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Enhancing MD simulations of proteins using vague and combinatorics information

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We have developed MELD, a method that ‘melds’ together replica-exchange molecular dynamics simulations with external information. Traditionally, accelerating MD simulations has only been possible by using information that is precise and correct. In contrast, MELD allows us to leverage information that is vague or corrupted. For example, we give generic instructives, such as ‘make a hydrophobic core’, ‘make good secondary structures’, or ‘search only compact structures’. Normally, such information implies a loss of ability to compute free energies and populations. But, MELD satisfies detailed balance. We show that it can fold small proteins much faster than brute-force MD can, that it gives reasonable populations, and that it can succeed in CASP, the blind protein-structure prediction event.