How to use MPI_GEVP_InvIter_qp and associated routines

This document is intended to describe the computationally fast Fortran 90+ quadruple precision (real(16)) portable parallel GRSDEP (generalized real symmetric-definite eigenvalue problem) package suitable for large (80,000 x 80,000 or greater) dense matrices discussed in [1]. The package itself consists of the subroutine MPI_GEVP_InvIter_qp (in the file MPI_GEVP_InvIter_qp.f) which solves the generalized eigenvalue problem (GEVP)

$$\mathbf{HC} = \mathbf{ESC} \tag{1}$$

using (shifted) inverse iteration, and the driver program MPI_GEVP_InvIter_solve_qp (in the file MPI_GEVP_InvIter_solve_qp.f) which reads the size of the problem (Nterms), an Etrial for the root of the GEVP to converge upon, and the Hamiltonian (H) and overlap (S) matrices for the GEVP to be solved. H (read from fort.7) and S (read from fort.8) must be stored in packed upper trianglar by columns format. A Makefile is provided which will compile the two fortran files and produce an executable MPI_GEVP_InvIter_solve_qp.exe. When executed,
MPI_GEVP_InvIter_solve_qp.exe runs the program MPI_GEVP_InvIter_solve_qp to perform the (shifted) inverse iteration used to convergence upon the desired eigenvalue.

To facilitate testing of the GEVP, the program Hatom4_qp (in file Hatom4_qp.f) is included. To compile the program Hatom4_qp and create the executable file Hatom4_qp.exe, the command is
fortran_compile_command -o Hatom4_qp.exe Hatom4_qp.f
When executed, Hatom4_qp.exe generates H and S matrices for solving the eigenvalue problem for 4 (non-interacting) hydrogen atoms (^{1}S states only), each of

which is represented by a one-electron basis of conventional un-normalized, non-orthogonal Slater-type orbital (STO) s orbitals:

$$\phi(\mathbf{r}) = \phi(r) = r^{n-1}e^{-\alpha r}, n = 1, 2, 3, ...m. \tag{2}$$

The interest in the 4 Hatom system is because it is easy to generate H and S and has interesting eigenvalues, especially excited states.[1]

For a concrete example, download the distribution MPI_GEVP.Package.tar.gz and unwrap it using:
gunzip MPI_GEVP.Package.tar.gz
tar xvof MPI_GEVP.Package.tar

Next use the commands:
make
and
fortran_compile_command -o Hatom4_qp.exe Hatom4_qp.f
to create the executables Hatom4_qp.exe and MPI_GEVP_InvIter_solve_qp.exe.

Now execute the program Hatom4_qp.exe. You will be prompted for m (size of STO set) and alpha (non-linear parameter of the STOs), see Equation 2. Hatom4_qp.exe first calculates the H (fort.7) and S (fort.8) matrices for a single H atom and then uses these matrices to build up H and S for the 4 atom case, hence the calculation will be for an Nterms $= m^4$ term expansion. Nterms will be printed by Hatom4_qp.exe.

Create the file aa containing the Nterms printed by Hatom_qp.exe and an Etrial, followed by the line 0 0 to terminate input (provision is made for more than one line to allow for truncations to be computed). Then execute the command
mpirun -np 8 ./MPI_GEVP_InvIter_solve_qp.exe
to run the eigensolver on 8 processes.

For example:

Hatom4_qp.exe input string	Screen output
3 0.95 -2.0002	Nterms = 81

File aa	Screen output
81 -2.0002d0	E = -1.9999 9998 6385

[1] There are roots for large N at -2.0, -1.625, -1.5555555555, -1.50, and so on if one of the H atoms is excited and corresponding roots if 2 H atoms are excited, etc.

In this way, letting m = 1,2,3,4,5,6,7 in successive runs, the following results were obtained:

Table 1: Code = MPI_GEVP_InvIter_solve_qp STO basis alpha = 0.95
Etrial = -2.0002

STO basis m	No. Terms	Eigenvalue (hartree)	Solve time[1] (sec.)
1	1	-1.9950 0000 0000 0000 0000 0000 0000	0.000
2	16	-1.9999 8965 5128 1311 5559 3320 6756	0.001
3	81	-1.9999 9998 6385 6790 4064 3612 6741	0.009
4	256	-1.9999 9999 9985 0785 4231 5306 2862	0.040
5	625	-1.9999 9999 9999 9852 8294 2287 5922	0.335
6	1296	-1.9999 9999 9999 9999 8645 2835 1441	2.353
7	2401	-1.9999 9999 9999 9999 9998 8123 8137	13.966

[1]All times are for 8 processors except m = 1 is for 1 processor.

Note the 20 digit accuracy with m = 7. To examine higher S states of the 4 H atom case, change alpha and use, for example, Etrial = -1.624 to converge on the first excited state. An interesting experiment with this basis is to attempt to represent the ground and first excited states with the same basis set. Using alpha = 0.65 and m = 10 (so Nterms = 10000), with aa:
10000 -2.0002
10000 -1.624
0 0
the results are
E(10000) = -1.9999 9999 9986 4935 7509 6677 6521 hartree
and
E(10000) = -1.6249 9999 9826 0000 6317 7097 8563 hartree,
so the two lowest states are calculated to about 11 digits with one alpha. The reason for not getting more converged roots in this case is that the STO basis has only one non-linear argument whereas the orbital exponents for the first 4 H atom states are 0.5, 0.5/4, 0.5/9, 0.5/14, ... So it is hard to satisfy the STO requirements for more than one state with one alpha.

When doing runs, after generating the H and S matrices on units 7 and 8, be sure

to edit the file aa accordingly. As we pointed out in [1], it is sufficient to know the trial eigenvalue Etrial to 5 digits. When this is not known, one can use NAG [2] or LAPACK [3] libraries with short expansions to get the starting value.

References

[1] J. S. Sims and M. B. Ruiz. Parallel Generalized Real Symmetric-Definite Eigenvalue Problem. *J. Res. NIST*, 2020. to be published.

[2] The NAG Library, The Numerical Algorithms Group, Oxford, United Kingdom, www.nag.com.

[3] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen. *LAPACK Users' Guide*. Society for Industrial and Applied Mathematics, Philadelphia, PA, third edition, 1999.