Liouville's Theorem

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Liouville's Theorem

- **Phase-space trajectory as a mapping**

$$\underset{t}{(x,p)} \rightarrow \underset{t+\Delta}{(x',p')}$$

- **Phase-space volume conservation: Jacobian of the mapping (areal enlargement factor) = 1**

$$\frac{\partial(x',p')}{\partial(x,p)} = 1$$

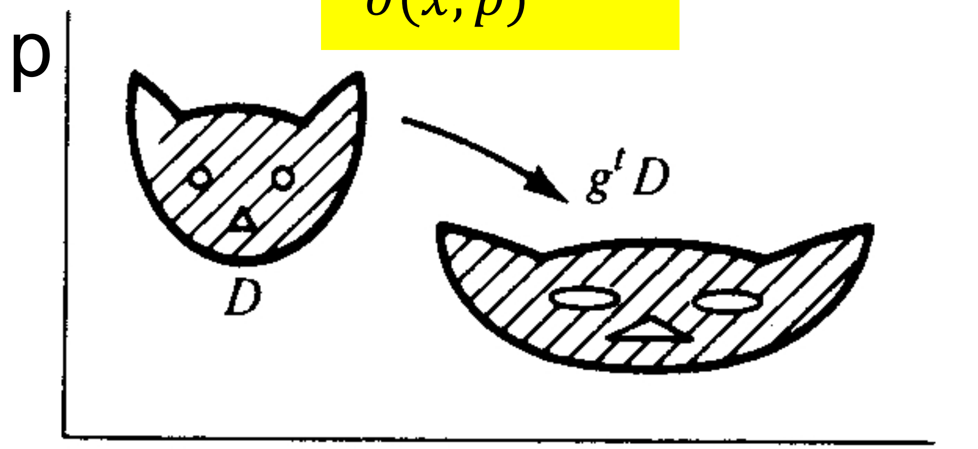

Figure 48 Conservation of volume

V.I. Arnold, *Mathematical Methods of Classical Mechanics, 2nd Ed.* (Springer, '89)

- **The cat is a phase-space volume occupied by an ensemble of phase-space points, each representing a specific instance of the initial condition (see `anim_spring.c`)**

Velocity Verlet Algorithm in 1D

$$\begin{cases} x' \leftarrow x + p\Delta + \frac{1}{2}a(x)\Delta^2 \equiv x'(x,p) \\ p' \leftarrow p + \dfrac{a(x) + a(x + p\Delta + \frac{1}{2}a(x)\Delta^2)}{2}\Delta \equiv p'(x,p) \end{cases}$$

Bottom-line: Velocity Verlet algorithm "exactly" satisfies Liouville's theorem

Prove phase-space volume conservation: $\dfrac{\partial(x',p')}{\partial(x,p)} = 1$

What phase-space volume conservation means? It's ensemble!

Compare an algorithm variant, Euler:

$$\begin{cases} x' \leftarrow x + p\Delta + \frac{1}{2}a(x)\Delta^2 \\ p' \leftarrow p + a(x)\Delta \end{cases} \rightarrow \frac{\partial(x',p')}{\partial(x,p)} \neq 1$$

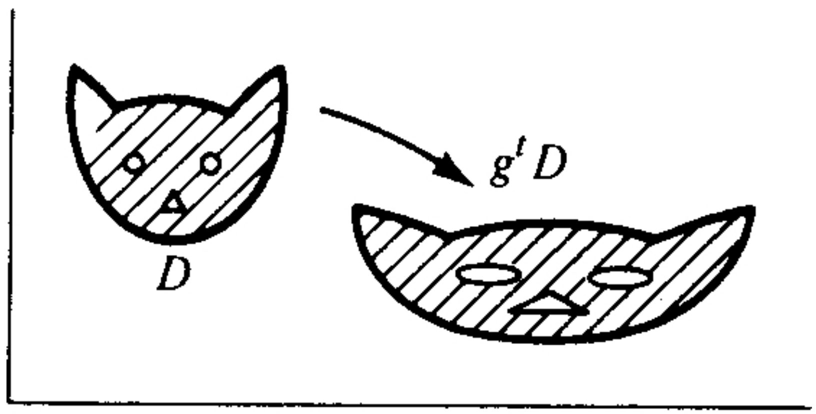

Figure 48 Conservation of volume

Algorithm Variants

(Velocity Verlet Algorithm)

Given a configuration, $\{\vec{r}_i(t), \vec{v}_i(t) \mid i = 1, \ldots, N_{\text{atom}}\}$

1. (Compute the acceleration, $\vec{a}_i(t)$)
2. $\vec{v}_i(t + \Delta/2) \leftarrow \vec{v}_i(t) + \vec{a}_i(t)\Delta/2$
3. $\vec{r}_i(t + \Delta) \leftarrow \vec{r}_i(t) + \vec{v}_i(t + \Delta/2)\Delta$
4. Compute the updated acceleration, $\vec{a}_i(t + \Delta)$
5. $\vec{v}_i(t + \Delta) \leftarrow \vec{v}_i(t + \Delta/2) + \vec{a}_i(t + \Delta)\Delta/2$

(Explicit Euler Algorithm)

Only modify SingleStep()!

Given a configuration, $\{\vec{r}_i(t), \vec{v}_i(t) \mid i = 1, \ldots, N_{\text{atom}}\}$

1. Compute the acceleration, $\vec{a}_i(t)$
2. Update the positions, $\vec{r}_i(t + \Delta) \leftarrow \vec{r}_i(t) + \vec{v}_i(t)\Delta\left[+\vec{a}_i(t)\Delta^2/2\right]$
3. Update the velocities, $\vec{v}_i(t + \Delta) \leftarrow \vec{v}_i(t) + \vec{a}_i(t)\Delta$

Algorithm Variants

Energy conservation: Velocity-Verlet *vs*. explicit-Euler algorithms