Figure 2

(*a*) Schematic of a coarse time-stepper-based bifurcation analysis. IC, initial condition; PDE, partial differential equation; RPM, recursive projection method. (*b*) Coarse bifurcation diagram (C-KMC) of the CO coverage of system (Equation 12) with respect to β (a parameter that contains the oxygen partial pressure) compared to its mean field (MFA) and quasichemical (QCA) approximations. Triangles give the long time average of full kinetic Monte Carlo simulations. Simulation details and parameters can be found in Reference 67. (*c*) Schematic view of a dynamic renormalization procedure using the coarse time-stepper. Starting with a probability density function (PDF) coarse description, through its cumulative density function (CDF), we lift to particle realizations; after fine-scale evolution, the coarse description is obtained and appropriately rescaled. (*d*) Application to the two-dimensional molecular dynamics simulation of self-diffusion, starting from a coarsely one-dimensional piecewise linear CDF. (*Inset*) A snapshot around the center of the domain at $t = 300$ (*top panel*) and the result of its restriction, rescaling, and lifting (*bottom panel*). Simulation details can be found in Reference 82.