CONTINUUM MODELS FOR FLOWS ON COMPLEX NETWORKS

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Introduction: Network Examples: Some examples of ’real world’ networks + theoretical structure.

Part I:

- **Multi agent models:** Define a generic agent based model with random rules.
- **Kinetic theory for agent based models:** Continuum models and separation of time scales.

PART II:

- **Reorganization and homogenization:** Reorder the graph such that the continuum model gives a ’smooth’ problem.
- **Questions:** Criteria for reorganization.
Example I (the easy case): Battiston - Stiglitz Network
(Flow of products and capital from raw material to customer)
Survivors after bankruptcies and optimizing the final capital.
Generating Small World networks

Method of preferential attachment.

- Start with $K$ nodes.
- Link the nodes.
- Successively add new nodes with $K$ random links.
- Probability of a link between new node and existing node $\propto$ to the number of links of the existing node.
- Creates ’hubs’. Older nodes are more likely to be linked than newer nodes.
- Number of links to hubs grows exponentially $\Rightarrow \phi(N) = \ln(N)$.

Example II: (the hard case)
Small World network with 50 nodes and $K = 3$.

Usage: Toy model for spread of information or disease in a closed society, or for traffic flow.
Example III (the hard case): Small World Network
(Air traffic networks, from D. Brockmann et. al. European J. Phys, 2011.)
Agent models

- Agents travel along links of a graph.
- Goal: Develop continuum (PDE) models for the dynamics (homogenization).
- Reason:
  - Computational efficiency.
  - Separate different mechanisms on different time scales.
Different mechanisms on different time scales: A simple example

- One dimensional graph with nodes 1, .., N.
- In a time interval $\Delta t$ an agent at node $n$ moves from to node $n - 1$ with probability $\Delta t a$, and to node $n + 1$ with probability $\Delta t b$, and stays at node $n$ with probability $1 - \Delta t a - \Delta t b$.
- Let $u_n(t)$ be the probability that the agent is at node $n$ at time $t$.

$$u_n(t + \Delta t) = a\Delta t u_{n-1}(t) + (1 - a\Delta t - b\Delta t)u_n(t) + b\Delta t u_{n+1}(t)$$

$$\Delta t \to 0 \Rightarrow$$

$$\partial_t u_n(t) = au_{n-1} - (a + b)u_n + bu_{n+1}$$

Put the nodes on a line with coordinates $x_n$ and a spacing $\Delta x$.

$$\partial_t u(x,t) = (b - a)\Delta x \partial_x u + \frac{(a + b)\Delta x^2}{2} \partial^2_x u + \text{HOT}$$
Problems

- Problem 2: Rearrange space (the graph) such that stochastic effects become visible on large time scales.
- Problem 1: Given a multi agent model, find a transport equation in $\mathbb{R}^2$, representing the model.
THE GENERIC AGENT MODEL (MONTE CARLO)

- **Graph** with nodes $x = z_n, n = 1 : N$ and (possible) arcs of length $d_{mn} = z_n - z_m$.
- **Wait**: An agent (particle) arrives at $z_n$ at time $t$, and waits a random time $\tau$ to be processed. $dP[\tau = s] = u(s, n) \, ds$.
- **Choice**: It then chooses the next node $z_k$ to go to. $P[k = m] = A(m, n)$.
- **Flight**: It chooses a random travel time $a$. $dP[a = s] = T(s, k, n) \, ds$.
- Arrives at $z_k$ at time $t + \tau + a$. 
Kinetic equations for multi agent systems

- State of the agent described by a state vector $q$.
- Continuous change: $\frac{dq}{dt} = E$
- Random discontinuous change with frequency $\omega$:

\[
q(t + \Delta t) = q', \quad \mathcal{P} = \Delta t \omega(q), \quad d\mathcal{P}[q' = p] = P(p, q) \, dp
\]
\[
q(t + \Delta t) = q(t), \quad \mathcal{P} = 1 - \Delta t \omega(q)
\]

The probability density $f(q, t) \, dq$ of $q$ at time $t$ satisfies

\[
\partial_t f(q, t) = -\nabla_q \cdot (Ef) + \int P(q, p) \omega(p) f(p) \, dp - \omega(q)f(q, t)
\]

Remarks:
- This is a linear theory if the agents do not interact.
- For $N$ interacting agents the theory is still linear if $q = (q_1, \ldots, q_N)$.
- Nonlinearity arises from approximations and effective one-agent equations.
THE PROBLEM WITH STANDARD KINETIC MODELS:

Natural choice: $q = (x, m, n)$

$$\partial_t f(x, m, n, t) = -\nabla_x \cdot (vf) + \sum_{m'n'} P(x, m, n, m', n') \omega' f(x, m', n') - \omega f$$

$v(q)$: velocity

- Collisions (the changes of the state $q$) are instantaneous.
- Mean free path and mean collision frequency.
  Particles travel for an exponentially distributed time.

$$q(t + \Delta t) = (1 - r)q + rp, \quad r \in \{0, 1\}, \quad \mathbb{P}[r = 1] = \Delta t \omega(q)$$

$$d\mathbb{P}[T = t \mid q] = \omega(q)e^{-\omega(q)t}dt, \quad \frac{d\mathbb{P}}{dy} [|\Delta x| = y] = \int \omega(q)\left|\frac{\omega(q)}{|v(q)|}e^{-\frac{y\omega(q)}{|v|}}\right|dq$$

- Particles reach the next node only on average!

*Poissonparticlemoviehere*
**Goal:** Derive a kinetic equation in $\mathbb{R}^d$, such that the network structure enters only in the scattering cross sections, and the PDF stays concentrated on the nodes and arcs.

**State:** $(x, v, m, a, \tau)$

- $x$: position, $v$: velocity
- $m$: node to travel to ($\rightarrow \frac{v}{|v|}$)
- $a$: flight time ($\rightarrow |v|$)
- Clock variable:
  - $\tau$: time elapsed since leaving the last node.

Derive kinetic equation from a Monte Carlo model.
FREE FLIGHT PHASE: $\tau < a$

\[ x(t + \Delta t) = x(t) + \Delta t v(t) \]

\[ v(t + \Delta t) = v(t) \]

\[ m(t + \Delta t) = m(t) \]

\[ a(t + \Delta t) = a(t) \]

\[ \tau(t + \Delta t) = \tau(t) + \Delta t \quad \text{(clock)} \]
Monte Carlo:

$r$: Decision variable whether to go to the next node $m'$ with a new $a = a'$ and a new $v = v'$

\[
\begin{align*}
  r & \in \{0, 1\}, \quad \mathcal{P}[r = 1] = \Delta t \omega, \quad \mathcal{P}[r = 0] = 1 - \Delta t \omega \\
  x(t + \Delta t) &= x(t) \\
  v(t + \Delta t) &= (1 - r)v(t) + rv' \\
  m(t + \Delta t) &= (1 - r)m(t) + rm' \\
  a(t + \Delta t) &= (1 - r)a(t) + ra' \\
  \tau(t + \Delta t) &= (1 - r)(\tau(t) + \Delta t) + r0
\end{align*}
\]
THE RANDOM PARTICLE MODEL

\[ q = (x, v, m, a, \tau) \]

\[ m: \text{node to travel to} \]

\[ a: \text{flight time} \]

\[ \tau: \text{time elapsed since we left the last node.} \]

\[
x(t + \Delta t) = x(t) + H(a - \tau)\Delta tv(t) + H(\tau - a)0
\]

\[
v(t + \Delta t) = H(a - \tau)v(t) + H(\tau - a)((1 - r)v(t) + rv')
\]

\[
m(t + \Delta t) = H(a - \tau)m(t) + H(\tau - a)((1 - r)m(t) + rm')
\]

\[
a(t + \Delta t) = H(a - \tau)a(t) + H(\tau - a)((1 - r)a(t) + ra')
\]

\[
\tau(t + \Delta t) = H(a - \tau)(\tau(t) + \Delta t) + H(\tau - a)((1 - r)(\tau(t) + \Delta t) + r0)
\]

Particle travels precisely a time \( a \) and a distance \( av! \)
PROBABILITIES OF THE NEW STATE

\[ q = (x, v, a, \tau, m) \]

\[ d\mathcal{P}[(v, a, \tau, m)_{\text{new}} = (v', a', \tau', m')] |_{x=z_n} = \]

\[ A(m', n)T(a', m', n)\delta(\tau')\delta(v' - \frac{z_{m'}-z_n}{a}) \, dv' a' m' \tau' \]

Waiting time given by an imbedded Markov process for a general waiting time distribution \( u(n, \tau) \, d\tau \). (Larsen 2010).

\[ \mathcal{P}[r = 1] = \Delta t \omega(n, \tau) = \Delta t \frac{\int_{\tau}^{\infty} u(n, \tau) \, ds}{\int_{\tau}^{\infty} u(n, s) \, ds} \]

Particle travels precisely a time \( a \) and a distance \( av \)!
THE KINETIC EQUATION

Probability density: $f(x, v, a, \tau, m)$

$$\partial_t f = -\nabla_x \cdot [H(a - \tau)vf] - \partial_\tau f + Q[f] = 0$$

$$Q[f](x) = \delta(\tau) \sum_m A^I(m, x) \delta(v - \frac{d^I_m(x)}{a}) \int T(a, m, x) \omega^I f' dv' da' \eta' - \omega^I f$$

$$\omega = H(\tau - a)\omega^I(x, \tau)$$

$A^I(x)$, $d^I_m(x)$, $\omega^I$: interpolants of $A$ and the arc vectors:

$$A^I(m, z_n) = A(m, n), \quad d_m(z_n) = z_m - z_n$$

(???: How to construct the interpolants?)
CONCENTRATION:

\[
\partial_t f = -\nabla_x \cdot [H(a - \tau)vf] - \partial_\tau f + Q[f]
\]

Theorem

If \( f \) is initially concentrated on the nodes

\[
f(x, v, a, \tau, m, t = 0) = \sum_n \delta(x - z_n)f^n_i(v, a, \tau, m)
\]

then the density function \( f \) will stay concentrated on the nodes and the arcs for all time.

⇒ On the kinetic level the choice of interpolants is irrelevant!, since \( Q \) is only evaluated at the nodes!

particlemoviehere
LARGE TIME AVERAGES

Assume large graph and large time scale

\[ x \rightarrow \frac{x}{\varepsilon}, \quad t \rightarrow \frac{t}{\varepsilon} \]

\[ \varepsilon \partial_t f = -\varepsilon \nabla_x \cdot [H(a - \tau)vf}] + C[f] \]

\[ C[f]|_{x=z_n} = -\partial_\tau f + \int P(x, q, q') \omega' f' dq' - \omega f \]

\[ q = (v, a, \tau, m) \]

\[ P(x, q, q')|_{x=z_n} = \delta(\tau) \sum_{m} A(m, n) \delta(v - \frac{z_m - z_n}{a}) T(a, m, n) \]
THE CHAPMAN - ENSKOG EXPANSION

\[ \varepsilon (\partial_t f(q, t) + Lf) = C[f] \]

- \( f \) relaxes on a fast time scale against the kernel manifold of \( C \).
- Find a coordinate system on the kernel manifold, corresponding to slowly variant ’macroscopic variables’ (observables).
- Yields a convection - diffusion system for the macroscopic variables.
- Original work for fluids: Maxwell, Chapman+Enskog. Refinements: Poupaud, Cercignani, Gamba, Levermore, C.R.
RESULT OF THE CHAPMAN - ENSKOG EXPANSION

Manifold coordinate:

\[ \rho(x, t) = \sum_m \int f(x, v, a, \tau, m, t) \, dv_a \tau \]

Result: Yields a convection - diffusion equation of the form

\[ \partial_t \rho(x, t) + \nabla_x \cdot [V \rho - \varepsilon D \nabla_x \rho] = 0 \]

Remark: Analogy to derivation of compressible Navier - Stokes. So, no Nobel Prize here.
TRANSPORT COEFFICIENTS:

\[ \partial_t \rho(x, t) + \nabla_x \cdot [V \rho - \varepsilon D \nabla_x \rho] = 0 \]

Mean velocity:

\[ V(x) = \frac{\mathbb{E}[d(x)]}{\mathbb{E}[a + \tau](x)} \]

The diffusion matrix \( D \):

Lemma

\( D(x) \) is positive semi-definite. So, this is a well posed problem.

\[ r^T D s = \frac{(r + s)^T K(r + s) - (r - s)^T K(r - s)}{8 \mathbb{E}[a + \tau]}, \quad \forall r, s \in \mathbb{R}^2 \]

\[ K = \text{cov}[d] + \frac{\text{var}[a + \tau]}{\mathbb{E}[a + \tau]^2} \mathbb{E}[d] \mathbb{E}[d]^T \]

\[ \mathbb{E}[d] = \sum_m A^I(m, x)d_m(x), \quad \text{cov}[d] = \sum_m A^I(m, x)d_m(x) d_m(x)^T - \mathbb{E}[d] \mathbb{E}[d]^T \]
Kinetic model, for stochastic transport, restricted to an arbitrary network.

Large time behavior ($O(\frac{t}{\varepsilon})$ time scale) given by asymptotics

$$\partial_t \rho(x, t) + \nabla_x \cdot [V \rho - \varepsilon D \nabla_x \rho] = 0$$

Possibly even larger $O(\frac{t}{\varepsilon^2})$ time scale if $V = O(\varepsilon)$ (depends on arrangement of nodes).

Requires the computation of the interpolants of the Kirchhoff matrix and the distance vectors $A^l(m, x), d^l_m(x)$.

Not relevant on the kinetic microscopic level, since collisions only happen at the nodes.

Necessary for computing large time averages.
To compute on large scales the fine structured geometry of the network has to be approximated (interpolation, least squares, averaging).

\[ A^I(m, x) : A^I(x, z_n) \approx A(m, n), \quad d^I_m(x) : d^I_m(z_n) \approx d_{mn}, \]

\[ d_{mn} = z_m - z_n \]

Would in general lead to measure valued transport coefficients. (Bouchitte, Fragala, 2001.)

One approach: compute basis functions for a finite element method from microscopic models in each cell. (DellaRossa, D’Angelo, Quarteroni 2010). Requires some uniformity or quasi-periodicity.

More applicable to problems where distances in the network have a physical meaning (porous media...).
IDEA: Re-arrange the nodes (compute a metric) such that $d^I(x)$, $A^I(x)$ become as uniform as possible.
Given \( A(m, n), \ T(a, m, n), \ u(\tau, m, n) \), choose the \( z_n \) such that the transport coefficients in the convection - diffusion equation become uniform.

(Nonlinear) least squares or optimization problem for the node coordinates \( z_n \).
Cost functionals

\[ |z_n - z_m| \] should be proportional to the average time it takes to get from node \( n \) to node \( m \), weighted by the probability of the path.

- **1 step velocity:**
  \[
  J_1 = \sum_n \left( \sum_m A_{mn} (|z_m - z_n| - v_0 \mathbb{E}[a + \tau]_{mn}) \right)^2
  \]

  \( v_0 = O(1) \) gives scale of the graph.

- **2 step velocity:**
  \[
  J_2 = \sum_n \left( \sum_{mkn} A_{mk} A_{kn} (|z_m - z_n| - v_0 (\mathbb{E}[a + \tau]_{mk} + \mathbb{E}[a + \tau]_{kn})) \right)^2
  \]

- \( |V| \) should be small to give diffusion regime
  \[
  J_V = \langle V^2 \rangle
  \]

minimize \( J_1 + J_2 + J_3 + J_4 + J_V \)
Small World with 10 nodes
Small World with 10 nodes reordered.

Topologically equivalent!!
Flow field for Small World with 10 nodes
Flow field for Small World with 10 nodes reordered
'Large' World with 6000 nodes
'Large' World with 6000 nodes reordered
'Large' World flow field with 6000 nodes reordered
Relative Diffusivity per node

\[ \varepsilon \lambda_{\text{max}}(D) \]

\[ \frac{|D|}{|V|} \]
Map onto a cartesian grid by averaging over grid cells.

o: holes in the grid with zero flux
PART I:
Multi agent system (random) $\rightarrow$ convection - diffusion equation.

\[ (1) \quad \partial_t \rho(x, t) + \nabla_x \cdot [V \rho - \varepsilon D \nabla_x \rho] = 0 \]

- Nonlinear problem via mean fields, \[ V(x, \rho) = \frac{\mathbb{E}[d(x)]}{\mathbb{E}[a+\tau](x,\rho)}. \]
- Transport coefficients dependent on density via clearing functions (Graves, Piccoli, Missbauer, Armbruster, Herty, Degond, CR).
- Discretizing (1) on a mesh gives

\[ \partial_t \rho = L_\rho(z) \rho \]

with $L_\rho(z)$ an M - matrix (the nonlinear 'network Laplacian'), dependent on the coordinates $\overrightarrow{z}$ of the nodes.
Clustering: Replace a given network by a smaller ’similar’ network by grouping nodes together.

- Group them together in computational cells after rearranging the graph.
- Make $L(z)$ look like a discrete Laplacian

$$L(z)u = \lambda u \Rightarrow u = e^{ik \cdot x}$$

- Approximate the range of $L(z)$ by a low rank matrix.

$$L(z) \approx RS(y), \quad \text{range}(RS) \approx \text{range}(L)$$

$$\int ||[L(z) - RS(y)]x||^2 dP(x) \rightarrow \min$$