The simple spatial SIR model The case - 1D queue Consider a gueue of people waiting in front of a drugstore. Some of them are ill, some have just come to buy medicine for their beloved ones. Some are standing alone, some are couples or whole families... What is the probability that the susceptible people would get infected? A 1D queue example shall allows us to observe the spatial effects and make some general conclusions before setting up a more real, 2D How does the people behave? Do they swap their places in the queue? What is the distance at which an individual may get infected? Let us start with the already presented SIR system: $\frac{\partial}{\partial t}S = -\beta \frac{S}{N}I$ $\frac{\partial}{\partial t}I = \beta \frac{S}{N}I - \gamma I$ $\frac{\partial}{\partial t}R = \gamma I$ The spatial effect The disease may spread to neighbours with some probability P(r), where r is the "infectious" distance. Various functions can be choosen to model P(r). Comparing to 0D SIR, we have to take into account interaction between two functions. First accounts for the spatial distribution of infected individuals I(x), while the second describes the distance at which infection may occour P(r), where $r=x-x_0$ From a mathematical perspective, the resulting interaction can be writen as a convolution of these two functions. Now, the *viral load*, W, can be defined as: $W = I \star P(r)$ Next, the rate of change of infected people can be generalized as: $\frac{\partial}{\partial t}I = \beta \frac{S}{N}W - \gamma I$ Notice, that the 0D case corresponds to $P(r) = \delta$, where δ is the Dirac distribution. Choice of the "infectious" operator Let us investigate four basic distributions. 1) The simplest choice is to assume, that an individual can get become infected (with constant probability) if he/she is located within a *circe* of radius r. $W = I \star [\operatorname{disc of radius r}],$ 2) which can be (explicitly) approximated as [1], $Wpprox I+rac{r^2}{8}\Delta I.$ 3) An alternative (implicit) approximation is, $W-rac{r^2}{8}\Delta Wpprox I$ 4) Finally, assuming, that the probability of getting infected at some distance has a normal distribution, $W = I \star Gaussian(\sigma)$ [1] "Continuous and discrete SIR-models with spatial distributions" Seong-Hun Paeng and Jonggul Lee, Journal of Mathematical Biology, 2016 Comparison of "infectious" operators in the frequency domain Let us remind basic properties of the Fourier transform: $\mathcal{F}(
abla u) = -k^2 \mathcal{F}(u)$ $\mathcal{F}(u\star v)=\mathcal{F}(u)\mathcal{F}(v)$ $\mathcal{F}(C_1u+C_2v)=C_1\mathcal{F}(u)+C_2\mathcal{F}(v)$ The frequency responce, G, (Transmitancja widmowa) describes the ratio of the output amplitude, Y, to the input amplitude, Y, for each frequency ω . The *gain* is defined as absolute value of the system frequency response. (Moduł transmitancji widmowej opisuje wzmocnienie układu.) $G(j\omega) = rac{Y}{Y}$ where X and Y denote the Fourier transform of the *input* and *output* signal respectively. The frequency responce for each of the "infectious" operators can be calculated as follows: $G_1=rac{\mathcal{F}(I+rac{r^2}{8}\Delta I)}{F(I)}=rac{\mathcal{F}(I)-k^2rac{r^2}{8}\mathcal{F}(I))}{\mathcal{F}(I)}=1-k^2rac{r^2}{8}$ $G_2=rac{\mathcal{F}(I)}{\mathcal{F}(I-rac{r^2}{8}\Delta I)}=rac{1}{1+k^2rac{r^2}{8}}$ $G_3 = rac{\mathcal{F}(I \star [ext{disc of radius r}])}{\mathcal{F}(I)} = rac{2 * besselJ(kr,1)}{kr}$ $G_4 = rac{\mathcal{F}(I \star Gaussian(\sigma = r/2)}{\mathcal{F}(I)} = exp\left((-kr)^{2/8}
ight)$ Notice: • the input, X, in G_2 is implicit. • the frequency responce is related to the continous (not discrete) operator. Operators Remarks Q1 What is the interpretation of the negative values? • A1 For frequencies where negative values occurs, the spread of the disease may become unphysical. The high frequency for $W=I+rac{r^2}{8}\Delta I$ continous operator tends to infinity, thus such IC is expected to diverge. Q2 Does the frequency responce for the discrete operators follows the same plot? • A2 No. The responce for higher frequencies becomes flattened by a discrete operator. The lower the order of a FD stencil, the more flattened the responce. Q3 What are the pros / cons of convolution with some reasonable function (like Gaussian) vs its approximation? A3 Approximation (laplacian term) is more local than convolution. As a result, the algorithm is computationally faster. Moreover, imposing BC for an equation which includes a laplacian term is far easier than with convolution. • Q4 Are there any other differences between $W=I+rac{r^2}{8}\Delta I$ and $W-rac{r^2}{8}\Delta W=I$ approximations apart from frequency The spatial SIR system Let us use the simplest approximation [1], $rac{\partial}{\partial t}S = -etarac{S}{N}(I + rac{r^2}{8}\Delta I)$ $\frac{\partial}{\partial t}I = \beta \frac{S}{N}(I + \frac{r^2}{8}\Delta I) - \gamma I$ $\frac{\partial}{\partial t}R = \gamma I$ Substituting $W=I+rac{r^2}{8}\Delta I$, $\frac{\partial}{\partial t}S = -\beta \frac{S}{N}W$ $rac{\partial}{\partial t}I=etarac{S}{N}W-\gamma I$ $\frac{\partial}{\partial t}R = \gamma I$ Notice that the diffusivity depends on S, which is decreasing in time. The low diffusivity issue and the spatial WSIR remedy Low values of the diffusivity coefficient can lead to stability problems in the numerical algorithms. To avoid numerical issues, the W, is simulated as an additional field. W is relaxed (with eta_W coefficient) to $W - \Delta W rac{r^2}{8} = I$. The WSIR system reads: $rac{\partial}{\partial t}W=eta_W\left[rac{r^2}{8}\Delta W+(I-W)
ight]$ $\frac{\partial}{\partial t}S = -\beta \frac{S}{N}W$ $\frac{\partial}{\partial t}I = \beta \frac{S}{N}W - \gamma I$ $\frac{\partial}{\partial t}R = \gamma I$ The nondimensional form equations - revisited Again, we can rescale the time as $au=\gamma t$, then the set of equations can be described by single similarity number $R_0=rac{eta}{\gamma}$ $\frac{\partial}{\partial \tau}S = -R_0 \frac{S}{N} (I + \frac{r^2}{8} \Delta I)$ $rac{\partial}{\partial au} I = R_0 rac{S}{N} (I + rac{r^2}{8} \Delta I) - I$ $\frac{\partial}{\partial \tau}R = I$ The WSIR system reads: $rac{\partial}{\partial au}W=rac{eta_W}{\gamma}igg[rac{r^2}{8}\Delta W+(I-W)igg]$ $rac{\partial}{\partial au}S = -R_0rac{S}{N}W$ $rac{\partial}{\partial au} I = R_0 rac{S}{N} W - \ I$ $\frac{\partial}{\partial \tau}R = I$ Remarks on other SIR-diffusion models There are models [2], in which the diffusion acts as an independent operator for each of the compartments, $rac{\partial}{\partial t}S = -etarac{S}{N}I + k_S\Delta S$ $rac{\partial}{\partial t}I=etarac{S}{N}I-\gamma I+k_I\Delta I$ $rac{\partial}{\partial t}R=\gamma I+k_R\Delta R$ where $k_{S,I,R}$ denotes the diffusion coefficient for particular compartment. According to [1], such models does not capture physics of the epidemy because: • a) almost all humans moves within a small fixed radius and does not disperse in a manner such as Brownian motion. b) equation cannot explain the spatial transmission by infection if individuals are at rest. c) humans would move away from an increasing gradient of the infected. d) humans would move away from over-crowded locations. Consequently, the spatial transmission described by [2] is caused not by infection but by the dispersion of patients. Inspired by the heat transfer equation: $rac{\partial}{\partial t}
ho T =
abla \cdot k
abla T + \dot{q}$ One can mitigate the escape of humans from *over-crowded* locations by using fractions in the laplacian term. Notice, that this will be a different model: $\frac{1}{N}
abla \cdot k_s
abla S
eq
abla \cdot k_s
abla s because <math>N$ is a spatial variable: $rac{\partial}{\partial au}S = rac{\partial}{\partial au}Ns =
abla \cdot k_s
abla s - eta rac{S}{N}I$ $rac{\partial}{\partial t}I = rac{\partial}{\partial t}Ni =
abla \cdot k_i
abla i + eta rac{S}{N}I - \gamma I$ $rac{\partial}{\partial t}R = rac{\partial}{\partial t}Nr =
abla \cdot k_r
abla r + \gamma I$ Anyway, the drawbacks mentioned in a)-c) still apply. [2] Modeling epidemics by the lattice Boltzmann method, De Rosis, Alessandro, Phys. Rev. E, 2020 Similarity numbers in SIR-like models Let us define dimensionless variables, $ar{x}=rac{x}{x_c}, \qquad ar{t}=rac{t}{t_c}, \qquad ar{N}=rac{N}{N_c}, \qquad ar{S}=rac{S}{N_c}, \qquad ar{I}=rac{I}{N_c},$ where the *c*-subscript denotes a characteristics scale. The Fourier number The Fourier number, Fo, is the ratio of the diffusive term to the temporal term. It can can be viewed as a non-dimensional-time. The (second) Damköhler number The (second) Damköhler number is defined as the ratio of the reaction rate to the diffusive transfer rate. $Da = rac{\dot{R}x_c^2}{\iota}$ where: • R[1/s] denotes the reaction rate • $x_c[m]$ is the characteristics lenght • $k[m^2/s]$ is the diffusion coefficient SIR with *independent* (naive) diffusion First, we will analyze a SIR model with independent (naive) diffusion. Its dimensions are $\overbrace{rac{\partial}{\partial t}}^{[1/s]}[individual] = \overbrace{S}^{[1/s]}\underbrace{S}[individual] = \overbrace{K_S}^{[m^2/s]}[individual] + \overbrace{K_S}^{[m^2/s]}\underbrace{\Delta}^{[individual]}$ In terms of the characteristic scales $rac{1}{t_c}rac{\partial}{\partialar{t}}\overline{S}N_c = -etarac{SN_c}{\overline{N}N}ar{I}N_c + k_Srac{N_c}{x_c^2}rac{\partial^2}{\partial\overline{x}^2}ar{S} \hspace{1cm}//\cdot t_c,:N_c$ $rac{\partial}{\partialar{t}}\overline{S} = -eta t_c rac{S}{\overline{N}}ar{I} + k_S rac{t_c}{x_c^2} rac{\partial^2}{\partial\overline{m}^2} \overline{S}$ $egin{aligned} &= -eta rac{x_c^2rac{I}{\overline{N}}}{k_S}rac{k_St_c}{x_c^2} \overline{S} + rac{k_St_c}{x_c^2}rac{\partial^2}{\partial \overline{x}^2} \overline{S} \end{aligned}$ In this model, the diffusion coefficient are independent for each fo the S,I,R compartments. As a consequence, this model will be described by three Damkohnler numbers, Da_S, Da_I, Da_R . SIR-Peng Notice, that in the SIR-Peng model, the only field with diffusive term is the I compartment. $rac{\partial}{\partial t}I = eta rac{S}{N}(I + rac{r^2}{8}\Delta I) - \gamma I$ Repeating the analysis. $rac{1}{t_c}rac{\partial}{\partialar{t}}ar{I}N_c=etarac{SN_c}{\overline{N}N}igg[ar{I}N_c+N_crac{r^2}{8}rac{1}{x_c^2}rac{\partial^2}{\partialar{r}^2}ar{I}igg]-\gammaar{I}N_c \hspace{1cm}//\cdot t_c,:N_c$ and denoting $k=etarac{r^2}{8}rac{\overline{S}}{N}$ $\frac{\partial}{\partial \bar{t}} \bar{I} = \left(\beta \frac{\overline{S}}{\overline{N}} - \gamma\right) t_c \bar{I} + \underbrace{\frac{r^2}{8} \beta \frac{\overline{S}}{\overline{N}}}_{\overline{N}} \frac{t_c}{r^2} \frac{\partial^2}{\partial z^2} \bar{I}$ leads to the final form $rac{\partial}{\partial ar{t}}ar{I} = rac{x_c^2\left(etarac{S}{\overline{N}} - \gamma
ight)}{k} \underbrace{rac{kt_c}{x_c^2}ar{I}}_{R_L} + rac{kt_c}{x_c^2}rac{\partial^2}{\partial ar{x}^2}ar{I}$ **WSIR** Notice, that in the WSIR model, the only field with diffusive term is the W field. $\left | rac{\partial}{\partial t} W = eta_W \left | rac{r^2}{8} \Delta W + (I-W)
ight |$ Repeating the analysis, $rac{1}{t_c}rac{\partial}{\partialar{t}}\overline{W}N_c=eta_WN_c\left[rac{r^2}{8}rac{1}{x_c^2}rac{\partial^2}{\partial\overline{x}^2}\overline{W}+(ar{I}-\overline{W})
ight] \qquad //\cdot t_c,:N_c$ $rac{\partial}{\partial ar{t}} \overline{W} = eta_W t_c ar{I} - eta_W t_c \overline{W} + \overbrace{rac{r^2}{8} eta_W}^\kappa rac{t_c}{r^2} rac{\partial^2}{\partial \overline{z}^2} \overline{W}$ and denoting $k=eta_Wrac{r^2}{8}$ $rac{\partial}{\partial ar{t}} \overline{W} = eta_W t_c ar{I} - rac{eta_W x_c^2}{k} rac{k t_c}{x^2} \overline{W} + rac{k t_c}{x^2} rac{\partial^2}{\partial ar{z}^2} \overline{W}$ $egin{aligned} &=eta_W t_c ar{I} - \underbrace{rac{8x_c^2}{r^2}}_{Da} \underbrace{rac{kt_c}{x_c^2}}_{F_c} \overline{W} + \underbrace{rac{kt_c}{x_c^2}}_{F_c} rac{\partial^2}{\partial \overline{x}^2} \overline{W} \end{aligned}$ Finally, the Damkohler number for WSIR model is $Da_W = rac{8x_c^2}{r^2}$ **Exercise** Implement a FD solver for both SIR-Peng and WSIR model. In [2]: import numpy as np import os from numba import jit import sys sys.path.append("..") from utils.sir_plot_utils import * %matplotlib inline In [3]: dx = domain length / (nx-1)xspace = np.linspace(0, domain length, nx) r0 = 5.5 # infectious radius beta sir = 3.01 # the average number of contacts per person per time gamma sir = 1/2.8 # 1 over days to recovery beta W = 1e3total time = 1e-0dt = 1e-5ntimesteps = int(total time / dt) In [4]: # Spatially uniform population density $I_IC = np.ones(nx)*0.01$ # numpy function ones() $I_IC[int((nx-1)/4):int(nx/2 + 1)] = 0.05$ # setting u = 2 between 0.5 and 1 as per our I.C.s $S_{IC} = np.ones(nx) - I_{IC}$ $R_IC = np.zeros(nx)$ $N = S_IC + I_IC + R_IC$ make_wsir_plot_1D(S_IC, I_IC, R_IC, xspace, 0, 0, 'SIR IC') SIR IC @ nt: 0 dt 0 1.0 0.8 No of people 0.4 Susceptible Infected Recovered Total population 0.2 0.0 0 10 20 30 40 50 60 х In [5]: # @jit(cache=True, nopython=True) @jit(nopython=True) def SIR_Peng_1D_FD_btcs(S, I, R, nx, dx, r0, beta_sir, gamma_sir, nt, dt): N = S + I + Rc ind = np.arange(0, nx) $l_{ind} = np.roll(c_{ind}, -1)$ r_ind = np.roll(c_ind, 1) hist_of_diffusivity = np.zeros((nt, nx), dtype=np.float64) for n in range(nt): # iterate through time lap I = $(I[l_ind] - 2 * I[c_ind] + I[r_ind]) / dx ** 2$ $qS2I_spatial = (r0 * r0 / 8.) * lap_I$ # qS2I_spatial = np.zeros(nx) hist_of_diffusivity[n] = beta_sir * S * qS2I_spatial qS2I = dt * beta sir * S * (qS2I spatial + I) / N qI2R = dt * gamma sir * I S = S - qS2II = I + qS2I - qI2RR = R + qI2Rreturn S, I, R, hist of diffusivity @jit(nopython=True) def WSIR_1D_FD_btcs(S, I, R, nx, dx, r0, beta_sir, gamma_sir, nt, dt, beta_W=1e2): W = np.zeros(nx)N = S + I + Rc_ind = np.arange(0, nx) $l_{ind} = np.roll(c_{ind}, -1)$ r_ind = np.roll(c_ind, 1) for n in range(nt): # iterate through time $lap W = (W[l_ind] - 2 * W[c_ind] + W[r_ind]) / dx ** 2$ $qW_spatial = (r0 * r0 / 8.) *lap W$ $\# qW_spatial = np.zeros(nx)$ $qW = dt * beta_W * (qW_spatial + (I - W))$ qS2I = dt * beta sir * S * W/NqI2R = dt * gamma sir * I W = W + qWS = S - qS2II = I + qS2I - qI2RR = R + qI2Rreturn S, I, R, W In [6]: S, I, R, _ = SIR_Peng_1D_FD_btcs(S_IC, I_IC, R_IC, nx, dx, r0, beta_sir, gamma_sir, ntimesteps, dt) make wsir plot 1D(S, I, R, xspace, ntimesteps, dt, 'SIR-Peng 1D') SIR-Peng 1D @ nt: 99999 dt 1e-05 1.0 0.8 No of people 0.4 Susceptible Infected Recovered Total population 0.2 0.0 10 20 0 30 40 50 60 Х In [7]: Sw, Iw, Rw, compare_sir_vs_wsir_plot((S, I, R), (Sw, Iw, Rw, Ww), beta_W, xspace, ntimesteps, 'SIR-Peng vs WSIR', dt) SIR-Peng vs WSIR dt=1.00e-05beta W=1e+03 @ ntimesteps=1.00e+05 1.0 0.8 No of people 0.0 0.4 S* ₩ 0.2 0.0 10 20 50 60 30 Х Effect of varing spatial density In [8]: # signal = 2* np.pi*xspace/max(xspace) # signal = 10*np.ones(nx) + 500*np.sin(signal)# signal += abs(min(signal)) +1 # N = signal# N[int((nx-1)/4):int(nx/2 + 1)] = 1.2*signal[int((nx-1)/4):int(nx/2 + 1)]# I IC = 0.05* signalN = np.ones(nx)N[int((nx-1)/4):int(nx/2 + 1)] *= 10I IC = 0.05* np.ones(nx) $I_{C[int(3*(nx-1)/8):int(6*nx/8 + 1)]} = 10$ $S_IC = N - I_IC$ $R_{IC} = np.zeros(nx)$ $y_{lim} = [-0.05, 1.05*max(N)]$ from utils.sir_plot_utils import make_wsir_plot_1D make_wsir_plot_1D(S_IC, I_IC, R_IC, xspace, 0, 0, 'SIR IC', w=None, y_lim=y_lim) SIR IC @ nt: 0 dt 0 10 Susceptible Infected Recovered 8 Total population No of people 6 2 0 10 20 30 50 40 60 Х In [9]: S, I, R, hist_of_diffusivity = SIR_Peng_1D_FD_btcs(S_IC, I_IC, R_IC, nx, dx, r0, beta_sir, gamma_sir, ntimester Sw, Iw, Rw, Ww = WSIR 1D FD btcs(S IC, I IC, R IC, nx, dx, r0, beta sir, gamma sir, ntimesteps, dt, beta W) compare_sir_vs_wsir_plot((S, I, R), (Sw, Iw, Rw, Ww), beta_W, xspace, ntimesteps, 'SIR-Peng vs WSIR', dt, y_lim SIR-Peng vs WSIR @ ntimesteps=1.00e+05 dt=1.00e-05beta W=1e+03S 10 R 8 S* N* No of people W* 2 20 10 30 40 50 60 Х Influence of the β_W relaxation coefficient For $eta_W o \infty$ the W-SIR model converges to the Peng-SIR one. Exercise Experiment with different β_W and check the output. Tip: You may need to decrease dt. In [10]: $beta_W = 10*1e3$ total_time = 1e-0 dt = 0.1*1e-5ntimesteps = int(total_time / dt) S, I, R, hist_of_diffusivity = SIR_Peng_1D_FD_btcs(S_IC, I_IC, R_IC, nx, dx, r0, beta_sir, gamma_sir, ntimester Sw, Iw, Rw, Ww = WSIR_1D_FD_btcs(S_IC, I_IC, R_IC, nx, dx, r0, beta_sir, gamma_sir, ntimesteps, dt, beta_W) compare_sir_vs_wsir_plot((S, I, R), (Sw, Iw, Rw, Ww), beta_W, xspace, ntimesteps, 'SIR-Peng vs WSIR', dt, y_lim SIR-Peng vs WSIR @ ntimesteps=1.00e+06 dt=1.00e-06 beta W=1e+04S 10 1 S* N* No of people W* 2 0 30 10 20 40 50 60 Х Numbers or fractions - revisited (for curious readers only) This time, the task is more difficult. First, let us remind the quotient rule for laplace operator: https://math.stackexchange.com/questions/652730/laplacian-identity $\Delta\left(rac{f}{q}
ight) = rac{1}{q}\Delta f - rac{2}{q}
abla\left(rac{f}{q}
ight)\cdot
abla g - rac{f}{q^2}\Delta g$ $ho
ho rac{1}{a} \Delta f = \Delta \left(rac{f}{a}
ight) + rac{2}{a}
abla \left(rac{f}{a}
ight) \cdot
abla g + rac{f}{a^2} \Delta g$ Again, we can divide each of the equations by N to represent them in terms of fractions instead of numbers. Consider the spatial equation for S from [1]: $rac{\partial}{\partial t}S = -etarac{S}{N}igg(I + rac{r^2}{8}\Delta Iigg)$ dividing each side by N... (1) $rac{\partial}{\partial t}rac{S}{N}=-etarac{S}{N}igg(rac{I}{N}+rac{r^2}{8}rac{1}{N}\Delta Iigg)$ (2)Substituting the quotient rule for laplace operator: $rac{\partial}{\partial t}rac{S}{N} = -etarac{S}{N}igg[rac{I}{N} + rac{r^2}{8}igg[\Delta\left(rac{I}{N}
ight) + rac{2}{N}
abla\left(rac{I}{N}
ight) \cdot
abla N + rac{I}{N^2}\Delta Nigg]igg]$ Introducing fractions $s=\frac{S}{N}, i=\frac{I}{N}, r=\frac{r}{N}$: $\left|rac{\partial}{\partial t}s = -eta s \left|i + rac{r^2}{8}igg(\Delta i + 2
abla i\cdotrac{
abla N}{N} + irac{\Delta N}{N}igg)
ight|$ $rac{\partial}{\partial t}i = eta s \left[i + rac{r^2}{8}igg(\Delta i + 2
abla i \cdot rac{
abla N}{N} + irac{\Delta N}{N}igg)
ight] - \gamma i \cdot rac{\partial}{\partial t}i = eta s \left[i + rac{r^2}{8}igg(\Delta i + 2
abla i \cdot rac{
abla N}{N} + irac{\Delta N}{N}igg)
ight]$ $\frac{\partial}{\partial t}r = \gamma i$ Alternatively, one can easily rewrite the initial equation as: $rac{\partial}{\partial t}s = -eta s \left(i + rac{r^2}{8}rac{1}{N}\Delta(iN)
ight)$ $rac{\partial}{\partial t}i = eta s \left(i + rac{r^2}{8}rac{1}{N}\Delta(iN)
ight) - \gamma i .$ $\frac{\partial}{\partial t}r = \gamma i$ Notice that $\Delta(iN) = i\Delta N + 2\nabla i \cdot \nabla N + N\Delta i$. Conclusion The attempt to switch from numbers to fractions in spatial model results in more complex form of the equations. According to the authors' experience, the LBM scheme for the latter form is expected to be unstable for large ratio of N (~100-1000).