Goal of Molecular Dynamic Simulations

To find trajectories of molecules being a part of a complex system

Trajectory: position versus time

We have three Cartesian coordinates x,y,z

x(t), y(t), z(t)

– vector describing position of a molecule

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The second Newton law:

a=F/m

a – acceleration

F-force

m-mass

F=ma

y(x)

(y(x+)-y(x))/

When goes to zero, the ratio gives the derivative of y(x) over x, denoted as y’(x)

**r**(t) position as a function of time

**v**(t)= (**r**(t+)-**r**(t))/ velocity as a function of time

for very small one gets the velocity at time t

**v**(t)= **r’**(t)

velocity – (first) derivative of position over time

**a**(t) = (**v**(t+)-**v**(t))/ acceleration as a function of time

**a**(t)=**v**’(t)

acceleration – (first) derivative of velocity over time

**a**(t)=**r**’’(t)

acceleration – (second) derivative of position

Taylor expansion

Rozwinięcie w szereg Taylora

There is a function y(x), and we want to approximate this function around x0

y(x)= y(x0)+(x-x0) + (x-x0)2+(x-x0)3+ ….

3!=1\*2\*3

5!=1\*2\*3\*4\*5…

Please expand y(x)=exp(x) around x0=0 up to the second term

Important remark: the derivative of an exponential function is the function itself

(exp(x))’=exp(x)

exp(0)=1

y(x)=exp(0)+(exp(x))’ (for x=0) \*(x-0)+ 0.5\*(exp(x))’’ (for x=0) \*(x-0)2+ …

y(x)=1+x+0.5x2+ …