

The program *epidesim* (written in FORTRAN 95) was used to generate the simulations used in the paper "The spread of infections from a physics perspective" which was accepted for publication in the *Journal Biology Methods and Protocols* as a part of the ongoing collection of Covid-19 related papers presented by the Journal. The program performs a Monte-Carlo simulation of the evolution/spread of an epidemic on a 2D square lattice of 2001x2001 nodes. The lattice represents the entire population with each node representing an individual member. The spread of infection takes place in a SIR context. As such, there are nodes that represent individuals susceptible to infection (labelled 1 in/by the program), active infections (labelled 2) and removed infection (labelled 3). In addition the program allows for nodes to be immune/vaccinated (labelled 4).

The program allows the user to choose between different types of social environments/bubbles of the population members (the program asks for the user's choice in this respect upon start-up ("WHICH CALCULATION (1,2,3,4,5)"). Option 1 is for contacts made throughout the population, option 3 for nearest-neighbour contacts only, and option 5 for contacts made in a $(2N+1) \times (2N+1)$ square of nodes surrounding each single node (the typical size parameter of the square (N) is asked as input upon selecting this option). Options 2 and 4 were only used by the author for evaluation and testing purposes, but not for generating data that were included in the paper.

Relevant model parameters must be given by the user as constants (real numbers) in the source code before compilation. Simulations for different model parameters can only be performed by changing the parameters in the source code and subsequent recompilation of the code. These model parameters are:

s0: initial rate of accumulated infections
 sr0: initial rate of recoveries/removed infections
 sa0: initial rate of active infections
 pi0: infection probability upon contact (be aware that $\pi = 2 * \pi_0$, with π being the parameter accounting for the infection rate in the ODEs)
 pr: probability of infection removal upon addressing a node (equal to π in the ODEs)

The section of the code for adjusting these parameters (starting at line 35) is:

```
s0=1.24875d-4      ! INITIAL NUMBER OF ACCUMULATED INFECTIONS
sr0=0.0d0         ! INITIAL NUMBER OF RECOVERIES
sa0=s0-sr0        ! INITIAL NUMBER OF ACTIVE INFECTIONS
pi0=5.0d-1        ! INFECTION PROBABILITY UPON CONTACT (REMINDE THAT  $\pi = 2 * \pi_0$  !!!)
pr=2.5d-2         ! PROBABILITY OF INFECTION-REMOVAL UPON ADDRESSING
a=1.0d-9          ! CONTROLS THE CONTACT DISTANCE BIAS
```

The parameter a (controlling the "distance bias") should be left as is, or chosen very close to zero (a was only relevant for code and model evaluation and is actually not used in most calculations).

The following additional user-input and user-choices are asked for by the program upon start-up¹:

DESCRIPTION OF REQUIRED INPUT	PROGRAM PROMPT TEXT
Type of social-bubble of a node (see above):	'WHICH CALCULATION (1,2,3,4,5)?' (input: integer)
Apply vaccination:	'VACCINATION (TYPE Y/N)?'
Degree of vaccination xv (when vaccination is chosen):	'GIVE DEGREE OF VACCINATION $xv \leq 1$ ' (input: real)

¹N.B. In each "cycle", every population member has contacted one other population member (on average). As such a cycle corresponds to a total of 2001^2 individual contacts made.

Length of time interval related to a single cycle:	'LENGTH OF TIME-INTERVAL ACCOUNTED FOR BY A SINGLE CYCLE IN NORMALISED TIME UNITS) ?' (input: real)
Number of cycles:	'NUMBER OF CYCLES?' (input: integer)
Determine the (average) coordination of nodes:	'DETERMINE COORDINATION (TYPE Y/N)?'
Explicit counting of s-a pairs (susceptible-infected pairs):	'COUNT s-a PAIRS EXPLICITELY (TYPE Y FOR YES, ANY OTHER CHARACTER FOR NO)?'
Ignore regimes with (unphysical) fluctuations:	'IGNORE REGIMES WITH FLUCTUATIONS' (TYPE y FOR yes or n FOR NO)' (meant are fluctuations in average coordination numbers due to vanishing number of active infections, however input n is recommended)
Bubble size in case of social-environment option 5:	'GIVE N=N _n (SPECIFIES SIZE OF 2N _x 2N _y GRID)?' (input: integer)
Write population status after epidemic to file:	'WRITESTATUS (TYPE y/n)?'
Write status of a smaller population section to file:	'INCLUDE A FILE WITH A SMALL SECTION OF POPULATION (TYPE y/n)?'

When the social bubble of a node consists of the entire population (option 1), extra input is asked for by the program via the prompt: REMOVAL CYCLE BASED ON SELECTION OF A SINGLE NODE FOR INFECTION REMOVEDAL (TYPE s), OR SELECTION OF NODES WITH A WEIGHTED EFFECTIVE pr-VALUE (TYPE ANY SYMBOL NON-EQUAL TO s)? It is emphasised that the option s (single node) should be entered here, other options were used only by the author for evaluation purposes and analysis during development of the code and the underlying model.

The program evaluates the following (relevant) data, used for output written to user specified files:

i:	number of cycles: integer
i*dt:	elapsed time: real
Ni:	number of cumulative infections: integer
Na:	number of active infections: integer
Nr:	number of removed infections: integer
s:	cumulative infection rate: real
s-s0:	increase in cumulative infection rate since start of epidemic: real
sa:	active infection rate: real
sra:	average number of receptives/susceptibles in contact with an active infection: real
sar:	average number of active infections in contact with a receptive/susceptible population member: real
sna:	average number of removed infections in contact with a an active infection (n stands for neutral): real
sva:	average number of vaccinated nodes in contact with an active infection: real
sa*sra:	normalised number of active-susceptible pairs: real
sr*sar:	normalised number of active-susceptible pairs: real
nra:	number of active-susceptible pairs: integer
pop(i,j):	(end) status of a node

There are 5 files to be specified by the user for output. Their names and paths must be typed into the code before compilation. Note that while running, the program overwrites previous versions of an existing file! The files are opened and given a name and path specification in the following sections of the code (presented here with comments on the contents of each file as given in the code listing):

```

OPEN(10, FILE='filename1.dat')      ! CONTAINS DATA ON NUMBERS OF TOTAL INFECTIONS,
                                     ACTIVE- AND REMOVED INFECTIONS VS CYCLE-NUMBER.
OPEN(20, FILE='filename2.dat')      ! CONTAINS THE STATUS OF EACH INDIVIDUAL IN THE POPULATION
                                     (POPULATION STORED AS 2-D ARRAY/NETWORK)
OPEN(30, FILE='filename3.dat')      ! CONTAINS COORDINATION DATA: i,s,sra,sar (IN RESPECTIVE
                                     COLUMNS)
OPEN(40, FILE='filename4.dat')      ! CONTAINS COORDINATION DATA: t=i*dt,s,sa,ds/dt,dsa/dt
                                     (IN RESPECTIVE COLUMNS)
OPEN(50, FILE='filename5.dat')      ! CONTAINS THE STATUS OF EACH INDIVIDUAL IN A LIMITED
                                     POPULATION-SECTION (MxM ARRAY, M < 1001)

```

The files identified by 'filename1', 'filename3', and 'filename5' contain columns with the following data (in the order indicated) depending on the choice of the type of calculation/simulation indicated in brackets (different social bubbles (user options/input 1,3,5), or evaluation and testing purposes (user options/input 2,4)):

```

'filename1':  i,i*dt,Ni,Na,Nr (ALL)
               i,i*dt,s0,ds (2&4)
'filename3':  i*dt,s,sa,sra,sar,sa*sra,sna,sva,s-s0,nra,sra/REAL((2*Nn+1)**2),1-(s+xv) (5, count s-a pairs option chosen)
               i*dt,s,sa,sra,sar,sa*sra,sna,sva,s-s0,sra/REAL((2*Nn+1)**2),1-(s+xv) (5, count s-a pairs option NOT chosen)
               i,s,sra,sar,sa*sra,sr*sar (1&3)
'filename4':  i*dt,s,sa,sa*2*pi0*sra,sa*(2*pi0*sra-pr) (1&3&5)

```

N.B. Options 2 and 4 are not recommended for general use, they were only used by the author for the purpose of testing the code and certain aspects of the algorithm.

The file identified as 'filename2' contains the status of the population after the last contact cycle has been evaluated by the program. The file identified as 'filename5' contains the status of a smaller segment of the population after the last contact cycle has been evaluated by the program. The files contain 3 columns, together listing the status of all the nodes in the population/section. The format used is (i,j,"status"), where i and j (resp. 1st and 2nd column) are integers representing the coordinates of a node on the population lattice, whereas "status" (3rd column) represents the status of the node by an integer (1: susceptible, 2: active infection, 3: removed infection, 4: vaccinated node).