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Created on May 28, 2011
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@author: neugebauer
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```
from PyQt4 import QtGui, QtCore
from projectCreatorUI import Ui_MainWindow as Dlg
from ProjectAdministrator import AtomProject, pRange, ProjectDatabase, JobDatabase
#from databaseUtilities import *
from KMCHamilton import atomKMC
from job_queue import JobQueue
import utilities as u
import os
```

```
class MainWindow(QtGui.QMainWindow, Dlg):
```

```
    def __init__(self, project, parent = None):
```

```
        print "parent", parent
```

```
        QtGui.QMainWindow.__init__(self, parent)
```

```
        self.setupUi(self)
```

```
        self.StepSpinBox.setMinimum(1)
```

```
        self.StepSpinBox.setValue(1)
```

```
        self.StartSpinBox.setMaximum(10000.)
```

```
        self.StopSpinBox.setMaximum(10000.)
```

```
        for i in range(1,3):
```

```
            self.NumParaBox.insertItem(i, str(i))
```

```
        self.project = project
```

```
        if self.project.hamilton == None:
```

```
            self.HamiltonInfoLabel.setText("None")
```

```
            self.ProjectTypeBox.enabled = False
```

```
            self.qDataBox.enabled = False
```

```
        else:
```

```
            ham = self.project.hamilton
```

```
            self.HamiltonInfoLabel.setText(ham.Type+ " "+ham.Version)
```

```
            pars = ham.control.paraDict.keys()
```

```
            for i,par in enumerate(pars):
```

```
                # TODO: select only useful ones, split up arrays, ... (should be done in
                #       Hamiltonian class)
```

```
                #       provide predefined values for start, stop, steps
```

```
                self.ParaBox.insertItem(i, par)
```

```
        self.ProjectTypeBox.enabled = True
```

```
        self.qDataBox.enabled = True
```

```
        #TODO: should be connected to a database so that it can be easily extended without
        #       programming
```

```
        if ham.Type == "KMC":
```

```
            self.ProjectTypeComboBox.insertItem(1, "KMC")
```

```
        self.ProjectViewerButton.setEnabled(False)
```

```

# connections
self.connect(self.closeButton, QtCore.SIGNAL("clicked(bool)"),
              self.exitAction)
self.connect(self.submitButton, QtCore.SIGNAL("clicked(bool)"),
              self.submit)
self.connect(self.StartQueueButton, QtCore.SIGNAL("clicked(bool)"),
              self.startQueue)
self.connect(self.ShowQueueButton, QtCore.SIGNAL("clicked(bool)"),
              self.showQueue)
self.connect(self.InspectHamiltonButton, QtCore.SIGNAL("clicked(bool)"),
              self.showStructure)

#TODO: relace by Hamilton creator form
self.connect(self.CreateHamiltonButton, QtCore.SIGNAL("clicked(bool)"),
              self.createStructure)
self.connect(self.DBViewerButton, QtCore.SIGNAL("clicked(bool)"),
              self.showDatabase)
self.connect(self.ProjectViewerButton, QtCore.SIGNAL("clicked(bool)"),
              self.showProjectViewer)

def showDatabase(self, status):
    import DatabaseViewerGUI
    projectDB = ProjectDatabase()
    self.dialog = DatabaseViewerGUI.MainWindow(projectDB)
    self.dialog.show()

def showProjectViewer(self, status):
    print "show project viewer"
    import ProjectViewerGUI

    # if self.project.projectDB == None:
    #     self.projectDB = ProjectDatabase()

    jobDB = JobDatabase("KMC" + str(self.projectID))
    self.dialog = ProjectViewerGUI.MainWindow(jobDB)
    self.dialog.show()

def showStructure(self, status):
    print "show structure viewer"
    import StructureInspectorGUI
    self.dialog = StructureInspectorGUI.MainWindow(self.project.hamilton.structure)
    self.dialog.show()

def createStructure(self,status):
    print "create structure button"
    import StructureCreatorGUI
    # must be changed later
    self.dialog = StructureCreatorGUI.MainWindow(self.project.hamilton.structure)
    self.dialog.show()

def checkQueueDeamon(self):
    #TODO: this routine should be implemented (e.g. by checking for a specific file)
    print "check"

```

```

try:
    f = open(u.srcDir("queueRunning"), "r")
except:
    print "No activity (queuing daemon not running)"
    return False

txt = f.read()
f.close()
if txt == "running":
    return True
else:
    return False

def stopQueueDaemon(self):
    if self.checkQueueDaemon():
        os.remove(u.srcDir("queueRunning"))
        print "stop", self.checkQueueDaemon()

def exitAction(self):
#     print "exit ProjectCreator"
    self.stopQueueDaemon() # TODO: should be called by a separate queue manager
    self.close()
#     QtGui.QApp.quit()

def submit(self, status):
    steps = self.StepSpinBox.value()
    start = self.StartSpinBox.value()
    stop = self.StopSpinBox.value()

    ind1 = self.ProjectTypeComboBox.currentIndex()
    projectType = self.ProjectTypeComboBox.itemData(ind1, 2).toString()
    ind2 = self.ParaBox.currentIndex()
    parameter = str(self.ParaBox.itemData(ind2, 2).toString())
    print "pRange: ", start, stop, steps, projectType, parameter, type (parameter)

    projectID = self.project.run(task = projectType,
                                parameters = pRange(start, stop, steps, symbol=parameter))
    self.projectID = projectID
    self.ProjectViewerButton.setEnabled(True)

def showQueue(self, status):
    import manageTable as db

    queue = JobQueue()
    queue.dbTable.setTimer(1)

    prog = db.app(0, queue.dbTable)
    prog.MainLoop()

    print "show queue"

```

```
def startQueue(self,status):
# TODO: before starting queueDeamon check whether it is already active
# otherwise threads will be created that never finish!!
    self.pid = u.runCommand("python " + u.srcDir("runQueueDemon.py"))

#from hamilton import AtomHamilton
if __name__ == '__main__':
    import pickle
    from KMCHamilton import KMC_control

#    kmc = atomKMC(u.DumpDir("kmcTest.dat"))
    kmc = atomKMC(dictProject = {"Name" : "kmcTest.dat"})
    project = AtomProject(kmc, name = "kmcTest.dat") # just a dummy name is needed, should be
    improved
    project.showGUI()
```