

DrugLevelsMain.java

Friday, June 30, 2023 11:24 AM

ModelingComplexSystems.net
Collection: Model Construction
Title: Methodology
Section: Drug Levels Model.Preview.code

```
1:  /** *****
2:  *
3:  * Main Class ID:      DrugLevelsMain
4:  * Creation Date:      2023-01-09
5:  * Updated:            2023-02-21
6:  * Version:            v1.5.8
7:  *
8:  * Diagram Versions
9:  *   Causal Inference:  v1.0.2
10: *   Flow Diagram:      v1.2.2
11: *
12: * Programmer: Garrett A. Hughes
13: *
14: * Purpose: Show levels of a prescription drug in a patient's blood serum
15: *           over the course of ingestion and through the elimination period.
16: *
17: * I/O: User Defined
18: *
19: * NOTE: This class (DrugLevelsMain) has its version number shown above.
20: *
21: *           The title and version number of this program are entered below as
22: *           static members of this class and are printed as part of the header
23: *           at runtime. The program version number changes whenever changes are
24: *           made to any of the classes.
25: *
26: *           If this program implements a model, then the programTitle entered
27: *           below, should be the same as the name of the model.
28: *
29:  ***** */
30:
31:  /* Ruler
32:      1          2          3          4          5          6          7
33: 12456789012345678901234567890123456789012345678901234567890123456789
34:  */
35:
36:  // from docs.oracle.com/javase/8/docs/api
37:  import java.time.LocalDate;
38:  import java.time.LocalDateTime;
39:  import java.time.Instant;
40:  import java.time.Duration;
41:
42:
43:  import xsd.*;
44:
45:  public class DrugLevelsMain
46:  {
47:      // INSTANCE FIELDS
48:      static String programTitle = "Drug Levels";
49:      static String programCreationDate = "2023-01-02";
50:      static String lastModified = "2023-03-14";
51:      static String version = "v2.2.3";
52:      static String runDescription =
53:          "Stable Version, ran all feasible DT values";
54:      static LocalDate LD;
55:      static LocalDateTime LT;
56:
57:  }
```

```
58:      // INITIALIZATION BLOCKS
59:
60:
61:      // CONSTRUCTORS
62:
63:
64:      // METHODS
65:
66:
67:      public static void main(String[] args)
68:      {
69:          System.out.printf("\nProgram Title: %s \nCreated: %s",
70:              programTitle, programCreationDate);
71:          System.out.printf("\nLast Modified: %s", lastModified);
72:          System.out.printf("\nVersion: %s ",version);
73:
74:          System.out.printf("\n\nRun Description: %s", runDescription);
75:          System.out.printf ("\nDate: %s   \nTime: %s\n",
76:              LD.now().toString(),
77:              LT.now().toString());
78:
79:          // *****BEGIN optional timer
80:          Instant start = Instant.now();
81:
82:          // Insert timed code here
83:
84:          // Create objects
85:          EventGenerator evgn = new EventGenerator();
86:          MasterClockRate msclrt = new MasterClockRate();
87:          MasterClock mscl = new MasterClock();
88:          Patient pt = new Patient();
89:          Prescription pr = new Prescription();
90:          IngestionRate inrt = new IngestionRate();
91:          DrugLevel drlv = new DrugLevel();
92:          EliminationRate elrt = new EliminationRate();
93:          BloodSerumConcentration blsrcn = new BloodSerumConcentration();
94:
95:          evgn.updateLinks(msclrt, mscl, pt, pr, inrt, drlv, elrt, blsrcn);
96:
97:          // Begin Simulation
98:          evgn.simulate();
99:
100:          Instant end = Instant.now();
101:          // compute and output duration
102:          Duration elapsedTime = Duration.between(start,end);
103:          long milliseconds = elapsedTime.toMillis();
104:          long seconds = elapsedTime.toSeconds();
105:          System.out.printf("\nelapsed time = %10d milliseconds",
106:              milliseconds);
107:          System.out.printf("\nelapsed time = %10d seconds", seconds);
108:          // *****END optional timer
109:
110:
111:      } // END method: main
112:
113: } // END class: DrugLevelsMain
```

EventGenerator.java

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ModelingComplexSystems.net

Collection: Model Construction

Title: Methodology

Section: Drug Levels Model.Preview.code

```

1: package xsd;;
2:
3: /** *****
4: *
5: * Class ID:          EventGenerator
6: * Creation Date:     2023-01-09
7: * Updated:          2023-03-14
8: * Version:          v2.1.5
9: *
10: * Programmer:       Garrett A. Hughes
11: *
12: * Purpose:          Initiate events for Drug Levels model
13: *
14: * I/O:
15: *   Input           User defined variables
16: *   Output          User defined at runtime
17: *
18: * NOTE: HOW TIME IS KEPT IN AN XSD MODEL
19: * The passage of time is recorded as ticks on a "MasterClock" object.
20: * Each tick represents the end of one time interval and the beginning of
21: * another. The interval of real time between ticks is kept in the variable
22: * referred to as "DT". You get to choose the value of DT. Note that DT
23: * is the smallest time increment that can be represented in any given model
24: * run. The units of time associated with DT can be of any convenient type:
25: * nanoseconds, hours, years, whatever. DT can be declared as any numerical
26: * primitive: usually a double or an integer.
27: *
28: ***** */
29:
30: /* Ruler
31:      1          2          3          4          5          6          7
32: 12456789012345678901234567890123456789012345678901234567890123456789
33: */
34:
35: // from docs.oracle.com/javase/8/docs/api
36: import java.time.Instant;
37: import java.time.Duration;
38: import java.io.*;
39:
40:
41: public class EventGenerator
42: {
43:     // INSTANCE FIELDS
44:     String name ="EventGenerator";
45:
46:     // object identifiers
47:     BloodSerumConcentration blsrcn;
48:     DrugLevel               drlv;
49:     EliminationRate         elrt;
50:     IngestionRate           inrt;
51:     MasterClockRate         msclrt;
52:     MasterClock             mscl;
53:     Patient                 pt;
54:     Prescription            pr;
55:
56:     // simulation runtime parameters
57:     int runtime;           // weeks

```

```
58:     int daysInWeek;        // days/week
59:     int runlength;         // ticks
60:
61:     double hoursInDay;      // hours/day
62:     double runtimeHours;    // hours
63:     double DT;              // hours
64:
65:     // class variables
66:     int remainder;
67:     int numberTicksPerDay;
68:     int numberTicksPerHour;
69:     int ticksElapsed;       // dimensionless
70:     int elapsedTimeInDays;  // days
71:     int interarrivalTime;   // ticks
72:
73:
74:     double elapsedTimeInHours; // hours
75:
76:     // output file
77:     File file;
78:
79:
80:     // INITIALIZATION BLOCK
81:     {
82:         DT = 1.0; // hours
83:         ticksElapsed = 1;
84:         hoursInDay = 24.0; // hours/day
85:         runtime = 4; // weeks
86:         daysInWeek = 7; // days/week
87:
88:         // convert runtime in weeks to runtime in hours
89:         runtimeHours = runtime * daysInWeek * hoursInDay;
90:
91:         // compute runlength in ticks
92:         runlength = (int)Math.round(runtimeHours / DT);
93:
94:         // determine number ticks per day
95:         numberTicksPerDay = (int)Math.round(hoursInDay / DT);
96:
97:         // determine number ticks per hour
98:         numberTicksPerHour = (int)Math.round(1.0 / DT);
99:
100:        // define output file instance
101:        file = new File("DrugLevels_v2.2.3.txt");
102:
103:    }
104:
105:
106:    // CONSTRUCTORS
107:
108:
109:    // METHODS
110:    public void simulate()
111:    {
112:        // view runtime parameters
113:        System.out.println( "\nModel Parameters");
114:        System.out.printf( "    runtime:    %d (weeks)\n", runtime);
```

```
115:         System.out.printf( "      DT:          %f (hours)\n", DT);
116:         System.out.printf( "      runlength:  %d (ticks)\n" , runlength);
117:
118:         // view patient's prescription
119:         pr.showPrescription();
120:
121:         interarrivalTime = numberTicksPerDay/pr.frequency;
122:
123:         System.out.println("\nSIMULATION HAS BEGUN AT ticks = "
124:             + mscl.ticks + "\n");
125:
126:         // open file in which to write results
127:         try
128:         {
129:             FileWriter fw = new FileWriter(file);
130:             BufferedWriter bf = new BufferedWriter(fw);
131:             PrintWriter out = new PrintWriter(bf)
132:         }
133:
134:         // update PrintWriter in DrugLevel object
135:         drlv.updatePrintWriter(out);
136:
137:         // write column headings to file
138:         out.printf("      time          drug      elimination  concentration\n");
139:
140:         do
141:         {
142:             // UPDATE RATES:
143:             inrt.updateIngestionRate();
144:             elrt.updateEliminationRate();
145:
146:             // UPDATE LEVELS:
147:             drlv.updateDrugLevel();
148:
149:
150:             // UPDATE PASSIVE AUXILIARIES
151:             // passive auxiliaries not used to compute rates or levels
152:             blsrcn.updateBloodSerumConcentration();
153:
154:
155:             // OUTPUT SYSTEM STATES
156:             remainder = mscl.ticks % numberTicksPerHour;
157:             if ( remainder == 0)
158:             {
159:                 // compute elapsed time in hours
160:                 elapsedTimeInHours = mscl.ticks / numberTicksPerHour;
161:
162:                 out.printf
163:                 ("%7.0f %13.6f %13.6f %13.6f\n",
164:                     elapsedTimeInHours, drlv.drugLevel, elrt.eliminationRate,
165:                     blsrcn.bloodSerumConcentration);
166:             }
167:
168:
169:             // END ONE TIME INTERVAL BEGIN THE NEXT
170:
171:             // UPDATE MasterClock
```

```
172:         if (mscl.ticks >= runlength) break;
173:         msclrt.updateMasterClockRate(ticksElapsed);
174:         mscl.updateMasterClock();
175:
176:     } while (true); // END do:
177:
178:
179:     System.out.println("\nSIMULATION HAS ENDED AT ticks = "
180:         + mscl.ticks);
181:
182:     System.out.printf("    time          drug          elim_rt
cncntrtn\n");
183:
184:     System.out.printf("(%7.0f %13.6f %13.6f %13.6f\n",
185:         elapsedTimeInHours, drlv.drugLevel, elrt.eliminationRate,
186:         blsrcn.bloodSerumConcentration);
187:
188:     // close BufferedWriter and PrintWriter
189:     bf.close();
190:     out.close();
191: } // END - try
192:
193: catch (IOException e)
194: {
195:
196: } // END - CATCH
197:
198: } // END method: simulate
199:
200:
201: public void reportName()
202: {
203:     System.out.println("\n" + name);
204: }
205:
206:
207: public void updateLinks(MasterClockRate msclrt, MasterClock mscl,
208:     Patient pt, Prescription pr, IngestionRate inrt, DrugLevel drlv,
209:     EliminationRate elrt, BloodSerumConcentration blsrcn)
210: {
211:     this.msclrt = msclrt;
212:     this.mscl = mscl;
213:     this.pt = pt;
214:     this.pr = pr;
215:     this.inrt = inrt;
216:     this.drlv = drlv;
217:     this.elrt = elrt;
218:     this.blsrcn = blsrcn;
219:
220:     // update links of other objects
221:
222:     msclrt.updateLinks(mscl);
223:     mscl.updateLinks(msclrt);
224:     pt.updateLinks(this, pr, mscl, inrt, elrt);
225:     pr.updateLinks(pt);
226:     inrt.updateLinks(drlv, pr, pt, mscl, this);
227:     drlv.updateLinks(this, mscl, inrt, elrt, pt);
```

```
228:         elrt.updateLinks(this, drlv, mscl, pr);
229:         blsrcn.updateLinks(drlv, pt);
230:
231:     }
232:
233: } // END class: EventGenerator
234:
```

MasterClock.java

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ModelingComplexSystems.net

Collection: Model Construction

Title: Methodology

Section: Drug Levels Model.Preview.code

```
1: package xsd;
2:
3: /** *****
4: *
5: * Class ID:      MasterClock
6: * Creation Date: 2023-01-09
7: * Updated:      2023-02-06
8: * Version:      v1.2.8
9: *
10: * Programmer:   Garrett A. Hughes
11: *
12: * Purpose:      Keep track of the time in "tick" units.
13: *
14: *
15: * I/O:
16: *   Input       clock is updated by updateMasterClock() message
17: *                which is sent from the MasterClockRate object
18: *
19: *   Output      on demand when receiving getMasterClockTime() message
20: *
21: ***** */
22:
23: /* Ruler
24:      1          2          3          4          5          6          7
25: 12456789012345678901234567890123456789012345678901234567890123456789
26: */
27:
28:
29: public class MasterClock
30: {
31:     // INSTANCE FIELDS
32:     String name = "MasterClock";
33:     MasterClockRate msclrt;
34:     int ticks = 0;           // time on Masterclock in ticks
35:
36:
37:     // INITIALIZATION BLOCKS
38:
39:
40:     // CONSTRUCTORS
41:
42:
43:     // METHODS
44:     public void reportName()
45:     {
46:         System.out.println("\n" + name);
47:
48:
49:     } public void updateLinks(MasterClockRate msclrt)
50:     {
51:         this.msclrt = msclrt;
52:
53:     } // END method: shareLinks
54:
55:
56:     public void updateMasterClock()
57:     {
```

```
58:         ticks += msclrt.ticksElapsed;
59:
60:     }
61:
62:     public int getMasterClockTime()
63:     {
64:         return ticks;
65:     }
66:
67:
68:
69: } // END class: MasterClock
70:
```

MasterClockRate.java

Friday, June 30, 2023 11:38 AM

ModelingComplexSystems.net

Collection: Model Construction

Title: Methodology

Section: Drug Levels Model.Preview.code

```
1: package xsd;
2:
3: /** *****
4: *
5: * Class ID:      MasterClockRate
6: * Creation Date: 2023-01-09
7: * Updated:      2023-02-06
8: * Version:      v1.2.3
9: *
10: * Programmer:    Garrett A. Hughes
11: *
12:
13: *
14: * Purpose: MasterClock mechanism for updating the time in "tick" units
15: *
16: * I/O:
17: *
18: ***** */
19:
20: /* Ruler
21:      1          2          3          4          5          6          7
22: 12456789012345678901234567890123456789012345678901234567890123456789
23: */
24:
25: // from docs.oracle.com/javase/8/docs/api
26: import java.time.Instant;
27: import java.time.Duration;
28:
29:
30: public class MasterClockRate
31: {
32:     // INSTANCE FIELDS
33:
34:     String name = "MasterClockRate";
35:     MasterClock mscl;
36:     int ticksElapsed;
37:
38:
39:     // INITIALIZATION BLOCKS
40:
41:
42:     // CONSTRUCTORS
43:
44:
45:     // METHODS
46:     public void reportName()
47:     {
48:         System.out.println("\n" + name);
49:
50:     }
51:
52:
53:     public void updateLinks(MasterClock mscl)
54:     {
55:         this.mscl = mscl;
56:
57:     } // END method: shareLinks
```

```
58:
59:
60:     public void updateMasterClockRate( int ticksElapsed)
61:     {
62:         this.ticksElapsed = ticksElapsed;
63:
64:     }
65:
66:
67: } // END class: MasterClockRate
68:
```

Patient.java

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ModelingComplexSystems.net
Collection: Model Construction
Title: Methodology
Section: Drug Levels Model.Preview.code

```

1: package xsd;
2:
3: /** *****
4: *
5: * Class ID:      Patient
6: * Creation Date: 2023-01-16
7: * Updated:      2023-02-23
8: * Version:      v1.1.2
9: *
10: * Programmer:    Garrett A. Hughes
11: *
12: * Purpose:       Ingest a prescribed drug on a scheduled basis
13: *
14: *                Eliminate that drug from their system based on the
15: *                the drug's normal half life in a human body.
16: *
17: * I/O
18: *
19: ***** */
20:
21: /* Ruler
22:      1      2      3      4      5      6      7
23: 12456789012345678901234567890123456789012345678901234567890123456789
24: */
25:
26: public class Patient
27: {
28:     // INSTANCE FIELDS
29:     String name = "Patient";
30:
31:     int startTime;          // ticks
32:
33:     boolean active = false;
34:
35:     double bloodVolume;     // liters
36:     double hoursInDay;      // hours/day
37:
38:     EventGenerator evgn;
39:     Prescription pr;
40:     MasterClock mscl;
41:     IngestionRate inrt;
42:     EliminationRate elrt;
43:
44:     Prescription prescrip;
45:
46:
47:     // INITIALIZATION BLOCKS
48:     {
49:
50:         startTime = 0;      // ticks
51:         bloodVolume = 5.0;  //liters
52:
53:     }
54:
55:
56:     // CONSTRUCTORS
57:

```

```
58:
59:     // METHODS
60:     public void updateLinks(EventGenerator evgn, Prescription pr,
61:         MasterClock mscl, IngestionRate inrt, EliminationRate elrt)
62:     {
63:         this.evgn = evgn;
64:         this.pr = pr;
65:         this.mscl = mscl;
66:         this.inrt = inrt;
67:         this.elrt = elrt;
68:     }
69:
70:
71:     public boolean updatePatientActivity()
72:     {
73:         if (mscl.ticks >= startTime)
74:             active = true;
75:         return active;
76:     }
77:
78:
79:
80: } // END class: Patient
81:
```

Prescription.java

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ModelingComplexSystems.net
Collection: Model Construction
Title: Methodology
Section: Drug Levels Model.Preview.code

```
1: package xsd;
2:
3: /** *****
4: *
5: * Class ID:      Prescription
6: * Creation Date: 2023-01-16
7: * Updated:      2023-03-05
8: * Version:      v1.1.8
9: *
10: * Programmer:    Garrett A. Hughes
11: *
12: * Purpose:       Provide description of current prescription for patient
13: *
14: ***** */
15:
16: /* Ruler
17:      1           2           3           4           5           6           7
18: 12456789012345678901234567890123456789012345678901234567890123456789
19:
20: */
21:
22: public class Prescription
23: {
24:     // INSTANCE FIELDS
25:     String name = "Prescription";
26:
27:     Patient pt;
28:
29:     String drugName = "clonazepam";
30:     String drugHalfLife = "35 hours";
31:     String drugDose = "0.25 milligrams";
32:     String drugFrequency = "3x daily";
33:     double halfLife; // hours
34:     double dose = 0.25; // milligrams
35:     int frequency = 3; // doses/day
36:
37:
38:     // INITIALIZATION BLOCK
39:     {
40:         halfLife = 35.0; // hours
41:
42:     }
43:
44:
45:     // CONSTRUCTORS
46:
47:
48:     // METHODS
49:     public void updateLinks(Patient pt)
50:     {
51:         this.pt = pt;
52:
53:     }
54:
55:
56:     public void showPrescription()
57:     {
```

```
58:         // show patient's current prescription
59:         System.out.println( "\nPatient's Current Prescription");
60:         System.out.println ( "    name:      " + drugName);
61:         System.out.println ( "    halflife:  " + drugHalflife);
62:         System.out.println ( "    dose:    " + drugDose);
63:         System.out.println ( "    frequency: " + drugFrequency);
64:
65:     }
66:
67: } // END class: Prescription
68:
```

DrugLevel.java

Friday, June 30, 2023 11:50 AM

ModelingComplexSystems.net
Collection: Model Construction
Title: Methodology
Section: Drug Levels Model.Preview.code

```
1: package xsd;
2:
3: /** *****
4: *
5: * Class ID:      DrugLevel
6: * Creation Date: 2023-01-02
7: * Updated:      2023-03-09
8: * Version:      v1.1.3
9: *
10: * Programmer:   Garrett A. Hughes
11: *
12: * Purpose:      Keep track of total drug amount in body of patient while
13: *               patient is ingesting that drug. This component holds a
14: *               state variable "drugLevel".
15: *
16: * I/O:
17: *
18: ***** */
19:
20: /* Ruler
21:      1          2          3          4          5          6          7
22: 12456789012345678901234567890123456789012345678901234567890123456789
23: */
24:
25: // from docs.oracle.com/javase/8/docs/api
26: import java.time.Instant;
27: import java.time.Duration;
28: import java.io.*;
29:
30:
31: public class DrugLevel
32: {
33:     // INSTANCE FIELDS
34:
35:     String name = "DrugLevel";
36:
37:     EventGenerator evgn;
38:     MasterClock mscl;
39:     IngestionRate inrt;
40:     EliminationRate elrt;
41:     Patient pt;
42:
43:     double drugLevel;
44:     double eliminationRate;
45:     double conversionFactor = 1000.0; // milligrams/liter to
nanograms/milliliter
46:     double blsrcn; // nanograms/milliliter
47:     int elapsedTimeInHours;
48:
49:     PrintWriter out;
50:
51:
52:     // INITIALIZATION BLOCKS
53:
54:     {
55:         drugLevel = 0.0; // (milligrams)
56:
```

```
57:     }
58:
59:
60:     // CONSTRUCTORS
61:
62:
63:     // METHODS
64:
65:     public void updateLinks(EventGenerator evgn, MasterClock mscl,
66:         IngestionRate inrt, EliminationRate elrt, Patient pt)
67:     {
68:         this.evgn = evgn;
69:         this.mscl = mscl;
70:         this.inrt = inrt;
71:         this.elrt = elrt;
72:         this.pt = pt;
73:     }
74:
75:
76:
77:     public void updateDrugLevel()
78:     {
79:         if( (inrt.ingesting > 0.0) )
80:         {
81:             drugLevel = drugLevel - (elrt.eliminationRate * evgn.DT);
82:
83:             elapsedTimeInHours = (mscl.ticks / evgn.numberTicksPerHour);
84:
85:
86:             eliminationRate = elrt.eliminationRate;
87:
88:             blsrcn = (drugLevel / pt.bloodVolume) * conversionFactor;
89:
90:             // output drug level afer elimination but before ingesting to
avoid conflating the two
91:             out.printf("%7d %13.6f %13.6f %13.6f\n", elapsedTimeInHours,
92:                 drugLevel, eliminationRate, blsrcn);
93:
94:             drugLevel = drugLevel + inrt.ingesting;
95:
96:         }
97:         else
98:         {
99:             drugLevel = drugLevel - (elrt.eliminationRate * evgn.DT);
100:
101:         }
102:
103:     }
104:
105:
106:     public void updatePrintWriter(PrintWriter out)
107:     {
108:         this.out = out;
109:
110:     }
111:
112:
```

```
113: } // END class: DrugLevel
114:
```

IngestionRate.java

Friday, June 30, 2023 11:53 AM

ModelingComplexSystems.net
Collection: Model Construction
Title: Methodology
Section: Drug Levels Model.Preview.code

```
1: package xsd;
2:
3: /** *****
4: *
5: * Class ID:      IngestionRate
6: * Creation Date: 2023-01-16
7: * Updated:      2023-03-06
8: * Version:      v1.1.1
9: *
10: * Programmer:    Garrett A. Hughes
11: *
12: * Purpose:       Ingest dose and increment drug level
13: *
14: * I/O:
15: *
16: ***** */
17:
18: /* Ruler
19:      1          2          3          4          5          6          7
20: 12456789012345678901234567890123456789012345678901234567890123456789
21: */
22:
23: // from docs.oracle.com/javase/8/docs/api
24: import java.time.Instant;
25: import java.time.Duration;
26:
27:
28: public class IngestionRate
29: {
30:     // INSTANCE FIELDS
31:
32:     String name = "IngestionRate";
33:     DrugLevel drlv;
34:     Prescription pr;
35:     Patient pt;
36:     MasterClock mscl;
37:     EventGenerator evgn;
38:
39:     double ingesting; // milligrams
40:
41:
42:     // INITIALIZATION BLOCKS
43:
44:
45:     // CONSTRUCTORS
46:
47:
48:     // METHODS
49:
50:     public void updateLinks(DrugLevel drlv, Prescription pr, Patient pt,
51:         MasterClock mscl, EventGenerator evgn)
52:     {
53:         this.drlv = drlv;
54:         this.pr = pr;
55:         this.pt = pt;
56:         this.mscl = mscl;
57:         this.evgn = evgn;
```

```
58:
59:     }
60:
61:
62:     public void updateIngestionRate()
63:     {
64:         if (pt.active) // if patient is already active
65:         {
66:             if (mscl.ticks == evgn.runlength)
67:                 // don't ingest anything at end of run
68:                 {
69:                     ingesting = 0.0;
70:                 }
71:             else if ((mscl.ticks - pt.startTime) % evgn.interarrivalTime == 0)
72:             {
73:                 ingesting = pr.dose;
74:             }
75:             else
76:             {
77:                 ingesting = 0.0;
78:             }
79:         }
80:         else // modify patient status if criteria are met
81:         {
82:             if (pt.updatePatientActivity() == true)
83:                 ingesting = pr.dose;
84:         }
85:
86:     } // END method: updateIngestionRate()
87:
88:
89: } // END class: IngestionRate
90:
```

EliminationRate.java

Friday, June 30, 2023 11:55 AM

ModelingComplexSystems.net

Collection: Model Construction

Title: Methodology

Section: Drug Levels Model.Preview.code

```
1: package xsd;
2:
3: /** *****
4: *
5: * Class ID:      EliminationRate
6: * Creation Date: 2023-01-27
7: * Updated:      2023-03-05
8: * Version:      v1.0.5
9: *
10: * Programmer:   Garrett A. Hughes
11: *
12: * Purpose:      Eliminate drug from patient's system.
13: *
14: *
15: * I/O:
16: *
17: ***** */
18:
19: /* Ruler
20:      1          2          3          4          5          6          7
21: 12456789012345678901234567890123456789012345678901234567890123456789
22: */
23:
24: // from docs.oracle.com/javase/8/docs/api
25: import java.time.Instant;
26: import java.time.Duration;
27:
28:
29: public class EliminationRate
30: {
31:     // INSTANCE FIELDS
32:
33:     String name = "EliminationRate";
34:
35:     DrugLevel drlv;
36:     MasterClock mscl;
37:     Prescription pr;
38:     EventGenerator evgn;
39:
40:     double eliminationFraction; // 1/hours
41:     double eliminationRate;     // milligrams/hour
42:
43:     // INITIALIZATION BLOCKS
44:
45:
46:     // CONSTRUCTORS
47:
48:
49:     // METHODS
50:     public void updateLinks(EventGenerator evgn, DrugLevel drlv,
51:         MasterClock mscl, Prescription pr)
52:     {
53:         this.evgn = evgn;
54:         this.drlv = drlv;
55:         this.mscl = mscl;
56:         this.pr = pr;
57:     }
}
```

```
58:     }
59:
60:
61:     public void updateEliminationRate()
62:     {
63:         /*
64:         The elimination rate depends on the halflife of the drug being
65:         ingested. The range of the halflife is given as 30 to 40 hours
66:         in NDA 017533 of the Food and Drug Administration dated
67:         October 2013. We use 35 hours for purposes of analysis.
68:
69:         Elimination is assumed to be continuous, therefore we compute
70:         the amount being eliminated at each DT of the model run using
71:         numerical integration. The elimination rate is assumed to be
72:         proportional to the drug level remaining in the patient's blood
73:         serum.
74:
75:         We compute the constant of proportionality, the
76:         eliminationFraction, from the drug halflife.
77:         */
78:
79:
80:         eliminationFraction = Math.abs(Math.log(0.5)/pr.halflife);
81:
82:         // We will return the negative sign when we use the
83:         // elimination rate to reduce the drug level
84:
85:         eliminationRate = drlv.drugLevel * eliminationFraction;
86:
87:
88:     }
89:
90:
91:
92:
93: } // END class: EliminationRate
94:
```

BloodSerumConcentration.java

Friday, June 30, 2023 11:05 AM

ModelingComplexSystems.net

Collection: Model Construction

Title: Methodology

Section: Drug Levels Model.Preview.code

```
1: package xsd;
2:
3: /** *****
4: *
5: * Class ID:      BloodSerumConcentration
6: * Creation Date: 2023-02-21
7: * Updated:      2023-02-21
8: * Version:      v1.0.0
9: *
10: * Programmer:   Garrett A. Hughes
11: *
12: * Purpose:      Compute the concentration of the drug in the blood serum
13: *
14: * I/O:          no class members required
15: *
16: ***** */
17:
18: /* Ruler
19:      1          2          3          4          5          6          7
20: 12456789012345678901234567890123456789012345678901234567890123456789
21: */
22:
23: // from docs.oracle.com/javase/8/docs/api
24: import java.time.Instant;
25: import java.time.Duration;
26:
27:
28: public class BloodSerumConcentration
29: {
30:     // INSTANCE FIELDS
31:
32:     DrugLevel drlv;
33:     Patient pt;
34:
35:     double bloodSerumConcentration; // (nanograms/milliliter)
36:
37:
38:     // INITIALIZATION BLOCKS
39:
40:
41:     // CONSTRUCTORS
42:
43:
44:     // METHODS
45:
46:     public void updateLinks(DrugLevel drlv, Patient pt)
47:     {
48:         this.drlv = drlv;
49:         this.pt = pt;
50:
51:     }
52:
53:
54:     public void updateBloodSerumConcentration()
55:     {
56:         bloodSerumConcentration = drlv.drugLevel / pt.bloodVolume;
57:     }
```

```
58:          // NOTE: concentration is currently in milligrams/liter
59:          //          convert concentration to nanograms per milliliter
60:          //          multiply by 1000
61:
62:          bloodSerumConcentration *= 1000.0;
63:
64:      }
65:
66:
67:
68:
69: } // END class: BloodSerumConcentration
70:
```
