

Project Team INRIA : HiePACS

Authors of the post-doctoral research subject : O. Coulaud, L. Giraud

Title of the post-doctoral research subject :

Parallel eigensolvers in Computational Chemistry

Scientific priorities :

Modeling, Simulation and Optimization of Complex Dynamic Systems

Scientific Research context :

The calculation of the physical properties of large molecules requires the computation of the eigenpairs (eigenvalue and associated eigenvectors) of large sparse structured symmetric non-Hermitian matrices arising from the discretization by variational or perturbational method of the vibrational schrodinger equation in the anharmonic case. The size of the matrices depends on the complexity of the molecule of interest and can be up-to a few tens of millions while the number of states (i.e., eigenpairs) range from a few unities to a few hundreds.

In that framework, advanced and efficient parallel eigensolvers are required such as those based on Krylov subspace techniques. Because the targeted eigenvalues are often clustered, block-variants of these solvers should be favored.

Finally, due the problem size the use of large parallel platform is mandatory to tackle this challenging calculation.

Post-doctoral researcher work description :

The candidate will primary work on block-Krylov subspace methods such as block Arnoldi and block Jacobi-Davidson techniques. She/He will first review the most recent developments on this subject in order to indentify what variants are the most promising according to the features of the targeted application. For this purpose, some basic code prototypes will be developed to assess the relevance of the selected schemes. The scheme offering the best trade-off between the numerical performance and intrinsic parallel characteristics will be implemented in a parallel package. The robustness of the design parallel numerical schemes will be assessed on large challenging applications and simulations will be performed on large computing platforms.

Required Knowledge and background :

The successful development of the scientific work described above requires a strong background in applied mathematics (to design/adapt numerical schemes) and in computer science (to perform an efficient parallel implementation); therefore a PhD in computational sciences (applied maths and/or computer science) would be ideal.

Former experiences in parallel code development (MPI, muti-threading) and a good knowledge in parallel numerical linear algebra algorithms is a requirement. A strong interest in large numerical simulation would surely be an additional asset.

References :

1. Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide. SIAM 2000, Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and Henk van der Vorst .
2. Matrix Algorithms Volume II: Eigensystems. SIAM 2001, G. W. Stewart.
- 3 New parallel software (P_Anhar) for Anharmonic vibrational calculations: application to (CH₃Li)₂, N. Gohaud, D. Begue, C. Darrigan, C. Pouchan.

Keywords : Block eigensolver, computational chemistry, large scale parallel simulation.

Duration : 12 months