www.simiode.org
SIMIODE Systemic Initiative for Modeling Investigations and Opportunities with Differential Equations

,

STUDENT VERSION
CONDENSATION OPTIMIZATION

Chris McCarthy
Borough of Manhattan Community College
New York NY USA

Brian Winkel
Director SIMIODE
Cornwall NY USA

STATEMENT

Prologue Describing Simulation

Consider the random motion of 200 particles in a 50 by 50 square with vertices $(0,0),(0,50)$, $(50,50),(0,50)$ in a plane. At each iteration, $n=0,1,2,\ldots$ each particle moves a fixed step size in one direction only, due north, due east, due south, or due west, and it must move.

Particles are initially randomly distributed on points with integer coordinates, but not on the boundaries, i.e. from within the set $S=\{(m,n)\,|\,m,n\in\{1,2,3,\ldots,49\}\,\}$ and at each iteration each particle moves. The number of condensed particles is tallied at each iteration.

If a particle comes in contact with the west, east, or north wall it bounces off by returning to the position just before the bump. If the particle comes in contact with the south or bottom wall it condenses and stays exactly at the position of contact, thus depleting the number of particles which are still randomly moving in the square. In Figures 2-4 we show a snapshot of several iterations of the particles and the plot of the number of condensed particles at each iteration using a step size of 1 unit. We reproduce here the activities from Modeling Scenario 1-47-S-Condensation-StudentVersion for completeness. We provide several animations for different runs of the simulation and we offer several data sets from such simulations.

1. Offer up a difference or differential equation which models $y(t)$ the number of condensed particles at iteration t.
2. Using the data set with step size 1 in Table 1 (and shown in Figure 1) or from one of the data sets provided estimate the parameter(s) in your model.

Iteration	0	1000	2000	3000	4000	5000	6000	7000	8000	9000	10000	11000	12000
# Condensed	1	75	103	121	129	136	150	160	170	173	179	182	188

Table 1. Sampled data at increments of 1000 iterations from a simulation of duration 10,000 iterations, with step size 1.

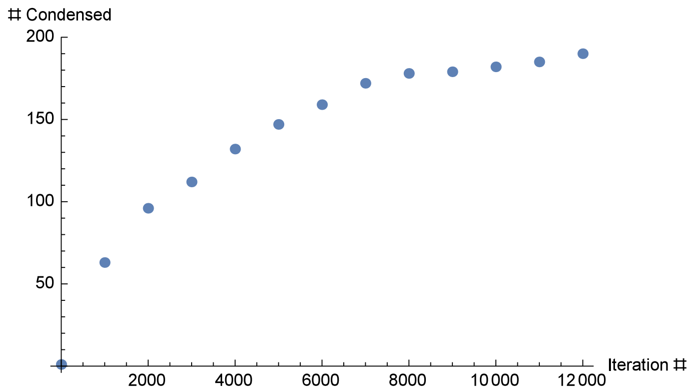

Figure 1. Plot of data in Table 1 of number of condensed particles at iterations, 1000, 2000, 3000, . . . , 11,000, 12000.

3. Confirm in some way the correctness of your model.

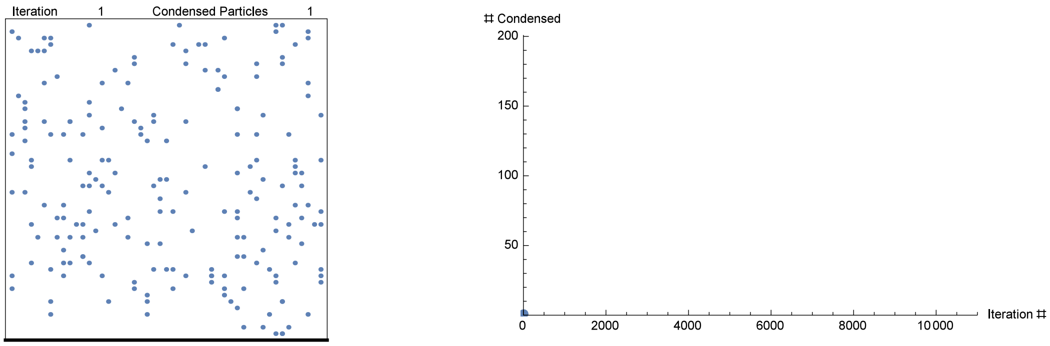

Figure 2. On the left we see the particles in the box at iteration 1 with 1 of the particles condensed on the bottom wall and on the right we see a plot of the accumulated number of condensed particles at given iteration.

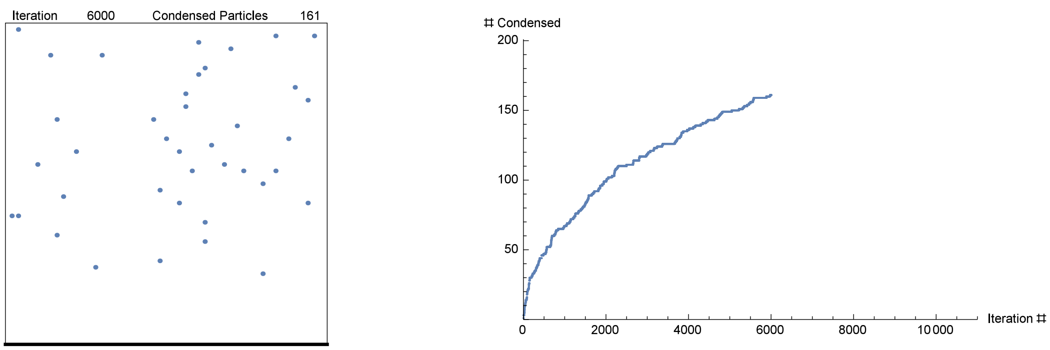

Figure 3. On the left we see the particles in the box at iteration 6000 with 161 of the particles condensed on the bottom wall and on the right we see a plot of the accumulated number of condensed particles at given iteration.

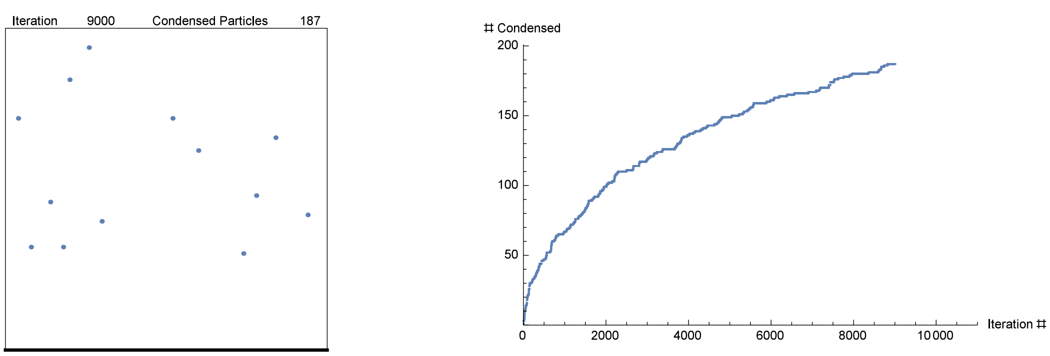

Figure 4. On the left we see the particles in the box at iteration 9000 with 187 of the particles condensed on the bottom wall and on the right we see a plot of the accumulated number of condensed particles at given iteration.

Optimization

In industrial applications it is often desirable to extract or separate particles, e.g., purification or collection for sale or re-use. Indeed, our condensation efforts are but one example of extraction.

Cost is a significant concern in all industrial efforts and we would like to examine our process in light of minimizing costs associated with condensation of particles. Accordingly, we can alter variables for a goal of separating out 90% of our 200 particles, i.e. 180 particles.

A reasonable assumption is that our process of condensation needs more heat for the particles to take a larger step size (more energy means more excitation) and so doing the condensation will be faster, i.e. the time for condensation will be reduced.

For our process let us ignore the "purchase costs" of particles and possible "reimbursements" for unused particles, the 20 particles not condensed in each operation. Also we will ignore set up and tear down costs for the apparatus.

Suppose the energy cost to produce a step size, h, in our particle motion is EnergyCost(h). A reasonable relationship between energy and step size might be linear, i.e. EnergyCost(h) $= \alpha h$, meaning for each additional unit of increase in step size our costs go up by α.

Further, suppose the cost to run the experiment for time $\mathrm{T}(h)$ as a function of h, step size, i.e. the time until, say, 90% or 180 of our particles are condensed, is TimeCost(h).

Then the total cost to run our process could be written as a function of our step size, h,

$$\mathrm{TotalCost}(h) = \mathrm{EnergyCost}(h) + \mathrm{TimeCost}(h)\,. \tag{1}$$

We will need to determine $\mathrm{T}(h)$, the time our process takes to condense 180 of our 200 particles as a function of step size, h, and then TimeCost(h) $= \beta\mathrm{T}(h)$ and EnergyCost(h) $= \alpha h$ where β is a constant for the cost per unit of time of running our process and α is the incremental cost in energy in order to raise the step size one unit.

Suppose our cost constants are $\beta = 0.0012$ and $\alpha = 1.5$.

Modeling $\mathrm{T}(h)$

We ran the condensation simulation using several different step sizes, $h = 1, 2, 3, 4, 5, 6$. For each step size we ran 50 simulations and we averaged the time it took for a simulation to reach exactly 180 condensed particles. So, for example, with step size $h = 3$ the average amount of time it took the simulation to reach exactly 180 condensed particles was 955.34 units of time. Complete data is offered in Table 2.

Incidental - Modeling the relationship between step size h **and parameter** k

We used the differential equation model, (2), quite successfully, to model, $y(t)$, the number of condensed particles at time t

$$y'(t) = k(200 - y(t)\,, \quad y(0) = 0\,. \tag{2}$$

Step size (h)	1	2	3	4	5	6
Duration of simulation (T(h))	8245.34	2161.48	955.34	551.68	371.57	264.24

Table 2. Empirical data on step size h and T(h), the average time (of 50 runs for each step size) for the condensation process to yield exactly 90% of the original 200 particles or 180 particles condensed.

Data on step size and the resulting parameter k using model (2) was collected from 10 runs of the simulation for condensation, each of duration 10,000 iterations, to determine 10 values of k. These values were averaged for each step size and the results are summarized in Table 3.

Step size (h)	1	2	1.5	2.5	3
Parameter k	0.0003491	0.001241	0.0006743	0.001699	0.00265

3.5	4	4.5	5	5.5	6
0.003465	0.004958	0.00605	0.006953	0.008286	0.009922

Table 3. Empirical data on step size h and the parameter k from model (2) which resulted from 10 simulations of duration 10,000 iterations for each step size. For each step size the 10 obtained values of k were averaged.

Questions to Address

1. From the data in Table 2 determine a functional relationship for T(h), the average time (of 50 runs for each step size) for the condensation process to yield exactly 90% of the original 200 particles or 180 particles condensed.
2. From the data in Table 3 determine a functional relationship between step size h and the corresponding parameter k. Explain the reasonableness of this relationship.
3. Construct the Total Cost function TotalCost(h) from (1).
4. Determine the step size, h, which gives minimum TotalCost(h).