Hamilton Institute

Integrated Stoichiometric, Thermodynamic and Kinetic Modelling of Steady State Metabolism

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Abstract:

In the modelling of biochemical networks at steady state, equations representing mass conservation, energy conservation, the second law of thermodynamics and reversible enzyme kinetics can be formulated as a single system of linear equalities and inequalities, in addition to linear equalities on exponential variables.The reformulation is exact and amenable to large scale nonlinear numerical analysis using linear algebra, a prerequisite for computationally feasible genome scale modelling. Integrating flux, concentration and kinetic parameters in a unified constraint-based formulation is aimed at increasing the quantitative predictive capacity of flux balance analysis.

Incorporation of experimental and theoretical bounds on thermodynamic and kinetic variables ensures that steady state fluxes are both thermodynamically and biochemically feasible. Preliminary numerical results are demonstrated for a genome scale E.coli model with ~1600 metabolites and ~2300 fluxes. Connections between the current approach and the mathematics of differential geometry and algebraic geometry are highlighted.

Venue: Seminar Room, Hamilton Institute, Rye Hall, NUI Maynooth

Time: 2.00 - 3.00pm (followed by tea/coffee)

Travel directions are available at www.hamilton.ie

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