Detailed implementation of the Particle-based simulator.

The epidemic states are enumerated as follows: Susceptible (0), Exposed (1), Infected (2), True Quarantined (5), False Quarantined (9), True Isolated (6), False Isolated (8), Severe Infected (7), Recovery Immunized (3), Vaccination Immunized (10), Dead (4).

The epidemic spread is modeled using the contact threshold distance between the particles. Particles with the distance in between less that x_{thr} are assumed to be contacted. First, we find the indices of the contagious particles considering the disease transmission rates. Let's define a vector ($\boldsymbol{\kappa_C} \in \mathbb{R}^n$) where $\kappa_{C_i} = 1$ or 0 for contagious and susceptible particles, respectively. Similarly, we can define vectors for the following states: susceptible particles ($\boldsymbol{\kappa_S} \in \mathbb{R}^n$), exposed particles ($\boldsymbol{\kappa_E} \in \mathbb{R}^n$), infected particles ($\boldsymbol{\kappa_I} \in \mathbb{R}^n$), true quarantined ($\boldsymbol{\kappa_{TQ}} \in \mathbb{R}^n$), true isolated ($\boldsymbol{\kappa_{TI}} \in \mathbb{R}^n$), and severely infected particles ($\boldsymbol{\kappa_{SI}} \in \mathbb{R}^n$).
Then, contagious particles are filtered as follows:

$$\kappa_{\boldsymbol{C}} = \kappa_{\boldsymbol{I}} \,|(\kappa_{\boldsymbol{E}} \odot (\boldsymbol{r} < \epsilon_{exp}))|(\kappa_{\boldsymbol{TQ}} \odot (\boldsymbol{r} < \epsilon_{qua}))| (\kappa_{\boldsymbol{TI}} \odot (\boldsymbol{r} < \epsilon_{qua}))|\big(\kappa_{\boldsymbol{SI}} \odot (\boldsymbol{r} < \epsilon_{sev})\big) \qquad (1)$$

Here $\boldsymbol{r} \in \mathbb{R}^n$ is represents uniformly distributed random numbers from 0 to 1, | and ⊙ are logical OR and pointwise multiplication operators, respectively.

Next, all contacts of the contagious particles are estimated using the MATLAB function [1] $\mathrm{rangesearch}\ (X,\ X_C, x_{thr})$. Here X and X_C are position matrices of all particles and contagious particles, respectively.

$$P_{C_j} = P_i \text{ if } \kappa_{C_i} = 1 \text{ for } i = 1, \dots, n, j = 1, \dots m. \qquad (2)$$

Then, susceptible contacts of the contagious particles are extracted as

$$\boldsymbol{\kappa_S^c} = \boldsymbol{\kappa_A} \,\&\, \boldsymbol{\kappa_S} \qquad (3)$$

where $\boldsymbol{\kappa_A} \in \mathbb{R}^n$ is a vector representing the contacts of the contagious particles. $\boldsymbol{\kappa_{A_i}} = 1$ or $\boldsymbol{\kappa_{A_i}} = 0$ if the particle was in contact or not, respectively.
Now, we transition these susceptible particles to Exposed state based on the following conditions, and time is reset to zero for the new state:

$$e_i = \begin{cases} 1, & if\ \boldsymbol{\kappa}_{Si}^c = 1 \\ e_i, & otherwise. \end{cases} \qquad (4)$$

$$t_i = \begin{cases} 0, & if\ \boldsymbol{\kappa}_{Si}^c = 1 \\ t_i, & otherwise. \end{cases}$$

Particles whose time in the Exposed state reaches t_{exp} move to the Infected state and their time is reset to zero, respectively:

$$e_i = \begin{cases} 2, & if\ e_i = 1 \,\&\, t_i \geq t_{exp} \\ e_i, & otherwise. \end{cases} \qquad (5)$$

$$t_i = \begin{cases} 0, & if\ e_i = 1\ \&\ t_i \geq t_{exp} \\ t_i, & otherwise. \end{cases}$$

Particles in the Susceptible, Exposed and Infected states are randomly tested according to the daily tests per thousand people. The test sensitivity (sn) and specificity (sp) parameters enable to imitate true-positive and false-positive cases:

$$e_i = \begin{cases} d, & if\ (e_i = 1\ |\ e_i = 2)\ \&\ ts_i = 0\ \&\ r_i \leq \theta sn\Delta t \\ d, & if\ e_i = 0\ \&\ ts_i = 0\ \&\ r_i \leq \theta(1 - sp)\Delta t \\ ts_i, & otherwise. \end{cases} \quad (6)$$

Next, certain infected particles transition to Severe Infected sub-state based on the following conditions:

$$e_i = \begin{cases} 7, & if\ e_i = 2\ \&\ r_i \leq sir\Delta t \\ e_i, & otherwise. \end{cases} \quad (7)$$

$$ts_i = \begin{cases} d, & if\ e_i = 2\ \&\ r_i \leq sir\Delta t \\ ts_i, & otherwise. \end{cases}$$

The transition in eq. 14 is done for each age group in a loop ascending the age order since the sir parameter is age-dependent.
Here, the vector of the uniformly distributed random numbers between 0 and 1 is defined by $\boldsymbol{r} \in \mathbb{R}^n$. Date, d, when the particle was tested positive is stored in vector $\boldsymbol{ts} \in \mathbb{R}^n$.

Infected particles that reach the time t_{inf} move to the recovered state.

$$e_i = \begin{cases} 3, & if\ e_i = 2\ \&\ t_i \geq t_{inf} \\ e_i, & otherwise. \end{cases} \quad (7)$$

Particles that reach t_{inf} in the Severely Infected state transition to the Dead state based on the mortality rate, γ_{mor}, and the rest move to the Recovered state:

$$e_i = \begin{cases} 4, & if\ e_i = 7\ \&\ t_i \geq t_{inf}\ \&\ r_i \leq \gamma_{mor} \\ 3, & if\ e_i = 7\ \&\ t_i \geq t_{inf}\ \&\ r_i > \gamma_{mor} \\ ts_i, & otherwise. \end{cases} \quad (8)$$

Exposed and infected particles that were tested true-positive transition to the True Quarantined and True Isolated sub-states, respectively:

$$e_i = \begin{cases} 5, & if\ e_i = 1\ \&\ ts_i = d\ \&\ r_i \leq \theta sn\Delta t \\ 6, & if\ e_i = 2\ \&\ ts_i = d\ \&\ r_i \leq \theta sn\Delta t \\ e_i, & otherwise. \end{cases} \quad (10)$$

False-positive tested susceptible particles transition to the False Isolated sub-state:

$$e_i = \begin{cases} 8, & if\ e_i = 0\ \&\ ts_i = d\ \&\ r_i \leq \theta(1 - sp)\Delta t \\ e_i, & otherwise. \end{cases} \quad (11)$$

Next, considering the testing results, the contact tracing module extracts the ids of the particles that were in contact with the positive tested particles within the last 14 days of the simulation. Contacts in the Exposed or Infected state then transition to the True Quarantined and True Isolated sub-states, respectively. Contacts of the false-positive tested particles (susceptible particles) move to the False Quarantined sub-state.

Similar to the Exposed to Infected transition, particles that reach a time t_{exp} in the True Quarantined state move to the True Isolated state:

$$e_i = \begin{cases} 6, & if\ e_i = 5\ \&\ t_i \geq t_{exp} \\ e_i, & otherwise. \end{cases} \quad (12)$$

$$t_i = \begin{cases} 0, & if\ e_i = 5\ \&\ t_i \geq t_{exp} \\ t_i, & otherwise. \end{cases}$$

False quarantined particles transition back to the Susceptible super-state after the exposure period t_{exp}:

$$e_i = \begin{cases} 0, & if\ e_i = 9\ \&\ t_i \geq t_{exp} \\ e_i, & otherwise. \end{cases} \quad (13)$$

$$t_i = \begin{cases} 0, & if\ e_i = 9\ \&\ t_i \geq t_{exp} \\ t_i, & otherwise. \end{cases}$$

Similarly, false isolated particles transition back to the Susceptible super-state after the infection period t_{inf} :

$$e_i = \begin{cases} 0, & if\ e_i = 8\ \&\ t_i \geq t_{inf} \\ e_i, & otherwise. \end{cases} \quad (16)$$

$$t_i = \begin{cases} 0, & if\ e_i = 8\ \&\ t_i \geq t_{inf} \\ t_i, & otherwise. \end{cases}$$

Similar to the infected particles certain particles in the True Isolated sub-state transition to the Severely Infected state until the infection period t_{exp} is reached:

$$e_i = \begin{cases} 7, & if\ e_i = 6\ \&\ r_i \leq sir\Delta t \\ e_i, & otherwise. \end{cases} \quad (14)$$

The transition in eq. 14 is done for each age group in a loop ascending the age order since the sir parameter is age-dependent.

The rest of the particles in the True Isolated state move to the Recovered state after t_{inf} days:

$$e_i = \begin{cases} 3, & if\ e_i = 6\ \&\ \ t_i \geq t_{inf} \\ e_i, & otherwise. \end{cases} \quad (15)$$

Sterilizing vaccination (random-all case): susceptible, exposed, infected, and recovered particles above age group 2 are randomly vaccinated based on the number of daily vaccines per thousand people υ:

$$v_i = \begin{cases} t_i, & (if\ (e_i = 0 \mid e_i = 1 \mid e_i = 2\ \mid e_i = 3)\ \&\ ag >\ 2)\ > \upsilon \\ 0, & otherwise. \end{cases} \quad (15)$$

For exposed, infected, and recovered particles vaccine is assumed to be wasted. Randomly selected susceptible particles that reach the time t_{imm1} transition to the Vaccination Immunized state based on the first dose immunization rate γ_{imm1}:

$$e_i = \begin{cases} 10, & r_i \leq \gamma_{imm1}\ \&\ v_i \geq t_{imm1} \\ e_i, & otherwise. \end{cases}$$

Susceptible particles that do not transition to the Vaccination Immunized state after the first dose might get contacted by the contagious particles and transition to an Exposed state before they reach the time t_{imm2}. In this case, they continue with the regular flow of the SEIR model.

Susceptible particles that reach the time t_{imm2} in the Susceptible super-state transition to the Vaccination Immunized state, according to the second dose vaccination efficiency γ_{imm2}:

$$e_i = \begin{cases} 10, & r_i \leq \gamma_{imm2}\ \&\ v_i \geq t_{imm2} \\ e_i, & otherwise. \end{cases} \quad (10)$$

The rest of the susceptible particles do not gain immunity and continue with the regular flow of the SEIR model.

For the age-based vaccination case, particles vaccinated descending the age groups:

$$v_i = \begin{cases} t_i, & (\sum_{ag \leq 9}^{3} (e_i = 0 \mid e_i = 1 \mid e_i = 2\ \mid e_i = 3)) > \upsilon \\ 0, & otherwise \end{cases} \quad (15)$$

Here, υ is the daily vaccination rate per thousand people.

Effective vaccination (random-all case): susceptible, exposed, infected and recovered particles are vaccinated based on the number of daily vaccines per thousand people υ:

$$v_i = \begin{cases} t_i, & (if\ (e_i = 0 \mid e_i = 1 \mid e_i = 2\ \mid e_i = 3)\ \&\ ag >\ 2)\ > \upsilon \\ 0, & otherwise. \end{cases} \quad (15)$$

For exposed, infected, and recovered particles the vaccine is assumed to be wasted. Susceptible particles that reach the time t_{imm1} become vaccination immunized, according to the vaccine efficacy γ_{imm1}:

$$vac_{imm} = \begin{cases} 1, & r_i \leq \gamma_{imm1}\ \&\ v_i \geq t_{imm1} \\ 0, & otherwise. \end{cases}$$

Susceptible particles that did not become immunized after the first dose at a time t_{imm1} and reach time t_{imm2} become vaccination immunized, according to the vaccine efficacy γ_{imm2}:

$$vac_{imm} = \begin{cases} 1, & r_i \leq \gamma_{imm2} \ \& \ v_i \geq t_{imm2} \\ 0, & otherwise. \end{cases}$$

Susceptible particles that are vaccination immunized and not immunized go through the regular flow of the SEIR model, except they have a much smaller rate of transitioning from the Infected state and to the Severe Infected sub-state. For each age group the following transitions occur:

$$e_i = \begin{cases} 7, & if\ e_i = 6 \ \& \ r_i \leq sir\Delta t \ \& \ vac_{imm} = 0 \\ 7, & if\ e_i = 6 \ \& \ r_i \leq sir_{ev}\Delta t \ \& \ vac_{imm} = 1 \\ e_i, & otherwise. \end{cases}$$

$$e_i = \begin{cases} 7, & if\ e_i = 2 \ \& \ r_i \leq sir\Delta t \ \& \ vac_{imm} = 0 \\ 7, & if\ e_i = 2 \ \& \ r_i \leq sir_{ev}\Delta t \ \& \ vac_{imm} = 1 \\ e_i, & otherwise. \end{cases}$$