Benchmark characteristics

Standard MD benchmarks

Tab. 1: Specifications of the "standard" benchmarks.

MD system	MEM	RIB	PEP
# atoms	81,743	2,136,412	12,495,503
system size / nm	$10.8 \times 10.2 \times 9.6$	31.2^3	50.0^3
time step / fs	2	4	2
cutoff radii / nm	1.0	1.0	1.2
PME grid spacing / nm	0.12	0.135	0.16

Useful command line arguments for benchmarking

Run the MEM benchmark for 10,000 steps, reset cycle counters after half of the steps:
`mdrun -s MEM.tpr -nsteps 10000 -resethway`

Run the MEM benchmark for 4,000 steps, reset cycle counters at 3,000 steps:
`mdrun -s MEM.tpr -nsteps 4000 -resetstep 3000`

Run the MEM benchmark for an hour, reset cycle counters after 30 minutes:
`mdrun -s MEM.tpr -nsteps -1 -maxh 1.0 -resethway`

Same as above, but suppress output of the last configuration (which we don't need anyway):
`mdrun -s MEM.tpr -nsteps -1 -maxh 1.0 -resethway -noconfout`

Free energy benchmarks

Tab. 2: Specifications of the "solvation free energy" benchmarks.

MD system	SFI	SFC	STI	STC	SNI	SNC
# atoms	3,363					
# perturbed atoms	48					
system size / nm	$3.65 \times 3.65 \times 2.58$					
time step / fs	2					
cutoff radii / nm	1.2					
PME grid spacing / nm	0.1					
nstcalcenergy	1	100	1	100	1	100
free-energy	yes	yes	slow-growth	slow-growth	no	no

Three letter code for the free energy benchmarks:

- first letter: S = solvation free energy, B = binding free energy MD system, N = no free energy

Tab. 3: Specifications of the "binding free energy" benchmarks.

MD system	BFI	BFC	BTI	BTC	BNI	BNC
# atoms			43,952			
# perturbed atoms			48			
system size / nm			$8.55 \times 8.55 \times 6.04$			
time step / fs			2			
cutoff radii / nm			1.2			
PME grid spacing / nm			0.1			
nstcalcenergy	1	100	1	100	1	100
free-energy	yes	yes	slow-growth	slow-growth	no	no

- second letter: T = TI, F = FEP
- third letter: value of nstcalcenergy, I = 1 step, C = 100 steps

The following two different simulation systems are part of the free energy benchmark suite:

S **solvation** – bromosporine solvation in water

B **binding** – absolute binding affinity of bromosporine to bromodomain

Simulation modes:

NI `noFreeEnergy_nstcalcenergy1` – no free energy, energy evaluations done every step

NC `noFreeEnergy_nstcalcenergy100` – no free energy, energy evaluations done every 100 steps

TI `ti_constLambda_nstcalcenergy1` – free energy is controlled with init-lambda, (delta-lambda set to 0.0 to allow for longer running benchmarks as well), energy evaluations done every step

TC `ti_constLambda_nstcalcenergy100` – free energy is controlled with init-lambda, (delta-lambda set to 0.0 to allow for longer running benchmarks as well), energy evaluations done every 100 steps

FI `fep_nstcalcenergy1` – free energy is controlled with init-lambda-state, coul-lambdas and vdw-lambdas vectors, all 20 lambda neighbors are calculated, energy evaluations done every step

FC `fep_nstcalcenergy100` – free energy is controlled with init-lambda-state, coul-lambdas and vdw-lambdas vectors, all 20 lambda neighbors are calculated, energy evaluations done every 100 steps

Free energy benchmark results

Tab. 9: Solvation free energy benchmarks (48 of 3,363 atoms are perturbed). Single-node performances for CUDA 8.0 and GROMACS 2018.

processor Intel	sockets × cores	clock (GHz)	GPUs GTX	SFI (ns/d)	SFC (ns/d)	STI (ns/d)	STC (ns/d)	SNI (ns/d)	SNC (ns/d)
E3-1240v6	1 × 4	3.7	–	6.1	62.9	59.4	70.3	148.1	208.4
E3-1240v6	1 × 4	3.7	1080	6.7	85.1	87.6	94.2	701	912.1
E3-1240v6	1 × 4	3.7	1080			PME on CPU:		645.7	799.9

Tab. 10: Binding free energy benchmarks (48 of 43,952 atoms are perturbed). Single-node performances for CUDA 8.0 and GROMACS 2018.

processor Intel	sockets × cores	clock (GHz)	GPUs GTX	BFI (ns/d)	BFC (ns/d)	BTI (ns/d)	BTC (ns/d)	BNI (ns/d)	BNC (ns/d)
E3-1240v6	1 × 4	3.7	–	3.2	9	7.1	9	9.9	13.3
E3-1240v6	1 × 4	3.7	1080	4.4	22.4	21.2	22.7	74.7	95.9
E3-1240v6	1 × 4	3.7	1080			PME on CPU:		58.4	73.5