Table 1: **Model description language**. A summary of the main elements of the Morpheus description language and their most important sub-elements. Required (sub)elements are printed in boldface.

| Element | Description | Sub-elements |
|---|---|---|
| **`Description`** | Sets the name (`Title`) of the model, used for naming the destination folder. May include model annotation (`Details`), used for human-readable annotation only. | **`Title`**<br>`Details` |
| **`Space`** | Sets the size, structure and boundary conditions of the lattice (`Lattice`). Optionally, sets a symbols for the lattice size and current location (`Lattice/Size/symbol` and `SpaceSymbol`). | **`Lattice`**<br>`SpaceSymbol` |
| **`Time`** | Set the duration of a simulation (`StartTime` and `StopTime`) defining the global time. Optionally, sets a symbol for current time (`TimeSymbol`). May specify the interval to save the simulation state (`SaveInterval`). May set a random seed for stochastic simulations (`RandomSeed`). | **`StartTime`**<br>**`StopTime`**<br>`TimeSymbol`<br>`SaveInterval`<br>`RandomSeed` |
| `CellTypes`<br>**`CellType`** | Allows multiple cell types to be defined. Each cell type (`CellType`) sets a name and type (i.e. biological or medium).<br>May define multiple properties (`Property`) for use in mathematical expressions (`Equation`, ...). May contain reporters for spatial mapping (`Reporter`). May define systems of ordinary differential equations (ODE) (`System/DiffEqn`). May specify a diversity of cellular behaviors (`Chemotaxis`, `Proliferation`, ...). | `Property`<br>`System`<br>`Constant`<br>`Function`<br>`Equation`<br>`Event`<br>`Reporter`<br>`Chemotaxis`<br>`Proliferation`<br>... |
| `CPM` | Sets the time-scale of a Monte Carlo step (`MCSDuration`), the parameters for the cellular Potts model (`MetropolisKinetics`) and the parameters of interactions between cells (`Interaction`). Optionally, for constant boundary condition, sets a cell type at a boundary (`BoundaryValue`). | **`Interaction`**<br>**`MetropolisKin.`**<br>**`MCSDuration`**<br>`BoundaryValue` |
| `PDE` | Sets the symbol and diffusion coeffients for species (`Layer`) in a reaction-diffusion model for use in mathematical expressions (`Equation`, ...). May set a system of differential equations (`System/DiffEqn`) for reactions. | **`Layer`**<br>`Constant`<br>`System`<br>`Function`<br>`Equation` |
| `CellPopulations`<br>**`Population`** | Allows multiple populations to be defined. Each population sets a cell type and size (`Population`). May set initializers (e.g. `Initrectangle`). May explicitly specify multiple cells with properties and positions (`Cell`). When saving the simulation state, state of each cell is specified here. | `Cell`<br>`Initrectangle`<br>`TIFFReader`<br>... |
| `Analysis` | Sets the visualization and analysis tools. May contain various loggers and plotters (`Gnuplotter`, `Logger`). Executed at user-specified intervals. | `Gnuplotter`<br>`TIFFPlotter`<br>`Logger`<br>`HistogramLogger` |

Table 2: **Mathematical constructs**. Overview of the mathematical constructs available in model description language (• = symbol definition, ○ = symbol reference).

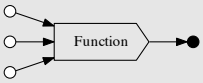
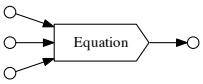
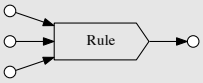
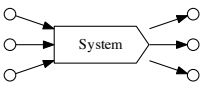
| Element | Description | Symbol graph |
|---|---|---|
| | **Containers** | |
| `Constant` | Constant value of type double with local scope, i.e. valid within the `CellType` or `System` it is defined in. |   |
| `Global` | Variable value of type double with global scope. |   |
| `Property`<br>`PropertyVector`<br>`DelayProperty` | Cell-bound variable. `Property` and `DelayProperty` are of type double. `DelayProperty` has attribute `delay` to set the lag between assignment and return of value. `PropertyVector` defines Euclidean vector in space delimited format "x y z". |   |
| `Layer` | `PDE` model variable, i.e. species in reaction-diffusion system. Diffusivity of a `Layer` is specified in attribute `diffusion`. |   |
| | **Expressions** | |
| `Function` | Mathematical expression. Computes a value (double) for the output symbol it defines, but does not assign it to a variable. Updated whenever when output symbol is referenced. May not contain algebraic loop. |   |
| `Equation` | Mathematical expression. Computes a value (double) and assigns it to the variable it references. Updates are scheduled depending on its symbol dependencies. May not contain algebraic loop. |   |
| `Rule` | Mathematical expression that defines a (recurrence) equation for use in environments such as `System` and `Event`. Scheduled according to `System/time-step`. May contain algebraic loop and self-references. |   |
| `DiffEqn` | Mathematical expression that defines a differential equation. Only allowed in `System` environment. May contain algebraic loop and self-references. |   |
| | **Reporters** | |
| `Reporter`<br>`NeighborsReporter`<br>`PDEReporter`<br>`...` | Explicit data mappings. Computes a statistic (average, mean, etc.) of the input data and assigns this to the output symbol. Updates are scheduled depending on its symbol dependencies. |   |
| | **Environments** | |
| `System` | Environment for tightly coupled sets of differential equations and rules that are synchronously updated (see section **??**). Scheduled according to user-specified `System` `time-step` and `time-scaling`. |   |
| `Event` | Environment for conditional or timed events. Triggered periodically or, if `Condition` is specified, whenever the condition changes from false to true. Updates are scheduled according to `time-step` if specified or depending on its symbol dependencies otherwise. |   |

Table 3: **User-defined and pre-defined symbols** in Morpheus model description language.

| Context | Element | Type | Description |
|---|---|---|---|
| | | **Simulation symbols** | |
| Space | Lattice/Size | vector | Size of lattice |
| | SpaceSymbol | vector | Current location |
| | NodeLength | double | Spatial discretization |
| Time | StartTime | double | Initial simulation time |
| | StopTime | double | Termination time of simulation |
| | SaveInterval | double | Interval between checkpointing |
| | TimeSymbol | double | Current time |
| | | **Model symbols** | |
| Various | Global | double | Constant with global scope |
| | Constant | double | Constant with local scope |
| | ConstantVector | vector | Constant vector with local scope |
| | Function | double | Mathematical expression |
| Celltype | Property | double | Cell-bound variable |
| | PropertyVector | vector | Cell-bound variable vector |
| | DelayProperty | double | Cell-bound variable with delay |
| CPM | MCSDuration | double | Time of single Monte Carlo step |
| PDE | Layer | double | Reaction-diffusion species |
| | | **Predefined symbols** | |
| cell | cell.id | integer | Unique cell index |
| | cell.type | integer | Cell type index |
| | cell.volume | integer | Number of lattice sites cell occupies |
| | cell.surface | integer | Number of lattice sites of cell boundary |
| | cell.center | vector | Center of mass of cell |
| | cell.length | double | Cell length of major axis |
| | cell.orientation | vector | Orientation of major axis |
| vectors | [symbol].x/y/z | double | Cartesian vector coordinates |
| | [symbol].abs | double | Magnitude of vector |
| | [symbol].phi/theta | double | Polar coordinates of vector |

Table 4: **Operators and predefined functions** available in mathematical expressions.

| Class | Description | Syntax |
|---|---|---|
| **Operators** | Addition | `+` |
| | Subtraction | `-` |
| | Multiplication | `*` |
| | Division | `/` |
| | Power | `^` |
| **Logical operators** | Logical and | `and` |
| | Logical or | `or` |
| | Exclusive or | `xor` |
| **Comparison** | Equal | `==` |
| | Not equal | `!=` |
| | Smaller | `< or <` |
| | Greater | `> or >` |
| | Smaller or equal | `<= or <=` |
| | Greater or equal | `>= or >=` |
| **Functions** | Sine | `sin(...)` |
| | Cosine | `cos(...)` |
| | Tangens | `tan(...)` |
| | Arc sine | `asin(...)` |
| | Arc cosine | `acos(...)` |
| | Arc tangens | `atan(...)` |
| | Hyperbolic sine | `sinh(...)` |
| | Hyperbolic cosine | `cosh(...)` |
| | Hyperbolic tangens | `tanh(...)` |
| | Arc hyperbolic sine | `asinh(...)` |
| | Arc hyperbolic cosine | `acosh(...)` |
| | Arc hyperbolic tangens | `atanh(...)` |
| | Logarithm base 2 | `log2(...)` |
| | Logarithm base 10 | `log(...)` |
| | Natural logarithm | `ln(...)` |
| | Exponent | `exp(...)` |
| | Power | `pow([base], [exponent])` |
| | Square root | `sqrt(...)` |
| | Sign, -1 if x<0, 1 if x>0 | `sign(...)` |
| | Round nearest integer | `rint(...)` |
| | Absolute | `abs(...)` |
| | Minimum of arguments | `min(..., ..., ...)` |
| | Maximum of arguments | `max(..., ..., ...)` |
| | Sum of arguments | `sum(..., ..., ...)` |
| | Average of arguments | `avg(..., ..., ...)` |
| | Modulus, remainder | `mod([numer], [denom])` |
| **Random number** | Uniform distribution | `rand_uni([min], [max])` |
| | Normal distribution | `rand_norm([mean], [stdev])` |
| | Gamma distribution | `rand_gamma([shape], [scale])` |
| | Boolean (0 or 1) | `rand_bool()` |
| **Condition** | Conditional statement | `if([condition], [then], [else])` |