A summary of the genome simulated by TEgenomeSimulator

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Contents

1	Simulation information													
2	Loaded files for creating this report													
3 The proportion of the TE/nonTE sequence														
4	Breaking down the simulated TEs by superfamily 4.1 Total simulated TE loci categorised by TE superfamily	4												
5	5 Extracting full information from TE's gff file													
6	Simulation of nested TE insertions 6.1 Nested and non-nested Copia 6.2 TE loci cut by nested Copia 6.3 Nested and non-nested Gypsy 6.4 TE loci cut by nested Gypsy													
7	The distribution of TE loci identity	8												
8	The distribution of TE loci integrity	9												

1 Simulation information

Simulated genome: donghong

Range of simulated TE loci per TE family: 5-10

CPU	RAM	Time	$Timestamp_of_completion$
1	$842.30~\mathrm{MB}$	00:00:51	2024-02-21 14:14:22

In this simulation, TEgenomeSimulator did the followings:

- 1. It took the TE library file, combined_curated_TE_lib_ATOSZM_selected.fasta, which comprises curated TE family sequences from A. thalian, Z. maize and O. sativa, and simulates multiple TE copies with sequence variations depending on the parameters specified in the table: TElib_sim_list_5_10.table. In addition to nucleotide substitution and INDEL, it also simulated fragmentation (as a proportion of TE truncated from 5' end), nested insertion (only for Copia and Gypsy), as well as target site duplication.
- 2. The simulated TE copies were then randomly inserted into the user-provided TE-depleted genome, **Donghong.chromosomes.only.fa.nonTE**, where TE sequences had been exhaustively detected by multiple TE annotators (e.g. EDTA, RepeatModeler, and EarlGrey) and removed. The final simulated genome can be utilised for benchmarking TE annotators.

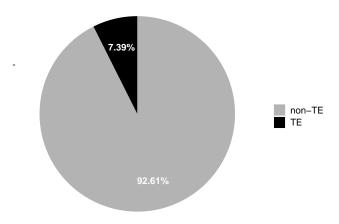
2 Loaded files for creating this report

- All TE fasta index file: donghong_5_10_repeat_sequence_out_nest.fasta.fai
- All TE gff file: donghong_5_10_repeat_annotation_out_nest.gff

3 The proportion of the TE/nonTE sequence

Total simulated genome size: 306,230,938 bp
Total simulated TE bases: 22,638,471 bp

Simulated genome: donghong_5_10 Genome size: 306,230,938 bp



High quality image saved in

/workspace/cflthc/scratch/2022_Actinidia_TE/10.01_TEgenomeSimulator_output/sim_donghong_5_10_genome/report/

File name: 001_sim_genome_size_donghong_5_10.png

4 Breaking down the simulated TEs by superfamily

There are total 16 TE superfamilies included in the curated TE library. The following table shows the number of loci, bases and family of each superfamily, as well as the percentage of loci, bases and family.

TE_superfamily	loci	bp	family_count	loci_percentage	bp_percentage	family_percentage
01_LTR/Copia	920	2907611	139	7.51	12.84	8.44
02 _LTR/Gypsy	753	2476491	109	6.15	10.94	6.62
03_LTR/Solo	21	28080	3	0.17	0.12	0.18
04_LTR/unknown	84	110541	11	0.69	0.49	0.67
05 _LINE/L1	89	312729	12	0.73	1.38	0.73
06_LINE/unknown	710	1470449	94	5.80	6.50	5.71
07 _SINE/tRNA	38	8237	5	0.31	0.04	0.30
08_SINE/unknown	307	153493	43	2.51	0.68	2.61
09_DNA/CACTA	789	2109253	110	6.44	9.32	6.68
10_DNA/hAT	1891	1627563	249	15.44	7.19	15.12
11_DNA/MuDR	2993	6228941	393	24.43	27.51	23.86
12_DNA/Harbinge	r 23	68688	3	0.19	0.30	0.18
13_DNA/Mariner	58	32961	7	0.47	0.15	0.43
14_RC/Helitron	2424	4835648	314	19.79	21.36	19.06
15_MITE/Stow	286	60556	40	2.33	0.27	2.43
16_MITE/Tourist	865	207940	115	7.06	0.92	6.98
Total	12251	22639181	1647	100.00	100.00	100.00

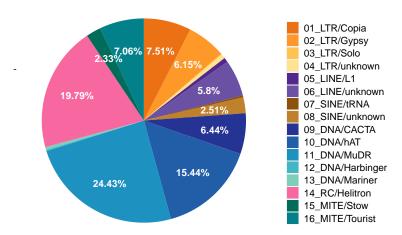
Table saved in

 $/work space/cflthc/scratch/2022_Actinidia_TE/10.01_TE genome Simulator_output/sim_donghong_5_10_genome/report/File name: sim_genome_summary_TE superfamily_donghong_5_10.csv$

4.1 Total simulated TE loci categorised by TE superfamily

• Total simulated TE loci: 12,251 loci

Simulated genome: donghong_5_10 Simulated loci: 12,251



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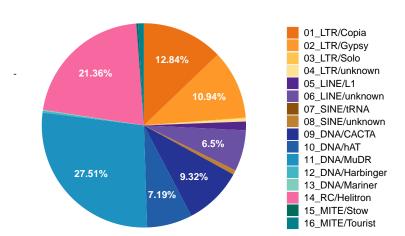
/workspace/cflthc/scratch/2022 Actinidia TE/10.01 TEgenomeSimulator output/sim donghong 5 10 genome/report/

File name: 002_sim_te_loci_donghong_5_10.png

4.2 Total simulated TE bases categorised by TE superfamily

• Total simulated TE bases: 22,639,181 bp

Simulated genome: donghong_5_10 Simulated TE bases: 22,639,181 bp



High quality image saved in

/workspace/cflthc/scratch/2022_Actinidia_TE/10.01_TEgenomeSimulator_output/sim_donghong_5_10_genome/report/

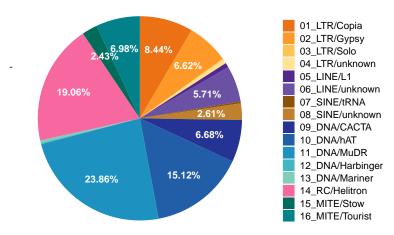
File name: 003_sim_te_bp_donghong_5_10.png

4.3 Simulated TE family per superfamily

This part only depends on the curated TE library. It shouldn't make any difference between simulations.

• Total simulated TE families: 1647 families

Simulated genome: donghong_5_10 Simulated families: 1,647



High quality image saved in

/workspace/cflthc/scratch/2022_Actinidia_TE/10.01_TEgenomeSimulator_output/sim_donghong_5_10_genome/report/

File name: 004 sim te family donghong 5 10.png

5 Extracting full information from TE's gff file

Have a look at the full info extracted from TE's gff file (row 100 to 109):

	Chr	Start	End	strand	TE_rename	ID
100	chr1	2573750	2574278	-	16_MITE/Tourist	Os0702#MITE/Tourist_TE0000096
101	chr1	2595879	2596849	-	14_RC/Helitron	Os2409#DNAnona/Helitron_TE0000097
102	chr1	2608489	2608619	+	$11_DNA/MuDR$	Os0372#DNAnona/MULE_TE0000098_1
103	chr1	2608625	2613534	+	01_LTR/Copia	ATCOPIA13#LTR/Copia_TEn000003
104	chr1	2613539	2613734	+	$11_DNA/MuDR$	$Os0372\#DNAnona/MULE_TE0000098_2$
105	chr1	2625733	2629620	-	09_DNA/CACTA	Os1544#DNAnona/CACTA_TE0000099
106	chr1	2633990	2639706	-	01_LTR/Copia	ATCOPIA76#LTR/Copia_TE0000100
107	chr1	2705427	2705731	+	16_MITE/Tourist	$Os1928\#MITE/Tourist_TE0000101$
108	chr1	2740223	2741792	+	14_RC/Helitron	$Os 0980 \# DNA auto/Helitron_TE 0000102$
109	chr1	2766526	2770040	+	$11_DNA/MuDR$	Os0896#DNAauto/MULE_TE0000103

	TE_id	TE_family	Subclass
100	TE0000096	Os0702	MITE
101	TE0000097	Os2409	Helitron
102	$TE0000098_1$	Os0372	TIR_transposon
103	TEn000003	ATCOPIA13	$LTR_retrotransposon$
104	$TE0000098_2$	Os0372	$TIR_transposon$
105	TE0000099	Os1544	$TIR_transposon$
106	TE0000100	ATCOPIA76	$LTR_retrotransposon$
107	TE0000101	Os1928	MITE
108	TE0000102	Os0980	Helitron
109	TE0000103	Os0896	TIR_transposon

	Identity	Integrity	Nested_in	Cut_at	Cut_by	chrid
100	0.86	1.0	NA	NA	NA	1
101	0.87	0.58	NA	NA	NA	1
102	0.94	0.9	NA	0.4	ATCOPIA13#LTR/Copia_TEn000003	1
103	0.94	1.0	TE0000098	NA	NA	1
104	0.94	0.9	NA	0.4	ATCOPIA13#LTR/Copia_TEn000003	1
105	0.71	0.84	NA	NA	NA	1
106	0.91	1.0	NA	NA	NA	1
107	0.66	0.98	NA	NA	NA	1
108	0.94	0.58	NA	NA	NA	1
109	0.76	1.0	NA	NA	NA	1

Full table saved in

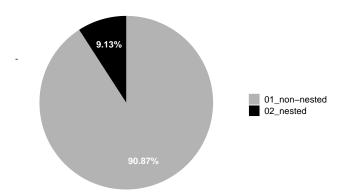
 $/work space/cflthc/scratch/2022_Actinidia_TE/10.01_TE genome Simulator_output/sim_donghong_5_10_genome/report/sim_donghong_5$

 $File \ name: \ sim_genome_TE_insertion_info_donghong_5_10.csv$

6 Simulation of nested TE insertions

6.1 Nested and non-nested Copia

Simulated genome: donghong_5_10 TE superfamily: Gypsy Total loci: 920 Nested loci: 84



6.2 TE loci cut by nested Copia

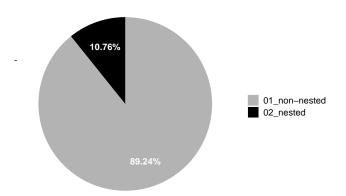
TE loci cut by nested Copia

40 36 34 34 Count of TE loci 18 16 12 8 8 10 0 0 0 0 0 0 SWEINKOWN J'Alsolo SINEHRIVA InElinkrown DWACACTA LINEL ON DANGE HELD THE WEST OF THE WIFE STON OUTS

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Nested and non-nested Gypsy 6.3

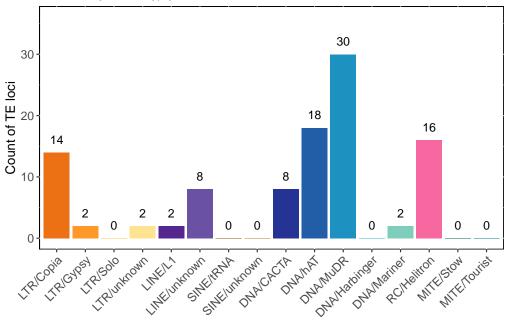
Simulated genome: donghong_5_10 TE superfamily: Gypsy Total loci: 753 Nested loci: 81



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6.4TE loci cut by nested Gypsy

TE loci cut by nested Gypsy

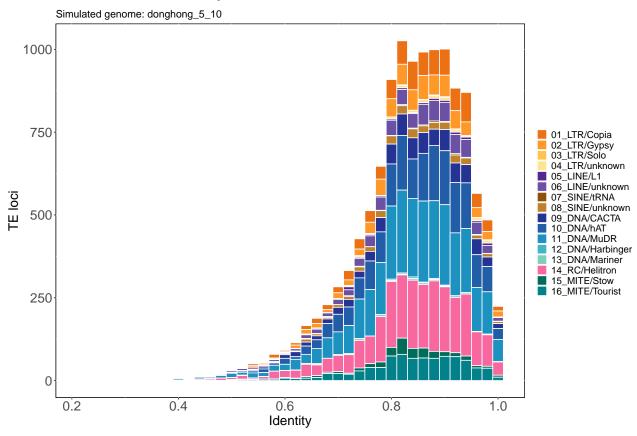


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7 The distribution of TE loci identity

How did TEgenomeSimulator simulate sequence identity in this simulation?

- 1. The distribution of sequence identity of each TE family was defined by the **idn** and **sd** values (user provided) stored in **TElib_sim_list_5_10.table**.
- 2. TEgenomeSimulator took the **idn** as mean identity and **sd** as standard deviation to create a distribution, from which a value was sampled as the **simulated identity** of a TE member. Therefore, **simulated divergence** = 1 **simulated identity**
- 3. Inherited from it's predecessor, denovoTE-eval, TEgenomSimulator broke down the simulated divergence into substitution and INDELs (i.e. divergence = substitution % + INDEL %).
- 4. The INDEL % was defined by the indels value from TElib_sim_list_5_10.table.

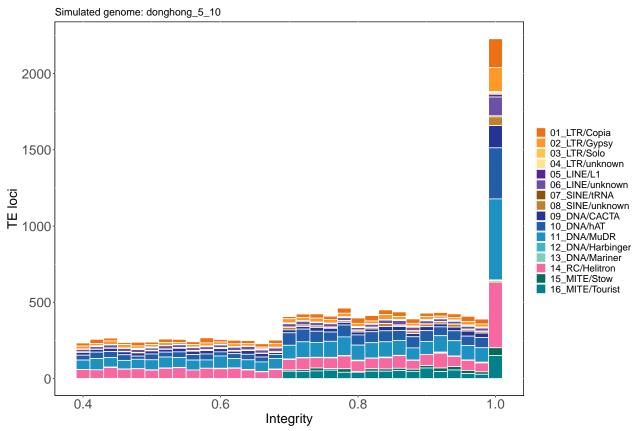


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8 The distribution of TE loci integrity

How did TEgenomeSimulator simulate sequence integrity in this simulation?

- 1. TEgenomeSimulator considers sequence integrity as **integrity** = (1 (TE locus length / full length))
- 2. The length of a TE locus is decided by INDELs and fragmentation.
- 3. In the fragmentation step, if a TE length is shorter than 500 bp, TEgenomeSimulator would randomly select a value between 70 and 90 as the fraction of the sequence to be removed from 5' end; otherwise the simulator randomly chooses a value between 40 and 90. (This is the same as in denovoTE-eval)
- 4. The number of fragmented loci was defined by the value of **frag** in **TElib_sim_list_5_10.table**. This value was taken as a proportion of total TE loci to undergo fragmentation step.



High quality image saved in /workspace/cflthc/scratch/2022_Actinidia_TE/10.01_TEgenomeSimulator_output/sim_donghong_5_10_genome/report/File name: 010 sim te loci integrity donghong 5 10.png