An example of the Drexel beamer template

Exploring color schemes and graphics

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Variational Enhanced Sampling

- A free energy surface, $F(\mathbf{s})$, associated with set of collective variables, $\mathbf{s}$, is defined as

$$F(\mathbf{s}) = -(1/\beta)\log\int \mathrm{d}\mathbf{R}\delta(\mathbf{s}-\mathbf{s}(\mathbf{R})e^{-\beta U(\mathbf{R})} \tag{1}$$

- Valsson and Parrinello introduce a functional of bias potential $V(\mathbf{s})$,

$$\Omega[V] = \frac{1}{\beta}\log\frac{\int \mathrm{d}\mathbf{s}e^{-\beta[F(\mathbf{s})+V(\mathbf{s})]}}{\int \mathrm{d}\mathbf{s}e^{-\beta F(\mathbf{s})}} + \int \mathrm{d}\mathbf{s}p(\mathbf{s})V(\mathbf{s}) \tag{2}$$

where $p(\mathbf{s})$ is an arbitrary probability distribution (normalized).
$\Rightarrow \Omega[V]$ is convex!

- The potential which renders $\Omega[V]$ stationary is (to within a constant):

$$V(\mathbf{s}) = -F(\mathbf{s}) - (1/\beta)\log p(\mathbf{s}) \tag{3}$$

Valsson, Parrinello. (2014) PRL 113,090601

Variational Enhanced Sampling

1. Write bias potential $V(\mathbf{s};\boldsymbol{\alpha})$ as function of variational parameters $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, ..., \alpha_K)$
2. Minimize $\Omega[V(\boldsymbol{\alpha})]$ with respect to $\boldsymbol{\alpha}$ using the gradient $\Omega'(\boldsymbol{\alpha})$ and Hessian $\Omega''(\boldsymbol{\alpha})$,

$$\frac{\partial \Omega}{\partial \alpha_i} = -\left\langle \frac{\partial V(\mathbf{s};\boldsymbol{\alpha})}{\partial \alpha_i} \right\rangle_{V(\boldsymbol{\alpha})} + \left\langle \frac{\partial V(\mathbf{s};\boldsymbol{\alpha})}{\partial \alpha_i} \right\rangle_{p} \tag{4}$$

$$\frac{\partial^2 \Omega(\boldsymbol{\alpha})}{\partial \alpha_j \partial \alpha_i} = \beta \mathrm{Cov}\left[\frac{\partial V(\mathbf{s};\boldsymbol{\alpha})}{\partial \alpha_j}; \frac{\partial V(\mathbf{s};\boldsymbol{\alpha})}{\partial \alpha_i}\right]_{V(\boldsymbol{\alpha})} - \left\langle \frac{\partial^2 V(\mathbf{s};\boldsymbol{\alpha})}{\partial \alpha_j \partial \alpha_i} \right\rangle_{V(\boldsymbol{\alpha})} + \left\langle \frac{\partial^2 V(\mathbf{s};\boldsymbol{\alpha})}{\partial \alpha_j \partial \alpha_i} \right\rangle_{p} \tag{5}$$

   where $\langle ... \rangle_{V(\boldsymbol{\alpha})}$ and $\langle ... \rangle_{p(\mathbf{s})}$ are the expectation value obtained in a biased simulation with potential $V(\mathbf{s};\boldsymbol{\alpha})$ and distribution $p(\mathbf{s})$, respectively
3. Use stochastic gradient descent-based algoritm to iterate $\boldsymbol{\alpha}$
   $\Rightarrow$ In practice, only the diagonal of the Hessian is used during optimization

Valsson, Parrinello. (2014) PRL 113,090601

Block copolymers are awesome

They can assemble into so many different morphologies

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This title is approximately 47 characters. ABCD

Note no logo!