Initialisation of conserved moiety tutorials

Conserved moiety decomposition consists of several sequential live scripts

1. driver_initConservedMoietyPaths.mlx (this script)
2. tutorial_buildAtomTransitionMultigraph.mlx
3. tutorial_identifyConservedMoieties.mlx
4. tutorial_analyseConservedMoieties.mlx
5. tutorial_visualiseConservedMoieties.mlx

Decide whether to recompute everything from scratch or try to load cached intermediate results

```
recompute = 1;
```

Define the model that will be used for conserved moiety decomposition

```
if ~exist('modelName','var')
    %modelName = 'centralMetabolism_fastCore';
    %modelName = 'centralMetabolism';
    %modelName = 'iDopaNeuroC';
    modelName = 'DAS'
end
```

Setup the paths

```
switch modelName
    case 'DAS'
        projectDir = strrep(which('tutorial_identifyConservedMoieties'),'/
tutorial_identifyConservedMoieties.mlx','')
        %projectDir = ['~' filesep 'work' filesep 'sbgCloud' filesep
'programExperimental' filesep 'projects' filesep 'tracerBased']
    case 'iDopaNeuro1'
        %projectDir = '~/work/sbgCloud/programReconstruction/projects/
exoMetDN/results/codeResults/iDN1/iDopaNeuro1';
        projectDir = ['~' filesep 'work' filesep 'sbgCloud' filesep
'programExperimental' filesep 'projects' filesep 'tracerBased']
    case 'iDopaNeuroC'
        projectDir = ['~' filesep 'work' filesep 'sbgCloud' filesep
'programExperimental' filesep 'projects' filesep 'tracerBased']
    case
{'centralMetabolism','centralMetabolism_thermoKernel','centralMetabolism_fast
Core'}
        projectDir = ['~' filesep 'work' filesep 'sbgCloud' filesep
'programExperimental' filesep 'projects' filesep 'tracerBased']
end
```

```
projectDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties'
```

```
dataDir = [projectDir filesep 'data']
```

```
dataDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/data'
```

```
addpath(genpath(dataDir));
softwareDir = [projectDir filesep 'software']
```

```
softwareDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/software'
```

```
visDataDir = [projectDir filesep 'data' filesep 'visualisation']
```

```
visDataDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/data/visualisation'
```

```
resultsDir = [projectDir filesep 'results' filesep modelName]
```

```
resultsDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/results/DAS'
```

A collection of pre-existing chemical table files in vmh namespace, including atom mapped reactions are here: https://github.com/opencobra/ctf, otherwise use a local directory.

```
switch modelName
    case 'DAS'
        %ctfRxnfileDir ='~/work/sbgCloud/code/fork-ctf/rxns/atomMapped'
        ctfRxnfileDir = [projectDir filesep 'data' filesep 'mini-ctf'
filesep 'rxns' filesep 'atomMapped']
        %ctfRxnfileDir = [projectDir filesep 'data' filesep 'mini-ctf2'
filesep 'rxns' filesep 'atomMapped']
    case
{'iDopaNeuro1','iDopaNeuroC','centralMetabolism','centralMetabolism_thermoKer
nel','centralMetabolism_fastCore'}

        %rxnfileDir = [resultsDir 'fluxCobra' filesep 'dataBase' filesep
'rxn', filesep 'atomMapped']
        %rxnfileDir = '~/work/sbgCloud/programReconstruction/projects/
exoMetDN/papers/v20/SM/SM5'; %%% temporal
        %rxnfileDir ='~/work/sbgCloud/data/rxnDatabase/explicitH/
atomMapped/RDT/rxnFiles'

        %system('git clone git@github.com:opencobra/ctf.git ~/work/sbgCloud/
code/fork-ctf/rxns/atomMapped')
        ctfRxnfileDir ='~/work/sbgCloud/code/fork-ctf/rxns/atomMapped'
end
```

```
ctfRxnfileDir =
'/home/rfleming/work/sbgCloud/code/fork-COBRA.tutorials/analysis/conservedMoieties/data/mini-ctf/rxns/atom
```

```
if ~exist(resultsDir,'dir')
    mkdir(resultsDir)
end
cd(resultsDir)
```