Lecture LV-Nr. 21357

Molecular dynamics

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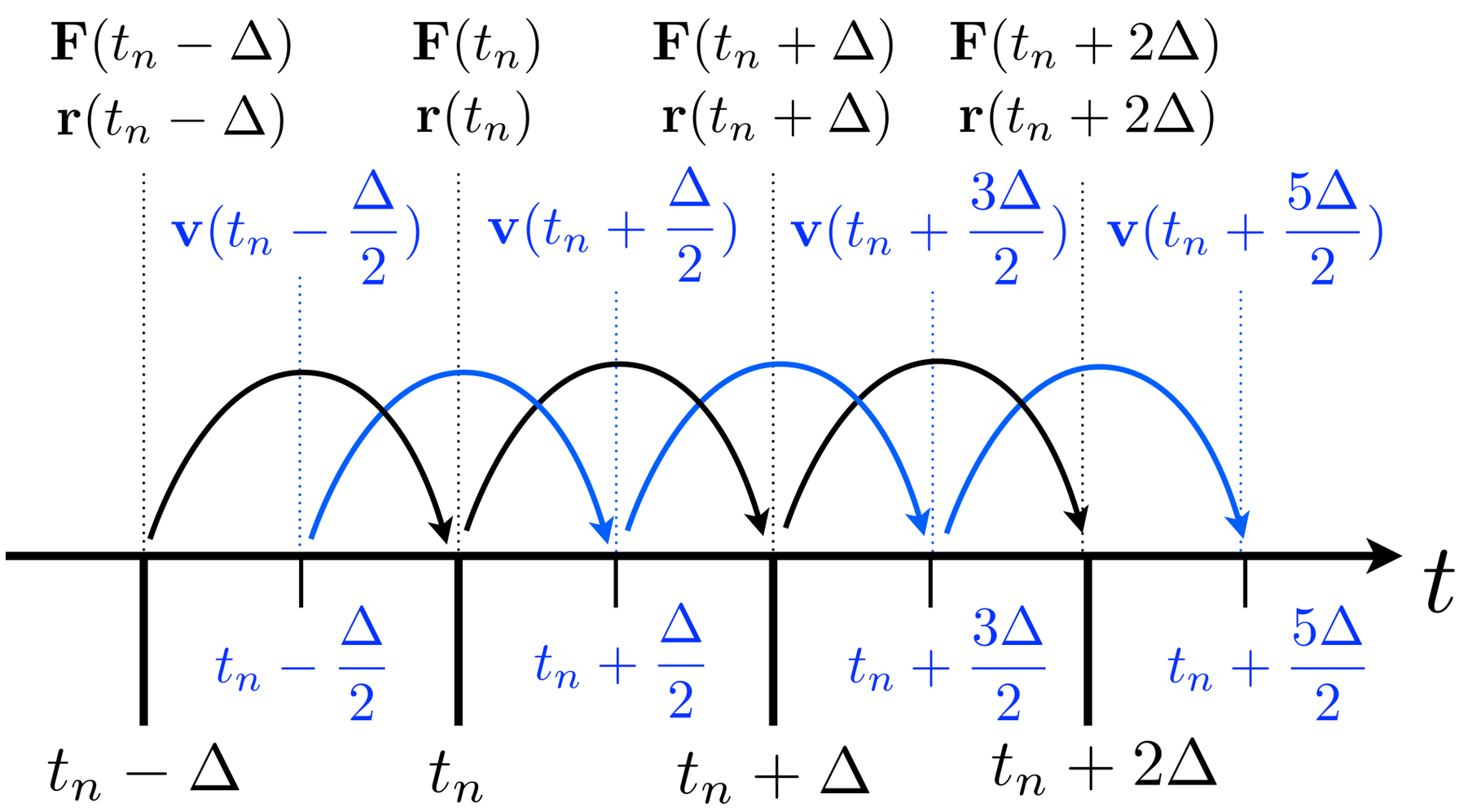
Lecture 3:
Integrators

Leap frog algorithm



GROMACS input file - the .mdp file

```
; VARIOUS PREPROCESSING OPTIONS =
title                    = Yo
cpp                      = /lib/cpp
include                  = -I../top
define                   =

; RUN CONTROL PARAMETERS =
integrator               = md
; start time and timestep in ps =
tinit                    = 0
dt                       = 0.002
nsteps                   = 500000
; number of steps for center of mass motion removal =
nstcomm                  = 1
comm-grps                =

; LANGEVIN DYNAMICS OPTIONS =
; Temperature, friction coefficient (amu/ps) and random seed =
bd-temp                  = 300
bd-fric                  = 0
ld-seed                  = 1993

; ENERGY MINIMIZATION OPTIONS =
; Force tolerance and initial step-size =
emtol                    = 100
emstep                   = 0.01
; Max number of iterations in relax-shells =
niter                    = 20
; Frequency of steepest descents steps when doing CG =
nstcgsteep               = 1000

; OUTPUT CONTROL OPTIONS =
; Output frequency for coords (x), velocities (v) and forces (f)
=
nstxout                  = 5000
nstvout                  = 5000
nstfout                  = 0
...
```

Run control parameters

```
; RUN CONTROL PARAMETERS =
integrator   =   md            Leap frog integrator.
                 md-vv         Velocity Verlet integrator.
                 md-vv-avek    Velocity Verlet integrator with improved estimation of the kinetic
                               energy.
; start time and timestep in ps =
tinit        =   0             Starting time of this simulation run.
dt           =   0.002         Time step Δ in ps. Should be set to 2 fs = 0.002 ps.
nsteps       =   500000        Number of time steps, i.e. the length of the simulation.
initstep     =   0             initstep ≠ 0 only if tinit ≠ 0 and the index of the integration step
                               has to be shifted accordingly.
; number of steps for center of mass motion removal =
comm-mode    =   Linear        Remove center-of-mass translation.
                 Angular       Remove center-of-mass translation and rotation around the center of
                               mass
                 None          Center-of-mass motion is not removed.
nstcomm      =   100           Frequency at which the center-of-mass motion is removed. Default:
                               100.
comm-grps    =                 Group(s) for the removal of the center-of-mass motion. Default: the
                               whole system.
```

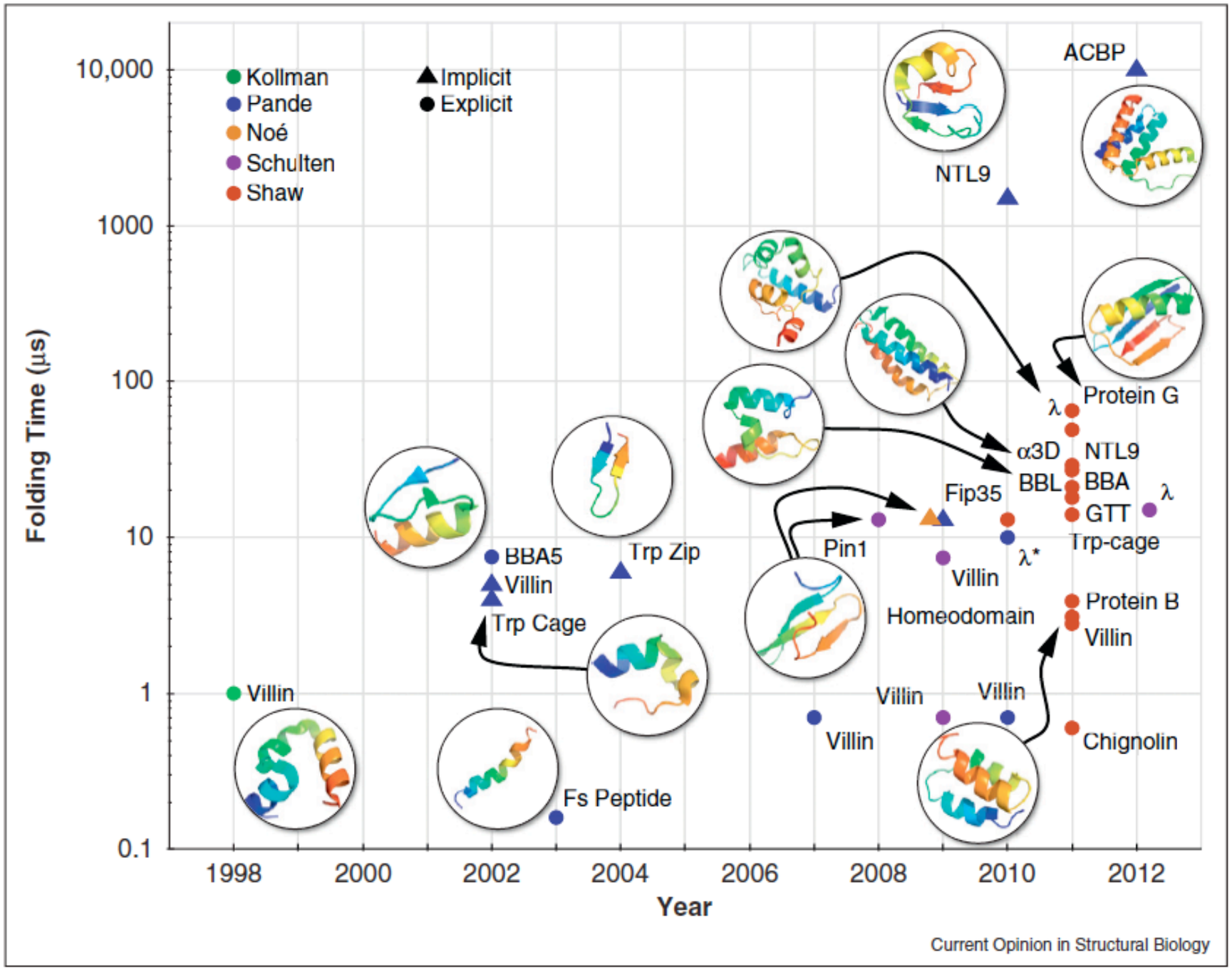
Velocity generation

```
; GENERATE VELOCITIES FOR STARTUP RUN =
gen-vel    =   no       Do not generate velocities. If no velocities are given in the input file,
                        all velocities are set to zero.
               yes      Generate velocities according to a Maxwell distribution at tempera-
                        ture gen-temp, with random-seed gen-seed.
gen-temp   =   300      Temperature of the Maxwell distribution in K.
gen-seed   =   314159   Seed for the random number generator (integer). If gen-seed is set
                        to -1, the seed is calculated from the process ID
```

Output control

```
; OUTPUT CONTROL OPTIONS =
; Output frequency for coords (x), velocities (v) and forces (f) =
nstxout          =   5000          Frequency at which the coordinates are written to the trajectory file.
nstvout          =   5000          Frequency at which the velocities are written to the trajectory file.
nstfout          =   0             Frequency at which the forces are written to the trajectory file.
; Output frequency for energies to log file and energy file =
nstlog           =   5000          Frequency at which the energies are written to the log file.
nstcalcenergy    =   100           Frequency at which the energies are calculated
nstenergy        =   250           Frequency at which the energies are written to the energy file.
; Output frequency and precision for xtc file =
nstxtcout        =   250           Frequency at which the energies are written to the xtc file.
xtc-precision    =   1000          Precision of the output in the xtc-file
; This selects the subset of atoms for the xtc file.  You can =
; select multiple groups.  By default all atoms will be written.  =
xtc-grps         =   Protein       Select the groups which should be written to the xtc-file
; Selection of energy groups =
energygrps       =   Protein SOL   Select the groups which should be written to the energy-file
```

Folding times accessible with classical MD



The folding times accessible by simulation have increased exponentially over the past decade. Shown are all protein folding simulations conducted using unbiased, all-atom MD in empirical force-fields reported in the literature. Some folding times for the same protein differ, due to various mutations. For lambda marked with a (*), the longest timescale seen in that simulation, which was not the folding time, occurred on the order of 10 ms [18,23]. Data are same as Figure 1, with [93].

T. Lane et. al., Current opinion in structural biology, 23, pp- 58-65 (2013).