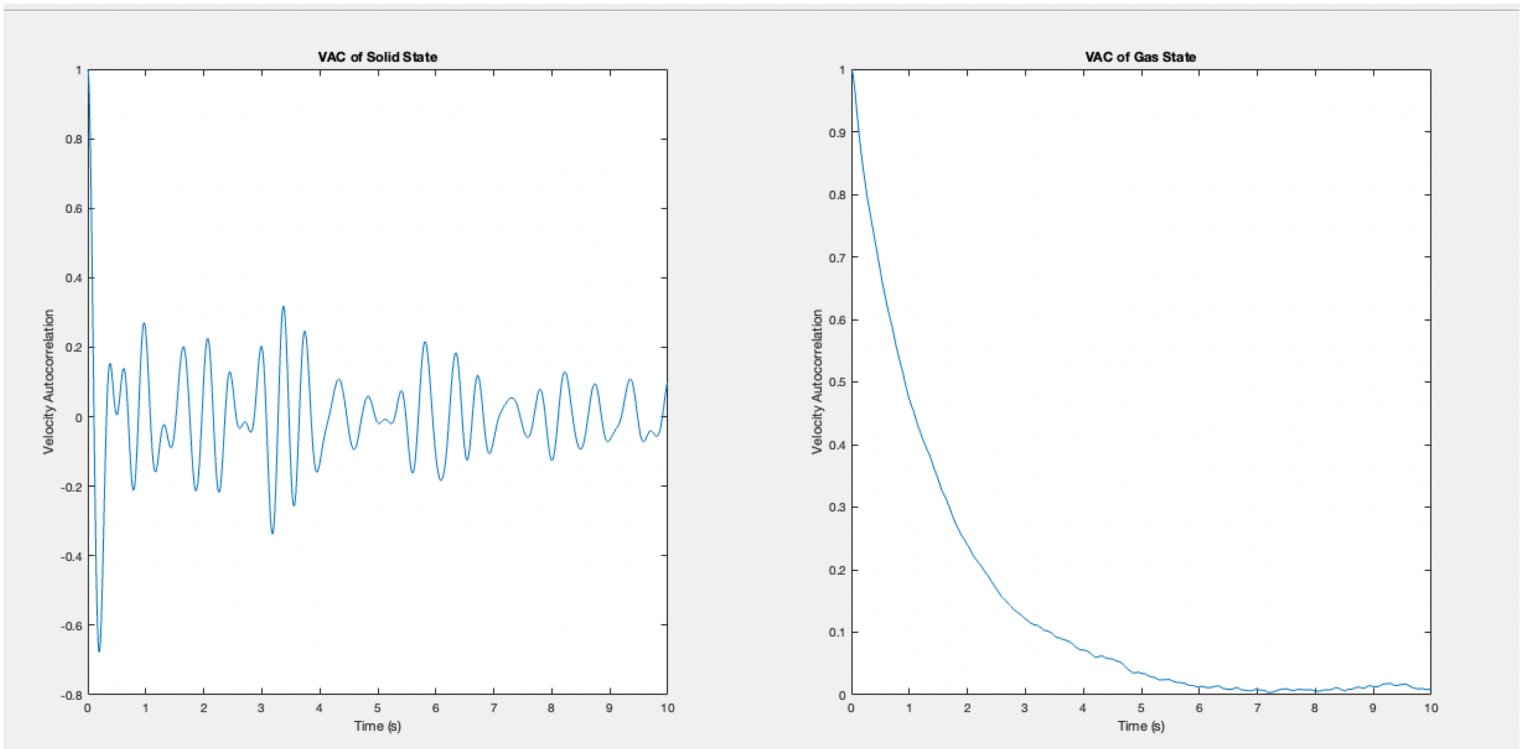
[Link to md-vac.c](md-vac.c)
[Link to md-vac.h](md-vac.h)



The velocity verlet algorithm is a method of numerical integration for newton's laws of motion under discretized time.

The position $\vec{x}$ and momentum $\vec{p}$ at step $i+1$ are given by

$$\vec{x}_{i+1} = \vec{x}_i + \vec{p}_i \Delta t + \frac{1}{2}\vec{a}_i \Delta t^2$$

$$\vec{p}_{i+1} = \vec{p}_i + \frac{1}{2}(\vec{a}_i + \vec{a}_{i+1})\Delta t$$

a_i depends on x_i and a_{i+1} depends on x_{i+1}

We denote x_{i+1} as x', p_{i+1} as p', x_i as simply x and p_i as p

In 2D space, the Jacobian defines the areal transformation.

$$J = \begin{bmatrix} \frac{\partial x'}{\partial x} & \frac{\partial x'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{bmatrix}$$

Therefore, demonstrating that the Jacobian $\frac{\partial(x', p')}{\partial(x, p)}$ is 1 is sufficient to prove that the velocity verlet algorithm preserves area in phase space.

$$\frac{\partial x'}{\partial x} = 1 + \frac{1}{2}\frac{\partial a}{\partial x}\Delta t^2$$

$$\frac{\partial x'}{\partial p} = \Delta t$$

$$\frac{\partial p'}{\partial x} = \frac{1}{2}\left(\frac{\partial a}{\partial x} + \frac{\partial x'}{\partial x}\cdot\frac{\partial a'}{\partial x'}\right)\Delta t$$

$$= \frac{1}{2}\left(\frac{\partial a}{\partial x} + \frac{\partial a'}{\partial x'}\left(1 + \frac{1}{2}\left(\frac{\partial a}{\partial x}\right)\Delta t^2\right)\Delta t\right.$$

$$\frac{\partial p'}{\partial p} = 1 + \frac{1}{2}\left(\frac{\partial a'}{\partial x'}\cdot\Delta t\right)\Delta t$$

Now, the Jacobian determinant is:

$$\left(1+\frac{1}{2}\frac{\partial a}{\partial x}\Delta t^2\right)\left(1+\frac{1}{2}\left(\frac{\partial a'}{\partial x'}\cdot\Delta t\right)\Delta t\right) -$$

$$\left[\frac{1}{2}\left(\frac{\partial a}{\partial x} + \frac{\partial a'}{\partial x'}\left(1+\frac{1}{2}\left(\frac{\partial a}{\partial x}\right)\Delta t^2\right)\Delta t\right]\Delta t$$

$$= 1 + \frac{1}{2}\left(\frac{\partial a'}{\partial x'}\Delta t^2\right) + \left(\frac{1}{2}\frac{\partial a}{\partial x}\Delta t^2\right) + \frac{1}{4}\left(\frac{\partial a}{\partial x}\frac{\partial a'}{\partial x'}\Delta t^4\right)$$

$$- \frac{1}{2}\frac{\partial a}{\partial x}\Delta t^2 - \frac{1}{2}\frac{\partial a'}{\partial x'}\Delta t^2 - \frac{1}{4}\frac{\partial a'}{\partial x'}\frac{\partial a}{\partial x}\Delta t^4$$

Since $\frac{\partial a'}{\partial x'} = \frac{\partial a}{\partial x}$, the terms all cancel out, leaving only 1.

Thus, the area scaling factor is 1, and phase space area is conserved by the verlet velocity algorithm

3.

$$\vec{x}_{i+1} = \vec{x}_i + \vec{p}_i \Delta t + \frac{1}{2}\vec{a}_i \Delta t^2$$

$$\vec{p}_{i+1} = \vec{p}_i + \frac{1}{2}(\vec{a}_i + \vec{a}_{i+1})\Delta t$$

The Liouville operator L is defined as $iL = \sum_{j=1}^{f} \left[\dot{x}_j \frac{\partial}{\partial x_j} + F_j \frac{\partial}{\partial p_j}\right]$

where f is the number of degrees of freedom of the system, x is the position, p is the momentum, and F is the force on th jth degree of freedom

Since L is a linear, Hermitian operator, its corresponding classical propogator is $U(t) = e^{iLt}$, a unitary operator.

If we define $\Gamma = \{x_j, p_j\}$ as the state of the system, then the state at time t is $\Gamma(t) = U(t)\Gamma(0)$

Now, Trotter's expansion of $U(t)$ is defined as

$$e^{i(L_1+L_2)t} = \left[e^{iL_1(\Delta t/2)} e^{iL_2\Delta t} e^{iL_1(\Delta t/2)}\right]^P + O(t^3/P^2)$$

where $\Delta t = t/P$ and $O(t^3/P^2)$ is a term on the order t^3/P^2, and

$iL = iL_1 + iL_2$

Using this, we can define a discrete time propogator

$$G(\Delta t) = U_1\left(\frac{\Delta t}{2}\right) U_2(\Delta t) U_1\left(\frac{\Delta t}{2}\right) = e^{iL_1(\Delta t/2)} e^{iL_2\Delta t} e^{iL_1(\Delta t/2)}$$

Since $U_1(t)$, $U_2(t)$ are unitary, $G(\Delta t)$ is also unitary.

Remember that due to the Trotter expansion, $G(\Delta t)$ is equivalent

to the original unitary propogator, but discrete.

Now, we set $iL_1 = F(x)\frac{\partial}{\partial p}$ and $iL_2 = \dot{x}\frac{\partial}{\partial x}$

Thus $G(\Delta t) = e^{(\Delta t/2)F(x)\partial/\partial p}\, e^{\Delta t\, \dot{x}\,\partial/\partial x}\, e^{(\Delta t/2)F(x)\partial/\partial p}$.

Using the property that $e^{c\,\partial/\partial q} f(q) = f(q+c)$ given c independent of q,

we can apply $G(\Delta t)$ to $x(0)$ and $p(0)$ to get $x(\Delta t)$ and $p(\Delta t)$

Taking the taylor expansions, we get that $G(\Delta t) = \underbrace{\left[1 + \frac{\Delta t}{2}F(x)\frac{\partial}{\partial p} + \left(\frac{\Delta t}{2}\right)^2 F^2(x)\frac{\partial^2}{\partial p^2}\right]}_{C}$

$$\underbrace{\left[1 + \Delta t\,\dot{x}\frac{\partial}{\partial x} + \Delta t^2 \dot{x}^2 \frac{\partial^2}{\partial x^2}\right]}_{B}\underbrace{\left[1 + \frac{\Delta t}{2}F(x)\frac{\partial}{\partial p} + \left(\frac{\Delta t}{2}\right)^2 F^2(x)\frac{\partial^2}{\partial p^2}\right]}_{A} + O(t^3)$$

We will apply A, then B, then C to $x(0)$ and $p(0)$, starting with $x(0)$

$A\,x(0) = x(0)$ Derivatives W.R.T p result in 0 for $x(0)$

$$BA\,x(0) = x(0) + \Delta t\,\dot{x}\underbrace{\frac{\partial x}{\partial x}}_{1} + \Delta t^2 \dot{x}^2 \underbrace{\frac{\partial^2 x}{\partial x^2}}_{0}$$

$$= x(0) + \Delta t\,\dot{x} = x(0) + \Delta t\frac{p}{m}$$ $\dot{x}$ is rewritten as $\frac{p}{m}$ here

$$CBA\,x(0) = x(0) + \Delta t\frac{p}{m} + \frac{\Delta t}{2}F(x)\frac{\partial}{\partial p}\left(\Delta t\frac{p}{m}\right) + \left(\frac{\Delta t}{2}\right)^2 F^2(x)\underbrace{\frac{\partial^2}{\partial p^2}\left(\Delta t\frac{p}{m}\right)}_{0}$$

$$= x(0) + \Delta t\frac{p}{m} + \frac{\Delta t^2}{2}\frac{F(x)}{m}$$

$$x(\Delta t) \;\boxed{= x(0) + \Delta t\,\dot{x} + \ddot{x}\cdot\frac{\Delta t^2}{2}}$$ $\frac{F(x)}{m}$ is rewritten as $\ddot{x}$ and $\frac{p}{m}$ as $\dot{x}$ here.

This is identical to the velocity verlet alg. for position.

Now, we apply A, B, and C to p(0) sequentially.

$$A\,p(0) = p(0) + \frac{\Delta t}{2}F(x)\underbrace{\frac{\partial p}{\partial p}}_{1} + \left(\frac{\Delta t}{2}\right)^2 F^2(x)\underbrace{\frac{\partial^2 p}{\partial p^2}}_{0}$$

$$= p(0) + \frac{\Delta t}{2}F(x)$$

$$BA\,p(0) = \underbrace{e^{\Delta t \dot{x}\frac{\partial}{\partial x}}p(0)}_{p(0)} + e^{\Delta t \dot{x}\frac{\partial}{\partial x}}\frac{\Delta t}{2}F(x)$$

Using the earlier property that $e^{c\frac{\partial}{\partial q}}f(q) = f(q+c)$, we can conclude the following

$$= p(0) + \frac{\Delta t}{2}F\left(x(0) + \Delta t\frac{p}{m}\right)$$

$$CBA\,p(0) = e^{\left(\frac{\Delta t}{2}F(x)\frac{\partial}{\partial p}\right)}BA\,p(0)$$

Applying the same property again, we can replace each p with $\left(p + \frac{\Delta t}{2}F(x)\right)$ and get

$$= p(0) + \frac{\Delta t}{2}F(x) + \frac{\Delta t}{2}F\left(x(0) + \frac{\Delta t}{m}\left(p(0) + \frac{\Delta t}{2}F(x)\right)\right)$$

$$= p(0) + \frac{\Delta t}{2}F(x) + \frac{\Delta t}{2}F\underbrace{\left(x(0) + \dot{x}\Delta t + \frac{1}{2}\Delta t^2\cdot\ddot{x}\right)}$$

By rewriting $\frac{p(0)}{m}$ as $\dot{x}$ and $\frac{F(x)}{m}$ as $\ddot{x}$, this becomes $x(\Delta t)$ from earlier.

So, the whole eq. becomes:

$$p(\Delta t) = p(0) + \frac{\Delta t}{2}\left[F(x(0)) + F(x(\Delta t))\right]$$

Thus, both parts of the velocity verlet alg. emerge from the Liouville operator.