Document of ELSES Matrix Library

(http://www.elses.jp/matrix/)

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Contents

1 Introduction

1.1 About ELSES Matrix Library

ELSES Matrix Library (`http://www.elses.jp/matrix/`) is the collection of matrix data generated by ELSES (`http://www.elses.jp`, ELSES=Extra-Large-Scale Electrnic Structure calculation). The matrices are sparse real-symmetric or Hermitian and appear in generalized and standard eigen-value equations.

If you use the matrix data in a publication, please cite our paper(s), as shown in the below examples:

Example 1

The used matrix data are stored at ELSES Matrix Library (http://www.elses.jp/matrix/) [1].

Example 2

The used matrix data are stored at ELSES Matrix Library (http://www.elses.jp/matrix/) [1] and were generated by ELSES (http://www.elses.jp/) [2], a quantum mechanical nanomaterial simulator.

1.2 Brief explanation of data

- The package name contains the size. For example, the matrix package " BNZ30 " contains matrices with the size of N=30.
- The matrices appear in generalized or standard eigenvalue equations of

$$A\boldsymbol{x}_k = \lambda_k B\boldsymbol{x}_k \quad (\boldsymbol{x}_k^{\mathrm{T}} B\boldsymbol{x}_k = 1). \tag{1}$$

  The matrices of A and B are sparse, real-symmetric or Hermitian and the matrix B is positive definite. In the standard eigenvalue equations, the matrix B is reduced to the unit matrix ($B = I$).
- Several packages include the calculated eigenvalue data of $\{\lambda_k\}$, as well as the input matrices of A and B. Several packages also include the data of the inverse participation ratio (IPR) for the calculated eigenvectors (IPR($\boldsymbol{x}_k$)). The inverse participation ratio is defined for a vector $\boldsymbol{v} \equiv (v_1, v_2, ..., v_N)$ as

$$\mathrm{IPR}(\boldsymbol{v}) \equiv \sum_j^N |v_j|^4. \tag{2}$$

  The values were obtained by the LAPACK or ScaLAPACK routines, except where indicated.
  Note : The participation ratio appears in quantum localization theory of condensed matter physics and its inverse is called inverse participation ratio. See a review [3] for the physical origin.
- The matrix data is recorded in the Matrix-Market format [1]. The atomic unit is used for energy unit.
- Some packages are presented as an encrypted zip file that contains matrix data and a README file (README.txt). The password for decryption is " ELSES2007 " .
- The library is maintained mainly by Takeo Hoshi [2].

[1] `http://math.nist.gov/MatrixMarket/index.html`
[2] `http://www.damp.tottori-u.ac.jp/~hoshi/`

1.3 History

The library was built by the request of numerical researchers who need sparse matrices in real problems. The efficiency of linear algebraic solvers, in particular sparse matrix solvers, can depend on the matrix properties and it is important to compare the solver algorithms with the same test problems. The above fact motivated us to build this library.

Figure 1 shows, as examples, the matrices of APF4686 in Sec. 2.1.8 and AUNW9180 in Sec. 2.1.11. The two matrices are significantly different in the number of non-zero elements. These matrices are used in in Ref. [4], before the foundation of this library. 'Test problem 1' and '2' in Ref. [4] are the cases of APF4686 and AUNW9180, respectively.

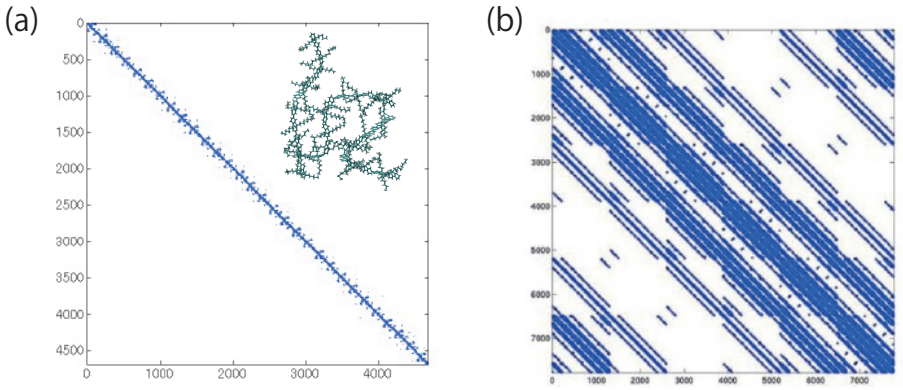

Figure 1: Examples of the matrices; The non-zero elements are plotted for (a) APF4686 and (b) AUNW9180.

Several matrix data were generated as a 'series', because numerical researches would like to use them as a systematic investigation. One example is the data of vibrating carbon nanotube (VCNT); VCNT900, VCNT1800, VCNT4500, VCNT9000, VCNT22500, VCNT90000, VCNT225000, VCNT900000, VCNT1008000. They are different in the size but similar in the non-zero element pattern.

1.4 Theory and a simplest case with 2 x 2 matrices

This subsection is devoted to an elementary explanation of the physical theory for numerical researchers. We will demonstrate the problem in a simplest case with 2 x 2 matrices for hydrogen molecule (H_2). Such explanation appears among many elementary textbooks of quantum mechanics for material science.

The fundamental Schrödinger-type equation is written for an electronic wavefunction $\phi(\boldsymbol{r})$ as

$$\hat{H}\phi(\boldsymbol{r}) = \lambda\phi(\boldsymbol{r}) \tag{3}$$

where $\hat{H}$ is the Hamilton operator or Hamitonian

$$\hat{H} \equiv -\frac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}). \tag{4}$$

Here, Δ is Laplacian, m is the mass of electron and $\hbar$ is the Planck constant, a physical constant ($\hbar \approx 1.05^{-34}$Js). $V(\boldsymbol{r})$ is the effective potential, a scalar funtion. In general, the potential V depends on the positions of atomic nucleus and the electronic waves but is considered to be a given scalar function, for simplicity, at the present subsection.

Now $\phi(\boldsymbol{r})$ is expressed as a linear combination of given basic functions

$$\phi(\boldsymbol{r}) = \sum_j^M v_j\chi_j(\boldsymbol{r}). \tag{5}$$

The basis functions $\{\chi_j(\boldsymbol{r})\}$ are normalized to be

$$\int \chi_j^*(\boldsymbol{r})\chi_j(\boldsymbol{r})d\boldsymbol{r} = 1. \tag{6}$$

A typical method is called Linear Combination of Atomic Orbital (LCAO), in which a basis functions is localized and its localization center is the position of an atomic nucleus.

A generalized eigenvalue equation appears, when Eq (5) is substituted for Eq. (3);

$$A\boldsymbol{v} = \lambda B\boldsymbol{v} \tag{7}$$

with the $M \times M$ matrices of

$$A_{ij} \equiv \int \chi_i^*(\boldsymbol{r})\hat{H}\chi_j(\boldsymbol{r})d\boldsymbol{r} \tag{8}$$

$$B_{ij} \equiv \int \chi_i^*(\boldsymbol{r})\chi_j(\boldsymbol{r})d\boldsymbol{r}. \tag{9}$$

The matrices A and B are Hermitian. The matrix B is positive definite and satisfies $B_{jj} = 1$ and $|B_{ij}| < 1 (i \neq j)$. When the basis functions are real, the matrices A and B are real-symmetric.

A simplest case is one for hydrogen molecule (H_2). The atomic nucleus of the first or second hydrogen atom is located at $\boldsymbol{r} = \boldsymbol{R}_1$ or $\boldsymbol{R}_2$, respectively. We consider a localized function $f(\boldsymbol{r})$ of which localization center is located as $\boldsymbol{r} = 0$. Two basis functions $\chi_1(\boldsymbol{r})$ and $\chi_2(\boldsymbol{r})$ are prepared as

$$\chi_1(\boldsymbol{r}) \equiv f(\boldsymbol{r} - \boldsymbol{R}_1), \quad \chi_2(\boldsymbol{r}) \equiv f(\boldsymbol{r} - \boldsymbol{R}_2). \tag{10}$$

The generalized eigenvalue problem of Eq. (7) appears with the 2 × 2 real-symmetric matrices of

$$A \equiv \begin{pmatrix} a & -t \\ -t & a \end{pmatrix}, \quad B \equiv \begin{pmatrix} 1 & s \\ s & 1 \end{pmatrix}. \tag{11}$$

Here, a, t, s are given positive real parameters and $s < 1$. The eigenvalue λ is determined by

$$0 = \left|A - \lambda B\right| = \begin{vmatrix} a-\lambda & -t-\lambda s \\ -t-\lambda s & a-\lambda \end{vmatrix} = (a-\lambda)^2 - (t+\lambda s)^2 \tag{12}$$

or

$$a - \lambda = \pm(t + \lambda s). \tag{13}$$

Then we obtain the eigenvalues $\lambda = \lambda_1, \lambda_2$ of

$$\lambda_1 \equiv \frac{a-t}{1+s}, \quad \lambda_2 \equiv \frac{a+t}{1-s}. \tag{14}$$

The eigenvectors are obtained by

$$\boldsymbol{v}_1 = \frac{1}{\sqrt{2(1+s)}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \boldsymbol{v}_2 = \frac{1}{\sqrt{2(1-s)}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{15}$$

and satisfies

$$A\boldsymbol{v}_i = \lambda_i B \boldsymbol{v}_i. \tag{16}$$

It is noteworthy that the matrix B has the eigenvalues of $1 \pm s$ and will be not positive definite in the limiting situation of $s \to 1$. Such limiting situation appears in an unphysical case, in which the distance between the atom nuclei is almost zero ($d \equiv |\boldsymbol{R}_1 - \boldsymbol{R}_2| \to 0$).

2 List of ELSES matrices

2.1 Real-symmetric matrices for generalized eigen-value equations

2.1.1 BNZ30 (updated at 27. Feb. 2018)

The present package gives tiny matrices for a tutorial. The data appears in an electronic structure calculation of benzene (C_6H_6).

This is the detailed explanation of the package:

```
ELSES_MATRIX_BNZ30_20180227.tgz
from ELSES matrix library (http://www.elses.jp/matrix/)
-----------------------------------------------
Matrix data "BNZ30"
  generated by ELSES
          T. Hoshi, 27. Feb. 2018
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A, B: N x N real-symmetric matrix with N = 30
B : positive definite
e_k : eigenvalue
y_k : eigenvector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_BNZ30_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_BNZ30_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_BNZ30_ev.txt
 list of eigenvalues
ELSES_MATRIX_BNZ30_ipr.txt
 list of inverse participation ratio
-----------------------------------------------
```

2.1.2 PPE354

The matrix data appears for an organic polymer poly-(phenylene-ethynylene) (PPE) in the para (linear-chain) structure with 10 monomers or 120 atoms. See Refs. [10, 12] for details. 'Rotational disorders' or random numbers on the dihedral angles between benzene rings are introduced like Fig. 4.11 (b) of Ref. [12].

```
-------------------------------------------
Original problem:
-------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 354
B : positive definite
e_k : eigen value
y_k : eigen vector
-------------------------------------------
Files
-------------------------------------------
ELSES_MATRIX_PPE354_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_PPE354_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_PPE354_ev.txt
 list of eigen values
ELSES_MATRIX_PPE354_ev.txt
 list of inverse participation ratio
-------------------------------------------
```

2.1.3 VCNT900

The matrix data appears for a vibrating carbon nanotube within a supercell with spd orbitals. [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT900_20130820.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT900"
  generated by ELSES
          T. Hoshi, 20. Aug. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 900
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT900_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT900_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_VCNT900_E.txt
 list of eigen values
-----------------------------------------------
```

Note: The used atomic structure is the one in VCNT400std, generated with sp orbitals.

2.1.4 VCNT1800

The matrix data appears for a vibrating carbon nanotube within a supercell with spd orbitals. [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT1800_20130820.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT1800"
  generated by ELSES
          T. Hoshi, 20. Aug. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 1800
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT1800_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT1800_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_VCNT1800_E.txt
 list of eigen values
-----------------------------------------------
```

Note: The used atomic structure is the one in VCNT800std, generated with sp orbitals.

2.1.5 ICNT1800

The matrix data appears for an ideal carbon nanotube within a supercell with spd orbitals. [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_ICNT1800_20130828.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "ICNT1800"
  generated by ELSES
          T. Hoshi, 28. Aug. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 1800
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_ICNT1800_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_ICNT1800_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_ICNT1800_E.txt
 list of eigen values
-----------------------------------------------
```

2.1.6 PPE3594

The matrix data appears for an organic polymer poly-(phenylene-ethynylene) (PPE) See the explanation of PPE354 in Sec. 2.1.2.

```
-------------------------------------------
Original problem:
-------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 3594
B : positive definite
e_k : eigen value
y_k : eigen vector
-------------------------------------------
Files
-------------------------------------------
ELSES_MATRIX_PPE3594_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_PPE3594_B.mtx
 matrix B in the Matrix-Market format
-------------------------------------------
```

2.1.7 VCNT4500

The matrix data appears for a vibrating carbon nanotube within a supercell with spd orbitals. [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT4500_20131206.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT4500"
  generated by ELSES
          T. Hoshi, 06. Dec. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 4500
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT4500_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT4500_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_VCNT4500_E.txt
 list of eigen values
-----------------------------------------------
```

Note: The used atomic structure is the one in VCNT2000std, generated with sp orbitals.

2.1.8 APF4686 (updated at 5. May. 2017)

The matrix data appears in an electronic structure calculation of a nanoscale amourphous-like conjugated polymer, poly-(9,9 dioctyl-fluorene) [2].

The package includes the files of

```
(1) ELSES_MATRIX_APF4686_A.mtx
 matrix A in the Matrix-Market format
(2) ELSES_MATRIX_APF4686_B.mtx
 matrix B in the Matrix-Market format
(3) ELSES_MATRIX_APF4686_ev.mtx
 list of eigen values
(4) ELSES_MATRIX_APF4686_ipr.mtx
 list of inverse participation ratio
```

Note : The package was updated with the date stamp of 5. May. 2017; The values of the eigenvalues and the inverse participation ratio were added. The input matrices were not updated.

2.1.9 PPE7194

The matrix data appears for an organic polymer poly-(phenylene-ethynylene) (PPE) See the explanation of PPE354 in Sec. 2.1.2.

```
-------------------------------------------
Original problem:
-------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 7194
B : positive definite
e_k : eigen value
y_k : eigen vector
-------------------------------------------
Files
-------------------------------------------
ELSES_MATRIX_PPE7194_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_PPE7194_B.mtx
 matrix B in the Matrix-Market format
-------------------------------------------
```

2.1.10 VCNT9000

The matrix data appears for a vibrating carbon nanotube within a supercell with spd orbitals. [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT9000_20130820.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT4500"
  generated by ELSES
          T. Hoshi, 20. Aug. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 9000
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT9000_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT9000_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_VCNT9000_E.txt
 list of eigen values
-----------------------------------------------
```

Note: The used atomic structure is the one in VCNT4000std, generated with sp orbitals.

2.1.11 AUNW9180

The matrix data appears in an electronic structure calculation of a helical multishell gold nanowire with defects [6].

```
ELSES_MATRIX_AUNW9180_20120718.tgz
from ELSES matrix library (http://www.elses.jp/matrix/)
-----------------------------------------------
Matrix data "AUNW9180"
  generated by ELSES
          T. Hoshi, 18. Jul. 2012
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A, B: N x N real-symmetric matrix with N = 9180
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_AUNU9180_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_AUNW9180_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_AUNW9180_E.txt
 list of eigen values
-----------------------------------------------
```

2.1.12 PPE17994

The matrix data appears for an organic polymer poly-(phenylene-ethynylene) (PPE) with 500 monomers or 6000 atoms. See the explanation of a shorter polymer of PPE354 in Sec. 2.1.2.

```
-------------------------------------------
Original problem:
-------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 17994
B : positive definite
e_k : eigen value
y_k : eigen vector
-------------------------------------------
Files
-------------------------------------------
ELSES_MATRIX_PPE17994_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_PPE17994_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_PPE17994_ev.txt
 list of eigen values
ELSES_MATRIX_PPE17994_ev.txt
 list of inverse participation ratio
-------------------------------------------
```

2.1.13 PENTF20400

The matrix data stems from a disordered pentacene thin-film with one atomic layer. The package includes the files of

```
(1) ELSES_MATRIX_PENTF20400_A.mtx
 matrix A in the Matrix-Market format
(2) ELSES_MATRIX_PENTF20400_B.mtx
 matrix B in the Matrix-Market format
(3) ELSES_MATRIX_PENTF20400_ev.txt
 list of eigen values
(4) ELSES_MATRIX_PENTF20400_ipr.txt
 list of inverse participation ratio
```

2.1.14 VCNT22500 (updated at 6. Aug. 2017)

The matrix data appears for a vibrating carbon nanotube (VCNT) within a supercell with spd orbitals. [9] The package includes the files of

```
(1) ELSES_MATRIX_VCNT22500_A.mtx
 matrix A in the Matrix-Market format
(2) ELSES_MATRIX_VCNT22500_B.mtx
 matrix B in the Matrix-Market format
(3) ELSES_MATRIX_VCNT22500_ev.txt
 list of eigen values
(4) ELSES_MATRIX_VCNT22500_ipr.txt
 list of inverse participation ratio
```

Note : The used atomic structure is the same as the one in VCNT10000std.
Note : The package was updated at 6. Aug. 2017. The data of the eigenvalues and the inverse participation ratio were added. The data were calculated with four nodes of the K computer by EigenKernel [11] with ScaLAPACK routines. The input matrices were not updated.

2.1.15 CPPE32346

The matrix data appears for condensed (nine, bundle-like) organic polymers poly-(phenylene-ethynylene) (PPE) . See Refs. [10, 12] for details.

```
-------------------------------------------
Original problem:
-------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 32346
B : positive definite
e_k : eigen value
y_k : eigen vector
-------------------------------------------
Files
-------------------------------------------
ELSES_MATRIX_CPPE32346_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_CPPE32346_B.mtx
 matrix B in the Matrix-Market format
-------------------------------------------
```

2.1.16 VCNT90000

The matrix data appears for a vibrating carbon nanotube within a supercell with spd orbitals. [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT90000_20130829.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT90000"
  generated by ELSES
          T. Hoshi, 29. Aug. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 90000
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT90000_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT90000_B.mtx
 matrix B in the Matrix-Market format
-----------------------------------------------
```

The used atomic structure is the one in VCNT40000std, generated with sp orbitals.

2.1.17 PENTF98736

The matrix data stems from a disordered pentacene thin-film with one atomic layer. The package includes the files of

```
(1) ELSES_MATRIX_PENTF98736_A.mtx
 matrix A in the Matrix-Market format
(2) ELSES_MATRIX_PENTF98736_B.mtx
 matrix B in the Matrix-Market format
(3) ELSES_MATRIX_PENTF98736_ev.txt
 list of eigen values
(4) ELSES_MATRIX_PENTF98736_ipr.txt
 list of inverse participation ratio
```

2.1.18 PPE107994

The matrix data appears for an organic polymer poly-(phenylene-ethynylene) (PPE) with 3,000 monomers or 36,000 atoms. See the explanation of a shorter polymer of PPE354 in Sec. 2.1.2.

```
-------------------------------------------
Original problem:
-------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 107994
B : positive definite
e_k : eigen value
y_k : eigen vector
-------------------------------------------
Files
-------------------------------------------
ELSES_MATRIX_PPE107994_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_PPE107994_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_PPE107994_ev.txt
 list of eigen values
ELSES_MATRIX_PPE107994_ipr.txt
 list of inverse participation ratio
-------------------------------------------
```

2.1.19 PPE107994MD

The matrix data appears for an organic polymer poly-(phenylene-ethynylene) (PPE) in the para (linear-chain) structure with 3,000 monomers or 36,000 atoms. See Refs. [10, 12] for details. The structure was obtained after the quantum-mechanical molecular dynamics simulation for 1 ps under the temperature condition of 500 K. For the initial structure of the simulation, 'rotational disorders' or random numbers on the dihedral angles between benzene rings are introduced like Fig. 4.11 (b) of Ref. [12].

```
-------------------------------------------
Original problem:
-------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 107994
B : positive definite
e_k : eigen value
y_k : eigen vector
-------------------------------------------
Files
-------------------------------------------
ELSES_MATRIX_PPE107994MD_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_PPE107994MD_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_PPE107994MD_ev.txt
 list of eigen values
ELSES_MATRIX_PPE107994MD_ipr.txt
 list of inverse participation ratio
-------------------------------------------
```

2.1.20 PENTF183600

The matrix data stems from a disordered pentacene thin-film with one atomic layer. The package includes the files of

```
(1) ELSES_MATRIX_PENTF183600_A.mtx
 matrix A in the Matrix-Market format
(2) ELSES_MATRIX_PENTF183600_B.mtx
 matrix B in the Matrix-Market format
(3) ELSES_MATRIX_PENTF183600_ev.txt
 list of eigen values
(4) ELSES_MATRIX_PENTF183600_ipr.txt
 list of inverse participation ratio
```

2.1.21 VCNT225000

The matrix data appears for a vibrating carbon nanotube within a supercell with spd orbitals. [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT225000_20130831.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT225000"
  generated by ELSES
          T. Hoshi, 31. Aug. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 225000
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT225000_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT225000_B.mtx
 matrix B in the Matrix-Market format
-----------------------------------------------
```

The used atomic structure is the one in VCNT100000std, generated with sp orbitals.

2.1.22 NCCS430080 (updated at 7. May. 2017)

The matrix data appears in an electronic structure calculation of an sp2-sp3 nano-composite carbon solid (NCCS). [5]
The package includes the files of

```
(1) ELSES_MATRIX_NCCS430080_A.mtx
 matrix A in the Matrix-Market format
(2) ELSES_MATRIX_NCCS430080_B.mtx
 matrix B in the Matrix-Market format
(3) ELSES_MATRIX_NCCS430080_ev.mtx
 list of eigen values
(4) ELSES_MATRIX_NCCS430080_ipr.mtx
 list of inverse participation ratio
```

Note : The package was updated with the date stamp of 7. May. 2017; The values of the eigenvalues and the inverse participation ratio were added. The input matrices were not updated.

2.1.23 VCNT900000

The matrix data appears for a vibrating carbon nanotube within a supercell with spd orbitals. [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT900000_20130907.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT900000"
  generated by ELSES
          T. Hoshi, 07. Sep. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 900000
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT900000_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT900000_B.mtx
 matrix B in the Matrix-Market format
-----------------------------------------------
```

The used atomic structure is the one in VCNT400000std, generated with sp orbitals.

2.1.24 VCNT1008000

The matrix data appears for a vibrating carbon nanotube within a supercell with spd orbitals. [9] The used atomic structure is generated with the sp-orbital theory, as in VCNT400000std.
The detailed explanation of the package is shown below;

```
ELSES_MATRIX_VCNT1008000_20140906.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-------------------------------------------
Matrix data "VCNT1008000"
  generated by ELSES
          T. Hoshi, 06. Sep. 2014
-------------------------------------------
Note:
-------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-------------------------------------------
Original problem:
-------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A,B : N x N real-symmetric matrix with N = 1008000
B : positive definite
e_k : eigen value
y_k : eigen vector
-------------------------------------------
Files
-------------------------------------------
ELSES_MATRIX_VCNT1008000_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT1008000_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_VCNT1008000_README.mtx
 short explanation
-------------------------------------------
```

(Added at 20. Dec. 2014) The calculated result was added. All the eigen values and the lowest ten eigen vectors were stored as files. The calculation was carried out with all the nodes (4800 nodes) on the supercomputer Oakleaf-FX (U Tokyo). The detailed explanation of the package is shown below;

```
ELSES_MATRIX_VCNT1008000_20140906_result.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Calculated result for the problem of  "VCNT1008000"
           T. Hoshi, 20. Dec. 2014
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem of "VCNT1008000"
See the document on the web.
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT1008000_E.txt
 eigen values
ELSES_MATRIX_VCNT1008000_V01.txt
 the first lowest eigen vector
ELSES_MATRIX_VCNT1008000_V02.txt
 the second lowest eigen vector
ELSES_MATRIX_VCNT1008000_V03.txt
 the third lowest eigen vector
ELSES_MATRIX_VCNT1008000_V04.txt
 the 4-th lowest eigen vector
ELSES_MATRIX_VCNT1008000_V05.txt
 the 5-th lowest eigen vector
ELSES_MATRIX_VCNT1008000_V06.txt
 the 6-th lowest eigen vector
ELSES_MATRIX_VCNT1008000_V07.txt
 the 7-th lowest eigen vector
ELSES_MATRIX_VCNT1008000_V08.txt
 the 8-th lowest eigen vector
ELSES_MATRIX_VCNT1008000_V09.txt
 the 9-th lowest eigen vector
ELSES_MATRIX_VCNT1008000_V10.txt
 the 10-th lowest eigen vector
-----------------------------------------------
```

2.2 Hermitian matrices for generalized eigen-value equations

2.2.1 DIAB18h

The present package gives tiny matrices for a tutorial.

The data appears at a Brillouin zone point in the band diagram of diamond with s-, p-, d-type orbitals [9]

This is the detailed explanation of the package:

```
ELSES_MATRIX_DIAB18h_20130430.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "DIAB18h"
  generated by ELSES
          T. Hoshi, 30. Apr. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A, B: N x N Hermitian matrix with N = 18
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_DIAB18h_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_DIAB18h_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_DIAB18h_E.txt
 list of eigen values
-----------------------------------------------
```

2.2.2 VCNT900h

The matrix data appears for a vibrating carbon nanotube within a supercell, at a Brillouin zone point in the band diagram with s-, p-, d-type orbitals [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT900h_20130501.tgz
  from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT900h"
  generated by ELSES
          T. Hoshi, 1. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A, B: N x N Hermitian matrix with N = 900
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT900h_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT900h_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_VCNT900h_E.txt
 list of eigen values
-----------------------------------------------
```

2.2.3 VCNT10800h

The matrix data appears for a vibrating carbon nanotube within a supercell, at a Brillouin zone point in the band diagram with s-, p-, d-type orbitals [9]
This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT10800h_20130501.tgz
  from ELSES matrix library ( http://www.elses.jp/matrix/ )
-------------------------------------------
Matrix data "VCNT900h"
  generated by ELSES
          T. Hoshi, 1. May. 2013
-------------------------------------------
Note:
-------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-------------------------------------------
Original problem:
-------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A, B: N x N Hermitian matrix with N = 10800
B : positive definite
e_k : eigen value
y_k : eigen vector
-------------------------------------------
Files
-------------------------------------------
ELSES_MATRIX_VCNT10800h_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT10800h_B.mtx
 matrix B in the Matrix-Market format
ELSES_MATRIX_VCNT10800h_E.txt
 list of eigen values
-------------------------------------------
```

2.3 Real-symmetric matrices for standard eigen-value equations

2.3.1 VCNT400std

The matrix data appears for a vibrating carbon nanotube within a supercell. The description of carbon system is found in Ref. [7].

This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT400std_20130515.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT400std"
  generated by ELSES
          T. Hoshi, 15. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k y_k
A : N x N Hermitian matrix with N = 400
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT400std_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT400std_E.txt
 list of eigen values
-----------------------------------------------
```

2.3.2 VCNT800std

The matrix data appears for a vibrating carbon nanotube within a supercell. The description of carbon system is found in Ref. [7].

This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT800std_20130517.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT800std"
  generated by ELSES
          T. Hoshi, 17. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k y_k
A : N x N Hermitian matrix with N = 800
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT800std_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT800std_E.txt
 list of eigen values
-----------------------------------------------
```

2.3.3 VCNT2000std

The matrix data appears for a vibrating carbon nanotube within a supercell. The description of carbon system is found in Ref. [7].

This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT2000std_20130517.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT2000std"
  generated by ELSES
          T. Hoshi, 17. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k y_k
A : N x N Hermitian matrix with N = 2000
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT2000std_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT2000std_E.txt
 list of eigen values
-----------------------------------------------
```

2.3.4 VCNT4000std

The matrix data appears for a vibrating carbon nanotube within a supercell. The description of carbon system is found in Ref. [7].

This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT4000std_20130517.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT4000std"
  generated by ELSES
          T. Hoshi, 17. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k y_k
A : N x N Hermitian matrix with N = 4000
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT4000std_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT4000std_E.txt
 list of eigen values
-----------------------------------------------
```

2.3.5 CLIQ6912std

See the attached README file for details.

2.3.6 VCNT10000std

IThe matrix data appears for a vibrating carbon nanotube within a supercell. The description of carbon system is found in Ref. [7].

This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT10000std_20130517.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT10000std"
  generated by ELSES
          T. Hoshi, 17. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k y_k
A : N x N Hermitian matrix with N = 10000
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT10000std_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_VCNT10000std_E.txt
 list of eigen values
-----------------------------------------------
```

2.3.7 VCNT40000std

The matrix data appears for a vibrating carbon nanotube within a supercell. The description of carbon system is found in Ref. [7].

This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT40000std_20130517.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT40000std"
  generated by ELSES
          T. Hoshi, 17. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k y_k
A : N x N Hermitian matrix with N = 40000
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT40000std_A.mtx
 matrix A in the Matrix-Market format
-----------------------------------------------
```

2.3.8 CLIQ55296std

See the attached README file for details.

2.3.9 VCNT100000std

The matrix data appears for a vibrating carbon nanotube within a supercell. The description of carbon system is found in Ref. [7].

This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT100000std_20130518.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT100000std"
  generated by ELSES
          T. Hoshi, 18. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k y_k
A : N x N Hermitian matrix with N = 100000
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT100000std_A.mtx
 matrix A in the Matrix-Market format
-----------------------------------------------
```

2.3.10 VCNT400000std

The matrix data appears for a vibrating carbon nanotube within a supercell. The description of carbon system is found in Ref. [7].

This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT400000std_20130518.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT400000std"
  generated by ELSES
          T. Hoshi, 18. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k y_k
A : N x N Hermitian matrix with N = 400000
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT400000std_A.mtx
 matrix A in the Matrix-Market format
-----------------------------------------------
```

2.3.11 NCCS430080std

The matrix data appears in an electronic structure calculation of an sp2-sp3 nano-composite carbon solid (NCCS). [5]
The matrix is formulated by the theory in Ref. [8].
This is the detailed explanation of the package:

```
ELSES_MATRIX_NCCS430080std_20140221.tgz.zip
from ELSES matrix library (http://www.elses.jp/matrix/)
-----------------------------------------------
Matrix data "NCCS430080std"
  generated by ELSES
          T. Hoshi, 21. Feb. 2014.
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k B y_k
A, B: N x N real-symmetric matrix with N = 430,080
B : positive definite
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_AUNU430080_A.mtx
 matrix A in the Matrix-Market format
ELSES_MATRIX_AUNW430080_B.mtx
 matrix B in the Matrix-Market format
-----------------------------------------------
Note
-----------------------------------------------
Details are found in the document on the web page
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
```

2.3.12 VCNT1000000std

The matrix data appears for a vibrating carbon nanotube within a supercell. The description of carbon system is found in Ref. [7].

This is the detailed explanation of the package:

```
ELSES_MATRIX_VCNT1000000std_20130522.tgz
from ELSES matrix library ( http://www.elses.jp/matrix/ )
-----------------------------------------------
Matrix data "VCNT1000000std"
  generated by ELSES
          T. Hoshi, 22. May. 2013
-----------------------------------------------
Note:
-----------------------------------------------
Details are found in the document;
http://www.elses.jp/matrix/document_ELSES_Matrix_Library.pdf
If you use the matrix data in a publication,
please cite the paper(s) indicated in the document
-----------------------------------------------
Original problem:
-----------------------------------------------
A generalized eigen-value problem
    A y_k = e_k y_k
A : N x N real-symmetric matrix with N = 1000000
e_k : eigen value
y_k : eigen vector
-----------------------------------------------
Files
-----------------------------------------------
ELSES_MATRIX_VCNT1000000std_A.mtx
 matrix A in the Matrix-Market format
-----------------------------------------------
```

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A Update log

- (12. Jun. 2019) Add the section 'About ELSES Matrix Library' .
- (24. Nov. 2018) Add matrix data package PPE3594, PPE7194
- (27. Feb. 2018) Update the data package of BNZ30.
- (24. Feb. 2018) Add matrix data package PENTF183600.
- (15. Feb. 2018) The direct links to the matrix data are prepared. For example, the link to BNZ30 is `http://www.elses.jp/matrix/index.html#BNZ30`
- (15. Feb. 2018) Add matrix data package PENTF98736.
- (18. Jan. 2018) Add matrix data package PENTF20400.
- (7. Jan. 2018) Add matrix data package CPPE32346.
- (29. Dec. 2017) Add matrix data package PPE107994MD.
- (6. Aug. 2017) Update the data package of VCNT22500.
- (2. Jul. 2017) Modify slightly.
- (1. Jul. 2017) Add Sec. 1.4 (Theory).
- (29. Jun. 2017) Add Sec. 1.3 (History).
- (28. Jun. 2017) Add matrix data packages of PPE354, PPE17994 and PPE107994.
- (20. Dec. 2016) The documentation is simplified.
- (20. Dec. 2014) Added result data to the package of VCNT1008000.
- (06. Sep. 2014) Added matrix data package: VCNT1008000.
- (09. Mar. 2013) Added matrix data package: NCCS430080std. Minor update on explanation (No existing numerical data was changed).
- (13. Feb. 2013) Updated package: VCNT225000. No numerical data is changed.
- (06. Dec. 2013) Updated package: VCNT4500. No numerical data is changed.
- (20. Sep. 2013) Updated package: BNZ30. No numerical data is changed.
- (07. Sep. 2013) Added matrix data: VCNT900000
- (31. Aug. 2013) Added matrix data: VCNT225000
- (29. Aug. 2013) Added matrix data: VCNT22500, VCNT90000
- (28. Aug. 2013) Added matrix data: VCNT1800, VCNT4500, VCNT9000, ICNT1800
- (20. Aug. 2013) Added matrix data: VCNT900
- (30. May. 2013) Added matrix data: G-WAT7,
- (22. May. 2013) Added matrix data: VCNT1000000std.
- (18. May. 2013) Added matrix data: VCNT800std, VCNT2000std, VCNT4000std, VCNT10000std, VCNT40000std, VCNT100000std, VCNT400000std

- (15. May. 2013) Updated package: VCNT400std
- (7. May. 2013) Minor revision.
- (2. May. 2013) Minor revision.
- (1. May. 2013) Added matrix data: VCNT900h, VCNT10800h.
- (30. Apr. 2013) Added matrix data: DIAB18h.
- (29. Apr. 2013) Minor revision.
- (11. Mar. 2013) Initial release of the collection. Added matrix data: BNZ30, APF4686, AUNW9180, NCCS430080, VCNT400std, CLIQ6912std, CLIQ55296std.