

Package ‘MeDiChISeq’

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Type Package

Title Model-based peak caller for epigenomic profiles

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Description Self-learning, model-based peak caller

License GPL

LazyLoad yes

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Suggests lattice (>= 0.20-15), Matrix (>= 1.0-12), zoo (>= 1.7-10)

LinkingTo Rcpp

R topics documented:

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chip.deconv.seq	<i>High-resolution model-based deconvolution of ChIP-seq data in WIG format.</i>
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Description

Deconvolves a subset of data on one chromosome. Used to deconvolve an entire data set across multiple chromosomes, see [deconv.entire.genome.seq](#).

Usage

```
chip.deconv.seq(data, center = NA, window = 20000, kernel = NA,
quant.cutoff = "q1e-5", fit.res = 50,
max.steps = 100, post.proc.factor = 2, selection.method = "bic",
verbose = T, trace = F, nr.boots = 1,
boot.sample.opt = "residual", max.peak = NA, boot.vary.res = F,
tile.distance = NA, where = NA,
min.npeaks = 0, max.npeaks = 99999, ...)
```

Arguments

data	data.frame or matrix containing genome coordinates (column 1) and intensities (column 2), or a path to a WIG file.
center	Central coordinate of the data subset to deconvolve.
window	Size of the data chunk to deconvolve.
kernel	data.frame or matrix which is one of the outputs of fit.peak.profile.seq , describing the peak shape.
quant.cutoff	Intensity or quantile cutoff for data to be processed. Limits the locations of potential sites to those that are above this threshold.
fit.res	Numeric for base pairs. Desired deconvolution resolution.
max.steps	Limit the number of LARS steps taken.
post.proc.factor	Post-processing filter for combining deconvolution coefficients. When equal 2, means that all the coefficients that are separated by maximum 2*fit.res will be merged.
selection.method	In LARS regression the accurate model is chosen based on AIC or BIC criterion. Default is "bic".
verbose	If TRUE, print out status messages.
trace	If TRUE, print out LARS progress.
nr.boots	Number of bootstrap iterations to perform. Attention: in contrast to chip.deconv, this version does not produce local p-values at all, since they are calculated in different manner by deconv.entire.genome.seq . See details.
boot.sample.opt	Bootstrap resampling option. See Details. Default is "residual".
max.peak	Any coefficient with an intensity above this threshold is set to this value. Default is NA - no cutoff.

boot.vary.res	If TRUE, vary the resolution during bootstraps. By default FALSE.
tile.distance	Distance in bp which for ChIP-seq data corresponds to the WIGS resolution. If NA (the default) then this is computed from the data.
where	The chromosome of the subset of data to deconvolve. Inactive (NA) for ChIP-seq data.
min.npeaks	Optionally limit the minimum number of coefficients. Default is 0 - no lower limit.
max.npeaks	Optionally limit the maximum number of coefficients. Default is 99999 - no upper limit.
...	All the other parameters of original chip.deconv from MeDiChI package such as: boot.sample.opt = "residual", max.peak = NA, boot.vary.res = F, tile.distance = NA, where = NA, min.npeaks = 0, max.npeaks = 99999 and smooth=FALSE can be also changed. Nevertheless in deconv.entire.genome.seq and fit.peak.profile.seq they are set up to the default values.

Details

See details of chip.deconv from MeDiChI package.

Author(s)

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References

http://archive.igbmc.fr/recherche/Prog_FGC/Eq_HGron/bioinfotools.html

Mendoza-Parra MA, Walia M, Sankar M, Gronemeyer H. Dissecting the retinoid-induced differentiation of F9 embryonal stem cells by integrative genomics. Mol Syst Biol. 2011 Oct 11;7:538. doi: 10.1038/msb.2011.73. PubMed PMID: 21988834; PubMed Central PMCID: PMC3261707. URL: <http://www.nature.com/msb/journal/v7/n1/full/msb201173.html>

Mendoza-Parra MA, Sankar M, Walia M, Gronemeyer H. POLYPHEMUS: R package for comparative analysis of RNA polymerase II ChIP-seq profiles by non-linear normalization. Nucleic Acids Res. 2012 Feb;40(4):e30. doi: 10.1093/nar/gkr1205. Epub 2011 Dec 7. PubMed PMID: 22156059; PubMed Central PMCID: PMC3287170. URL: <http://nar.oxfordjournals.org/content/40/4/e30.long>

David J. Reiss, Marc T. Facciotti, and Nitin S. Baliga. Model-based deconvolution of genome-wide DNA binding. Bioinformatics, pages btm592+, 2007. doi: 10.1093/bioinformatics/btm592. URL: <http://bioinformatics.oxfordjournals.org/cgi/content/abstract/btm592v1>

See Also

[deconv.entire.genome.seq](#), [fit.peak.profile.seq](#), [chip.deconv](#)

Examples

```
# one window deconvolution for CTCF

dir <- system.file("extdata/CTCF", package="MeDiChISeq")
data <- read.table(file.path(dir,
"chr19_IP_GSM646314_GM12878_CTCF_rep1_rcd_res-10_dist-150_both.wig"), skip=2)
kernel <- read.table(file.path(dir, "MeDiChISeq_CTCF_kernel.txt"))

out <- chip.deconv.seq(data = data, center = 461582, window = 20000,
kernel = kernel, quant.cutoff = 10, fit.res = 50)

coef(out)

plot(out)

# one window deconvolution for H3K4me3

dir <- system.file("extdata/H3K4me3", package="MeDiChISeq")
data <- read.table(file.path(dir,
"chr19_IP_GSM646424_Huvec_H3K4me3_rep1_rcd_res-10_dist-150_both.wig"), skip=2)
kernel <- read.table(file.path(dir, "MeDiChISeq_H3K4me3_kernel.txt"))

out <- chip.deconv.seq(data = data, center = 469384, window = 50000,
kernel = kernel, quant.cutoff = 10, fit.res = 50)

coef(out)

plot(out)

plot(out, center = 483241, window = 5000)
```

```
deconv.entire.genome.seq
```

High-resolution model-based deconvolution of normalized ChIP-Seq data

Description

Deconvolves an entire ChIP-Seq data set, across all chromosomes by running adjusted version of chip.deconv function from MeDiChI package on multiple, contiguous, overlapping subsets of the data and combining the results.

Usage

```
deconv.entire.genome.seq(file.IP, file.Control=NULL,
format="bed", genome="hg19", output.dir=NULL, output.name=NULL,
chrom.list=NULL, limL=0, limU=Inf, potential.peaks=NULL,
reads.elong=150, kernel, frag.length,
quant.cutoff="q1e-5", window=20000, wig.res=10, fit.res=50,
max.steps=100, selection.method="bic", post.proc.factor=2,
nr.boots=5, local.windows=c(1000, 2000, 5000),
Control.corr.param=0.01, nr.cores=1,
```

```
remove.clonal.reads=TRUE, clonal.reads.to.keep=3,
verbose.console=TRUE, overwrite.wigs=FALSE, keep.wigs=TRUE, ...)
```

Arguments

<code>file.IP</code>	Path to the ChIP-Seq file.
<code>file.Control</code>	Path to the Control file.
<code>format</code>	Format of the ChIP-Seq file. By default "bed". Other accepted formats: "sam", "bam", "bowtie", "soap".
<code>genome</code>	Character specifying the genome "hg18", "hg19", "mm8", "mm9", "dm2", "dm3", "ce4", "ce6", "rn3", "rn4", "danRer4", "danRer6".
<code>output.dir</code>	Directory to the folder where all the output should be saved. If such a path does not exist, it will be created. By default <code>output.dir = NULL</code> and a folder named "MeDiChISeq_output" is created in the current working directory.
<code>output.name</code>	Character. Experiment name used when output files are generated. By default <code>output.name = NULL</code> .
<code>chrom.list</code>	Character vector of chromosomes to be deconvolved. If <code>chrom.list = NULL</code> , whole genome is deconvolved.
<code>limL</code>	Lowest boundary of the region to deconvolve, by default <code>limL = 0</code>
<code>limU</code>	Upper boundary of the region to deconvolve, by default <code>limU = Inf</code> . Default values for <code>limL</code> and <code>limU</code> result in deconvolving entire chromosomes.
<code>potential.peaks</code>	Path or data.frame that should have columns "chromosome", "start", "end". This is a list of regions in which potential peaks can be located.
<code>reads.elong</code>	Path or numeric. Reads are elongated by this value in order to create intensity wig files. Should correspond to the length of the sonicated DNA fragments and can be estimated with fit.peak.profile.seq function. Should be the same value which was used for reads elongation when kernel was generated.
<code>kernel</code>	Path, data.frame or matrix which is one of the outputs of fit.peak.profile.seq , describing the peak shape.
<code>frag.length</code>	Path or numeric value which is one of the outputs of fit.peak.profile.seq . This value is used to calculate the base of annotated peaks.
<code>quant.cutoff</code>	Intensity threshold that defines the regions of potential peaks. By assigning a numeric value it will be constant for a whole genome, when defined as quantile the threshold for each window will be calculated based on a Poisson approach. Default value <code>quant.cutoff = "q1e-5"</code> corresponds to $1 - 1e-5 = 0.99999$ th quantile from Poisson distribution with lambda equal to the average intensity in that window, as if it was equally distributed.
<code>window</code>	Numeric in base pairs. Whole genome is divided into overlapping windows of this size in which the deconvolution takes place. When <code>quant.cutoff</code> is defined as quantile, the Poisson background is estimated based on the information from such windows. By default <code>window=20000</code> . It is suggested to use bigger window for broader profiles. See vignette.
<code>wig.res</code>	Resolution of the wigs that are created.
<code>fit.res</code>	Numeric in base pairs. Desired deconvolution resolution.
<code>max.steps</code>	Limit the number of LARS steps taken.

selection.method	In LARS regression the accurate model is chosen based on AIC or BIC criterion. Default is "bic".
post.proc.factor	Post-processing filter for combining deconvolution coefficients. When equal 2, means that all the coefficients that are separated by maximum $2 * \text{fit.res}$ will be merged. When equal 0, no merging is performed, but usually this results in profile overfitting. The value $\text{post.proc.factor} * \text{fit.res}$ can be interpreted as minimal allowed distance between two neighbor peaks.
nr.boots	Number of bootstrap iterations to perform. If $\text{nr.boots} = 1$, no bootstraps are performed and no p-values will be generated. Suggested value $\text{nr.boots} = 5$.
local.windows	Numeric vector specifying the size of windows used for local assessment of confidence of putative peaks. By default $\text{local.windows} = c(1000, 2000, 5000)$.
Control.corr.param	Numeric value from [0,1] interval. If Control sample is available this value is the percentage of overlap that is necessary to conclude that two peaks from IP and Control are located in the same position. Consequently the confidence of IP peak is reduced.
nr.cores	Numeric. The number of cores to be used for parallel processing. This argument is passed directly to the <code>mclapply</code> function.
remove.clonal.reads	Logical. Whether the clonal reads should be removed before creating WIG files.
clonal.reads.to.keep	Numeric. Number of reads that are accepted to have exactly the same position. Additional reads are removed.
verbose.console	Logical. If $\text{verbose.console} = \text{TRUE}$, than the progress of fitting is displayed in console and saved in <code>output.dir</code> .
overwrite.wigs	Logical. Whether to overwrite WIG files with the existing ones. When FALSE one can save time on WIG construction.
keep.wigs	Logical. Whether to keep or delete the generated WIG files.
...	

Value

Generated output consists of the following object:

- `All.coeffs.IP` that contains a list of all annotated peaks with their intensities, global, local and combined p-values and coefficients after control correction,

This object is saved in `output.dir`. Moreover you can find there a BED file with annotated peaks and their intensities and WIG files which can be loaded to any genome browser for visual verification of obtained results. In order to facilitate the choice of p-values cutoff a plot of intensities versus p-values is generated. The console output of `deconv.entire.genome.seq` is also saved.

Author(s)

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References

http://archive.igbmc.fr/recherche/Prog_FGC/Eq_HGron/bioinfotools.html

Mendoza-Parra MA, Walia M, Sankar M, Gronemeyer H. Dissecting the retinoid-induced differentiation of F9 embryonal stem cells by integrative genomics. *Mol Syst Biol.* 2011 Oct 11;7:538. doi: 10.1038/msb.2011.73. PubMed PMID: 21988834; PubMed Central PMCID: PMC3261707. URL: <http://www.nature.com/msb/journal/v7/n1/full/msb201173.html>

Mendoza-Parra MA, Sankar M, Walia M, Gronemeyer H. POLYPHEMUS: R package for comparative analysis of RNA polymerase II ChIP-seq profiles by non-linear normalization. *Nucleic Acids Res.* 2012 Feb;40(4):e30. doi: 10.1093/nar/gkr1205. Epub 2011 Dec 7. PubMed PMID: 22156059; PubMed Central PMCID: PMC3287170. URL: <http://nar.oxfordjournals.org/content/40/4/e30.long>

David J. Reiss, Marc T. Facciotti, and Nitin S. Baliga. Model-based deconvolution of genome-wide DNA binding. *Bioinformatics*, pages btm592+, 2007. doi: 10.1093/bioinformatics/btm592. URL: <http://bioinformatics.oxfordjournals.org/cgi/content/abstract/btm592v1>

See Also

[chip.deconv.seq](#), [fit.peak.profile.seq](#)

Examples

```
# if possible increase the number of cores used for parallelization
nr.cores=2
# deconvolve a small chunk of chromosome 19 from CTCF profile

dir <- system.file("extdata/CTCF", package="MeDiChISeq")
file.IP <- file.path(dir, "GSM646314_GM12878_CTCF_rep1_rcd.bed")
kernel <- file.path(dir, "MeDiChISeq_CTCF_kernel.txt")
reads.elong <- file.path(dir, "MeDiChISeq_CTCF_reads_elong.txt")
frag.length <- file.path(dir, "MeDiChISeq_CTCF_frag_length.txt")

CTCF.deconv <- deconv.entire.genome.seq(file.IP,
output.name="CTCF", genome="hg18",
quant.cutoff="q1e-5", window=20000,
chrom.list="chr19", limL=0, limU=500000,
reads.elong=reads.elong, kernel=kernel, frag.length=frag.length,
nr.cores=nr.cores, nr.boots=2,
remove.clonal.reads=FALSE)
```

fit.peak.profile.seq *Learn deconvolution kernel - peak shape - from ChIP-Seq data.*

Description

Learn the peak shape, to be further used for the deconvolution via `deconv.entire.genome.seq`.

Usage

```
fit.peak.profile.seq(file.IP, format="bed", genome="hg19", output.dir=NULL,
output.name=NULL, chrom.fit=NULL, limL=0, limU=Inf,
reads.elong=150, quant.cutoff="q1e-7", window=20000, mini.window=2000,
wig.res=10, fit.res=50, reads.length=50,
n.peaks = 50, n.skip = 20, re.fit=100, max.iter=500,
selection.method="bic", post.proc.factor=2,
start.pars =c(shape =10, scale = 20), to.be.fit=c("shape", "scale"),
method = "Nelder-Mead", nr.cores=1,
remove.clonal.reads=TRUE, clonal.reads.to.keep=3,
write.pdf=TRUE, save.kernel=TRUE, verbose.console=TRUE,
overwrite.wigs=FALSE, keep.wigs=TRUE, ...)
```

Arguments

file.IP	Path to the ChIP-Seq file.
format	Format of the ChIP-Seq file. By default "bed". Other accepted formats are "sam", "bam", "bowtie", "soap".
genome	Character specifying the genome "hg18", "hg19", "mm8", "mm9", "dm2", "dm3", "ce4", "ce6", "rn3", "rn4", "danRer4", "danRer6".
output.dir	Directory to the folder where all the output should be saved. If such a path does not exist, it will be created. By default output.dir = NULL and a folder named "MeDiChISeq_output" is created in the current working directory.
output.name	Character. Experiment name used when output files are generated. By default output.name = NULL.
chrom.fit	Character specifying the chromosome on which the learning should be performed. If fit.chrom = NULL, the shortest chromosome is taken.
limL	Lowest boundary of the region to deconvolve, by default limL = 0
limU	Upper boundary of the region to deconvolve, by default limU = Inf. Default values for limL and limU result in entire chromosomes deconvolution.
reads.elong	Numeric. Reads are elongated by this value in order to create intensity WIG files. Should correspond to the average length of sonicated DNA fragments. When reads.elong = NULL, average fragment length is estimated based on forward and reverse profiles. See vignette.
quant.cutoff	Intensity threshold that defines the regions of potential peaks. By assigning a numeric value it will be constant for a whole genome, when defined as quantile the threshold for each window will be calculated based on Poisson approach. Default value quant.cutoff = "q1e-7" corresponds to 1 - 1e-7 = 0.9999999th quantile from Poisson distribution with lambda equal to the average intensity in that window, as if it was equally distributed.
window	Numeric in base pairs. Whole genome is divided into overlapping windows of this size in which the deconvolution takes place. When quant.cutoff is defined as quantile, the Poisson background is estimated based on the information from such windows. By default window=20000. It is suggested to use bigger window for broader profiles. See vignette.
mini.window	Numeric in base pairs. Size of the window to be plotted around each of the bright peaks.
wig.res	Resolution of the wigs that are created.

fit.res	Numeric in base pairs. Desired deconvolution resolution.
reads.length	Length of aligned reads. This value is used during the estimation of reads.elong. See vignette.
n.peaks	Number of regiones with biggest peaks to learn from.
n.skip	Number of regiones with worst-fitting to skip. Enables filtering out of peaks that do not agree with the majority of isolated peaks.
re.fit	Re-run deconv.entire.genome.adj on input data using current best-fit profile, every re.fit iterations.
max.iter	Maximum number of iterations for "Nelder-Mead", "BFGS", "CG" methods. See optim function.
selection.method	In LARS regression the accurate model is chosen based on AIC or BIC criterion. Default is "bic".
post.proc.factor	Post-processing filter for combining deconvolution coefficients. When equal 2, means that all the coefficients that are separated by maximum 2*fit.res will be merged. When equal 0, no merging is performed, but usually this results with profile overfitting. The value post.proc.factor * fit.res can be interpreted as minimal allowed distance between two neighbor peaks.
start.pars	Starting parameters for model profile. By default c(shape =10, scale = 20), which corresponds to the average DNA fragment length of 200bp.
to.be.fit	Names of parameters to be learned.
method	Optimization method, by default method = "Nelder-Mead". See optim function.
nr.cores	Numeric. The number of cores to be used for parallel processing. This argument is passed directly to the mclapply function.
remove.clonal.reads	Logical. If the clonal reads should be removed before creating WIG files.
clonal.reads.to.keep	Numeric. Number of reads that are accepted to have exactly the same position. Additional reads are removed.
write.pdf	Logical. Whether pdf plots of fitted kernels should be generated and saved in the output.dir.
save.kernel	Logical. Whether the files with kernel and frag.length should be saved in the output.dir.
verbose.console	Logical. If verbose.console = TRUE, than the progress of fitting is displayed in console and saved in output.dir.
overwrite.wigs	Logical. Whether to overwrite WIG files with the existing ones. When FALSE one can save time on WIGs construction.
keep.wigs	Logical. Whether to keep or delete the generated WIG files.
...	

Value

A list of 3 objects:

- reads.elong: see above.

- kernel: data.frame with the final peak profile.
- frag.length: estimated fragment length. Base of the peak profile is assumed to be equal to 2*frag.length.

Moreover, if kernel=TRUE, verbose.console=TRUE, keep.wigs=TRUE, then in the directory output.dir all the above outputs will be saved together with generated WIG files, console display of work progress and the PDF files with kernel plots.

Author(s)

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References

http://archive.igbmc.fr/recherche/Prog_FGC/Eq_HGron/bioinfotools.html

Mendoza-Parra MA, Walia M, Sankar M, Gronemeyer H. Dissecting the retinoid-induced differentiation of F9 embryonal stem cells by integrative genomics. Mol Syst Biol. 2011 Oct 11;7:538. doi: 10.1038/msb.2011.73. PubMed PMID: 21988834; PubMed Central PMCID: PMC3261707. URL: <http://www.nature.com/msb/journal/v7/n1/full/msb201173.html>

Mendoza-Parra MA, Sankar M, Walia M, Gronemeyer H. POLYPHEMUS: R package for comparative analysis of RNA polymerase II ChIP-seq profiles by non-linear normalization. Nucleic Acids Res. 2012 Feb;40(4):e30. doi: 10.1093/nar/gkr1205. Epub 2011 Dec 7. PubMed PMID: 22156059; PubMed Central PMCID: PMC3287170. URL: <http://nar.oxfordjournals.org/content/40/4/e30.long>

David J. Reiss, Marc T. Facciotti, and Nitin S. Baliga. Model-based deconvolution of genome-wide DNA binding. Bioinformatics, pages btm592+, 2007. doi: 10.1093/bioinformatics/btm592. URL: <http://bioinformatics.oxfordjournals.org/cgi/content/abstract/btm592v1>

See Also

[chip.deconv.seq](#), [deconv.entire.genome.seq](#)

Examples

```
# if possible increase the number of cores used for parallelization
nr.cores=2

# finds kernel for CTCF profile

dir <- system.file("extdata/CTCF", package="MeDiChISeq")
file.IP <- file.path(dir, "GSM646314_GM12878_CTCF_rep1_rcd.bed")

CTCF.peak.profile <- fit.peak.profile.seq(file.IP, genome="hg18", chrom.fit="chr19",
output.name="CTCF", window=20000, mini.window=2000, quant.cutoff=20,
limL=0, limU=1000000, re.fit=15, max.iter=20,
start.pars =c(shape = 17, scale = 10), nr.cores=nr.cores,
remove.clonal.reads=FALSE)
```

remove.clons	<i>Remove clonal reads</i>
--------------	----------------------------

Description

Removes reads that starts in exactly the same position.

Usage

```
remove.clons(file, reads.to.keep, output.dir, format)
```

Arguments

file	Path to the file containing aligned reads.
reads.to.keep	Numeric. Defines number of reads that are allowed to have exactly the same position.
output.dir	Directory to the folder where new BED file will be saved.
format	Format of the ChIP-Seq file. Accepted formats: "sam", "bam", "bowtie", "soap".

Details

It can happen that profile will have a lot of reads starting in exactly the same position. Such reads are usually considered as artefacts resulting from "clonal" amplification during the PCR phase in ChIP-seq experiment. If this is a frequent phenomena they can have an influence on the shape of peaks. Such peaks follow a square pattern. That is why we suggest to remove so called clonal reads.

Value

Produces new cleaned BED file in pointed directory. Output of `remove.clons` a path to the generated BED file.

Author(s)

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Examples

```
dir <- system.file("extdata/CTCF", package="MeDiChISeq")
file <- file.path(dir, "GSM646314_GM12878_CTCF_rep1_rcd.bed")

remove.clons(file, reads.to.keep=2, output.dir=getwd(), format="bed")
```

write.wigs.parallel	<i>WIG generator</i>
---------------------	----------------------

Description

Produces WIG files from files containing aligned reads.

Usage

```
write.wigs.parallel(file, output.dir, chromosomes, sample.type,
wig.res, reads.elong, split = FALSE, genome, format, zeros = F,
nr.cores = 1, overwrite.wigs = FALSE, verbose = T)
```

Arguments

file	Path to the file containing aligned reads.
output.dir	Directory to the folder where all the WIGS will be saved.
chromosomes	List of chromosomes for which the WIGS will be produced.
sample.type	Name prefix of the new WIG files.
wig.res	Resolution of the wigs.
reads.elong	Numeric. Reads are elongated by this value in order to create intensity wig files.
split	Logical. If TRUE, separate wigs for forward and reverse strand will be produced.
genome	Character specifying the genome "hg18", "hg19", "mm8", "mm9", "dm2", "dm3", "ce4", "ce6", "rn3", "rn4", "danRer4", "danRer6".
format	Format of the ChIP-Seq file. Accepted formats: "sam", "bam", "bowtie", "soap".
zeros	Logical. Whether to produce the entries with intensity zero.
nr.cores	Numeric. The number of cores to be used for parallel processing.
overwrite.wigs	Logical. Whether to overwrite wig files with the existing ones. When FALSE one can save time on wig construction.
verbose	Logical. Whether to display processing status.

Value

Produces the WIG files in pointed directory. Output of write.wigs.parallel is a list of paths to the generated WIGS.

Author(s)

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Examples

```
dir <- system.file("extdata/CTCF", package="MeDiChISeq")
file <- file.path(dir, "GSM646314_GM12878_CTCF_rep1_rcd.bed")

write.wigs.parallel(file, output.dir=getwd(), chromosomes="chr19", sample.type="IP",
wig.res=10, reads.elong=150, split = FALSE, genome="hg18", format="bed", zeros = FALSE,
nr.cores = 1, overwrite.wigs = FALSE, verbose = TRUE)
```

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