Parameter Files

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The structure of parameter file is adapted from the C++/CUDA version of PSCF, and contain one `System` block as shown below.

```
System{
  Mixture{
    nMonomer   ...
    monomers   ...  ...
               ...  ...
    nPolymer   ...
    Polymer{
      nBlock  ...
      nVertex ...
      blocks  ...  ... ... ...  ...
              ...  ... ... ...  ...
      phi     ...
    }
    DPolymer{
      nBlock  ...
      nVertex ...
      bonds   ...  ... ... ...  ...  ...
              ...  ... ... ...  ...  ...
      phi     ...
    }
    [ns        ...]
  }
  Interaction{
     chi ... ... ...
         ... ... ...
     [kappa    ...]
     sigma     ...
  }
  unitCell ... ... ...
  mesh ....
  groupName ...
  AmIterator{
     maxItr  ...
     epsilon ...
     maxHist ...
     isMinimized ...
  }
}
```

Each sub-block and required parameter (represented by ...) is explained as follows:

- **Mixture**: Description of molecular components (each is considered as a block copolymer in general with each block being a linear homopolymer) and composition in the system (which is considered as a mixture in general).
    - **nMonomer**: Number of monomer (segment) types in the system; this includes solvent molecules.
    - **monomers**: Description of each segment type in a seperate line (thus a total of `nMonomer` lines). The first parameter in each line is a unique integer index starting from 0 for the segment type, and the second parameter specifies its statistical segment length.
    - **nPolymer**: Number of molecular components in the system.
    - **Polymer** (only used for continuous-Gaussian-chain models): Description of each molecular component in a seperate sub-block (thus a total of `nPolymer` sub-blocks), which includes its chain architecture (specified by `nBlock`, `nVertex`, and `blocks` as explained below) and its overall volume fraction `phi` in the system.

        - **nBlock**: Number of blocks of this molecular component.
        - **nVertex**: Number of vertices of this molecular component. A vertex is either a joint (where at least two blocks meet) or a free end.
        - **blocks**: Description of each block in a seperate line (thus a total of `nBlock` lines). The first parameter in each line is a unique integer index starting from 0 for the block, the second parameter specifies its segment type, the next two parameters are the indices of the two vertices it connects, and the last parameter specifies its length.
    - **DPolymer** (only used for discrete-chain models): Description of each molecular component in a seperate sub-block (thus a total of `nPolymer` sub-blocks), which includes its chain architecture (specified by `nBond`, `nVertex`, and `bonds` as explained below; see Models.pdf for details.) and its overall volume fraction `phi` in the system.
        - **nBond**: Number of v-bonds (including both block bonds and joint bonds) of this molecular component.
        - **nVertex**: Number of vertices of this molecular component. A vertex here is either a joint (which is connected by at least two v-bonds) or a free end (which is connected by one v-bond).
        - **bonds**: Description of each v-bond in a seperate line (thus a total of `nBond` lines). The first parameter in each line is a unique integer index starting from 0 for the bond, the second and the third parameters are the indices of the two vertices it connects, the next two parameters specify the types of these vertices (segments), and the last parameter is its number of segments (0 for a joint bond).
    - **ns**: Total number of discretization steps along the chain contour of length 1. This line is used only for continuous-Gaussian-chain models, and is omitted for discrete-chain models.
- **Interaction**: Description of non-bonded interactions in the system.
    - **chi**: Value of the (generalized) Flory-Huggins χ parameter for each pair of different segment types in a seperate line. The first two parameters in each line are the segment-type indices, and the third one is the corresponding value of χ. By default, the value between segments of the same type is 0, and thus not needed.
    - **kappa**: Compressibility parameter κ, used only for compressible systems and omitted for incompressible systems.
    - **sigma**: Interaction range of the non-bounded potential, which is 0 for Dirac δ-function interaction.
- **unitCell**: The first parameter in this line is the lattice system of the unit cell and the following is a list of real numbers needed to describe the unit cell.
- **mesh**: Description of the mesh size used for spatial discretization, given by D integer numbers with D being the dimensionality of the system.
- **groupName**: Name of the crystallographic space group.
- **AmIterator**: Parameters required by Anderson mixing for iteratively solving the SCF equations; see *Matsen*, **Eur. Phys. J. E 53**, 361 (2009) for details.
    - **maxItr**: Maximum number of iterations.
    - **epsilon**: Criterion of convergence for SCF equations.
    - **maxHist**: A positive integer for the maximum size of the history matrix used in Anderson mixing.
    - **isMinimized**: 1 for finding the bulk period of the ordered phase, and 0 otherwise.

Below are two examples of the parameter file:

- ***Example for SCF calculations of the BCC phase formed by the "Standard" model of compositionally asymmetric A-B diblock copolymer***

```
System{
  Mixture{
    nMonomer  2
    monomers  0   A   1.0
              1   B   1.0
    nPolymer  1
    Polymer{
      nBlock  2
      nVertex 3
      blocks  0  0  0  1  2.50000000E-01
              1  1  1  2  7.50000000E-01
      phi     1.0
    }
    ns        128
  }
  Interaction{
    chi   1   0   20.0
    sigma 0.0
  }
  unitCell cubic      4.6662857614e+00
  mesh      64   64  64
  groupName         I_m_-3_m
  AmIterator{
    maxItr 5000
    epsilon 1e-9
    maxHist 20
    isMinimized 1
  }
}
```

- ***Example for SCF calculations of the σ phase formed by the DPDC model of conformationally asymmetric A-B diblock copolymer***

```
System{
  Mixture{
    nMonomer  2
    monomers  0   A   3.0
              1   B   1.0
    nPolymer  1
    DPolymer{
      nBond   3
      nVertex 4
      bonds   0  0  1  0  0   3
              1  2  3  1  1   7
              2  1  2  0  1   0
      phi     1.0
    }
  }
  Interaction{
    chi   1   0   2.0
    kappa 0.06366197723676
    sigma 0.89442719099992
  }
  unitCell tetragonal      2.8767371691e+01      1.5168759856e+01
  mesh    128  128  64
  groupName         P_42%m_n_m
  AmIterator{
    maxItr 5000
    epsilon 1e-8
    maxHist 20
    isMinimized 1
  }
}
```