Numerical methods and uncertainty quantification for kinetic equations

Lecture 3: Appendix on Asymptotic Preserving schemes
On the spread of a virus

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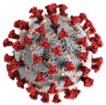
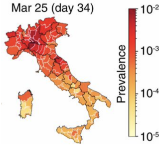
Outline

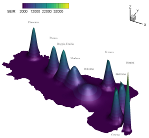
Outline



The ongoing COVID-19 pandemic has led to a strong interest from researchers around the world in building and studying new epidemiological models capable of describing the progress of the epidemic[1]

Most classical compartmental models represent the spread of the epidemic only concerning the temporal evolution of the disease among the population, but not taking into account spatial effects

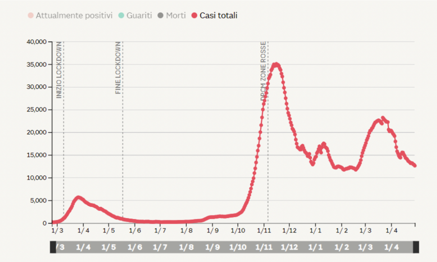


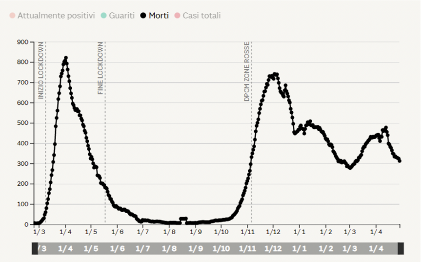


Spatial effects can be modeled using networks of interacting components (cities, regions, ...) or more in general by considering a fully two-dimensional space dynamics

Bellomo et al. '20; Buonuomo, Della Marca '20; Colombo et al. '20; Gatto et a al. 2020; Giordano et al. '20; Peirlinck et al. '20; Tang et al. 2020; Viguerie et al. '20; Vollmer at al. '20; and many many more....

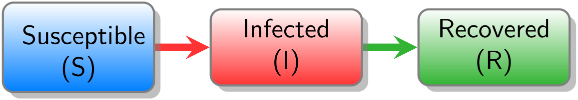
Additionally, any realistic data-driven model must take into account the large uncertainty in the values reported by official sources, such as the amount of infectious individuals

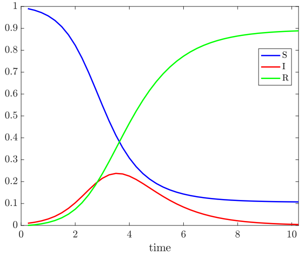




Detected cases (left) and deaths (right) in Italy from the beginning of the pandemic

The SIR model[2]





$$\frac{dS}{dt} = -\beta \frac{SI}{N}$$
$$\frac{dI}{dt} = \beta \frac{SI}{N} - \gamma I$$
$$\frac{dR}{dt} = \gamma I$$

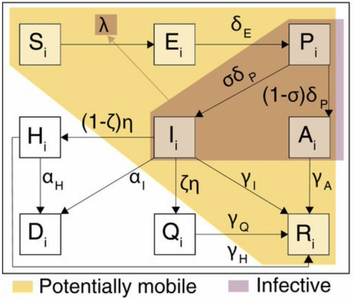
- $N = S + I + R \Rightarrow$ total population (normalized $N = 1$)
- β, $\gamma \Rightarrow$ transmission and recovery rates
- $R_0 = \beta/\gamma \Rightarrow$ basic reproduction number

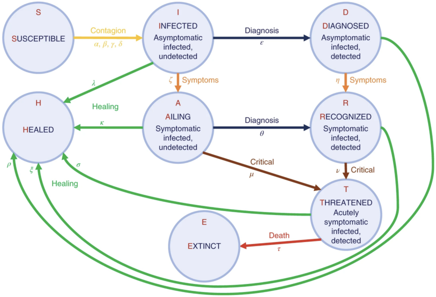
Deterministic model with no spatial information on the epidemic spread

[2] Kermack, McKendrick '27; Hethcote '00

The compartmentalization game

More realistic models involve additional compartmentalizations depending on the specific characteristic of the infectious disease[3]





Matching models with available data may be a real challenge (data-driven models). Introducing some degree of uncertainty into the data is an essential feature of analyzing realistic scenarios.

[3]Hethcote '00; Gatto et al. '20; Giordano et al. '20

The parabolic SIR model[4]

$$\frac{\partial S}{\partial t} = -\beta S I + \frac{\partial}{\partial x}\left(D_S \frac{\partial S}{\partial x}\right)$$
$$\frac{\partial I}{\partial t} = \beta S I - \gamma I + \frac{\partial}{\partial x}\left(D_I \frac{\partial I}{\partial x}\right)$$
$$\frac{\partial R}{\partial t} = \gamma I + \frac{\partial}{\partial x}\left(D_R \frac{\partial R}{\partial x}\right)$$

- $S = S(x,t)$, $I = I(x,t)$, $R = R(x,t)$, $x \in \Omega \subset \mathbb{R}$
- D_S, D_I, $D_R \Rightarrow$ self-diffusion coefficients
- $D_S > D_I$ (population dynamics), $D_I > D_S = 0$ (infection dynamics)
- the diffusion coefficients might also be space-dependent (or nonlinear)

The parabolic character of the model may lead the disease to propagate instantaneously over large distances

[4] Webb '86; Murray '01; Berestycki, Roquejoffre, Rossi '21

Outline

A compartmental kinetic transport model for commuters

We consider a population of commuters at position $x \in \Omega$ moving with velocity directions $v \in \mathbb{S}^1$. The kinetic densities of the commuters satisfy the transport equations

$$\begin{aligned}
\frac{\partial f_S}{\partial t} + \nabla_x \cdot (v_S f_S) &= -F_I(f_S, I_T) - F_A(f_S, A_T) + \frac{1}{\tau_S}(S - f_S) \\
\frac{\partial f_E}{\partial t} + \nabla_x \cdot (v_E f_E) &= F_I(f_S, I_T) + F_A(f_S, A_T) - a f_E + \frac{1}{\tau_E}(E - f_E) \\
\frac{\partial f_I}{\partial t} + \nabla_x \cdot (v_I f_I) &= a\sigma f_E - \gamma_I f_I + \frac{1}{\tau_I}(I - f_I) \\
\frac{\partial f_A}{\partial t} + \nabla_x \cdot (v_A f_A) &= a(1-\sigma) f_E - \gamma_A f_A + \frac{1}{\tau_A}(A - f_A) \\
\frac{\partial f_R}{\partial t} + \nabla_x \cdot (v_R f_R) &= \gamma_I f_I + \gamma_A f_A + \frac{1}{\tau_R}(R - f_R)
\end{aligned} \qquad (1)$$

The number of Susceptible, Exposed, Infected and Recovered is

$$S(x,t) = \frac{1}{2\pi}\int_{\mathbb{S}^1} f_S(x,v,t)\,dv,\;\; E(x,t) = \frac{1}{2\pi}\int_{\mathbb{S}^1} f_E(x,v,t)\,dv,\;\; R(x,t) = \frac{1}{2\pi}\int_{\mathbb{S}^1} f_R(x,v,t)$$

$$I(x,t) = \frac{1}{2\pi}\int_{\mathbb{S}^1} f_I(x,v,t)\,dv,\;\; A(x,t) = \frac{1}{2\pi}\int_{\mathbb{S}^1} f_A(x,v,t)\,dv,$$

A diffusion compartmental model for non commuters

The unknowns $S_u(x,t)$, $E_u(x,t)$, $I_u(x,t)$, $A_u(x,t)$, $R_u(x,t)$ are the density fractions of the non-commuters who, by assumption, move only on an urban scale and satisfy

$$
\begin{aligned}
\frac{\partial S_u}{\partial t} &= -F_I(S_u, I_T) - F_A(S_u, A_T) + \nabla_x \cdot (D_S^u \nabla_x S_u) \\
\frac{\partial E_u}{\partial t} &= F_I(S_u, I_T) + F_A(S_u, A_T) - aE_u + \nabla_x \cdot (D_E^u \nabla_x E_u) \\
\frac{\partial I_u}{\partial t} &= a\sigma E_u - \gamma_I I_u + \nabla_x \cdot (D_I^u \nabla_x I_u) \\
\frac{\partial A_u}{\partial t} &= a(1-\sigma)E_u - \gamma_A A_u + \nabla_x \cdot (D_A^u \nabla_x A_u) \\
\frac{\partial R_u}{\partial t} &= \gamma_I I_u + \gamma_A A_u + \nabla_x \cdot (D_R^u \nabla_x R_u).
\end{aligned}
\tag{2}
$$

The velocities $v_i = \lambda_i(x)v$ in the kinetic model, the diffusion coefficients $D_i^u = D_i^u(x)$, $i \in \{S, E, I, A, R\}$ and the relaxation times $\tau_i = \tau_i(x)$, $i \in \{S, E, I, A, R\}$ take into account the heterogeneity of geographical areas.

The coupled model

The total densities are defined by

$$S_T(x,t) = S(x,t) + S_u(x,t), \;\; E_T(x,t) = E(x,t) + E_u(x,t), \;\; R_T(x,t) = R(x,t) + R_u(x,t),$$

$$I_T(x,t) = I(x,t) + I_u(x,t), \;\; A_T(x,t) = A(x,t) + A_u(x,t).$$

The transmission of the infection is governed by the incidence functions $F_I(\cdot, I_T)$ and $F_A(\cdot, A_T)$. We assume local interactions to characterize the nonlinear incidence functions

$$F_I(g, I_T) = \beta_I \frac{g I_T^p}{1 + \kappa_I I_T}, \qquad F_A(g, A_T) = \beta_A \frac{g A_T^p}{1 + \kappa_A A_T},$$

Alternative incidence functions are

$$F_I(g, I_T) = \beta_I \frac{g I_T^p}{1 + \kappa_I \int_{\bar{\Omega}} I_T \, dx}, \qquad F_A(g, A_T) = \beta_A \frac{g A_T^p}{1 + \kappa_A \int_{\bar{\Omega}} A_T \, dx},$$

$\beta_I = \beta_I(x,t)$ and $\beta_A = \beta_A(x,t)$ characterize the contact rates of highly symptomatic and mildly symptomatic/asymptomatic infectious individuals.
$\kappa_I = \kappa_I(x,t)$ and $\kappa_A = \kappa_A(x,t)$ are the incidence damping coefficients based on the self-protective behavior.

Commuters behavior in urban areas

A diffusion behavior can be recovered when $\tau_{S,I,R} \to 0$ while the diffusion coefficients

$$D_S = \frac{1}{2}\lambda_S^2\tau_S, \quad D_E = \frac{1}{2}\lambda_E^2\tau_E, \quad D_I = \frac{1}{2}\lambda_I^2\tau_I, \quad D_A = \frac{1}{2}\lambda_A^2\tau_A, \quad D_R = \frac{1}{2}\lambda_R^2\tau_R.$$

Let us introduce the flux functions

$$J_S = \frac{\lambda_S}{2\pi}\int_{\mathbb{S}^1} v f_S(x,v,t)\,dv, \quad J_E = \frac{\lambda_E}{2\pi}\int_{\mathbb{S}^1} v f_E(x,v,t)\,dv, \quad J_I = \frac{\lambda_I}{2\pi}\int_{\mathbb{S}^1} v f_I(x,v,t)\,dv$$

$$J_A = \frac{\lambda_A}{2\pi}\int_{\mathbb{S}^1} v f_A(x,v,t)\,dv, \quad J_R = \frac{\lambda_R}{2\pi}\int_{\mathbb{S}^1} v f_R(x,v,t)\,dv.$$

Integrating system (1) in v we see that the macroscopic densities of commuters obey to

$$\begin{aligned}
\frac{\partial S}{\partial t} + \nabla_x \cdot J_S &= -F_I(S, I_T) - F_A(S, A_T)\\
\frac{\partial E}{\partial t} + \nabla_x \cdot J_E &= F_I(S, I_T) + F_A(S, A_T) - aE\\
\frac{\partial I}{\partial t} + \nabla_x \cdot J_I &= a\sigma E - \gamma_I I\\
\frac{\partial A}{\partial t} + \nabla_x \cdot J_A &= a(1-\sigma)E - \gamma_A A\\
\frac{\partial R}{\partial t} + \nabla_x \cdot J_R &= \gamma_I I + \gamma_A A
\end{aligned}$$

Diffusion limit

The flux functions satisfy

$$
\begin{aligned}
\frac{\partial J_S}{\partial t} + \nabla_x \cdot \left(\frac{\lambda_S^2}{2\pi} \int_{\mathbb{S}^1} ((v \otimes v) f_S)\, dv \right) &= -F_I(J_S, I_T) - F_A(J_S, A_T) - \frac{1}{\tau_S} J_S \\
\frac{\partial J_E}{\partial t} + \nabla_x \cdot \left(\frac{\lambda_E^2}{2\pi} \int_{\mathbb{S}^1} ((v \otimes v) f_E)\, dv \right) &= \frac{\lambda_E}{\lambda_S} \left(F_I(J_S, I_T) + F_A(J_S, A_T) \right) - a J_E - \frac{1}{\tau_E} J_E \\
\frac{\partial J_I}{\partial t} + \nabla_x \cdot \left(\frac{\lambda_I^2}{2\pi} \int_{\mathbb{S}^1} ((v \otimes v) f_I)\, dv \right) &= \frac{\lambda_I}{\lambda_E} a\sigma J_E - \gamma_I J_I - \frac{1}{\tau_I} J_I \\
\frac{\partial J_A}{\partial t} + \nabla_x \cdot \left(\frac{\lambda_A^2}{2\pi} \int_{\mathbb{S}^1} ((v \otimes v) f_A)\, dv \right) &= \frac{\lambda_A}{\lambda_E} a(1-\sigma) J_E - \gamma_A J_A - \frac{1}{\tau_A} J_A \\
\frac{\partial J_R}{\partial t} + \nabla_x \cdot \left(\frac{\lambda_R^2}{2\pi} \int_{\mathbb{S}^1} ((v \otimes v) f_R)\, dv \right) &= \frac{\lambda_R}{\lambda_I} \gamma_I J_I + \frac{\lambda_R}{\lambda_A} \gamma_A J_A - \frac{1}{\tau_R} J_R.
\end{aligned}
$$

Letting $\tau_{S,I,R} \to 0$, we get from the r.h.s. in (1)

$$
f_S = S, \quad f_E = E, \quad f_I = I, \quad f_A = A, \quad f_R = R,
$$

and

$$
J_S = -D_S \nabla_x S, \quad J_E = -D_E \nabla_x E, \quad J_I = -D_I \nabla_x I, \quad J_A = -D_A \nabla_x A, \quad J_R = -D_R \nabla_x R,
$$

Diffusion limit II

Thus, the following diffusion system for the population of commuters is obtained

$$
\begin{aligned}
\frac{\partial S}{\partial t} &= -F_I(S, I_T) - F_A(S, A_T) + \nabla_x \cdot (D_S \nabla_x S) \\
\frac{\partial E}{\partial t} &= F_I(S, I_T) + F_A(S, A_T) - aE + \nabla_x \cdot (D_E \nabla_x E) \\
\frac{\partial I}{\partial t} &= a\sigma E - \gamma_I I + \nabla_x \cdot (D_I \nabla_x I) \\
\frac{\partial A}{\partial t} &= a(1-\sigma)E - \gamma_A A + \nabla_x \cdot (D_A \nabla_x A) \\
\frac{\partial R}{\partial t} &= \gamma_I I + \gamma_A A + \nabla_x \cdot (D_R \nabla_x R)
\end{aligned} \tag{3}
$$

The capability of the model to account for different regimes, hyperbolic or parabolic, accordingly to the space dependent relaxation times τ_i, $i \in \{S, E, I, A, R\}$, makes it suitable for describing the dynamics of human beings.

Including data uncertainty

- To extend the model to the case of uncertainties, let us suppose that the population depend on an additional random vector $\boldsymbol{z} = (z_1, \ldots, z_d)^T \in \Omega_{\boldsymbol{z}} \subseteq \mathbb{R}^d$.
- Possible sources of uncertainty are due to lack of information on the actual number of infected or specific epidemic characteristics.
- This gives the following high-dimensional unknowns

$$f_S(x, v, t, \boldsymbol{z}),\ f_E(x, v, t, \boldsymbol{z}),\ f_I(x, v, t, \boldsymbol{z}),\ f_A(x, v, t, \boldsymbol{z}), f_R(x, v, t, \boldsymbol{z}).$$

$$S_u(x, t, \boldsymbol{z}),\ E_u(x, t, \boldsymbol{z}),\ I_u(x, t, \boldsymbol{z}), A_u(x, t, \boldsymbol{z}), R_u(x, t, \boldsymbol{z}).$$

- Notice that, the structure of the model does not change, i.e. there is no direct variation of the unknowns with respect to $\boldsymbol{z}$.
- One common choice is to consider the parameters acting inside the incidence function to have a dependence of the form

$$\beta_I = \beta_I(x, t, \boldsymbol{z}),\ \beta_A = \beta_A(x, t, \boldsymbol{z}).$$

$$k_I = k_I(x, t, \boldsymbol{z}),\ k_A = k_A(x, t, \boldsymbol{z}),$$

Outline

The numerical method

- For the commuters, the numerical scheme for the deterministic case is based on a discrete ordinate method in velocity in which the even and odd parity formulation is employed [5].
- Then a finite volume method working on two-dimensional unstructured meshes [6] approximate the discrete ordinate formulation.
- The full discretization of the equations is obtained through the use of suitable IMEX Runge-Kutta schemes [7].
- The above choices permit to obtain a scheme which consistently captures the diffusion limit from the kinetic system when the scaling parameters $\tau_{S,I,R}$ tends toward zero.
- The discretization of the stochastic part is performed by standard generalized Polynomial Chaos (gPC) expansion technique [8].

[5] Jin-Pareschi '00, Klar '98, D.-Pareschi-Rispoli '14
[6] Boscheri-D. '20
[7] Boscarino-Pareschi-Russo '13, D.-Pareschi-Rispoli '14
[8] Xiu '10

Even and odd parities formulation

We rewrite the commuters system denoting $v = (\eta, \xi) \in \mathbb{S}^1$. This gives

$$r_i^{(1)}(\xi,\eta) = \frac{1}{2}(f_i(\xi,-\eta) + f_i(-\xi,\eta)), \quad r_i^{(2)}(\xi,\eta) = \frac{1}{2}(f_i(\xi,\eta) + f_i(-\xi,-\eta))$$

while for the scalar fluxes one has

$$j_i^{(1)}(\xi,\eta) = \frac{\lambda_i}{2}(f_i(\xi,-\eta) + f_i(-\xi,\eta)), \quad j_i^{(2)}(\xi,\eta) = \frac{\lambda_i}{2}(f_i(\xi,\eta) + f_i(-\xi,-\eta))$$

with $i = S, E, I, A, R$. An equivalent formulation with respect to (1) can then be obtained thanks to this change of variables

$$\frac{\partial r_S^{(1)}}{\partial t} + \xi \frac{\partial j_S^{(1)}}{\partial x} - \eta \frac{\partial j_S^{(1)}}{\partial y} = -F_I(r_S^{(1)}, I_T) - F_A(r_S^{(1)}, A_T) + \frac{1}{\tau_S}\left(S - r_S^{(1)}\right)$$

$$\frac{\partial r_S^{(2)}}{\partial t} + \xi \frac{\partial j_S^{(2)}}{\partial x} + \eta \frac{\partial j_S^{(2)}}{\partial y} = -F_I(r_S^{(2)}, I_T) - F_A(r_S^{(2)}, A_T) + \frac{1}{\tau_S}\left(S - r_S^{(2)}\right)$$

$$\frac{\partial r_E^{(1)}}{\partial t} + \xi \frac{\partial j_E^{(1)}}{\partial x} - \eta \frac{\partial j_E^{(1)}}{\partial y} = F_I(r_S^{(1)}, I_T) + F_A(r_S^{(1)}, A_T) - a r_E^{(1)} + \frac{1}{\tau_E}\left(E - r_E^{(1)}\right)$$

$$\frac{\partial r_E^{(2)}}{\partial t} + \xi \frac{\partial j_E^{(2)}}{\partial x} + \eta \frac{\partial j_E^{(2)}}{\partial y} = F_I(r_S^{(2)}, I_T) + F_A(r_S^{(2)}, A_T) - a r_E^{(2)} + \frac{1}{\tau_E}\left(E - r_E^{(2)}\right)$$

Even and odd parities formulation II

$$\frac{\partial r_I^{(1)}}{\partial t} + \xi \frac{\partial j_I^{(1)}}{\partial x} - \eta \frac{\partial j_I^{(1)}}{\partial y} = a\sigma r_E^{(1)} - \gamma_I r_I^{(1)} + \frac{1}{\tau_I}\left(I - r_I^{(1)}\right)$$

$$\frac{\partial r_I^{(2)}}{\partial t} + \xi \frac{\partial j_S^{(2)}}{\partial x} + \eta \frac{\partial j_I^{(2)}}{\partial y} = a\sigma r_E^{(2)} - \gamma_I r_I^{(2)} + \frac{1}{\tau_I}\left(I - r_I^{(2)}\right)$$

$$\frac{\partial r_A^{(1)}}{\partial t} + \xi \frac{\partial j_A^{(1)}}{\partial x} - \eta \frac{\partial j_A^{(1)}}{\partial y} = a(1-\sigma) r_E^{(1)} - \gamma_A r_A^{(1)} + \frac{1}{\tau_A}\left(A - r_A^{(1)}\right)$$

$$\frac{\partial r_A^{(2)}}{\partial t} + \xi \frac{\partial j_A^{(2)}}{\partial x} + \eta \frac{\partial j_A^{(2)}}{\partial y} = a(1-\sigma) r_E^{(2)} - \gamma_A r_A^{(2)} + \frac{1}{\tau_A}\left(A - r_A^{(2)}\right)$$

$$\frac{\partial r_R^{(1)}}{\partial t} + \xi \frac{\partial j_R^{(1)}}{\partial x} - \eta \frac{\partial j_R^{(1)}}{\partial y} = \gamma_I r_I^{(1)} + \gamma_A r_A^{(1)} + \frac{1}{\tau_R}\left(R - r_R^{(1)}\right)$$

$$\frac{\partial r_R^{(2)}}{\partial t} + \xi \frac{\partial j_R^{(2)}}{\partial x} + \eta \frac{\partial j_R^{(2)}}{\partial y} = \gamma_I r_I^{(2)} + \gamma_A r_A^{(2)} + \frac{1}{\tau_R}\left(R - r_R^{(2)}\right)$$

In addition we have

Even and odd parities formulation III

$$\frac{\partial j_S^{(1)}}{\partial t} + \lambda_S^2 \xi \frac{\partial r_S^{(1)}}{\partial x} - \lambda_S^2 \eta \frac{\partial r_S^{(1)}}{\partial y} = -F_I(j_S^{(1)}, I_T) - F_A(j_S^{(1)}, A_T) - \frac{1}{\tau_S} j_S^{(1)}$$

$$\frac{\partial j_S^{(2)}}{\partial t} + \lambda_S^2 \xi \frac{\partial r_S^{(2)}}{\partial x} + \lambda_S^2 \eta \frac{\partial r_S^{(2)}}{\partial y} = -F_I(j_S^{(2)}, I_T) - F_A(j_S^{(1)}, A_T) - \frac{1}{\tau_S} j_S^{(2)}$$

$$\frac{\partial j_E^{(1)}}{\partial t} + \lambda_E^2 \xi \frac{\partial r_E^{(1)}}{\partial x} - \lambda_E^2 \eta \frac{\partial r_E^{(1)}}{\partial y} = \frac{\lambda_E}{\lambda_S} \left(F_I(j_S^{(1)}, I_T) + F_A(j_S^{(1)}, A_T) \right) - a j_E^{(1)} - \frac{1}{\tau_E} j_E^{(1)}$$

$$\frac{\partial j_E^{(2)}}{\partial t} + \lambda_E^2 \xi \frac{\partial r_E^{(2)}}{\partial x} + \lambda_E^2 \eta \frac{\partial r_E^{(2)}}{\partial y} = \frac{\lambda_E}{\lambda_S} \left(F_I(j_S^{(2)}, I_T) + F_A(j_S^{(2)}, A_T) \right) - a j_E^{(2)} - \frac{1}{\tau_E} j_E^{(2)}$$

$$\frac{\partial j_I^{(1)}}{\partial t} + \lambda_I^2 \xi \frac{\partial r_I^{(1)}}{\partial x} - \lambda_I^2 \eta \frac{\partial r_I^{(1)}}{\partial y} = \frac{\lambda_I}{\lambda_E} a\sigma j_E^{(1)} - \gamma_I j_I^{(1)} - \frac{1}{\tau_I} j_I^{(1)}$$

$$\frac{\partial j_I^{(2)}}{\partial t} + \lambda_I^2 \xi \frac{\partial r_I^{(2)}}{\partial x} + \lambda_I^2 \eta \frac{\partial r_I^{(2)}}{\partial y} = \frac{\lambda_I}{\lambda_E} a\sigma j_E^{(2)} - \gamma_I j_I^{(2)} - \frac{1}{\tau_I} j_I^{(2)}.$$

$$\frac{\partial j_A^{(1)}}{\partial t} + \lambda_A^2 \xi \frac{\partial r_A^{(1)}}{\partial x} - \lambda_A^2 \eta \frac{\partial r_A^{(1)}}{\partial y} = \frac{\lambda_A}{\lambda_E} a(1-\sigma) j_E^{(1)} - \gamma_A j_A^{(1)} - \frac{1}{\tau_A} j_A^{(1)}$$

$$\frac{\partial j_A^{(2)}}{\partial t} + \lambda_A^2 \xi \frac{\partial r_A^{(2)}}{\partial x} + \lambda_A^2 \eta \frac{\partial r_A^{(2)}}{\partial y} = \frac{\lambda_A}{\lambda_E} a(1-\sigma) j_E^{(2)} - \gamma_A j_A^{(2)} - \frac{1}{\tau_A} j_A^{(2)}$$

$$\frac{\partial j_R^{(1)}}{\partial t} + \lambda_R^2 \xi \frac{\partial r_R^{(1)}}{\partial x} - \lambda_R^2 \eta \frac{\partial r_R^{(1)}}{\partial y} = \frac{\lambda_R}{\lambda_I} \gamma_I j_I^{(1)} + \frac{\lambda_R}{\lambda_A} \gamma_A j_A^{(1)} - \frac{1}{\tau_R} j_R^{(1)}$$

$$\frac{\partial j_R^{(2)}}{\partial t} + \lambda_R^2 \xi \frac{\partial r_R^{(2)}}{\partial x} + \lambda_R^2 \eta \frac{\partial r_R^{(2)}}{\partial y} = \frac{\lambda_R}{\lambda_I} \gamma_I j_I^{(2)} + \frac{\lambda_R}{\lambda_A} \gamma_A j_A^{(2)} - \frac{1}{\tau_R} j_R^{(2)}.$$

Space discretization on unstructured grids

- We consider a spatial two-dimensional computational domain Ω discretized by a set of non overlapping polygons $P_i, i = 1, \dots N_p$.
- Each element P_i exhibits an arbitrary number N_{S_i} of edges e_{ji}. The boundary of the cell is given by $\partial P_i = \bigcup_{j=1}^{N_{S_i}} e_{ji}$.
- The governing equations discretized by means of a finite volume scheme

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla_x \cdot \mathbf{F}(\mathbf{Q}) = \mathbf{S}(\mathbf{Q}), \qquad (x, y) \in \Omega \subset \mathbb{R}^2, \quad t \in \mathbb{R}_0^+,$$

where $\mathbf{Q}$ is the vector of conserved variables

$$\mathbf{Q} = \left(r_i^{(1)}, \, r_i^{(2)}, j_i^{(1)}, \, j_i^{(2)} \right)^\top, \quad i = S, E, I, A, R$$

while $\mathbf{F}(\mathbf{Q})$ is the linear flux tensor and $\mathbf{S}(\mathbf{Q})$ represents the stiff source term.
- A first order in time finite volume method is obtained by

$$\mathbf{Q}_i^{n+1} = \mathbf{Q}_i^n - \frac{\Delta t}{|P_i|} \sum_{P_j \in \mathcal{N}_{S_i}} \int_{e_{ij}} \mathbf{F}_{ij}^n \cdot \mathbf{n}_{ij} \, d\mathbf{l} + \int_{P_i} \mathbf{S}_i^n \, d\mathbf{x}.$$

Space discretization on unstructured grids II

- Higher order in space is then achieved by substituting the cell averages by piecewise high order polynomials: $\mathbf{w}_i(\mathbf{x})$.
- These are obtained from the given cell averages relying on a second order Central WENO (CWENO) reconstruction procedure.
- The numerical flux function $\mathbf{F}_{ij} \cdot \mathbf{n}_{ij}$ is a simple and robust local Lax-Friedrichs flux

$$\mathbf{F}_{ij} \cdot \mathbf{n}_{ij} = \frac{1}{2}\left(\mathbf{F}(\mathbf{w}_{i,j}^{+}) + \mathbf{F}(\mathbf{w}_{i,j}^{-})\right) \cdot \mathbf{n}_{ij} - \frac{1}{2} s_{\max}\left(\mathbf{w}_{i,j}^{+} - \mathbf{w}_{i,j}^{-}\right),$$

  where $\mathbf{w}_{i,j}^{+}, \mathbf{w}_{i,j}^{-}$ are the high order boundary extrapolated data evaluated through the CWENO reconstruction procedure.
- In the diffusion limit, i.e. as $(\tau_S, \tau_I, \tau_R) \to 0$, the source term $\mathbf{S}(\mathbf{Q})$ becomes stiff, therefore in order to avoid prohibitive time steps we need to discretize the commuters system partly implicitly.
- A second order IMEX method which preserves the asymptotic limit given by the diffusion equations is proposed.

Time integration

We consider again system (1) formulated using the parities. We assume $\tau_{S,I,R} = \tau$ and rewrite it in partitioned form as

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{v})}{\partial x} + \frac{\partial \mathbf{g}(\mathbf{v})}{\partial y} = \mathbf{E}(\mathbf{u}) + \frac{1}{\tau}(\mathbf{U} - \mathbf{u})$$
$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{\Lambda}^2 \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} + \mathbf{\Lambda}^2 \frac{\partial \mathbf{g}(\mathbf{u})}{\partial y} = \mathbf{E}(\mathbf{v}) - \frac{1}{\tau}\mathbf{v},$$

where

$$\mathbf{u} = \left(r_S^{(1)}, r_S^{(2)}, r_E^{(1)}, r_E^{(2)}, r_I^{(1)}, r_I^{(2)}, r_A^{(1)}, r_A^{(2)}, r_R^{(1)}, r_R^{(2)}\right)^T,$$

$$\mathbf{v} = \left(j_S^{(1)}, j_S^{(2)}, j_E^{(1)}, j_E^{(2)}, j_I^{(1)}, j_I^{(2)}, j_A^{(1)}, j_A^{(2)}, j_R^{(1)}, j_R^{(2)}\right)^T,$$

$$\mathbf{f}(\mathbf{v}) = \xi \mathbf{v}, \quad \mathbf{g}(\mathbf{v}) = \eta \mathbf{J}\mathbf{v}, \quad \mathbf{J} = \mathrm{diag}\{-1, 1, -1, 1, -1, 1, -1, 1, -1, 1\},$$

$$\mathbf{E}(\mathbf{u}) = \Big(-F_I(r_S^{(i)}, I_T) - F_A(r_S^{(i)}, A_T), F_I(r_S^{(i)}, I_T) + F_A(r_S^{(i)}, A_T) - a r_E^{(i)}, a\sigma r_E^{(i)} - \gamma_I r_I^{(i)},$$
$$a(1-\sigma) r_E^{(i)} - \gamma_A r_A^{(i)}, \gamma_I r_I^{(i)} \gamma_A r_A^{(i)}\Big)^T, \; i = 1, 2$$

$$\mathbf{U} = (S, S, E, E, I, I, A, A, R, R)^T, \quad \mathbf{\Lambda} = \mathrm{diag}\{\lambda_S, \lambda_S, \lambda_E, \lambda_E, \lambda_I, \lambda_I, \lambda_A, \lambda_A, \lambda_R, \lambda_R\},$$

and $\mathbf{f}(\mathbf{u})$, $\mathbf{g}(\mathbf{u})$, $\mathbf{E}(\mathbf{v})$ are defined similarly.

Time integration II

The Implicit-Explict Runge-Kutta (IMEX-RK) approach applied to the partitioned system reads as

$$\mathbf{u}^{(k)} = \mathbf{u}^n - \Delta t \sum_{j=1}^{k} a_{kj} \left(\frac{\partial \mathbf{f}(\mathbf{v}^{(j)})}{\partial x} + \frac{\partial \mathbf{g}(\mathbf{v}^{(j)})}{\partial y} - \frac{1}{\tau} \left(\mathbf{U}^{(j)} - \mathbf{u}^{(j)} \right) \right) + \Delta t \sum_{j=1}^{k-1} \tilde{a}_{kj} \mathbf{E} \left(\mathbf{u}^{(j)} \right)$$

$$\mathbf{v}^{(k)} = \mathbf{v}^n - \Delta t \sum_{j=1}^{k-1} \tilde{a}_{kj} \left(\boldsymbol{\Lambda}^2 \frac{\partial \mathbf{f}(\mathbf{u}^{(j)})}{\partial x} + \boldsymbol{\Lambda}^2 \frac{\partial \mathbf{g}(\mathbf{u}^{(j)})}{\partial y} - \mathbf{E}(\mathbf{v}^{(j)}) \right) + \Delta t \sum_{j=1}^{k} a_{kj} \frac{1}{\tau} \mathbf{v}^{(j)},$$

where $\mathbf{u}^{(k)}, \mathbf{v}^{(k)}$ are the so-called internal stages. The numerical solution reads

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \Delta t \sum_{k=1}^{s} b_k \left(\frac{\partial \mathbf{f}(\mathbf{v}^{(k)})}{\partial x} + \frac{\partial \mathbf{g}(\mathbf{v}^{(k)})}{\partial y} - \frac{1}{\tau} \left(\mathbf{U}^{(k)} - \mathbf{u}^{(k)} \right) \right) + \Delta t \sum_{k=1}^{s} \tilde{b}_k \mathbf{E} \left(\mathbf{u}^{(k)} \right)$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n - \Delta t \sum_{k=1}^{s} \tilde{b}_k \left(\boldsymbol{\Lambda}^2 \frac{\partial \mathbf{f}(\mathbf{u}^{(k)})}{\partial x} + \boldsymbol{\Lambda}^2 \frac{\partial \mathbf{g}(\mathbf{u}^{(k)})}{\partial y} - \mathbf{E}(\mathbf{v}^{(k)}) \right) + \Delta t \sum_{k=1}^{s} b_k \frac{1}{\tau} \mathbf{v}^{(k)}.$$

Furthermore, we choose the Runge-Kutta scheme in such a way that the following relations hold true

$$a_{kj} = b_j, \qquad j = 1, \ldots, s, \qquad \tilde{a}_{kj} = \tilde{b}_j, \qquad j = 1, \ldots, s-1.$$

Numerical diffusion limit

Assuming for simplicity $D_{S,I,R}$ independent from space, we can write

$$\tau \mathbf{v}^{(k)} = \tau \mathbf{v}^n - \Delta t \sum_{j=1}^{k-1} \tilde{a}_{kj} \left(\tau \mathbf{\Lambda}^2 \frac{\partial \mathbf{f}(\mathbf{u}^{(j)})}{\partial x} + \tau \mathbf{\Lambda}^2 \frac{\partial \mathbf{g}(\mathbf{u}^{(j)})}{\partial y} - \tau \mathbf{E}(\mathbf{v}^{(j)}) \right) + \Delta t \sum_{j=1}^{k} a_{kj} \mathbf{v}^{(j)},$$

therefore the limit $\tau \to 0$ yields

$$\sum_{j=1}^{k} a_{kj} \mathbf{v}^{(j)} = \sum_{j=1}^{k-1} \tilde{a}_{kj} \left(2\mathbf{D} \frac{\partial \mathbf{f}(\mathbf{U}^{(j)})}{\partial x} + 2\mathbf{D} \frac{\partial \mathbf{g}(\mathbf{U}^{(j)})}{\partial y} \right),$$

where we used $\mathbf{u}^{(j)} = \mathbf{U}^{(j)}$ as $\tau \to 0$. Using now the same identity $\mathbf{u}^{(j)} = \mathbf{U}^{(j)}$ we get

$$\mathbf{U}^{(k)} = \mathbf{U}^n - \Delta t \sum_{j=1}^{k} a_{kj} \left(\frac{\partial \mathbf{f}(\mathbf{v}^{(j)})}{\partial x} + \frac{\partial \mathbf{g}(\mathbf{v}^{(j)})}{\partial y} \right) + \Delta t \sum_{j=1}^{k-1} \tilde{a}_{kj} \mathbf{E} \left(\mathbf{U}^{(j)} \right),$$

Numerical diffusion limit II

Thanks to the definitions of **f** and **g** we get

$$\mathbf{U}^{(k)} = \mathbf{U}^n - 2\Delta t \mathbf{D} \sum_{j=1}^{k-1} \tilde{a}_{kj} \left(\xi^2 \frac{\partial^2 \mathbf{U}^{(j)}}{\partial x^2} + 2\xi\eta \mathbf{J} \frac{\partial^2 \mathbf{U}^{(j)}}{\partial x \partial y} + \eta^2 \frac{\partial^2 \mathbf{U}^{(j)}}{\partial y^2} \right)$$
$$+ \Delta t \sum_{j=1}^{k-1} \tilde{a}_{kj} \mathbf{E}\left(\mathbf{U}^{(j)}\right).$$

Finally, integrating over the velocity field one has

$$S^{(k)} = S^n - \Delta t D_S \sum_{j=1}^{k-1} \tilde{a}_{kj} \left(\frac{\partial^2 S^{(j)}}{\partial x^2} + \frac{\partial^2 S^{(j)}}{\partial y^2} \right) - \Delta t \sum_{j=1}^{k-1} \tilde{a}_{kj} F_I(S^{(j)}, I_T^{(j)}) + F_A(S^{(j)}, A_T^{(j)}),$$
$$R^{(k)} = R^n - \Delta t D_R \sum_{j=1}^{k-1} \tilde{a}_{kj} \left(\frac{\partial^2 R^{(j)}}{\partial x^2} + \frac{\partial^2 R^{(j)}}{\partial y^2} \right) + \Delta t \sum_{j=1}^{k-1} \tilde{a}_{kj} \gamma_I I^{(j)} + \gamma_A A^{(j)}$$

and the same for $A^{(k)}, I^{(k)}$ and $E^{(k)}$.
Thus, the internal stages correspond to the stages of the explicit scheme applied to the reaction-diffusion system. Moreover, the last stage is equivalent to the numerical solution.

Stochastic collocation method

- We restrict to the case in which there is only one stochastic variable z in the system.
- The probability density function is supposed known. The approximate solution for the commuters $\mathbf{Q}_M(x, v, t, z)$ and the non commuters $\mathbf{Q}^u_M(x, t, z)$ are represented as truncations of the series of the orthonormal polynomials, i.e.

$$\mathbf{Q}_M(x, v, t, z) = \sum_{j=1}^{M} \hat{\mathbf{Q}}_j(x, v, t)\phi_j(z), \quad \mathbf{Q}^u_M(x, t, z) = \sum_{j=1}^{M} \hat{\mathbf{Q}}^u_j(x, t)\phi_j(z)$$

  where M is the number of terms of the truncated series and $\phi_j(z)$ are orthonormal polynomials, with respect to the measure $\rho_z(z)\,dz$.
- The expansion coefficients are obtained by

$$\hat{\mathbf{Q}}_j(x, v, t) = \int_\Gamma \mathbf{Q}(x, v, t, z)\,\phi_j(z)\,\rho_z(z)\,dz,\ \ j = 1, \dots, M.$$

$$\hat{\mathbf{Q}}^u_j(x, t) = \int_\Gamma \mathbf{Q}^u(x, t, z)\,\phi_j(z)\,\rho_z(z)\,dz,\ \ j = 1, \dots, M.$$

Stochastic collocation method II

- The exact integrals for the expansion coefficients are replaced by a suitable quadrature formula characterized by the set $\{z_n, w_n\}_{n=1}^{N_p}$, z_n the collocation point, w_n the corresponding weight, N_p the number of quadrature points

$$\hat{\mathbf{Q}}_j(x,v,t) \approx \sum_{n=1}^{N_p} \mathbf{Q}(x,v,t,z_n)\,\phi_j(z_n)\,w_n, \;\; \hat{\mathbf{Q}}_j^u(x,t) \approx \sum_{n=1}^{N_p} \mathbf{Q}^u(x,t,z_n)\,\phi_j(z_n)\,w_n,$$

  where $\mathbf{Q}(x,v,t,z_n)$ and $\mathbf{Q}^u(x,t,z_n)$ with $n = 1,\ldots,N_p$ are the solutions of the problem evaluated at the n-th collocation point.

- All quantities of interest concerning the random variable can then be computed. For example, the expectations are approximated as

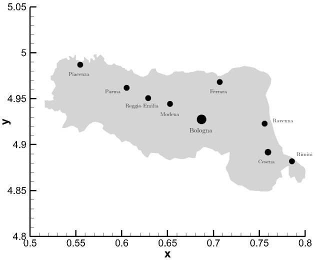
$$\mathbb{E}[\mathbf{Q}] \approx \mathbb{E}[\mathbf{Q}_M] = \int_\Gamma \mathbf{Q}_M(x,v,t,z)\,\rho_z(z)\,dz \approx \sum_{n=1}^{N_p} \mathbf{Q}(x,v,t,z_n)\,w_n,$$

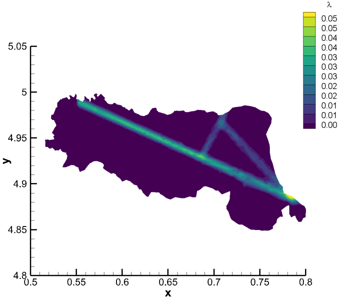
$$\mathbb{E}[\mathbf{Q}^u] \approx \mathbb{E}[\mathbf{Q}_M^u] = \int_\Gamma \mathbf{Q}_M^u(x,t,z)\,\rho_z(z)\,dz \approx \sum_{n=1}^{N_p} \mathbf{Q}^u(x,t,z_n)\,w_n.$$

Outline

Application to the spread of COVID-19 in a realistic geographical scenario

COVID-19 outbreak in Emilia-Romagna (Italy), 1-10 March 2020





From \ To	PC	PR	RE	MO	BO	FE	RA	FC	RN	$\mathcal{C}$ [%]
PC	-	4178	-	-	-	-	-	-	-	1.45
PR	1707	-	5142	-	-	-	-	-	-	1.51
RE	-	8969	-	19841	-	-	-	-	-	5.42
MO	-	-	11488	-	13034	1173	-	-	-	3.63
BO	-	-	-	6842	-	5983	3887	-	-	1.64
FE	-	-	-	2682	16865	-	2610	-	-	6.80
RA	-	-	-	-	9808	1016	-	9211	-	5.14
FC	-	-	-	-		-	6646	-	6944	3.41
RN	-	-	-	-		-	-	6075	-	1.79

Population

Initial distribution of a generic population $f(x, y)$ assigned to each main city c

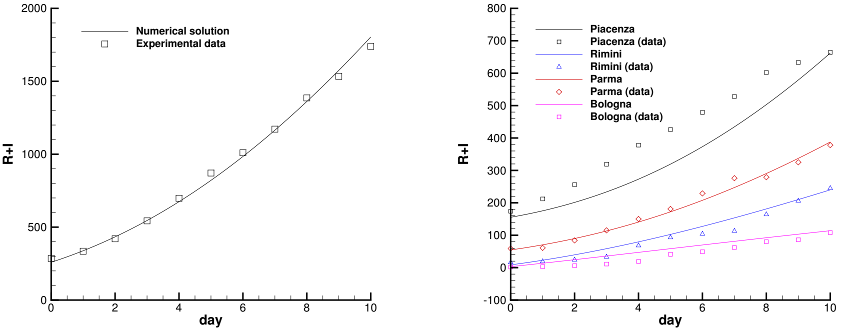
$$f(x,y) = \frac{1}{2\pi r_c} e^{-\frac{(x-x_c)^2+(y-y_c)^2}{2r_c^2}} f_c$$

where r_c is the radius of the urban area.

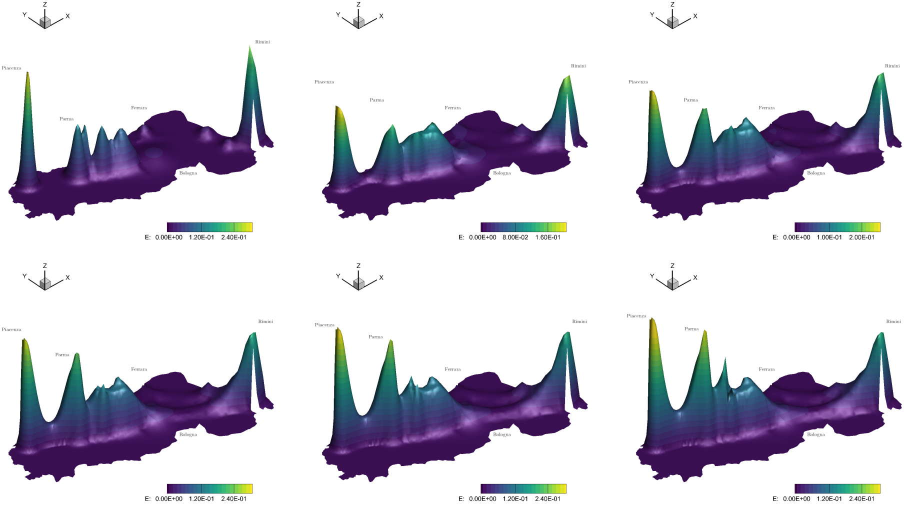
Model calibration

Using the connection matrix and the road distances for the traveling speed λ_i, $i \in \{S, E, I, R\}$

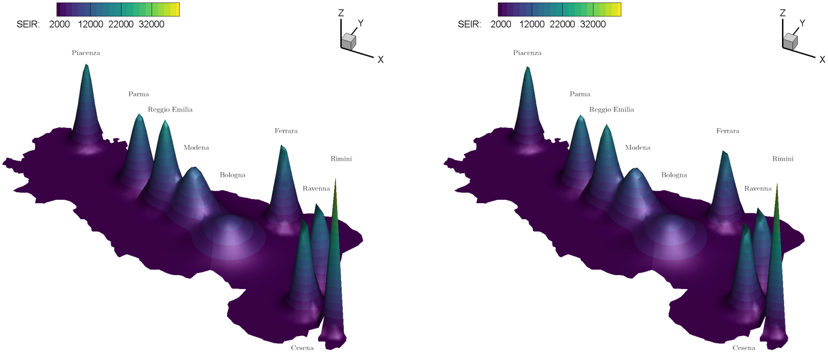
Using the corresponding SEIR ODE model for the epidemic parameters



Time evolution of total infected and recovered population $(R + I)$ **compared against experimental data** for the region Emilia-Romagna. Right: time evolution of total infected and recovered population $(R + I)$ compared against experimental data.



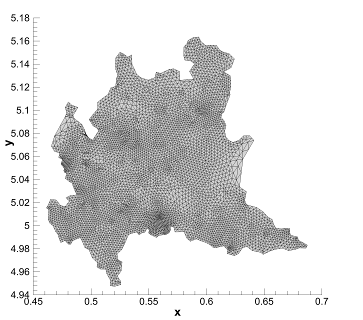
Distribution of exposed population E including asymptomatic at times $t = 0$, $t = 2$, $t = 4$ (top), $t = 6$, $t = 8$ and $t = 10$ (bottom).



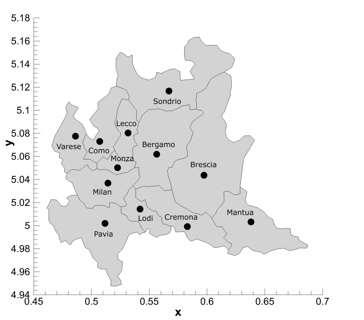
Distribution of total population $(S+S_u)+(E+E_u)+(I+I_u)+(R+R_u)$ at initial time $t=0$ (left) and at the final time $t=10$ (right). The model bring back at regular intervals from day to day the situation to the initial condition in which all commuters and non-commuters are located in the main urban areas.

The Lombardy network

From/To	LO	MI	BG	BS	CR	Total commuters
LO	–	56717 (80.53%)	–	–	13712 (19.47%)	70429 (30.97%)
MI	55397 (31.14%)	–	74168 (41.69%)	26709 (15.01%)	21622 (12.15%)	177896 (5.45%)
BG	–	76337 (45.79%)	–	78348 (47.00%)	12016 (7.21%)	166701 (15.04%)
BS	–	26594 (23.24%)	70879 (61.93%)	–	16967 (14.83%)	114440 (9.12%)
CR	13264 (20.06%)	23142 (35.00%)	12025 (18.19%)	17681 (26.75%)	–	66112 (18.58%)

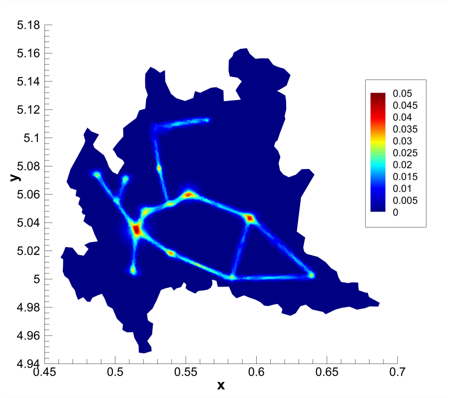


mesh grid

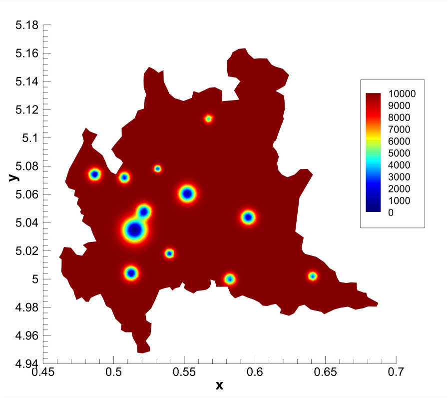


provinces

The Lombardy network II

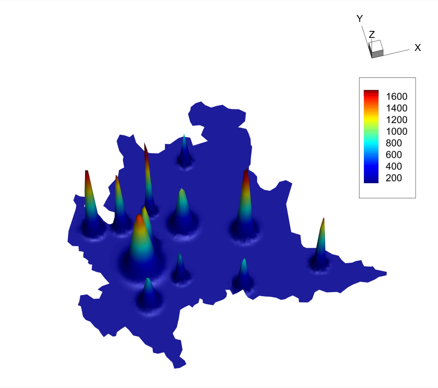


$\lambda_i,\ i \in \{S, E, A, R\}$

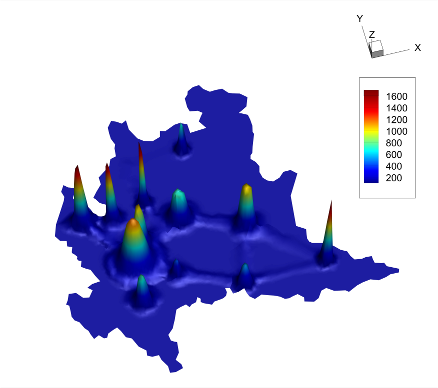


$\tau_i,\ i \in \{S, E, I, A, R\}$

Figure: Left initial condition imposed for characteristic speeds λ. Right relaxation times τ.



$\mathrm{Exp}[S_{T,0}(x,y)]$



$\mathrm{Exp}[S_T(x,y)]$

Figure: Numerical results of the simulation of the first outbreak of COVID-19 in Lombardy, Italy. Left expectation of the susceptible population S_T on the initial day simulated (February 27, 2020) and right at the end of the simulation (March 22, 2020).

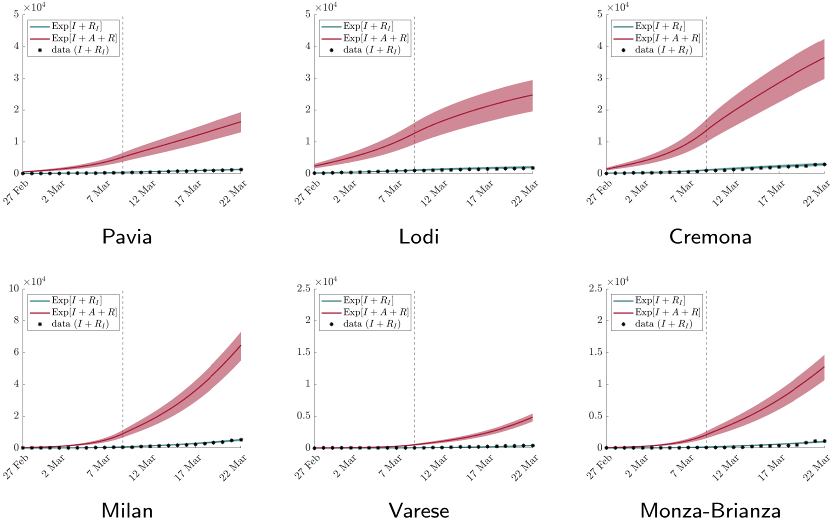


Figure: Numerical results, with 95% confidence intervals, of the simulation of the first outbreak of COVID-19 in Lombardy, Italy. Data are taken from the COVID-19 repository of the Civil Protection Department of Italy. Vertical dashed lines identify the onset of governmental lockdown restrictions.

Research perspectives

Conclusions

- Multiscale kinetic models for the description of the spread of an epidemic disease in a spatially heterogeneous context
- Introduction of commuters and non-commuters population.
- Application to a real epidemic spread (COVID-19 outbreak in Emilia-Romagna and Lombardy).
- Second order asymptotic preserving time discretization and finite volume spatial discretization made of unstructured meshes of arbitrary shape.

Outlook

- Multidimensional uncertainty quantification.
- Data fitting for extrapolation of the model parameter and construction of data driven models.
- Incorporation of an age-structured population.
- Control.

The material for this part is mostly based on the recent survey: "Kinetic modelling of epidemic dynamics: social contacts, control with uncertain data, and multiscale spatial dynamics." G. Albi, G. Bertaglia, W. Boscheri, G.D., L. Pareschi, G. Toscani, M. Zanella. Predicting Pandemics in a Globally Connected World, Vol. 1, Birkhauser-Springer Series: Modeling and Simulation in Science, Engineering and Technology, 2022.