Build Atom Transition Multigraph

```
tutorial_initConservedMoietyPaths
```

```
projectDir =
'~/work/sbgCloud/programExperimental/projects/tracerBased'
dataDir =
'~/work/sbgCloud/programExperimental/projects/tracerBased/data/'
softwareDir =
'~/work/sbgCloud/programExperimental/projects/tracerBased/software/'
visDataDir =
'~/work/sbgCloud/programExperimental/projects/tracerBased/data/visualisation/'
resultsDir =
'~/work/sbgCloud/programExperimental/projects/tracerBased/results/iDopaNeuro1_ConservedMoieties/'
rxnfileDir =
'~/work/sbgCloud/code/fork-ctf/rxns/atomMapped'
```

```
if ~recompute
    load([resultsDir modelName '_dATM.mat'])
    return
end
```

Load the model and input data

```
switch modelName
    case 'DAS'
        load('DAS.mat')
    otherwise
        load([dataDir 'models' filesep modelName '.mat'])
        model = iDopaNeuro1;
end
```

Find the flux consistent subset

```
%% Identify the flux consistent set
paramConsistency.epsilon = 1e-5;
paramConsistency.method = 'fastcc';
[~, fluxConsistentRxnBool] = findFluxConsistentSubset(model, paramConsistency);

%remove any flux inconsistent reactions and the corresponding metabolites
%and coupling constraints if necessary
model = removeRxns(model, model.rxns(~fluxConsistentRxnBool),'metRemoveMethod','exclusi
```

1.2.1. Atom transition multigraph

Calculate the atom transition multigraph in order to follow the path of all the atoms in the network (this may take some time).

```
options.directed=0;
options.sanityChecks=1;
currentDir=pwd;
cd(rxnfileDir)
dATM = buildAtomTransitionMultigraph(model, rxnfileDir, options);
```

```
Atom mappings found for 910 model reactions.
Generating atom transition network for reactions with atom mappings.
Error using buildAtomTransitionMultigraph (line 237)
Transition 3 in reaction 5 maps between atoms of different elements
```

```
cd(resultsDir)
save([resultsDir modelName '_dATM.mat'],'dATM')
```