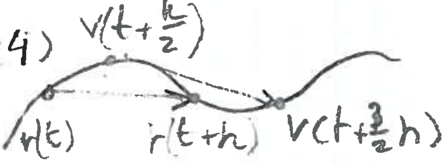
Other Verlet incarnations

leap-frog

$$v(t+h/2) = v(t-h/2) + h\,a(t) \quad (3)$$
$$r(t+h) = r(t) + h\,v(t+h/2) \quad (4)$$



(4) is similar to (2) with $h \to 2h$

(3) is reformulation of (1)

Velocity verlet

$$r(t+h) = r(t) + h\,v(t) + h^2\,a(t)/2$$
$$v(t+h) = v(t) + h\underbrace{[\underline{a(t+h)} + a(t)]/2}_{\text{average of forward backward}}$$

implement as
$\tilde{v}(t) = v(t) + h\,a(t)$,
$r(t+h) = r(t) + h\,\tilde{v}(t)$
$v(t+h) = \tilde{v}(t) + h\,\underline{a(t+h)}/2$

This was for simple eqs of motion with Hamiltonian dynamics.

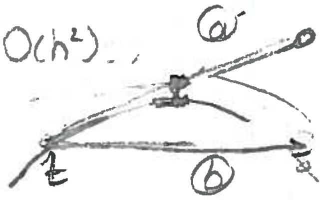
Can include in Verlet $\dot{v}(t) = a(r(t)) - \eta\,v(t)$ viscous friction
(common addition in models, for instance Langevin thermostat)

Problem: other non-Hamiltonian terms not always easy. $\dot{\gamma} = f(\gamma, t)$ ← for time dependence, see appendix

ⓐ $\gamma(t+h) = \gamma(t) + h\,f(\gamma(t))$ error $O(h^2)$..

ⓑ $\gamma(t+\frac{1}{2}h) = \gamma(t) + \overbrace{\tfrac{1}{2}h\,f(\gamma(t))}^{k_1}$

$\gamma(t+h) = \gamma(t) + h f(\gamma(t+\frac{1}{2}h))$ midpoint rule



Taylor expansion: $= \gamma(t) + k_2 + O(h^3)$, $k_2 = h f(\gamma(t) + \frac{1}{2}k_1)$

$$\gamma(t+h) = \gamma(t) + h\,f(\gamma(t) + \tfrac{1}{2}h\,f(\gamma(t)))$$
$$= \gamma(t) + h\left[f(\gamma(t)) + \frac{\partial f}{\partial \gamma}\,\tfrac{1}{2}h f(\gamma(t))\right]$$
$$= \gamma(t) + h\,\dot{\gamma}(t) + \tfrac{1}{2}h^2\,\ddot{\gamma}(t)$$

error is $O(h^3)$

ⓒ Even more midpoints:

$k_1 = h\,f(\gamma(t))$ $\quad k_2 = h\,f(\gamma(t) + \frac{1}{2}k_1)$

$k_3 = h\,f(\gamma(t) + \frac{1}{2}k_2)$ $\quad k_4 = h\,f(\gamma(t) + k_3)$

$\gamma(t+h) = \gamma(t) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) + O(h^5)$

4th order Runge-Kutta.
(you can take this further)

big advantage: efficient with variable time step (so that you can save computation time in intermittent systems like dilute gasses)
RK-Fehlberg compare RK4, RK5

very general method
more work than Verlet

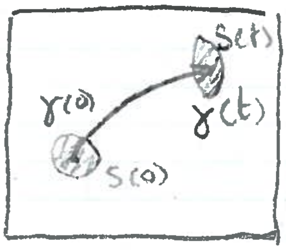
FK7029 2014 (13)

Symplectic dynamics (

recall dynamical system:

$$\begin{cases} \text{phase space } \Gamma, \text{ coordinate } \gamma \\ \text{eqs of motion } \dot{\gamma} = f(\gamma, t) \end{cases}$$

γ in our case $= r_1, r_2 \dots r_N \; v_1, v_2 \dots v_N$

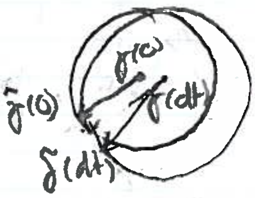


small volume $S(0)$ around $\gamma(0)$

$\gamma(0) \to \gamma(t) \quad : S(0) \to S(t)$

$\dot{S}(t)$?

$$\boxed{\begin{aligned} \gamma(dt) &= \gamma(0) + dt \left.\frac{\partial \gamma}{\partial t}\right|_{\gamma=\gamma_0} \text{ th} \\ &= \gamma(0) + dt\, f(\gamma(0)) \\ \tilde{\gamma}(dt) &= \tilde{\gamma}(0) + dt\, f(\tilde{\gamma}(0)) \end{aligned}}$$



$$\gamma(t) + \delta\gamma(t) = \tilde{\gamma}(t)$$

$$\begin{aligned} \delta\gamma(dt) &= \tilde{\gamma}(dt) - \gamma(dt) \\ &= \tilde{\gamma}(0) + dt\, f(\tilde{\gamma}(0)) - \gamma(0) - dt\, f(\gamma(0)) \\ &= \delta\gamma(0) + dt\left[f(\tilde{\gamma}(0)) - f(\gamma(0))\right] \quad \text{taylor in } \gamma(0) \\ &= \delta\gamma(0) + dt \left.\frac{\partial f}{\partial \gamma}\right|_{\gamma=\gamma(0)} \cdot \delta\gamma(0) = \underbrace{\left(\mathbb{1} + dt \left.\frac{\partial f}{\partial \gamma}\right|_{\gamma=\gamma_0}\right)}_{M} \cdot \delta\gamma(0) \end{aligned}$$

volume spanned by $\delta\gamma$ vectors is multiplied by $\det M$ $\quad S(t) = S(0) \det M$

$$\frac{d}{dt} \ln S = \frac{1}{dt}\left[\ln S(dt) - \ln S(0)\right] \overset{\text{th.o}}{=} \frac{1}{dt} \ln \det M$$

$$= \frac{1}{dt} \ln \prod_i (1 + dt\,\lambda_i) = \frac{1}{dt} \sum_i dt\,\lambda_i = \operatorname{Tr} \left.\frac{\partial f}{\partial \gamma}\right|_{\gamma=\gamma(0)}$$

eigenvalues of $\left.\frac{\partial f}{\partial \gamma}\right|_{\gamma=\gamma(0)}$ are $\lambda_1, \lambda_2, \dots$

Hamiltonian dynamical systems (conserved E)

$$\dot{p} = -\frac{\partial H}{\partial q} \quad \dot{q} = \frac{\partial H}{\partial p} \qquad \gamma = (p, q) \quad f(\gamma) = \left(-\frac{\partial H}{\partial q}, \frac{\partial H}{\partial p}\right)$$

$$\frac{\dot{S}(t)}{S} = \frac{\partial}{\partial \gamma} \cdot f(\gamma, t) = \frac{\partial}{\partial p} \cdot \left(-\frac{\partial H}{\partial q}\right) + \frac{\partial}{\partial q} \cdot \frac{\partial H}{\partial p} = 0$$

conserving phase space volume = symplectic

- if contraction: areas the system eventually will no longer visit.
- time reversal symmetry

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Verlet integration and phase space volume

$$\left.\begin{aligned} r(t+h) &= r(t) + h\,v(t) + h^2 a(t)/2 \\ v(t+h) &= v(t) + h\,[a(t+h) + a(t)]/2 \end{aligned}\right\}\ \text{velocity verlet}$$

volume change: jacobian:

$$\det \begin{pmatrix} \frac{\partial r(t+h)}{\partial r(t)} & \frac{\partial v(t+h)}{\partial r(t)} \\ \frac{\partial r(t+h)}{\partial v(t)} & \frac{\partial v(t+h)}{\partial v(t)} \end{pmatrix} =$$

$$1 + \tfrac{1}{2}h^2 \frac{\partial a}{\partial r}(t)$$

$$\det \begin{bmatrix} 1 + \frac{1}{2}h^2 \frac{\partial a}{\partial r}(t) & \frac{1}{2}h\left[\frac{\partial a}{\partial r}(t+h)\frac{\partial r(t+h)}{\partial r(t)} + \frac{\partial a}{\partial r}(t)\right] \\ h & 1 + \frac{1}{2}h^2 \frac{\partial a}{\partial r}(t+h) \end{bmatrix}$$

$= 1$ + everything else cancels

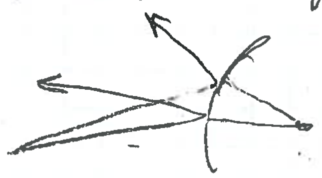
$\Rightarrow$ conserves phase space volume exactly, dynamics really act hamiltonian

$\Rightarrow$ there is another hamiltonian, $\hat{H}$ similar to H, which describes the calculated trajectory exactly.

$\Rightarrow$ error in E is bounded. $\Rightarrow$ no silly blowups.

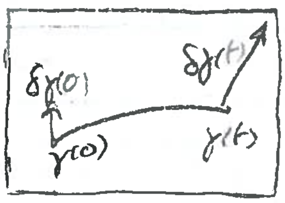
Finally: phase space and numerical errors.

Consider as an example the sinai billiard or Lorentz gas

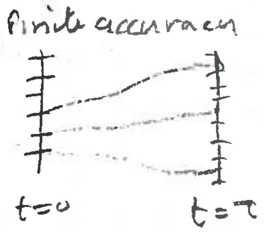


small difference in direction of velocity grows after every collision

(almost) all our systems have this



growing perturbations in phase space:
<u>sensitivity to initial conditions</u>
<u>Lyapunov instability (exponent)</u>
<u>butterfly effect</u> = <u>chaos</u>



indistinguishable points become distinguishable
(this is why weather is inherently unpred. in long term)

can be used as <u>random number generator</u>

variables are stored with <u>finite numerical accuracy</u>.
$\Rightarrow$ after a while <u>everything becomes result of numerical errors</u> that have blown up!

shadowing theorem: there was a real initial condition that would have looked almost the same.

Verlet (robust)	vs	RK (flexible)
less work / time step, error $O(h^4)$		better accuracy, so time step can be larger (error $O(h^5)$)
only Hamiltonian systems (or with simple modification)		any eqs. of motion
symplectic $\Rightarrow$ robust		suitable for variable time step (RK-Fehlberg)
recommend, use if E should be conserved or you have only viscous friction		otherwise

There are other options as well

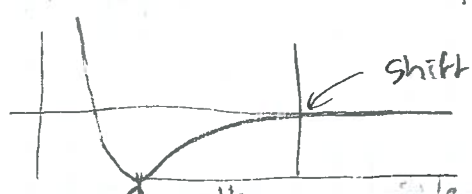
endlecture 3 (must still do Lyapunov

NEXT: interactions

- Already looked at Lennard-Jones $U_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$

often used for weak-ish interactions, f.e v.d. Waals

Falls off rapidly: cutoff, speeds things up



shift by $U(r_{cutoff})$ to avoid discontinuity

other possible cutoff, purely repulsive

Weeks-Chandler-Andersen

$$U = \begin{cases} U_{LJ} + \epsilon & \text{if } r < 2^{1/6}\sigma \\ 0 & \text{otherwise} \end{cases}$$

warning:

time step across cutoff has problem, because

non-smooth $\Rightarrow$ less accurate integration

$\dot{y} = f(y,t)$ $\quad y(t+h) = y(t) + hf(y,t) + h^2 \dot{f}(y,t) + \dots$

Taylor expansion

- other potentials, various cutoffs. Morse $U = U_0(1-e^{-a(r-r_e)})^2$