An Example Calculation of the Distributed Replica Potential Energy (DRPE):

There are five possible temperatures in this case (λ_i) which are exponentially spaced. There are five corresponding values for $\lambda_{i,\,unit}$ which are uniformly spaced:

$\lambda_{i,\,unit}$ (uniform spacing)	1	2	3	4	5
λ_i (temperatures, K)	280	288	296	305	314

There are five replicas of the system, and their temperatures currently are: 305K, 296K, 288K, 280K, and 288K. The move which will be attempted will be for replica 1 to change its temperature from 305K to 296K. First we compute the DRPE for the current state:

STEP 1: Sort the current temperatures into ascending order.

$$\boxed{\begin{array}{c}\mathbf{305}\\\mathbf{296}\\\mathbf{288}\\\mathbf{280}\\\mathbf{288}\end{array}} \Longrightarrow \boxed{\begin{array}{c}\mathbf{280}\\\mathbf{288}\\\mathbf{288}\\\mathbf{296}\\\mathbf{305}\end{array}}$$

STEP 2: Transform this list into the corresponding uniformly spaced values.

$$\boxed{\begin{array}{c}\mathbf{280}\\\mathbf{288}\\\mathbf{288}\\\mathbf{296}\\\mathbf{305}\end{array}} \Longrightarrow \boxed{\begin{array}{c}\mathbf{1}\\\mathbf{2}\\\mathbf{2}\\\mathbf{3}\\\mathbf{4}\end{array}}$$

STEP 3: Compute the DRPE

$$DRPE = c_1 \sum_{m=1}^{M} \sum_{n=1}^{M} \left[\left(\lambda_{m,unit} - \lambda_{n,unit} \right) - \left(m - n \right) \right]^2 + c_2 \left[\sum_{m=1}^{M} \lambda_{m,unit} - \sum_{m=1}^{M} m \right]^2$$

$$DRPE = c_1 \left\{ \begin{array}{l} \left[(1-1)-(1-1)\right]^2 + \left[(1-2)-(1-2)\right]^2 + \left[(1-2)-(1-3)\right]^2 + \\ \left[(1-3)-(1-4)\right]^2 + \left[(1-4)-(1-5)\right]^2 + \left[(2-1)-(2-1)\right]^2 + \\ \left[(2-2)-(2-2)\right]^2 + \left[(2-2)-(2-3)\right]^2 + \left[(2-3)-(2-4)\right]^2 + \\ \left[(2-4)-(2-5)\right]^2 + \left[(2-1)-(3-1)\right]^2 + \left[(2-2)-(3-2)\right]^2 + \\ \left[(2-2)-(3-3)\right]^2 + \left[(2-3)-(3-4)\right]^2 + \left[(2-4)-(3-5)\right]^2 + \\ \left[(3-1)-(4-1)\right]^2 + \left[(3-2)-(4-2)\right]^2 + \left[(3-2)-(4-3)\right]^2 + \\ \left[(3-3)-(4-4)\right]^2 + \left[(3-4)-(4-5)\right]^2 + \left[(4-1)-(5-1)\right]^2 + \\ \left[(4-2)-(5-2)\right]^2 + \left[(4-2)-(5-3)\right]^2 + \left[(4-3)-(5-4)\right]^2 + \\ \left[(4-4)-(5-5)\right]^2 \end{array} \right\} +$$

$$c_2 \left[(1+2+2+3+4)-(1+2+3+4+5)\right]^2$$

We use c_1=0.02 and c_2=0.05, and we find the DRPE is:

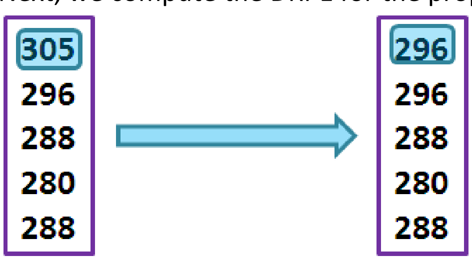
$$DRPE = c_1 \left\{ \begin{array}{l} (0+0+1+1+1)+(0+0+1+1+1)+(1+1+0+0+0) \\ +(1+1+0+0+0)+(1+1+0+0+0) \end{array} \right\} + c_2 \left[(1+2+2+3+4)-(1+2+3+4+5)\right]^2$$

$$DRPE = (0.02)(12)+(0.05)(9)$$

$$DRPE = 0.24 + 0.45$$

$$DRPE = 0.69$$

Next, we compute the DRPE for the proposed move:



STEP 1: Sort the temperatures into ascending order.

STEP 2: Transform this list into the corresponding uniformly spaced values.

$$\begin{array}{|c|}\hline 280\\ 288\\ 288\\ 296\\ 296\\ \hline\end{array} \Longrightarrow \begin{array}{|c|}\hline 1\\ 2\\ 2\\ 3\\ 3\\ \hline\end{array}$$

STEP 3: Compute the DRPE

$$DRPE = c_1 \sum_{m=1}^{M} \sum_{n=1}^{M} \left[\left(\lambda_{m,unit} - \lambda_{n,unit} \right) - \left(m - n \right) \right]^2 + c_2 \left[\sum_{m=1}^{M} \lambda_{m,unit} - \sum_{m=1}^{M} m \right]^2$$

$$DRPE = c_1 \left\{ \begin{array}{l} \left[(1-1)-(1-1)\right]^2 + \left[(1-2)-(1-2)\right]^2 + \left[(1-2)-(1-3)\right]^2 + \\ \left[(1-3)-(1-4)\right]^2 + \left[(1-3)-(1-5)\right]^2 + \left[(2-1)-(2-1)\right]^2 + \\ \left[(2-2)-(2-2)\right]^2 + \left[(2-2)-(2-3)\right]^2 + \left[(2-3)-(2-4)\right]^2 + \\ \left[(2-3)-(2-5)\right]^2 + \left[(2-1)-(3-1)\right]^2 + \left[(2-2)-(3-2)\right]^2 + \\ \left[(2-2)-(3-3)\right]^2 + \left[(2-3)-(3-4)\right]^2 + \left[(2-3)-(3-5)\right]^2 + \\ \left[(3-1)-(4-1)\right]^2 + \left[(3-2)-(4-2)\right]^2 + \left[(3-2)-(4-3)\right]^2 + \\ \left[(3-3)-(4-4)\right]^2 + \left[(3-3)-(4-5)\right]^2 + \left[(3-1)-(5-1)\right]^2 + \\ \left[(3-2)-(5-2)\right]^2 + \left[(3-2)-(5-3)\right]^2 + \left[(3-3)-(5-4)\right]^2 + \\ \left[(3-3)-(5-5)\right]^2 \end{array} \right\} +$$

$$c_2 \left[(1+2+2+3+3) - (1+2+3+4+5) \right]^2$$

$$DRPE = c_1 \left\{ \begin{array}{l} (0+0+1+1+4)+(0+0+1+1+4)+(1+1+0+0+1) \\ +(1+1+0+0+1)+(4+4+1+1+0) \end{array} \right\} + c_2 \left[(1+2+2+3+3) - (1+2+3+4+5) \right]^2$$

$$DRPE = (0.02)(28) + (0.05)(16)$$

$$DRPE = 1.36$$

The difference in the DRPEs is:
DRPE(proposed move) – DRPE(current) = 1.36 – 0.69 = 0.67

Since the acceptance ratio in STDR has the form:

$$p\left(T_i \rightarrow T_j\right) = \min \left\{ \begin{array}{c} 1 \\ e^{-\left(\beta_j - \beta_i\right)E + \left(a_j - a_i\right) - \left(DRPE_j - DRPE_i\right)} \end{array} \right.$$

the addition of the DRPE is the same as multiplying the acceptance ratio of ST by a factor of $e^{-0.67}$, decreasing the likelihood of the move by approximately 51%, which is the same as applying a penalty of -0.67kcal/mol. This move is unfavourable because there is already a replica at 296K, and because it would cause more replicas to be at the lower end of the temperature range. The constants c_1 and c_2 control the degree of energetic penalty imposed for these unfavourable moves.