```
  _/_/          _/_/_/_/_/  _/_/_/    _/_/_/
 _/  _/   _/    _/      _/  _/    _/  _/   _/
_/   _/  _/_/   _/_/_/_/_/  _/    _/  _/   _/
_/   _/ _/  _/  _/      _/  _/    _/  _/   _/
 _/_/  _/    _/ _/      _/  _/_/_/    _/_/_/
```

Preprocessor of 3D Wang Tiles
with Ellipsoidal Inclusions for T3D

Version 1.0

User Guide

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Daniel Rypl

Czech Technical University in Prague
Faculty of Civil Engineering, Department of Mechanics

Thákurova 7, 166 29, Prague
Czech Republic

e-mail: drypl@fsv.cvut.cz
http://mech.fsv.cvut.cz/~dr/dr.html

1 Introduction

Wang3d4t3d processes a given geometry of three-dimensional Wang Tiles with ellipsoidal inclusions subjected to generalized periodic conditions and produces input file for finite element mesh generator T3d (version 1.11 or higher). The inclusions are allowed neither to overlap nor to touch. In order to prevent too small elements (induced by the Wang tiles geometry) to appear in the finite element mesh produced by T3d, inclusions close to or intersecting tile boundary may be slightly shifted to satisfy proximity criteria with respect to tile sides, edges, and corners. Magnitude of this shifting is controlled by command line parameters and some compilation directives (see Sections 4 and 6).

2 Synopsis

Wang3d4t3d is generally executed as

`wang3d4t3d geometry_file t3d_input_file [ epsilon [ subdivisions ]]`

where

geometry_file – is an obligatory parameter specifying the name of the input file describing geometry of 3D Wang tiles to be processed (see Section 3).

t3d_input_file – is an obligatory parameter specifying the name of the output file containing the geometry in the format of T3d finite element mesh generator.

epsilon – is an optional parameter specifying tolerance for the evaluation of proximity criteria of inclusion with respect to tile sides, edges, and corners (see Section 4). While positive value of epsilon is considered as an absolute tolerance, negative value of epsilon is considered as an relative tolerance with respect to tile size. If zero value of epsilon is specified or if epsilon specification is missing, the default relative tolerance is applied. If the specified or computed absolute tolerance is smaller than problem dependent tolerance, it is replaced by this problem dependent tolerance.

subdivisions – is an optional integer parameter (expected only if epsilon is specified) defining how many times epsilon may be halved to satisfy proximity criteria of inclusion with respect to tile edges, and corners. Missing specification is considered as zero value. Negative value should be used to prevent inclusion shifting (see Section 4).

Basic usage can be obtained by executing wang3d4t3d without any parameter. Basic usage together with concise description of the format of the geometry file and with the actual setting of relevant compilation directives can be obtained by executing wang3d4t3d -h.

3 Format of Geometry File

Empty lines and comment lines (starting by #) in the geometry file are ignored. Length of each not ignored line in the geometry file may not reach or exceed BUFFER_SIZE (see Section 6). The numbers in individual records (except for the problem identification record) must be separated by at least one space or tabulator.

The geometry file is organised into several sections. The first section contains a record (single line) with an arbitrary (but not empty and not starting by #) problem identification string:

PROBLEM IDENTIFICATION STRING

In the second section, there is a record containing the number of Wang tiles, the number of reference inclusions, and the number of side codes:

NWT NRI NSC

The number of Wang tiles `NWT` must be larger than zero and smaller than `MAX_TILES` (see Section 6). The number of reference inclusions `NRI` must be zero or larger. Note that not all inclusions must be used in processed Wang tiles. The number of side codes `NSC`, corresponding to the number of generalized periodic conditions, must be zero or larger. Note that different side codes must be considered for different directions and that not all side codes must be used in processed Wang tiles.

The third section contains a record describing the reference Wang tile:

XTC YTC ZTC TDX TDY TDZ MMAT MIMSZ MBMSZ

The reference tile is placed in a global right-handed Cartesian coordinate system xyz with sides aligned with the coordinate system axes. Position of the center of the reference Wang tile is defined by three coordinates `XTC`, `YTC`, and `ZTC` in the global coordinate system. The (positive) dimensions of the reference Wang tile in the directions of individual axes of the global coordinate system are defined by `TDX`, `TDY`, and `TDZ`. The identification number of the material of the matrix phase `MMAT` must be larger than zero. Specifications of the internal and boundary mesh size `MIMSZ` and `MBMSZ` of the matrix phase may not be negative. Zero mesh size specification correspond to maximal possible element size. Note that the size of actually generated finite elements may be (even significantly) smaller than the specified non-zero values depending on other mesh density control specifications.

The fourth section contains `NRI` records describing individual inclusions of (exclusively) ellipsoidal shape:

IID XIC YIC ZIC X1 Y1 Z1 X2 Y2 Z2 MAX MIN MID IIMSZ IBMSZ IMAT IFMAT

Absolute value of the identification number of the inclusion must be integer number in the range $\langle 1; \text{NRI} \rangle$. The position and orientation of the inclusion is defined by coordinates `XIC`, `YIC`, and `ZIC` of its center, by coordinates `X1`, `Y1`, and `Z1` of a point P_1 on its major positive half-axis, and by coordinates `X2`, `Y2`, and `Z2` of a point P_2 in the half-plane given by the ellipsoid major axis and minor positive half-axis. While coordinates of inclusion center are specified in the global coordinate system, coordinates of points P_1 and P_2 are given either in the global coordinate system if the identification number of the inclusion is positive or in the local coordinate system, aligned with the global coordinate system and with origin at inclusion center, if the number is negative. Note that the center of the inclusion is expected to be inside or on the boundary of the reference tile. If directive `ALLOW_OUTSIDE` (see Section 6) is defined, then the center of the inclusion can be also outside of the reference tile but not by more than `epsilon`. In this case the inclusion is shifted in appropriate direction(s) by corresponding dimension of the reference tile so that the center falls inside the tile. Simultaneously, specifications of periodic repetition of all instances of this inclusion in all tiles corresponding to directions in which the shifts were performed are swapped to opposite (see the fifth section of the geometry file). The shape of the inclusion is defined by sizes of the major, minor, and middle half-axes `MAX`, `MIN`, and `MID`, respectively. Note that size of the major half-axis `MAX` may not be larger than minimum dimension of the tile reduced by epsilon divided

by `MAX_RADIUS_RATE` (see Section 6) and that the size of the minor half-axis must be larger than 10 times `epsilon`. Specifications of the internal and boundary mesh size `IIMSZ` and `IBMSZ` of the inclusion may not be negative. Zero mesh size specification corresponds to the maximal possible element size. Note that the size of actually generated finite elements may be (even significantly) smaller than the specified non-zero values depending on other mesh density control specifications. The identification number of the material of the inclusion `IMAT` must be larger than zero or zero if the inclusion is a hole. Similarly, the identification number of the material of the interface between the matrix and (non-hole) inclusion `IFMAT` must be larger than zero or zero if there is no interface. Note that in the current version of wang3d4t3d, the interface material specification is ignored and the connection between the matrix and (non-hole) inclusion is always without interface. The ordering of the inclusions is irrelevant.

If the directive `ALLOW_OVERLAP` is defined, the defined inclusions are allowed to touch or even overlap in the reference tile (which normally serves only as a container of individual inclusions and is not subjected to the disrectization). If the directive `ALLOW_OVERLAP` is not defined, while the directive `CHECK_OVERLAP` (see Section 6) is defined, the individual inclusions including all their periodic repetitions (see the fifth section of the geometry file) are checked against their overlapping. Note that the overlapping is identified whenever points on two inclusions are closer to each other than `epsilon`. Currently, there is no space search optimization adopted. This makes the check computationally very demanding if large number of inclusions is involved.

The fifth section contains description of individual Wang tiles. The ordering of Wang tiles is irrelevant. For each of the `NWT` Wang tiles, three sets of records need to be defined.

The first set contains just a single record containing side codes of the tile, number of inclusions related to the tile, and number of control points related to the tile:

`TID  CXN CXP CYN CYP CZN CZP  NTI  NCP`

If the directive `ARBITRARY_TILE_ID` (see Section 6) is defined, then the identification number of the tile `TID` can be arbitrary non-negative integer, otherwise positive integer number in range $\langle 1;\texttt{NWT}\rangle$ is expected. The codes corresponding to tile sides with outer normal in the direction of negative and positive x-, y-, and z-axes `CXN`, `CXP`, `CYN`, `CYP`, `CZN`, and `CZP` are integer numbers in range $\langle 0;\texttt{NSC}\rangle$. Non-zero code is used for matching sides of different tiles or for matching (opposite) sides of the same tile on which identical finite element mesh is required. Zero code is used for those sides that are not matching any other side of all tiles or for sides that are matching other side(s) but identical finite element mesh is not required. Two sides are considered matching if their normals are aligned with the same global coordinate system axis and if they are geometrically identical (except for a shift along that axis). Note that only limited check is applied to sides marked as matching to verify their compatibility. The number of tile inclusions `NTI` related to the tile can be larger than the number of reference inclusions `NRI` because up to eight instances of the same inclusion may be related to a single tile due to the periodic repetition of the inclusion. Note also that an inclusion touching the tile from outside (unless touching it at the tile corner) must be included in `NTI` and present later in the enumeration of inclusions. Since the inclusions may be shifted to comply with proximity criteria (see Section 4), it is desirable to account also for inclusions that are outside of the tile up to a reasonable distance (typically an appropriate multiple of `epsilon`). The density of the mesh over the tile can be controlled by additional control points number of which is specified as `NCP`.

The second set contains `NTI` records enumerating all inclusions (including their periodic repetitions). The format of the records depends on the directive `SEPARATE_PER_REP` (see Section 6). If the directive is defined, the format of the record is:

```
IID    PRX PRY PRZ
```

Inclusion identification number `IID` must be in the range $\langle 1;$`NRI`$\rangle$. The flags of periodic repetition in $x-$, $y-$, and $z-$directions `PRX`, `PRY`, and `PRZ`, being either zero or one, indicate whether that particular instance of the inclusion is or is not shifted by the dimension of the tile in the corresponding direction with respect to its reference position defined in the fourth section. Note that the shift is always performed towards the tile center. The ordering of the inclusions and their periodic repetitions is irrelevant.

If the directive `SEPARATE_PER_REP` is not defined, the record is expected in a concise format:

```
IID    PRXYZ
```

Specification `PRXYZ` is defined as `PRX` $<< 0 +$ `PRY` $<< 1 +$ `PRZ` $<< 2$, where $<<$ stands for binary shift. Thus `PRXYZ` is the integer number ranging from 0 to 7.

If directive `CHECK_OVERLAP` is defined, then specified inclusions including applied periodic repetitions are checked against their overlapping. The overlapping of two inclusions is identified whenever points on these two inclusions are closer to each other than `epsilon`. Note that the check works with inclusions shifted in order to satisfy the proximity criteria (see Section 4). This is also the reason, why the check is performed even if directive `ALLOW_OVERLAP` is not defined, in which case, however, only those pairs of inclusions, in which at least one is shifted, are investigated. Currently, there is no space search optimization adopted. This makes the check computationally very demanding if large number of inclusions is involved.

The third set contains `NCP` specifications of mesh density at individual control points:

```
XCP YCP ZCP   MSZ
```

The coordinates of the control point `XCP`, `YCP`, and `ZCP` in the global coordinate system may not fall outside the tile by more than `epsilon`. The required size of elements `MSZ` at the control point and in its immediate vicinity must be positive.

For an example of the geometry file see Section 7.

4 Proximity Criteria

In order to prevent undesirable mesh refinement induced by the Wang tiles or even a mesh generation failure, the inclusions close to or intersecting tile boundary may be subjected to slight shift to comply with three kinds of proximity criteria. The first proximity criterion is related to tile sides. Generally, if the inclusion is closer[1] to a tile side than `epsilon`, then the inclusion is shifted in appropriate direction (inclusion fully inside the tile is shifted towards the side, otherwise towards tile center) to enforce its touching the tile side. If directive `DETOUCH` (see Section 6) is

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[1]The distance of an inclusion from a tile side is considered as the smaller from distances between the tile side and plane parallel to the side and touching the inclusion on either or other side.

defined, inclusion fully inside the tile (but closer to the tile side than `epsilon`) or touching the tile side is shifted towards the tile center to make its distance from the tile side exactly `epsilon`, and inclusion intersecting the tile side (but closer to the tile side than `epsilon`) is shifted outwards from the tile center to make its distance from the tile side exactly `epsilon`. If (except directive `DETOUCH`) also directive `OVERDETOUCH` (see Section 6) is defined, then inclusion touching or intersecting the tile side (but closer to the tile side than `epsilon`) is shifted towards the tile center to make its distance from the tile side exactly `epsilon`. The second proximity criterion is related to tile edges. If the intersection (an ellipse or a single point, which is treated as an ellipse degenerated into a point) of the inclusion with a particular tile side is closer[2] to tile edges in the plane of that side than `epsilon`, then the inclusion is shifted in the plane parallel to the tile side to make the ellipse either touching the tile edge, if directive `DETOUCH` is not defined, or distant from the edge by at least `epsilon`, no matter whether intersecting the edge or not. The shift is however limited in the sense that the overall shift of the inclusion with respect to its reference position may not exceed in either direction maximal shift defined as `MULTIPLE_EPS`×`epsilon` (see Section 6). If such shift does not exist, the tolerance (initially `epsilon`) is halved and a new attempt to compute an appropriate shift is made. Note that halving is applied repeatedly but not more than `subdivisions` times and also until the problem dependent tolerance is reached. If appropriate shift is not found for any of the considered tolerances, an error message is issued and the program is prematurely terminated. The third proximity criterion is related to tile corners. If the intersection of the inclusion with relevant tile edges is closer to tile corner than current (possibly reduced) tolerance, the inclusion is further shifted in appropriate direction, while not exceeding the maximal shift, to pass through the tile corner. If such shift does not exist, an error message is issued and the program is prematurely terminated. The same happens if the inclusion intersects a tile edge at two points closer to each other than twice the problem dependent tolerance. Note that the reduced tolerance is reset back to `epsilon` before other inclusion is processed. The problem dependent tolerance is influenced by the size of the complete problem, when all processed tiles are distributed in space in order to not interfere with each other when being discretized in T3d. In order to prevent overlapping of inclusions as a consequence of their shifting, it is recommended to distribute inclusions in individual tiles so that they are far enough from each other to allow for their safe shifting. This safety distance can be roughly estimated as (`MULTIPLE_EPS` + 1)×2×`epsilon`. Alternatively, the `epsilon` to be passed to wang3d4t3d can be estimated as the smallest distance between inclusions distributed in individual tiles divided by 2×(`MULTIPLE_EPS`+1). Note that the shifting can be suppressed by using negative value of the command line parameter `subdivisions`. In such a case, whenever a proximity criterion is not satisfied for given `epsilon`, an error message is issued and the program is prematurely terminated.

5   Compilation

The source code is written in plain C without dependence on any non-standard libraries. For compilation on Linux/Unix platforms, change to the directory containing wang3d4t3d.c and use (typically) command

```
gcc -O2 -o wang3d4t3d wang3d4t3d.c -lm
```

Should you prefer other compiler, replace `gcc` by the name of your preferred compiler and follow its syntax for proper specification of command line options. For compilation on Windows/Mac

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[2]The distance of an intersection ellipse from a tile edge (in the plane of the ellipse) is considered as the smaller from distances between the tile edge and line parallel to the edge and touching the ellipse on either or other side.

platforms, create a project for console application in you favourite development environment or use you favourite command line compiler for Windows/Mac.

Note that all other source files are included in wang3d4t3d.c and should be therefore kept in a directory searched for header files (ideally in the same directory as wang3d4t3d.c). They should not be compiled separately.

6   Compilation Directives

There are several compilation directives influencing the behaviour and performance of wang3d4t3d. While some of the directives can be customized by basic users, the other should be modified by advanced user only or should not be modified at all. The default values of the directives can be obtained by executing `wang3d4t3d -h`. The directives are placed at the top of the source code (wang3d4t3d.c) and should not be therefore used as command line options of the compiler.

MAX_RADIUS_RATE – defines the minimum ratio between the minimum dimension of the tile reduced by `epsilon` and the size of the major half-axis. The value MAX_RADIUS_RATE may not be smaller than 2. Recommended value is 2.5.

MAX_TILES – controls the maximum number of tiles that can be processed by wang3d4t3d. It is expected that MAX_TILES is an integer power (at least the first power) of 10, in which case the maximum number of tiles is equal to MAX_TILES - 1. The larger value of MAX_TILES, the smaller number of inclusions intersecting individual sides of a tile are allowed. The most common value for MAX_TILES is 100.

DEF_REL_EPSILON – is the default relative tolerance. It should not exceed the maximal relative tolerance MAX_REL_EPSILON.

MAX_REL_EPSILON – is the maximal relative tolerance. It should be much smaller than 1.

ARBITRARY_TILE_ID – allows to number tiles arbitrarily by non-negative integer identification numbers.

SEPARATE_PER_REP – enforces specification of periodic repetitions of inclusions separately for each direction of global coordinate system.

DETOUCH – forces inclusion closer to the tile side than `epsilon` to be shifted so that its distance from the tile side is exactly `epsilon` and simultaneously the shift is minimized. If the inclusion is touching the tile side, then it is shifted inside the tile.

OVERDETOUCH – forces inclusion intersecting the tile side and being closer to that side than `epsilon` to be shifted inside tile so that its distance from the tile side is exactly `epsilon`. Note that directive OVERDETOUCH can be defined only if directive DETOUCH is defined.

ALLOW_OVERLAP – allows inclusions (including all their periodic repetitions) in the reference tile to freely overlap.

CHECK_OVERLAP – forces a check that inclusions (including all their periodic repetitions) in reference tile, if directive ALLOW_OVERLAP is not defined, do not overlap and that inclusions (including applied periodic repetitions) used in individual tiles do not overlap. The overlap is checked with respect to `epsilon`.

ALLOW_OUTSIDE – allows to accept also reference inclusions with center outside the reference tile but not by more than `epsilon`.

FIX_HOLE – enforces T3d (via command line parameter) to fix degeneration (on the level of mesh) of not only solid regions but also of holes.

CHECK_ISOLATED – checks for setups resulting in isolated nodes at tile corners in the generated finite element mesh. Generally these nodes must be present in the mesh to allow for tile mesh assembly after which these nodes usually become not isolated. In some cases, however, these nodes may remain isolated even in the assembled mesh and should be removed by postprocessing. If such setup is identified, a warning is issued.

USE_TILE – forces that each t3d model entity (except virtual ones) refers to a particular tile. This directive must be defined.

USE_SIDE – forces explicit side specification for t3d patches on tile sides. This directive may not be defined.

USE_CODE – forces explicit code specification for t3d tiles. This directive may not be defined.

USE_SIMPLE – forces simple mirroring between sides of tiles with the same code in order to override discrepancies due to round-off error or numerical instabilities. This directive may not be defined.

MULTIPLE_EPS – defines the multiple of the `epsilon` up to which the shift of the inclusion in each particular direction is performed when resolving intersection of the inclusion with tile sides, edges, and corners. The value `MULTIPLE_EPS` may not be smaller than 1. Recommended value is 2. Note that value less than 2 may prevent overdetouching (see directive `OVERDETOUCH`).

SETUP – controls the way how the individual tiles are arranged in space in order to not interfere with each other when being discretized in T3d. The possible values are `GRID_3D` or `GRID_2D` resulting in distribution of tiles in a regular 3D or 2D grid (if there are not enough tiles to fill the grid fully, some of its entries will remain empty), or `DIAGONAL`, in which case the tiles are distributed along spatial diagonal of a cube. Obviously, the setting of `SETUP` is irrelevant if only one tile is processed. Note that no matter whether `GRID_3D`, `GRID_2D` or `DIAG` is used, the resulting meshes of individual tiles are placed in the position of the reference tile. Keep in mind however, that the resulting meshes are generally different depending on the setting of `SETUP`. Note also that the `GRID_3D` (`DIAGONAL`) setup results in the smallest (largest) problem dependent tolerance.

USE_VIRTUAL_ELLIPSOID – enables to overcome singularity of biquadratic rational Bezier surface approximating in some cases the exact ellipsoidal shape of the inclusion by using also the exact but virtual geometry to allow for proper curvature evaluation. This feature is not necessary.

HALF_MAX_TILES – reduces the number of tiles defined by `MAX_TILES` to half in order to allow for larger number of inclusions (including their periodic repetitions) to intersect each particular side of individual tiles when interfaces between matrix and inclusions are considered. This feature is not recommended.

MIN_MAX_HALVING – allows to split intersection ellipse (intersection of the inclusion with the tile side) also with respect to the major and minor axes. The feature is currently not fully implemented and should not be used.

EXCESS_SIZE – defines in which way the size by which inclusions may exceed the tile is considered. The possible values are `MAX_ALLOWED_SIZE`, assuming maximal possible inclusion size (see directive `MAX_RADIUS_RATE`), and `MAX_PRESENT_SIZE`, assuming the largest (in terms of the size of the major axis) reference inclusion no matter whether the inclusion is used in individual tiles or whether it is intersecting the tile side. Note that `MAX_PRESENT_SIZE` setting results in smaller problem dependent tolerance.

OFFSET – defines the relative distance between tiles (with respect to the minimal tile dimension) to ensure that the individual tiles arranged in the space do not interfere with each other when being discretized in T3d. The value of `OFFSET` should be in range $\langle 0.5; 1.0 \rangle$. Recommended

value is 0.5. Note that the distance between tiles is further enlarged to account for inclusions exceeding the tiles. Although the part of the inclusion outside the tile is obviously not subjected to the discretization, it may influence the mesh density control space. The real distance between the tiles may be further increased due to arrangement of tiles in space which must comply with certain criteria to minimize the dispersion of specified mesh density along the corresponding pairs of matching sides.

MAX_RATE – defines what portion of the inclusion can be inside the tile (with respect to its particular side) so that the ellipsoidal shape of the part of the inclusion inside the tile can be safely approximated by a single biquadratic rational Bezier surface. The value of MAX_RATE should be close to 1. Recommended value is 0.95.

INC_RATE – defines the position of a plane splitting an inclusion intersecting a particular tile side to the part approximated by a single biquadratic rational Bezier surface so that the singularity of the surface is safely outside of the tile. The position is defined relatively with respect to the portion of the inclusion outside the tile with zero being on the tile side. The value of INC_RATE should be close to 0. Recommended value is 0.05.

BUFFER_SIZE – defines the size of the input line buffer. Recommended value is 1024.

7 Example of Geometry File

```
Arbitrary comment

# Overall numbers
2 5 6

# Reference tile
0 0 0  1 1 1  1  0.5 0.2

# Reference inclusions
1  0.31 -0.09 -0.05  0.37 0.01 -0.27  0.23 -0.04 -0.04 0.25 0.1 0.15 0.2 0.1 0 0
3 -0.05  0.45 -0.03  0.16 0.34 -0.07 -0.09  0.41 -0.11 0.25 0.1 0.15 0.2 0.1 0 0
4 -0.13  0.27 -0.50 -0.36 0.19 -0.44 -0.16  0.29 -0.59 0.25 0.1 0.15 0.2 0.1 0 0
5 -0.17  0.07  0.50 -0.41 0.02  0.48 -0.17  0.07  0.59 0.25 0.1 0.15 0.2 0.1 0 0
2 -0.43  0.03 -0.03 -0.35 0.20  0.13 -0.51  0.01  0.03 0.25 0.1 0.15 0.2 0.1 0 0

# Tile 1
1  1 1 2 2 4 5  5 0
1  0 0 0
3  0 1 0
3  0 0 0
4  0 0 0
5  0 0 0

# Tile 2
2  3 3 6 6 5 4  4 0
2  0 0 0
2  1 0 0
4  0 0 1
5  0 0 1
```

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