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Dissipation and irreversibility for models of mechanochemical machines AIDAN BROWN, DAVID SIVAK, Simon Fraser University — For biological systems to maintain order and achieve directed progress, they must overcome fluctuations so that reactions and processes proceed forwards more than they go in reverse. It is well known that some free energy dissipation is required to achieve irreversible forward progress, but the quantitative relationship between irreversibility and free energy dissipation is not well understood. Previous studies focused on either abstract calculations or detailed simulations that are difficult to generalize. We present results for mechanochemical models of molecular machines, exploring a range of model characteristics and behaviours. Our results describe how irreversibility and dissipation trade off in various situations, and how this trade-off can depend on details of the model. The irreversibility-dissipation trade-off points towards general principles of microscopic machine operation or process design. Our analysis identifies system parameters which can be controlled to bring performance to the Pareto frontier.

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