A Tour of the Sparse Linear Algebra Functionality in Intel® Math Kernel Library

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Agenda

Intel® MKL Sparse BLAS

Intel® MKL PARDISO

Intel® MKL Parallel Direct Sparse Solver for Clusters

Intel® MKL Iterative Sparse Solvers

Intel® MKL Extended Eigensolver

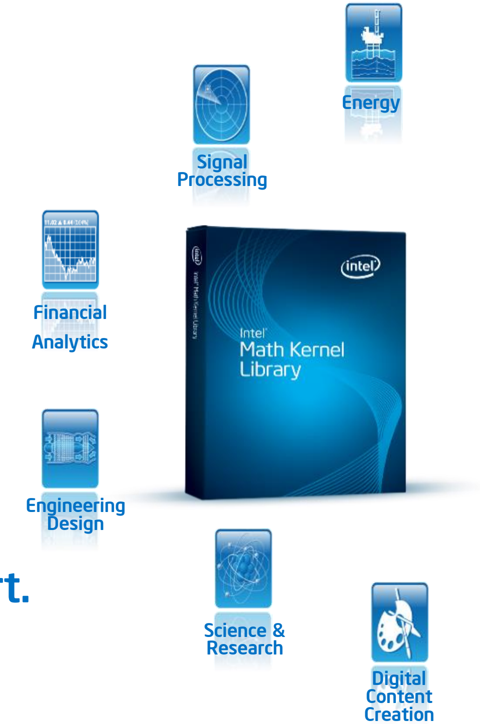
Intel® Math Kernel Library (Intel® MKL)

A feature-rich mathematical library designed with scientific, engineering and financial applications in mind.

Always optimized for the latest Intel® Xeon® and Intel® Xeon Phi™ product families.

Provides scientific programmers and domain scientists:

- Interfaces to de-facto standard APIs.
- Support for Linux*, Windows* and OS X* operating systems.
- The ability to extract great parallel performance with minimal effort.



Intel® MKL Used on the World's Fastest Supercomputers*

*http://www.top500.org

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Intel® MKL Sparse BLAS

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Functionality

x, y –vectors

A - sparse matrix

B, C – dense matrices

alpha, beta – scalars

op(A)=A or AT or conjg(AT)

Level 1

- y=a*x+y
- Dot products
- Rotation of points
- Gather/scatter

Level 2

- y=A*x
- y=alpha*op(A)*x+beta*y
- y= alpha*inv(op(A))*x

Level 3

- C=alpha*op(A)*B +beta*C
- Operations with parts L, D, U of matrix A decomposed as A=L+D+U
- C= alpha*inv(op(A))*B

  only for triangular matrix A

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Supported Sparse Matrix Storage Formats

CSR – Compressed Sparse Row storage format

CSC - Compressed Sparse Column storage format

DIA - Diagonal storage format

SKY - Skyline storage format

BSR - Block compressed sparse row storage format

COO - Coordinate storage format

Intel MKL provides subroutines to convert from one format to another.

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Important Features

Provides C and FORTRAN interface.

Supports 0-based and 1-based indexing.

Supports operations with partial matrices – *L, U, D*

```
char transa = 't';
char matdescra[6];
matdescra[0] = 't';  /* triangular */
matdescra[1] = 'l';  /* lower */
matdescra[2] = 'n';  /* non-unit diagonal*/
matdescra[3] = 'c';  /* 0-based indexing */

mkl_dcsrmm( &transa, &m, &n, &m,
            &alpha, matdescra,
            values, cols, rowIdx,
            &b, &n, &beta, &res, &n);
```

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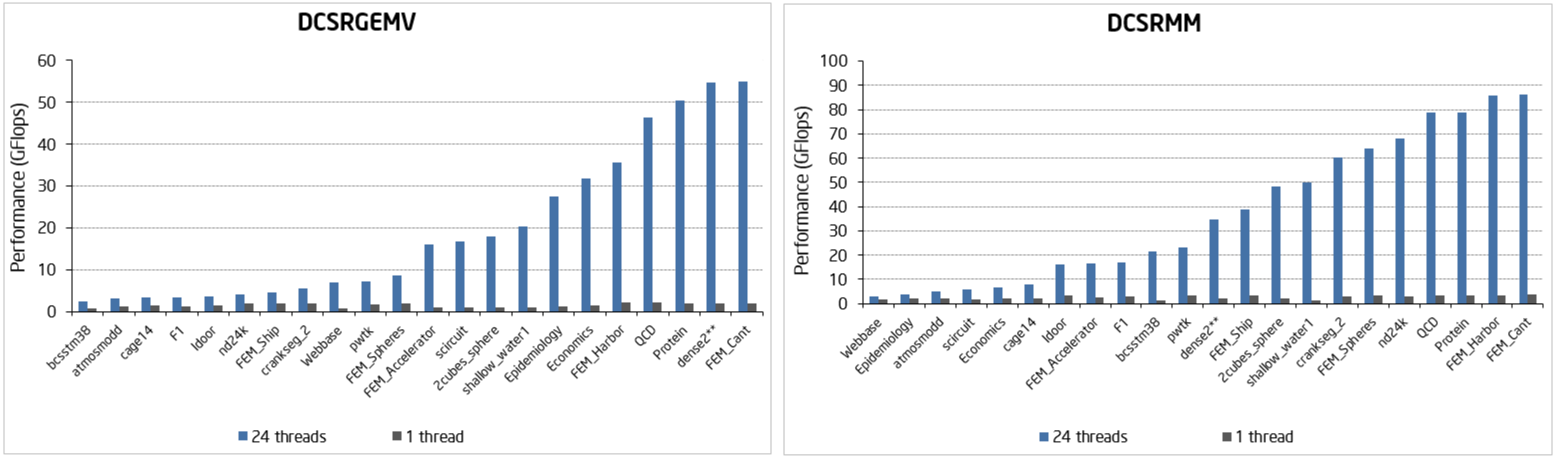
Performance

Excellent Performance and Scalability Using Intel® Math Kernel Library Sparse BLAS

DCSRGEMV and CDSRMM on Intel® Xeon® Processor E5-2697 v2



Configuration Info - Versions: Intel® Math Kernel Library (Intel® MKL) 11.1; Hardware: Intel® Xeon® Processor E5-2697 v2, 2 Twelve-Core CPUs (30MB LLC, 2.7GHz), 32GB of RAM; Operating System: RHEL 6 GA x86_64.

Software and workloads used in performance tests may have been optimized for performance only on Intel microprocessors. Performance tests, such as SYSmark and MobileMark, are measured using specific computer systems, components, software, operations and functions. Any change to any of those factors may cause the results to vary. You should consult other information and performance tests to assist you in fully evaluating your contemplated purchases, including the performance of that product when combined with other products. * Other brands and names are the property of their respective owners. Benchmark Source: Intel Corporation. ** All matrices except dense2 are from "The University of Florida Sparse Matrix Collection"(http://www.cise.ufl.edu/research/sparse/matrices/index.html)

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Performance greatly depends on matrix structure.

On Intel® Xeon Phi coprocessors, performance is optimized for CSR format.

- But, see the "Intel MKL SpMV Format Technology Preview Package"
- https://software.intel.com/en-us/articles/the-intel-math-kernel-library-sparse-matrix-vector-multiply-format-prototype-package

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Intel® MKL PARDISO

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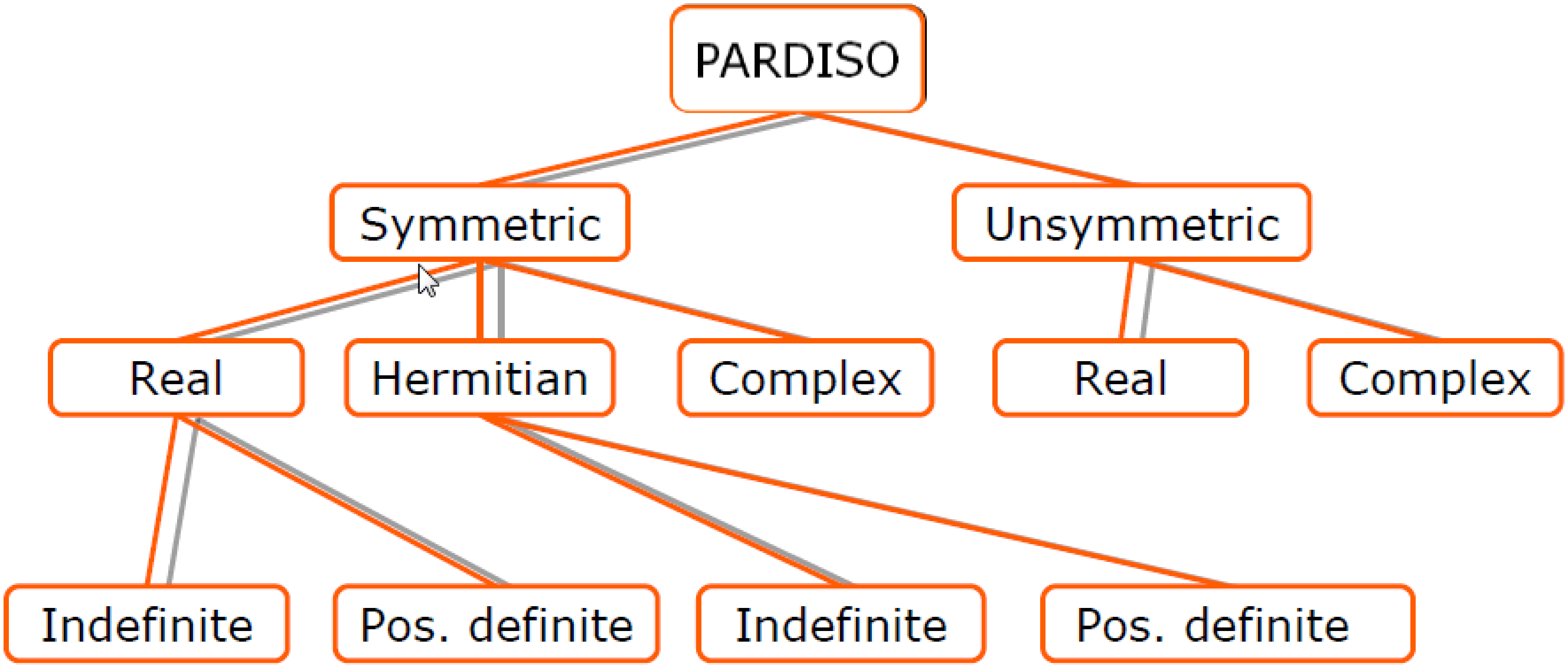
Intel® MKL PARDISO



$A = LDL^T$ $A = LL^T$ $A = LDL^H$ $A = LL^H$ $A = LU$

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Main Features

FORTRAN and C interfaces.

Supports 0-based and 1-based indexing.

CSR format only.

Comes with a matrix checker.

Solves multiple matrices at the same time.

- Matrices with the same portrait.

Solves system with multiple RHS at the same time.

- Effectively using multiple threads

Supports direct-iterative preconditioning.

- Many matrices to be solved with identical sparsity pattern but gradually changing of the nonzero coefficients.

OOC – Out-of-Core PARDISO.

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Usage Model

pardiso (pt, maxfct, mnum, mtype, phase, n, a, ia, ja, perm, nrhs, iparm, msglvl, b, x, error);

Initialization and parameters setting. Most important parameters:

- mtype – matrix type.
- phase – solution phases.
- iparm[64] – control various aspects of the solver.

Phase 1: Fill-in reduction analysis & reordering.

Phase 2: Numerical factorization.

Phase 3: Forward and Backward solve + Iterative refinement.

Termination and memory release.

User code can further control and fine tune each step.

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PARDISO Example

```
iparm[0] = 0; iparm[1] = 2; …… iparm[9] = 13; iparm[10] = 1; ……
iparm[34] = 1; …… iparm[59] = 0;
phase = 12;
pardiso( pt,                  → opaque handle
        &maxfct,              } number of matrices and the current matrix to solve
        &mnum,
        &mtype,               → matrix type
        &phase,               → solution phase
        &n,                   } number of rows, and the matrix in the CSR format
        a, ia, ja,
        &perm,                → permutation vector
        &nrhs                 → number of right-hand sides
        iparm;                → the iparm array
        &msglvl,              → message level
        &b, &x, &error);
phase = 33; iparm[7] = 2;
pardiso( pt, ……,
        &b,                   → right-hand side
        &x,                   → solution vector
        &error);
phase = -1;
pardiso(……);
```

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Direct Sparse Solver (DSS) Interface

DSS is a simplified interface of Intel® MKL PARDISO.

- Simpler and easier to use.
- Not as many fine tuning options.

A group of routines used in step-by-step solving process. Six steps:

- Initialization (dss_create)
- Matrix structure definition (dss_define_structure)
- Reordering (dss_reorder)
- Factorization (dss_factor_real, dss_factor_complex)
- Solve (dss_solve_real, dss_solve_complex)
- Release resource (dss_delete)

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Intel® MKL Parallel Direct Sparse Solver for Clusters

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Parallel Direct Sparse Solver for Clusters

A new feature in MKL 11.2 (coming out Q3'2014).

- Available for evaluation now in MKL 11.2 Beta.

Extends Intel® MKL PARDISOT to distributed memory systems.

Very competitive performance, comparing to MUMPS*, VSS*, and PETSc*.

Scales up to 1000 cores.

Familiar API to PARDISO users → Easy migration!

```
{
…
PARDISO (pt, &maxfct, &mnum, &mtype,
   &phase, &n, a, ia, ja, &idum,
   &nrhs, iparm, &msglvl, b, x,
   &error);
…
}
```

```
{
…
int comm =
   MPI_Comm_c2f(MPI_COMM_WORLD);
cluster_sparse_solver (pt, &maxfct,
   &mnum, &mtype, &phase, &n, a, ia,
   ja, &idum, &nrhs, iparm, &msglvl, b,
   x, &comm, &error);
…
}
```

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Distribution of Input Matrix (Example)

Subset1 =

6	-1	*	-3	*
-1	5	*	*	*
*	*	3	*	2

Rows from 1 to 3

Values	6	-1	-3	5	3	2
Column	1	2	4	2	3	5
rowInd	1	4	5	7		

Stored on MPI rank 1

Subset2 =

*	*	8	6	2
-3	*	6	10	*
*	*	4	*	5

Rows from 3 to 5

Values	8	6	2	10	5
Column	3	4	5	4	5
rowInd	1	4	5	6	

Stored on MPI rank 2

A=

6	-1	*	-3	*
-1	5	*	*	*
*	*	11	6	4
-3	*	6	10	*
*	*	4	*	5

The resulted matrix to be solved

Values	6	-1	-3	5	11	6	4	10	5
Column	1	2	4	2	3	4	5	4	5
rowInd	1	4	5	8	9	10			

Note: A is symmetric, only upper-triangular part is stored.

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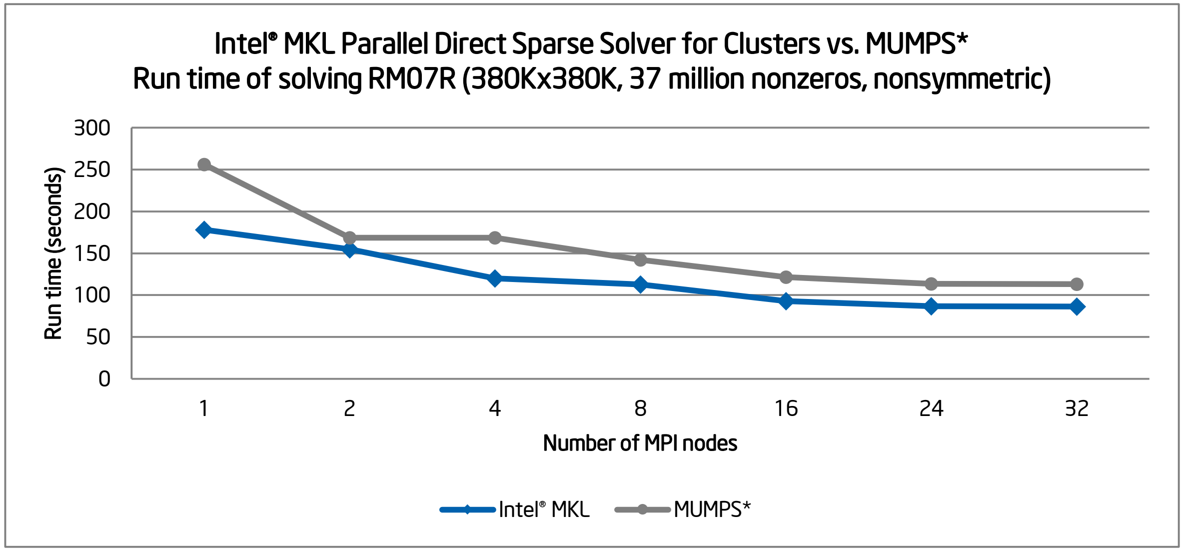
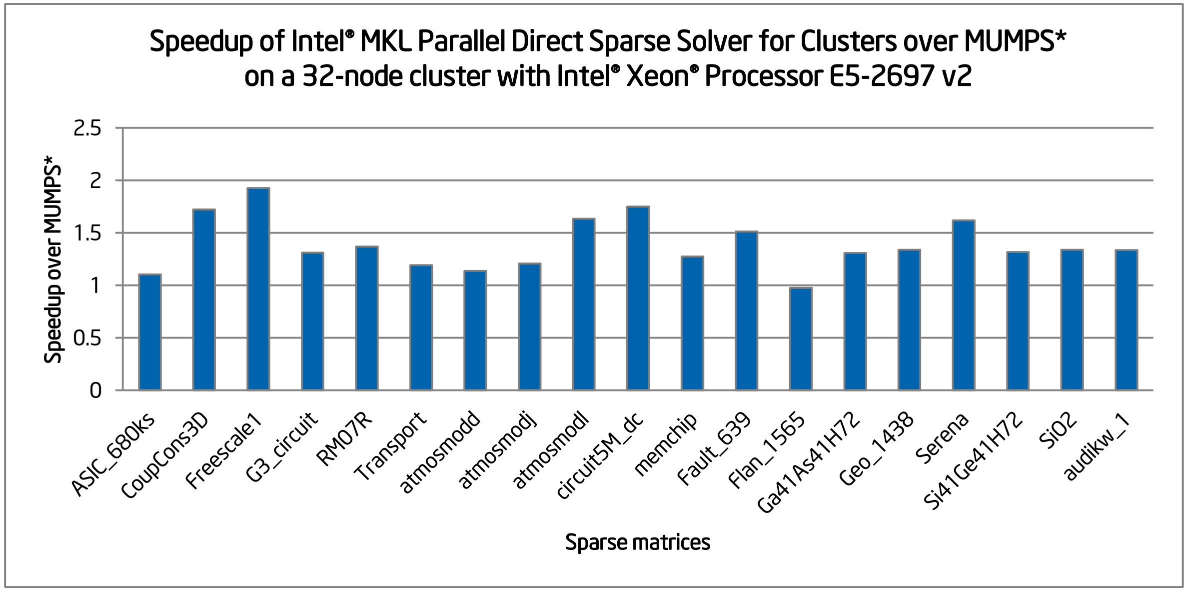
Performance Comparison





Versions: Intel® Math Kernel Library (Intel® MKL) 11.2 beta; Intel® MPI 4.1.

Hardware of cluster nodes: Intel® Xeon® Processor E5-2697 v2, 2 Twelve-Core CPUs (30MB LLC, 2.7GHz), 64GB of RAM. Interconnect: FDR Infiniband.

Operating System: RHEL 6.1 GA x86_64

Benchmark Source: Intel Corporation.

Theses matrices are from "The University of Florida Sparse Matrix Collection" (http://www.cise.ufl.edu/research/sparse/matrices/index.html).

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Intel® MKL Iterative Sparse Solvers

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Intel® MKL Iterative Sparse Solvers

MKL provides two iterative solvers:

- RCI Conjugate Gradient Solver - Symmetric Positive Definite matrices.
- RCI Flexible Generalized Minimal Residual Solver (FGMRES) – Nonsymmetric indefinite.
- Supports only real-valued matrices.

Preconditioners:

- ILU0: Less effective, less computation
- ILUT: More effective, more computation

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Reverse Communication Interface (RCI)

```
    initialize
        |
        |
        |
change parameters (manually)
        |
        |
        |
      check <--+
        |      |
        |      |
        |      |
      solve <--+
        |      |
        |      |
        |      |
       get <---+
```

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Intel® MKL Extended Eigensolver for Sparse Symmetric/Hermitian Eigen Problems

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An Innovative Method for Eigen Problems

Intel® MKL Extended Eigensolver is based on the FEAST algorithm:

- http://www.ecs.umass.edu/~polizzi/feast/
- Inspired by the contour integration technique in quantum mechanics.
- Subspace iteration method + Approximate spectral projection.
- Given a search interval [λ_min, λ_max], computes ALL eigenvalues and corresponding eigenvectors.

Symmetric/Hermitian standard Eigenproblem

$$Au = \lambda u,\ \lambda \in [\lambda_{\min}, \lambda_{\max}], A = A^*$$

Symmetric/Hermitian generalized Eigenproblem

$$Au = \lambda Bu, \lambda \in [\lambda_{\min}, \lambda_{\max}], A = A^*, B = B^* > 0$$

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Functionality

Predefined driver routines for ease-of-use:

- Supports only CSR format and 1-based indexing.
- Internally depends on PARDISO for solving sparse linear systems (90% of computation).

RCI based routines for customizability:

- User to provide linear system solver and matrix multiplication routine.
- More flexibility for specific application needs.

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Advantages

Efficiently solve Eigen problems for sparse matrices (symmetric or Hermitian).

Capture all multiplicities of Eigen values.

Highly parallelized algorithm:

- Great performance on multicore systems.
- Scalability depends on the internal linear sparse system solver.

Customizable:

- The RCI interface allows flexibility in solving special and challenging systems.
- E.g. users can use specialized iterative sparse solver and preconditioners.

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Predefined Driver Routine Usage Model

dfeast_scsrev (uplo, n, a, ia, ja, fpm, epsout, loop, emin, emax, m0, e, x, m, res, info);

User to provide:

- Search interval ***(emin, emax)*** and an estimation of the number of eigenvalues within a given search interval ***m0***
- The input matrix stored in the CSR format ***(uplo, n, a, ia, ja)***
- ***fpm*** – Controls number of contour points, stopping criteria, refinement loops, etc.

On output:

- ***epsout*** – Error on trace.
- ***loop*** – Number of refinement loops executed.
- ***e*** – Eigenvalues found in the search interval.
- ***x*** – Eigenvectors.
- ***m*** – Number of eigenvalues found.
- ***res*** – relative residuals.

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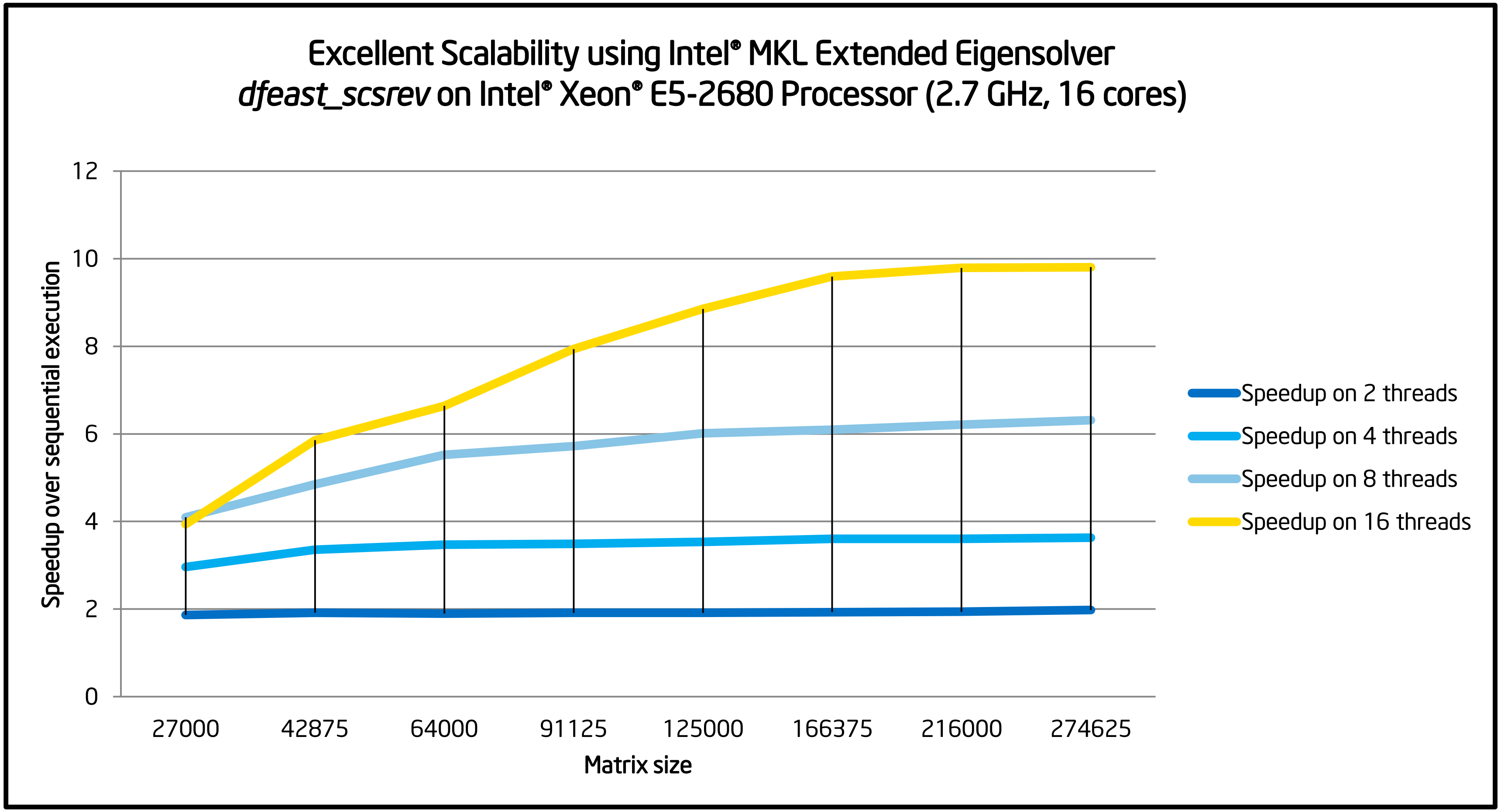
Performance



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Intel® MKL Provides Optimized Mathematical Building Blocks

Linear Algebra

- BLAS
- LAPACK
- Sparse Solvers
  - Iterative
  - Pardiso*
- ScaLAPACK

Fast Fourier Transforms

- Multidimensional
- FFTW interfaces
- Cluster FFT

Vector Math

- Trigonometric
- Hyperbolic
- Exponential, Log
- Power / Root

Vector RNGs

- Congruential
- Wichmann-Hill
- Mersenne Twister
- Sobol
- Neiderreiter
- Non-deterministic

Summary Statistics

- Kurtosis
- Variation coefficient
- Order statistics
- Min/max
- Variance-covariance

And More

- Splines
- Interpolation
- Trust Region
- Fast Poisson Solver

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Additional Resources

See PARDISO and Sparse BLAS in action:

- Code sample: Finding an approximate solution to a stationary nonlinear heat equation
  http://pages.cs.wisc.edu/~holzer/cs412/lecture03.pdf

Intel® MKL Cookbook:

- https://software.intel.com/en-us/mkl_cookbook

Intel® MKL User Forum:

- https://software.intel.com/en-us/forums/intel-math-kernel-library

Intel® MKL product site:

- https://software.intel.com/en-us/intel-mkl

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