Supporting Information

Fast Solver for Large Scale Multistate Bennett Acceptance Ratio Equations

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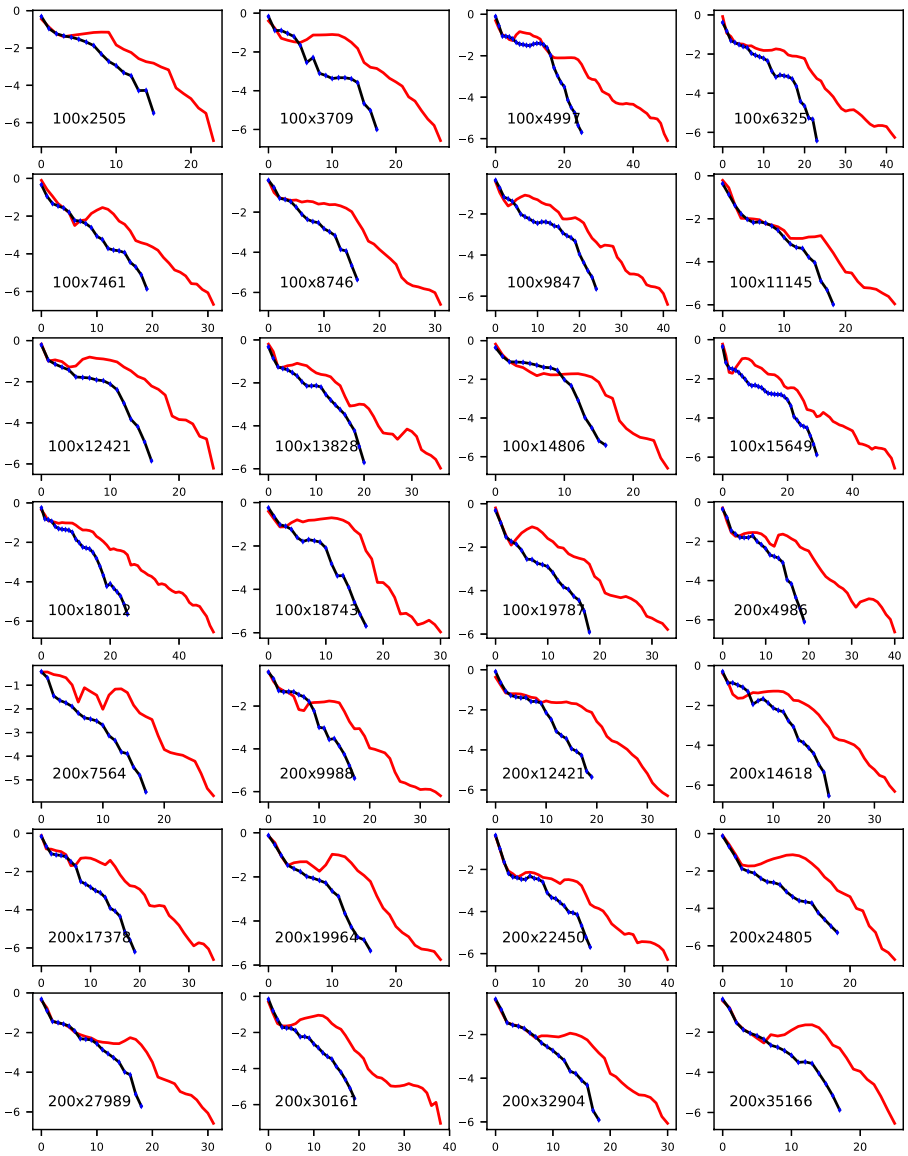

Figure S1: Estimator precision changes with the number of iterations for pymbar (red line), FastMBAR-CPU (black line), and FastMBAR-GPU (blue diamond) to solve MBAR/UWHAM equations of different sizes. All graphs use a log-10 scale for the Y axis. The numbers inside each subplot represent the size of the energy matrix.

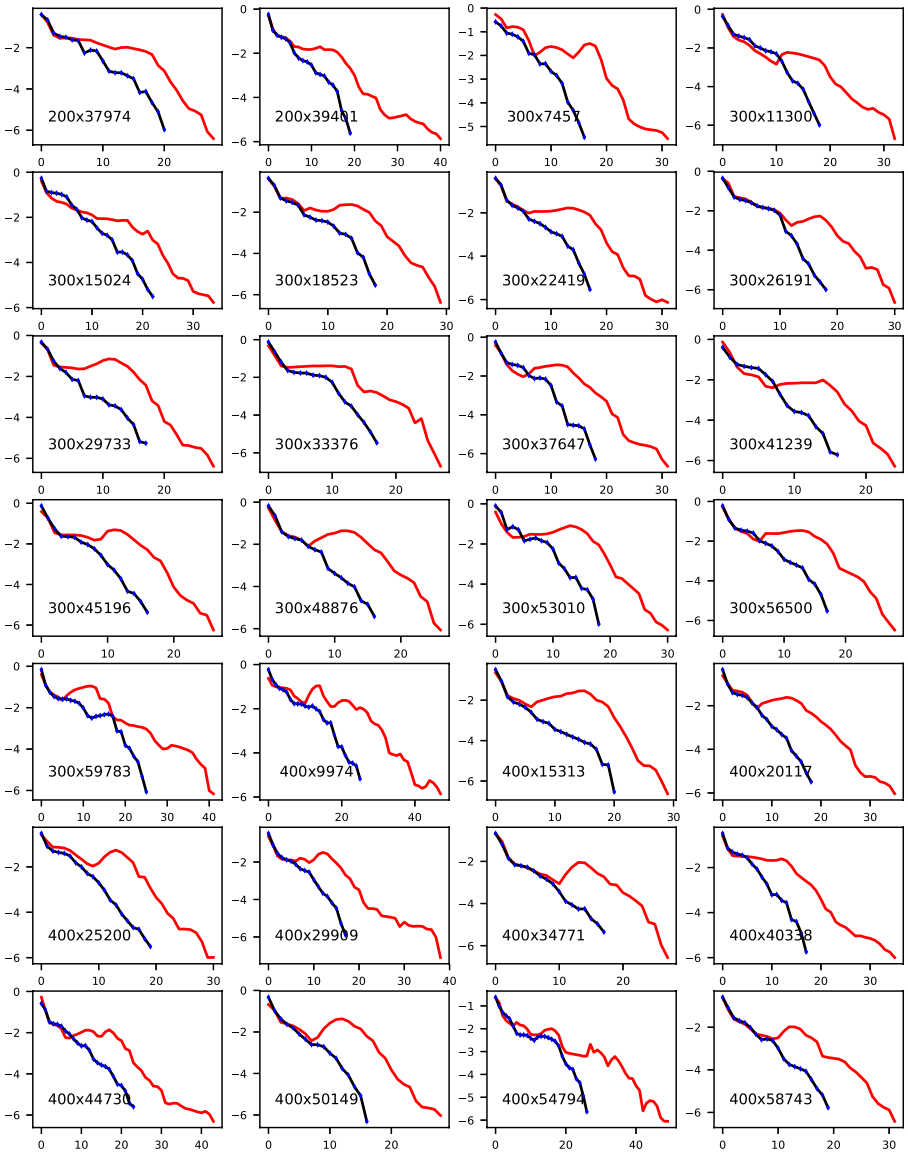

Figure S2: Estimator precision changes with the number of iterations for pymbar (red line), FastMBAR-CPU (black line), and FastMBAR-GPU (blue diamond) to solve MBAR/UWHAM equations of different sizes. All graphs use a log-10 scale for the Y axis. The numbers inside each subplot represent the size of the energy matrix.

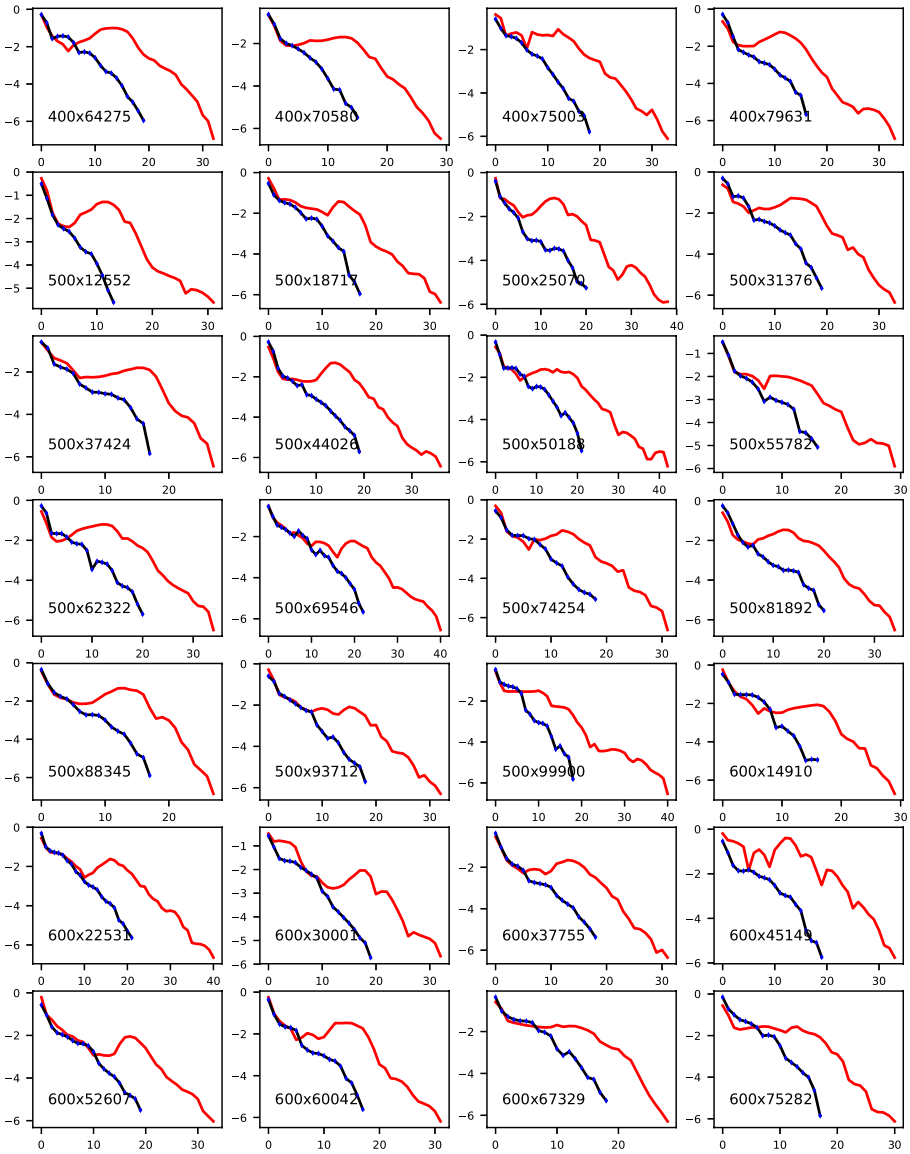

Figure S3: Estimator precision changes with the number of iterations for pymbar (red line), FastMBAR-CPU (black line), and FastMBAR-GPU (blue diamond) to solve MBAR/UWHAM equations of different sizes. All graphs use a log-10 scale for the Y axis. The numbers inside each subplot represent the size of the energy matrix.

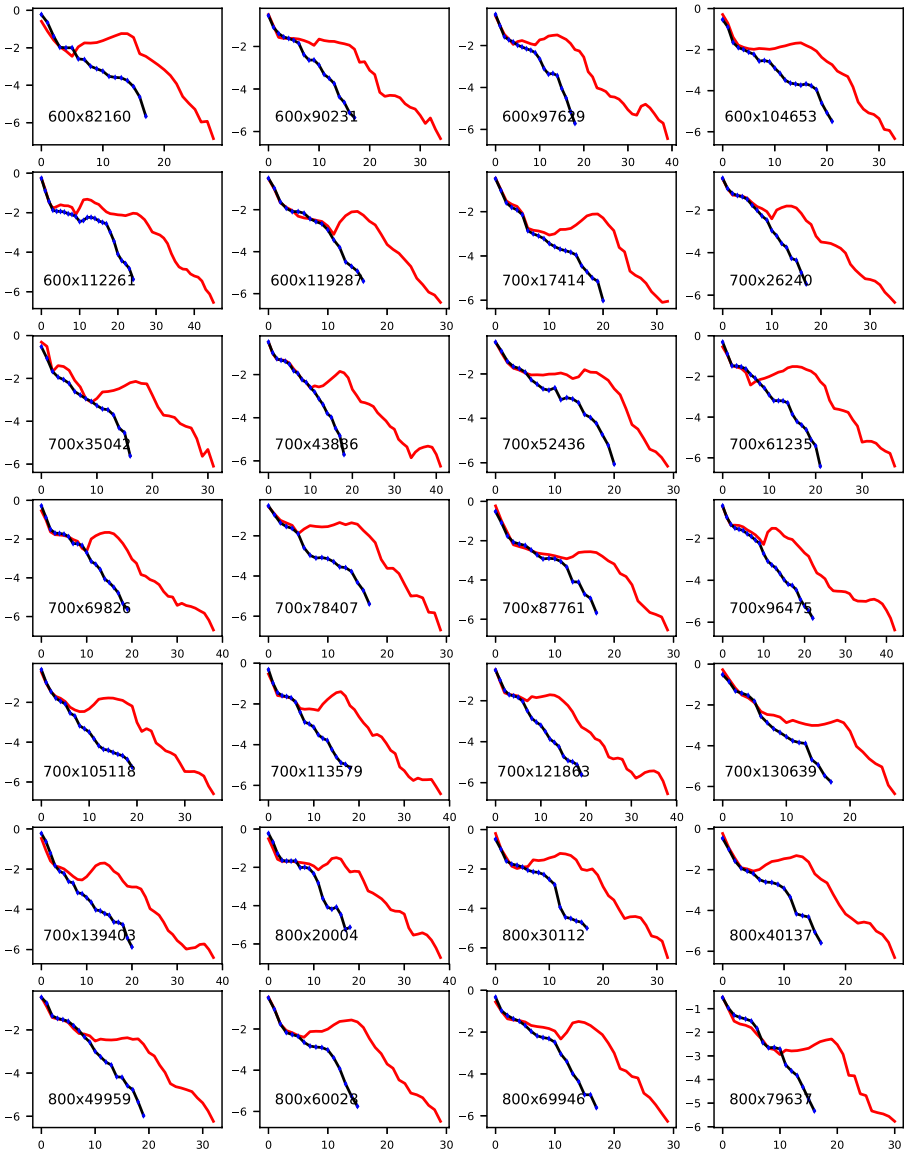

Figure S4: Estimator precision changes with the number of iterations for pymbar (red line), FastMBAR-CPU (black line), and FastMBAR-GPU (blue diamond) to solve MBAR/UWHAM equations of different sizes. All graphs use a log-10 scale for the Y axis. The numbers inside each subplot represent the size of the energy matrix.

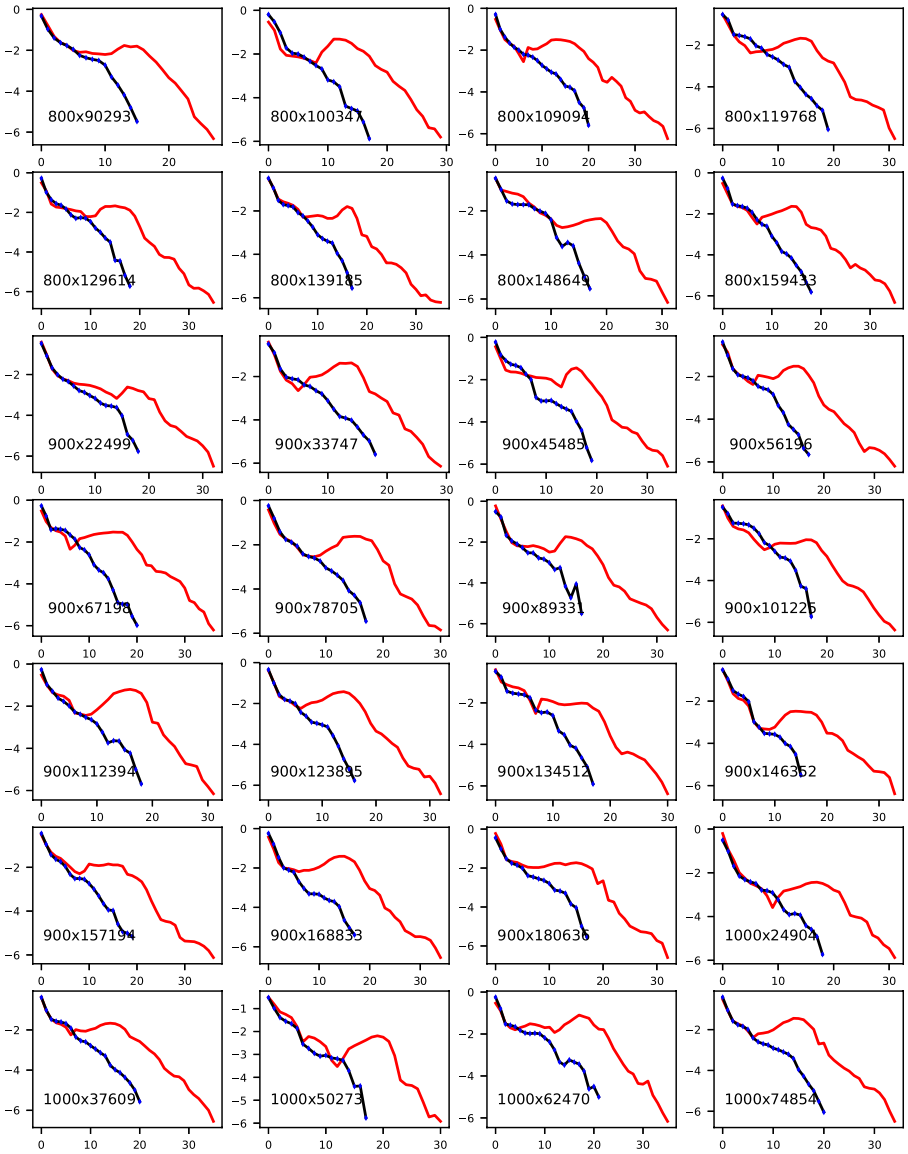

Figure S5: Estimator precision changes with the number of iterations for pymbar (red line), FastMBAR-CPU (black line), and FastMBAR-GPU (blue diamond) to solve MBAR/UWHAM equations of different sizes. All graphs use a log-10 scale for the Y axis. The numbers inside each subplot represent the size of the energy matrix.

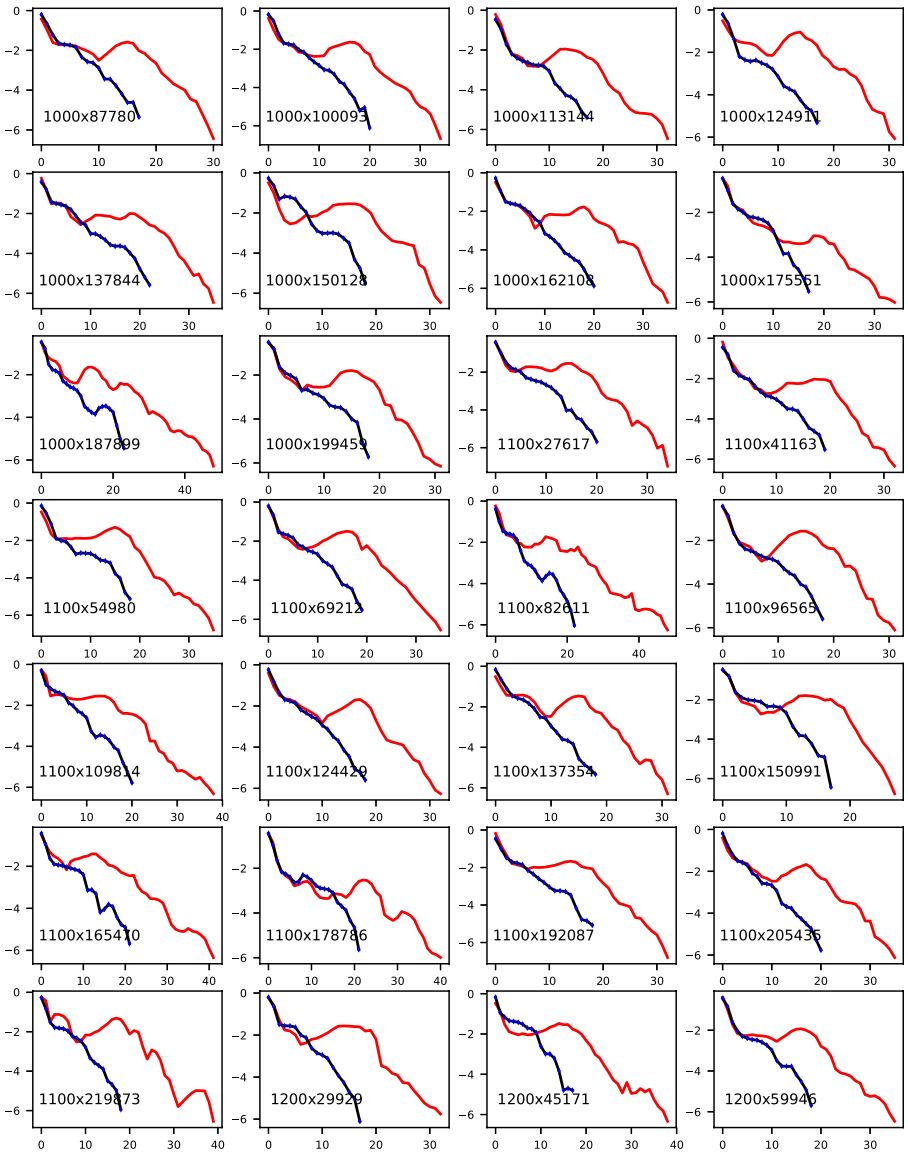

Figure S6: Estimator precision changes with the number of iterations for pymbar (red line), FastMBAR-CPU (black line), and FastMBAR-GPU (blue diamond) to solve MBAR/UWHAM equations of different sizes. All graphs use a log-10 scale for the Y axis. The numbers inside each subplot represent the size of the energy matrix.

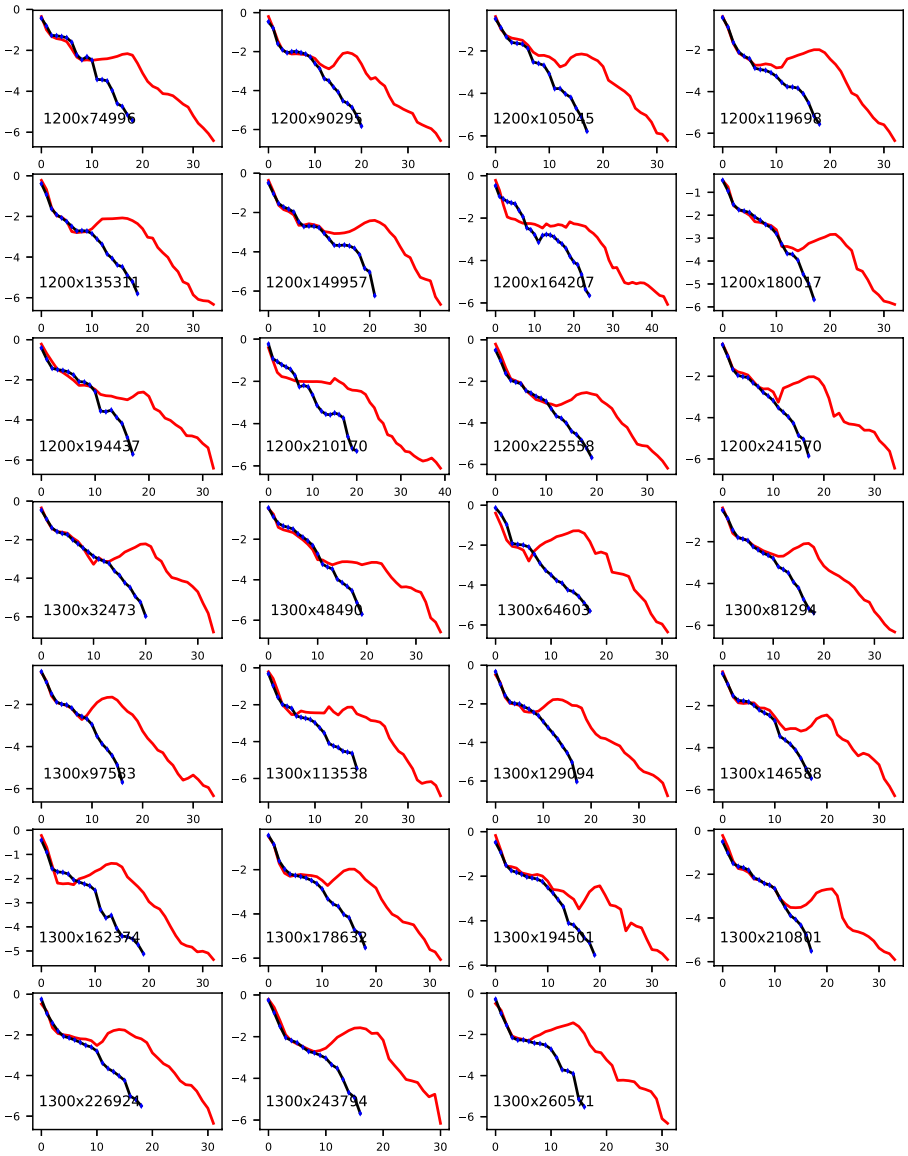

Figure S7: Estimator precision changes with the number of iterations for pymbar (red line), FastMBAR-CPU (black line), and FastMBAR-GPU (blue diamond) to solve MBAR/UWHAM equations of different sizes. All graphs use a log-10 scale for the Y axis. The numbers inside each subplot represent the size of the energy matrix.