

Title: Graphs and the dynamics of reaction networks

Abstract: The mathematical foundation for Chemical Reaction Network Theory (CRNT) is generally attributed to Feinberg, Horn and Jackson in the 70ies. A fundamental notion is that of relating dynamical properties of a reaction network to its underlying reaction graph. Perhaps the best known example is the deficiency zero theorem that relates the structure of the reaction graph to the existence of stable steady states and the non-existence of periodic orbits.

In this talk I will discuss a few examples of how graphs can be used to infer dynamical properties of reaction networks. Graphs are not only mathematically appealing, but also pleasant to work with; and often it is much easier to check properties of a graph than analytical properties of a parameterised ODE system.

The first example is a graphical procedure to simplify a reaction network, and its relationship to the QSSA procedure. In its simplest form it amounts to contract reaction paths, for example by eliminating intermediate species. In its general form it amounts to eliminate species that occur in loops of reactions. The method is akin to early work by King and Altman. Furthermore, it will be shown that this graphical procedure might be interpreted in terms of the QSSA procedure by dividing the reactions in the original network into fast and slow reactions. Using results by Walcher (Aachen) and co-workers, it will be shown that the trajectories of the reduced system approximates the trajectories of the full system.

The second example, builds on work by Angeli (ICL) and collaborators. They gave sufficient graphical conditions to ensure that a reaction network is persistent (concentrations are bounded from below for all times). I will give an algorithm to construct an equivalent reduced reaction network where the graphical conditions are much easier to check; in fact in important examples the reduced reaction network has no reactions at all ! Additionally, the reduced reaction network might often be interpreted in biological terms.

The talk is based on joint work with Elisenda Feliu, Meritxell Sàez, Michael Marcondes de Freitas and Sebastian Walcher.