

Initial conditions – there are several instructive choices

- (1) R_{bc} at potential energy minimum, atom A
given an incident velocity (try different velocities)
- (2) R_{bc} at inner turning point of BC, atom A
given an incident velocity (try different velocities)
- (3) R_{bc} at outer turning point of BC, atom A
given an incident velocity (try different velocities)

Possible outcomes

$A + BC(v = 0) \rightarrow A + BC(v = 0)$	elastic
$A + BC(v = 0) \rightarrow A + BC(v = v')$	inelastic
$A + BC(v = 0) \rightarrow AB(v = 0) + C$	reactive
$\rightarrow AB(v = v') + C$	reactive with vibr. excitation

Which outcome do you expect?

How can we keep track of vibrational excitation in a classical simulation?

What would happen if we put a barrier on the reaction path?

What sort of averaging do we need to do to get meaningful results?