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 (\cite{2}). 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 (\cite{2}). 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 (\cite{2}).

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.