POSITION PAPER ON "HIERARCHICAL AGGREGATION OF COMPLEX SYSTEMS"

R.S.MACKAY

1. Introduction

The forthcoming call from EC Future and Emerging Technologies – Proactive on "Dynamics of Multi-level Complex Systems" aims to develop "new mathematical and computational formalism on dynamics of multi-level systems developed and validated on real-world applications involving large and heterogeneous data sets".

One important strand of investigation that fits this objective is that of hierarchical aggregation procedures for complex systems. It is a theme that goes back to Herbert Simon [SA], but which has great potential for further development now.

I consider a "complex system" to be a large collection of interdependent units. Given a description at the level of individual units it can be fruitful to partition the collection into groups of units that can be considered as "super-units" and to derive effective interactions between them. Thus one obtains a description at a higher level.

The description at the higher level need not preserve all the information at the lower level, but ideally the effective interactions at the higher level produce exactly the same effect as that of observing the aggregated units for the original system. If a record is kept of the aggregation procedure then it may be possible to infer the lower level description from the higher level one.

Aggregation can be iterated, producing a hierarchy of levels of description. Going from the bottom to the top achieves the "micro to macro" transition.

2. Contexts

There are many contexts to which such aggregation ideas can be applied, and varieties of ways in which the procedure can be implemented.

The oldest application is probably to equilibrium statistical mechanics, in which aggregation is known as "real-space renormalisation". For some types of such system, the approach leads to deep understanding (the case I know best is Frenkel-Kontorova models, e.g. [CM] for the last in a series). For others, it appears to be a dead end [E], though I'm not convinced of this. Physicists believe in its applicability way beyond where mathematicians can justify it, and I think the right response is for the mathematicians to try harder.

Another application is to finding shortest paths in a graph. This is something that satellite navigation designers want to be able to do efficiently in order to be able to respond in real-time to traffic updates. A hierarchical representation could also facilitate

Date: August 24, 2011.

dealing with such updates, as only the parts containing the updated roads would need updating.

A step beyond that is to computing selfish traffic flows. This is a problem that traffic planners face when they wish to find the effects of proposed changes to the road network. Again it can be treated by hierarchical aggregation. One thing to note is that if one starts with a model of costs on edges only then aggregating will in general produce a systems with junction costs, not just edge costs. Edge costs can be trivially absorbed into junction costs. But aggregating systems with junction costs produces only junction costs again.

The context in which Herbert Simon proposed aggregation schemes is Markov processes. The approach was to lump states of a Markov process together in groups and propose a Markov process on the set of groups which has the aggregated stationary probability. This can be extended to the question of computing mean first passage time between two states or sets of states. Advances have been made on the latter problem by Wales [W] but I have proposed what I believe are some further improvements. It is not possible in general to aggregate in such a way as to respect the general dynamics, but one can do this by working in the Laplace-transform of time.

Multi-agent games is an excellent context for aggregation. If the interests of a group of individuals are sufficiently aligned it could make sense to replace them by one super-agent with an effective preference order. A key thing to notice here is that in general if each agent has a complete preference order the aggregated agent will in general have only an incomplete preference order. But aggregating agents with incomplete preference order produces ones of the same type.

Lastly, for something that really is dynamics I mention oscillator networks. By an oscillator let us understand a continuous-time dynamical system with an attracting limit cycle. In a network of oscillators there may be some a group of n oscillators which synchronise together. By this I mean that in their joint state space there is not just an attracting n-torus but the dynamics on this n-torus has an attracting periodic orbit. Or there could be partial synchronisation, meaning that the dynamics on the n-torus has an attracting m-torus for some $1 < m < n$. This does not suffice as an aggregation procedure, however, because the group of oscillators in general has inputs from others. Thus the way I look at an oscillator is in extended state space, with the addition of time to take into account input functions of time. Instead of being a limit cycle, an oscillator is an attracting cylinder for each set of input functions of time. A group of n oscillators subject to input functions of time produces an attracting n-torus cross time. The dynamics on this n-torus cross time may possess an attracting m-torus cross time for some $0 \leq m < n$, in which case we say the group synchronises (partially if $m > 1$). In the case $m = 0$ I say the group synchronises to its inputs. Aggregation consists in recognising groups of oscillators that are likely to synchronise in the presence of inputs in some expected class, making a rigorous verification that they do have a lower dimensional attracting submanifold, using normal hyperbolicity theory, and then replacing them by the lower-dimensional submanifold (which depends of course on the input functions).

The same ideas could apply to more general dynamics than oscillators, where some dimension reduction can occur.

3. Potential outcomes

There are at least two potential outcomes from such aggregation procedures.

The first is efficient ways to compute desired quantities for complex systems. "Divide and conquer" strategies have been extremely effective in for example computing Fourier transforms, multiplying large numbers, and testing conditions in a parameter space. The same is probably true for complex systems, and hierarchical aggregation is the essence of divide and conquer strategies.

The second is to provide insight into the macroscopic behaviour. This is the main success of the renormalisation group. Some asymptotically universal features may take hold at the high levels, which depend on only a few aspects of the low level system. Perhaps the scope for this is more limited in complex systems than equilibrium statistical mechanics, because the range of scales may not be so wide (whereas from Angstroms to millimetres is a factor of 10^7) and there may not be such a domination of local interactions. But there may still be some scope. For example, waves of activity are seen in the brain, despite its having a very complex network of short and long connections.

4. Challenges

There are many challenges for such a programme of research.

One is the choice of which units to aggregate. An a priori promising looking partition is required, but to choose it needs some rationale. It is somewhat easier to generate a hierarchical partition top-down, because one can do "community detection" iteratively.

Also one should not think purely in terms of partitions. There are successful schemes that are based instead on elimination. This approach is used in several of the above examples. Eliminated sites are not directly aggregated with any other particular sites, but their effects are absorbed into all sites that were linked to it.

Similarly, it may be appropriate to consider higher level units which are based mainly on some group of units but are affected by some effect of others. For example in the theory of uniformly hyperbolic dynamics in discrete time, a small perturbation of a product of uniformly hyperbolic systems is topologically conjugate to the uncoupled case. Thus a partition of the original system into groups is preserved under perturbation with a weaker sense of groups, where a homeomorphism is applied to the whole system. Another example is a representation of some condensed matter systems by quasiparticles.

The biggest challenges are probably those of practical implementation. The ideas may sound nice, but only those that can be implemented without too much trouble will have much effect.

References

[CM] Catarino N, MacKay RS, Renormalization and quantum scaling of Frenkel-Kontorova models, J Stat Phys 121 (2005) 995–1014.

[E] Enter ACD van, Renormalization group, non-Gibbsian states, their relationship and further developments, Kyoto workshop (2006?)

[SA] Simon HA, Ando A, Aggregation of variables in dynamic systems, Econometrica 29 (1961) 111-

[W] Wales DJ, Calculating rate constants and committor probabilities for transition networks by graph transformation, J Chem Phys 130 (2009) 204111

Centre for Complexity Science,, University of Warwick, Coventry CV4 7AL, U.K.
E-mail address: R.S.MacKay@warwick.ac.uk