Supporting information to "Simultaneous modeling of chromatin conformation changes from multiple single-cell interaction maps"

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S1 Appendix

Frame force coefficient

Parameters used for the ChromMovie frame force coefficient study (Figure 1B of the manuscript). The full configuration file (`config.yaml`) is provided below.

```yaml
descriptions:
  general:
    input: 'Folder containing input scHi-C contacts in csv format. If None simulated
      scHi-C maps are going to be used.'
    output: 'Output folder for storing simulation results.'
    genome: 'Genome assembly of the input data. Currently supported assemblies: hg19,
      hg38, mm10, GRCm39, GRCg6a.'
    pdf_report: 'Whether to save the simulation diagnostics in a pdf format.'
    remove_problematic: 'A flag indicating whether at each resolution round
      problematic contacts that the simulation was unable to resolve,
      should be removed.'
  simulation:
    platform: 'Available platoforms: CPU, CUDA and OpenCL.'
    resolutions: 'Resolutions to be used for hierarchical modeling. Expected to be
      in the form of comma separated integer of float numbers in the units of Mb.'
    N_steps: 'Number of simulation steps to take at every resolution.'
    burnin: 'Number of simulation steps before starting collecting the simulation
      diagnostic data.'
    MC_step: 'Simulation diagnostic data is going to be collected every MC_step.'
    sim_step: 'The simulation step of Langevin integrator.'
  forcefield:
    ev_formula: 'Type of the Excluded Volume (EV) repulsion. Available types:
      harmonic.'
    ev_min_dist: 'Excluded Volume (EV) minimal distance.'
    ev_coef: 'Excluded Volume (EV) force coefficient.'
    ev_coef_evol: 'Enable or disable the changing EV coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ev_coef at the end.

      If False the coefficient will have stable value of ev_coef.'
    bb_formula: 'Type of the Backbone (BB) potential. Available types:
      harmonic, gaussian.'
    bb_opt_dist: 'Backbone (BB) optimal distance.'
    bb_lin_thresh: 'Backbone (BB) distance after which the potential grows linearly.

```

```
      Must be strictly greater than bb_opt_dist.

      Only applicable if bb_formula is harmonic.'
    bb_coef: 'Backbone (BB) force coefficient.'
    bb_coef_evol: 'Enable or disable the changing BB coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach bb_coef at the end.

      If False the coefficient will have stable value of bb_coef.'
    sc_formula: 'Type of the Single cell contact (SC) potential. Available types:
      harmonic, gaussian.'
    sc_opt_dist: 'Single cell contact (SC) optimal distance.'
    sc_lin_thresh: 'Single cell contact (SC) distance after which the potential grows
      linearly.

      Must be strictly greater than sc_opt_dist.

      Only applicable if sc_formula is harmonic.'
    sc_coef: 'Single cell contact (SC) force coefficient.'
    sc_coef_evol: 'Enable or disable the changing SC coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach sc_coef at the end.

      If False the coefficient will have stable value of sc_coef.'
    ff_formula: 'Type of the Frame force (FF) potential. Available types: harmonic,
      gaussian.'
    ff_opt_dist: 'Frame force (FF) optimal distance.'
    ff_lin_thresh: 'Frame force (FF) distance after which the potential grows
      linearly.

      Must be strictly greater than ff_opt_dist.

      Only applicable if ff_formula is harmonic.'
    ff_coef: 'Frame force (FF) force coefficient.'
    ff_coef_evol: 'Enable or disable the changing FF coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ff_coef at the end.

      If False the coefficient will have stable value of ff_coef.'
general:
  input: data/data_ff_study
  output: ./results/tests/test17/
  genome: mm10
  pdf_report: false
  remove_problematic: false
simulation:
  platform: OpenCL
  resolutions: 5,2
  N_steps: 100
  burnin: 5
  MC_step: 1
```

```
  sim_step: 20
forcefield:
  ev_formula: harmonic
  ev_min_dist: 1.0
  ev_coef: 1000.0
  ev_coef_evol: false
  bb_formula: harmonic
  bb_opt_dist: 1.0
  bb_lin_thresh: 2.0
  bb_coef: 1000.0
  bb_coef_evol: false
  sc_formula: harmonic
  sc_opt_dist: 1.0
  sc_lin_thresh: 2.0
  sc_coef: 1000.0
  sc_coef_evol: false
  ff_formula: harmonic
  ff_opt_dist: 1.0
  ff_lin_thresh: 2.0
  ff_coef: 90.77494998747494
  ff_coef_evol: false
```

Single-cell contact violation

Parameters used for the ChromMovie single-cell contact violation study (Figure 1D and 1E of the manuscript). The full configuration file (`config.yaml`) is provided below.

```
descriptions:
  general:
    input: 'Folder containing input scHi-C contacts in csv format. If None simulated
      scHi-C maps are going to be used.'
    output: 'Output folder for storing simulation results.'
    genome: 'Genome assembly of the input data. Currently supported assemblies: hg19,
      hg38, mm10, GRCm39, GRCg6a.'
    pdf_report: 'Whether to save the simulation diagnostics in a pdf format.'
    remove_problematic: 'A flag indicating whether at each resolution round
      problematic contacts that the simulation was unable to resolve,
      should be removed.'
  simulation:
    platform: 'Available platoforms: CPU, CUDA and OpenCL.'
    resolutions: 'Resolutions to be used for hierarchical modeling. Expected to be
      in the form of comma separated integer of float numbers in the units of Mb.'
    N_steps: 'Number of simulation steps to take at every resolution.'
    burnin: 'Number of simulation steps before starting collecting the simulation
      diagnostic data.'
    MC_step: 'Simulation diagnostic data is going to be collected every MC_step.'
    sim_step: 'The simulation step of Langevin integrator.'
  forcefield:
    ev_formula: 'Type of the Excluded Volume (EV) repulsion. Available types:
      harmonic.'
    ev_min_dist: 'Excluded Volume (EV) minimal distance.'
    ev_coef: 'Excluded Volume (EV) force coefficient.'
    ev_coef_evol: 'Enable or disable the changing EV coefficient value.
```

```
      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ev_coef at the end.

      If False the coefficient will have stable value of ev_coef.'
    bb_formula: 'Type of the Backbone (BB) potential. Available types:
      harmonic, gaussian.'
    bb_opt_dist: 'Backbone (BB) optimal distance.'
    bb_lin_thresh: 'Backbone (BB) distance after which the potential grows linearly.

      Must be strictly greater than bb_opt_dist.

      Only applicable if bb_formula is harmonic.'
    bb_coef: 'Backbone (BB) force coefficient.'
    bb_coef_evol: 'Enable or disable the changing BB coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach bb_coef at the end.

      If False the coefficient will have stable value of bb_coef.'
    sc_formula: 'Type of the Single cell contact (SC) potential. Available types:
      harmonic, gaussian.'
    sc_opt_dist: 'Single cell contact (SC) optimal distance.'
    sc_lin_thresh: 'Single cell contact (SC) distance after which the potential grows
      linearly.

      Must be strictly greater than sc_opt_dist.

      Only applicable if sc_formula is harmonic.'
    sc_coef: 'Single cell contact (SC) force coefficient.'
    sc_coef_evol: 'Enable or disable the changing SC coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach sc_coef at the end.

      If False the coefficient will have stable value of sc_coef.'
    ff_formula: 'Type of the Frame force (FF) potential. Available types: harmonic,
      gaussian.'
    ff_opt_dist: 'Frame force (FF) optimal distance.'
    ff_lin_thresh: 'Frame force (FF) distance after which the potential grows
      linearly.

      Must be strictly greater than ff_opt_dist.

      Only applicable if ff_formula is harmonic.'
    ff_coef: 'Frame force (FF) force coefficient.'
    ff_coef_evol: 'Enable or disable the changing FF coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ff_coef at the end.

      If False the coefficient will have stable value of ff_coef.'
general:
  input: examples/example1_cell_cycle
  output: ./results/results_sccv/
```

```
  genome: mm10
  pdf_report: true
  remove_problematic: false
simulation:
  platform: OpenCL
  resolutions: 5,2
  N_steps: 50
  burnin: 0
  MC_step: 1
  sim_step: 20
forcefield:
  ev_formula: harmonic
  ev_min_dist: 2.0
  ev_coef: 50.0
  ev_coef_evol: false
  bb_formula: harmonic
  bb_opt_dist: 1.0
  bb_lin_thresh: 2.0
  bb_coef: 1000.0
  bb_coef_evol: false
  sc_formula: harmonic
  sc_opt_dist: 1.0
  sc_lin_thresh: 2.0
  sc_coef: 100.0
  sc_coef_evol: false
  ff_formula: harmonic
  ff_opt_dist: 1.0
  ff_lin_thresh: 2.0
  ff_coef: 100.0
  ff_coef_evol: false
```

Comparison with NucDynamics

Parameters used for the ChromMovie comparison with NucDynamics study (Figure 2 and Figure 3 of the manuscript). The full configuration file (`config.yaml`) is provided below.

```
descriptions:
  general:
    input: 'Folder containing input scHi-C contacts in csv format. If None simulated
      scHi-C maps are going to be used.'
    output: 'Output folder for storing simulation results.'
    genome: 'Genome assembly of the input data. Currently supported assemblies: hg19,
      hg38, mm10, GRCm39, GRCg6a.'
    pdf_report: 'Whether to save the simulation diagnostics in a pdf format.'
    remove_problematic: 'A flag indicating whether at each resolution round
      problematic contacts that the simulation was unable to resolve,
      should be removed.'
  simulation:
    platform: 'Available platoforms: CPU, CUDA and OpenCL.'
    resolutions: 'Resolutions to be used for hierarchical modeling. Expected to be
      in the form of comma separated integer of float numbers in the units of Mb.'
    N_steps: 'Number of simulation steps to take at every resolution.'
    burnin: 'Number of simulation steps before starting collecting the simulation
      diagnostic data.'
```

```
    MC_step: 'Simulation diagnostic data is going to be collected every MC_step.'
    sim_step: 'The simulation step of Langevin integrator.'
  forcefield:
    ev_formula: 'Type of the Excluded Volume (EV) repulsion. Available types:
      harmonic.'
    ev_min_dist: 'Excluded Volume (EV) minimal distance.'
    ev_coef: 'Excluded Volume (EV) force coefficient.'
    ev_coef_evol: 'Enable or disable the changing EV coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ev_coef at the end.

      If False the coefficient will have stable value of ev_coef.'
    bb_formula: 'Type of the Backbone (BB) potential. Available types:
      harmonic, gaussian.'
    bb_opt_dist: 'Backbone (BB) optimal distance.'
    bb_lin_thresh: 'Backbone (BB) distance after which the potential grows linearly.

      Must be strictly greater than bb_opt_dist.

      Only applicable if bb_formula is harmonic.'
    bb_coef: 'Backbone (BB) force coefficient.'
    bb_coef_evol: 'Enable or disable the changing BB coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach bb_coef at the end.

      If False the coefficient will have stable value of bb_coef.'
    sc_formula: 'Type of the Single cell contact (SC) potential. Available types:
      harmonic, gaussian.'
    sc_opt_dist: 'Single cell contact (SC) optimal distance.'
    sc_lin_thresh: 'Single cell contact (SC) distance after which the potential grows
      linearly.

      Must be strictly greater than sc_opt_dist.

      Only applicable if sc_formula is harmonic.'
    sc_coef: 'Single cell contact (SC) force coefficient.'
    sc_coef_evol: 'Enable or disable the changing SC coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach sc_coef at the end.

      If False the coefficient will have stable value of sc_coef.'
    ff_formula: 'Type of the Frame force (FF) potential. Available types: harmonic,
      gaussian.'
    ff_opt_dist: 'Frame force (FF) optimal distance.'
    ff_lin_thresh: 'Frame force (FF) distance after which the potential grows
      linearly.

      Must be strictly greater than ff_opt_dist.

      Only applicable if ff_formula is harmonic.'
    ff_coef: 'Frame force (FF) force coefficient.'
```

```
    ff_coef_evol: 'Enable or disable the changing FF coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ff_coef at the end.

      If False the coefficient will have stable value of ff_coef.'
general:
  input: ./data/cell_cycle/chr12
  output: ./results/results_k562_chr12/
  genome: hg38
  pdf_report: false
  remove_problematic: false
simulation:
  platform: OpenCL
  resolutions: 2,0.5,0.1
  N_steps: 50
  burnin: 0
  MC_step: 1
  sim_step: 20
forcefield:
  ev_formula: harmonic
  ev_min_dist: 2.0
  ev_coef: 40.0
  ev_coef_evol: false
  bb_formula: harmonic
  bb_opt_dist: 1.0
  bb_lin_thresh: 2.0
  bb_coef: 1000.0
  bb_coef_evol: false
  sc_formula: harmonic
  sc_opt_dist: 1.0
  sc_lin_thresh: 2.0
  sc_coef: 20.0
  sc_coef_evol: false
  ff_formula: harmonic
  ff_opt_dist: 1.0
  ff_lin_thresh: 2.0
  ff_coef: 1000.0
  ff_coef_evol: false
```

Mitotic chromosome formation

Parameters used for the ChromMovie mitotic chromosome formation study (Figure 4A of the manuscript). The full configuration file (`config.yaml`) is provided below.

```
descriptions:
  general:
    input: 'Folder containing input scHi-C contacts in csv format. If None simulated
      scHi-C maps are going to be used.'
    output: 'Output folder for storing simulation results.'
    genome: 'Genome assembly of the input data. Currently supported assemblies: hg19,
      hg38, mm10, GRCm39, GRCg6a.'
    pdf_report: 'Whether to save the simulation diagnostics in a pdf format.'
    remove_problematic: 'A flag indicating whether at each resolution round
```

```
    problematic contacts that the simulation was unable to resolve,
    should be removed.'
simulation:
  platform: 'Available platoforms: CPU, CUDA and OpenCL.'
  resolutions: 'Resolutions to be used for hierarchical modeling. Expected to be
    in the form of comma separated integer of float numbers in the units of Mb.'
  N_steps: 'Number of simulation steps to take at every resolution.'
  burnin: 'Number of simulation steps before starting collecting the simulation
    diagnostic data.'
  MC_step: 'Simulation diagnostic data is going to be collected every MC_step.'
  sim_step: 'The simulation step of Langevin integrator.'
forcefield:
  ev_formula: 'Type of the Excluded Volume (EV) repulsion. Available types:
    harmonic.'
  ev_min_dist: 'Excluded Volume (EV) minimal distance.'
  ev_coef: 'Excluded Volume (EV) force coefficient.'
  ev_coef_evol: 'Enable or disable the changing EV coefficient value.

    If True the coefficient will start as 0 at the beginning of the simulation and
    reach ev_coef at the end.

    If False the coefficient will have stable value of ev_coef.'
  bb_formula: 'Type of the Backbone (BB) potential. Available types:
    harmonic, gaussian.'
  bb_opt_dist: 'Backbone (BB) optimal distance.'
  bb_lin_thresh: 'Backbone (BB) distance after which the potential grows linearly.

    Must be strictly greater than bb_opt_dist.

    Only applicable if bb_formula is harmonic.'
  bb_coef: 'Backbone (BB) force coefficient.'
  bb_coef_evol: 'Enable or disable the changing BB coefficient value.

    If True the coefficient will start as 0 at the beginning of the simulation and
    reach bb_coef at the end.

    If False the coefficient will have stable value of bb_coef.'
  sc_formula: 'Type of the Single cell contact (SC) potential. Available types:
    harmonic, gaussian.'
  sc_opt_dist: 'Single cell contact (SC) optimal distance.'
  sc_lin_thresh: 'Single cell contact (SC) distance after which the potential grows
    linearly.

    Must be strictly greater than sc_opt_dist.

    Only applicable if sc_formula is harmonic.'
  sc_coef: 'Single cell contact (SC) force coefficient.'
  sc_coef_evol: 'Enable or disable the changing SC coefficient value.

    If True the coefficient will start as 0 at the beginning of the simulation and
    reach sc_coef at the end.

    If False the coefficient will have stable value of sc_coef.'
  ff_formula: 'Type of the Frame force (FF) potential. Available types: harmonic,
```

```
      gaussian.'
    ff_opt_dist: 'Frame force (FF) optimal distance.'
    ff_lin_thresh: 'Frame force (FF) distance after which the potential grows
      linearly.

      Must be strictly greater than ff_opt_dist.

      Only applicable if ff_formula is harmonic.'
    ff_coef: 'Frame force (FF) force coefficient.'
    ff_coef_evol: 'Enable or disable the changing FF coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ff_coef at the end.

      If False the coefficient will have stable value of ff_coef.'
general:
  input: data/data_mitotic
  output: results/results_mitotic
  genome: GRCg6a
  pdf_report: true
  remove_problematic: true
simulation:
  platform: OpenCL
  resolutions: 5,2,1,0.2,0.05
  N_steps: 100
  burnin: 10
  MC_step: 1
  sim_step: 100
forcefield:
  ev_formula: harmonic
  ev_min_dist: 2.0
  ev_coef: 10.0
  ev_coef_evol: true
  bb_formula: harmonic
  bb_opt_dist: 1.0
  bb_lin_thresh: 2.0
  bb_coef: 10.0
  bb_coef_evol: false
  sc_formula: harmonic
  sc_opt_dist: 2.0
  sc_lin_thresh: 2.5
  sc_coef: 10.0
  sc_coef_evol: false
  ff_formula: harmonic
  ff_opt_dist: 1.0
  ff_lin_thresh: 1.5
  ff_coef: 10.0
  ff_coef_evol: false
```

Downsampling

Parameters used for the ChromMovie downsampling study (Figure 4B of the manuscript). The full configuration file (`config.yaml`) is provided below.

```
descriptions:
```

```
general:
  input: 'Folder containing input scHi-C contacts in csv format. If None simulated
    scHi-C maps are going to be used.'
  output: 'Output folder for storing simulation results.'
  genome: 'Genome assembly of the input data. Currently supported assemblies: hg19,
    hg38, mm10, GRCm39, GRCg6a.'
  pdf_report: 'Whether to save the simulation diagnostics in a pdf format.'
  remove_problematic: 'A flag indicating whether at each resolution round
    problematic contacts that the simulation was unable to resolve,
    should be removed.'
simulation:
  platform: 'Available platoforms: CPU, CUDA and OpenCL.'
  resolutions: 'Resolutions to be used for hierarchical modeling. Expected to be
    in the form of comma separated integer of float numbers in the units of Mb.'
  N_steps: 'Number of simulation steps to take at every resolution.'
  burnin: 'Number of simulation steps before starting collecting the simulation
    diagnostic data.'
  MC_step: 'Simulation diagnostic data is going to be collected every MC_step.'
  sim_step: 'The simulation step of Langevin integrator.'
forcefield:
  ev_formula: 'Type of the Excluded Volume (EV) repulsion. Available types:
    harmonic.'
  ev_min_dist: 'Excluded Volume (EV) minimal distance.'
  ev_coef: 'Excluded Volume (EV) force coefficient.'
  ev_coef_evol: 'Enable or disable the changing EV coefficient value.

    If True the coefficient will start as 0 at the beginning of the simulation and
    reach ev_coef at the end.

    If False the coefficient will have stable value of ev_coef.'
  bb_formula: 'Type of the Backbone (BB) potential. Available types:
    harmonic, gaussian.'
  bb_opt_dist: 'Backbone (BB) optimal distance.'
  bb_lin_thresh: 'Backbone (BB) distance after which the potential grows linearly.

    Must be strictly greater than bb_opt_dist.

    Only applicable if bb_formula is harmonic.'
  bb_coef: 'Backbone (BB) force coefficient.'
  bb_coef_evol: 'Enable or disable the changing BB coefficient value.

    If True the coefficient will start as 0 at the beginning of the simulation and
    reach bb_coef at the end.

    If False the coefficient will have stable value of bb_coef.'
  sc_formula: 'Type of the Single cell contact (SC) potential. Available types:
    harmonic, gaussian.'
  sc_opt_dist: 'Single cell contact (SC) optimal distance.'
  sc_lin_thresh: 'Single cell contact (SC) distance after which the potential grows
    linearly.

    Must be strictly greater than sc_opt_dist.

    Only applicable if sc_formula is harmonic.'
```

```
    sc_coef: 'Single cell contact (SC) force coefficient.'
    sc_coef_evol: 'Enable or disable the changing SC coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach sc_coef at the end.

      If False the coefficient will have stable value of sc_coef.'
    ff_formula: 'Type of the Frame force (FF) potential. Available types: harmonic,
      gaussian.'
    ff_opt_dist: 'Frame force (FF) optimal distance.'
    ff_lin_thresh: 'Frame force (FF) distance after which the potential grows
      linearly.

      Must be strictly greater than ff_opt_dist.

      Only applicable if ff_formula is harmonic.'
    ff_coef: 'Frame force (FF) force coefficient.'
    ff_coef_evol: 'Enable or disable the changing FF coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ff_coef at the end.

      If False the coefficient will have stable value of ff_coef.'
general:
  input: data/data_downsample
  output: results/results_downsample
  genome: GRCg6a
  pdf_report: false
  remove_problematic: false
simulation:
  platform: OpenCL
  resolutions: 5,2,1,0.2
  N_steps: 100
  burnin: 10
  MC_step: 1
  sim_step: 100
forcefield:
  ev_formula: harmonic
  ev_min_dist: 2.0
  ev_coef: 10.0
  ev_coef_evol: true
  bb_formula: harmonic
  bb_opt_dist: 1.0
  bb_lin_thresh: 2.0
  bb_coef: 10.0
  bb_coef_evol: false
  sc_formula: harmonic
  sc_opt_dist: 2.0
  sc_lin_thresh: 2.5
  sc_coef: 10.0
  sc_coef_evol: false
  ff_formula: harmonic
  ff_opt_dist: 1.0
  ff_lin_thresh: 1.5
```

```
  ff_coef: 10.0
  ff_coef_evol: false
```

Ensemble

Parameters used for the ChromMovie ensemble study (Figure 4C of the manuscript). The full configuration file (`config.yaml`) is provided below.

```
descriptions:
  general:
    input: 'Folder containing input scHi-C contacts in csv format. If None simulated
      scHi-C maps are going to be used.'
    output: 'Output folder for storing simulation results.'
    genome: 'Genome assembly of the input data. Currently supported assemblies: hg19,
      hg38, mm10, GRCm39, GRCg6a.'
    pdf_report: 'Whether to save the simulation diagnostics in a pdf format.'
    remove_problematic: 'A flag indicating whether at each resolution round
      problematic contacts that the simulation was unable to resolve,
      should be removed.'
  simulation:
    platform: 'Available platoforms: CPU, CUDA and OpenCL.'
    resolutions: 'Resolutions to be used for hierarchical modeling. Expected to be
      in the form of comma separated integer of float numbers in the units of Mb.'
    N_steps: 'Number of simulation steps to take at every resolution.'
    burnin: 'Number of simulation steps before starting collecting the simulation
      diagnostic data.'
    MC_step: 'Simulation diagnostic data is going to be collected every MC_step.'
    sim_step: 'The simulation step of Langevin integrator.'
  forcefield:
    ev_formula: 'Type of the Excluded Volume (EV) repulsion. Available types:
      harmonic.'
    ev_min_dist: 'Excluded Volume (EV) minimal distance.'
    ev_coef: 'Excluded Volume (EV) force coefficient.'
    ev_coef_evol: 'Enable or disable the changing EV coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ev_coef at the end.

      If False the coefficient will have stable value of ev_coef.'
    bb_formula: 'Type of the Backbone (BB) potential. Available types:
      harmonic, gaussian.'
    bb_opt_dist: 'Backbone (BB) optimal distance.'
    bb_lin_thresh: 'Backbone (BB) distance after which the potential grows linearly.

      Must be strictly greater than bb_opt_dist.

      Only applicable if bb_formula is harmonic.'
    bb_coef: 'Backbone (BB) force coefficient.'
    bb_coef_evol: 'Enable or disable the changing BB coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach bb_coef at the end.

      If False the coefficient will have stable value of bb_coef.'
```

```
    sc_formula: 'Type of the Single cell contact (SC) potential. Available types:
      harmonic, gaussian.'
    sc_opt_dist: 'Single cell contact (SC) optimal distance.'
    sc_lin_thresh: 'Single cell contact (SC) distance after which the potential grows
      linearly.

      Must be strictly greater than sc_opt_dist.

      Only applicable if sc_formula is harmonic.'
    sc_coef: 'Single cell contact (SC) force coefficient.'
    sc_coef_evol: 'Enable or disable the changing SC coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach sc_coef at the end.

      If False the coefficient will have stable value of sc_coef.'
    ff_formula: 'Type of the Frame force (FF) potential. Available types: harmonic,
      gaussian.'
    ff_opt_dist: 'Frame force (FF) optimal distance.'
    ff_lin_thresh: 'Frame force (FF) distance after which the potential grows
      linearly.

      Must be strictly greater than ff_opt_dist.

      Only applicable if ff_formula is harmonic.'
    ff_coef: 'Frame force (FF) force coefficient.'
    ff_coef_evol: 'Enable or disable the changing FF coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ff_coef at the end.

      If False the coefficient will have stable value of ff_coef.'
general:
  input: data/data_ensemble
  output: results/results_ensemble_00
  genome: GRCg6a
  pdf_report: false
  remove_problematic: false
simulation:
  platform: OpenCL
  resolutions: 5,2,1,0.2
  N_steps: 100
  burnin: 10
  MC_step: 1
  sim_step: 100
forcefield:
  ev_formula: harmonic
  ev_min_dist: 2.0
  ev_coef: 10.0
  ev_coef_evol: true
  bb_formula: harmonic
  bb_opt_dist: 1.0
  bb_lin_thresh: 2.0
  bb_coef: 10.0
```

```
  bb_coef_evol: false
  sc_formula: harmonic
  sc_opt_dist: 2.0
  sc_lin_thresh: 2.5
  sc_coef: 10.0
  sc_coef_evol: false
  ff_formula: harmonic
  ff_opt_dist: 1.0
  ff_lin_thresh: 1.5
  ff_coef: 10.0
  ff_coef_evol: false
```

Computational time

Parameters used for the ChromMovie computational time benchmarking study (Figure 5 of the manuscript). The full configuration file (`config.yaml`) is provided below.

```
descriptions:
  general:
    input: 'Folder containing input scHi-C contacts in csv format. If None simulated
      scHi-C maps are going to be used.'
    output: 'Output folder for storing simulation results.'
    genome: 'Genome assembly of the input data. Currently supported assemblies: hg19,
      hg38, mm10, GRCm39, GRCg6a.'
    pdf_report: 'Whether to save the simulation diagnostics in a pdf format.'
    remove_problematic: 'A flag indicating whether at each resolution round
      problematic contacts that the simulation was unable to resolve,
      should be removed.'
  simulation:
    platform: 'Available platoforms: CPU, CUDA and OpenCL.'
    resolutions: 'Resolutions to be used for hierarchical modeling. Expected to be
      in the form of comma separated integer of float numbers in the units of Mb.'
    N_steps: 'Number of simulation steps to take at every resolution.'
    burnin: 'Number of simulation steps before starting collecting the simulation
      diagnostic data.'
    MC_step: 'Simulation diagnostic data is going to be collected every MC_step.'
    sim_step: 'The simulation step of Langevin integrator.'
  forcefield:
    ev_formula: 'Type of the Excluded Volume (EV) repulsion. Available types:
      harmonic.'
    ev_min_dist: 'Excluded Volume (EV) minimal distance.'
    ev_coef: 'Excluded Volume (EV) force coefficient.'
    ev_coef_evol: 'Enable or disable the changing EV coefficient value.

      If True the coefficient will start as 0 at the beginning of the simulation and
      reach ev_coef at the end.

      If False the coefficient will have stable value of ev_coef.'
    bb_formula: 'Type of the Backbone (BB) potential. Available types:
      harmonic, gaussian.'
    bb_opt_dist: 'Backbone (BB) optimal distance.'
    bb_lin_thresh: 'Backbone (BB) distance after which the potential grows linearly.

      Must be strictly greater than bb_opt_dist.
```

```
38
39        Only applicable if bb_formula is harmonic.'
40      bb_coef: 'Backbone (BB) force coefficient.'
41      bb_coef_evol: 'Enable or disable the changing BB coefficient value.
42
43        If True the coefficient will start as 0 at the beginning of the simulation and
44        reach bb_coef at the end.
45
46        If False the coefficient will have stable value of bb_coef.'
47      sc_formula: 'Type of the Single cell contact (SC) potential. Available types:
48        harmonic, gaussian.'
49      sc_opt_dist: 'Single cell contact (SC) optimal distance.'
50      sc_lin_thresh: 'Single cell contact (SC) distance after which the potential grows
51        linearly.
52
53        Must be strictly greater than sc_opt_dist.
54
55        Only applicable if sc_formula is harmonic.'
56      sc_coef: 'Single cell contact (SC) force coefficient.'
57      sc_coef_evol: 'Enable or disable the changing SC coefficient value.
58
59        If True the coefficient will start as 0 at the beginning of the simulation and
60        reach sc_coef at the end.
61
62        If False the coefficient will have stable value of sc_coef.'
63      ff_formula: 'Type of the Frame force (FF) potential. Available types: harmonic,
64        gaussian.'
65      ff_opt_dist: 'Frame force (FF) optimal distance.'
66      ff_lin_thresh: 'Frame force (FF) distance after which the potential grows
67        linearly.
68
69        Must be strictly greater than ff_opt_dist.
70
71        Only applicable if ff_formula is harmonic.'
72      ff_coef: 'Frame force (FF) force coefficient.'
73      ff_coef_evol: 'Enable or disable the changing FF coefficient value.
74
75        If True the coefficient will start as 0 at the beginning of the simulation and
76        reach ff_coef at the end.
77
78        If False the coefficient will have stable value of ff_coef.'
79  general:
80    input: data/data_benchmark_001
81    output: results/results_benchmark_001
82    genome: mm10
83    pdf_report: false
84    remove_problematic: false
85  simulation:
86    platform: OpenCL
87    resolutions: 5,2,0.5,0.2,0.1
88    N_steps: 100
89    burnin: 99
90    MC_step: 1
91    sim_step: 20
```

```yaml
forcefield:
  ev_formula: harmonic
  ev_min_dist: 1.0
  ev_coef: 100.0
  ev_coef_evol: true
  bb_formula: harmonic
  bb_opt_dist: 1.0
  bb_lin_thresh: 2.0
  bb_coef: 100.0
  bb_coef_evol: false
  sc_formula: harmonic
  sc_opt_dist: 1.0
  sc_lin_thresh: 1.5
  sc_coef: 50.0
  sc_coef_evol: false
  ff_formula: harmonic
  ff_opt_dist: 1.0
  ff_lin_thresh: 1.5
  ff_coef: 50.0
  ff_coef_evol: false
```