# Large-Time Behavior of Averaged Kinetic Models on Networks

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# LARGE–TIME BEHAVIOR OF AVERAGED KINETIC MODELS ON NETWORKS

MICHAEL HERTY AND CHRISTIAN RINGHOFER

Abstract. We are interested in flows on general networks and derive a kinetic equation describing general production, social or transportation networks. Corresponding macroscopic transport equations for large time and homogenized behavior are obtained and studied numerically. This work continues a recent discussion [20] and provides additionally explicit equilibrium solutions, second–order macroscopic approximations as well as numerical simulations on a large-scale homogenized network.
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## 1. Introduction

This paper is concerned with models for agent flows on general networks. The investigation of flows on networks is motivated by production, social or traffic flow networks where on a given graph dynamics on arcs and at vertices are prescribed. Flows on structured media have been studied widely in the literature and we refer to the review article [4] and to the textbooks on traffic flow [14, 28] and production processes [2], respectively. They have also been studied in the context of structured media in the work [10] and [13].

Normally, very little attention is paid to the detailed description of the stochastic effects on the underlying dynamics on arcs and the modeling of suitable conditions at the vertices in averaged large time scale models. In the case of large–scale networks stochastic agent based models involve a tremendous computational effort.

Possible applications are production networks. Here, a good is flowing from a raw material supplier through a certain number of layers (nodes in the networks) of intermediate producers to a final consumer. Due to possible machine breakdowns and service distributions travel and waiting times of goods maybe described using probability distributions. Production networks of this type have been introduced originally in [6, 11], and optimized in [15, 16].

Another application might be air traffic where we consider passengers arriving and leaving airports. The links are the possible flight routes and waiting times reflect delays at airports due to for example stochastic weather conditions.

A description of effects of possible network structures in application examples for traffic and social networks has been studied in [7]. Therein, the so–called small world

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network structure is discussed. Those networks are constructed by a process described in [5] and the mean connection between nodes grows at most logarithmic with the number of nodes [30].

Within this paper we want to explore the connection between a simple dynamics with possible applications in production and air traffic and the structure of the network more closely. To this end we consider a general mathematical model for transport on graphs described as a multi–agent model. We apply asymptotic techniques (borrowed from classical kinetic theory) to derive a simplified model for flows on large networks on large time scales. This reduces the computational complexity of the study of long time phenomena in such flows. We develop a kinetic model for flows on arbitrary graphs, originally proposed in [20], under some simplifying assumptions, which make the large time scale model practically applicable. The macroscopic model consists of a convection - diffusion equation for the agent density, posed on a continuum in space, representing the graph of the network. In order for this model to be 'reasonably smooth', i.e not to involve measure valued transport coefficients, it is necessary to locate the nodes of the graph in a certain way, i.e. to 'draw the graph in $\mathbb{R}^2$' in a special way. Reorganizing the network this way results in the solution of an optimization problem for the coordinates of the network nodes. This represents the generalization of an idea, originally proposed in [7] to higher dimensions. The final macroscopic model is a convection - diffusion equation for the agent density on the reorganized graph. It allows for the computationally efficient simulation of large time phenomena on arbitrarily complex networks. The computations leading to the mean–field equation for the macroscopic variables are purely formal. In order to proceed we always assume the solution to be as smooth as necessary to allow for the manipulations in the computations. The best functional analytic setting for the presented problem is still open and left for future investigations.

This paper is organized as follows: In Section 2 we define the stochastic agent based model and derive the kinetic equation for the probability distribution of the agent density. In Section 3 we derive long time averaged equations for the agent density. In order for the transport coefficients for these equations to be as smooth as possible, we choose the node coordinates ('draw the graph') optimally in Section 4. Some of the technically more involved proofs are given in the Appendix in Section 6.

## 2. The multi–agent and the kinetic model

We start by formulating a multi–agent model for the transport picture on an arbitrary network, where agents travel on randomly chosen arcs of a graph. Travel on each arc takes a randomly chosen time, and the agents spend a random time at each node, waiting to continue their journey. The final result of this section is the formal theorem 2.1 which gives a kinetic equation for the probability distribution of the agents, suitable for large time averaging and homogenization in Sections 3 and 4. All the computations are formal in the sense that we assume the regularity required to proceed with the computations.

In order to derive the kinetic model, it is necessary to reformulate the multi agent model below as a Monte Carlo algorithm in Section 2.2.

### 2.1. **The multi–agent model.**

The general multi–agent model we consider is similar to [20] and of the following form:

- We consider an oriented graph $\mathcal{G}$ with $n = 1, \dots, N$ nodes. The weighted $N \times N$ adjacency matrix of the graph $\mathcal{G}$ is $A$. $A$ is a Markov matrix $\sum_{m=1}^{N} A_{mn} = 1$ for all $n$.
- Each node $n \in \{1, \dots, N\}$ is assigned a coordinate $x = Z_n \in \mathbb{R}^2$. Given the coordinates $Z_n$, we introduce as $e_{mn} = Z_m - Z_n$ the edge vectors between two nodes. The length of arc $e_{mn}$ is $\|e_{mn}\|_2$.
- Agents move in $\mathbb{R}^2$ between the nodes along the arcs. Each agent has as state variables the flight time $\tau$ in between nodes and the index $m$ of the target node.

The dynamics are described by the following mechanism.

- The agent arrives at time $t$ at position $x = Z_n$
- The agent chooses a waiting time $w$ at the node $x = Z_n$ according to a given probability density $W$
$$dP[w = s] = W(s, n)ds$$
where $\int W(s, n)ds = 1$ for all $m$. We assume the waiting time $w$ to be always non–negative and enforce this by assuming that $W(s, n) = 0$ for $s \leq 0$ holds.
- The agent decides on the next node $Z_m$ to visit. The decision is random with probability according to the weighted adjacency matrix $A$.
$$P[m = k] = A_{kn} \ .$$
- At time $t + w$ the agent leaves node $n$ traveling to node $m$. The flight time $\tau$ to this node is described by a random variable distributed with probability density function $T$
$$dP[\tau = s] = T(s, m, n) \ ds$$
where $\int T(s, m, n)ds = 1$ for all $m, n$, and where $T(s, m, n) = 0$ for $s < 0$. Since we do not model where the agent is located on the arc $(n \to m)$ at any particular time, we might as well decide on a linear motion with constant velocity during the time of the flight. For the continuum model in Section 2.3 below this velocity has to be included in the state space. So, we set the flight velocity $v$ to
$$v = \frac{e_{m,n}}{\tau} \ .$$
- At time $t + w + \tau$ the agent arrives at node $m$ (with position $x = Z_m$) and the process is repeated.

We assume the graph of the network is given which introduces already the arcs and the nodes as well as the connectivity via the matrix $A$. The independent state variables of an agent are its flight time $\tau$, its position $x$ and its target node $m$. The flight velocity $v$ is introduced as additional variable for the state space for convenience but is not an independent variable. It is defined by the arc $e_{m,n}$ and the flight time $\tau$. The flight time $\tau$ is supposed to be non–negative. However, we treat the variable as belonging to the real–line and set the probability $T(s, m, n) = 0$ for $s \leq 0$.

**Remark 1.** The above model presents a slight simplification over the previous model, presented in [20], in the following sense. The probability of the next target node $m$ does, other than in [20], *not* depend on the node $n$ the agent came from. This simplification will allow us to explicitly compute transport coefficients in the macroscopic models in

Section 3. It is motivated by applications to large air traffic networks, where available data consist usually of flow rates. There, usually the only data available is how many agents travel from point $A$ to point $B$ per week. In [20] the corresponding data required would be on how many agents coming from point $A$ , arriving at point $B$ and leaving for point $C$ would be required. In this sense $A_{mn}$ is independent of the origin of the agent, it only depends on its current position $n$ and the target node $m$. Similarly, the waiting time $W$ in this model does not dependent on the target airport or the airport of origin of the agent, but only on the airport the agent is waiting at. This would cover for example delays common to all travelers at a given airport. Obviously, the model may be refined to take into account delays at destination airports leading to $W = W(s, n, m)$.

The restriction $x \in \mathbb{R}^2$ is not necessary. We may study the problem also in $\mathbb{R}^d$. However, for the numerical simulations and the homogenization the number of vertices per volume should be sufficiently large.

2.2. **A Monte Carlo algorithm.** In the next section we will formulate a kinetic equation for the probability density that the agent is at certain point in space $x$ at a given time $t$. To do so, we first reformulate the recipe in Section 2.1 as a Monte Carlo (MC) algorithm. This gives rise to a minor complication, since neither of the probability densities $W$ and $T$ can be assumed to be exponential, and MC algorithms are usually formulated for Markov processes, i.e. for exponential distributions of the time between events. In general a MC algorithm is governed by a event frequency $\omega$. So, to change a state $q$ of a system, we 'toss a coin' at each infinitesimal time step $\Delta t$ and evolve the state $q$ according to

$$q(t + \Delta t) = (1 - \xi)q(t) + \xi p(q(t)),\ \xi \in \{0, 1\},\ P[\xi = 1] = \Delta t\omega(q(t)) \ . \tag{1}$$

So, with probability $\Delta t\omega(q)$ ('heads') we choose a new state $p(q)$ and with probability $1 - \Delta t\omega(q)$ ('tails') we keep the old state. Taking the limit $\Delta t \to 0$ and some straight forward calculations give that the time $a(q)$ to the next change of state is distributed according to the exponential distribution

$$dP[a(q) = t] = \omega(q)e^{-t\omega(q)}\ dt \ .$$

So, a Markov process of the form (1) leads to an exponential distribution of the times $a$ between changes of state. To include non - Markov processes into the model, we have to include memory in the form of adding the time elapsed since the last change of state to the state variable, i.e. we imbed a non-Markov process into a Markov process of higher dimension. Defining the time elapsed since the last change of state as $\eta$, we reformulate the above process by making the frequency $\omega$ dependent on the elapsed time $\eta$:

$$q(t+\Delta t) = (1-\xi)q(t)+\xi p(q(t)),\ \eta(t+\Delta t) = (1-\xi)(\eta(t)+\Delta t),\ P[\xi = 1] = \Delta t\omega(\eta(t), q(t)). \tag{2}$$

So, the elapsed time $\eta$ is advanced by $\Delta t$ as long as $\xi = 0$ holds, and reset to $\eta = 0$ as soon as the state $q$ changes if $\xi = 1$ holds. This gives the discrete probability $P[\eta = n\Delta t]$ as

$$\begin{aligned} P[\eta = n\Delta t] &= \Delta t\omega(n\Delta t, q)[1 - \Delta t\omega(0, q)][1 - \Delta t\omega(\Delta t, q)]...[1 - \Delta t\omega((n - 1)\Delta t, q)] \\ &\approx \Delta t\omega(n\Delta t, q) \exp[-\int_0^{n\Delta t} \omega(s, q)\ ds] \end{aligned}$$

and, in an obvious limit $n \to \infty,\ \Delta t \to 0,\ n\Delta t = t$, the continuous version $dP[\eta = t] = \omega(t,q)\exp[-\int_0^t \omega(s,q)\ ds]\ dt$. To match the above to a given distribution of scattering times $W(t,q)\ dt$ between changes of state, we choose the scattering frequency $\omega(t,q)$ in (2) such that $\omega(t,q)\exp[-\int_0^t \omega(s,q)\ ds] = W(t,q)$ holds. This relation can be inverted to express $\omega(t,q)$ as

$$\omega(t,q) = \frac{W(t,q)}{\int_t^\infty W(s,q)\ ds}\ . \tag{3}$$

We note that, if $W(t,q)$ is an exponential distribution, i.e. if $W(t,q) = \alpha(q)e^{-t\alpha(q)}$ holds, formula (3) reduces to $\omega(t,q) = \alpha(q)$. So, in this case $\omega(\eta,q)$ in the Monte Carlo algorithm (2) is independent of $\eta$, and , consequently, so is the evolution of the state q. Therefore, the algorithm (2) represents a generalization of a classical Monte Carlo procedure to non - Markov processes with arbitrarily distributed scattering times. This 'imbedding trick' is, to our knowledge, due to E. Larsen and coworkers [22],[25] and has also been applied in [20].

We now reformulate the multi–agent model in Section 2.1 for a continuous spatial variable $x$ and a discrete time step $\Delta t$. All variables

- If $\eta(t) < \tau$, then the agent is in free flight on the arc $n \to m$. In this case we advance the position $x$ and the elapsed time $\eta$ and leave the rest of the state unchanged:

$$x(t+\Delta t) = x(t) + \Delta t v,\ \eta(t+\Delta t) = \eta(t) + \Delta t\ . \tag{4}$$

  The velocity vector $v$ is then given by the current edge vector divided by the free flight time: $v = \frac{e_{mn}}{\tau}$.
- If $\eta(t) \geq \tau$, then the agent is waiting at the node at $x = Z_m$. In this case we leave $x$ unchanged and start to update the other variables with the frequency $\omega$ as defined in equation (3).

$$(a)\ x(t+\Delta t) = x(t),\ \eta(t+\Delta t) = (\eta(t)+\Delta t)(1-\xi) \tag{5}$$

$$(b)\ m(t+\Delta t) = m(t)(1-\xi)+\xi m',\ n(t+\Delta t) = n(t)(1-\xi)+\xi m(t),\ \tau(t+\Delta t) = \tau(t)(1-\xi)+\xi\tau'$$

with the frequency $\omega$ and the 'heads or tails variable' $\xi$ chosen, according to (2), as

$$P[\xi = 1] = \Delta t\omega(\eta-\tau, m),\ P[\xi = 0] = 1 - \Delta t\omega(\eta-\tau, m), \tag{6}$$

$$\omega(\eta, n) = \frac{W(\eta, n)}{\int_\eta^\infty W(s, n)\ ds}$$

and the new state values chosen randomly from to the probability distributions

$$P[m' = k] = A_{km},\ dP[\tau' = s] = T(s, m', m)\ ds,\ v = \frac{e_{m'm}}{\tau'} \tag{7}$$

Note, that we have retarded the argument $\eta$ for the frequency $\omega$ in (6) by the value $\tau$, due to the fact that, arriving from the free flight phase, we already start the waiting process with $\eta = \tau$. The above algorithm is equivalent to the one in Section 2.1 and a simplification of the algorithm stated in [20]. We rewrite the algorithm combining both phases. Note, that the distribution $W(t, n)$ vanishes for $t < 0$ (i.e. the waiting times are always nonnegative). Therefore also the frequency $\omega(\eta, n)$ vanishes for $\eta < 0$.

$$(a)\ x(t+\Delta t) = x(t) + \Delta t H(\tau-\eta)v,\ \eta(t+\Delta t) = (\eta(t)+\Delta t)(1-\xi), \tag{8}$$

$$(b)\ m(t+\Delta t) = m(t)(1-\xi)+\xi m',\ n(t+\Delta t) = n(t)(1-\xi)+\xi m(t),\ \tau(t+\Delta t) = \tau(t)(1-\xi)+\xi\tau'$$

$$(c)\ P[\xi = 1] = \Delta t\omega(\eta-\tau, m),\ P[\xi = 0] = 1-\Delta t\omega(\eta-\tau, m),\ \omega(\eta, m) = \frac{W(\eta, m)}{\int_\eta^\infty W(s, m)\ ds},$$

$$(d)\ P[m' = k] = A_{km},\ dP[\tau' = s] = T(s, m', m)\ ds,\ v(t+\Delta t) = v(t)(1-\xi) + \xi\frac{e_{m'm}}{\tau'}$$

So, for $\eta < \tau$ we have $\omega = 0$ and $\xi = 0$ with probability one, and we recover phase 1 from above, whereas for $\eta > \tau$ we have $x(t+\Delta t) = x(t)$ and we recover phase 2.

In order to define the process for continuous spatial variables we define interpolants. We note that the probability distributions $A, T$ and $W$ in (7) and (8) are only used for $\eta > \tau$, when the position $x$ equals $Z_m$. To reduce the dimension of the state variable

space we define the interpolants $\mathbf{A}(k,x), \mathbf{T}(t,m',x), \mathbf{W}(t,x), \mathbf{e}(m',x)$ for $x \in \mathbb{R}^2$ and such that

$$\mathbf{A}(k,Z_m) = A_{km},\ \mathbf{T}(t,m',Z_m) = T(t,m',m),\ \mathbf{W}(t,Z_n) = W(t,x),\ \mathbf{e}(m',Z_m) = e_{m'm}$$

With these definitions (8) reads

$$(9) \qquad (a)\ x(t+\Delta t) = x(t) + \Delta t H(\tau-\eta)v,\ \eta(t+\Delta t) = (\eta(t)+\Delta t)(1-\xi),$$

$$(b)\ m(t+\Delta t) = m(t)(1-\xi)+\xi m',\ n(t+\Delta t) = n(t)(1-\xi)+\xi m(t),\ \tau(t+\Delta t) = \tau(t)(1-\xi)+\xi\tau'$$

$$(c)\ P[\xi=1] = \Delta t\omega(\eta-\tau,x),\ P[\xi=0] = 1-\Delta t\omega(\eta-\tau,x),\ \omega(\eta,x) = \frac{\mathbf{W}(\eta,x)}{\int_\eta^\infty \mathbf{W}(s,x)\ ds}$$

$$(d)\ P[m'=k] = \mathbf{A}(k,x),\ dP[\tau'=s] = \mathbf{T}(s,m',x)\ ds,\ v(t+\Delta t) = v(t)(1-\xi)+\xi\ \frac{\mathbf{e}(m',x)}{\tau'}$$

2.3. **The kinetic equation for the probability density.** In this section we derive an equation for the probability density $f(x,v,\eta,\tau,m,t)\ dxdvd\eta d\tau$. Note, that the probability density is independent of the state $n$ since the dynamics is independent of this state.

In order to simplify the notation, we will denote with $q = (q_1,q_2,q_3,q_4)$ the microscopic variables of the state

$$q = (\tau, m, v, \eta).$$

Here $v$ is in $\mathbb{R}^2$ and $\eta,\tau$ are in $\mathbb{R}$, whereas the index $m = 1:N$ is discrete. Note that due to the assumption on $T$ we have that there is zero probability for $\tau < 0$. Similarly, by definition of the dynamics of $\eta$ we have $\eta \geq 0$. Therefore, provided the initial data for $\eta,\tau$ is non–negative the values for $\eta,\tau$ will always be non–negative even so $\eta,\tau \in \mathbb{R}$.

With a slight abuse of notation we will write $\int f(x,q,t)\ dq$ for $\sum_{m=1}^N \int f(x,v,\eta,\tau,m,t)\ dvd\eta d\tau$ in the following. We have

**Theorem 2.1** (Formal)**.** *Let $f(x,q,t)\ dxq$ be the probability density that the agent occupies the state $(x,q) = (x,v,\eta,\tau,m)$ at time $t$. The density $f$ satisfies the equation*

$$(10)$$

$$\partial_t f(x,q,t) + H(\tau-\eta)v\cdot\nabla_x f + \partial_\eta f + \omega(\eta-\tau,x)f - \Gamma(x,q)\int \omega(\eta'-\tau',x)f(x,q',t)\ dq' = 0$$

*with the probability density $\Gamma(x,q)\ dq$ given by*

$$\Gamma(x,v,\eta,\tau,m) = \delta(\frac{\mathbf{e}(m,x)}{\tau} - v)\delta(\eta)\mathbf{T}(\tau,m,x)\mathbf{A}(m,x)$$

**Formal computation leading to Theorem 2.1.** According to the algorithm (9) in Section 2.2, we have for the transition probability $\mathcal{P}(x',q',x,q)$ that the state $x,q$ changes to the state $x',q'$

$$\mathcal{P}(x',q',x,q) =$$

$$\Delta t\omega(\eta-\tau,x)\delta(x+\Delta t H(\tau-\eta)v - x')\delta(\frac{\mathbf{e}(m',x)}{\tau'} - v')\delta(\eta')\mathbf{T}(\tau',m',x)\mathbf{A}(m',x)$$

$$+[1-\Delta t\omega(\eta-\tau,x)]\delta(x+\Delta t H(\tau-\eta)v - x')\delta(v-v')\delta(\eta+\Delta t-\eta')\delta(\tau-\tau')\delta(m-m')\ ,$$

where the first term denotes the case $\xi = 1$ (with probability $\Delta t\omega$ and the second term denotes the case $\xi = 0$ (with probability $1 - \Delta t\omega$) and $q = (v, \eta, \tau, m)$ and $q = (v', \eta', \tau', m')$ holds. Therefore the evolution of $f$ in a time step $\Delta t$ is given by

$$f(x', q', t + \Delta t) = \int \mathcal{P}(x', q', x, q) f(x, q, t)\ dxdq$$

Integrating against a smooth compactly supported test function $\psi(x', q')$ gives

$$\int \psi(x', q') f(x', q', t+\Delta t)\ dx'dq' = \sum_{m'} \int \psi(x', v', \eta', \tau', m') \mathcal{P}(x', q', x, q) f(x, q, t)\ dxdqdx'dv'd\eta'd\tau'$$

$$= \sum_{m'} \int \Delta t\omega(\eta - \tau, x)\psi(x + \Delta t H(\tau - \eta)v, \frac{\mathbf{e}(m', x)}{\tau'}, 0, \tau', m')\mathbf{T}(\tau', m', x)\mathbf{A}(m', x) f(x, q, t)\ dxdqd\tau'$$

$$+ \int [1 - \Delta t\omega(\eta - \tau, x)]\psi(x + \Delta t H(\tau - \eta)v, v, \eta + \Delta t, \tau, m) f(x, q, t)\ dxdq$$

Expanding this in $\Delta t$ and neglecting second order terms gives

$$\int \psi(x', q') f(x', q', t)\ dx'q' + \Delta t \int \psi(x', q')\partial_t f(x', q', t)\ dx'dq'$$

$$= \sum_{m'} \int \Delta t\omega(\eta - \tau, x)\psi(x, \frac{\mathbf{e}(m', x)}{\tau'}, 0, \tau', m')\mathbf{T}(\tau', m', x)\mathbf{A}(m', x) f(x, q, t)\ dxdqd\tau'$$

$$+ \int \psi(x, q) f(x, q, t)\ dxdq + \int \Delta t H(\tau - \eta) v \cdot \nabla_x \psi(x, q) f(x, q, t)\ dxdq + \int \Delta t \partial_\eta \psi(x, q) f(x, q, t)\ dxdq$$

$$- \int \Delta t\omega(\eta - \tau, x)\psi(x, q) f(x, q, t)\ dxdq + O(\Delta t^2)$$

Interchanging the primed and unprimed variables, dividing by $\Delta t$ and $\Delta t \to 0$ gives the relation

$$\int \psi(x, q)\partial_t f(x, q, t)\ dxdq =$$

$$\sum_{mm'} \int \omega(\eta' - \tau', x)\psi(x, \frac{\mathbf{e}(m, x)}{\tau}, 0, \tau, m)\mathbf{T}(\tau, m, x)\mathbf{A}(m, x) f(x, v', \eta', \tau', m', t)\ dxdv'd\eta'd\tau d\tau'$$

$$+ \int H(\tau - \eta) v \cdot \nabla_x \psi(x, q) f(x, q, t)\ dxdq + \int \partial_\eta \psi(x, q) f(x, q, t)\ dxdq$$

$$- \int \omega(\eta - \tau, x)\psi(x, q) f(x, q, t)\ dxdq$$

for all test functions $\psi$. This represents the weak formulation of (10).

∎

## 3. Large time asymptotic

After re - scaling and formulating the dimensionless version of the kinetic equation from Section 2.3 in Section 3.1, we derive a convection - diffusion equation for the macroscopic agent density $\rho(x,t) = \int f(x,q,t)\ dq$, in the limit for large times and large networks where the state $q = (v,\eta,\tau,m)$ . To do so, we employ a well known methodology, the so called Chapman - Enskog expansion (see c.f. [9]). We summarize the general idea of this procedure, adapted to our problem, in Section 3.2. To make the result practically applicable, it is necessary to compute the transport coefficients, i.e. the convection velocity and the diffusion matrix, from the microscopic model parameters in Section 2. Not surprisingly, this turns out to be quite elaborate, and is done in Section 3.3, with the final result of this section being Theorem 3.4.

3.1. **Scaling and dimensionless formulation.** We now consider the solution of the transport equation (10) for large time and spatial scales. That is we consider a large graph ($N >> 1$) over long periods of time. We assume that the nodes $Z_n,\ n = 1:N$ are located in a domain $\Omega \subset \mathbb{R}^2$ and choose units such that the area of $\Omega$ equals unity, i.e. we set $x = Lx_s$ with $L^2 = \int_\Omega 1\ dx$. We scale the probability distributions $\mathbf{T}$ and $\mathbf{W}$ such that their mean is $O(1)$ in scaled variables, setting $\mathbf{T}(\tau,m,x) = \frac{1}{\tau_0}\mathbf{T}_s(\frac{\tau}{\tau_0},m,x_s)$ and $\mathbf{W}(\eta,x) = \frac{1}{\tau_0}\mathbf{W}_s(\frac{\eta}{\tau_0},x_s)$. We scale the state variables $\eta$ and $\tau$ by $\eta = \tau_0\eta_s$ and $\tau = \tau_0\tau_s$. Correspondingly, we have to scale the scattering frequency $\omega$ as $\omega(\eta,x) = \frac{1}{\tau_0}\omega_s(\eta_s,x_s) = \frac{\mathbf{W}_s(\eta_s,x_s)}{\tau_0\int_{\eta_s}^\infty \mathbf{W}_s(t,x_s)\ dt}$. Finally we choose a time scale $t_0$ and scale $t = t_0 t_s$ and $v = \frac{L}{t_0}v_s$. This gives for the scaled probability density $f_s(x_s,v_s,\eta_s,\tau_s,m) = \frac{L\tau_0^2}{t_0}f(x,v,\eta,\tau,m)$ in (10)

$$\partial_{t_s} f_s(x_s,q_s,t_s) + \nabla_{x_s}\cdot\big(H(\tau_s-\eta_s)v_s f_s\big) + \frac{t_0}{\tau_0}\partial_{\eta_s} f_s \tag{11}$$

$$+\frac{t_0}{\tau_0}\omega_s(\eta_s-\tau_s,x_s)f_s - \frac{t_0}{\tau_0}\Gamma_s(x_s,q_s)\int \omega_s(\eta_s'-\tau_s',x_s)f_s(x_s,q_s',t_s)\ dq_s' = 0$$

with the scaled probability density $\Gamma_s(x_s,q_s)\ dq_s$ given by

$$\Gamma_s(x_s,v_s,\eta_s,\tau_s,m) = \delta(\frac{\mathbf{e}_s(m,x_s)}{\tau_s} - v_s)\delta(\eta_s)\mathbf{T}_s(\tau_s,m,x_s)\mathbf{A}(m,x_s),\ \mathbf{e}_s(m,x_s) = \frac{\mathbf{e}(m,x)t_0}{\tau_0 L}$$

We next want to study scenarios where the average flight time $\tau_0$ is small compared with the characteristic time $t_0$ and the network size $L$ is large compared with the average flight time. Therefore, we introduce the small dimensionless parameter $\varepsilon = \frac{\mathbf{e}(m,x)}{L} << 1$ since $L$ is supposedly large. Assume also that the typical time–scale as $t_0 = \frac{\tau_0}{\epsilon}$. Then, $\frac{L\tau_0}{t_0} = O(1)$ and $\mathbf{e}_s(m,x_s) = O(1)$.

Introducing the small dimensionless parameter $\varepsilon$ (and dropping the subscript $s$ from here on) we write (11) as

$$\partial_t f(x,q,t) + \nabla_x\cdot\big(H(\tau-\eta)vf\big) + \frac{1}{\varepsilon}\mathcal{C}[f] = 0 \tag{12}$$

with the collision operator $\mathcal{C}$ and the probability density $\Gamma$ given by

$$(a)\ \mathcal{C}[f] = \partial_\eta f + \omega(\eta-\tau,x)f - \Gamma(x,q)\int \omega(\eta'-\tau',x)f(x,q',t)\ dq', \tag{13}$$

$$(b)\ \Gamma(x,v,\eta,\tau,m) = \delta(\frac{\mathbf{e}(m,x)}{\tau} - v)\delta(\eta)\mathbf{T}(\tau,m,x)\mathbf{A}(m,x),$$

3.2. **Formal asymptotic.** In zero order the solution of equation (12) obviously has to satisfy $\mathcal{C}[f] = 0$. On the other hand, the operator $\mathcal{C}$ has unity as an integral invariant. In other words, $\int \mathcal{C}[f]\ dq = 0,\ \forall f$ holds. Noting that the operator $\mathcal{C}$ does not act on the $x,\ t$ variables, is dependent on $x$, but independent of the time $t$, we first consider the equilibrium problem

$$\mathcal{C}[G](x,q) = 0,\ \int G(x,q)\ dq = 1\ \forall x. \tag{14}$$

$G(x,q)$ is sometimes referred to as the Gibbs measure of the collision operator $\mathcal{C}$. Assuming that the problem (14) has a unique solution, a solution of $\mathcal{C}[f] = 0$ will therefore be of the form $f(x,q,t) = \rho(x,t)G(x,q)$ for an arbitrary density function $\rho(x,t)$ with $\int f(x,q,t)\ dq = \rho(x,t)$. This leads to the definition of the projection operator

$$\mathbf{\Pi}[f](x,q,t) = G(x,q)\int f(x,q',t)\ dq' = G(x,q)\rho(x,t)$$

$\mathbf{\Pi}$ is a projection operator, $\mathbf{\Pi}^2 = \mathbf{\Pi}$ holds, and conserves the integral $dq$, $\int \mathbf{\Pi}[f]\ dq = \int f\ dq,\ \forall f$ holds. Since the Gibbs measure is the solution of (14), and $\int \mathcal{C}[f]\ dq = 0,\ \forall f$ holds, $\mathbf{\Pi}$ and $\mathcal{C}$ satisfy the left and right annihilation properties $\mathbf{\Pi}\circ\mathcal{C} = \mathcal{C}\circ\mathbf{\Pi} = 0$.

We split the solution of the transport equation (12) into

$$f = f_0 - \varepsilon f_1,\ f_0 = \mathbf{\Pi}[f],\ \varepsilon f_1 = \mathbf{\Pi}[f] - f\ ,$$

where we have already re - scaled the component $-\varepsilon f_1$ of the solution $f$, belonging to the orthogonal complement of the null space of $\mathcal{C}$, to order $O(\varepsilon)$. Further, note that with the previous splitting $\int f_1 dq = 0$. Applying the operators $\mathbf{\Pi}$ and $id - \mathbf{\Pi}$ to equation (12) gives the split equations

$$(a)\ \partial_t f_0 + \mathbf{\Pi}[\nabla_x \cdot \big(H(\tau-\eta)v(f_0 - \varepsilon f_1)\big)] = 0 \tag{15}$$

$$(b)\ -\varepsilon\partial_t f_1 + (id - \mathbf{\Pi})[\nabla_x \cdot \big(H(\tau-\eta)v(f_0 - \varepsilon f_1)\big)] - \mathcal{C}[f_1] = 0\ .$$

The large scale approximation now consists of retaining only the $O(1)$ terms in equation (15)(b) and solving (15)(a) and

$$(b)\ \mathcal{C}[f_1] = (id - \mathbf{\Pi})[\nabla_x \cdot \big(H(\tau-\eta)vf_0\big)]\ . \tag{16}$$

which gives, since we have committed an $O(\varepsilon)$ error in (15)(b), an order $O(\varepsilon^2)$ error in (15)(a). Note that the operator in equation (16) involves the spatial derivative of $f_0$. Therefore, we assume that $G$ has the required spatial regularity in order to obtain a well-defined operator $\mathcal{C}[f_1]$.

Integrating (16)(a) w.r.t. the microscopic variables $q$, and using the projection property $\int \mathbf{\Pi}[f]\ dq = \int f\ dq$ gives

$$(a)\ \partial_t\rho(x,t) + \nabla_x \cdot \big(\int H(\tau-\eta)v(\rho G - \varepsilon f_1)\ dq\big) = 0 \tag{17}$$

$$(b)\ (id - \mathbf{\Pi})\nabla_x \cdot [H(\tau-\eta)v\rho G] = \mathcal{C}[f_1]\ .$$

So, the process of deriving the approximate macroscopic equation consists of computing the Gibbs measure $G$ in (14), solving the constitutive relation (17)(b) for $f_1$ in terms

of $f_0 = \rho G$, and inserting the solution into (17)(a). This produces (17)(a) as a closed conservation law for the density $\rho$ on the $O(1)$ time scale $t$.

In order to carry out the above general recipe, we need the following assumption, which has to be verified for a particular collision operator $\mathcal{C}$:

**Assumption 3.1** (Gibbs measure and pseudo inverse)**.** The problem (14) for the Gibbs measure $G(x,q)$ has a unique solution. Furthermore, the problem

$$(a)\ \mathcal{C}[f] = g,\ (b)\ \int f(x,q)\ dq = 0,\ \forall x \tag{18}$$

has a unique solution for all right hand sides $g(x,q)$ satisfying $\int g(x,q)\ dq = 0,\ \forall x$, if the additional condition (18)(b) is imposed. That is, $\mathcal{C}$ has a pseudo inverse $\mathcal{C}^+$ on the subspace of all functions satisfying $\int f\ dq = 0$.

The averaged conservation law (17)(a) will be of a convection - diffusion type with an $O(\varepsilon)$ diffusion term. After computing the Gibbs measure and the pseudo-inverse of $\mathcal{C}$, we obtain an equation of the form

$$\partial_t \rho + \nabla_x \cdot \big((V - \varepsilon p)\rho - \varepsilon D \nabla_x \rho\big) = 0 \tag{19}$$

with the mean velocity $V(x)$, the diffusion matrix $D$, and the velocity correction vector $p$ given by

$$(a)\ V(x) = \int H(\tau - \eta) v G(x,q)\ dq, \tag{20}$$

$$(b)\ D(x)\nabla_x \rho + p(x)\rho = \int H(\tau-\eta) v (\mathcal{C}^+ \circ (id - \mathbf{\Pi}))[\nabla_x \cdot \big(H(\tau-\eta) v \rho G\big)]\ dq$$

The diffusion matrix $D(x)$ is given by $D = \int H(\tau-\eta) v (\mathcal{C}^+ \circ (id - \mathbf{\Pi}))[\big(H(\tau-\eta) v^T G\big)]\ dq$, and the first order correction $p$ to the mean velocity $V$ arises from the fact that we are dealing with a highly nonhomogeneous medium, i.e. the Gibbs measure $G$ is dependent on the spatial variable $x$ as well.

3.3. **Transport Coefficients.** We now apply the methodology from Section 3.2 to the specific collision operator $\mathcal{C}$ given by the definition (13), and compute the transport coefficients $V, D$ and $p$ in (19). The final result of this section is Theorem 3.4, giving the transport coefficients in the macroscopic diffusion convection equation. The formal proofs for this section consist of lengthy exercises in integration, and are deferred to the Appendix in Section 6.

Since the operator $\mathcal{C}$, although dependent on $x$, *does not act* on $x$ and $t$, we will drop the dependence on the variables $x$ and $t$ occasionally for the rest of this section for notational convenience.

As in [20] we decompose the operator $\mathcal{C}$ into $\mathcal{C} = \mathcal{B} \circ \mathcal{A}$ with $\mathcal{A}$ and $\mathcal{B}$ given by

$$\mathcal{A}[f](q) = \partial_\eta f + \omega(\eta - \tau) f,\ \mathcal{B}[f](q) = f - \Gamma(q) \int f(q')\ dq'\ .$$

The operator $\mathcal{A}$ has an inverse (given essentially by using an integrating factor), and the operator $\mathcal{B}$ is a simple relaxation operator, whose kernel and pseudo inverse are easy to compute. We introduce the antiderivative $\mathbf{U}(\eta) = \int_\eta^\infty \mathbf{W}(t)\ dt$ (the probability that

$w > \eta$ holds), and write $\omega$ as $\omega(\eta) = -\frac{\partial_\eta \mathbf{U}}{\mathbf{U}}$. Solving the problem $\mathcal{A}[f] = g$ gives (using the integrating factor $\frac{1}{\mathbf{U}}$)

$$\partial_\eta[\frac{f(q)}{\mathbf{U}(\eta-\tau)}] = \frac{g(q)}{\mathbf{U}(\eta-\tau)}$$

which gives the inverse of $\mathcal{A}$ as

$$\mathcal{A}^{-1}[g](q) = f(q) = \int H(\eta-\eta')\frac{\mathbf{U}(\eta-\tau)}{\mathbf{U}(\eta'-\tau)} g(v,\eta',\tau,m)\ d\eta' \ . \tag{21}$$

The null space of $\mathcal{B}$ consists obviously of multiples of the measure $\Gamma$ since $\int \Gamma(q)dq = 1$. The pseudo inverse $\mathcal{B}^+$ on the subspace of functions $\{f : \int f dq = 0\}$ of $\mathcal{B}$ reduces to the identity operator.

**Definition 3.1.** We define expectations of quantities with respect to the measure $\Gamma$ as

$$\mathbb{E}[w](x) = \int_0^\infty \eta \mathbf{W}(\eta, x)\ d\eta,\ \mathbb{E}[\tau](x) = \sum_m \mathbf{A}(m,x) \int_0^\infty \tau \mathbf{T}(\tau, m, x)\ d\tau,$$

$$\mathbb{E}[\mathbf{e}](x) = \sum_m \mathbf{A}(m,x)\mathbf{e}(m,x)\ , \mathbb{E}[\tau\mathbf{e}](x) = \sum_m \mathbf{A}(m,x)\mathbf{e}(m,x) \int_0^\infty \tau \mathbf{T}(\tau,m,x)\ d\tau\ .$$

**Lemma 3.2** (The Gibbs measure )**.** *Let the expectations of travel and waiting times and edge vectors be defined as in Definition 3.1. Then the Gibbs measure in problem (14) is of the form*

$$G(q) = \frac{1}{\mathbb{E}[w] + \mathbb{E}[\tau]} H(\eta)\mathbf{U}(\eta-\tau)\delta(\frac{\mathbf{e}(m)}{\tau} - v)\mathbf{T}(\tau,m)\mathbf{A}(m) \tag{22}$$

*and the mean velocity $V = \int H(\tau-\eta) v G\ dq$ in equation (19) is given by*

$$V = \frac{\mathbb{E}[\mathbf{e}]}{\mathbb{E}[w] + \mathbb{E}[\tau]} \tag{23}$$

**Remark 2.** The existence of the equilibrium distribution $G$ is given by the explicit formula (22). Usually, existence of equilibrium distribution may be proven by the Krein–Rutman theorem [21] that requires a positive compact operator. The integral operator $\Gamma(x,q)\int \omega(\eta'-\tau', x) f(x, q', t) dq'$ is a positive and compact operator on some Banach space $X$ to $X$ under suitable growth conditions on $s \to \omega(s,x)$. However, this argument does not easily give existence of $f \geq 0$ for the operator $C$ since $f \to \partial_\eta f$ is not bounded operator on some Banach space $X$. Therefore, a careful definition of suitable spaces for the solution of $f$ is required. We leave this point aside and explicitly compute $G$ in the appendix. However, those computations are formal.

**Lemma 3.3** (The pseudo inverse)**.** *Consider the Gibbs measure defined in equation (22). Then, $G$ is a probability measure with respect to $q$ and the pseudo inverse $\mathcal{C}^+$ on the subspace $\{f : \int f dq = 0\}$ is given by*

$$\mathcal{C}^+[g](q) = \mathcal{A}^{-1}[g](q) - \gamma[g]G(q),\ \gamma[g] = \int \mathcal{A}^{-1}[g](q)\ dq \tag{24}$$

*with the operator $\mathcal{A}^{-1}$ defined as in equation (21).*

**Theorem 3.4** (Transport coefficients (formal))**.** *The probability density* $\rho(x,t) = \int f(x,q,t)\,dq$ *satisfies the convection - diffusion equation*

$$\partial_t \rho(x,t) + \nabla_x \cdot \big(\rho(V - \varepsilon p) - \varepsilon D \nabla_x \rho\big) = 0\ , \tag{25}$$

*where the mean velocity*

$$V(x) = \frac{\mathbb{E}[\mathbf{e}]}{\mathbb{E}[w] + \mathbb{E}[\tau]}$$

*and the diffusion matrix* $D(x)$ *and the velocity correction* $p(x)$ *are given by*

$$(a)\ D = \frac{1}{2(\mathbb{E}[w] + \mathbb{E}[\tau])}\{\mathbb{E}[\mathbf{e}\mathbf{e}^T] - V\mathbb{E}[\tau\mathbf{e}]^T - \mathbb{E}[\tau\mathbf{e}]V^T + \big(\mathbb{E}[\tau^2] - \mathbb{E}[w^2]\big)VV^T\} \tag{26}$$

$$(b)\ p = \frac{1}{2}\nabla_x \cdot \big(\frac{\mathbb{E}[\mathbf{e}\mathbf{e}^T]}{\mathbb{E}[w] + \mathbb{E}[\tau]}\big) - \frac{1}{2}V\nabla_x \cdot \big(\frac{\mathbb{E}[\tau\mathbf{e}]}{\mathbb{E}[w] + \mathbb{E}[\tau]}\big) - \mathbb{E}[w]V\nabla_x \cdot V$$
$$+\big(\frac{1}{2}V\mathbb{E}[\tau^2] + \frac{1}{2}V\mathbb{E}[w^2] + V\mathbb{E}[\tau]\mathbb{E}[w] - \frac{1}{2}\mathbb{E}[\tau\mathbf{e}]\big)\frac{\nabla_x \cdot V}{\mathbb{E}[w] + \mathbb{E}[\tau]}$$

**Remark 3.** The presence of the drift term $\rho V$ in the equation (25) is due to the fact that the equilibrium $G$ is space dependent. Another possibility to have the drift term in the diffusion approximation of the kinetic equation would be the fact that the bulk velocity of the equilibrium is non–zero.

Also, in the work by E. Larsen and others already investigated the asymptotic regime of kinetic equation leading to diffusion equations [22, 24, 17]. In particular, it has already been pointed out that the transport coefficients only depend on mean and standard deviations of the underlying probability distributions, here, on the ones of $T$ and $W$, respectively. This has also been analyzed for numerical schemes for example in [12, 23].

**Remark 4.** For the macroscopic transport equation to be well–posed, it is necessary that the diffusion matrix $D$ is positive semidefinite.

Assume that for all $z \in \mathbb{R}^2$ and $z \neq 0$ we have

$$\mathbb{E}[\|z^T(\mathbf{e} - \tau V)\|^2] \geq \mathbb{E}[w^2]\|V^T z\|^2. \tag{27}$$

Then, $D$ is positive semidefinite. Indeed, we obtain due to equation (26)(a)

$$\begin{aligned} z^T D z &= \frac{1}{2(\mathbb{E}[w] + \mathbb{E}[\tau])} z^T \Big(\mathbb{E}[\mathbf{e}\mathbf{e}^T] - V\mathbb{E}[\tau\mathbf{e}]^T - \mathbb{E}[\tau\mathbf{e}]V^T + \big(\mathbb{E}[\tau^2] - \mathbb{E}[w^2]\big)VV^T\Big) z \\ &= \frac{1}{2(\mathbb{E}[w] + \mathbb{E}[\tau])} z^T \Big(\frac{\mathbb{E}[(\mathbf{e} - \tau V)(\mathbf{e} - \tau V)^T] - \mathbb{E}[w^2]VV^T}{2(\mathbb{E}[w] + \mathbb{E}[\tau])}\Big) z \\ &= \frac{\mathbb{E}[\|z^T(\mathbf{e} - \tau V)\|^2] - \mathbb{E}[w^2]\|V^T z\|^2}{2(\mathbb{E}[w] + \mathbb{E}[\tau])} \geq 0. \end{aligned}$$

We offer the following interpretation of condition (27). In many applications waiting times are exponentially distributed with mean $\frac{1}{\lambda}$. In this case $\mathbb{E}(w^2) = \frac{1}{\lambda^2}$. Hence, provided we have a process with very small average waiting times $\frac{1}{\lambda} << 1$, then we may fulfill condition (27). Intuitively, the density has 'no time' to accumulate at the node and will therefore diffuse.

## 4. Network reorganization

Without making any further assumptions on the topology of the graph, the interpolated probability measures $\mathbf{A}(m,x), \mathbf{T}(\tau,m,x)$ and $\mathbf{W}(w,x)$ will become measure valued in the limit $\varepsilon \to 0$, that is in the homogenization limit for $x = Z_n$ approaching a continuum variable. One approach would be to assume a certain regularity of the graph structure, as c.f. proposed in [10] for a more or less rectangular street network. When discretizing the final convection–diffusion equation on a *regular* , rectangular grid we need to interpolate the probabilities leading to possibly large and difficult to estimate discretization errors.

Therefore, in this paper, we will use a different approach, namely to use the *freedom* we still have in choosing the node coordinates $Z_n \in \mathbb{R}^2,\ n = 1 : N$. So, we will try to 'draw the graph' in such a way that the probability measures $\mathbf{A}(m,x), \mathbf{T}(\tau,m,x)$ and $\mathbf{W}(w,x)$, and therefore also the transport coefficients $V, D, p$ in equation (25), are possible to discretize on a regular mesh. This is the subject of the reorganization procedure described below.

4.1. **Reorganization.** The basic idea is to choose the coordinates $Z_n$ in such a way that the distance $|e_{mn}| = |Z_n - Z_m|$ is proportional to the expected waiting and travel time, weighted with the probability $A_{mn}$ that the agent actually travels along this edge of the graph. This generalizes an idea, originally presented in [7], to higher dimensions. Ideally, we would choose the coordinates $Z_n$ such that

$$|e_{mn}| = |Z_m - Z_n| = \begin{pmatrix} v_0(E^\tau_{mn} + E^w_n) & for & A_{mn} \neq 0 \\ \infty & for & A_{mn} = 0 \end{pmatrix} \tag{28}$$

holds, with the expectations given by $E^\tau_{mn} = \int \tau T(\tau,m,n)\, d\tau$ and $E^w_n = \int w W(w,n)\, dw$. So the distance between $Z_n$ and $Z_m$ is proportional to the expected time spent in waiting and travel if the edge $n \to m$ is actually used. If $A_{mn} = 0$, then there is no link from $n \to m$ and we indicate this in the function $e_{mn}$ by setting its value to infinity. This value does not appear in the cost functional later on since those are multiplied by $A_{mn}$.

In equation (28) $v_0$ is an arbitrary parameter, determining the size of the graph. Enforcing (28) for a general graph for all $m, n$ is of course impossible, leading in the worst case, to $N^2$ equations for $2N$ unknowns. We can, however, try to solve (28) approximately by minimizing the functional

$$\mathcal{J}_1(\vec{Z}) = \sum_{mn} A_{mn}\big(|Z_m - Z_n| - v_0(E^\tau_{mn} + E^w_n)\big)^2,\ \vec{Z} = (Z_1, .., Z_N)\ .$$

So, we weigh the residual in (28) by the probability, that the path can actually be taken. It turns out, that just considering the functional $\mathcal{J}_1$ is not sufficient. This can be seen from the simple example of a chain graph, where $A_{mn} = \delta_{m,n+1}$ holds, i.e. the agents travel along a chain with certainty. Any choice of coordinates $Z_n$, which satisfies $|Z_{n+1} - Z_n| = v_0(E^\tau_{n,n+1} + E^w_n),\ n = 1 : N-1$, i.e. any curve in $\mathbb{R}^2$ with the correct arclengths, would minimize $\mathcal{J}_1$. In view of the discretization of the convection diffusion equation of the previous theorem we are more interested in reorganizations leading to a regular rectangular grid like structure.

We therefore consider not only paths of length one but general paths of length $K+1$ through the graph and the corresponding functional

$$\mathcal{J}_{K+1}(\vec{Z}) = \sum_m \sum_{k_1} .. \sum_{k_K} \sum_n A_{mk_1} A_{k_1k_2} .. A_{k_{K-1}k_K} A_{k_Kn} \times$$

$$\big(|Z_m - Z_n| - v_0(E^\tau_{mk_1} + E^w_{k_1} + ... + E^\tau_{k_Kn} + E^w_n)\big)^2,\ \vec{Z} = (Z_1, .., Z_N)\ .$$

The functional $\mathcal{J}_{K+1}$ considers all paths $n \to k_K \to .. \to k_1 \to m$ of length $K+1$ through the graph, and tries to assign them the arclength proportional to their total expected travel and waiting times, weighted with the probability $A_{mk_1}...A_{k_{K-1}k_K}A_{k_Kn}$ that this path is actually used. It can be easily seen, that considering only $\mathcal{J}_1 + \mathcal{J}_2$ in the example of a linear chain reduces the number of possible minima to straight lines, albeit with an arbitrary location in $\mathbb{R}^2$. For practical implementation, we impose the additional constraint $Z_1 = (0,0)$ and $Z_1 - Z_2 = |Z_1 - Z_2|(1,0)$, i.e. we fix the location and the orientation of the graph. Optimizing all possible paths of length $1, .., N$ results, in the worst case in an $NP$ complete problem, i.e. the functional $\mathcal{J}_N$ would contain possibly $O(N^N)$ nonzero terms. In practice, we will restrict ourselves to paths of a moderate length (optimizing $\mathcal{J}_1 + .. + \mathcal{J}_{K+1},\ K+1 = 3$ or 4), noting that the probabilities $A_{mk_1}...A_{k_{K-1}k_K}A_{k_Kn}$ decay rapidly with the path length.

To compute a solution to the kinetic equation (10) in Section 2.3 for a given real world network we would need data on the flow rates. In particular, information on how many agents per time unit at node $n$ travel to arc $m$ is required to compute $A_{mn}$. Furthermore, we would need histograms of the incurred travel and waiting times $\tau_{mn}, w_n$ to compute the probability densities $T(\tau, m, n)$ and $W(w, n)$. This would allow us to compute the probability density $\Gamma$ in Theorem 2.1 after we have computed the arc vectors $e_{mn}$ from the above optimization procedure. One of the advantages of an averaged model, as derived in Section 3.3 is that it requires less detailed information. To compute the transport coefficients in Theorem 3.4 we only need the means and the standard deviations of the distributions $T$ and $W$.

4.2. **Diffusive time scales.** The macroscopic model equation (25) in Theorem 3.4 is essentially convective with a small $O(\varepsilon)$ diffusive correction. So, the randomness of the travel and waiting times enters only as an $O(\varepsilon)$ term through the diffusion matrix $D$ and the velocity correction $p$. This statement holds true *unless the mean velocity* $V(x)$ *is very small*. If, c.f. the mean velocity $V$ were of order $O(\varepsilon)$ as well, then (25) would reduce to a diffusion equation on a much larger $t_1 = \frac{t}{\varepsilon}$ time scale of the form

$$\partial_{t_1}\rho + \nabla_x \cdot \big(\rho(V_1 - p) - D\nabla_x\rho\big) = 0\ , V = \varepsilon V_1\ . \tag{29}$$

There is of course no reason that, in the asymptotic regime considered in Section 3.1, the mean velocity $V$ is of order $O(\varepsilon)$. However, we can try to minimize $|V|$ by adding it to the functionals in the minimization procedure. So we arrange the nodes $Z_n$ such that the functional

$$\mathcal{J} = \mathcal{J}_1 + .. + \mathcal{J}_K + \mathcal{J}_V \tag{30}$$

is minimized, with $\mathcal{J}_V$ given by

$$\mathcal{J}_V = \frac{1}{N}\sum_n |V(Z_n)|$$

and $V(x)$ given by the definition (23) as $\frac{\mathbb{E}[e]}{\mathbb{E}[w]+\mathbb{E}[\tau]}$. That is, we try to arrange the nodes in such a way that the individual edge vectors cancel out when averaged with the weights $A$. This will actually work better for so called 'hubs', i.e. network nodes with a very high connectivity. So, we still solve the convection - diffusion equation (25) in Section 3.3 but the local time scale for the evolution will now, roughly speaking, be of the form $\frac{t}{\varepsilon+|V(x)|}$ which is much larger for nodes where $|V| << 1$ holds. So for network hubs with many connections the effects of the randomness in the system, entering through the diffusion term, will be much more pronounced. The stronger diffusion therefore reflects on a different time scale the many possibilities an agent have to choose new target nodes.

4.3. **Some reorganization examples.** The rearrangement of nodes produces some interesting results. To demonstrate the procedure, we first consider a small network of 10 nodes with randomly chosen expected travel times $E^{\tau}_{mn} \in [1,4]$ and waiting times $E^{w}_{n} \in [1,2]$. The connectivity matrix $A$ is generated by the method of preferred attachment, creating a small world network. We first arrange the nodes in a circle and then optimize their location by minimizing the functional $\mathcal{J}$ in equation (30) for $K = 3$. Figure 1 shows the network before and after optimization. In Figure 2 we show the individual

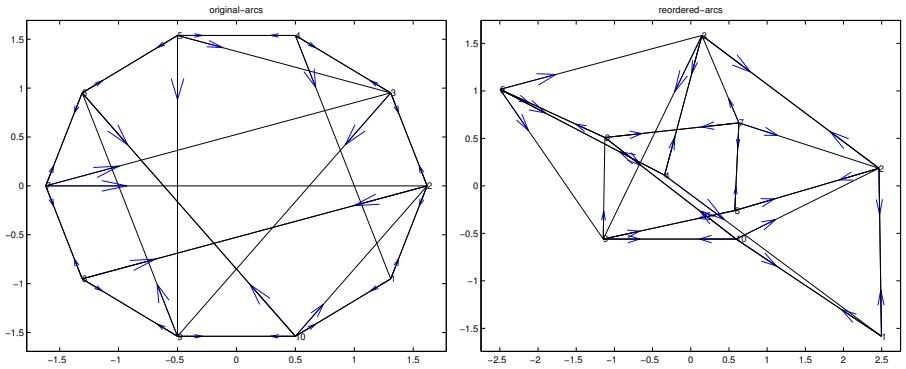


FIGURE 1. A small world network with ten nodes. Left and right panels: before and after optimization of $\mathcal{J}$. The arrows only indicate the direction of the arcs.

velocity vectors $v_{mn} = \frac{e_{mn}}{E^{\tau}_{mn}+E^{w}_{n}}$ before and after rearrangement. Note, that the $v_{mn}$ after reorganization are of approximately equal length and the highly connected nodes have been moved towards the center of the network. The mean velocity $V$ Theorem 3.4 will be small for these nodes, and the solution of equation (25) will evolve on a much larger time scale. (While already present, this effect is of course not very pronounced for a network with only ten nodes.) To demonstrate the scalability of the reorganization approach, we repeat the exercise with 4000 nodes. The left panel in Figure 3 shows the individual velocity vectors $v_{mn} = \frac{e_{mn}}{E^{\tau}_{mn}+E^{w}_{n}}$ before reorganization. The right panel shows the mean velocity vectors $V(Z_n)$ for the diffusion equation (25). Note, that they represent a reasonable flow field for a differential equation, i.e. after reorganization the transport coefficients have become reasonably smooth functions. Note also, that the mean velocities become much smaller in the center of the reorganized network. That is,

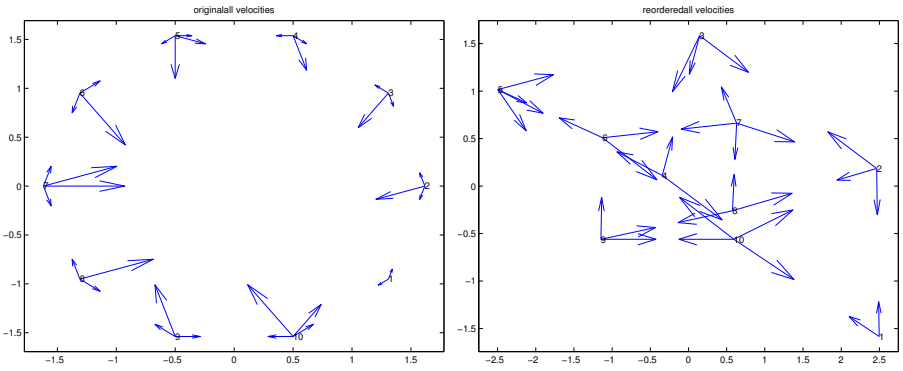


FIGURE 2. Arclength velocities, given by $v_{mn} = \frac{e_{mn}}{E^{\tau}_{mn}+E^{w}_{n}}$ for the 10 node network. Left and right panels: before and after optimization of $\mathcal{J}$. For nodes in the center the arclength velocities tend to average out to zero, making the mean velocity $V$ small.

the highly connected 'hubs' with small mean velocities tend to be placed into the center of the network.

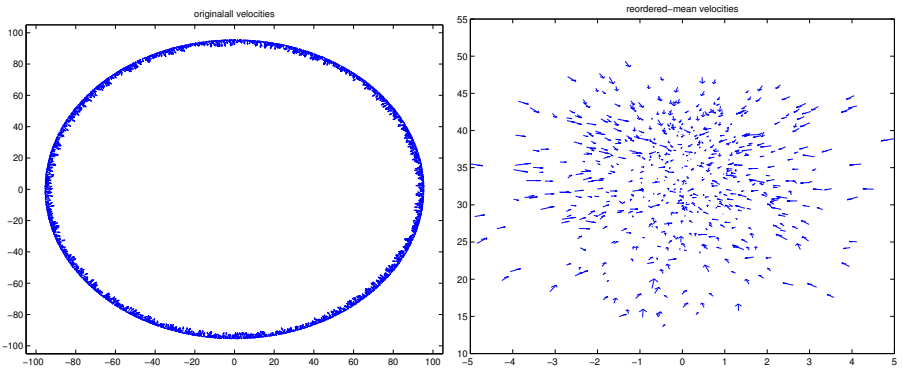


FIGURE 3. Left Panel: Arclength velocities, given by $v_{mn} = \frac{e_{mn}}{E^{\tau}_{mn}+E^{w}_{n}}$ for a network with 4000 nodes. Right panel: Mean velocities $V(x)$ after reorganization. For nodes in the center the arclength velocities tend to average out to zero, making the mean velocity $V$ small.

4.4. **Numerical solution of the transport equation.** Finally, we turn to the solution of the convection diffusion equation (25) in Section 3.3. This is not a completely straight forward task. For a randomly generated unstructured network the reorganized nodes $Z_n$ will not be at all uniformly distributed in $\mathbb{R}^2$. In particular, there will be subregions without any nodes present. As outlined above interpolation of the values of the transport coefficients in these regions is possible. However, this would generate additional interpolation errors which would be hard to estimate in general. We choose a different option, discretizing the transport equation (25) by a straight forward finite volume method on a *regular* rectangular mesh. This will result in computational grid

cells which do not contain any nodes. For such cells we simply set the computational fluxes across the cell boundaries equal to zero. The density $\rho$ will therefore remain equal to zero in these cells for all time, and we essentially solve the transport equation (25) on a 'domain with holes'. Further, we do not connect the resulting equations to possibly data from production networks but chose rectangular distributions for all arising probabilities to simplify the computational effort. An adaption to realistic networks and waiting and distribution rates will be studied in a forthcoming work.

Figure 4 shows the mean velocities $V(x)$ on the computational grid, where the circles denote 'holes' in the domain, i.e. grid cells which will remain empty for all time.

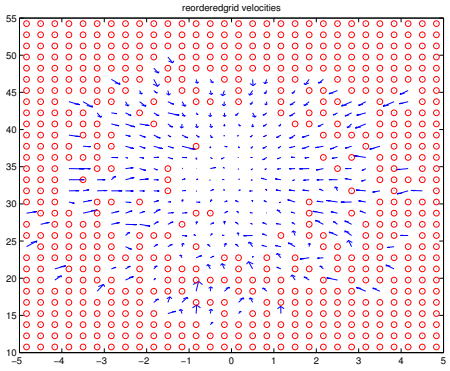


FIGURE 4. Mean velocities on the computational grid. The '$\circ$'s denote empty gridcells without any network nodes.

We solve the transport equation (25) in space by the finite volume method described above, and use a standard Cranck - Nicholson discretization in time. We consider the spread of a perturbation (i.e. a $\delta-$ function), starting in one of the outlying nodes towards the center (where the hubs are placed by the reorganization procedure). The time scale considered here is such that the dimensionless parameter $\varepsilon$ in Section 3.1 has a value of $\varepsilon = 0.05$. So, in physical units the average travel and waiting times are 20 times smaller than the time scale considered. Figures 5 and 6 show the time evolution of the density $\rho$ at selected times.

**Remark 5.** Clearly, due to the reorganization procedure minimizing $|V|$, the density $\rho$ evolves on an even larger time scale, at least locally in space. Thus, the transport equation (25) in Section 3.3 evolves, in unscaled variables, locally on a time scale of order $O(\frac{\tau_0}{\varepsilon^2})$, which allows for the study of phenomena, which would be impossible to consider, based on a direct solution of the multi - agent model in Section 2.

## 5. SUMMARY

We homogenized a recent model for general transport on networks to allow for an efficient simulation of large scale networks. Under mild simplifications we were able to derive a Chapman–Enskog expansion of the transport model introduced in [20] to derive a macroscopic convection–diffusion equation. We re–organized the coordinates of the nodes in the network in order to allow for a simulation of the macroscopic equation on a

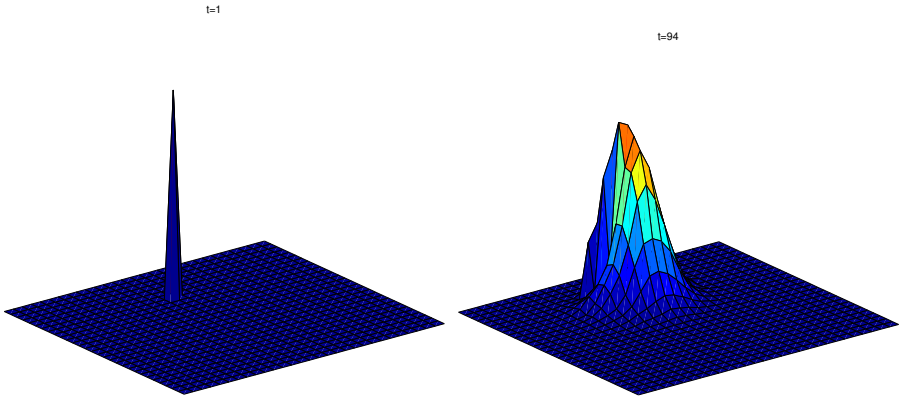


FIGURE 5. Time evolution: Left Panel: $\rho(x,0)$. Right Panel: $\rho(x,94)$. The kinks in the solution are due to the presence of holes in the domain, where $\rho(x,t)=0$ holds, and interpolation in the graphics routine.

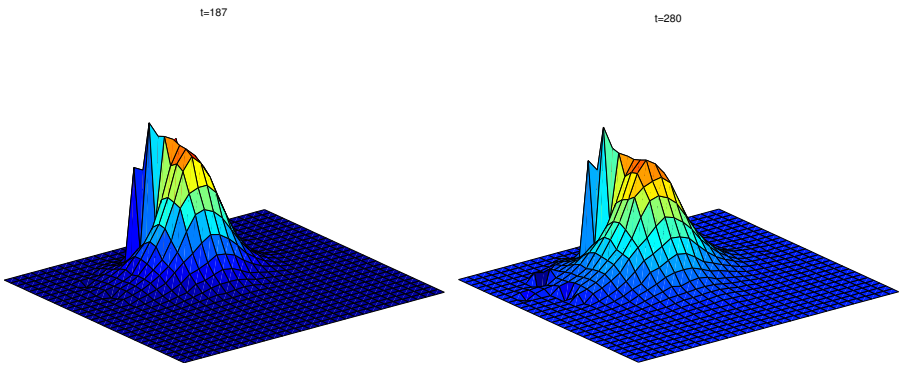


FIGURE 6. Time evolution: Left Panel: $\rho(x,187)$. Right Panel: $\rho(x,280)$. The kinks in the solution are due to the presence of holes in the domain, where $\rho(x,t)=0$ holds, and interpolation in the graphics routine.

regular grid. The convection and diffusion coefficients include the network structure as well as the mean and variance of the waiting and travel times of the microscopic model. The numerical example has been chosen only to highlight to possibility to compute the meanfield limit but has not yet been applied to a realistic problem. Also, the presented computations are so far purely formal. A rigorous assessment in terms of suitable function spaces for kinetic and macroscopic equation will be left for future work.

## 6. Appendix

**Proof of Lemma 3.2**

To solve for the Gibbs measure in problem (14) we have to solve the two problems $\mathcal{B}[G_1]=0$ and $\mathcal{A}[G]=G_1$. The later implies $G=\frac{1}{c}\mathcal{A}^{-1}[\Gamma]$. Here, $c$ is chosen such that

the solution is normalized, i.e., $\int G\ dq = 1$. This results in the formula

$$G(q) = \frac{1}{c}\int H(\eta-\eta')\frac{\mathbf{U}(\eta-\tau)}{\mathbf{U}(\eta'-\tau)}\Gamma(v,\eta',\tau,m)\ d\eta' \ .$$

Inserting the distribution $\Gamma$ given by (13)(b) yields

$$G(q) = \frac{1}{c}H(\eta)\frac{\mathbf{U}(\eta-\tau)}{\mathbf{U}(-\tau)}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m) \ .$$

Now, $\mathbf{W}(\eta)$ is supported only on $\eta > 0$. Therefore, $\mathbf{U}(\eta) = 1$ for $\eta < 0$. Since also $\mathbf{T}(\tau,m) = 0$ for $\tau < 0$ the previous formula simplifies

$$G(q) = \frac{1}{c}H(\eta)\mathbf{U}(\eta-\tau)\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m) \ ,$$

which gives (22). The normalization constant $c$ is computed by

$$c = \sum_m \int H(\eta)\mathbf{U}(\eta-\tau)\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\ dvd\eta d\tau =$$

$$\sum_m \int H(\eta)\mathbf{U}(\eta-\tau)\mathbf{T}(\tau,m)\mathbf{A}(m)\ d\eta d\tau$$

Further, we obtain for each fixed $m$

$$\int H(\eta)\mathbf{U}(\eta-\tau)\mathbf{T}(\tau,m)\ d\tau d\eta = \int H(\eta)\mathbf{U}(\eta)\mathbf{T}(\tau,m)\ d\tau d\eta + \int H(\eta)H(\tau-\eta)\mathbf{T}(\tau,m)\ d\tau d\eta =$$

$$\int H(\eta)\mathbf{U}(\eta)\ d\eta + \int H(\tau)\tau\mathbf{T}(\tau,m)\ d\tau$$

Integration by parts gives $\int H(\eta)\mathbf{U}(\eta)\ d\eta = \int H(\eta)\eta\mathbf{W}(\eta)\ d\eta$ and

$$\int H(\eta)\mathbf{U}(\eta-\tau)\mathbf{T}(\tau,m)\ d\tau\eta = \int H(\eta)\eta\mathbf{W}(\eta)\ d\eta + \int H(\tau)\tau\mathbf{T}(\tau,m)\ d\tau$$

Finally, summation over the index $m$ gives

$$c = \int H(\eta)\eta\mathbf{W}(\eta)\ d\eta + \sum_m \mathbf{A}(m)\int H(\tau)\tau\mathbf{T}(\tau,m)\ d\tau$$

which gives the form of normalization constant as in equation (22). To compute the mean velocity $V$ we observe

$$V = \int H(\tau-\eta)vG(q)\ dq = \sum_m \int \frac{1}{c}H(\eta)H(\tau-\eta)v\mathbf{U}(\eta-\tau)\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\ dvd\eta d\tau$$

$$= \sum_m \int \frac{1}{c}H(\eta)H(\tau-\eta)\frac{\mathbf{e}(m)}{\tau}\mathbf{T}(\tau,m)\mathbf{A}(m)\ d\eta d\tau$$

since $\mathbf{U}(\eta) = 1,\ \eta < 0$ holds. Integrating with respect to $\eta$ gives

$$V = \sum_m \int \frac{1}{c}\tau H(\tau)\frac{\mathbf{e}(m)}{\tau}\mathbf{T}(\tau,m)\mathbf{A}(m)\ d\tau = \sum_m \frac{1}{c}\mathbf{e}(m)\mathbf{A}(m)$$

which gives (23)

∎

**Proof of Lemma 3.3**
To compute $\mathcal{C}^+[g]$ we have to solve the problem $\mathcal{B}\circ\mathcal{A}[f] = g$ under the constraint $\int f\ dq = 0$. If $\int g\ dq = 0$ holds, then $f_1 = \mathcal{A}f$ is given by $f_1 = g - c\Gamma$ for an arbitrary constant $c$, and therefore $f$ is given by $f = \mathcal{A}^{-1}[g] - c\mathcal{A}^{-1}[\Gamma]$. $c$ has to be chosen such that $\int f\ dq = 0$ holds. So, we have $c = \frac{\int \mathcal{A}^{-1}[g]\ dq}{\int \mathcal{A}^{-1}[\Gamma]\ dq}$. If we define the normalized measure $\Gamma_0$ as $\Gamma_0[q] = \frac{\mathcal{A}^{-1}[\Gamma](q)}{\int \mathcal{A}^{-1}[\Gamma](q')\ dq'}$, we obtain

$$f(q) = \mathcal{C}^+[g](q) = \mathcal{A}^{-1}[g](q) - \gamma[g]\Gamma_0(q),\ \gamma[g] = \int \mathcal{A}^{-1}g\ dq$$

Using Lemma 3.2 we obtain that in fact $\Gamma_0 = G$.

To prove Theorem 3.4 we need to evaluate the term $\int H(\tau-\eta)v(\mathcal{C}^+\circ(id-\mathbf{\Pi}))[\nabla_x\cdot\big(H(\tau-\eta)v\rho G\big)]$. We proceed so by step by step in Propositions 1 and 2.

**Proposition 1.** *Let $\int g\ dq = 0$ hold. Then the identity*

$$\int H(\tau-\eta)v_k\mathcal{C}^+[g](q)\ dq = \int(\tau-\eta)H(\tau-\eta)v_k g(q)\ dq - \gamma[g]V_k\ . \tag{31}$$

*holds, with mean velocity $V$ given by equation (23).*

**Proof:** According to Lemma 3.3, we have

$$\int H(\tau-\eta)v_k\mathcal{C}^+[g](q)\ dq = \int H(\tau-\eta)v_k\mathcal{A}^{-1}[g](q)\ dq - \gamma[g]\int H(\tau-\eta)v_k G(q)\ dq\ . \tag{32}$$

To compute the first term in (32) we have, using the definition (21) of $\mathcal{A}^{-1}$,

$$\int H(\tau-\eta)v_k\mathcal{A}^{-1}[g](q)\ dq = \int H(\tau-\eta)v_k H(\eta-\eta')\frac{1}{\mathbf{U}(\eta'-\tau)}g(v,\eta',\tau,m)\ dvd\eta d\tau dmd\eta'$$

$$= \int(\tau-\eta')H(\tau-\eta')v_k\frac{1}{\mathbf{U}(\eta'-\tau)}g(v,\eta',\tau,m)\ dvd\tau dmd\eta' = \int(\tau-\eta')H(\tau-\eta')v_k g(v,\eta',\tau,m)\ dvd\tau dmd\eta'$$

$$\int H(\tau-\eta)v_k\mathcal{A}^{-1}[g](q)\ dq = \int(\tau-\eta)H(\tau-\eta)v_k g(q)\ dq \tag{33}$$

Due to Lemma 3.2 we obtain

$$\int H(\tau-\eta)v_k G(q)\ dq = V_k \tag{34}$$

This gives for (32), inserting from (33)

$$\int H(\tau-\eta)v_k\mathcal{C}^+[g](q)\ dq = \int(\tau-\eta)H(\tau-\eta)v_k g(q)\ dq - \gamma[g]V_k\ .$$

∎

**Proposition 2.** *Let $g$ be given by $g = (id-\mathbf{\Pi})[\nabla_x\cdot\big(H(\tau-\eta)v\rho G\big)]$. Then $\gamma[g]$ in equation (24) is given by*

$$\gamma[g] = \frac{1}{2}\nabla_x\cdot\big(\mathbb{E}[\tau\mathbf{e}]\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big) + \mathbb{E}[w]\nabla_x\cdot\big(\mathbb{E}[\mathbf{e}]\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big) \tag{35}$$

$$-\frac{1}{2}\beta\mathbb{E}[\tau^2]\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}-\frac{1}{2}\beta\mathbb{E}[w^2]\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}-\beta(\mathbb{E}[\tau]\mathbb{E}[w])\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}$$

*with the constant $\beta$ arising from the projection as $\beta = \int \nabla_x \cdot \big(H(\tau-\eta)v\rho G\big)\ dq = \nabla_x \cdot (\rho V)$.*

**Proof:** Now $g$ is given by

$$g(q) = \nabla_x \cdot \big(H(\tau-\eta)v\rho G\big) - \beta G(q),\ \beta = \int \nabla_x \cdot \big(H(\tau-\eta)v\rho G\big)\ dq$$

We compute the term $\gamma[g]$ in equation (24) as $\gamma[g] = \int \mathcal{A}^{-1}[g](q)\ dq$, with $\mathcal{A}^{-1}$ defined as in equation (21). We have for $\mathcal{A}^{-1}[g]$

$$\mathcal{A}^{-1}[g](q) = \int H(\eta-\eta')H(\tau-\eta')\mathbf{U}(\eta-\tau)\nabla_x \cdot \big(v\rho G(v,\eta',\tau,m)\big)\ d\eta'$$

$$-\beta\int H(\eta-\eta')\frac{\mathbf{U}(\eta-\tau)}{\mathbf{U}(\eta'-\tau)}G(v,\eta',\tau,m)\ d\eta'$$

and, inserting for $G$ from (22)

$$\mathcal{A}^{-1}[g](q) =$$

$$\int H(\eta-\eta')H(\tau-\eta')H(\eta')\mathbf{U}(\eta-\tau)\nabla_x \cdot \big(v\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\big)\ d\eta'$$

$$-\beta\int H(\eta-\eta')H(\eta')\mathbf{U}(\eta-\tau)\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\ d\eta'-$$

Integrating with respect to $\eta'$ gives

$$\mathcal{A}^{-1}[g](q) =$$

$$\min\{\tau,\eta\}H(\min\{\tau,\eta\})\mathbf{U}(\eta-\tau)\nabla_x \cdot \big(v\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\big)$$

$$-\beta\eta H(\eta)\mathbf{U}(\eta-\tau)\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m).$$

Next, we split the integration into $\eta<\tau$ and $\eta>\tau$ as follows:

$$\gamma[g] = \int \mathcal{A}^{-1}[g](q)\ dq =$$

$$\int \eta H(\eta)H(\tau-\eta)\nabla_x \cdot \big(v\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\big)\ dq$$

$$+\int \tau H(\tau)H(\eta-\tau)\mathbf{U}(\eta-\tau)\nabla_x \cdot \big(v\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\big)\ dq$$

$$-\beta\int \eta H(\eta)H(\tau-\eta)\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\ dq$$

$$-\beta\int \eta H(\eta)H(\eta-\tau)\mathbf{U}(\eta-\tau)\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\ dq.$$

Because $\mathbf{W} = -\partial_\eta \mathbf{U}$ the following identities hold true: $\int H(\eta-\tau)\mathbf{U}(\eta-\tau)\ d\eta = \mathbb{E}[w]$ and $\int \eta H(\eta)H(\eta-\tau)\mathbf{U}(\eta-\tau)\ d\eta = \frac{1}{2}\mathbb{E}[w^2] + \tau\mathbb{E}[w]$. The last equality is only true if $\eta^2\mathbf{U}(\eta) \to 0$ for $\eta \to \infty$. Applying the previous identities we simplify

$$\gamma[g] = \int \frac{\tau^2}{2} H(\tau)\nabla_x \cdot \big(v\rho \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau} - v)\mathbf{T}(\tau,m)\mathbf{A}(m)\big)\ dvd\tau dm$$
$$+ \int \tau H(\tau)\mathbb{E}[w]\nabla_x \cdot \big(v\rho \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau} - v)\mathbf{T}(\tau,m)\mathbf{A}(m)\big)\ dvd\tau dm$$
$$-\beta \int \frac{\tau^2}{2} H(\tau) \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau} - v)\mathbf{T}(\tau,m)\mathbf{A}(m)\ dvd\tau dm$$
$$-\beta \int (\frac{1}{2}\mathbb{E}[w^2] + \tau\mathbb{E}[w]) \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau} - v)\mathbf{T}(\tau,m)\mathbf{A}(m)\ dvd\tau dm$$

Integration on $dv$ yields

$$\gamma[g] = \int \frac{\tau}{2} H(\tau)\nabla_x \cdot \big(\mathbf{e}(m)\rho \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\mathbf{T}(\tau,m)\mathbf{A}(m)\big)\ d\tau dm$$
$$+ \int H(\tau)\mathbb{E}[w]\nabla_x \cdot \big(\mathbf{e}(m)\rho \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\mathbf{T}(\tau,m)\mathbf{A}(m)\big)\ d\tau dm$$
$$-\beta \int \frac{\tau^2}{2} H(\tau) \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\mathbf{T}(\tau,m)\mathbf{A}(m)\ d\tau dm$$
$$-\beta \int (\frac{1}{2}\mathbb{E}[w^2] + \tau\mathbb{E}[w]) \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\mathbf{T}(\tau,m)\mathbf{A}(m)\ d\tau dm$$

Integrating the remaining variables $\tau, m$ gives

$$\gamma[g] = \frac{1}{2}\nabla_x \cdot \big(\mathbb{E}[\tau\mathbf{e}]\rho \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big) + \mathbb{E}[w]\nabla_x \cdot \big(\mathbb{E}[\mathbf{e}]\rho \frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big) \tag{36}$$
$$-\frac{1}{2}\beta\mathbb{E}[\tau^2]\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]} - \frac{1}{2}\beta\mathbb{E}[w^2]\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]} - \beta(\mathbb{E}[\tau]\mathbb{E}[w])\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}$$

∎

Using Propositions 1 and 2, the results of Lemmas 3.2 and 3.3 we finally able to state the proof of Theorem 3.4.

**Proof of Theorem 3.4:** To compute the diffusion matrix $D$ and the velocity correction $b$ in (19) we have to set $g = (id - \mathbf{\Pi})[\nabla_x \cdot \big(H(\tau-\eta)v\rho G\big)]$ in Proposition 1, or

$$g(q) = \nabla_x \cdot \big(H(\tau-\eta)v\rho G\big) - \beta G(q),\ \beta = \int \nabla_x \cdot \big(H(\tau-\eta)v\rho G\big)\ dq = \nabla_x \cdot (\rho V)$$

this gives for the first term in (31)

$$\int (\tau-\eta)H(\tau-\eta)v_k g(q)\ dq = \int (\tau-\eta)H(\tau-\eta)v_k\nabla_x\cdot\big(H(\tau-\eta)v\rho G\big)\ dq - \beta\int (\tau-\eta)H(\tau-\eta)v_k G(q)\ dq\,.$$

Inserting for the Gibbs measure $G$ from Lemma 3.2, and using the fact that $H(\tau-\eta)\mathbf{U}(\eta-\tau) = H(\tau-\eta)$ holds, gives

$$\int (\tau-\eta)H(\tau-\eta)v_k g(q)\ dq =$$

$$\int (\tau-\eta)H(\tau-\eta)H(\eta)\nabla_x\cdot\big(vv_k\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\big)\ dq$$
$$-\beta\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\int(\tau-\eta)H(\tau-\eta)H(\eta)v_k\delta(\frac{\mathbf{e}(m)}{\tau}-v)\mathbf{T}(\tau,m)\mathbf{A}(m)\ dq\ .$$

Integrating out $\eta$ and $v$ gives

$$\int(\tau-\eta)H(\tau-\eta)v_kg(q)\ dq=$$
$$\int\frac{1}{2}H(\tau)\nabla_x\cdot\big(\mathbf{e}(m)\mathbf{e}_k(m)\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\mathbf{T}(\tau,m)\mathbf{A}(m)\big)\ d\tau dm$$
$$-\beta\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\int\frac{\tau}{2}H(\tau)\mathbf{e}_k(m)\mathbf{T}(\tau,m)\mathbf{A}(m)\ d\tau dm\ ,$$

or

$$\int(\tau-\eta)H(\tau-\eta)v_kg(q)\ dq=\frac{1}{2}\nabla_x\cdot\big(\mathbb{E}[\mathbf{e}\mathbf{e}_k]\frac{\rho}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)-\frac{1}{2}\beta\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\mathbb{E}[\tau\mathbf{e}_k]\ . \tag{37}$$

Combining (37) with the result (35) in Proposition 2 gives for the term $\int H(\tau-\eta)v_k\mathcal{C}^+[g]\ dq=\int(\tau-\eta)H(\tau-\eta)v_kg(q)\ dq-\gamma[g]V_k$ in Proposition 1

$$\int H(\tau-\eta)v_k\mathcal{C}^+[g]\ dq=\int(\tau-\eta)H(\tau-\eta)v_kg(q)\ dq-\gamma[g]V_k= \tag{38}$$
$$\frac{1}{2}\nabla_x\cdot\big(\mathbb{E}[\mathbf{e}\mathbf{e}_k]\frac{\rho}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)-\frac{1}{2}\beta\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\mathbb{E}[\tau\mathbf{e}_k]$$
$$-\frac{1}{2}V_k\nabla_x\cdot\big(\mathbb{E}[\tau\mathbf{e}]\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)-V_k\mathbb{E}[w]\nabla_x\cdot\big(\mathbb{E}[\mathbf{e}]\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)$$
$$+\frac{1}{2}\beta V_k\mathbb{E}[\tau^2]\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}+\frac{1}{2}\beta V_k\mathbb{E}[w^2]\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}+\beta V_k\mathbb{E}[\tau]\mathbb{E}[w]\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}$$

with $\beta$ given by $\beta=\int\nabla_x\cdot\big(H(\tau-\eta)v\rho G\big)\ dq=\nabla_x\cdot(\rho V)$. Rearranging terms in (38) gives

$$p_k\rho+\sum_j D_{kj}\partial_{x_j}\rho=\int H(\tau-\eta)v_k\mathcal{C}^+[g]\ dq=$$
$$\frac{1}{2}\nabla_x\cdot\big(\mathbb{E}[\mathbf{e}\mathbf{e}_k]\frac{\rho}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)-\frac{1}{2}V_k\nabla_x\cdot\big(\mathbb{E}[\tau\mathbf{e}]\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)-V_k\mathbb{E}[w]\nabla_x\cdot\big(\mathbb{E}[\mathbf{e}]\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)$$
$$+\frac{\nabla_x\cdot(\rho V)}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big(\frac{1}{2}V_k\mathbb{E}[\tau^2]+\frac{1}{2}V_k\mathbb{E}[w^2]+V_k\mathbb{E}[\tau]\mathbb{E}[w]-\frac{1}{2}\mathbb{E}[\tau\mathbf{e}_k]\big)$$

or, in matrix - vector notation

$$p\rho+D\nabla_x\rho=$$
$$\frac{1}{2}\nabla\cdot\big(\mathbb{E}[\mathbf{e}\mathbf{e}^T]\frac{\rho}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)-\frac{1}{2}V\nabla_x\cdot\big(\mathbb{E}[\tau\mathbf{e}]\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)-\mathbb{E}[w]V\nabla_x\cdot\big(\mathbb{E}[\mathbf{e}]\rho\frac{1}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)$$
$$+\frac{\nabla_x\cdot(\rho V)}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big(\frac{1}{2}V\mathbb{E}[\tau^2]+\frac{1}{2}V\mathbb{E}[w^2]+V\mathbb{E}[\tau]\mathbb{E}[w]-\frac{1}{2}\mathbb{E}[\tau\mathbf{e}]\big)$$

Differentiating out on the right hand side and comparing coefficients of $\rho$ and $\nabla_x\rho$ gives

$$(\mathbb{E}[w]+\mathbb{E}[\tau])D=$$

$$\frac{1}{2}\mathbb{E}[\mathbf{e}\mathbf{e}^T]-\frac{1}{2}V\mathbb{E}[\tau\mathbf{e}]^T-\frac{1}{2}\mathbb{E}[\tau\mathbf{e}]V^T-\mathbb{E}[w]V\mathbb{E}[\mathbf{e}]^T+\big(\frac{1}{2}\mathbb{E}[\tau^2]+\frac{1}{2}\mathbb{E}[w^2]+\mathbb{E}[\tau]\mathbb{E}[w]\big)VV^T$$

$$p=\frac{1}{2}\nabla_x\cdot\big(\frac{\mathbb{E}[\mathbf{e}\mathbf{e}^T]}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)-\frac{1}{2}V\nabla_x\cdot\big(\frac{\mathbb{E}[\tau\mathbf{e}]}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)-\mathbb{E}[w]V\nabla_x\cdot\big(\frac{\mathbb{E}[\mathbf{e}]}{\mathbb{E}[w]+\mathbb{E}[\tau]}\big)$$
$$+\big(\frac{1}{2}V\mathbb{E}[\tau^2]+\frac{1}{2}V\mathbb{E}[w^2]+V\mathbb{E}[\tau]\mathbb{E}[w]-\frac{1}{2}\mathbb{E}[\tau\mathbf{e}]\big)\frac{\nabla_x\cdot V}{\mathbb{E}[w]+\mathbb{E}[\tau]} \tag{39}$$

Using the fact that $\mathbb{E}[\mathbf{e}]=(\mathbb{E}[w]+\mathbb{E}[\tau])V$ holds in (39) gives (26). This finishes the proof of the theorem.

∎

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