# 3. Molecular Dynamics – Properties of Discretisation Schemes and Linked-Cells

*November 22, 2010*

# 3.1. Störmer-Verlet-Method

The **Störmer-Verlet** method is given by

$$\vec{r}(t+\Delta t) = 2\cdot\vec{r}(t) - \vec{r}(t-\Delta t) + \Delta t^2\cdot\vec{a}(t) \quad (1)$$

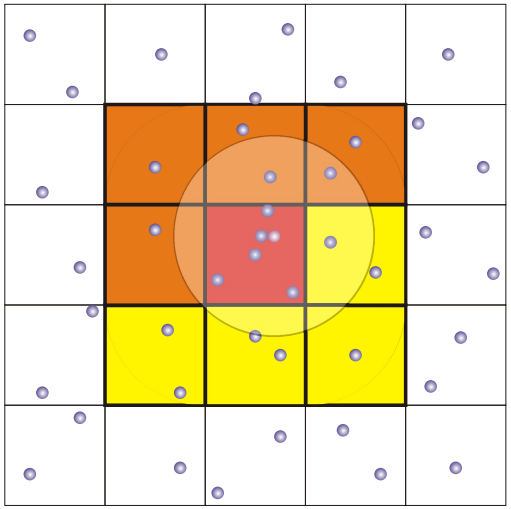
$$\vec{v}(t) = \frac{\vec{r}(t+\Delta t) - \vec{r}(t-\Delta t)}{2\Delta t} \quad (2)$$

The **Velocity-Störmer-Verlet** method is given by

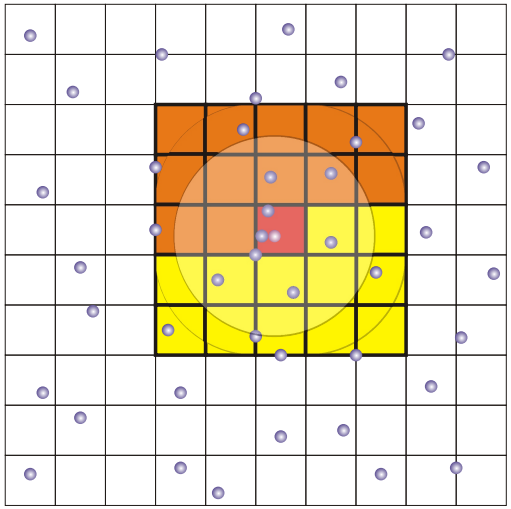
$$\vec{r}(t+\Delta t) = \vec{r}(t) + \Delta t\cdot v(t) + \frac{\Delta t^2}{2}\cdot\vec{a}(t) \quad (3)$$

$$\vec{v}(t+\Delta t) = \vec{v}(t) + \frac{\Delta t}{2}\cdot(\vec{a}(t) + \vec{a}(t+\Delta t)) \quad (4)$$

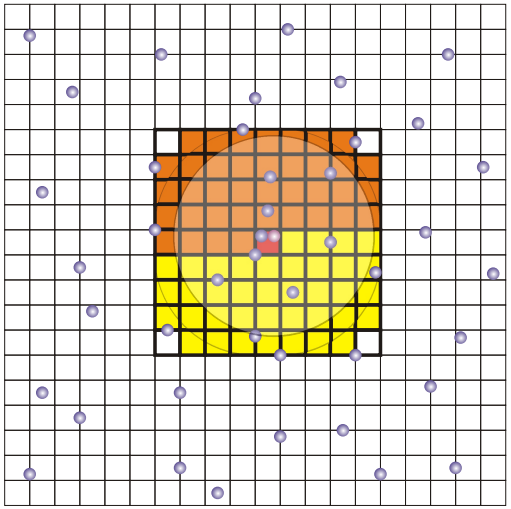
# 3.2. Exercise D: Linked-Cells



$t = 1$

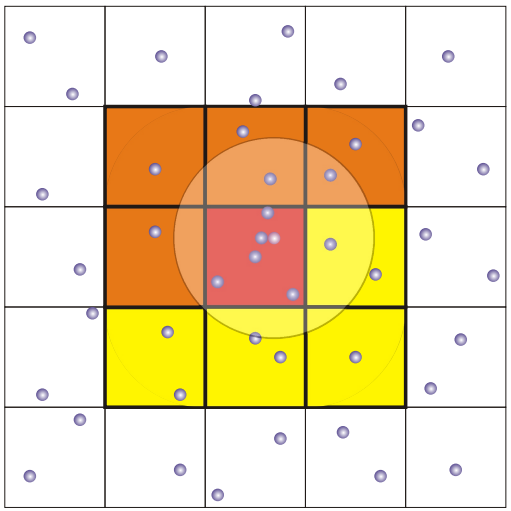


$t = 2$

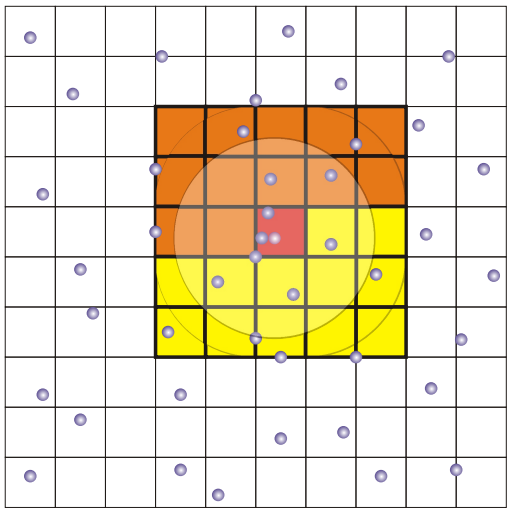


$t = 4$

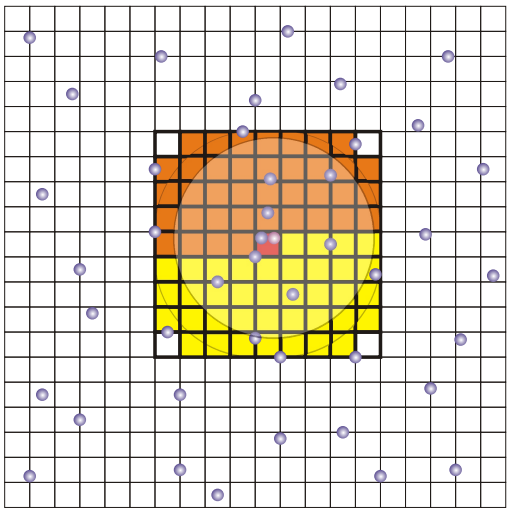
# 3.3. Exercise D: Linked-Cells



$t = 1$



$t = 2$



$t = 4$

| | $l = rc$ | $l = \frac{rc}{2}$ | $l = \frac{rc}{4}$ | $\cdots$ | $l \to \infty$ |
|---|---|---|---|---|---|
| 2D (total area) | $9rc^2$ | $6.25rc^2$ | $4.81rc^2$ | | $3.14rc^2$ |
| 2D (percentage unnecessary | 65 % | 50 % | 35 % | | 0 % |
| 3D (total volume) | $27rc^3$ | $15.63rc^3$ | $9.58rc^3$ | | $4.19rc^3$ |
| 3D (percentage unnecessary | 84 % | 73 % | 56 % | | 0 % |