Aggregation Procedures for Complex Systems

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Outline

- Equilibrium statistical mechanics
- Markov processes
- Traffic Flow
- Interacting Agents
- Oscillator Networks
- Conclusion

1.Equilibrium Statistical Mechanics

- e.g. Frenkel-Kontorova chains: balls $n \varepsilon Z$ at positions $x_n \varepsilon$ R connected by springs in a periodic potential
- Energy $H(x) = \Sigma_n h(x_n,x_{n+1})$
  with $h(x+1,x'+1)=h(x,x')$, $\partial_1\partial_2 h<0$,
  e.g. $h(x,x')=½(x'-x-a)^2+k \cos 2\pi x$
- Minimise energy, or compute properties of canonical ensemble $\exp\{-\beta H(x)\} \Pi dx_n$ or quantum version

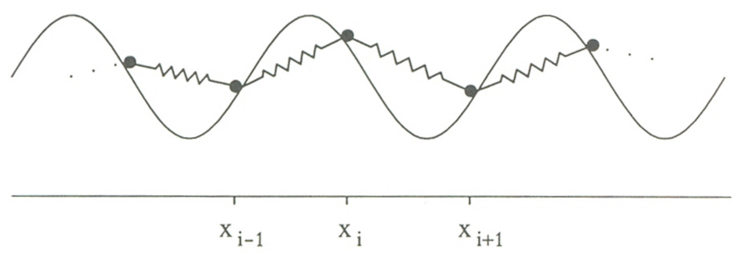


Fig. 1. The Frenkel–Kontorova model.

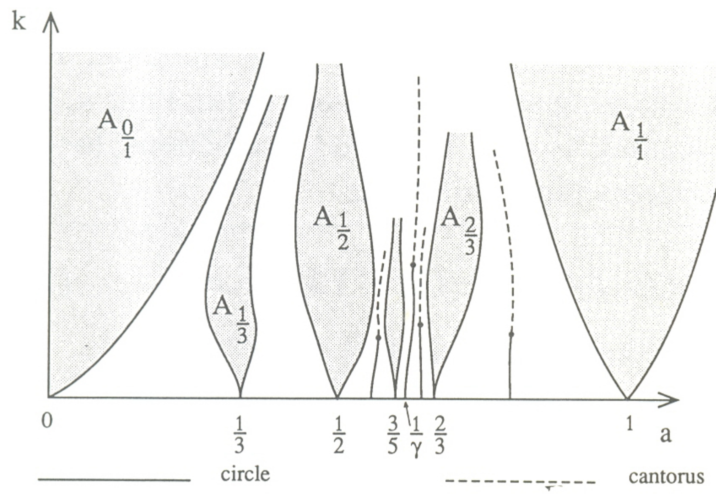


Fig. 2. A sketch phase diagram.

Minimum energy aggregation

- Eliminate ball n by aggregating its two bonds into one new type of bond: $\hat{h}(x_{n-1},x_{n+1}) = \min(h(x_{n-1},x_n)+h(x_n,x_{n+1}))$ over x_n.
- If interested in structures with mean spacing near ω, elimination of balls with nω ε [α,α+ω) mod 1 produces a chain with two types of bond: h and $\hat{h}$; one type occurs in singletons, say h (ω>½).
- Can iterate, aggregating every h with right neighbour $\hat{h}$ and leaving one type in singletons.
- If also rescale x,h,$\hat{h}$ (renormalisation), discover asymptotic self-similarity, e.g. ω=(√5-1)/2 has a fixed point of renormalisation with two unstable directions, hence many scaling exponents: MacKay, Physica D 50 (1991) 71
- Classical SM: MacKay, J Stat Phys 80 (1995) 45
- Quantum SM: Catarino & M, J Stat Phys 121 (2005) 995
- Much other literature on real space renormalisation in statistical mechanics, e.g. van Enter

2.Markov processes

- Continuous-time regular jump homogeneous Markov chain, state space S, mean waiting times T_s, transition probabilities P_{st} (wlog $P_{ss} = 0$); equivalently, transition rate matrix $q_{st} = P_{st}/T_s$, $q_{ss} = -\Sigma_{t\neq s}\, q_{st}$.
- Wish to aggregate states to get a smaller Markov chain, with equivalent stationary probability and mean first passage time (MFPT); cf H Simon, 1961, and many others, but most I've seen involve non-local computation.
- Two local schemes: Wales, 2006; MacKay
- They work for semi-Markov too (arbitrary waiting time distributions); best to think of as steady flows

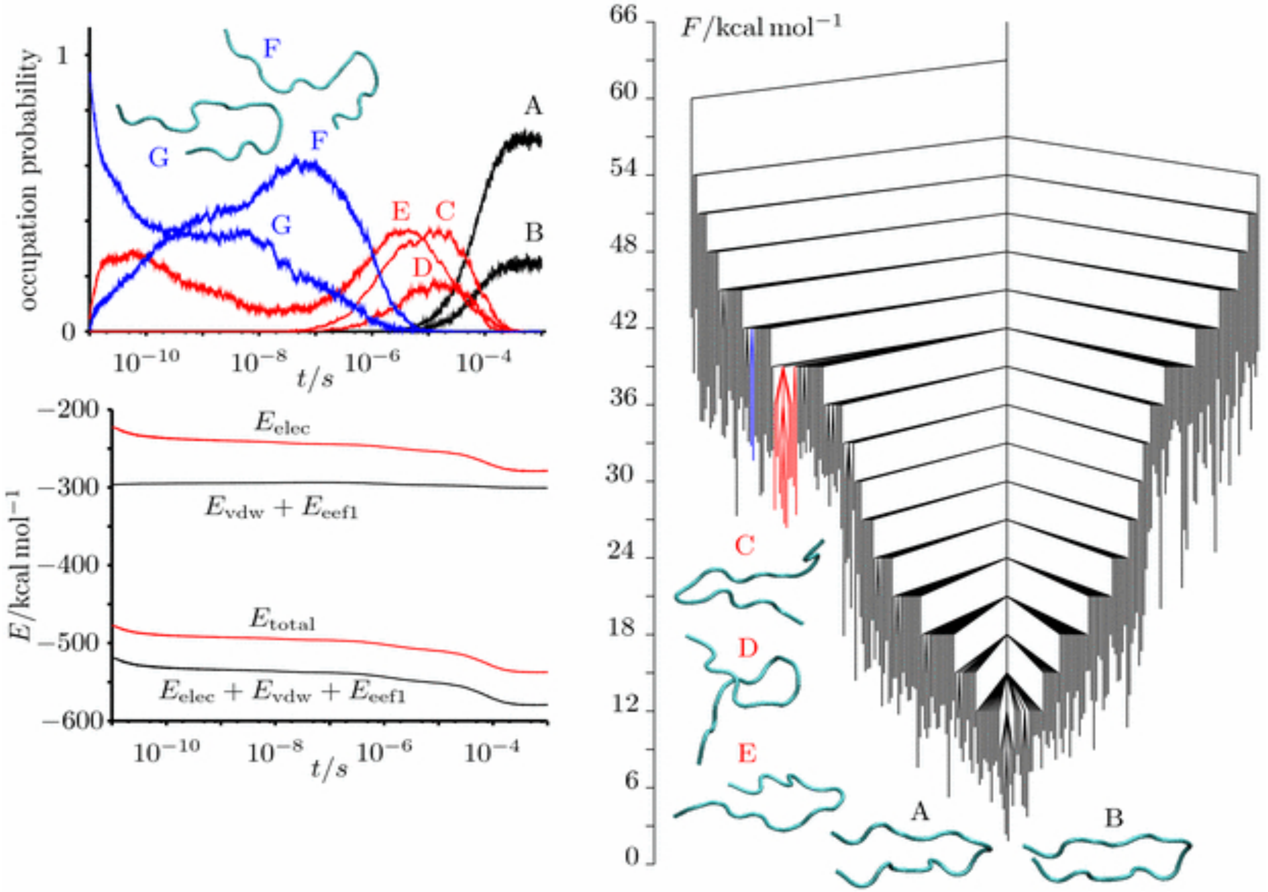
Wales, Int Rev Phys Chem 25 (2006) 237

- Eliminate node x, and put

  $T'_s = (T_s + P_{sx} T_x)/(1 - P_{sx} P_{xs})$

  $P'_{st} = (P_{st} + P_{sx} P_{xt})/(1 - P_{sx} P_{xs})$, $t \neq s$
- Then for any initial $s \neq x$ and subset B (not containing x nor s) with probability 1 of eventual hitting B from s, the new Markov chain computes correct MFPT T_{sB}.
- e.g. can eliminate all but s and B, then $T_{sB} = T'_s$; or reduce to B and a small A containing s and find vector $T_{AB} = (I - P'_{AA})^{-1} T'_A$.
- Also version allowing $P_{ss} \neq 0$ which also conserves T_{sB} for B containing s: J Chem Phys 130 (2009) 204111
- Uses to estimate chemical reaction rates for systems with many local minima: connect minima in a tree at energy where their basins merge and compute a transition rate from saddle.

Wales: GB1 (16 amino-acids)



Can get stationary probability from Wales 2009 version, by

$\pi_s = T_s/T_{s\{s\}}$ (0 if P{return}<1)

and $T_{s\{s\}} = T'_s + P'_{s\$}(I-P'_{\$\$})^{-1}\, T'_{\$}$,

where \$ = set of nodes remaining after aggregation minus s

Aggregation of Markov flows

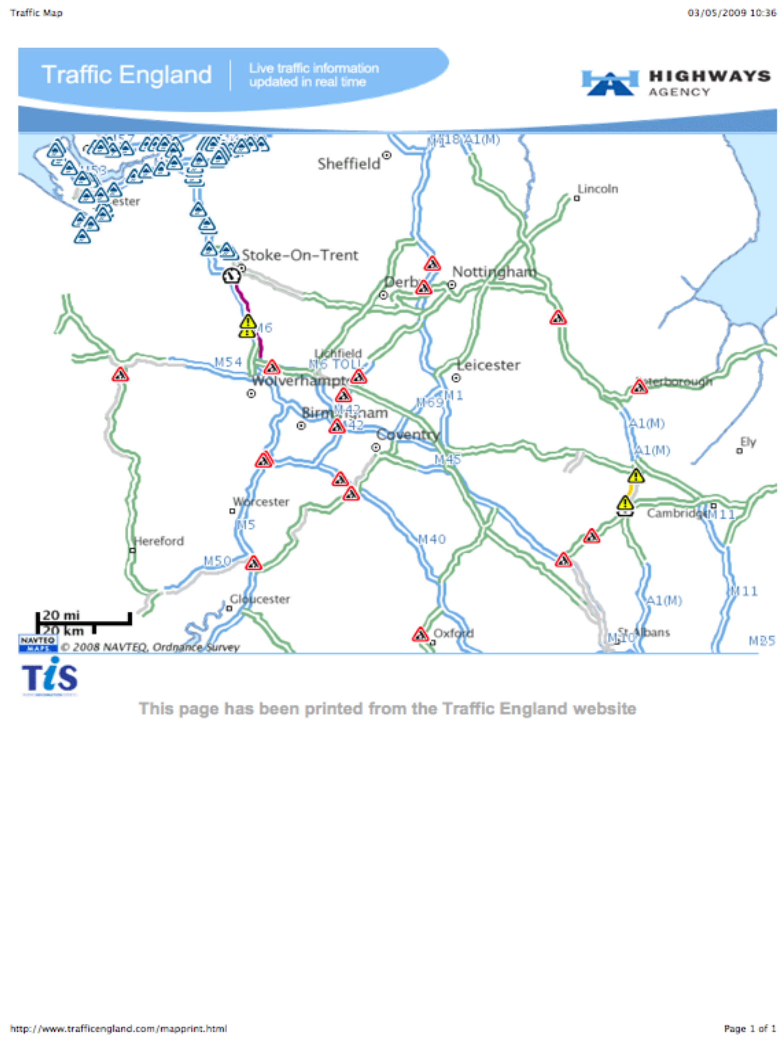
- Alternatively, can aggregate nodes $a \varepsilon A$ to a super-node A, at the expense of possible multiple edges $s \rightarrow A$, $A \rightarrow t$ and making mean waiting time T_e in A and transition probabilities P_{ef} depend on entry edge e.
- Can aggregate super-nodes just the same (and allow waiting time on edges too):

  $T'_e = T_e + P_{eA} (I-P_{AA})^{-1} T_A$ for e entering A

  $P'_{ef} = P_{ef} + P_{eA} (I-P_{AA})^{-1} P_{Af}$ for e entering A, f leaving A
- Get a Markov flow on space of remaining edges, hence e.g. MFPT $T_{eB} = T_e + \Sigma_f P_{ef} T_{fB}$.
- If desired, can aggregate its nodes etc.
- Want useful choices which decrease the complexity.

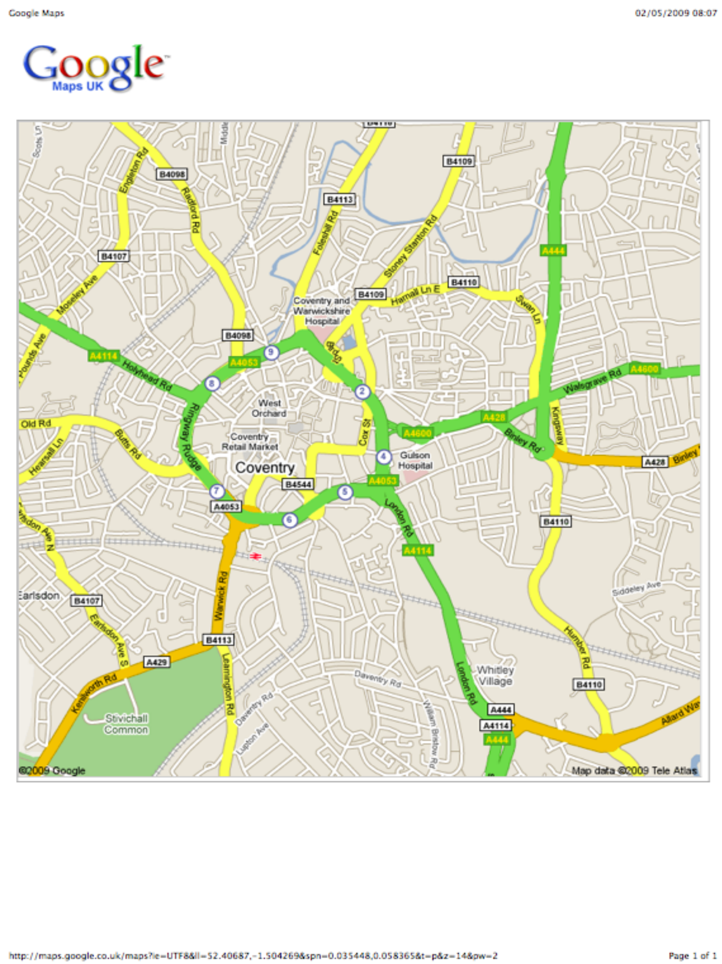
3.Traffic Flow

- Suppose each driver knows cost of each route under current conditions, and chooses route to minimise cost
- If cost of a route is just a sum of edge costs, each depending on flow on that edge, and know set of desired flow rates from origins to destinations, there is good theory to predict the resulting traffic (Nash flow), e.g. Roughgarden's 2005 book



Aggregation

- But might want to treat some subgraphs as single nodes, e.g. to simplify representation or for hierarchical computation: given entry➔exit flow rates $f_{ee'}$ and those for internal origins/destinations, compute Nash flow inside and call resulting costs $c_{ee'}(f)$, $c_{oe'}(f)$, $c_{ed}(f)$
- Introduces junction costs in addition to edge costs



Edge & Junction Costs

- In any case, real junctions incur costs too
- So work in class of models with edge and junction costs
- Further aggregation results in a model of the same type
- So can construct a hierarchy of aggregated models
- Can view as just edge costs on graph with edges as nodes but with dependence on other flows; allows extension of standard theory, and aggregation of edges.
- Looks useful for computation & planning
- Should start with simpler problem of aggregation methods for **shortest route planning**, on which there is a large literature.

4.Interacting Agents

- Standard view in economics is that we are expected-utility maximisers; this can be derived from assuming preferences form a complete pre-order:

  $x \geq y,\ y \geq z \Rightarrow x \geq z;\ x \geq x;\ x \geq y$ or $y \geq x$

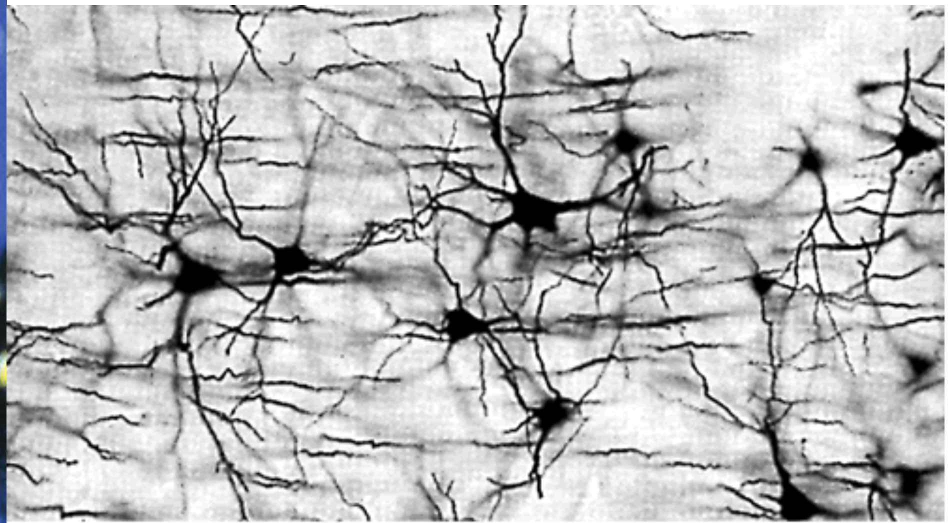
- Suppose the utilities of a group of agents are closely aligned or include cooperative trades, then might expect to be able to replace them by one super-agent with some effective utility function
- Sometimes; but in general the super-agent's preferences form just a partial order (incomplete pre-order):

  $x \geq y,\ y \geq z \Rightarrow x \geq z;\ x \geq x$

Aggregation of Partial-order Agents

- In any case, experiments show individual's preferences don't form a complete pre-order, so why not start from partial-order agents (incomplete preferences)?
- Aggregation of partial-order agents remains in same class
- Could be useful to understand behaviour of social and economic systems, e.g. conditions for "asabiya": capacity of a group for collective action.

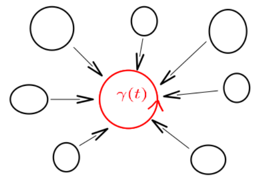
5.Oscillator Networks

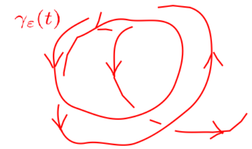


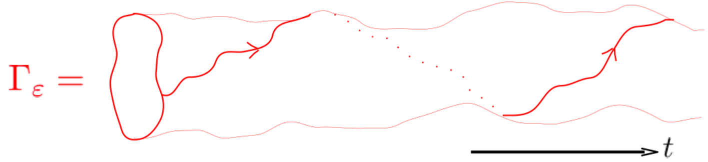
• e.g. Breathing is controlled by two groups of about 300 neurons each, generating robust, synchronised bursting

• 2 oscillators phase-lock if coupling exceeds frequency difference (Huygens): then could replace by a single oscillator

Normal Hyperbolicity







- In a network, oscillators have inputs, so consider an oscillator as an input-output device: for each set of (not too large) input functions of time there is an attracting invariant cylinder in state space x time, depending smoothly on the input functions (normal hyperbolicity), so a circle of output functions.
- With PhD student Stephen Gin we're developing theory for aggregation of oscillators as input-output systems
- 2 oscillators with input functions gives an attracting 2-torus x time; if dynamics on it contains an attracting cylinder then can replace the pair by one effective oscillator
- Special case of one-way coupling when attracting cylinder for forced oscillator may contain an attracting trajectory (phase-locked loop)
- If consider strong forcing, can also get quenching, but intermediate regime is complicated because normal hyperbolicity lost.
- Exploring conditions to aggregate into a large phase-locked cluster

Conclusion

- Aggregation of complex systems is a powerful procedure with a wide range of applications
- Some others: electricity networks, financial networks, shortest route planning
- Hierarchical aggregation produces multi-level dynamics
- But need good principles/heuristics to choose which bits to aggregate, e.g. community detection, highway hierarchies.
- There are lots of research opportunities here.
- I wrote a short paper for FET-Proactive