solver Routines	mkl_rci.f90 mkl_rci.fi <sup>†</sup>	mkl_rci.h <sup>‡</sup>
Vector Mathematical Functions	mkl_vml.90 mkl_vml.fi <sup>†</sup> mkl_vml.f77	mkl_vml.h <sup>‡</sup>
Vector Statistical Functions	mkl_vsl.f90 mkl_vsl.fi <sup>†</sup> mkl_vsl.f77	mkl_vsl.h <sup>‡</sup>
Fourier Transform Functions	mkl dfti.f90	mkl dfti.h <sup>‡</sup>

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Function domain	Fortran Include Files	C/C++ Include Files
Cluster Fourier Transform Functions	mkl_cdft.f90	mkl_cdft.h <sup>‡‡</sup>
Partial Differential Equations Support Routines		
Trigonometric Transforms	mkl_trig_transforms.f90	mkl_trig_transform.h <sup>‡</sup>
Poisson Solvers	mkl_poisson.f90	mkl_poisson.h <sup>‡</sup>
Data Fitting Functions	mkl_df.f90 mkl_df.f77	mkl_df.h <sup>‡</sup>
Extended Eigensolver Functions	mkl_solvers_ee.fi <sup>†</sup>	mkl_solvers_ee.h <sup>‡</sup>
Support functions	mkl_service.f90 mkl_service.fi <sup>†</sup>	mkl_service.h <sup>‡</sup>
Declarations for replacing memory allocation functions. See Redefining Memory Functions for details.		i_malloc.h

 $<sup>^{\</sup>dagger}$  You can use the  ${\tt mkl.fi}$  include file in your code instead.

## **See Also**

Language Interfaces Support, by Function Domain

<sup>&</sup>lt;sup>‡</sup> You can include the mkl.h header file in your code instead.

<sup>\*\*</sup> Also include the mkl.h header file in your code.



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# Support for Third-Party Interfaces

# **FFTW Interface Support**

Intel® Math Kernel Library (Intel® MKL) offers two collections of wrappers for the FFTW interface (www.fftw.org). The wrappers are the superstructure of FFTW to be used for calling the Intel MKL Fourier transform functions. These collections correspond to the FFTW versions 2.x and 3.x and the Intel MKL versions 7.0 and later.

These wrappers enable using Intel MKL Fourier transforms to improve the performance of programs that use FFTW without changing the program source code. See the "FFTW Interface to Intel® Math Kernel Library" appendix in the Intel MKL Reference Manual for details on the use of the wrappers.

#### **Important**

For ease of use, FFTW3 interface is also integrated in Intel MKL.



# **Directory Structure in Detail**

Tables in this section show contents of the Intel(R) Math Kernel Library (Intel(R) MKL) architecture-specific directories.

#### **Optimization Notice**

Intel's compilers may or may not optimize to the same degree for non-Intel microprocessors for optimizations that are not unique to Intel microprocessors. These optimizations include SSE2, SSE3, and SSSE3 instruction sets and other optimizations. Intel does not guarantee the availability, functionality, or effectiveness of any optimization on microprocessors not manufactured by Intel. Microprocessor-dependent optimizations in this product are intended for use with Intel microprocessors. Certain optimizations not specific to Intel microarchitecture are reserved for Intel microprocessors. Please refer to the applicable product User and Reference Guides for more information regarding the specific instruction sets covered by this notice.

Notice revision #20110804

# **Detailed Structure of the IA-32 Architecture Directories**

# Static Libraries in the lib/ia32 Directory

Some of the libraries in this directory are optional. However, some optional libraries are installed by default, while the rest are not. To get those libraries that are not installed by default, explicitly select the specified optional component during installation.

### NOTE

Cluster libraries for IA-32 architecture are deprecated and will be removed in a future release.

File	Contents	Optional Component	
		Name	Installed by Default
Interface Layer			
libmkl_intel.a	Interface library for the Intel compilers. Also use for other supported compilers that do not have a specialized Intel MKL interface library.		
libmkl_blas95.a	Fortran 95 interface library for BLAS for the Intel <sup>®</sup> Fortran compiler.	Fortran 95 interfaces for BLAS and LAPACK	Yes
libmkl_lapack95.a	Fortran 95 interface library for LAPACK for the Intel Fortran compiler.	Fortran 95 interfaces for BLAS and LAPACK	Yes

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File	Contents	Optional Component		
		Name	Installed by Default	
libmkl_gf.a	Interface library for the GNU* Fortran compiler.	GNU* Compiler Collection support	Yes	
Threading Layer				
libmkl_intel_thread.a	Threading library for the Intel compilers			
libmkl_gnu_thread.a	Threading library for the GNU Fortran and C compilers	GNU* Compiler Collection support	Yes	
libmkl_pgi_thread.a	Threading library for the PGI* compiler	PGI* compiler support		
libmkl_sequential.a	Sequential library			
Computational Layer				
libmkl_core.a	Kernel library for the IA-32 architecture			
Cluster Libraries				
libmkl_scalapack_core.a	ScaLAPACK routines	Cluster support		
libmkl_cdft_core.a	Cluster version of FFT functions	Cluster support		
libmkl_blacs.a	BLACS routines for MPICH.	Cluster support		
libmkl_blacs_intelmpi.a	BLACS routines for Intel MPI and MPICH2	Cluster support		
libmkl_blacs_openmpi.a	BLACS routines for OpenMPI	Cluster support		

# Dynamic Libraries in the lib/ia32 Directory

Some of the libraries in this directory are optional. However, some optional libraries are installed by default, while the rest are not. To get those libraries that are not installed by default, explicitly select the specified optional component during installation.

#### NOTE

Cluster libraries for IA-32 architecture are deprecated and will be removed in a future release.

File	Contents	Optional Con	Optional Component	
		Name	Installed by Default	
libmkl_rt.so	Single Dynamic Library	,		

## **Interface Layer**

File	Contents	Optional Component		
		Name	Installed by Default	
libmkl_intel.so	Interface library for the Intel compilers. Also use for other supported compilers that do not have a specialized Intel MKL interface library.			
libmkl_gf.so	Interface library for the GNU Fortran compiler	GNU* Compiler Collection support	Yes	
Threading Layer				
libmkl_intel_thread.so	Threading library for the Intel compilers			
libmkl_gnu_thread.so	Threading library for the GNU Fortran and C compilers	GNU* Compiler Collection support	Yes	
libmkl_pgi_thread.so	Threading library for the PGI* compiler	PGI* compiler support		
libmkl_sequential.so	Sequential library			
Computational Layer				
libmkl_core.so	Library dispatcher for dynamic load of processor-specific kernel library			
libmkl_p4.so	Pentium <sup>®</sup> 4 processor kernel library			
libmkl_p4m.so	Kernel library for Intel® Supplemental Streaming SIMD Extensions 3 (Intel® SSSE3) enabled processors			
libmkl_p4m3.so	Kernel library for Intel® Streaming SIMD Extensions 4.2 (Intel® SSE4.2) enabled processors			
libmkl_avx.so	Kernel library for Intel® Advanced Vector Extensions (Intel® AVX) enabled processors			
libmkl_avx2.so	Kernel library for Intel® Advanced Vector Extensions 2 (Intel® AVX2) enabled processors			



File	Contents	Optional Component	
		Name	Installed by Default
libmkl_avx512.so	Kernel library for Intel® Advanced Vector Extensions 512 (Intel® AVX-512) enabled processors		
libmkl_vml_p4.so	VML/VSL/DF part of Pentium® 4 processor kernel		
libmkl_vml_p4m.so	VML/VSL/DF for Intel® SSSE3 enabled processors		
libmkl_vml_p4m2.so	VML/VSL/DF for 45nm Hi-k Intel® Core™2 and Intel Xeon® processor families		
libmkl_vml_p4m3.so	VML/VSL/DF for Intel® SSE4.2 enabled processors		
libmkl_vml_avx.so	VML/VSL/DF optimized for Intel® AVX enabled processors		
libmkl_vml_avx2.so	VML/VSL/DF optimized for Intel® AVX2 enabled processors		
libmkl_vml_avx512.so	VML/VSL/DF optimized for Intel® AVX-512 enabled processors		
libmkl_vml_ia.so	VML/VSL/DF default kernel for newer Intel® architecture processors		
libmkl_vml_cmpt.so	VML/VSL/DF library for conditional numerical reproducibility		
Cluster Libraries			
libmkl_scalapack_core.so	ScaLAPACK routines	Cluster support	
libmkl_cdft_core.so	Cluster version of FFT functions	Cluster support	
libmkl_blacs_intelmpi.so	BLACS routines for Intel MPI and MPICH2	Cluster support	
Message Catalogs			
locale/en_US/mkl_msg.cat	Catalog of Intel® Math Kernel Library (Intel® MKL) messages in English		

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File	Contents	Optional Con	nponent
		Name	Installed by Default
locale/ja_JP/mkl_msg.cat	Catalog of Intel MKL messages in Japanese. Available only if Intel MKL provides Japanese localization. Please see the Release Notes for this information.		

# **Detailed Structure of the Intel® 64 Architecture Directories**

# Static Libraries in the lib/intel64 Directory

Some of the libraries in this directory are optional. However, some optional libraries are installed by default, while the rest are not. To get those libraries that are not installed by default, explicitly select the specified optional component during installation.

File	Contents	Optional Component	
		Name	Installed by Default
Interface Layer			
libmkl_intel_lp64.a	LP64 interface library for the Intel compilers. Also use for other supported compilers that do not have a specialized Intel MKL interface library		
libmkl_intel_ilp64.a	ILP64 interface library for the Intel compilers. Also use for other supported compilers that do not have a specialized Intel MKL interface library		
libmkl_intel_sp2dp.a	SP2DP interface library for the Intel compilers	SP2DP interface	
libmkl_blas95_lp64.a	Fortran 95 interface library for BLAS for the Intel® Fortran compiler. Supports the LP64 interface	Fortran 95 interfaces for BLAS and LAPACK	Yes
libmkl_blas95_ilp64.a	Fortran 95 interface library for BLAS for the Intel® Fortran compiler. Supports the ILP64 interface	Fortran 95 interfaces for BLAS and LAPACK	Yes



File	Contents	Optional Component		
		Name	Installed by Default	
libmkl_lapack95_lp64.a	Fortran 95 interface library for LAPACK for the Intel® Fortran compiler. Supports the LP64 interface	Fortran 95 interfaces for BLAS and LAPACK	Yes	
libmkl_lapack95_ilp64.a	Fortran 95 interface library for LAPACK for the Intel® Fortran compiler. Supports the ILP64 interface	Fortran 95 interfaces for BLAS and LAPACK	Yes	
libmkl_gf_lp64.a	LP64 interface library for the GNU Fortran compilers	GNU* Compiler Collection support	Yes	
libmkl_gf_ilp64.a	ILP64 interface library for the GNU Fortran compilers	GNU* Compiler Collection support	Yes	
Threading Layer				
libmkl_intel_thread.a	Threading library for the Intel compilers			
libmkl_gnu_thread.a	Threading library for the GNU Fortran and C compilers	GNU* Compiler Collection support	Yes	
libmkl_pgi_thread.a	Threading library for the PGI compiler	PGI* Compiler support		
libmkl_sequential.a	Sequential library			
Computational Layer				
libmkl_core.a	Kernel library for the Intel® 64 architecture			
Cluster Libraries				
libmkl_scalapack_lp64.a	ScaLAPACK routine library supporting the LP64 interface	Cluster support		
libmkl_scalapack_ilp64.a	ScaLAPACK routine library supporting the ILP64 interface	Cluster support		
libmkl_cdft_core.a	Cluster version of FFT functions.	Cluster support		
libmkl_blacs_lp64.a	LP64 version of BLACS routines for MPICH.	Cluster support		
libmkl_blacs_ilp64.a	ILP64 version of BLACS routines for MPICH.	Cluster support		

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File	Contents	Optional Component	
		Name	Installed by Default
libmkl_blacs_intelmpi_lp64.a	LP64 version of BLACS routines for Intel® MPI Library and MPICH2 or higher.	Cluster support	
<pre>libmkl_blacs_intelmpi_ilp64.a</pre>	ILP64 version of BLACS routines for Intel MPI Library and MPICH2 or higher.	Cluster support	
libmkl_blacs_openmpi_lp64.a	LP64 version of BLACS routines supporting Open MPI.	Cluster support	
libmkl_blacs_openmpi_ilp64.a	ILP64 version of BLACS routines supporting Open MPI.	Cluster support	
libmkl_blacs_sgimpt_lp64.a	LP64 version of BLACS routines supporting SGI Message-passing Interface Toolkit* (MPT).	Cluster support	
libmkl_blacs_sgimpt_ilp64.a	ILP64 version of BLACS routines supporting SGI MPT.	Cluster support	

# Dynamic Libraries in the lib/intel64 Directory

Some of the libraries in this directory are optional. However, some optional libraries are installed by default, while the rest are not. To get those libraries that are not installed by default, explicitly select the specified optional component during installation.

File	Contents	<b>Optional Component</b>	
		Name	Installed by Default
libmkl_rt.so	Single Dynamic Library		
Interface Layer			
libmkl_intel_lp64.so	LP64 interface library for the Intel compilers. Also use for other supported compilers that do not have a specialized Intel MKL interface library		
libmkl_intel_ilp64.so	ILP64 interface library for the Intel compilers. Also use for other supported compilers that do not have a specialized Intel MKL interface library		



File	Contents	Optional Component	
		Name	Installed by Default
libmkl_intel_sp2dp.so	SP2DP interface library for the Intel compilers	SP2DP interface	
libmkl_gf_lp64.so	LP64 interface library for the GNU Fortran compilers	GNU* Compiler Collection support	Yes
libmkl_gf_ilp64.so	ILP64 interface library for the GNU Fortran compilers	GNU* Compiler Collection support	Yes
Threading Layer			
libmkl_intel_thread.so	Threading library for the Intel compilers		
libmkl_gnu_thread.so	Threading library for the GNU Fortran and C compilers	GNU* Compiler Collection support	Yes
libmkl_pgi_thread.so	Threading library for the PGI* compiler	PGI* Compiler support	
libmkl_sequential.so	Sequential library		
Computational Layer			
libmkl_core.so	Library dispatcher for dynamic load of processor-specific kernel		
libmkl_def.so	Default kernel library		
libmkl_mc.so	Kernel library for Intel® Supplemental Streaming SIMD Extensions 3 (Intel® SSSE3) enabled processors		
libmkl_mc3.so	Kernel library for Intel® Streaming SIMD Extensions 4.2 (Intel® SSE4.2) enabled processors		
libmkl_avx.so	Kernel library for Intel® Advanced Vector Extensions (Intel® AVX) enabled processors		
libmkl_avx2.so	Kernel library for Intel® Advanced Vector Extensions 2 (Intel® AVX2) enabled processors		
libmkl_avx512.so	Kernel library for dispatching Intel® Advanced Vector		

File	Contents	Optional Compo	onent
		Name	Installed by Default
	Extensions 512 (Intel® AVX-512) on Intel® Xeon® processors		
libmkl_avx512_mic.so	Kernel library for dispatching Intel® Advanced Vector Extensions 512 (Intel® AVX-512) on Intel® Xeon Phi™ processors and coprocessors		
libmkl_vml_def.so	Vector Math Library (VML)/Vector Statistical Library (VSL)/Data Fitting (DF) part of default kernels		
libmkl_vml_mc.so	VML/VSL/DF for Intel® SSSE3 enabled processors		
libmkl_vml_mc2.so	VML/VSL/DF for 45nm Hi-k Intel® Core™2 and Intel® Xeon® processor families		
libmkl_vml_mc3.so	VML/VSL/DF for Intel® SSE4.2 enabled processors		
libmkl_vml_avx.so	VML/VSL/DF optimized for Intel® AVX enabled processors		
libmkl_vml_avx2.so	VML/VSL/DF optimized for Intel® AVX2 enabled processors		
libmkl_vml_avx512.so	VML/VSL/DF optimized for Intel® AVX-512 on Intel® Xeon® processors		
libmkl_vml_avx512_mic.so	VML/VSL/DF optimized for Intel® AVX-512 on Intel® Xeon Phi™ processors and coprocessors		
libmkl_vml_cmpt.so	VML/VSL/DF library for conditional numerical reproducibility		
Cluster Libraries			
libmkl_scalapack_lp64.so	ScaLAPACK routine library supporting the LP64 interface	Cluster support	



File	Contents	Optional Component	
		Name	Installed by Default
libmkl_scalapack_ilp64.so	ScaLAPACK routine library supporting the ILP64 interface	Cluster support	
libmkl_cdft_core.so	Cluster version of FFT functions.	Cluster support	
libmkl_blacs_intelmpi_lp64.so	LP64 version of BLACS routines for Intel® MPI Library and MPICH2 or higher.	Cluster support	
<pre>libmkl_blacs_intelmpi_ilp64.so</pre>	ILP64 version of BLACS routines for Intel MPI Library and MPICH2 or higher.	Cluster support	
Message Catalogs			
locale/en_US/mkl_msg.cat	Catalog of Intel® Math Kernel Library (Intel® MKL) messages in English		
locale/ja_JP/mkl_msg.cat	Catalog of Intel MKL messages in Japanese. Available only if Intel MKL provides Japanese localization. Please see the Release Notes for this information.		

# Detailed Directory Structure of the $\ensuremath{\mathtt{lib/mic}}$ Directory

File	Contents
Static Libraries	
libmkl_intel_lp64.a	LP64 interface library for the Intel compilers
libmkl_intel_ilp64.a	ILP64 interface library for the Intel compilers
libmkl_blas95_lp64.a	Fortran 95 interface library for BLAS and Intel® Fortran compiler. Supports the LP64 interface.
libmkl_blas95_ilp64.a	Fortran 95 interface library for BLAS and Intel Fortran compiler. Supports the ILP64 interface.
libmkl_lapack95_lp64.a	Fortran 95 interface library for LAPACK and Intel Fortran compiler. Supports the LP64 interface.
libmkl_lapack95_ilp64.a	Fortran 95 interface library for LAPACK and Intel Fortran compiler. Supports the ILP64 interface.
libmkl_intel_thread.a	Threading library for the Intel compilers
libmkl_sequential.a	Sequential library

File	Contents
libmkl_core.a	Core computation library
libmkl_scalapack_lp64.a	Static library with LP64 versions of ScaLAPACK routines
libmkl_scalapack_ilp64.a	Static library with ILP64 versions of ScaLAPACK routines
libmkl_cdft_core.a	Static library with cluster FFT functions
libmkl_blacs_intelmpi_lp64.a	Static library with LP64 versions of BLACS routines for Intel MPI
libmkl_blacs_intelmpi_ilp64.a	Static library with ILP64 versions of BLACS routines for Intel MPI
Dynamic Libraries	
libmkl_rt.so	Single Dynamic Library
libmkl_ao_worker.so	The Intel® MIC Architecture library to implement the Automatic Offload mode
libmkl_intel_lp64.so	LP64 interface library for the Intel compilers
libmkl_intel_ilp64.so	ILP64 interface library for the Intel compilers
libmkl_intel_thread.so	Threading library for the Intel compilers
libmkl_sequential.so	Sequential library
libmkl_core.so	Core computation library
libmkl_scalapack_lp64.so	Dynamic library with LP64 versions of ScaLAPACK routines
libmkl_scalapack_ilp64.so	Dynamic library with ILP64 versions of ScaLAPACK routines
libmkl_cdft_core.so	Dynamic library with cluster FFT functions
libmkl_blacs_intelmpi_lp64.so	Dynamic library with LP64 versions of BLACS routines for Intel MPI
libmkl_blacs_intelmpi_ilp64.so	Dynamic library with ILP64 versions of BLACS routines for Intel MPI
locale/en_US/mkl_msg.cat	Catalog of Intel® Math Kernel Library (Intel® MKL) messages in English
locale/ja_JP/mkl_msg.cat	Catalog of Intel MKL messages in Japanese. Available only if Intel MKL provides Japanese localization. Please see the Release Notes for this information.





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