

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
.../...

```

$$[i\underline{s}_i(\varepsilon) - \underline{c}_i(\varepsilon)]^{-1} \rightarrow p_jinvi$$

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

call invertMatrixBlock to get p_BlockMatrix

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

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

$$\underline{K}^{11}(\varepsilon) = \varepsilon [s^1(\varepsilon)]^{-1} (\underline{\tau}^{11}(\varepsilon) - t^1(\varepsilon)) [s^1(\varepsilon)]^{-T*} = \sqrt{\varepsilon} \left(\left[\underline{I} - \frac{1}{\sqrt{\varepsilon}} [i\underline{s}(\varepsilon) - \underline{c}(\varepsilon)]^{-1} \underline{g}(\varepsilon) \underline{s}(\varepsilon) \right]_{11}^{-1} - \underline{I} \right) \hat{\underline{\Omega}}^1(\varepsilon) = \sqrt{\varepsilon} \underline{W}^{11}(\varepsilon) \hat{\underline{\Omega}}^1(\varepsilon) \rightarrow \text{Tau00\%kau_1}$$

$$\underline{\tau}^{11}(\varepsilon) = \frac{1}{\varepsilon} s^1(\varepsilon) \underline{K}^{11}(\varepsilon) [s^1(\varepsilon)]^{T*} + t^1(\varepsilon) \rightarrow \text{Tau00\%tau_1}$$

$$\tau\text{-matrix: } \underline{\tau}^{11}(\varepsilon) = \begin{bmatrix} [t^1(\varepsilon)]^{-1} & -\underline{g}^{12}(\varepsilon) & L & -\underline{g}^{1M}(\varepsilon) \\ -\underline{g}^{21}(\varepsilon) & [t^2(\varepsilon)]^{-1} & L & -\underline{g}^{2M}(\varepsilon) \\ M & M & O & M \\ -\underline{g}^{M1}(\varepsilon) & -\underline{g}^{M2}(\varepsilon) & L & [t^M(\varepsilon)]^{-1} \end{bmatrix}_{11}^{-1}$$

$$= [t^{-1}(\varepsilon) - \underline{g}(\varepsilon)]_{11}^{-1}$$

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.

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

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

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

$$\underline{s}_i(\varepsilon) \rightarrow \text{p_sinej}$$

$$\underline{J}_i(\varepsilon) = [i\underline{s}_i(\varepsilon) - \underline{c}_i(\varepsilon)]^{-1} \rightarrow \text{p_jinvi}$$

$$\underline{\underline{J}}(\varepsilon) = \begin{bmatrix} \underline{J}_1(\varepsilon) & 0 & \text{L} & 0 \\ 0 & \underline{J}_2(\varepsilon) & \text{L} & 0 \\ \text{M} & \text{M} & \text{O} & \text{M} \\ 0 & 0 & \text{L} & \underline{J}_N(\varepsilon) \end{bmatrix} \quad \underline{\underline{s}}(\varepsilon) = \begin{bmatrix} \underline{s}_1(\varepsilon) & 0 & \text{L} & 0 \\ 0 & \underline{s}_2(\varepsilon) & \text{L} & 0 \\ \text{M} & \text{M} & \text{O} & \text{M} \\ 0 & 0 & \text{L} & \underline{s}_N(\varepsilon) \end{bmatrix}$$

$$\underline{\underline{g}}(\varepsilon) = \begin{bmatrix} 0 & \underline{g}_{12}(\varepsilon) & \text{L} & \underline{g}_{1N}(\varepsilon) \\ \underline{g}_{21}(\varepsilon) & 0 & \text{L} & \underline{g}_{2N}(\varepsilon) \\ \text{M} & \text{M} & \text{O} & \text{M} \\ \underline{g}_{N1}(\varepsilon) & \underline{g}_{N2}(\varepsilon) & \text{L} & 0 \end{bmatrix}$$

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

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

$$\underline{A}_{11}\underline{B}_{11} + \underline{A}_{12}\underline{B}_{21} = \underline{I}_{11}$$

$$\underline{A}_{11}\underline{B}_{12} + \underline{A}_{12}\underline{B}_{22} = \underline{0}$$

$$\underline{A}_{21}\underline{B}_{11} + \underline{A}_{22}\underline{B}_{21} = \underline{0}$$

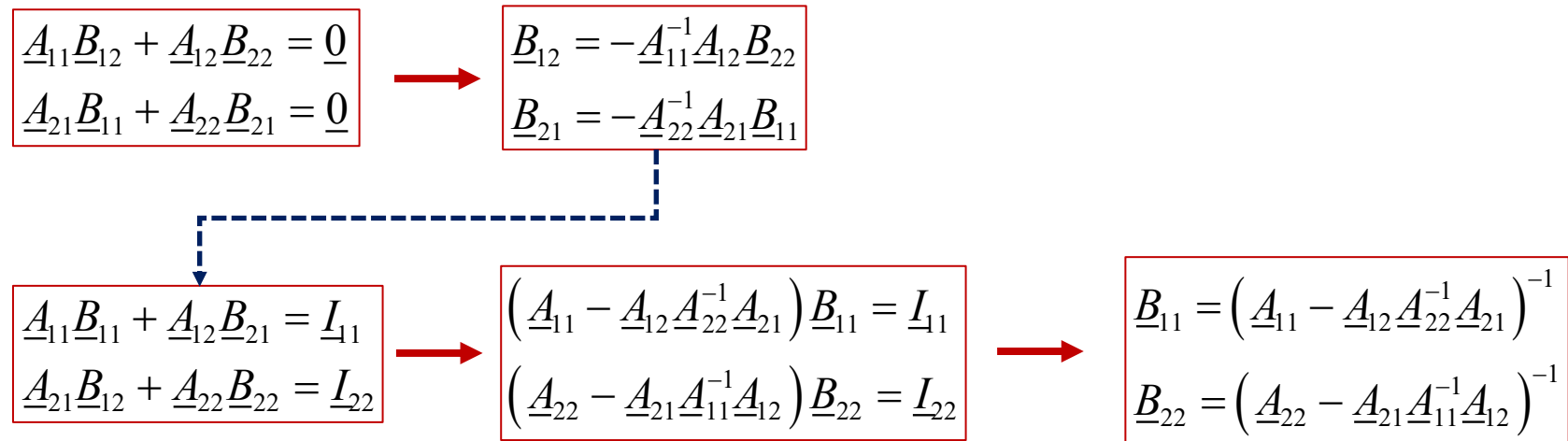
$$\underline{A}_{21}\underline{B}_{12} + \underline{A}_{22}\underline{B}_{22} = \underline{I}_{22}$$

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

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

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



Acceleration of LSMS

MuST/MST/src/ClusterMatrixModule.F90::
calClusterMatrix

```
#ifdef ACCEL
  pBigMatrix => aliasArray2_c(BigMatrix, dsize, dsize)
  call invertMatrixLSMS_CUDA(my_atom, pBlockMatrix, kkrasz_ns, &
    pBigMatrix, dsize )
#else
  call invertMatrixBlock( my_atom, pBlockMatrix, kkrasz_ns, kkrasz_ns, &
    BigMatrix, dsize, dsize )
#endif
```

Without GPU Acceleration

MuST/MST/src/MatrixBlockInversionModule.F90::
invertMatrixBlock

With GPU Acceleration

MuST/MST/Accelerator/invertMatrixLSMS_CUDA.F90

```
#ifdef CUDA
  ...,...
  call cusolver_lsms_c(dsize,pBigMatrix,kkrasz_ns,tmpmatrixC)
  ...,...
#else
  ! The following line under this condition seems from an unfinished
  ! work and needs to be corrected.
  ! However, under the current setting , this condition is not reached
  call zblock_lu_CPU(a,lda,blk_sz,nblk,ipvt,mp,idcol,k)
#endif
```

MuST/MST/Accelerator/cusolver_LSMS_c.cu

```
extern "C"
void cusolver_lsms_c_(int *m, double _Complex *a,
int *block_size, double _Complex *b)
{
  ...,...
}
```