Developing and Testing a Taskbased Approach for an High Performance Computing algorithm

Bachelor's thesis, Master's thesis, Student project
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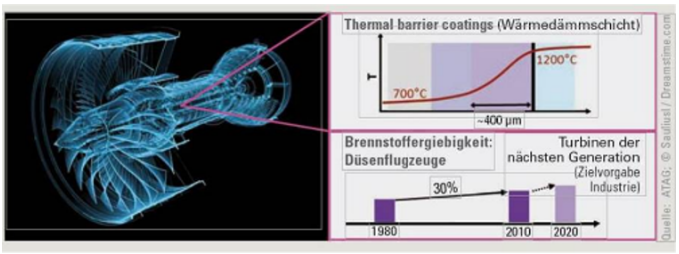
Abstract

For the transformation of the Generalized Eigenvalue Problem $Ax = \lambda Bx$ to the Standard Eigenvalue Problem $Ax = \lambda x$ we work on a novel algorithm. We want to test the application of a Task Based Approach for this transformation. Therefore an implementation of our novel algorithm for the Task Based Approach as well as the identification of a suitable Task Based Programming Framework is content of this project.

Global Picture

The solution of dense symmetric Eigenvalue problems is a crucial step in many simulations in science and engineering. Often solving a series of eigenvalue problems is the most expensive step in this simulations. Therefore powerful and highly scalable parallel algorithms are needed for this task.

Example: Electronic Structure Theory



- Prediction of material properties from atomic scale upwards
- Simulations are run on Supercomputers

Schrödinger equation

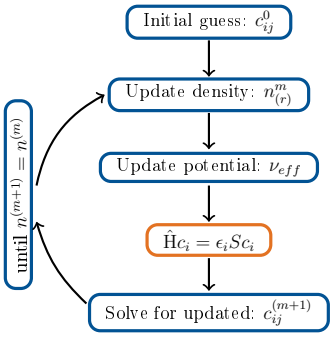
$$\hat{\mathcal{H}}\Phi_i = \mathrm{E}_i\Phi_i$$

$$\downarrow \text{Approx.} \downarrow \text{Discret.}$$

$$\hat{\mathrm{H}}c_i = \epsilon_i S c_i$$

$$\downarrow$$

Eigenproblem to solve in Iteration:



The ELPA library and the context

Together with our collaborators from other universities and several Max-Plank-institues we are working on ELPA [1, 2, 3], a highly scalable library for solving the Eigenvalue problem for dense symmetric matrices.
To solve the Eigenproblem we follow a two step approach: Transform the full matrix to banded form, transform the banded matrix to a tridiagonal matrix and solve the Eigenproblem on the tridiagonal matrix. Additionally, two backtransformations follow to get the correct Eigenvectors.

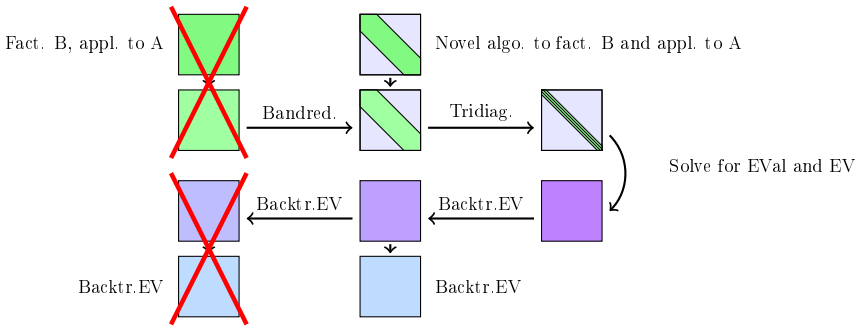


Figure 1: Algorithmic path of ELPA using the novel algorithm

However, in Electronic Structure Theory, a generalized Eigenvalue problem with banded matrices has to be solved. For this, we are working on a novel algorithm which will allow us to circumvent the expensive transformation to a banded matrix (see Figure 1). This algorithm has a structure that allows to use a Task Based Approach.

In standard programming model the path of the execution is well determined. The lines appearing first are executed first. In the **Task Based Approach** the algorithm is cut into tasks and the tasks are given to the framework manager. The manager decides upon certain criteria (is the task already executable? is it important to execute the task early?, etc.) which task is executed at a time.

In C/C++ exist libraries who allow to follow the Task Based Approach. The ELPA library, however, is written in Fortran90 and there are no libraries available.
To follow the Task Based Approach we want to implement the parts of our novel algorithm (only the transformation from the generalized Eigenproblem to the banded standard Eigenproblem) in C/C++ and test the Task Based Approach.

Tasks

- Find a suitable Task Based Programming Framework for parallel computing
- Implement parts of our novel algorithm for the transformation of the generalized to the banded Eigenproblem for the Task Based Framework

- Run performance measurements and compare the two approaches

Requirements

- Good programming skills
- Basic skills in parallel programming
- Knowledge in HPC and Computer Architecture
- Ideally background in Linear Algebra

Bibliography

[1] Elpa project website. http://elpa-aeo.mpcdf.mpg.de/.

[2] Thomas Auckenthaler. *Highly scalable eigensolvers for petaflop applications*. PhD thesis, PhD thesis. Fakultät für Informatik, Technische Universität München, 2012.

[3] Andreas Marek, Volker Blum, Rainer Johanni, Ville Havu, Bruno Lang, Thomas Auckenthaler, Alexander Heinecke, Hans-Joachim Bungartz, and Hermann Lederer. The elpa library: scalable parallel eigenvalue solutions for electronic structure theory and computational science. *Journal of Physics: Condensed Matter*, 26(21):213201, 2014.