Development of strategies for the optimal control in complex systems

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We present a newly developed "Field induced surface hopping" method (FISH) which combines quantum electronic state population dynamics with classical nuclear dynamics carried out "on the fly". This method can be combined with optimal control in order to steer molecular processes by optimizing laser fields using evolutionary algorithms. For the propagation of classical trajectories the whole spectrum of methods ranging from empirical force fields, semiempirical to ab initio quantum chemical methods can be employed, opening the possibility of broad application in complex systems. Furthermore our approach allows to gain a fundamental insight into the mechanisms underlying the control of molecular processes by direct application of experimentally optimized laser pulses. We illustrate our approach on the optimal control of multiphoton ionization, transcis isomerization and control of photodynamics in biochromophores such as flavins and adenine.