$$dF = -S \cdot dT - P \cdot dV + \mu \cdot dN \quad (1)$$

$$U = F + T \cdot S \quad (2)$$

$0.45 < T/T_c < 1.13$
T_c

$$V_{Lennard-Jones} = 4\epsilon \left[\left(\frac{\sigma}{4} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right] \quad (3)$$

?
?
$\eta =$
$\frac{N}{V}$
$\eta =$
$packingFraction$
$\Lambda =$

$$\frac{F}{N \cdot k \cdot T} = a^{IDEAL} + a^{HS} + \beta \cdot a_1^{SW} + \beta^2 \cdot a_2^{SW} \tag{5}$$

$$a^{IDEAL} = \ln\left(n \cdot \Lambda^3\right) - 1 \tag{6}$$

$$a^{HS} = -\ln(1 - 4 \cdot \eta) \tag{7}$$

$$a_1^{SW} = a_1^{VDW} \cdot g^{HS}(1; \eta_{eff}) \tag{8}$$

$$a_1^{VDW} = -4 \cdot \eta \cdot \epsilon \cdot (\lambda^3 - 1) \tag{9}$$

$$g^{HS}(1; \eta_{eff}) = \frac{1 - \eta_{eff}/2}{(1 - \eta_{eff})^3} \tag{10}$$

$$n_{eff} = c1 \cdot \eta + c_2 \cdot \eta^2 + c_3 \cdot \eta^3 \tag{11}$$

$$\left(c\right)_1{}^{c_2 c_3 = \left(2\right) .25855-1.503490.249434-0.6692701.40049-0.82773910.1576-15.04275.30827 \times \left(1\right) \lambda\lambda^2} \tag{12}$$

$$a_2^{SW} = \frac{1}{2} \cdot \epsilon K^{HS} \eta \cdot \frac{\partial a_1^{SW}}{\partial \eta} \tag{13}$$

$$K^{HS} = \frac{(1 - \eta)^4}{1 + 4 \cdot \eta + 4 \cdot \eta^2} \tag{14}$$

$$Z = Z_{ideal} \cdot Z_{HS} \cdot Z_{disp} \tag{15}$$

$$Z_{ideal} = Z_{ideal}^{SAFT} = N \cdot (1 - ln(n \cdot \Lambda^3)) \tag{16}$$

$$Z_{HS} = e^{-S_{HS}/k} \tag{17}$$

$$Z_{disp} = \frac{Z_{interaction}}{Z_{HS}} = \frac{\sum_i \alpha \cdot D(E_i) \cdot e^{-\beta \cdot E_i}}{\lim_{T \to \infty} \sum_i \alpha \cdot D(E_i) \cdot e^{-\beta \cdot E_i}} = \frac{\sum_i D(E_i) \cdot e^{-\beta \cdot E_i}}{\sum_i D(E_i)} \tag{18}$$

S_{HS}
?
$T =$
∞
$P_{success}$
$\Delta S_{HS} =$
$k \cdot$
$\ln(P_{success})$
S_{HS} $\frac{}{N! \sum_i e^{-\beta \cdot E_i} 19 = \frac{1}{N!} \int \cdots \int e^{-\beta \cdot [\{P_1^2/2m + P_2^2/2m + \ldots\} + V(\vec{R}_1, \vec{R}_2, \ldots)]} d\vec{P}_1 \cdot d\vec{P}_2 \cdots d\vec{P}_N \cdot d\vec{R}_1 \cdot d\vec{R}_2 \cdots d\vec{R}_N}$
V^N / V^N
$ideal \cdot$
$\frac{1}{V^N} \cdot$
$\int \cdot\cdot$
$\cdot \int e^{-\beta \cdot V(\vec{R}_1, \vec{R}_2, \ldots)} d\vec{R}_1 \cdot$
$d\vec{R}_2 \cdot$
$\cdot\cdot$

Here resolution reduction of the data is demonstrated. The data must be generated from a range of box sizes, and for each box size it is possible to run simulations From 2 atoms in a box all the way up to the desired filling fraction of 0.5; depending on the box size, a filling fraction of 0.5 can correspond to only 40 atoms or it could be as much as 100 atoms. Running simulations with every possible filling fraction will in-deed