```
ClusterMatrixModule:
calClusterMatrix(e)
```

```
…,…
do my_atom = 1, LocalNumAtoms
!  For each atom on my MPI process treated as a center atom
   do j = 0, Neighbor%NumAtoms
!     For each atom in the LIZ of the center atom
      …,…
      do i = 0, Neighbor%NumAtoms
!        For each atom in the LIZ of the center atom
         …,…
         rij = posj - posi
         gij => RSpaceStrConstModule:getStrConstMatrix(e,rij)
         …,…
!        Construct BigMatrix
         …,…
      enddo
   enddo
enddo
…,…
```

$$\left[i\underline{s}_i(\varepsilon)-\underline{c}_i(\varepsilon)\right]^{-1} \rightarrow \texttt{p\_jinvi}$$

$$\underline{\underline{I}}-\frac{1}{\sqrt{\varepsilon}}\left[i\underline{\underline{s}}(\varepsilon)-\underline{\underline{c}}(\varepsilon)\right]^{-1}\underline{\underline{g}}(\varepsilon)\underline{\underline{s}}(\varepsilon) \rightarrow \texttt{BigMatrix}$$

`call invertMatrixBlock` to get `p_BlockMatrix`

τ-matrix:
$$\underline{\tau}^{11}(\varepsilon)=\begin{bmatrix} \left[\underline{t}^{1}(\varepsilon)\right]^{-1} & -\underline{g}^{12}(\varepsilon) & \cdots & -\underline{g}^{1M}(\varepsilon) \\ -\underline{g}^{21}(\varepsilon) & \left[\underline{t}^{2}(\varepsilon)\right]^{-1} & \cdots & -\underline{g}^{2M}(\varepsilon) \\ \vdots & \vdots & \ddots & \vdots \\ -\underline{g}^{M1}(\varepsilon) & -\underline{g}^{M2}(\varepsilon) & \cdots & \left[\underline{t}^{M}(\varepsilon)\right]^{-1} \end{bmatrix}^{-1}_{11}$$
$$=\left[\underline{\underline{t}}^{-1}(\varepsilon)-\underline{\underline{g}}(\varepsilon)\right]^{-1}_{11}$$

Note: There are M atoms in the LIZ of the center atom. In this expression for the τ-matrix of the center atom, the center atom is numbered as atom 1, and the rest of the atoms in the LIZ are numbered as 2, 3, …, M.

Note: The diagonal blocks of `BigMatrix` are identity matrix.

$$\underline{t}^{i}(\varepsilon)=\left(i\sqrt{\varepsilon}\underline{I}-\sqrt{\varepsilon}\underline{c}^{i}(\varepsilon)\left[\underline{s}^{i}(\varepsilon)\right]^{-1}\right)^{-1}$$

$$\hat{\underline{\Omega}}^{i}(\varepsilon)=\left[\left[\underline{s}^{i}(\varepsilon)\right]^{T\bullet}\left(i\underline{s}^{i}(\varepsilon)-\underline{c}^{i}(\varepsilon)\right)\right]^{-1}$$

$\underline{J}(\varepsilon)=i\underline{s}^{i}(\varepsilon)-\underline{c}^{i}(\varepsilon)$ is called Jost matrix

$$\underline{p}^{1}(\varepsilon)=\underline{I}-\left(\left[\underline{\underline{I}}-\frac{1}{\sqrt{\varepsilon}}\left[i\underline{\underline{s}}(\varepsilon)-\underline{\underline{c}}(\varepsilon)\right]^{-1}\underline{\underline{g}}(\varepsilon)\underline{\underline{s}}(\varepsilon)\right]^{-1}_{11}\right)^{-1} \rightarrow \texttt{p\_BlockMatrix}$$

$$\underline{W}^{11}(\varepsilon)=\left[\underline{\underline{I}}-\frac{1}{\sqrt{\varepsilon}}\left[i\underline{\underline{s}}(\varepsilon)-\underline{\underline{c}}(\varepsilon)\right]^{-1}\underline{\underline{g}}(\varepsilon)\underline{\underline{s}}(\varepsilon)\right]^{-1}_{11}-\underline{I}=\left(\underline{I}-\underline{p}^{1}(\varepsilon)\right)^{-1}-\underline{I}=\left(\underline{I}-\underline{p}^{1}(\varepsilon)\right)^{-1}\underline{p}^{1}(\varepsilon) \rightarrow \texttt{wau\_g}$$

$$\underline{K}^{11}(\varepsilon)=\varepsilon\left[\underline{s}^{1}(\varepsilon)\right]^{-1}\left(\underline{\tau}^{11}(\varepsilon)-\underline{t}^{1}(\varepsilon)\right)\left[\underline{s}^{1}(\varepsilon)\right]^{-T\bullet}=\sqrt{\varepsilon}\left(\left[\underline{\underline{I}}-\frac{1}{\sqrt{\varepsilon}}\left[i\underline{\underline{s}}(\varepsilon)-\underline{\underline{c}}(\varepsilon)\right]^{-1}\underline{\underline{g}}(\varepsilon)\underline{\underline{s}}(\varepsilon)\right]^{-1}_{11}-\underline{I}\right)\hat{\underline{\Omega}}^{1}(\varepsilon)=\sqrt{\varepsilon}\underline{W}^{11}(\varepsilon)\hat{\underline{\Omega}}^{1}(\varepsilon) \rightarrow \texttt{Tau00\%kau\_l}$$

$$\underline{\tau}^{11}(\varepsilon)=\frac{1}{\varepsilon}\underline{s}^{1}(\varepsilon)\underline{K}^{11}(\varepsilon)\left[\underline{s}^{1}(\varepsilon)\right]^{T\bullet}+\underline{t}^{1}(\varepsilon) \rightarrow \texttt{Tau00\%tau\_l}$$

$$\underline{s}_i(\varepsilon) \rightarrow \texttt{p\_sinej}$$

$$\underline{J}_i(\varepsilon) = \left[i\underline{s}_i(\varepsilon) - \underline{c}_i(\varepsilon) \right]^{-1} \rightarrow \texttt{p\_jinvi}$$

$$\underline{\underline{J}}(\varepsilon) = \begin{bmatrix} \underline{J}_1(\varepsilon) & 0 & \cdots & 0 \\ 0 & \underline{J}_2(\varepsilon) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \underline{J}_N(\varepsilon) \end{bmatrix}$$

$$\underline{\underline{s}}(\varepsilon) = \begin{bmatrix} \underline{s}_1(\varepsilon) & 0 & \cdots & 0 \\ 0 & \underline{s}_2(\varepsilon) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \underline{s}_N(\varepsilon) \end{bmatrix}$$

$$\underline{\underline{g}}(\varepsilon) = \begin{bmatrix} 0 & \underline{g}_{12}(\varepsilon) & \cdots & \underline{g}_{1N}(\varepsilon) \\ \underline{g}_{21}(\varepsilon) & 0 & \cdots & \underline{g}_{2N}(\varepsilon) \\ \vdots & \vdots & \ddots & \vdots \\ \underline{g}_{N1}(\varepsilon) & \underline{g}_{N2}(\varepsilon) & \cdots & 0 \end{bmatrix}$$

$$\underline{\underline{M}}(\varepsilon) = \underline{\underline{I}} - \frac{1}{\sqrt{\varepsilon}} \underline{\underline{J}}(\varepsilon) \underline{\underline{g}}(\varepsilon) \underline{\underline{s}}(\varepsilon) \rightarrow \texttt{BigMatrix}$$

Given block matrix A: $\underline{\underline{A}} = \begin{bmatrix} \underline{A}_{11} & \underline{A}_{12} \\ \underline{A}_{21} & \underline{A}_{22} \end{bmatrix}$

Denote its inverse as B: $\underline{\underline{B}} = \underline{\underline{A}}^{-1} = \begin{bmatrix} \underline{B}_{11} & \underline{B}_{12} \\ \underline{B}_{21} & \underline{B}_{22} \end{bmatrix}$

$$\begin{aligned} \underline{A}_{11}\underline{B}_{11} + \underline{A}_{12}\underline{B}_{21} &= \underline{I}_{11} \\ \underline{A}_{11}\underline{B}_{12} + \underline{A}_{12}\underline{B}_{22} &= \underline{0} \\ \underline{A}_{21}\underline{B}_{11} + \underline{A}_{22}\underline{B}_{21} &= \underline{0} \\ \underline{A}_{21}\underline{B}_{12} + \underline{A}_{22}\underline{B}_{22} &= \underline{I}_{22} \end{aligned}$$

We have $\underline{\underline{A}} \cdot \underline{\underline{B}} = \begin{bmatrix} \underline{A}_{11} & \underline{A}_{12} \\ \underline{A}_{21} & \underline{A}_{22} \end{bmatrix} \begin{bmatrix} \underline{B}_{11} & \underline{B}_{12} \\ \underline{B}_{21} & \underline{B}_{22} \end{bmatrix} = \begin{bmatrix} \underline{A}_{11}\underline{B}_{11} + \underline{A}_{12}\underline{B}_{21} & \underline{A}_{11}\underline{B}_{12} + \underline{A}_{12}\underline{B}_{22} \\ \underline{A}_{21}\underline{B}_{11} + \underline{A}_{22}\underline{B}_{21} & \underline{A}_{21}\underline{B}_{12} + \underline{A}_{22}\underline{B}_{22} \end{bmatrix} = \begin{bmatrix} \underline{I}_{11} & \underline{0} \\ \underline{0} & \underline{I}_{22} \end{bmatrix}$

This gives rise to

$$\underline{A}_{11}\underline{B}_{11} + \underline{A}_{12}\underline{B}_{21} = \underline{I}_{11}, \quad \underline{A}_{11}\underline{B}_{12} + \underline{A}_{12}\underline{B}_{22} = \underline{0}, \quad \underline{A}_{21}\underline{B}_{11} + \underline{A}_{22}\underline{B}_{21} = \underline{0}, \text{ and } \underline{A}_{21}\underline{B}_{12} + \underline{A}_{22}\underline{B}_{22} = \underline{I}_{22}.$$

$$\begin{aligned} \underline{A}_{11}\underline{B}_{12} + \underline{A}_{12}\underline{B}_{22} &= \underline{0} \\ \underline{A}_{21}\underline{B}_{11} + \underline{A}_{22}\underline{B}_{21} &= \underline{0} \end{aligned} \quad \rightarrow \quad \begin{aligned} \underline{B}_{12} &= -\underline{A}_{11}^{-1}\underline{A}_{12}\underline{B}_{22} \\ \underline{B}_{21} &= -\underline{A}_{22}^{-1}\underline{A}_{21}\underline{B}_{11} \end{aligned}$$

$$\begin{aligned} \underline{A}_{11}\underline{B}_{11} + \underline{A}_{12}\underline{B}_{21} &= \underline{I}_{11} \\ \underline{A}_{21}\underline{B}_{12} + \underline{A}_{22}\underline{B}_{22} &= \underline{I}_{22} \end{aligned} \quad \rightarrow \quad \begin{aligned} \left(\underline{A}_{11} - \underline{A}_{12}\underline{A}_{22}^{-1}\underline{A}_{21}\right)\underline{B}_{11} &= \underline{I}_{11} \\ \left(\underline{A}_{22} - \underline{A}_{21}\underline{A}_{11}^{-1}\underline{A}_{12}\right)\underline{B}_{22} &= \underline{I}_{22} \end{aligned} \quad \rightarrow \quad \begin{aligned} \underline{B}_{11} &= \left(\underline{A}_{11} - \underline{A}_{12}\underline{A}_{22}^{-1}\underline{A}_{21}\right)^{-1} \\ \underline{B}_{22} &= \left(\underline{A}_{22} - \underline{A}_{21}\underline{A}_{11}^{-1}\underline{A}_{12}\right)^{-1} \end{aligned}$$

Acceleration of LSMS