Algorithm iteratively constructs a sequence of nested search spaces that are spanned by vectors of \( B \); Hermitian operator for which the orthonormal basis of eigenvectors \( B \) is analytically known. The newly proposed eigensolver consists in viewing the vibrational operator as a perturbation of an extensibility will be demonstrated on 7 atoms. Its scalability will be studied on mesoscale computers first (PlaFRIM, MCIA) and its extensibility will be demonstrated on national and European platforms. The scalable solver will be validated to efficiently compute vibrational spectra of molecules with 6 to 10 atoms. Its scalability will be studied on mesoscale computers first (PlaFRIM, MCIA) and its extensibility will be demonstrated on national and European platforms.

In this context, the purpose of the HiE PACS project is to perform efficiently frontier simulations arising from challenging research and industrial multiscale applications. The solution of these challenging problems require a multidisciplinary approach involving applied mathematics, computational and computer sciences. In applied mathematics, it essentially involves advanced numerical schemes. In computational science, it involves massively parallel computing and the design of highly scalable algorithms and codes to be executed on future petaflop (and beyond) platforms. Through this approach, HiE PACS intends to contribute to all steps that go from the design of new high-performance more scalable, robust and more accurate numerical schemes to the optimized implementations of the associated algorithms and codes on very high performance supercomputers.

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Context

Scientific priorities:
Computing the future: models, software and digital systems.

Scientific Research context:
Many applications (quantum chemistry, bio-diversity, ...) require the calculation of eigenpairs of very large matrices that arise either from the fine discretization of a given problem or from a problem defined in a very large dimensional space. The solution of those large problems can only be performed using numerical iterative schemes that often rely on matrix-vector product to project the problem in a lower dimensional space (a few tens of thousands) where the reduced problem becomes more tractable. The core of such a calculation is the solution of a small eigenvalue problem and efficient orthogonalization of a basis of the search space.

For the innermost eigenproblem dense linear kernel are considered to compute a part or the full spectrum of the projected matrix.

Assignment

The objective of this PhD is to develop an eigensolver on top of a task-based runtime system for parallel distributed heterogeneous platform. The building box will be the Chameleon [1] package for all dense linear algebra calculation that will be used to design the scalable implementation of a recently introduced eigensolver [2]. The runtime system StarPU, already used by Chameleon, will be considered to implement this new solver.

The scalable solver will be validated to efficiently compute vibrational spectra of molecules with 6 to 7 atoms. Its scalability will be studied on mesoscale computers first (PlaFRIM, MCIA) and its extensibility will be demonstrated on national and European platforms.

The newly proposed eigensolver consists in viewing the vibrational operator as a perturbation of an Hermitian operator for which the orthonormal basis of eigenvectors \( B \) is analytically known. The algorithm iteratively constructs a sequence of nested search spaces that are spanned by vectors of \( B \);
the expansion of the search space is monitored by selecting the dominating direction of the scaled residuals. At a given iteration, the Rayleigh quotient matrix associated with the current basis is computed that results in a large unsymmetric matrix whose eigenvalues in the interval of interest are computed using an Arnoldi or Krylov-Schur method. The implementation of these later numerical methods requires the construction of an orthonormal basis of a Krylov space and the calculation of Ritz pairs of a small dense matrix using numerical kernels from Chameleon.

Main activities

Keywords:
Linear algebra, eigensolver, runtime system, task parallelism

References:


Skills

Required Knowledge and background:
Knowledgeable in linear algebra and HPC, C/C++

Benefits package

- Subsidised catering service
- Partially-reimbursed public transport

Remuneration

1982€ / month (before taxes) during the first 2 years, 2085€ / month (before taxes) during the third year.