Electronic Supplementary Information

Large-scale benchmarks of the Time-Warp/Graph-Theoretical Kinetic Monte Carlo approach for distributed on-lattice simulations of catalytic kinetics

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Weak-scaling results

In Fig. S1 we reproduce the weak-scaling results of ref. 1 for distributed runs of Systems 1 and 2. The weak-scaling efficiency, η_{WS}, is plotted against the number of lattice sites, n_{sites}. Using the notation introduced in Section 3.2 of the main text, the weak-scaling efficiency can be defined as

$$\eta_{\mathrm{WS}} = \tau^*_{\mathrm{serial}}/\tau^*, \tag{S1}$$

where τ^*_{serial} is the elapsed clock time per unit of KMC time for a serial run of a 100×100 lattice (i.e., the size of one subdomain in the distributed runs).

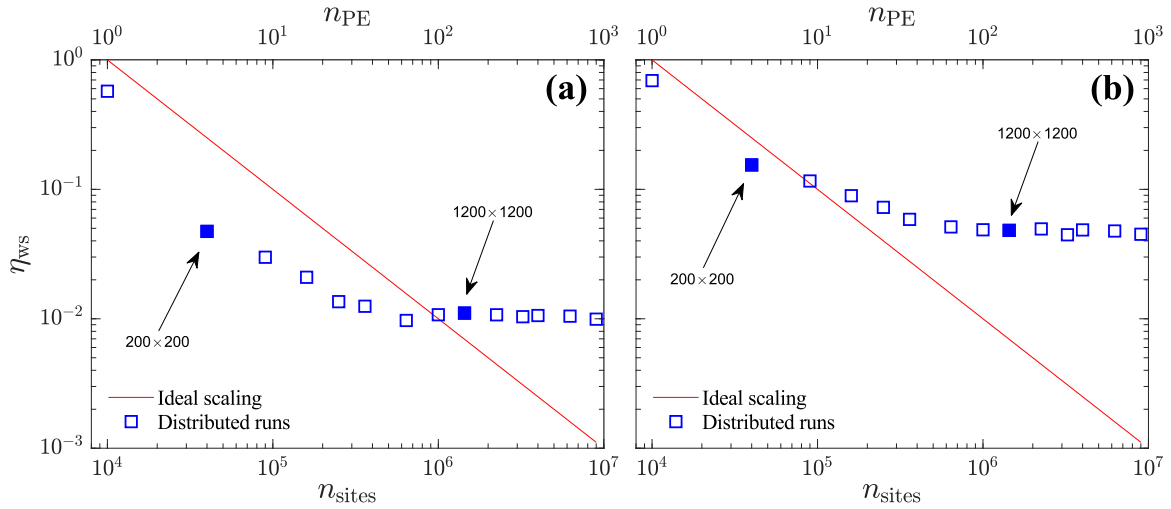

Figure S1 Weak-scaling results from Ref. 1 for distributed runs of (a) System 1 and (b) System 2, as defined in the main text. Desirable behaviour is represented by a constant weak-scaling efficiency, η_{WS}, such that no overheads are incurred as more processors are utilised to simulate progressively larger lattices. For both systems, we observe that a roughly constant efficiency is reached for sufficiently large runs, employing about 60 processors. The data points that correspond to the lattices used in the present study (200×200 and 1200×1200) are plotted using blue filled squares.

References

[1] S. Ravipati, G. D. Savva, I.-A. Christidi, R. Guichard, J. Nielsen, R. Réocreux and M. Stamatakis, *Comput. Phys. Commun.*, 2022, **270**, 108148.