KMATHLIB：
High Performance and Scalable Numerical Library for the K Computer

Large-scale Parallel Numerical Computing Technology Research Team, RIKEN AICS Research Division

KMATHLIB project

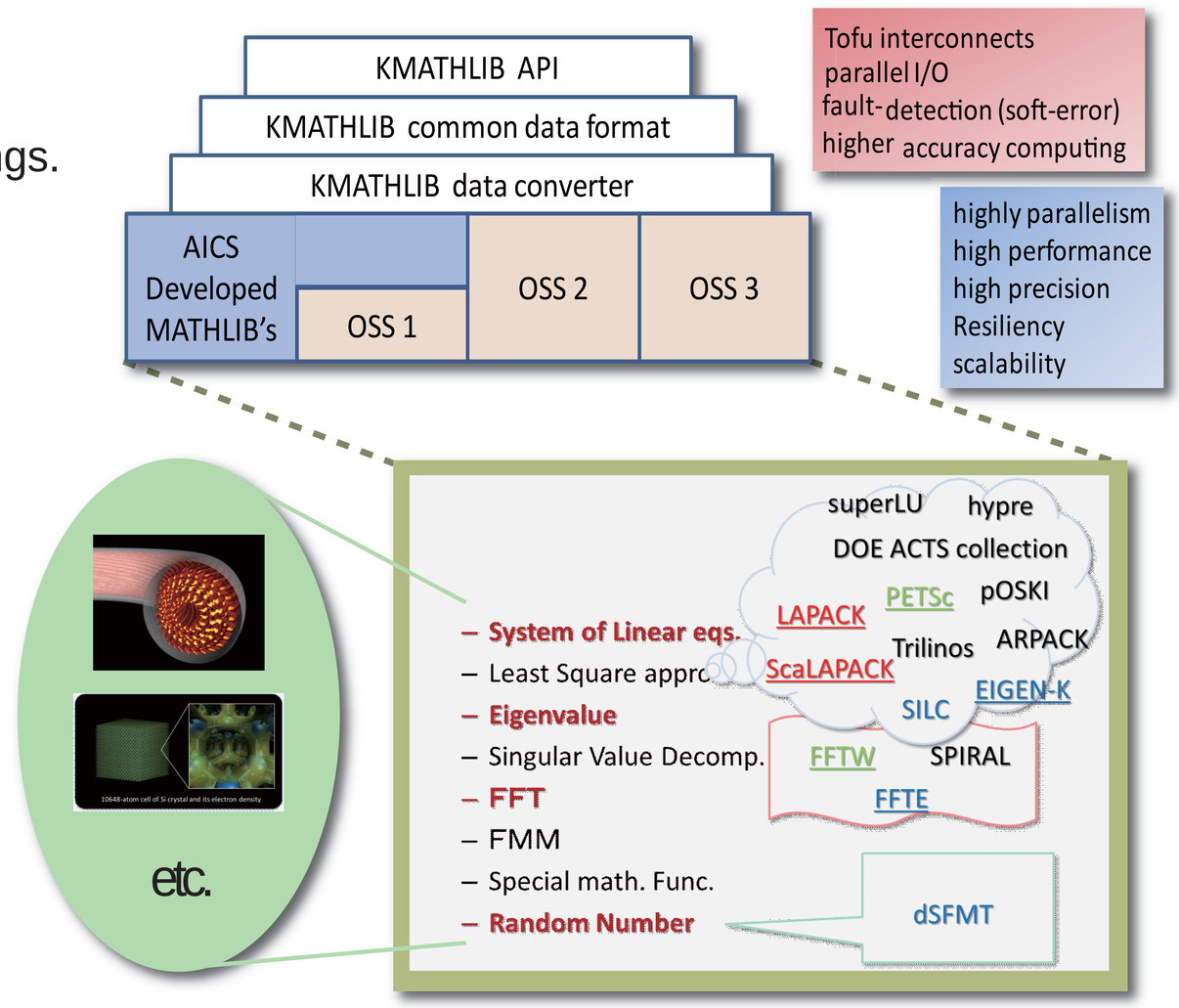
Our research team, the Large-scale Parallel Numerical Computing Technology Research Team, conducts research and development of large-scale, highly parallel and high-performance numerical software library on the K computer, named ‘KMATHLIB’. It comprises several components such as for

1) Solving linear systems, 2) Eigenvalue problems,
3) Singular value decomposition, 4) Fast Fourier transform,
5) Nonlinear equations, and other mathematical challengings.

Development of KMATHLIB

The purpose of KMATHLIB project is to manage HPC numerical software on the K computer. KMATHLIB is hierarchically structured and its development is made by the following steps:

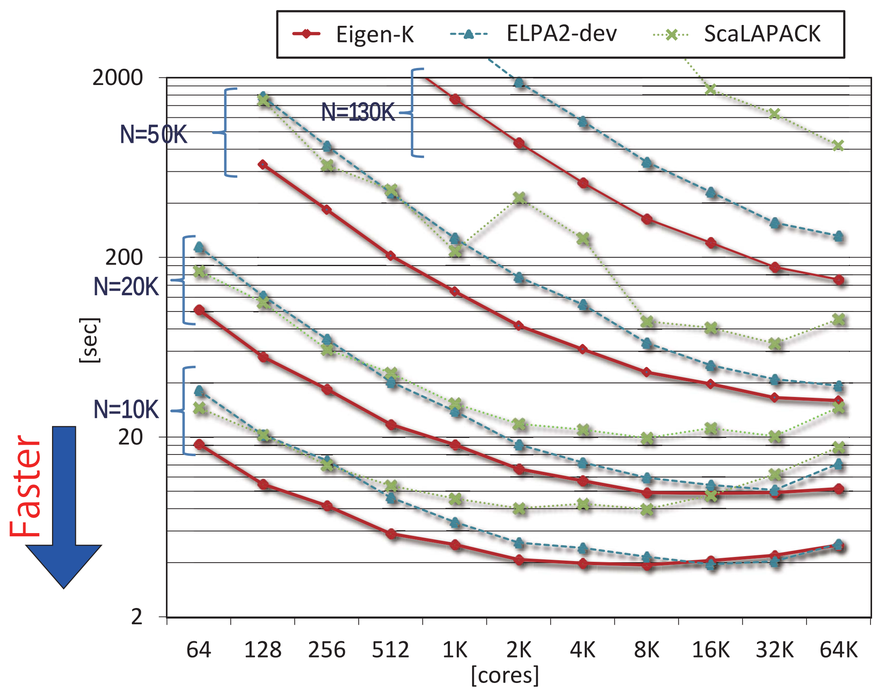
- Review the existing OSS features.
- Define API and common data format.
- Build data format converter and plugin mechanism.
- Develop extend features from OSS’s.
- Package successful OSS’s.



Current status of KMATHLIB

Followings are main components in the early stage development.

✔ Eigenvalue solver for dense matrices: Eigen-K
- Standard type (real symmetric and hermite)
- Generalized type (real symmetric and hermite)
- Non-symmetric type (developing)
- Sparse solver: z-Pares
  (developed by Prof. Sakurai, Tsukuba Univ.)

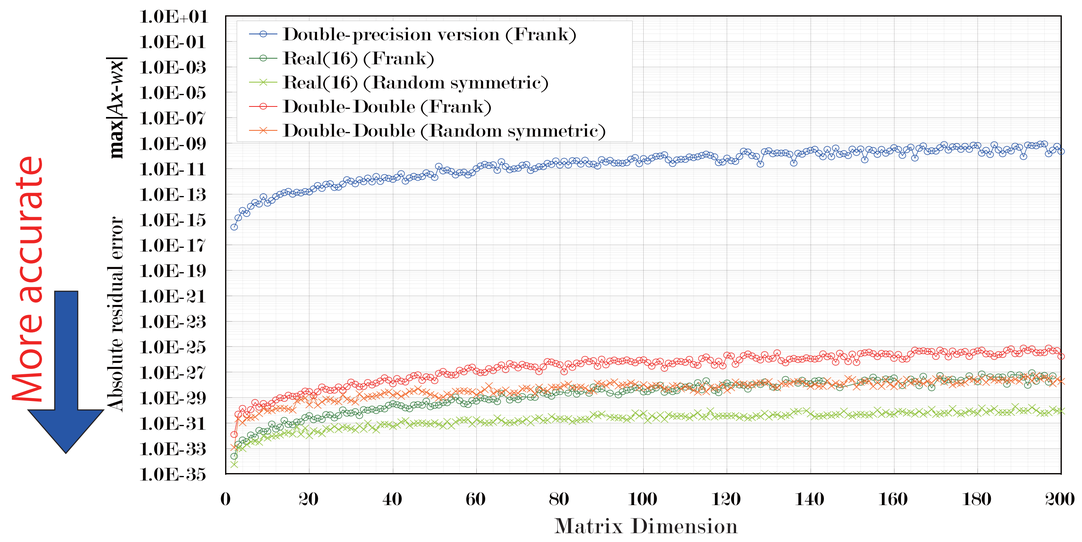


Standard type (real symmetric)

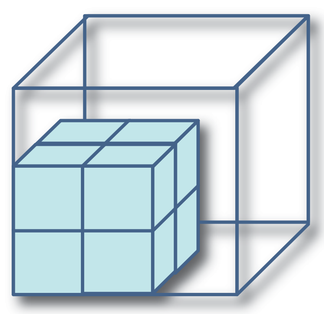
✔ Double-double precision eigenvalue solver: QPEigen-K

‘QPEigenK’ is now available on the K computer supporting the MPI and OpenMP hybrid parallelism. Accuracy improvement (16 digits) is confirmed by residual error as shown in the next Figure.

[1] T.Imamura S. Yamada, M. Machida, Preliminary report for a high precision distributed memory parallel eigenvalue solver, e-Poster presentation, SC12, Salt Lake City, Nov. 2012.



✔ FFT for 3D domain: FFTE or FFTW (developing)
- (3D-) Cubic decomposition FFT
  - We intend to increase parallelism compared to the existing (2D-) pencil decomposition.



✔ Random number generator: dsFMT
- MPI-distributed version
  - Mercenne twister engine

Part of KMATHLIB will be released soon.

Please contact us for further information.

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