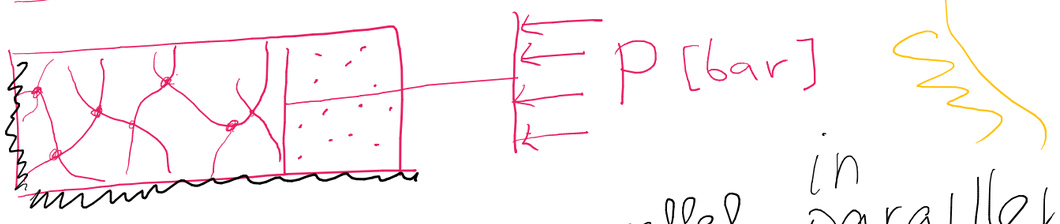
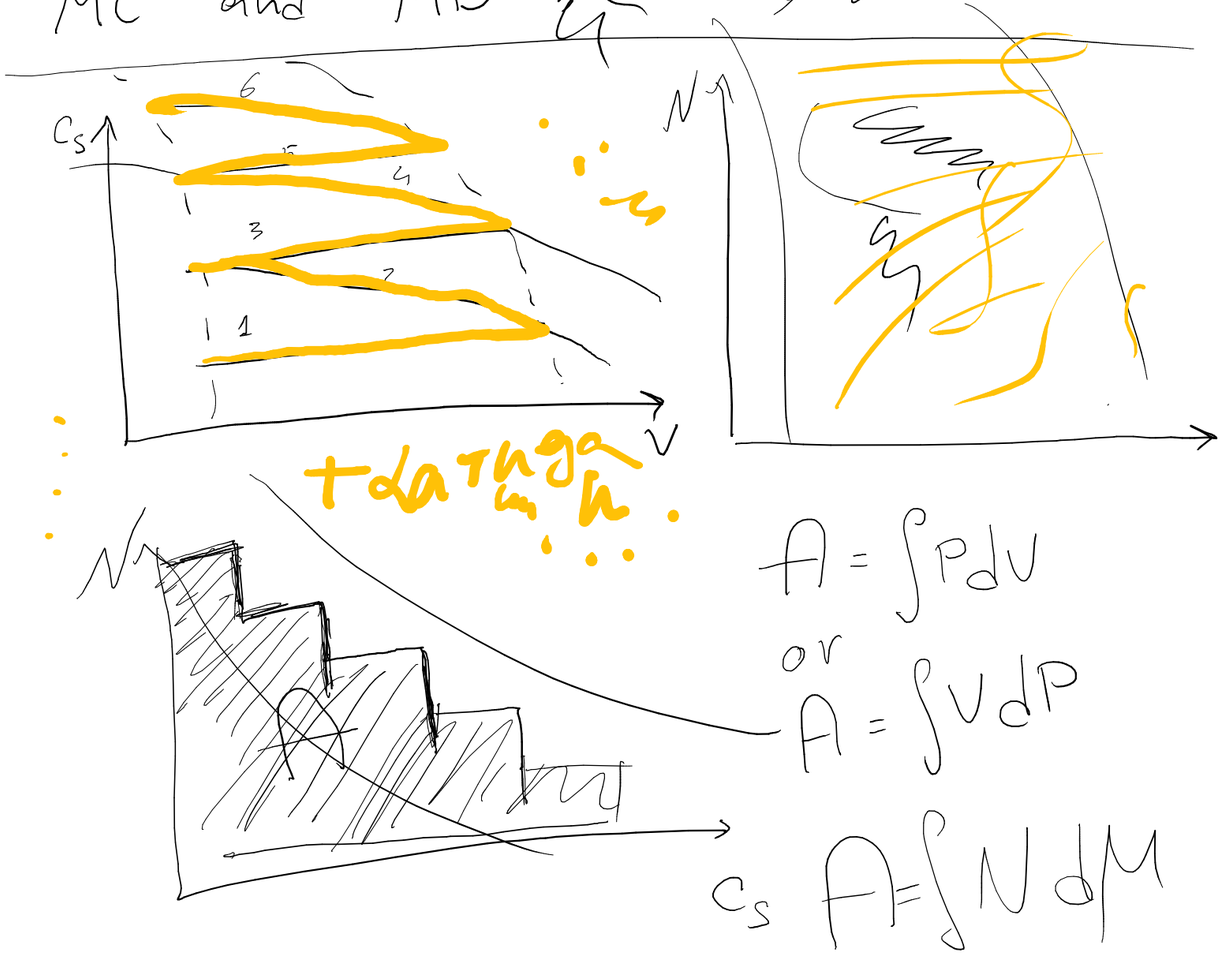
Gibbs ensemble simulation



Two simulations in parallel. in parallel

MC and MD

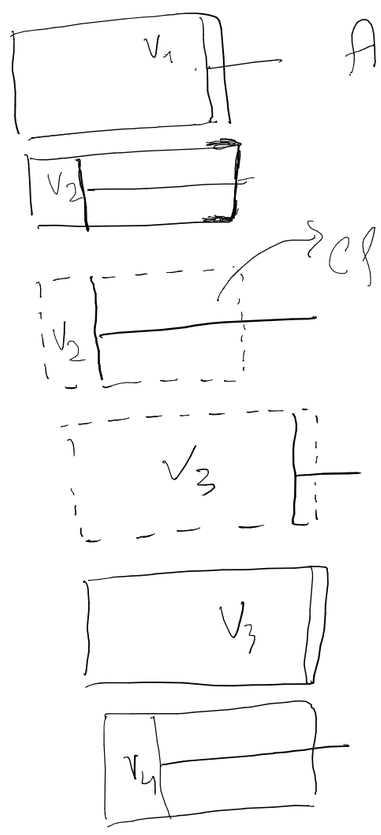


$A = \int p dV$

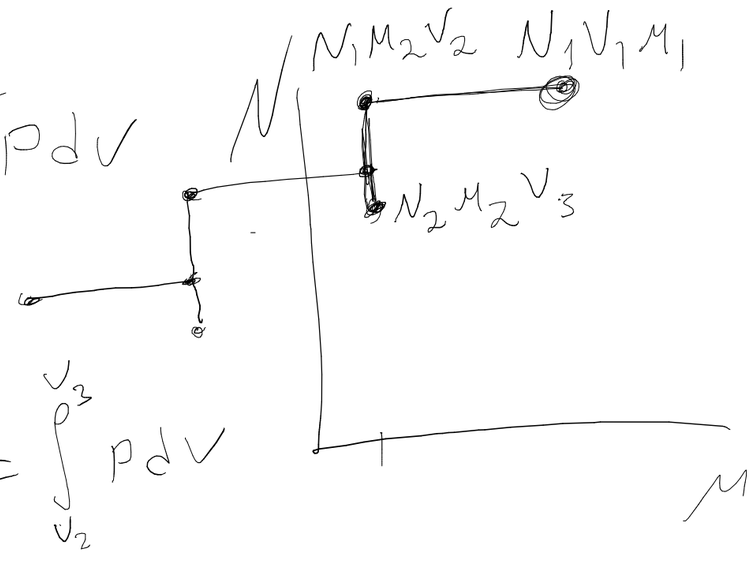
or

$A = \int V dP$

$A = \int N dM$



$A = \int N dM = \int_{V_1}^{V_2} p dV$



$A = \int M dN = \int_{V_2}^{V_3} p dV$

$\int N dM = \int_{V_3}^{V_2} p dV$

$pV = \nu RT$

$pV^{\kappa} = Const$

$V \sim \frac{\nu PT}{P}$

$P\left(\frac{\nu RT}{P}\right)^{\kappa} = P^{1-\kappa} T^{\kappa} = Const$

$pV = \nu RT$ $MN =$

$pdV + Vdp = \nu R dT$

$dU = pdV +$

$dU = \nu C_v dT = -p dV$ MdN

$pdV + \nu dp = \frac{dU}{\nu C_v} \nu R$

$pdV + \nu dp = dU \frac{R}{C_v} = -pdV \frac{R}{C_v}$

$pdV\left(1 + \frac{R}{C_v}\right) + \nu dp$

$K \frac{dV}{V} = -\frac{dP}{P}$