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1  -- vismol2-simple.hs
2
3  import Data.String
4  import Data.List
5  import Data.IORef
6  import Graphics.UI.GLUT
7  import System.Environment
8  import System.Exit ( exitWith, ExitCode(ExitSuccess) )
9
10 main = do
11     -- there may be many command line arguments in various formats (e.g. -screen 0 in X),
12     -- that's why we are looking for any .mol2 or .MOL2 suffix
13     args <- getArgs
14     let fileNames = filter ( \ fn -> or [isSuffixOf ".mol2" fn, isSuffixOf ".MOL2" fn] ) args
15     theText <- readFile $ fileNames !! 0 -- take 1st
16     let theLines = lines theText
17         theSplittedLines = map words theLines
18         theAtoms = filter ( \ aSplittedLine -> length aSplittedLine == 9 ) theSplittedLines
19     atomsRef <- newIORef theAtoms
20     -- glut --
21     -- ($=) is GLUT- and IORef-specific assignment operator of type
22     -- ($=) :: HasSetter s => s a -> a -> IO ()
23     getArgsAndInitialize
24     initialDisplayMode $= [ SingleBuffered, RGBMode, WithDepthBuffer ]
25     initialWindowSize $= Size 300 300
26     initialWindowPosition $= Position (-1) (-1)
27     createWindow $ fileNames !! 0
28     displayCallback $= (display atomsRef)
29     windowWidthRef <- newIORef (0::GLint)
30     windowHeightRef <- newIORef (0::GLint)
31     reshapeCallback $= Just (reshape windowWidthRef windowHeightRef)
32     xRef <- newIORef (0::GLint)
33     yRef <- newIORef (0::GLint)
34     keyboardMouseCallback $= Just (keyboardMouse xRef yRef)
35     motionCallback $= Just ( motion atomsRef xRef yRef windowWidthRef windowHeightRef)
36     clearColor $= Color4 0 0 0 1
37     shadeModel $= Smooth
38     materialAmbient Front $= Color4 1 1 1 1
39     lighting $= Enabled
40     position (Light 0) $= Vertex4 (-1) 1 1 0
41     light (Light 0) $= Enabled
42     depthFunc $= Just Less
43     {- closeCallback $= Just (exitWith ExitSuccess) -- present in freeglut only -}
44     mainLoop
45
46     keyboardMouse xRef yRef key@(MouseButton LeftButton) state@(Down) _ position@(Position x y) = do
47         xRef $= x
48         yRef $= y
49     keyboardMouse _ _ (Char '\27') Down _ _ = exitWith ExitSuccess -- on ESC, see closeCallback
50     keyboardMouse _ _ _ _ _ = return () -- to avoid crash?!
51
52     motion atomsRef xRef yRef windowWidthRef windowHeightRef position@(Position x y) = do
53         theAtoms <- get atomsRef
54         x0 <- get xRef
55         y0 <- get yRef
56         width <- get windowWidthRef
57         height <- get windowHeightRef
58         let dx = fromIntegral (x - x0)
59             dy = fromIntegral (y - y0)
60             w = fromIntegral width
61             h = fromIntegral height
62             angle1 = (180::Float) * dx / w
63             angle2 = (180::Float) * dy / h -- rather simplistic, but it works, really!
64         clear [ ColorBuffer, DepthBuffer ]
65         rotate angle1 $Vector3 0 (1::GLfloat) 0 -- ok, direction is correct
66         rotate angle2 $Vector3 (1::GLfloat) 0 0 -- ok, direction is correct
67         renderAtoms theAtoms
68         flush
69         xRef $= x
70         yRef $= y
71
72     display atomsRef = do
73         theAtoms <- get atomsRef
74         clear [ ColorBuffer, DepthBuffer ]

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75     renderAtoms theAtoms
76     flush
77
78     renderAtoms [] = do return ()
79     renderAtoms (atom:atoms) = do
80         renderAtom atom
81         renderAtoms atoms
82
83     renderAtom (_:_:x:y:z:atomType:_:_:charge) = do
84         let dx = (read x)::GLfloat
85             dy = (read y)::GLfloat
86             dz = (read z)::GLfloat
87         materialDiffuse Front $= atomColor4 atomType --Color4 1 1 1 1 --atomColor4 atomType
88         translate $ Vector3 dx dy dz
89         renderObject Solid (Sphere' (vdwRadius atomType) 32 32)
90         translate $ Vector3 (-dx) (-dy) (-dz)
91
92     reshape windowWidthRef windowHeightRef size@(Size width height) = do
93         windowWidth <- get windowWidthRef -- old value not used
94         windowHeight <- get windowHeightRef -- old value not used
95         viewport $= (Position 0 0, size)
96         matrixMode $= Projection
97         loadIdentity
98         let wf = fromIntegral width
99             hf = fromIntegral height
100         if width <= height
101             then ortho (-10) 10 (-10 * hf/wf) (10 * hf/wf) (-10) 10
102             else ortho (-10 * wf/hf) (10 * wf/hf) (-10) 10 (-10) 10
103         matrixMode $= Modelview 0
104         -- loadIdentity
105         windowWidthRef $= width
106         windowHeightRef $= height
107
108     vdwRadius atomType
109     | atomType == "H"   = 1.20
110     | atomType == "F"   = 1.47
111     | atomType == "Cl"  = 1.75
112     | atomType == "Br"  = 1.85
113     | atomType == "I"   = 1.98
114     | isPrefixOf "C." atomType = 1.70
115     | isPrefixOf "N." atomType = 1.55
116     | isPrefixOf "O." atomType = 1.52
117     | isPrefixOf "S." atomType = 1.80
118     | isPrefixOf "P." atomType = 1.80
119     | otherwise        = 2.0
120
121     atomColor4 atomType
122     | atomType == "H"   = Color4 1 1 1 1 -- white
123     | atomType == "F"   = Color4 0 1 0 1 -- green
124     | atomType == "Cl"  = Color4 0 1 0 1 -- green
125     | atomType == "Br"  = Color4 0 1 0 1 -- green
126     | atomType == "I"   = Color4 0 1 0 1 -- green
127     | isPrefixOf "C." atomType = Color4 0.5 0.5 0.5 1 -- gray
128     | isPrefixOf "N." atomType = Color4 0 0 1 1 -- blue
129     | isPrefixOf "O." atomType = Color4 1 0 0 1 -- red
130     | isPrefixOf "S." atomType = Color4 1 1 0 1 -- yellow
131     | isPrefixOf "P." atomType = Color4 1 0 1 1 -- magenta
132     | otherwise        = Color4 1 0 1 1 -- magenta

```