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package repressilator;

/*
 * Reconstruction of the Repressilator model found in
 * A Synthetic Oscillatory Network of Transcriptional
 * Regulators (Elowitz M, et al.) -- Nature vol. 403,
 * p. 335-338, 2000.
 */
public class deterministic
{
    // Setup
    static double[]    vals;
    static double[]    k1, k2, k3, k4;
    // Parameter values
    static final double hill        = 2;
    static final double prothalf    = 10;
    static final double mrnahalf    = 2;
    static final double h           = .0005;
    static final double alpha       = 10000;
    static final double alpha0      = 0;
    static final double beta        = prothalf / mrnahalf;
    static final double ttot        = 100;
    static final double STEPS       = ttot / h;

    public static void main(String[] args)
    {
        // Initialize stuff
        vals = new double[6];
        k1 = new double[6];
        k2 = new double[6];
        k3 = new double[6];
        k4 = new double[6];
        for (int i = 0; i < vals.length; i++)
            vals[i] = Math.random() * 600;

        System.out.print(0 + "\t");
        for (int i = 0; i < vals.length; i++)
            System.out.print(vals[i] + "\t");
        System.out.println();

        // Simulate development process.
        for (int i = 0; i < STEPS; i++)
        {
            double t = i * h;

            // Calculate RK coefficients.
            double[] dvals = derivs(t, vals);
            for (int j = 0; j < k1.length; j++)
                k1[j] = dvals[j];
            double[] tempvals = new double[6];
            for (int j = 0; j < tempvals.length; j++)
                tempvals[j] = vals[j] + h * k1[j] / 2;
            dvals = derivs(t + h / 2, tempvals);
            for (int j = 0; j < tempvals.length; j++)
                k2[j] = dvals[j];
            for (int j = 0; j < tempvals.length; j++)
                tempvals[j] = vals[j] + h * k2[j] / 2;
            dvals = derivs(t + h / 2, tempvals);

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        for (int j = 0; j < tempvals.length; j++)
            k3[j] = dvals[j];
        for (int j = 0; j < tempvals.length; j++)
            tempvals[j] = vals[j] + h * k3[j];
        dvals = derivs(t + h, tempvals);
        for (int j = 0; j < tempvals.length; j++)
            k4[j] = dvals[j];

        // Move all values one step in time according to 4th order RK.
        for (int j = 0; j < vals.length; j++)
            vals[j] += h * (k1[j] / 6 + k2[j] / 3 + k3[j] / 3 + k4[j] / 6);

        // Print output. Disallow negative values.
        System.out.print(t + "\t");
        for (int j = 0; j < vals.length; j++)
        {
            if (vals[j] < 0)
                vals[j] = 0;
            System.out.print(vals[j] + "\t");
        }
        System.out.println();
    }
}

/*
 * Computes derivatives according to the repressilator ODE's. Note that time
 * is completely aesthetical in this case.
 */
public static double[] derivs(double t, double[] vals)
{
    double[] dvals = new double[6];
    // compute p derivatives
    for (int i = 0; i < dvals.length / 2; i++)
        dvals[i] = -beta * (vals[i] - vals[i + 3]);
    // compute m derivatives
    for (int i = dvals.length / 2; i < dvals.length; i++)
        dvals[i] = -vals[i] + alpha / (1 + Math.pow(vals[(i + 2) % 3], hill))
            + alpha0;
    return dvals;
}
}

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