Noise Control for Molecular Computing

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With the advancement in nucleic-acid-based technology in general, and strand-displacement DNA computing in particular, a large class of abstract biochemical networks may be physically realized using nucleic acids [3, 4]. Mathematical and experimental methods for designing abstract biochemical circuits, and then physically realizing them, respectively, have been predominantly developed at the (less-detailed) deterministic level, when the circuits involve molecules in high-abundance and operate in well-mixed environments [2, 3, 4]. A proof-of-concept is a recently in-vitro man-made chemical oscillator, called the displacillator [5]. However, molecular circuits involving species in low-abundance, and operating in fluctuating environments, are increasingly found to play an important role in applications, such as when molecular computers are interfaced with cell-like vesicles, and when they are utilized in nanotechnology [6, 7, 8, 9, 10]. In such circumstances, methods for controlling the intrinsic noise in the system are necessary for a successful network design at the (more-detailed) stochastic level.

To bridge the gap, the *noise-control algorithm* for designing biochemical networks will be presented in this talk [1]. The algorithm structurally modifies any given reaction network under mass-action kinetics, in such a way that (i) controllable state-dependent noise is introduced into the stochastic dynamics (the chemical master equation), while (ii) the deterministic dynamics (reaction-rate equations) are preserved. The structural modification involves appropriately enlarging the input network, by adding suitable auxiliary species and chemical reactions. This allows for a hybrid approach when constructing reaction networks: the deterministic model may be used to guide the design, while the noise-control algorithm may be applied to favorably reprogram the intrinsic noise in the stochastic model. The deterministic-stochastic hybrid approach allows one to reshape the probability distributions of target chemical species, and gain control over their sample-paths, while inheriting the fixed mean-field behaviors. The capabilities of the algorithm are demonstrated by redesigning test reaction systems, enriching them with stochastic phenomena, such as noise-induced multimodality/multistability (coexistence of multiple maxima in the probability distributions) and oscillations (see also Figure 1).

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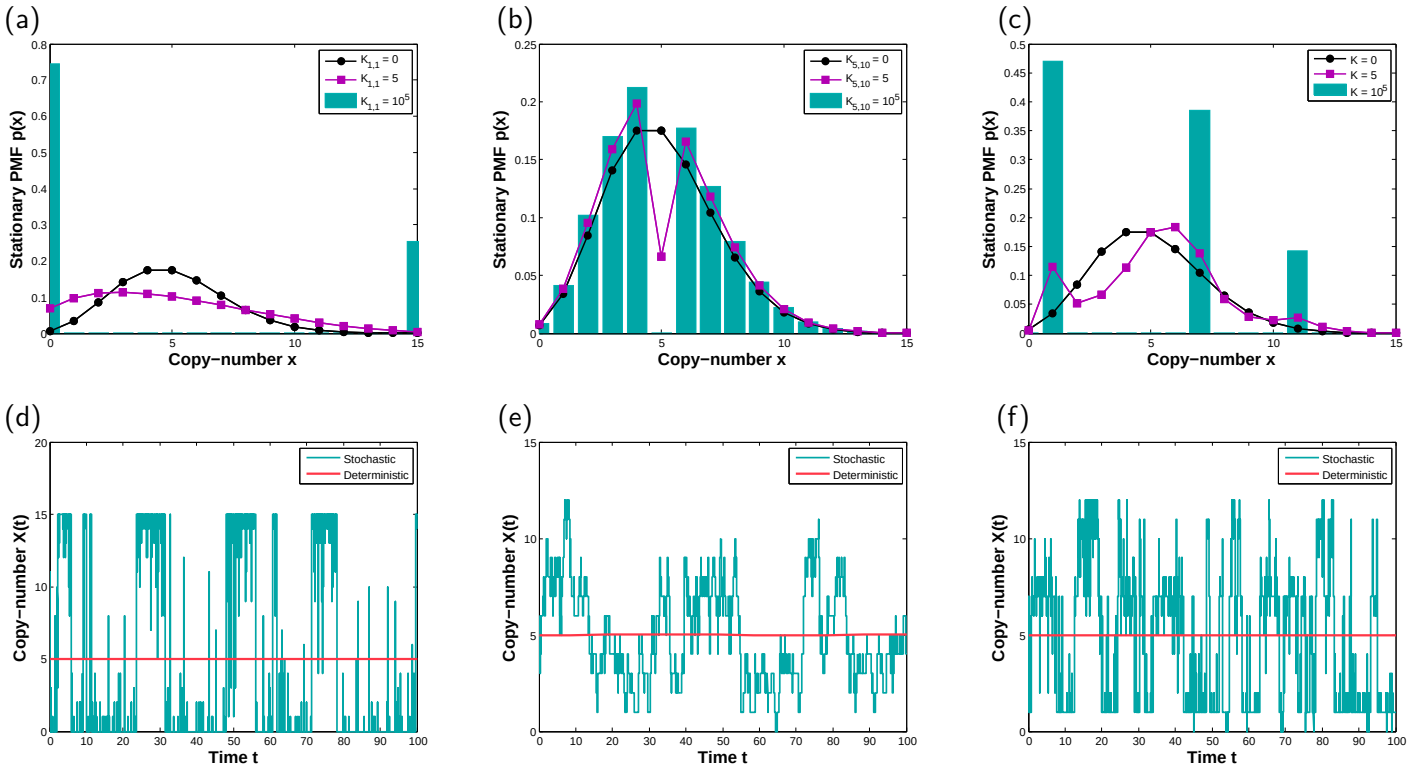

Figure 1: Panels (a), (b) and (c) display the stationary probability mass function (PMF) of a simple production-decay test reaction network without control as the black curve (a Poisson distribution), while with control (an application of the noise-control algorithm) as the blue histograms [1]. In particular, in panel (a), the noise is added to the whole interior of the state-space, while in panel (b) only at a single point, in both cases resulting in noise-induce bimodality. In panel (c), by adding the noise to specific points in the state-space, the network is redesigned to display noise-induced trimodality. Panels (d), (e) and (f) display in blue sample-paths corresponding to the blue histograms from panels (a), (b) and (c), respectively, while in red the underlying deterministic trajectories. One can notice that the noise-control algorithm has enriched the stochastic trajectories with multistability, while the red deterministic ones remain monostable and unchanged under the application of the algorithm.

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