Course 03/1

Integration algorithms for MD: Verlet algorithm

- Position Verlet
- Velocities with Verlet
- Leap-frog Verlet
- Velocity Verlet

Position Verlet

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \frac{f(t)}{2m}\Delta t^2 + \frac{\dddot{r}}{3!}\Delta t^3 + o(\Delta t^4)$$

$$r(t-\Delta t) = \text{"} - \text{"} + \text{"} - \text{"} + o(\Delta t^4)$$

By summing up the two Taylor series above, we obtain:

$$r(t+\Delta t) + r(t-\Delta t) = 2r(t) + \frac{f(t)}{m}\Delta t^2 + o(\Delta t^4)$$

$$\rightarrow \quad \boxed{r(t+\Delta t) = 2r(t) - r(t-\Delta t) + \frac{f(t)}{m}\Delta t^2 + o(\Delta t^4)}$$

position Verlet algorithm

Advantage: this algorithm satisfies the criteria for MD integration (1 force calculation & accuracy)

Only positions of steps n and $n-1$ need to be memorized to evolve.

Disadvantage: differences between large numbers – loss of accuracy

$r(t+\Delta t) = r(t) + r(t) - r(t-\Delta t) + \ldots.$

Velocities with Verlet

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \frac{f(t)}{2m}\Delta t^2 + \frac{\dddot{r}}{3!}\Delta t^3 + o(\Delta t^4)$$

$$r(t-\Delta t) = \text{"} - \text{"} + \text{"} - \text{"} + o(\Delta t^4)$$

By subtracting the two Taylor series above, we obtain:

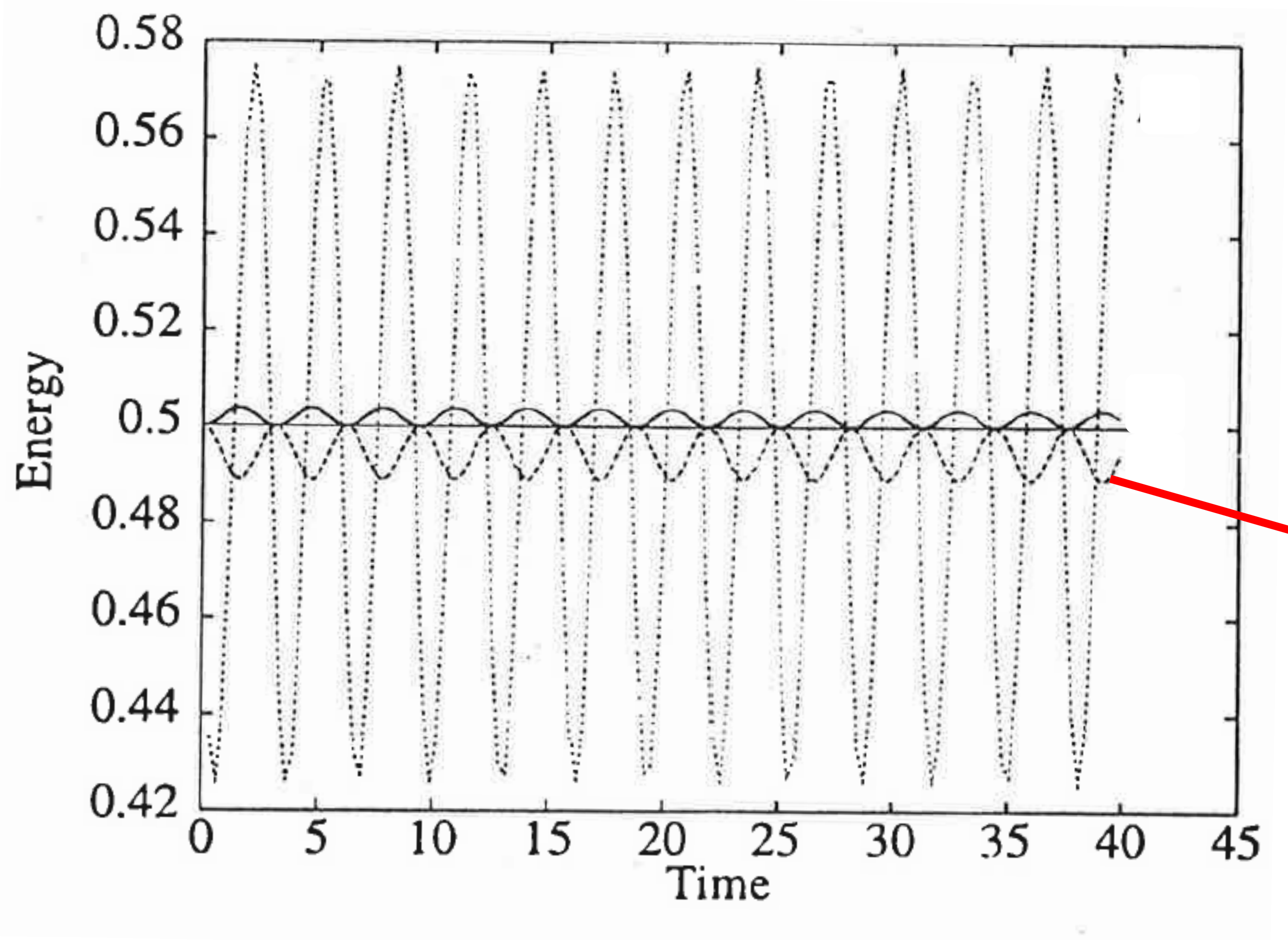
$$r(t+\Delta t) - r(t-\Delta t) = 2v(t)\Delta t + 2\frac{\dddot{r}}{3!}\Delta t^3 + o(\Delta t^5)$$

1. Low-order accuracy of velocity (neglecting $\dddot{r}$ term)

$$r(t+\Delta t) - r(t-\Delta t) = 2v(t)\Delta t + o(\Delta t^3)$$

$$\rightarrow \quad v(t) = \frac{r(t+\Delta t) - r(t-\Delta t)}{2\Delta t} + o(\Delta t^2)$$

Example: Harmonic oscillator



low-order
accuracy
velocities

Velocities with Verlet

2. Higher-order accuracy of velocity (including the $\dddot{r}$ term)

$$v(t) = \frac{r(t+\Delta t) - r(t-\Delta t)}{2\Delta t} - \frac{\dddot{r}}{6}\Delta t^2 + o(\Delta t^4)$$

For the $\dddot{r}$ term, we proceed as follows:

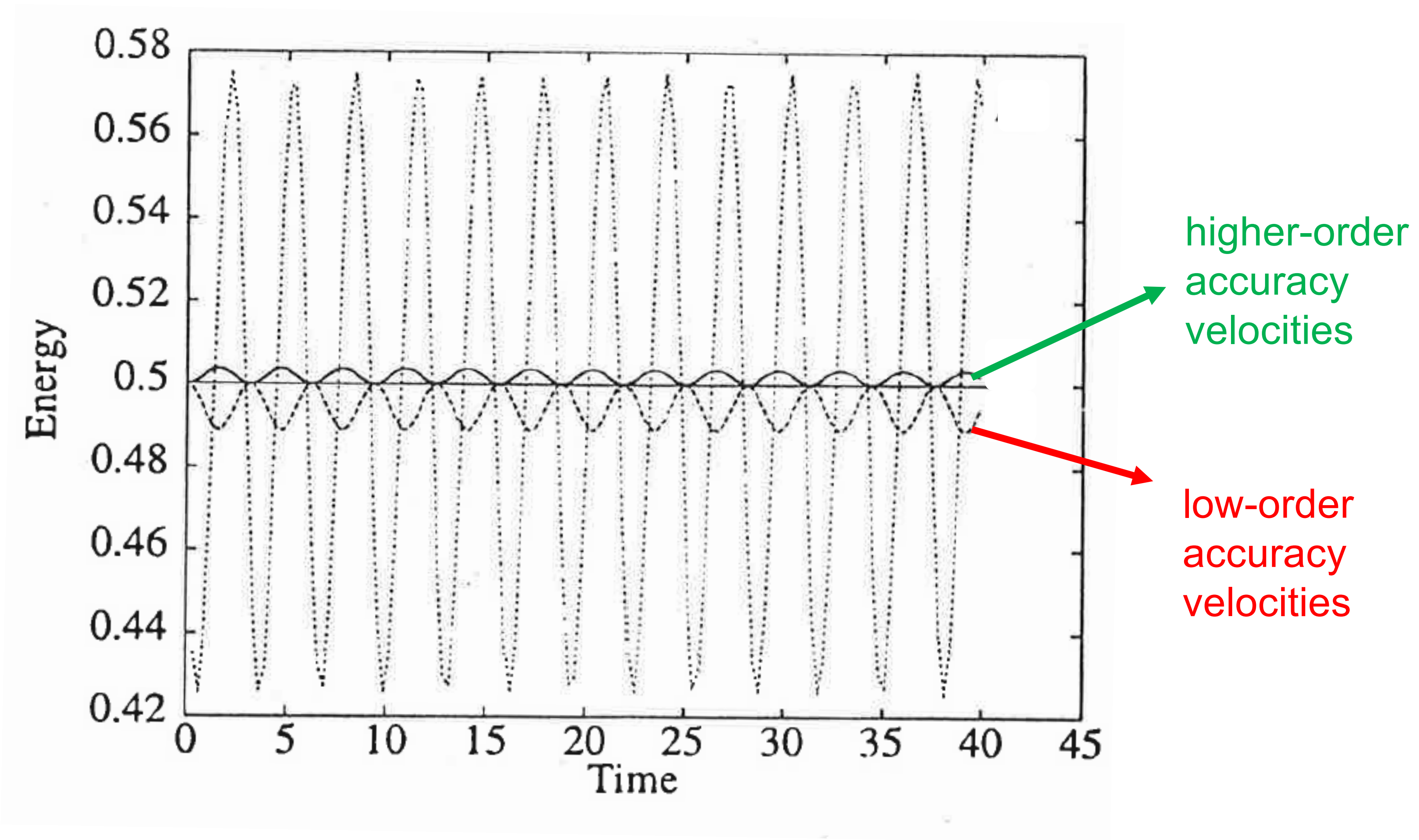
$$m\ddot{r} = f \qquad \Rightarrow \qquad \dddot{r} = \frac{\dot{f}}{m} \cong \frac{f(t+\Delta t) - f(t-\Delta t)}{2m\,\Delta t} + o(\Delta t^2)$$

symmetric difference

We obtain:

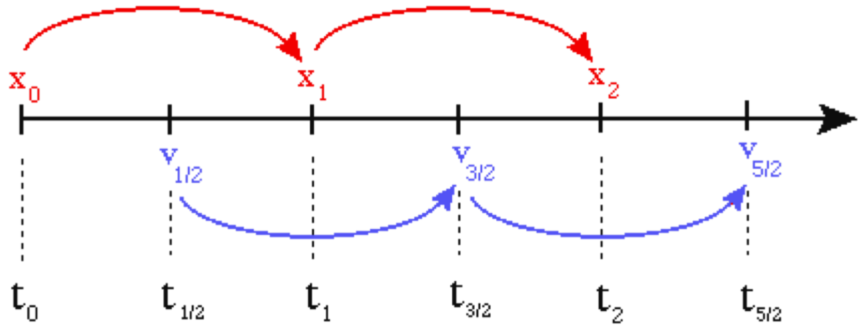
$$v(t) = \frac{r(t+\Delta t) - r(t-\Delta t)}{2\Delta t} - \frac{\Delta t}{12m}\left[f(t+\Delta t) - f(t-\Delta t)\right] + o(\Delta t^4)$$

Example: Harmonic oscillator



Leap-frog Verlet

$$\begin{cases} r(t+\Delta t) = r(t) + v\left(t+\frac{\Delta t}{2}\right)\Delta t \\ v\left(t+\frac{\Delta t}{2}\right) = v\left(t-\frac{\Delta t}{2}\right) + \frac{f(t)}{m}\Delta t \end{cases}$$



Sequence: $\ldots \rightarrow r(t) \rightarrow f(t) \rightarrow v(t+\Delta t/2) \rightarrow r(t+\Delta t) \rightarrow \ldots$

Equivalent to position Verlet

We write the equation for r at time steps $t - \Delta t$ and t :

$$r(t) = r(t-\Delta t) + v\left(t-\frac{\Delta t}{2}\right)\Delta t$$

$$r(t+\Delta t) = r(t) + v\left(t+\frac{\Delta t}{2}\right)\Delta t$$

By subtracting these equations, we obtain

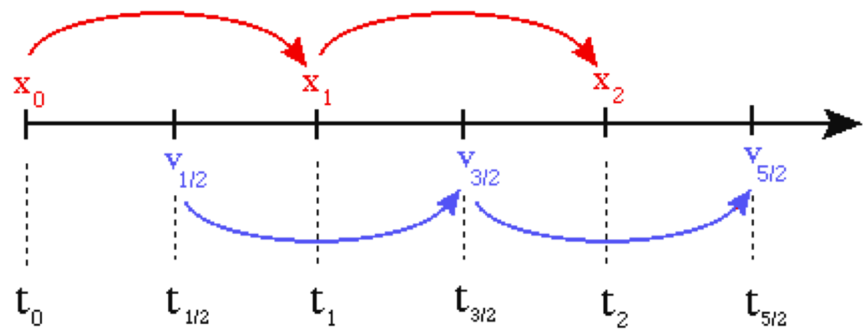
$$r(t+\Delta t) - r(t) = r(t) - r(t-\Delta t) + \Delta t\left[v\left(t+\frac{\Delta t}{2}\right) - v\left(t-\frac{\Delta t}{2}\right)\right]$$

and using the velocity evolution, we recover position Verlet:

$$r(t+\Delta t) = 2\,r(t) - r(t-\Delta t) + \frac{f(t)}{m}\Delta t^{2}$$

Leap-frog Verlet

$$\begin{cases} r(t+\Delta t) = r(t) + v\left(t+\frac{\Delta t}{2}\right)\Delta t \\ v\left(t+\frac{\Delta t}{2}\right) = v\left(t-\frac{\Delta t}{2}\right) + \frac{f(t)}{m}\Delta t \end{cases}$$



Advantage: this algorithm does not contain differences between large numbers.

Disadvantage: positions and velocities are not known at the same time steps.

In the leap-frog algorithm, the velocities are obtained by:

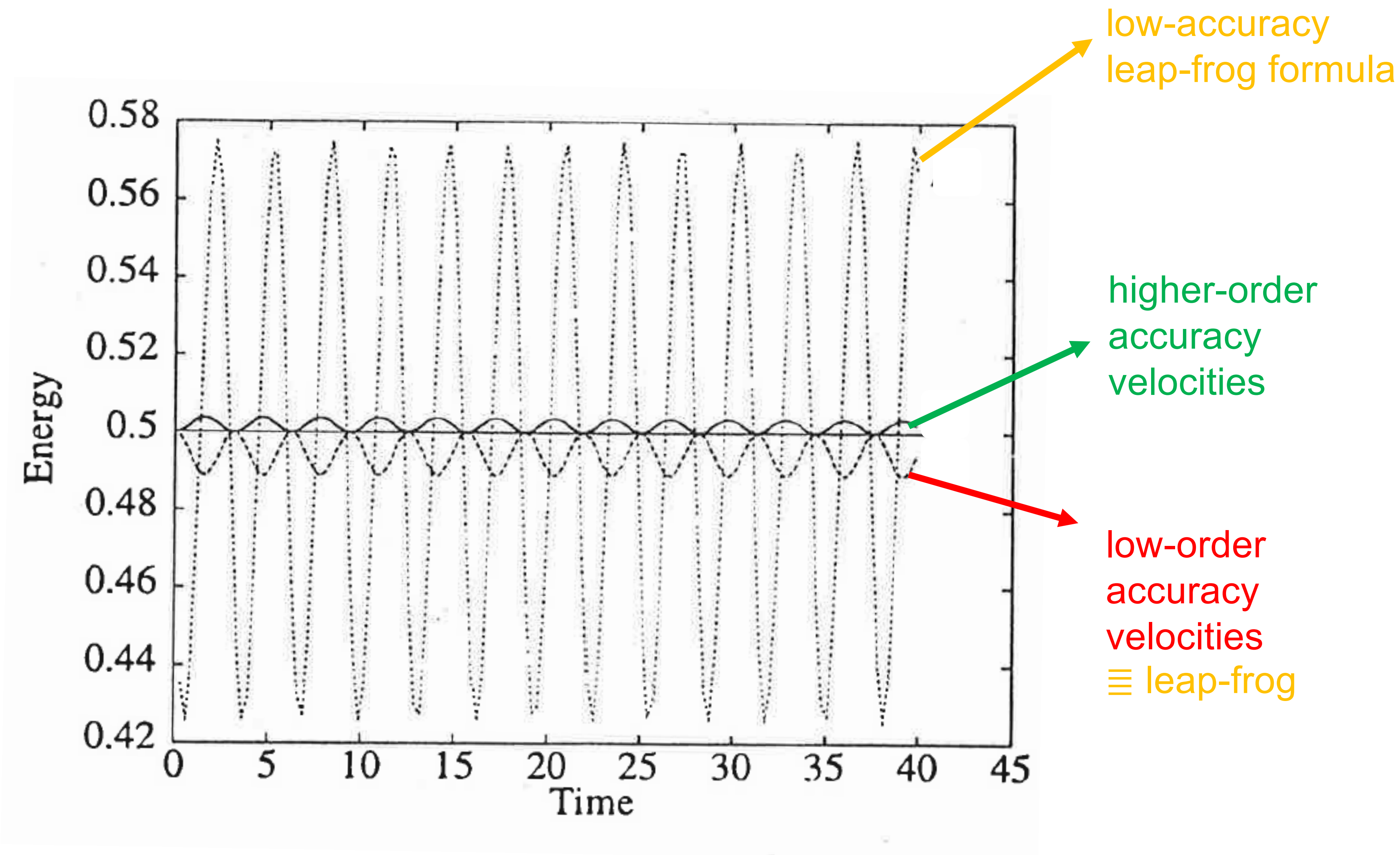
$$v(t) = \tfrac{1}{2}\left[v\left(t+\frac{\Delta t}{2}\right) + v\left(t-\frac{\Delta t}{2}\right)\right]$$

equivalent to low-accuracy velocities of position Verlet

Instead, the following expression shows dramatically larger errors:

$$v\left(t+\frac{\Delta t}{2}\right) = \frac{r(t+\Delta t) - r(t)}{\Delta t}$$

Example: Harmonic oscillator



Velocity Verlet

$$\begin{cases} r(t+\Delta t) = r(t) + v(t)\,\Delta t + \dfrac{f(t)}{2m}\Delta t^2 \\ v(t+\Delta t) = v(t) + \dfrac{f(t)+f(t+\Delta t)}{2m}\Delta t \end{cases}$$

Sequence:
$\ldots \to r(t+\Delta t)$
$\to f(t+\Delta t)$
$\to v(t+\Delta t) \to \ldots$

Equivalence with position Verlet

For $t+\Delta t$:
$$r(t+2\Delta t) = r(t+\Delta t) + v(t+\Delta t)\,\Delta t + \frac{f(t+\Delta t)}{2m}\Delta t^2$$

For t rearranging:
$$r(t) = r(t+\Delta t) - v(t)\,\Delta t - \frac{f(t)}{2m}\Delta t^2$$

Summing up:
$$r(t+2\Delta t) + r(t) = 2\,r(t+\Delta t) + [\,v(t+\Delta t) - v(t)\,]\,\Delta t + \frac{f(t+\Delta t) - f(t)}{2m}\Delta t^2$$

Feeding in the expressions for the velocity evolution:
$$r(t+2\Delta t) + r(t) = 2\,r(t+\Delta t) + \frac{f(t+\Delta t)}{m}\Delta t^2$$

which corresponds precisely to position Verlet for $t \to t-\Delta t$.

Course 03/1

Integration algorithms for MD: Verlet algorithm

- Position Verlet
- Velocities with Verlet
- Leap-frog Verlet
- Velocity Verlet