

分子动力学文件语法高亮 VScode 插件
v1.0
源程序文档

2025 年 9 月 23 日

一、 扩展配置模块

1.1 package.json - 扩展主配置文件

```
{
  "name": "md-highlighter",
  "displayName": "md-highlighter",
  "description": "Highlighting files about molecular modeling and dynamics simulation.",
  "version": "0.0.7",
  "publisher": "gxf1212",
  "repository": "https://github.com/gxf1212/md-highlighter",
  "engines": {
    "vscode": "^1.70.0"
  },
  "icon": "./images/benzene.png",
  "categories": [
    "Programming Languages"
  ],
  "contributes": {
    "languages": [
      {
        "id": "rtf",
        "aliases": [
          "NAMD force field",
          "rtf"
        ],
        "extensions": [
          ".rtf",
          ".str",
          ".inp",
          ".prm",
          ".par"
        ],
        "configuration": "./language-configuration.json"
      },
      {
        "id": "pdb",
        "aliases": [
          "PDB file",
          "pdb"
        ],
        "extensions": [
          ".pdb"
        ],
        "configuration": "./language-configuration.json"
      },
      {
        "id": "psf",
        "aliases": [
          "NAMD topology file"
        ],
        "extensions": [
          ".psf"
        ],
        "configuration": "./language-configuration.json"
      }
    ]
  }
}
```

```
},
{
  "id": "in",
  "aliases": [
    "Amber in file"
  ],
  "extensions": [
    ".in"
  ],
  "filenamePatterns": [
    "leaprc.*"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "prmtop",
  "aliases": [
    "Amber topology file",
    "prmtop"
  ],
  "extensions": [
    ".prmtop",
    ".parm7"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "inpcrd",
  "aliases": [
    "Amber coordinate file",
    "inpcrd"
  ],
  "extensions": [
    ".inpcrd",
    ".rst7"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "prepin",
  "aliases": [
    "Amber prepin file",
    "prepin"
  ],
  "extensions": [
    ".prepin",
    ".prepi"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "frcmod",
  "aliases": [
    "Amber parameter file",
    "frcmod"
  ],
  "extensions": [
```

```
    ".frcmod"
  ],
  "filenamePatterns": [
    "frcmod.*",
    "parm*.dat",
    "*parm.dat",
    "gaff*.dat",
    "lipid*.dat",
    "GLYCAM*.dat"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "lib",
  "aliases": [
    "Amber topology type file"
  ],
  "extensions": [
    ".lib",
    ".off"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "ac",
  "aliases": [
    "Antechamber file"
  ],
  "extensions": [
    ".ac",
    ".AC"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "mc",
  "aliases": [
    "Antechamber mainchain file"
  ],
  "extensions": [
    ".mc"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "gro",
  "aliases": [
    "Gromacs coordinate file"
  ],
  "extensions": [
    ".gro"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "atp",
  "aliases": [
```

```
    "Gromacs atomtype file"
  ],
  "extensions": [
    ".atp"
  ],
  "configuration": "../language-configuration.json"
},
{
  "id": "arn",
  "aliases": [
    "Gromacs atom renaming specification"
  ],
  "extensions": [
    ".arn"
  ],
  "configuration": "../language-configuration.json"
},
{
  "id": "rtp",
  "aliases": [
    "Gromacs residue type file"
  ],
  "extensions": [
    ".rtp"
  ],
  "configuration": "../language-configuration.json"
},
{
  "id": "hdb",
  "aliases": [
    "Gromacs hydrogen database"
  ],
  "extensions": [
    ".hdb"
  ],
  "configuration": "../language-configuration.json"
},
{
  "id": "r2b",
  "aliases": [
    "Gromacs r2b file"
  ],
  "extensions": [
    ".r2b"
  ],
  "configuration": "../language-configuration.json"
},
{
  "id": "tdb",
  "aliases": [
    "Gromacs terminal database"
  ],
  "extensions": [
    ".tdb"
  ],
  "configuration": "../language-configuration.json"
},
}
```

```
{
  "id": "mtp",
  "aliases": [
    "Gromacs mutation topology file"
  ],
  "extensions": [
    ".mtp"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "vsd",
  "aliases": [
    "Gromacs virtual site definition file"
  ],
  "extensions": [
    ".vsd"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "mol2",
  "aliases": [
    "mol2 file"
  ],
  "extensions": [
    ".mol2"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "sdf",
  "aliases": [
    "sdf file"
  ],
  "extensions": [
    ".sdf",
    ".mol"
  ],
  "configuration": "./language-configuration.json"
},
{
  "id": "plumed",
  "aliases": [
    "plumed input file",
    "plumed"
  ],
  "extensions": [
    ".plumed.dat"
  ],
  "configuration": "./language-configuration.json"
}
],
"grammars": [
  {
    "language": "rtf",
    "scopeName": "source.rtf",
```

```
    "path": "./syntaxes/rtf.tmLanguage.json"
  },
  {
    "language": "pdb",
    "scopeName": "source.pdb",
    "path": "./syntaxes/pdb.tmLanguage.json"
  },
  {
    "language": "psf",
    "scopeName": "source.psf",
    "path": "./syntaxes/psf.tmLanguage.json"
  },
  {
    "language": "in",
    "scopeName": "source.in",
    "path": "./syntaxes/in.tmLanguage.json"
  },
  {
    "language": "prmtop",
    "scopeName": "source.prmtop",
    "path": "./syntaxes/prmtop.tmLanguage.json"
  },
  {
    "language": "inpcrd",
    "scopeName": "source.inpcrd",
    "path": "./syntaxes/inpcrd.tmLanguage.json"
  },
  {
    "language": "prepin",
    "scopeName": "source.prepin",
    "path": "./syntaxes/prepin.tmLanguage.json"
  },
  {
    "language": "frcmod",
    "scopeName": "source.frcmod",
    "path": "./syntaxes/frcmod.tmLanguage.json"
  },
  {
    "language": "lib",
    "scopeName": "source.lib",
    "path": "./syntaxes/lib.tmLanguage.json"
  },
  {
    "language": "ac",
    "scopeName": "source.ac",
    "path": "./syntaxes/ac.tmLanguage.json"
  },
  {
    "language": "mc",
    "scopeName": "source.mc",
    "path": "./syntaxes/mc.tmLanguage.json"
  },
  {
    "language": "gro",
    "scopeName": "source.gro",
    "path": "./syntaxes/gro.tmLanguage.json"
  },
  }
```

```
{
  "language": "atp",
  "scopeName": "source.atp",
  "path": "./syntaxes/atp.tmLanguage.json"
},
{
  "language": "arn",
  "scopeName": "source.arn",
  "path": "./syntaxes/arn.tmLanguage.json"
},
{
  "language": "rtp",
  "scopeName": "source.rtp",
  "path": "./syntaxes/rtp.tmLanguage.json"
},
{
  "language": "hdb",
  "scopeName": "source.hdb",
  "path": "./syntaxes/hdb.tmLanguage.json"
},
{
  "language": "r2b",
  "scopeName": "source.r2b",
  "path": "./syntaxes/r2b.tmLanguage.json"
},
{
  "language": "tdb",
  "scopeName": "source.tdb",
  "path": "./syntaxes/tdb.tmLanguage.json"
},
{
  "language": "mtp",
  "scopeName": "source.mtp",
  "path": "./syntaxes/mtp.tmLanguage.json"
},
{
  "language": "vsd",
  "scopeName": "source.vsd",
  "path": "./syntaxes/vsd.tmLanguage.json"
},
{
  "language": "mol2",
  "scopeName": "source.mol2",
  "path": "./syntaxes/mol2.tmLanguage.json"
},
{
  "language": "sdf",
  "scopeName": "source.sdf",
  "path": "./syntaxes/sdf.tmLanguage.json"
},
{
  "language": "plumed",
  "scopeName": "source.plumed",
  "path": "./syntaxes/plumed.tmLanguage.json"
}
]
},
```



```
"__metadata": {  
  "id": "ea9482d2-d0dc-42fc-bbb3-a5e5f99d95ab",  
  "publisherId": "bacd9c21-e15d-4c96-a8e9-e7b218fadd67",  
  "publisherDisplayName": "XufanGao",  
  "targetPlatform": "undefined",  
  "updated": false,  
  "isPreReleaseVersion": false,  
  "hasPreReleaseVersion": false,  
  "installedTimestamp": 1706966519959,  
  "pinned": false  
}  
}
```

1.2 language-configuration.json - 语言通用配置

```
{  
  "comments": {  
    // symbol used for single line comment. Remove this entry if your language does  
    // not support line comments  
    "lineComment": "!",  
    // symbols used for start and end a block comment. Remove this entry if your  
    // language does not support block comments  
    "blockComment": [ "/*", "*/" ]  
  },  
  // symbols used as brackets  
  "brackets": [  
    ["{", "}"],  
    ["[", "]"],  
    ["(", ")"]  
  ],  
  // symbols that are auto closed when typing  
  "autoClosingPairs": [  
    ["{", "}"],  
    ["[", "]"],  
    ["(", ")"],  
    ["\\\"", "\"\\\""],  
    ["'", "'"]  
  ],  
  // symbols that can be used to surround a selection  
  "surroundingPairs": [  
    ["{", "}"],  
    ["[", "]"],  
    ["(", ")"],  
    ["\\\"", "\"\\\""],  
    ["'", "'"]  
  ]  
}
```

二、NAMD/CHARMM 格式支持模块

2.1 PDB 文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
  "name": "PDB file syntax highlighting",
  "scopeName": "source.pdb",
  "fileTypes": [
    "pdb"
  ],
  "patterns": [
    {
      "begin": "^(CRYST|REMARK|HEADER|TITLE|COMPND|SOURCE|KEYWDS|EXPDTA|AUTHOR|REVDAT|
        JRNL|ORIGX|SCALE\\S*|DBREF|CONECT|MASTER)\\b",
      "end": "$",
      "name": "comment.line.remark.pdb"
    },
    {
      "begin": "not for MODEL ENDMDL",
      "end": "$",
      "name": "keyword.other.record-name.pdb",
      "match": "\\b(CRYST1|TER|END|HELIX|SHEET|SSBOND)\\b"
    },
    {
      "begin": "^ATOM |^HETATM",
      "end": "$",
      "name": "keyword.atom.pdb",
      "patterns": [
        {
          "name": "constant.numeric.atom-number.pdb",
          "match": "(?<=^.{6}).{5}"
        },
        {
          "name": "entity.name.tag.atom-name.pdb",
          "match": "(?<=^.{12}).{4}"
        },
        {
          "name": "string.unquoted.alternate-location.pdb",
          "match": "(?<=^.{16}).{1}"
        },
        {
          "name": "entity.name.type.residue-name.pdb",
          "match": "(?<=^.{17}).{4}"
        },
        {
          "name": "support.type.chain-id.pdb",
          "match": "(?<=^.{21}).{1}"
        },
        {
          "name": "variable.other.residue-number.pdb",
          "match": "(?<=^.{22}).{4}"
        },
        {
          "name": "entity.name.function.code-for-insertions-of-residues.pdb",
          "match": "(?<=^.{26}).{1}"
        },
        {
          "name": "constant.numeric.x-coordinate.pdb",
          "match": "(?<=^.{30}).{8}"
        }
      ]
    }
  ]
}
```

```
    },
    {
      "name": "constant.numeric.y-coordinate.pdb",
      "match": "(?<=^.{38}).{8}"
    },
    {
      "name": "constant.numeric.z-coordinate.pdb",
      "match": "(?<=^.{46}).{8}"
    },
    {
      "name": "string.quoted.occupancy.pdb",
      "match": "(?<=^.{54}).{6}"
    },
    {
      "name": "storage.type.temperature-factor.pdb",
      "match": "(?<=^.{60}).{6}"
    },
    {
      "name": "support.type.segment-name.pdb",
      "match": "(?<=^.{72}).{4}"
    },
    {
      "name": "string.quoted.element-symbol.pdb",
      "match": "(?<=^.{76}).{2}"
    },
    {
      "name": "variable.other.charge.pdb",
      "match": "(?<=^.{78}).{2}"
    }
  ]
}
]
```

2.2 RTF 文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
  "name": "NAMD force field (atom, residue, parameter) file",
  "scopeName": "source.rtf",
  "fileTypes": [
    "rtf",
    "inp",
    "str",
    "prm"
  ],
  "patterns": [
    {
      "comment": "starting with exclamation",
      "name": "comment.line.exclamation",
      "match": "!.*$"
    },
    {
      "name": "comment.line.asterisk",
```

```

    "match": "^\\s*\\s*.*"
  },
  {
    "name": "keyword.rtf",
    "match": "\\b(MASS|RESI|PRES|DELETE|ATOM|BOND|ANGLE(S)?|DIHE(DRAL)?|IMPR|IMPH|(?i)IC|BILD|ACCE(PTOR)?|DONO(R)?|DOUBLE|DOUB|(?i)PATC(H)?|PATCHING|LONEPAIR|COLI|DIST|SCAL|DECL|DEFA|AUTO|FIRS|LAST|first|last|default)\\b"
  },
  {
    "name": "keyword.prm",
    "match": "(MASS|ATOMS|BONDS|ANGLES|DIHEDRALS|IMPROPER(S)?|CMAP|NONBONDED|NBFIX|HBOND|CUTHB)"
  },
  {
    "name": "entity.name.section.prm",
    "match": "\\b(BONDS|ANGLES|DIHEDRALS|IMPROPER(S)|CMAP|NONBONDED|NBFIX)\\b"
  },
  {
    "name": "support.type.end.rtf",
    "match": "^END|^GROUP"
  },
  {
    "/*": "floats in lines starting with those keywords",
    "name": "constant.numeric.rtf",
    "match": "(?<=\\b(MASS|ATOM|RESI|PRES|IC|BILD|LONEPAIR)\\b.*?)\\b(-?\\d+\\.\\d*)\\b"
  },
  {
    "/*": "the number after MASS, all -1, or 1,2,3...",
    "name": "string.mass_number.rtf",
    "match": "(?<=\\bMASS\\b.*?)\\s+~?\\d+\\s+"
  },
  {
    "/*": "element symbol in MASS line",
    "name": "string.quoted.element-symbol.rtf",
    "match": "(?<=^MASS\\s+~?\\d+\\s+\\s+\\s+\\b(-?\\d+\\.\\d*)\\b\\s+)\\s+"
  },
  {
    "/*": "the word after RESI|PRES",
    "name": "entity.name.type.resname.rtf",
    "match": "(?<=\\b(RESI|PRES)\\s)\\s+"
  },
  {
    "/*": "the number after RESI|PRES resname",
    "name": "string.quoted.charge.rtf",
    "match": "(?<=\\b(RESI|PRES)\\s+\\s+\\s+\\s+~?\\d+\\.\\d+"
  },
  {
    "/*": "the several words after a keyword",
    "note": "bond: variable length of pairs; impr: four strings",
    "/*": "Maybe atom names can be de",
    "name": "entity.name.tag.atom.rtf",
    "match": "(?<=\\bATOM\\s*)\\s+|(?<=\\bBOND\\s*)(\\s+\\s+\\s+\\s+)+|(?<=\\bANGLE\\s*)(\\s+\\s+\\s+\\s+){3}+|(?<=\\bIMPR\\s*)(\\s+\\s+\\s+\\s+){4}+|(?<=\\bIMPH\\s*)(\\s+\\s+\\s+\\s+){4}+|(?<=\\bCMAP\\s*)(\\s+\\s+\\s+\\s+){8}+|(?<=\\b\\s*(?i)IC\\s*)(\\s+\\s+\\s+\\s+){4}|(?<=\\b\\s*BILD\\s*)(\\s+\\s+\\s+\\s+){4}"
  },

```

```

{
  "///": "the several words after a keyword.",
  "name": "entity.name.tag.atom.rtf",
  "match": "(?<=\\bACCE(PTOR)?\\s*)(\\S+\\s*)+|(?<=\\bDONO(R)?\\s*)(\\S+\\s*)+|(?<=\\bDOUBLE\\s*)(\\S+\\s+\\S+\\s*)+|(?<=\\bPATC\\s*)(\\S+\\s+){4}|(?<=\\bPATCH\\s*)(\\S+\\s+){4}"
},
{
  "///": "rarer keywords",
  "name": "entity.name.tag.atom.rtf",
  "match": "(?<=\\bDECL\\s*)(?:[+-]\\S+\\s*)|(?<=\\bDEFA\\s*)(\\S+\\s*){4}|(?<=\\bLONEPAIR\\s+\\S+\\s+\\S+\\s+\\S+\\s+\\S+\\s+\\S+\\s+)"
},
{
  "///": "after charge, before atom-type.prm, otherwise overwritten...",
  "name": "constant.numeric.rtf",
  "match": "-?\\d+\\.\\d*"
},
{
  "///": "dihedral n",
  "name": "string.quoted.dihedral-n.prm",
  "match": "(?<=-?\\d+\\.\\d*\\s+)\\d(?:\\s+~?\\d+\\.\\d*)"
},
{
  "///": "all strings made up of capitalized letters (in special files there are lower case letters) and numbers. matching a lot of remaining strings...put them before this!",
  "name": "support.type.atom-type.prm",
  "match": "\\b([A-Za-z0-9]+)\\b"
},
{
  "///": "a special type",
  "name": "support.type.atomtype.prm",
  "match": "\\b(none)\\b|\\b(NONE)\\b"
}
]
}

```

2.3 PSF 文件语法定义

```

{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.json",
  "name": "PSF from GUI, that from vmd is different",
  "scopeName": "source.psf",
  "fileTypes": [
    "psf"
  ],
  "patterns": [
    {
      "name": "comment.line.psf",
      "match": "^\\s*.*$"
    },
    {
      "begin": "^\\s+REMARKS\\b",

```

```
"end": "$",
"name": "comment.line.remark.pdb"
},
{
  "///": "ATOM and BOND is missing...",
  "name": "keyword.psf",
  "match": "\\b(PSF|CMAP|NTITLE|NATOM|NBOND|NTHETA|NPHI|NIMPHI|NDON|NACC|NNB|NGRP|
NUMLP|NCRTERM)\\b"
},
{
  "name": "entity.name.function.total_number",
  "match": "(?<=^\\s+)\\d+(?= !N)"
},
{
  "begin": "(!NATOM\\s*$)",
  "end": "(!NBOND)",
  "name": "keyword.atom.psf",
  "///": "^\\s+\\d+\\s+\\s+\\s+\\s+\\d+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\b[A-Z0-9]+\\b\\s+(-?\\d+\\.\\d*(E-01)?)\\s+(-?\\d+\\.\\d*)\\s+\\d+$",
  "patterns": [
    {
      "///": "NATOM still not solved. see my notes",
      "name": "keyword.other.psf",
      "match": "NATOM|NBOND"
    },
    {
      "name": "entity.name.function.total_number",
      "match": "(?<=^\\s+)\\d+(?= !N)"
    },
    {
      "name": "constant.numeric.atom-number.psf",
      "match": "(?<=^\\s+)\\d+(?=\\s+\\s+\\s+\\s+\\d+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\b[A-Z0-9]+\\b\\s+(-?\\d+\\.\\d*(E-01)?)\\s+(-?\\d+\\.\\d*)\\s+\\d+$)"
    },
    {
      "name": "variable.other.segment-name.psf",
      "match": "(?<=^\\s+\\d+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\b[A-Z0-9]+\\b\\s+(-?\\d+\\.\\d*(E-01)?)\\s+(-?\\d+\\.\\d*)\\s+\\d+$)"
    },
    {
      "name": "support.type.residue-number.psf",
      "match": "(?<=^\\s+\\d+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\b[A-Z0-9]+\\b\\s+(-?\\d+\\.\\d*(E-01)?)\\s+(-?\\d+\\.\\d*)\\s+\\d+$)"
    },
    {
      "name": "entity.name.type.residue-name.psf",
      "match": "(?<=^\\s+\\d+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\b[A-Z0-9]+\\b\\s+(-?\\d+\\.\\d*(E-01)?)\\s+(-?\\d+\\.\\d*)\\s+\\d+$)"
    },
    {
      "name": "entity.name.tag.atom-name.psf",
      "match": "(?<=^\\s+\\d+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\b[A-Z0-9]+\\b\\s+(-?\\d+\\.\\d*(E-01)?)\\s+(-?\\d+\\.\\d*)\\s+\\d+$)"
    },
    {
      "name": "support.type.atom-type.psf",
      "match": "(?<=^\\s+\\d+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\s+\\b[A-Z0-9]+\\b(?:=
```

```

\\s+(-?\\d+\\.\\d*(E-01)?)\\s+(-?\\d+\\.\\d*)\\s+\\d+$)"
    },
    {
      "name": "string.quoted.charge.psf",
      "match": "(?<=^\\s+\\d+\\s+\\S+\\s+\\d+\\s+\\S+\\s+\\S+\\s+\\b[A-Z0-9]+\\b\\s+)(-?\\d+\\.\\d*(E-01)?)(?=\\s+(-?\\d+\\.\\d*)\\s+\\d+$)"
    },
    {
      "name": "constant.numeric.atomic-mass.psf",
      "match": "(?<=^\\s+\\d+\\s+\\S+\\s+\\d+\\s+\\S+\\s+\\S+\\s+\\b[A-Z0-9]+\\b\\s+)(-?\\d+\\.\\d*(E-01)?)\\s+(-?\\d+\\.\\d*)(?=\\s+\\d+$)"
    },
    {
      "name": "comment.line.unknown.psf",
      "match": "(?<=^\\s+\\d+\\s+\\S+\\s+\\d+\\s+\\S+\\s+\\S+\\s+\\b[A-Z0-9]+\\b\\s+)(-?\\d+\\.\\d*(E-01)?)\\s+(-?\\d+\\.\\d*)\\s+\\d+(?=$)"
    }
  ]
},
{
  "name": "constant.numeric.psf",
  "match": "\\b\\d+\\b|(?<=^\\s*)\\d+"
}
]
}

```

三、Amber 格式支持模块

3.1 PRMTOP 文件语法定义

```

{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.json",
  "name": "prmtop",
  "scopeName": "source.prmtop",
  "fileTypes": [
    "prmtop"
  ],
  "patterns": [
    {
      "match": "\\%VERSION|\\%FLAG|\\%FORMAT",
      "name": "keyword.prmtop"
    },
    {
      "match": "(?<=\\%FORMAT)\\S+",
      "name": "support.type.format.prmtop"
    },
    {
      "comment": "float",
      "match": "\\s+-?\\d+\\.\\d*",
      "name": "constant.numeric.float.prmtop"
    },
    {

```

```
"match": "\\s+-?\\d+",
"name": "constant.numeric.integer.primtop"
},
{
  "///": "use constant as itp?",
  "match": "E[+-]\\d\\d",
  "name": "entity.name.function.exponential.primtop"
},
{
  "begin": "ATOM\\_NAME",
  "end": "CHARGE",
  "///": "\\%FORMAT;\\s+\\n",
  "patterns": [
    {
      "name": "keyword.primtop",
      "match": "\\%VERSION|\\%FLAG|\\%FORMAT"
    },
    {
      "///": "use \\S+ instead of \\b([A-Z0-9a-z+-]+)\\b to include names with '+-',
      "match": "(?<=\\%FORMAT)\\S+",
      "name": "support.type.format.primtop"
    },
    {
      "match": "\\S+",
      "name": "entity.name.tag.atom-name.primtop"
    }
  ]
},
{
  "begin": "ATOMIC\\_NUMBER\\s+\\n",
  "end": "MASS",
  "patterns": [
    {
      "name": "keyword.primtop",
      "match": "\\%VERSION|\\%FLAG|\\%FORMAT"
    },
    {
      "match": "(?<=\\%FORMAT)\\S+",
      "name": "support.type.format.primtop"
    },
    {
      "match": "\\b\\d+\\b",
      "name": "constant.numeric.atom-name.primtop"
    }
  ]
},
{
  "begin": "MASS\\s+\\n",
  "end": "ATOM\\_TYPE\\_INDEX",
  "name": "string.quoted.primtop",
  "patterns": [
    {
      "name": "keyword.primtop",
      "match": "\\%VERSION|\\%FLAG|\\%FORMAT"
    },
    {
      "match": "(?<=\\%FORMAT)\\S+",

```



```

        "name": "support.type.format.primtop"
    }
  ],
},
{
  "begin": "RESIDUE\\_LABEL\\s+\\n",
  "end": "RESIDUE\\_POINTER",
  "/*": "values of fields",
  "patterns": [
    {
      "name": "keyword.primtop",
      "match": "\\%VERSION|\\%FLAG|\\%FORMAT"
    },
    {
      "match": "(?<=\\%FORMAT)\\s+",
      "name": "support.type.format.primtop"
    },
    {
      "/*": "todo: according to protein residue type?",
      "match": "\\s+",
      "name": "entity.name.type.residue-name.primtop"
    }
  ]
},
{
  "begin": "AMBER\\_ATOM\\_TYPE\\s+\\n",
  "end": "TREE\\_CHAIN\\_CLASSIFICATION",
  "/*": "values of fields",
  "patterns": [
    {
      "name": "keyword.primtop",
      "match": "\\%VERSION|\\%FLAG|\\%FORMAT"
    },
    {
      "match": "(?<=\\%FORMAT)\\s+",
      "name": "support.type.format.primtop"
    },
    {
      "match": "\\s+",
      "name": "support.type.atom-type.primtop"
    }
  ]
}
]
}
}

```

3.2 Amber 输入文件语法定义

```

{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
  "name": "Amber or AmberTools (like tleap, parmed) input file",
  "scopeName": "source.in",
  "fileTypes": [
    "in"
  ]
}

```

```
],
"patterns": [
  {
    "name": "comment.line.exclamation",
    "match": "!.*$"
  },
  {
    "name": "comment.line.numbersign",
    "match": "#.*$"
  },
  {
    "name": "entity.name.tag.asterisk",
    "match": "^\\s&\\S+"
  },
  {
    "name": "constant.numeric",
    "match": "\\s+-?\\d+\\.\\d+\\s+|\\s+\\d+\\s+"
  },
  {
    "name": "keyword.md",
    "match": "\\b(imin|iwrap|irest|ntx|cut|ntb|ntc|ntf|tempi|temp0|ntt|gamma_ln|ig|ntp|pres0|taup|barostat|nstlim|dt|ntpr|ntwx|ntwr)\\b"
  },
  {
    "name": "entity.name.function.format",
    "match": "\\b(pdb|mol2|prmtop|inpcrd|frcmod|itp|top|gro|psf|rtf)\\b"
  },
  {
    "name": "keyword.1.tleap",
    "match": "\\b(source|loadmol2|loadpdb|addAtomTypes|bond|combine|(?)loadamberparams|(?i)loadAmberPrep|(?i)loadOFF|(?i)addPdbAtomMap|(?i)addPdbResMap)\\b"
  },
  {
    "name": "keyword.2.tleap",
    "match": "\\b(charge|solvatebox|addIons(2|Rand)|savepdb|saveamberparm|quit)\\b"
  },
  {
    "name": "string.quoted.leap",
    "match": "\\b(leaprc\\.\\S+)\\b"
  },
  {
    "/*": "not matching + !",
    "name": "string.other.ions",
    "match": "\\b(Na+|Cl-|K+|Al3+|Mg2+|Ca2+)\\b"
  },
  {
    "name": "keyword.parmed",
    "match": "\\b(chamber|gromber|writeFrcmod|outparm|parmout)\\b"
  },
  {
    "name": "support.type.variable",
    "match": "^\\S+(?=\\s*=)"
  }
]
}
```

3.3 坐标文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
  "name": "inpcrd",
  "scopeName": "source.inpcrd",
  "fileTypes": [
    "inpcrd"
  ],
  "patterns": [
    {
      "name": "The second line",
      "match": "^\\s\\d+$",
      "name": "string.quoted.number-of-atom.inpcrd"
    },
    {
      "name": "all float numbers",
      "match": "\\d+\\.\\d+",
      "name": "constant.numeric.coordinates.inpcrd"
    }
  ]
}
```

3.4 预处理文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
  "name": "prepin",
  "scopeName": "source.prepin",
  "fileTypes": [
    "prepin"
  ],
  "patterns": [
    {
      "name": "comment.line.info.prepin",
      "match": "^.*(?)remark.*$"
    },
    {
      "name": "comment.line.dummy.prepin",
      "match": "DU(MM)?"
    },
    {
      "name": "entity.name.type.prepin",
      "match": "\\S+(?=\\s*(INT|XYZ))"
    },
    {
      "name": "variable.other.coord-type.prepin",
      "match": "INT|XYZ"
    },
    {
      "match": "CORRECT|CHANGE|OMIT|NOMIT|BEG|ALL|LOOP|IMPROPER|DONE|STOP",
      "name": "keyword.prepin"
    }
  ]
}
```

```

},
{
  "name": "constant.numeric.atom-number.prepin",
  "match": "(?<=\\s*)\\d+(?=\\s\\s\\s\\s\\s+\\s+\\s+\\s+[EMBS3456])"
},
{
  "name": "entity.name.tag.atom-name.prepin",
  "match": "(?<=\\s+)(\\s+\\s+){2}(?=$) | (?<=\\s+)(\\s+\\s+){4}(?=$) | (?<=\\s*\\d+\\s\\s)(\\s+)(?=\\s+\\s+\\s+[EMBS3456])"
},
{
  "name": "support.type.atom-type.prepin",
  "match": "(?<=\\s*\\d+\\s\\s\\s\\s\\s+\\s+\\s+\\s+)(?=\\s+[EMBS3456])"
},
{
  "//": "avoid the following three numbers",
  "name": "keyword.tree-symbol.prepin",
  "match": "(?<=\\s+\\d+\\s+\\s+\\s+\\s+\\s+\\s+)[EMBS3456](?!\\s+~?\\d*\\.\\d*|\\s+~?\\d*\\s+~?\\d*\\.\\d*)"
},
{
  "match": "(?<=~?\\d*\\.\\d*)\\s+~?\\d*\\.\\d*(?=$)",
  "name": "string.quoted.charge.prepin"
},
{
  "match": "\\s+~?\\d*\\.\\d*",
  "name": "constant.numeric.float.prepin"
}
]
}

```

3.5 力场修改文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
  "name": "frcmod",
  "scopeName": "source.frcmod",
  "fileTypes": [
    "frcmod"
  ],
  "patterns": [
    {
      "match": "MASS|BOND|ANGL(E)?|DIHE(DRAL)?|IMPROPER|IMPR|NONB(ON)?(D)?(ED)?|^CMAP|\\|\\%
FLAG|END|SOURCE\\d",
      "name": "keyword.frcmod"
    },
    {
      "///": "bug: some files like OPLS write values as integers/nothing after point",
      "begin": "^\\[A-Za-z0-9*\\]+\\ ]*-\\[A-Za-z0-9*\\]+\\ ]*-\\[A-Za-z0-9*\\]+\\ ]*-\\[A-Za-z0-9*\\]+\\ ]*
\\s+",
      "end": "$",
      "name": "support.type.atom-type.dihedral.frcmod",
      "patterns": [
        {
```

```

        "///": "sometimes phi = 180",
        "match": "\\s*\\d+(?=\\s+~?\\d*\\.\\.\\d*\\s+(-?\\d+\\.\\.\\d*|\\d+))",
        "name": "variable.other.redundancy.frcmod"
    },
    {
        "match": "(?<=\\s+\\d+\\s+~?\\d*\\.\\.\\d*\\s+(-?\\d+\\.\\.\\d*|\\d+)\\s+)-?\\d+",
        "name": "string.quoted.dihedral-n.frcmod"
    },
    {
        "///": "all previous in this line, correspond to above. sometimes no nonbond,
only one number",
        "match": "(?<=^[A-Za-z0-9*]+[ ]*-[A-Za-z0-9*]+[ ]*-[A-Za-z0-9*]+[ ]*-[A-Za-z0-9*]+[ ]*(\\s+\\d+)?\\s+~?\\d*\\.\\.\\d*\\s+(-?\\d+\\.\\.\\d*|\\d+)\\s+~?\\d+\\.?\\d*).*$",
        "name": "comment.line.dihedral-improper.frcmod"
    },
    {
        "match": "\\b(-?\\d*\\.\\.\\d*)\\b|\\b\\d+\\b",
        "name": "constant.numeric.parameter.frcmod"
    }
]
},
{
    "///": "angle incorrectly matches dihedral/... section",
    "begin": "^[A-Za-z0-9*]+[ ]*-[A-Za-z0-9*]+[ ]*-[A-Za-z0-9*]+[ ]*\\s+",
    "end": "$",
    "name": "support.type.atom-type.angle.frcmod",
    "patterns": [
        {
            "match": "(?<=^[A-Za-z0-9*]+[ ]*-[A-Za-z0-9*]+[ ]*-[A-Za-z0-9*]+[ ]*\\s+~?\\d*\\.\\.\\d*\\s+~?\\d*\\.\\.\\d*).*$",
            "name": "comment.line.angle.frcmod"
        },
        {
            "match": "\\b(-?\\d*\\.\\.\\d*)\\b|\\b\\d+\\b",
            "name": "constant.numeric.parameter.frcmod"
        }
    ]
},
{
    "///": "bond incorrectly matches angle/... section",
    "begin": "^[A-Za-z0-9*]+[ ]*-[A-Za-z0-9*]+[ ]*\\s+",
    "end": "$",
    "name": "support.type.atom-type.bond.frcmod",
    "patterns": [
        {
            "match": "(?<=^[A-Za-z0-9*]+[ ]*-[A-Za-z0-9*]+[ ]*\\s+~?\\d*\\.\\.\\d*\\s+~?\\d*\\.\\.\\d*).*$",
            "name": "comment.line.angle.frcmod"
        },
        {
            "match": "\\b(-?\\d*\\.\\.\\d*)\\b|\\b\\d+\\b",
            "name": "constant.numeric.parameter.frcmod"
        }
    ]
},
{
    "///": "ions may also contain +- but no bond/angle/...",

```

```
"begin": "^\\s*[A-Za-z0-9*+-]+\\s+",
"end": "$",
"name": "support.type.atom-type.atom.frcmod",
"patterns": [
  {
    "match": "\\b(?:\\d*\\.\\d*)\\b",
    "name": "constant.numeric.parameter.frcmod"
  },
  {
    "comment": "after float but not starting with number",
    "match": "(?<=\\.\\d*\\s+)[a-zA-Z#!;\\$].*$",
    "name": "comment.line.mass-nonbon.frcmod"
  }
]
},
{
  "match": "\\s+\\.\\d*",
  "name": "constant.numeric.cmap-float.frcmod"
},
{
  "name": "string.quoted.cmap-integer.frcmod",
  "match": "(?<=\\%FLAG\\s*\\S+\\s*)\\d+(?=\\s*$)"
}
]
}
```

3.6 库文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
  json",
  "name": "tLeap lib file",
  "scopeName": "source.lib",
  "fileTypes": [
    "lib"
  ],
  "patterns": [
    {
      "name": "comment.line.exclamation",
      "match": "(?<=\\!entry\\.[A-Z0-9]+).*$|\\!.*$"
    },
    {
      "name": "entity.name.type.residue-names.lib",
      "match": "(?<=\\s*)\\S+(?=\\s*$)"
    },
    {
      "name": "keyword.lib",
      "match": "!entry"
    },
    {
      "name": "entity.name.type.residue-name.lib",
      "match": "(?<=!entry.)[A-Z0-9]+"
    },
    {
      "comment": "overwritten by comment",

```

```
"name": "entity.name.tag.type.lib",
"match": "(?<!=!entry.[A-Z0-9]+.unit.)[a-z]+"
},
{
"name": "entity.name.tag.atom-name.lib",
"match": "(?<=^\\s+\\\"\\\\S+(?=\\\"\\\\s+\\\"\\\\S+\\\")\""
},
{
"name": "support.type.residue-number.lib",
"match": "(?<=^\\s+\\\"\\\\S+\\\"\\\\s+\\\"\\\\S+\\\"\\\\s\\\\d\\\\s)-?\\\\d+(?=\\\"\\\\s\\\\d+\\\\s\\\\d+\\\\s-?\\\\d+\\\\s-?\\\\d+\\\\.\\\\d*(E-0\\\\d)?)"
},
{
"name": "entity.name.function.atom-number.lib",
"match": "(?<=^\\s+\\\"\\\\S+\\\"\\\\s+\\\"\\\\S+\\\"\\\\s\\\\d\\\\s-?\\\\d+\\\\s\\\\d+\\\\s)\\\\d+(?=\\\"\\\\s-?\\\\d+\\\\s-?\\\\d+\\\\.\\\\d*(E-0\\\\d)?)"
},
{
"name": "entity.name.tag.element-number.lib",
"match": "(?<=^\\s+\\\"\\\\S+\\\"\\\\s+\\\"\\\\S+\\\"\\\\s\\\\d\\\\s-?\\\\d+\\\\s\\\\d+\\\\s\\\\d+\\\\s)-?\\\\d+(?=\\\"\\\\s-?\\\\d+\\\\.\\\\d*(E-0\\\\d)?)"
},
{
"name": "string.quoted.charge.lib",
"match": "(?<=^\\s+\\\"\\\\S+\\\"\\\\s+\\\"\\\\S+\\\"\\\\s\\\\d\\\\s-?\\\\d+\\\\s\\\\d+\\\\s\\\\d+\\\\s-?\\\\d+\\\\s)(-?\\\\d+\\\\.\\\\d*(E-0\\\\d)?)"
},
{
"name": "support.type.atom-type.lib",
"match": "(?<=^\\s+\\\"\\\\S+\\\"\\\\s+\\\"\\\\S+\\\"\\\\s+\\\"\\\\S+(?=\\\")\""
},
{
"/": "purely number lines. atom number in other places",
"match": "(?<=^)[\\\\s\\\\d+](?=\\\\s*$)",
"name": "variable.other.atom-number-index.lib"
},
{
"name": "constant.numeric.lib",
"match": "\\\\b\\\\d+\\\\b|(?<=^\\\\s*)\\\\d+|(\\\\\\\\b|\\\\\\\\- )\\\\d+\\\\. ?\\\\d*([eE][\\\\\\\\+\\\\\\\\-]?\\\\d+)?"
}
]
```

3.7 Antechamber 文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
  "name": "Amber ac file",
  "scopeName": "source.ac",
  "fileTypes": [
    "ac"
  ],
  "patterns": [
    {
```

```
"name": "keyword.ac",
"match": "\\b(CHARGE|Formula)\\b"
},
{
  "match": "(?<=CHARGE|Formula).*$",
  "name": "comment.line.remark.ac"
},
{
  "begin": "^ATOM |^HETATM",
  "end": "$",
  "name": "keyword.atom.ac",
  "patterns": [
    {
      "name": "constant.numeric.atom-number.ac",
      "match": "(?<=^.{6}).{5}"
    },
    {
      "name": "entity.name.tag.atom-name.ac",
      "match": "(?<=^.{12}).{4}"
    },
    {
      "name": "string.unquoted.alternate-location.ac",
      "match": "(?<=^.{16}).{1}"
    },
    {
      "name": "entity.name.type.residue-name.ac",
      "match": "(?<=^.{17}).{4}"
    },
    {
      "name": "support.type.chain-id.ac",
      "match": "(?<=^.{21}).{1}"
    },
    {
      "name": "variable.other.residue-number.ac",
      "match": "(?<=^.{22}).{4}"
    },
    {
      "name": "entity.name.function.code-for-insertions-of-residues.ac",
      "match": "(?<=^.{26}).{1}"
    },
    {
      "name": "constant.numeric.x-coordinate.ac",
      "match": "(?<=^.{30}).{8}"
    },
    {
      "name": "constant.numeric.y-coordinate.ac",
      "match": "(?<=^.{38}).{8}"
    },
    {
      "name": "constant.numeric.z-coordinate.ac",
      "match": "(?<=^.{46}).{8}"
    },
    {
      "name": "string.quoted.charge.ac",
      "match": "(?<=^.{55}).{10}"
    }
  ]
}
```



```
        "name": "support.type.atom-type.ac",
        "match": "(?<=^.{68}).{6}"
    }
]
},
{
    "begin": "^BOND",
    "end": "$",
    "name": "keyword.bond.ac",
    "patterns": [
        {
            "name": "string.other.bond-number.acconstant.numeric.atom-number.ac",
            "match": "(?<=^.{6}).{4}"
        },
        {
            "name": "constant.numeric.atom-number1.ac",
            "match": "(?<=^.{10}).{5}"
        },
        {
            "name": "constant.numeric.atom-number2.ac",
            "match": "(?<=^.{15}).{5}"
        },
        {
            "name": "entity.name.function.bond-type.ac",
            "match": "(?<=^.{20}).{5}"
        },
        {
            "name": "entity.name.tag.atom-name1.ac",
            "match": "(?<=^.{26}).{6}"
        },
        {
            "name": "entity.name.tag.atom-name2.ac",
            "match": "(?<=^.{32}).{4}"
        }
    ]
}
]
}
```

3.8 主链文件语法定义

```
{
    "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
    "name": "mc",
    "scopeName": "source.mc",
    "fileTypes": [
        "mc"
    ],
    "patterns": [
        {
            "match": "HEAD_NAME|TAIL_NAME|PRE_HEAD_TYPE|POST_TAIL_TYPE|CHARGE",
            "name": "keyword.other.mc"
        },
        {
```

```
    "match": "OMIT_NAME",
    "name": "string.other.mc"
  },
  {
    "name": "entity.name.tag.atom-name.mc",
    "match": "(?<=NAME\\s*)\\b\\S+\\b"
  },
  {
    "name": "support.type.atomtype.mc",
    "match": "(?<=TYPE\\s*)\\b\\S+\\b"
  },
  {
    "name": "constant.numeric.mc",
    "match": "\\b(-?\\d*\\.\\d*)\\b|\\b\\d+\\b"
  }
]
}
```

四、 Gromacs 格式支持模块

4.1 Gromacs 坐标文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
  json",
  "name": "Gromacs mutation file",
  "scopeName": "source.gro",
  "fileTypes": [
    "gro"
  ],
  "patterns": [
    {
      "name": "keyword.timestep",
      "match": "t=.*$"
    },
    {
      "comment": "the first line? not starting with number or space",
      "name": "comment.line.gro",
      "match": "^[^0-9 ].*$"
    },
    {
      "name": "keyword.total_number",
      "match": "\\d+\\s*"
    },
    {
      "name": "keyword.other.box-vector.gro",
      "match": "(\\s+-?\\d+\\.\\d+)+\\s*"
    },
    {
      "name": "support.type.residue-number.gro",
      "match": ".{5}"
    },
    {

```

```
    "name": "entity.name.type.residue-name.gro",
    "match": "(?<=^.{5}).{5}"
  },
  {
    "name": "entity.name.tag.atom-name.gro",
    "match": "(?<=^.{10}).{5}"
  },
  {
    "name": "constant.numeric.atom-number.gro",
    "match": ""
  },
  {
    "name": "constant.numeric.coordinate.gro",
    "match": "(?<=^.{20}).{8}|(?<=^.{28}).{8}|(?<=^.{36}).{8}"
  },
  {
    "name": "string.quoted.velocity.gro",
    "match": "(?<=^.{44}).{8}|(?<=^.{52}).{8}|(?<=^.{60}).{8}"
  }
]
```

4.2 原子类型文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.json",
  "name": "atp",
  "scopeName": "source.atp",
  "fileTypes": [
    "atp"
  ],
  "patterns": [
    {
      "name": "comment.line.semicolon",
      "match": ";.*$"
    },
    {
      "name": "constant.numeric.atp",
      "match": "-?\\d+\\.\\d*"
    },
    {
      "name": "support.type.atom-type.atp",
      "match": "\\b([A-Za-z0-9_]+)\\b"
    },
    {
      "name": "support.type.atomtype.atp",
      "match": "\\b(amber.*)\\b"
    }
  ]
}
```

4.3 原子重命名文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
  "name": "arn",
  "scopeName": "source.arn",
  "fileTypes": [
    "arn"
  ],
  "patterns": [
    {
      "name": "comment.line.semicolon",
      "match": ";.*$"
    },
    {
      "name": "constant.numeric.arn",
      "match": "-?\\d+\\.\\d*"
    },
    {
      "name": "entity.name.type.residue-name.rtf",
      "match": "(?<=^\\s*)\\S+"
    },
    {
      "name": "entity.name.tag.atom-name.tdb",
      "match": "(?<=^\\s*\\S+\\s*[0-9]*[A-Z]+[A-Z0-9_']*)*"
    },
    {
      "name": "support.type.atom-type.arn",
      "match": "(?<=^\\s*\\S+\\s*[0-9]*[A-Z]+[A-Z0-9_']*)*"
    }
  ]
}
```

4.4 残基类型文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
    json",
  "name": "Gromacs mutation file",
  "scopeName": "source.rtp",
  "fileTypes": [
    "rtp"
  ],
  "patterns": [
    {
      "name": "comment.line.semicolon",

```

```

    "match": ".*$"
  },
  {
    "name": "comment.line.other",
    "match": "torsion.*$|un.*$"
  },
  {
    "name": "section",
    "match": "\\[.*\\]",
    "name": "entity.name.class"
  },
  {
    "name": "atoms section; bonds",
    "name": "entity.name.tag.atom-name.rtp",
    "match": "[0-9]*[A-Z]+[A-Z0-9_']**(?=\\s+[0-9]*[A-Z]+[A-Z0-9_']*.*\\s+-?\\d+\\.\\d*)"
    | (\\s+-?\\s+[0-9]*[A-Z]+[A-Z0-9_']*\\s+){2}(?=\\s*($|;))"
  },
  {
    "name": "impropers/dihedrals; cmap",
    "name": "entity.name.tag.atom-name2.rtp",
    "match": "(\\s+-?\\s+[0-9]*[A-Z]+[A-Z0-9_']*\\s+){4}|(-?\\s+[0-9]*[A-Z]+[A-Z0-9_']*\\s+){4}-?\\s+[0-9]*[A-Z]+[A-Z0-9_']*\\s+"
  },
  {
    "name": "after atom name, match any of these strings",
    "name": "support.type.atom-type.rtp",
    "match": "[0-9]*[A-Z]+[A-Z0-9_']**(?=\\s+-?\\d+\\.\\d*)"
  },
  {
    "name": "string.quoted.charge.rtp",
    "match": "(?<=[0-9]*[A-Z]+[A-Z0-9_']*.*\\s+)-?\\d+\\.\\d*"
  },
  {
    "name": "number",
    "match": "(\\b|\\-\\.\\d+\\.\\d*([eE](\\+|\\-)?\\d+)?)",
    "name": "constant.language.rtp"
  }
]
}

```

4.5 氢数据库文件语法定义

```

{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.json",
  "name": "Gromacs hdb file",
  "scopeName": "source.hdb",
  "fileTypes": [
    "hdb"
  ],
  "patterns": [
    {
      "name": "comment.line.exclamation",
      "match": ".*$"
    },
  ],
}

```

```
{
  "name": "support.type.residue-name.hdb",
  "match": "(?<=^)\S+(?=\s*\d+\s*$)"
},
{
  "name": "string.other.count.hdb",
  "match": "(?<=^\S+\s*)\d+(?=\s*$)"
},
{
  "name": "entity.name.tag.atom-name.hdb",
  "match": "(?<=^\d+\s+\d+\s+)\S+\s+\S+(\s+\S+\s+\S+)?(\s+\S+)?(=\s*$)"
},
{
  "name": "constant.numeric.hdb",
  "match": "\\b\\d+\\b|(?<=^\\s*)\\d+|(\\b|\\-)\d+\\.?\d*([eE][\\+\\-]?\\d+)?"
}
]
```

4.6 残基到珠映射文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.json",
  "name": "Gromacs r2b file",
  "scopeName": "source.r2b",
  "fileTypes": [
    "r2b"
  ],
  "patterns": [
    {
      "name": "comment.line.exclamation",
      "match": ";.*$"
    },
    {
      "name": "entity.name.type.residue-name.r2b",
      "match": "\\S+"
    },
    {
      "name": "constant.numeric.r2b",
      "match": "\\b\\d+\\b|(?<=^\\s*)\\d+|(\\b|\\-)\d+\\.?\d*([eE][\\+\\-]?\\d+)?"
    }
  ]
}
```

4.7 终端数据库文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.json",
  "name": "Gromacs terminal database",
```

```

"scopeName": "source.tdb",
"fileTypes": [
  "tdb"
],
"patterns": [
  {
    "name": "comment.line.semicolon",
    "match": ".*$"
  },
  {
    "name": "section",
    "match": "\\[.*\\]",
    "name": "entity.name.class"
  },
  {
    "name": "deltete (one space); replace (before type mass charge)",
    "name": "entity.name.tag.atom-name.tdb",
    "match": "(?<=\\s)[0-9]*[A-Z]+[A-Z0-9_']*| [0-9]*[A-Z]+[A-Z0-9_']* (?=\\s+[0-9]*[A-Z]+[A-Z0-9_']*\\s+-?\\d+\\.\\d*)"
  },
  {
    "name": "add (4/5, after two numbers), improper (4)",
    "name": "entity.name.tag.atom-name2.tdb",
    "match": "(\\s*-?\\+?[0-9]*[A-Z]+[A-Z0-9_']*\\+){4}(\\s*-?\\+?[0-9]*[A-Z]+[A-Z0-9_']*\\+)*?"
  },
  {
    "name": "after atom name, match any of these strings",
    "name": "support.type.atom-type.tdb",
    "match": "[0-9]*[A-Z]+[A-Z0-9_']* (?=\\s+-?\\d+\\.\\d*)"
  },
  {
    "name": "constant.numeric.atomic-mass.tdb",
    "match": "(?<=[0-9]*[A-Z]+[A-Z0-9_']*\\s+-?\\d+\\.\\d*)"
  },
  {
    "name": "string.quoted.charge.tdb",
    "match": "(?<=[0-9]*[A-Z]+[A-Z0-9_']*\\s+-?\\d+\\.\\d*\\s+-?\\d+\\.\\d*)"
  },
  {
    "name": "number",
    "match": "(\\b|\\-|\\+|\\.)\\d+\\.?\\d*([eE](\\+|\\-)?\\d+)?",
    "name": "constant.language.tdb"
  }
]
}

```

4.8 突变拓扑文件语法定义

```

{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.json",
  "name": "Gromacs mutation file",
  "scopeName": "source.mtp",
  "fileTypes": [

```

```

    "mtp"
  ],
  "patterns": [
    {
      "name": "comment.line.semicolon",
      "match": ";.*$"
    },
    {
      "name": "keyword.mtp",
      "match": "default\\S+"
    },
    {
      "name": "entity.name.class",
      "match": "\\[.\\.\\]",
      "name": "entity.name.class"
    },
    {
      "name": "entity.name.tag.atom-name.mtp",
      "match": "[0-9]*[A-Z]+[A-Z0-9_']**(?=\\s+[0-9]*[A-Z]+[A-Z0-9_']**)|\\S+.gone\\S*|(\\s+
      +-?\\s+?[0-9]*[A-Z]+[A-Z0-9_']*){4}"
    },
    {
      "name": "support.type.atom-type.mtp",
      "match": "[0-9]*[A-Z]+[A-Z0-9_']**"
    },
    {
      "name": "string.quoted.charge.mtp",
      "match": "(?<=[0-9]*[A-Z]+[A-Z0-9_']*\\s+)-?\\d+\\.\\.\\d*"
    },
    {
      "name": "constant.language.mtp",
      "match": "(\\b|\\-\\.\\d+\\.\\.\\d*([eE][\\+\\-]?\\d+)?)",
      "name": "constant.language.mtp"
    }
  ]
}

```

4.9 虚拟位点定义文件语法定义

```

{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
  json",
  "name": "Gromacs virtual site definition file",
  "scopeName": "source.vsd",
  "fileTypes": [
    "vsd"
  ],
  "patterns": [
    {
      "name": "comment.line.semicolon",
      "match": ";.*$"
    },
  ],
}

```



```
{
  "name": "keyword.vsd",
  "match": "planar"
},
{
  "///": "section",
  "match": "\\[.*\\]",
  "name": "entity.name.class"
},
{
  "///": "aromatic section",
  "name": "entity.name.tag.atom-name.vsd",
  "match": "[0-9]*[A-Z]+[A-Z0-9_']*(?=.*\\s+\\d+\\.?.\\d*)"
},
{
  "///": "after atom name, match any of these strings",
  "name": "support.type.atom-type.vsd",
  "match": "[0-9]*[a-zA-Z]+[A-Z0-9_']*"
},
{
  "///": "number",
  "match": "(\\b|\\-)?\\d+\\.?.\\d*([eE][\\+\\-]?\\d+)?",
  "name": "constant.language.vsd"
}
]
```

五、 小分子格式支持模块

5.1 MOL2 文件语法定义

```
{
  "patterns": [
    {
      "include": "#structure"
    }
  ],
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.json",
  "scopeName": "source.mol2",
  "name": "mol2",
  "repository": {
    "structure": {
      "patterns": [
        {
          "begin": "^#",
          "end": "$",
          "name": "comment.line"
        },
        {
          "///": "not matching",
          "match": "(?<=(MOLECULE\\s*\\n))\\s+",
          "name": "entity.name.function.molname.mol2"
        }
      ]
    }
  }
}
```

```

},
{
  "begin": "^@",
  "end": "$",
  "name": "string.quoted.orange",
  "/*": "values of fields",
  "patterns": [
    {
      "match": "(?<=>)[A-Za-z\\_]+",
      "name": "keyword.mol2"
    }
  ]
},
{
  "/*": "in the following big section, the first number is matched and screened...
maybe use a new color",
  "match": "\\d+(?=\s+\\d+\\s+\\d+\\s+[0-9a-z]+$)",
  "name": "string.quoted.bond-number.mol2"
},
{
  "/*": "all lines beginning with a number, including bond section and mol info",
  "begin": "\\d+",
  "end": "$",
  "name": "constant.character.coordinates.mol2",
  "patterns": [
    {
      "/*": "the first number is not here at all, but we might not need to
highlight it.",
      "match": "(?<=\\s*)\\d+(?=\s+[A-Z]+[A-Za-z0-9_'\\".]*)",
      "name": "constant.numeric.atom-number.mol2"
    },
    {
      "match": "(?<=\\d+\\s+)[A-Z]+[A-Za-z0-9_'\\".]*+(?=(\\s+(-?\\d+\\\\".\\d*)\\s+
+(-?\\d+\\\\".\\d*)\\s+(-?\\d+\\\\".\\d*)))",
      "name": "variable.other.atom-name.mol2"
    },
    {
      "/*": "No ((?=(\\s+\\d+\\s+[a-zA-Z0-9\\_]+\\s+[\\\".0-9\\_]+[\\s\\s*]*$))|(?=[
\\s]*$)), sometimes no charge",
      "match": "(?<=(-?\\d+\\\\".\\d+\\s+-?\\d+\\\\".\\d+\\s+-?\\d+\\\\".\\d+\\s+)) [A-Z]+[
A-Za-z0-9_'\\".]*",
      "name": "support.type.atom-type.mol2"
    },
    {
      "match": "(?<=[A-Z]+[A-Za-z0-9_'\\".]*\\s+)\\d+(?=\s+[A-Z]+[A-Z0-9_'\\".]*)",
      "name": "variable.other.residue-number.mol2"
    },
    {
      "/*": "(?=(\\s+(-?\\d+\\\\".\\d*)+\\s*$)) charge is optional",
      "match": "(?<=\\s+\\d+\\s+)[A-Z]+[A-Z0-9_'\\".]*",
      "name": "entity.name.type.residue-name.mol2"
    },
    {
      "match": "(?<=\\s+\\d+\\s+[a-zA-Z0-9\\_]+\\s+)(-?\\d+\\\\".\\d+)(?<=$)",
      "name": "string.quoted.charge.mol2"
    },
    {

```

```
        "match": "(?<=^\\s*\\d+\\s+\\d+\\s+\\d+\\s+)[0-9a-z]+(?:\\s*$)",
        "name": "entity.name.function.bond-type.mo12"
    }
  ],
},
{
  "/*": "[a-zA-Z_]+, too blue!",
  "match": "",
  "name": "support.function.field"
}
]
}
}
```

5.2 SDF 文件语法定义

```
{
  "name": "sdf",
  "scopeName": "source.sdf",
  "fileTypes": [
    "sdf"
  ],
  "patterns": [
    {
      "/*": "float starting from column 1, no other",
      "match": "^\\d+(\\.\\d+)$",
      "name": "string.quoted.double.sdf"
    },
    {
      "/*": "string starting from column 1, no other",
      "match": "^(?!\\$\\{4}\\)\\S+$",
      "name": "string.quoted.double.sdf"
    },
    {
      "/*": "string starting from column very later, no other",
      "match": "^\\s+\\S+$",
      "name": "support.type.3d.sdf"
    },
    {
      "match": "\\bV2000\\b",
      "name": "keyword.other.sdf"
    },
    {
      "/*": "special string properties, 3/4 strings",
      "match": "^(\\S+\\s+){2}\\S+$|^(\\S+\\s+){3}\\S+$",
      "name": "string.quoted.double.sdf"
    },
    {
      "/*": "END and $$$$",
      "match": "^M\\s+END$|^\\$\\{4}$",
      "name": "support.type.end.sdf"
    },
    {
      "match": ">\\s<.+>$",

```

```
    "name": "keyword.other.sdf"
  },
  {
    "match": "\\s+(-?\\d+\\.\\d+)\\s+(-?\\d+\\.\\d+)\\s+(-?\\d+\\.\\d+)",
    "name": "constant.numeric.atom-coordinate.sdf"
  },
  {
    "match": "\\b([A-Za-z]+)\\b",
    "name": "string.quoted.element-symbol.sdf"
  },
  {
    "match": "\\s+\\d+\\s+\\d+",
    "name": "entity.name.tag.bond.sdf"
  },
  {
    "match": "(?<=\\s+\\d+\\s+\\d+)\\s+\\d+",
    "name": "string.quoted.bond-order.sdf"
  }
]
}
```

六、专业工具支持模块

6.1 PLUMED 输入文件语法定义

```
{
  "$schema": "https://raw.githubusercontent.com/martinring/tmlanguage/master/tmlanguage.
  json",
  "name": "plumed",
  "scopeName": "source.plumed",
  "fileTypes": [
    "plumed"
  ],
  "patterns": [
    {
      "name": "comment.line.plumed",
      "match": "^\\s*\\.\\s*"
    },
    {
      "name": "string.quoted.action.plumed",
      "match": "\\b(GROUP|MOLINFO|PRINT|ANGLE|TORSION|DISTANCE|COM|GYRATION|VOLUME)\\b"
    },
    {
      "name": "string.quoted.bias.plumed",
      "match": "\\b(LOWER_WALLS|UPPER_WALLS)\\b"
    },
    {
      "name": "keyword.common.plumed",
      "match": "\\b(ATOMS|ARG|FILE|STRIDE|NDX_FILE|NDX_GROUP|RESTRAINT|METAD)\\b"
    },
    {
      "name": "support.type.argument.plumed",
      "match": "\\b(AT|KAPPA|EXP|EPS|OFFSET)\\b"
    }
  ]
}
```

```
    },  
    {  
      "name": "variable.name.argument.plumed",  
      "match": "^\\S+(?:=)"  
    },  
    {  
      "name": "variable.name.plumed",  
      "match": "(?<=(ARG|ATOMS|FILE)=)\\S+(?=\s+)"  
    },  
    {  
      "name": "constant.numeric.plumed",  
      "match": "-?\\d+\\.?\d*"  
    }  
  ]  
}
```