CE 530 Molecular Simulation

Lecture 21

Histogram Reweighting Methods

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Histogram Reweighting

- Method to combine results taken at different state conditions
- Microcanonical ensemble

$$\Omega(E,V,N)=\sum_{\substack{micro\\states}} 1$$

- Canonical ensemble

$$\pi(\mathbf{r}^N,\mathbf{p}^N)=\frac{1}{Q}e^{-\beta E}$$

Probability of a microstate

$$\pi(E;\beta)=\Omega(E)\frac{e^{-\beta E}}{Q(\beta)}$$

Probability of an energy

Number of microstates having this energy

Probability of each microstate

- The big idea:
  - *Combine simulation data at different temperatures to improve quality of all data via their mutual relation to Ω(E)*

In-class Problem 1.

○ Consider three energy levels

$$\begin{aligned} \Omega_0 &= 1 & E_0 &= 0 = \ln 1 \\ \Omega_1 &= 100 & E_1 &= 2.3 = \ln 10 \\ \Omega_2 &= 1000 & E_2 &= 6.9 = \ln 1000 \end{aligned}$$

○ What are Q, distribution of states and <E> at $\beta = 1$?

In-class Problem 1A.

- ○ Consider three energy levels

$$\begin{aligned} \Omega_0 &= 1 & E_0 &= 0 = \ln 1 \\ \Omega_1 &= 100 & E_1 &= 2.3 = \ln 10 \\ \Omega_2 &= 1000 & E_2 &= 6.9 = \ln 1000 \end{aligned}$$

- ○ What are Q, distribution of states and <E> at β = 1?

$$\begin{aligned} Q &= \Omega_0 e^{-\beta E_0} + \Omega_1 e^{-\beta E_1} + \Omega_2 e^{-\beta E_2} \\ &= 1e^{-\ln 1} + 100e^{-\ln 10} + 1000e^{-\ln 1000} \\ &= 1\times 1 + 100\times 0.1 + 1000\times 0.001 \\ &= 12 \end{aligned}$$

$$\pi_0 = \frac{\Omega_0 e^{-\beta E_0}}{Q} = \frac{1}{12} = 0.083$$

$$\pi_1 = \frac{\Omega_1 e^{-\beta E_1}}{Q} = \frac{10}{12} = 0.833$$

$$\pi_2 = \frac{\Omega_2 e^{-\beta E_2}}{Q} = \frac{1}{12} = 0.083$$

$$\begin{aligned} \langle E \rangle &= \sum \pi_i E_i \\ &= 0.083\times 0 \\ &\quad +0.833\times 2.3 \\ &\quad +0.083\times 6.9 \\ &= 2.49 \end{aligned}$$

In-class Problem 1A.

- Consider three energy levels

$$\begin{aligned} \Omega_0 &= 1 & E_0 &= 0 = \ln 1 \\ \Omega_1 &= 100 & E_1 &= 2.3 = \ln 10 \\ \Omega_2 &= 1000 & E_2 &= 6.9 = \ln 1000 \end{aligned}$$

- What are Q, distribution of states and <E> at β = 1?

$$\begin{aligned} Q &= \Omega_0 e^{-\beta E_0} + \Omega_1 e^{-\beta E_1} + \Omega_2 e^{-\beta E_2} \\ &= 1e^{-\ln 1} + 100e^{-\ln 10} + 1000e^{-\ln 1000} \\ &= 1\times 1 + 100\times 0.1 + 1000\times 0.001 \\ &= 12 \end{aligned}$$

$$\pi_0 = \frac{\Omega_0 e^{-\beta E_0}}{Q} = \frac{1}{12} = 0.083$$

$$\pi_1 = \frac{\Omega_1 e^{-\beta E_1}}{Q} = \frac{10}{12} = 0.833$$

$$\pi_2 = \frac{\Omega_2 e^{-\beta E_2}}{Q} = \frac{1}{12} = 0.083$$

$$\begin{aligned} \langle E \rangle &= \sum \pi_i E_i \\ &= 0.083\times 0 \\ &\quad + 0.833\times 2.3 \\ &\quad + 0.083\times 6.9 \\ &= 2.49 \end{aligned}$$

- And at β = 3?

$$\begin{aligned} Q &= 1e^{-3\ln 1} + 100e^{-3\ln 10} + 1000e^{-3\ln 1000} \\ &= 1\times 1 + 100\times 0.001 + 1000\times 1000^{-3} \\ &= 1.1 \end{aligned}$$

$$\pi_0 = \frac{1}{1.1} = 0.91$$

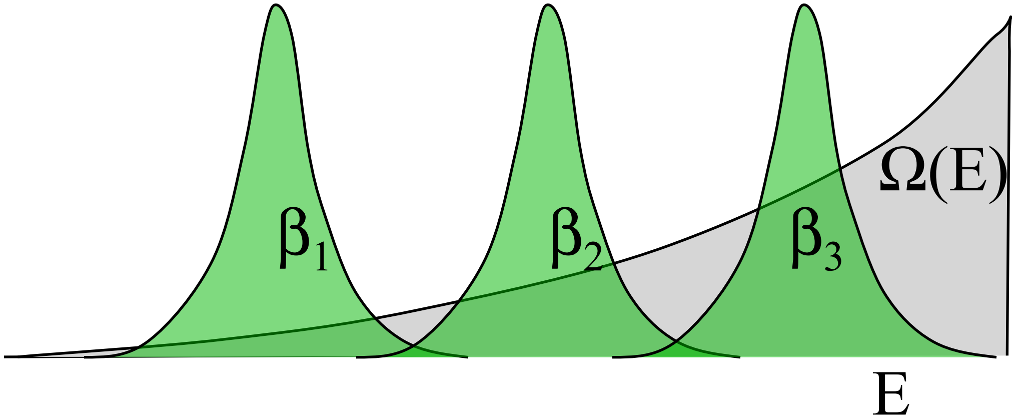
$$\pi_1 = \frac{1}{1.1} = 0.09$$

$$\pi_2 = \frac{0.0}{1.1} = 0.00$$

$$\begin{aligned} \langle E \rangle &= 0.91\times 0 \\ &\quad + 0.09\times 2.3 \\ &\quad + 0.00\times 6.9 \\ &= 0.21 \end{aligned}$$

Histogram Reweighting Approach

- Knowledge of Ω(E) can be used to obtain averages at any temperature



- Simulations at different temperatures probe different parts of Ω(E)
- But simulations at each temperature provides information over a range of values of Ω(E)
- Combine simulation data taken at different temperatures to obtain better information for each temperature

In-class Problem 2.

- Consider simulation data from a system having three energy levels
  - $M = 100$ samples taken at $\beta = 0.5$
  - m_i times observed in level i

$$m_0 = 4 \qquad E_0 = 0 = \ln 1$$
$$m_1 = 46 \qquad E_1 = 2.3 = \ln 100$$
$$m_2 = 50 \qquad E_2 = 9.2 = \ln 10000$$

- What is $\Omega(E)$?

In-class Problem 2.

- Consider simulation data from a system having three energy levels
  - *$M = 100$ samples taken at $\beta = 0.5$*
  - *m_i times observed in level i*

$m_0 = 4 \qquad E_0 = 0 = \ln 1$

$m_1 = 46 \qquad E_1 = 2.3 = \ln 100$

$m_2 = 50 \qquad E_2 = 9.2 = \ln 10000$

- What is Ω (E)?

Reminder $\pi(E) = \Omega(E)\dfrac{e^{-\beta E}}{Q(\beta)}$

In-class Problem 2.

- Consider simulation data from a system having three energy levels
  - *M = 100 samples taken at* $\beta = 0.5$
  - m_i *times observed in level i*

$$\begin{array}{ll} m_0 = 4 & E_0 = 0 = \ln 1 \\ m_1 = 46 & E_1 = 2.3 = \ln 100 \\ m_2 = 50 & E_2 = 9.2 = \ln 10000 \end{array}$$

- What is Ω (E)?

Hint $$\pi(E) = \left(\frac{\Omega(E)}{Q(\beta)}\right) e^{-\beta E}$$

Can get only relative values!

In-class Problem 2A.

- Consider simulation data from a system having three energy levels
  - *M = 100 samples taken at β = 0.5*
  - *m_i times observed in level i*

$m_0 = 4$	$E_0 = 0 = \ln 1$
$m_1 = 46$	$E_1 = 2.3 = \ln 100$
$m_2 = 50$	$E_2 = 9.2 = \ln 10000$

- What is Ω(E)?

$$\Omega_0 = \frac{m_0}{M} e^{+\beta U_0} Q_A = 0.04 \times 1^{0.5} Q = .04 Q_A$$

$$\Omega_1 = \frac{m_1}{M} e^{+\beta U_1} Q_A = 0.46 \times 100^{0.5} Q = 4.6 Q_A$$

$$\Omega_2 = \frac{m_2}{M} e^{+\beta U_2} Q_A = 0.50 \times 10000^{0.5} Q = 50 Q_A$$

$$Q_A \equiv Q(\beta = 0.5)$$

In-class Problem 3.

- Consider simulation data from a system having three energy levels
  - *M = 100 samples taken at* $\beta = 0.5$
  - m_i *times observed in level i*

$$\begin{array}{ll} m_0 = 4 & E_0 = 0 = \ln 1 \\ m_1 = 46 & E_1 = 2.3 = \ln 100 \\ m_2 = 50 & E_2 = 9.2 = \ln 10000 \end{array}$$

- What is Ω(E)?

$$\Omega_0 = \frac{m_0}{M} e^{+\beta U_0} Q_A = 0.04 \times 1^{0.5} Q_A = .04 Q_A$$

$$Q_A \equiv Q(\beta = 0.5)$$

$$\Omega_1 = \frac{m_1}{M} e^{+\beta U_1} Q_A = 0.46 \times 100^{0.5} Q_A = 4.6 Q_A$$

$$\Omega_2 = \frac{m_2}{M} e^{+\beta U_2} Q_A = 0.50 \times 10000^{0.5} Q_A = 50 Q_A$$

- Here's some more data, taken at β = 1 $m_0 = 50 \quad m_1 = 48 \quad m_2 = 2$
  - *what is* Ω(E)*?*

In-class Problem 3.

- Consider simulation data from a system having three energy levels
  - *M = 100 samples taken at β = 0.5*
  - *m_i times observed in level i*

$$\begin{array}{ll} m_0 = 4 & E_0 = 0 = \ln 1 \\ m_1 = 46 & E_1 = 2.3 = \ln 100 \\ m_2 = 50 & E_2 = 9.2 = \ln 10000 \end{array}$$

- What is Ω (E)?

$$\Omega_0 = \tfrac{m_0}{M} e^{+\beta U_0} Q_A = 0.04 \times 1^{0.5} Q_A = .04 Q_A$$

$$Q_A \equiv Q(\beta = 0.5)$$

$$\Omega_1 = \tfrac{m_1}{M} e^{+\beta U_1} Q_A = 0.46 \times 100^{0.5} Q_A = 4.6 Q_A$$

$$\Omega_2 = \tfrac{m_2}{M} e^{+\beta U_2} Q_A = 0.50 \times 10000^{0.5} Q_A = 50 Q_A$$

- Here's some more data, taken at β = 1 $m_0 = 50 \quad m_1 = 48 \quad m_2 = 2$
  - *what is Ω(E)?*

$$Q_B \equiv Q(\beta = 1.0)$$

$$\Omega_0 = 0.50 \times 1 Q_B = .50 Q_B$$

$$\Omega_1 = 0.48 \times 100 Q_B = 48 Q_B$$

$$\Omega_2 = 0.02 \times 10000 Q_B = 200 Q_B$$

Reconciling the Data

- We have two data sets

$$\begin{array}{ll} \Omega_0 = .04Q_A & \Omega_0 = .50Q_B \\ \Omega_1 = 4.6Q_A & \Omega_1 = 48Q_B \\ \Omega_2 = 50Q_A & \Omega_2 = 200Q_B \end{array}$$

- Questions of interest
  - *what is the ratio* Q_A/Q_B*? (which then gives us* ΔA*)*
  - *what is the best value of* Ω_1/Ω_0, Ω_2/Ω_0*?*
  - *what is the average energy at* $\beta = 2$*?*
- In-class Problem 4
  - *make an attempt to answer these questions*

In-class Problem 4A.

- We have two data sets

$$\Omega_0 = .04Q_A \qquad \Omega_0 = .50Q_B$$
$$\Omega_1 = 4.6Q_A \qquad \Omega_1 = 48Q_B$$
$$\Omega_2 = 50Q_A \qquad \Omega_2 = 200Q_B$$

- What is the ratio Q_A/Q_B? (which then gives us ΔA)
  - *Consider values from each energy level*

$$\frac{\Omega_0}{\Omega_0} = \frac{0.04Q_A}{0.50Q_B} \qquad \frac{\Omega_1}{\Omega_1} = \frac{4.6Q_A}{48Q_B} \qquad \frac{\Omega_2}{\Omega_2} = \frac{50Q_A}{200Q_B}$$

$$\frac{Q_A}{Q_B} = \frac{0.50}{0.04} = 12.5 \qquad \frac{Q_A}{Q_B} = \frac{48}{4.6} = 10.4 \qquad \frac{Q_A}{Q_B} = \frac{200}{50} = 4$$

- What is the best value of Ω_1/Ω_0, Ω_2/Ω_0?
  - *Consider values from each temperature*

$\beta = 0.5$	$\frac{\Omega_1}{\Omega_0} = \frac{4.6Q_A}{0.04Q_A} = 115$	$\frac{\Omega_2}{\Omega_0} = \frac{50Q_A}{0.04Q_A} = 1250$
$\beta = 1$	$\frac{\Omega_1}{\Omega_0} = \frac{48Q_B}{0.05Q_B} = 96$	$\frac{\Omega_2}{\Omega_0} = \frac{200Q_B}{0.5Q_B} = 400$

- What to do?

Accounting for Data Quality

- Remember the number of samples that went into each value

$$\Omega_0 = .04Q_A \quad m_0 = 4 \qquad \Omega_0 = .50Q_B \quad m_0 = 50$$
$$\Omega_1 = 4.6Q_A \quad m_1 = 46 \qquad \Omega_1 = 48Q_B \quad m_1 = 48$$
$$\Omega_2 = 50Q_A \quad m_2 = 50 \qquad \Omega_2 = 200Q_B \quad m_2 = 2$$

  - *We expect the A-state data to be good for levels 1 and 2*
  - *…while the B-state data are good for levels 0 and 1*
- Write each Ω as an average of all values, weighted by quality of result

$$\begin{aligned}\Omega_0^{est} &= w_A\Omega_{0,A}^{est} + w_B\Omega_{0,B}^{est}\\ &= w_A\left(e^{\beta_A U_0} Q_A \frac{m_{0,A}}{M_A}\right) + w_B\left(e^{\beta_B U_0} Q_B \frac{m_{0,B}}{M_B}\right)\end{aligned}$$

$$\pi(E) = \Omega(E)\frac{e^{-\beta E}}{Q(\beta)}$$

Histogram Variance

- Estimate confidence in each simulation result

$$\Omega_0 = .04Q_A \quad m_0 = 4 \qquad \Omega_0 = .50Q_B \quad m_0 = 50$$

$$\Omega_1 = 4.6Q_A \quad m_1 = 46 \qquad \Omega_1 = 48Q_B \quad m_1 = 48$$

$$\Omega_2 = 50Q_A \quad m_2 = 50 \qquad \Omega_2 = 200Q_B \quad m_2 = 2$$

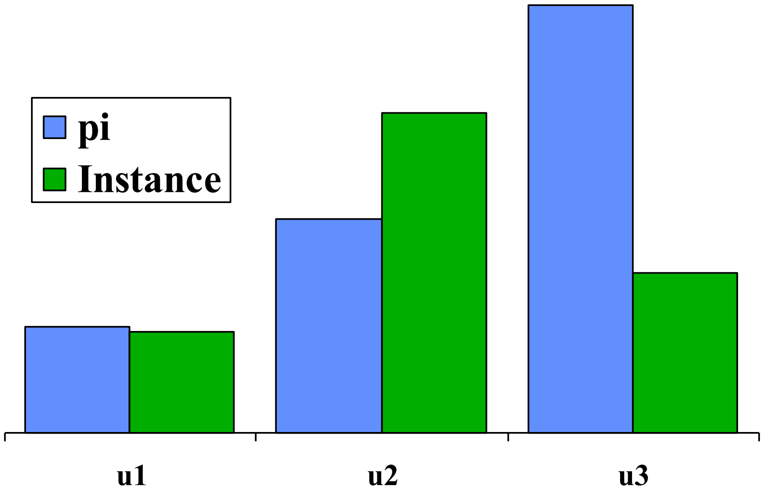
- Assume each histogram follows a Poisson distribution
  - *probability P to observe any given instance of distribution*

$$P[\{m_i\}] = M!\prod \frac{\pi_i^{m_i}}{m_i!}$$

$$P[\{m_1, m_2, m_3\}] = M!\frac{\pi_1^{m_1}\pi_2^{m_2}\pi_3^{m_3}}{m_1!m_2!m_3!}$$

  - *the variance for each bin is*

$$\sigma_{m_i}^2 = m_i = M\pi_i$$



Variance in Estimate of Ω

- Formula for estimate of Ω

$$\Omega_0^{est} = w_A e^{\beta_A E_0} Q_A \frac{m_{0,A}}{M_A} + w_B e^{\beta_B E_0} Q_B \frac{m_{0,B}}{M_B}$$

- Variance

$$\begin{aligned}\sigma^2_{\Omega_0^{est}} &= w_A^2 e^{2\beta_A E_0} Q_A^2 \frac{1}{M_A^2} \sigma^2_{m_{0,A}} + w_B^2 e^{2\beta_B E_0} Q_B^2 \frac{1}{M_B^2} \sigma^2_{m_{0,B}} \\ &= w_A^2 e^{2\beta_A E_0} Q_A^2 \frac{1}{M_A^2} \left(M_A \pi_{0,A} \right) + w_B^2 e^{2\beta_B E_0} Q_B^2 \frac{1}{M_B^2} \left(M_B \pi_{0,B} \right) \\ &= w_A^2 e^{2\beta_A E_0} Q_A^2 \frac{1}{M_A} \left(\frac{\Omega_0 e^{-\beta_A E_0}}{Q_A} \right) + w_B^2 e^{2\beta_B E_0} Q_B^2 \frac{1}{M_B} \left(\frac{\Omega_0 e^{-\beta_B E_0}}{Q_B} \right) \\ &= w_A^2 \Omega_0 e^{\beta_A E_0} Q_A \frac{1}{M_A} + w_B^2 \Omega_0 e^{\beta_B E_0} Q_B \frac{1}{M_B}\end{aligned}$$

$$\pi(E) = \Omega(E) \frac{e^{-\beta E}}{Q(\beta)}$$

Optimizing Weights

- Variance

$$\sigma^2_{\Omega_0^{est}} = w_A^2 \Omega_0 e^{\beta_A E_0} Q_A \frac{1}{M_A} + w_B^2 \Omega_0 e^{\beta_B E_0} Q_B \frac{1}{M_B}$$

- Minimize with respect to weight, subject to normalization
  - *In-class Problem 5*

    Do it!

Optimizing Weights

- Variance

$$\sigma^2_{\Omega_0^{est}} = w_A^2 \Omega_0 e^{\beta_A E_0} Q_A \frac{1}{M_A} + w_B^2 \Omega_0 e^{\beta_B E_0} Q_B \frac{1}{M_B}$$

- Minimize with respect to weight, subject to normalization
  - *Lagrange multiplier*

$$Min\left[\sigma^2_{\Omega_0^{est}} - \lambda\left(\sum w_a - 1\right)\right]$$

$$\pi(E) = \Omega(E)\frac{e^{-\beta E}}{Q(\beta)} \approx \frac{m_i}{M}$$

- Equation for each weight is $2 w_a \Omega_0 e^{\beta_a E_0} \frac{Q_a}{M_a} = \lambda$
- Rearrange

$$w_a = \lambda \frac{1}{2\Omega_0} \frac{e^{-\beta_a E_0} M_a}{Q_a}$$

- Normalize

$$w_a = \frac{e^{-\beta_a E_0} M_a / Q_a}{\frac{e^{-\beta_A E_0} M_A}{Q_A} + \frac{e^{-\beta_B E_0} M_B}{Q_B}}$$

Optimal Estimate

- Collect results

$$\Omega_0^{est} = w_A e^{\beta_A E_0} Q_A \frac{m_{0,A}}{M_A} + w_B e^{\beta_B E_0} Q_B \frac{m_{0,B}}{M_B}$$

$$w_a = \frac{e^{-\beta_a E_0} M_a / Q_a}{\frac{e^{-\beta_A E_0} M_A}{Q_A} + \frac{e^{-\beta_B E_0} M_B}{Q_B}}$$

- Combine

$$\Omega_0^{est} = \left[\frac{e^{-\beta_A E_0} M_A}{Q_A} + \frac{e^{-\beta_B E_0} M_B}{Q_B} \right]^{-1} \left[\left(\frac{e^{-\beta_A E_0} M_A}{Q_A} \right) e^{\beta_A E_0} Q_A \frac{m_{0,A}}{M_A} + \left(\frac{e^{-\beta_B E_0} M_B}{Q_B} \right) e^{\beta_B E_0} Q_B \frac{m_{0,B}}{M_B} \right]$$

$$= \left[\frac{e^{-\beta_A E_0} M_A}{Q_A} + \frac{e^{-\beta_B E_0} M_B}{Q_B} \right]^{-1} \left[m_{0,A} + m_{0,B} \right]$$

Calculating Ω

- Formula for Ω

$$\Omega_0^{est} = \left[\frac{e^{-\beta_A E_0} M_A}{Q_A} + \frac{e^{-\beta_B E_0} M_B}{Q_B} \right]^{-1} \left[m_{0,A} + m_{0,B} \right]$$

- In-class Problem 6
  - *explain why this formula cannot yet be used*

Calculating Ω

- Formula for Ω

$$\Omega_0^{est} = \left[\frac{e^{-\beta_A E_0} M_A}{Q_A} + \frac{e^{-\beta_B E_0} M_B}{Q_B}\right]^{-1} \left[m_{0,A} + m_{0,B}\right]$$

- We do not know the Q partition functions

$$Q_a = \Omega_0 e^{-\beta_a E_0} + \Omega_1 e^{-\beta_a E_1} + \Omega_2 e^{-\beta_a E_2}$$

$$\Omega_0^{est} = \left[\frac{e^{-\beta_A E_0} M_A}{\Omega_0 e^{-\beta_A E_0} + \Omega_1 e^{-\beta_A E_1} + \Omega_2 e^{-\beta_A E_2}} + \frac{e^{-\beta_B E_0} M_B}{\Omega_0 e^{-\beta_B E_0} + \Omega_1 e^{-\beta_B E_1} + \Omega_2 e^{-\beta_B E_2}}\right]^{-1} \left[m_{0,A} + m_{0,B}\right]$$

- One equation for each Ω
- Each equation depends on all Ω
- Requires iterative solution

In-class Problem 7

- Write the equations for each Ω using the example values

$$\Omega_0^{est} = \left[\frac{e^{-\beta_A E_0} M_A}{\Omega_0 e^{-\beta_A E_0} + \Omega_1 e^{-\beta_A E_1} + \Omega_2 e^{-\beta_A E_2}} + \frac{e^{-\beta_B E_0} M_B}{\Omega_0 e^{-\beta_B E_0} + \Omega_1 e^{-\beta_B E_1} + \Omega_2 e^{-\beta_B E_2}} \right]^{-1} \left[m_{0,A} + m_{0,B} \right]$$

$\underline{\beta = 0.5}$	$\underline{\beta = 1}$		
$m_0 = 4$	$m_0 = 50$	$E_0 = 0 = \ln 1$	$M_A = M_B = 100$
$m_1 = 46$	$m_1 = 48$	$E_1 = 2.3 = \ln 100$	
$m_2 = 50$	$m_2 = 2$	$E_2 = 9.2 = \ln 10000$	

In-class Problem 7

- Write the equations for each Ω using the example values

$$\Omega_0^{est}=\left[\frac{e^{-\beta_A E_0}M_A}{\Omega_0 e^{-\beta_A E_0}+\Omega_1 e^{-\beta_A E_1}+\Omega_2 e^{-\beta_A E_2}}+\frac{e^{-\beta_B E_0}M_B}{\Omega_0 e^{-\beta_B E_0}+\Omega_1 e^{-\beta_B E_1}+\Omega_2 e^{-\beta_B E_2}}\right]^{-1}\left[m_{0,A}+m_{0,B}\right]$$

$$\begin{array}{llll}
\underline{\beta=0.5} & \underline{\beta=1} & & \\
m_0=4 & m_0=50 & E_0=0=\ln 1 & M_A=M_B=100 \\
m_1=46 & m_1=48 & E_1=2.3=\ln 100 & \\
m_2=50 & m_2=2 & E_2=9.2=\ln 10000 &
\end{array}$$

$$\Omega_0^{est}=\left[\frac{1\times100}{1\Omega_0+0.1\Omega_1+0.01\Omega_2}+\frac{1\times100}{1\Omega_0+0.01\Omega_1+0.0001\Omega_2}\right]^{-1}[4+50]$$

$$\Omega_1^{est}=\left[\frac{0.1\times100}{1\Omega_0+0.1\Omega_1+0.01\Omega_2}+\frac{0.01\times100}{1\Omega_0+0.01\Omega_1+0.0001\Omega_2}\right]^{-1}[46+48]$$

$$\Omega_2^{est}=\left[\frac{0.01\times100}{1\Omega_0+0.1\Omega_1+0.01\Omega_2}+\frac{0.0001\times100}{1\Omega_0+0.01\Omega_1+0.0001\Omega_2}\right]^{-1}[50+2]$$

- Solution

$$\frac{\Omega_1}{\Omega_0}=94.7 \qquad \frac{\Omega_2}{\Omega_0}=943.2$$

In-class Problem 7A.

- Solution

$$\frac{\Omega_1}{\Omega_0} = 94.7 \quad \frac{\Omega_2}{\Omega_0} = 943.2$$

(?)

$\beta = 0.5$	$\beta = 1$
$m_0 = 4$	$m_0 = 50$
$m_1 = 46$	$m_1 = 48$
$m_2 = 50$	$m_2 = 2$

- Compare

$$\beta = 0.5 \quad \frac{\Omega_1}{\Omega_0} = \frac{4.6Q_A}{0.04Q_A} = 115 \quad \frac{\Omega_2}{\Omega_0} = \frac{50Q_A}{0.04Q_A} = 1250$$

$$\beta = 1 \quad \frac{\Omega_1}{\Omega_0} = \frac{48Q_B}{0.05Q_B} = 96 \quad \frac{\Omega_2}{\Omega_0} = \frac{200Q_B}{0.5Q_B} = 400$$

- "Exact" solution

$$\frac{\Omega_1}{\Omega_0} = 100 \quad \frac{\Omega_2}{\Omega_0} = 1000$$

- Free energy difference

$$\frac{Q_A}{Q_B} = \frac{1\Omega_0 + 0.1\Omega_1 + 0.01\Omega_2}{1\Omega_0 + 0.01\Omega_1 + 0.0001\Omega_2} = 9.74$$

"Design value" = 10

Extensions of Technique

○ Method is usually used in multidimensional form

○ Useful to apply to grand-canonical ensemble

$$\Xi = \sum_N e^{\beta\mu N} \frac{1}{h^{3N} N!} \int d\mathbf{r}^N d\mathbf{p}^N e^{-\beta E}$$

$$= \sum_N \sum_U \Omega(U,V,N) e^{\beta\mu N} e^{-\beta E}$$

○ Can then be used to relate simulation data at different temperature and chemical potential

○ Many other variations are possible