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$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		
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(10)		Conserves canonical dishibution in coordinate space.
	,	100
7/10		

	& 8.4 Proportional Timescaling: Berendsen thomostat
	Volocity resculing made top will Tourse here is
	Velocity rescaling works too well. Temporature is really fixed, while in the canonical ensemble, the avoye energy is fixed and allowed fluctuations also tremslate into fluctuations of the instantaneous temperature.
	into fluxtuctions of the instantaneous temporative.
	Idea: Use a weaker compling and try to drive the system dynamics towards the desired To
	How? Velocities are scaled at each time-step in such a way that the rate of change of temperature is proportional to the difference in
	temperateure:
	dT 1 (To-T) (*)
	i: compling parameter
	=> T=To-Ge-4E
	exponential decay of It to To. (x) in discrete resion:
-()-	$\Delta T = \frac{\Delta t}{T} (T_0 - T)$
U	and modification of momenta Pi > 1 Pi
	with $\lambda = 1 + \frac{\Delta E}{\Gamma} \left(\frac{T_0}{\Gamma} - 1 \right)$
	$/\Lambda$

	89. Barostats
	As with demperature couldol, there are
	different ways of how to ensure ountent
	different ways of how to ensure ourtent pressure in Molecular Dynamics Simulations.
	The obvious quarion to start from is how to measure pressure?
()	how to measure pressure?
\	
	89.1 The Vinial
	Starting from the equations of motion
	m: q: = t
-	we multiply this with q:
	=> m; q; q; - q; t; (*)
	11 d (2 c)
_(Now consider: 99: - d (99) -
/ .	
	$\frac{\partial}{\partial t} \left(m_1 q_1 q_1 \right) - m_2 q_1^2 = F_1 q_2$
	Ot (11 11 11 11 11 11 11 11 11 11 11 11 1
	Surveying and over all on dealers and intercontinue
	Summing ext over all particles and integrations over the president, leads to
(
	(W> = (Z, q, F; > = - (m, q; >
	= -2. Esin
1	$/\Lambda$

Why did we write Ftot? macroscopically internal In addition to the forces preson bed by the force-field, the walls cause an extra force Fext me the box is the a parallel epipedic ainer withe Lx, Ly, Lz. the average viral caused by the external Three is -plyl2)+Ly(-pLxl2)+L2(-pLxly \(\subseteq \) = \(\subseteq \) \(\text{T int} \) \(> - 3pV \) = -2 \(\text{Epin} \) Oz if rearranged: $P = \frac{2}{21/2} - E \sin \frac{1}{2}$ > Indicates two possible dials the adjust - hanging Enin

	Adjusting the lanetic energy means modifying particle relocities
	particle relocities
	particle reloaities > changing temporature of the simulated system
	§ 9.2 Berendsen barostat
	Citations - sustain is usually considered to an
	Situation: - system is weakly compled to an external bath, allowing for a pressure
	change
	$\frac{\partial P}{\partial t} = \frac{Po - P}{To}$
-(
	Lp: some time constant for the coupling
	- make modifications so that the local
-(pertubulions are small
/	Berendsen achieved this by modifying the
	equation,
	q = v
	into 9 = V + XX
	This corresponds to a simple resculing of coordinates - and concornitantly. The volume
	- and concomitantly - the volume
	$\dot{V} = 3\alpha V$
	What is a?
-	/3

Let's consider the pressure change again! $ \frac{dP}{dt} = \frac{1}{dV} \text{Re isothernal compressibility} \\ dt $		
de pv de = -3 = Po - P = -3 = Po - P = -3 = B (Po - P) = a = -3 = B (Po - P) = v - B (Po - P) q = v - B (Po - P) q = v - B (Po - P) q = v - B (Po - P) At q = scaling of all coordinates with factor \(\mu = 1 - \frac{BAt}{V} \) \(\mu = \frac{Po - P}{V} \) \(\mu = \f		Let's consido the pressure change again!
= -\frac{3\pi}{B} = \frac{70 - 7}{\text{F}} = \frac{3\pi}{B} = \frac{70 - 7}{\text{F}} = \frac{3}{\text{F}} = \frac{70 - 7}{3\text{F}} = \frac{3}{\text{F}} = \frac{3}{\text{F}} = \frac{10}{3\text{F}} = \		
=> $\alpha = -\frac{\beta(p_0 - p)}{3 \epsilon_p}$ => in Eq. for α $q = V - \beta(p_0 - p)$ $q = V - \beta(p_0 - p)$ Nia $q(t = t + t) = av \Delta t - \beta(p_0 - p) \Delta t$ => scaling of all coordinates with factor $\mu = 1 - \frac{\beta \Delta t}{p_0 - p}$ But one should know some good value for β . => generalizations to anisotropic systems		
⇒ in Eq. 40 g g = V - B(Po-P) 3 Tp Na g(####) = &VAL - B(Po-P) At q => scaling of all coordinates with factor µ = 1 - BLE Po-P) P -> µq But one should know some good value for B. ⇒ generalizations to anisotropic systems		$= \frac{3\alpha}{\beta} = \frac{\beta - \beta}{\zeta - \beta}$
⇒ in Eq. 40 g g = V - B(Po-P) 3 Tp Na g(####) = &VAL - B(Po-P) At q => scaling of all coordinates with factor M = 1 - BLE Po-P) P -> Mg But one should know some good value for B. => generalizations to anisotropic systems		$\Omega \left(0, -2 \right)$
ig = V - B(Po-P) q 3 Zp Nia glant) = &VAL - B(Po-P) At q > scaling of all coordinates with factor \(\mu = 1 - \frac{\beta \perp}{2} \) [Po-P) P But one should know some good value for B. => generalizations to anisotropic systems		$\Rightarrow d = -\frac{10000}{300}$
ig = V - B(Po-P) q 3 Zp Nia g(*****) = &VAL - B(Po-P) At q > Scaling of all coordinates with factor $\mu = 1 - \frac{\beta A \pm}{2} [Po-P]$ Po p But one should know some good value for B. -> generalizations to anisotropic systems	7	
hia gland = avit = B(Po-P) At q => scaling of all coordinates with factor u = 1 - BAt Po-P) P - Mq But one should know some good value for B. => generalizations to anisotropic systems		≥ in Eq. for of
=> scaling of all coordinates with factor $\mu = 1 - \frac{1}{12} \frac{1}{$	7	$\frac{\dot{q} = V - \beta(p_0 - p)}{3z_p} q$
=> scaling of all coordinates with factor $\mu = 1 - \beta A + \beta O - p$ Por one should know some good value for β . => generalizations to anisotropic systems		B(B, zB)
mith factor $\mu = 1 - \frac{\beta \Delta t}{Lp} [Po - p]$ 9 - Mg But one should know some good value for β . => generalizations to anisotropic systems	<u> </u>	
mith factor $\mu = 1 - \frac{\beta \Delta t}{Lp} [Po - p]$ 9 - Mg But one should know some good value for β . => generalizations to anisotropic systems		=> scaling of all coordinates
But one should know some good value for B. => generalizations to anisotropic systems		
But one should know some good value for B. > generalizations to anisotropic systems		with factor u = 1 - To -pl
But one should know some good value for B. > generalizations to anisotropic systems		
But one should know some good value for B. > generalizations to anisotropic systems		9 -> µg
=> generalizations to anisotropic systems		
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