Kinetic Simulation Algorithm Ontology

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Nick Juty, Camille Laibe and
Nicolas Le Novère

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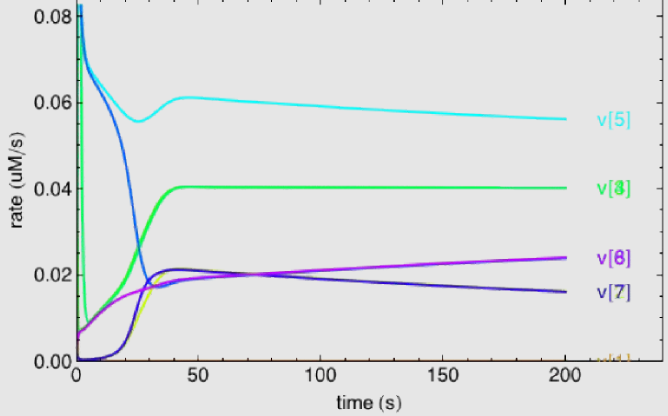
EMBL-EBI



MIASE

Modeling

Simulation

- Algorithm used
- Initial set-up

Numerical Results

KiSAO

SED ML

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KiSAO 2.0 vs 1.0

KiSAO 1.0 (OBO)

- algorithm using adaptive timesteps
  - Bortz-Kalos-Liebowitz method
  - tau-leaping method
- algorithm using discrete variables
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  - deterministic cellular automata
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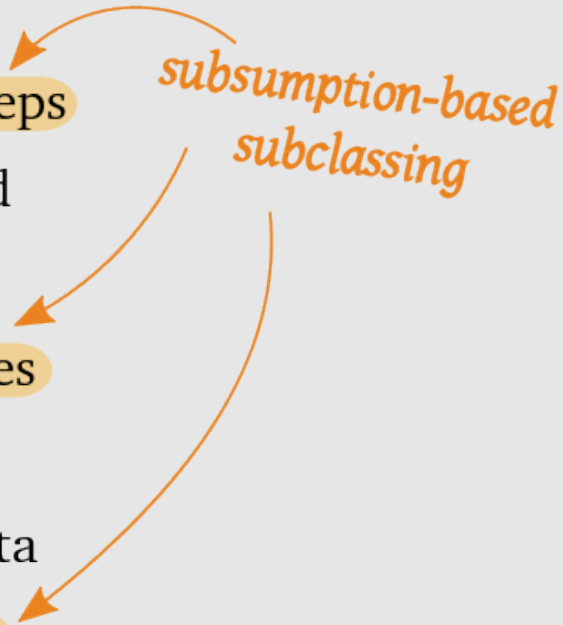

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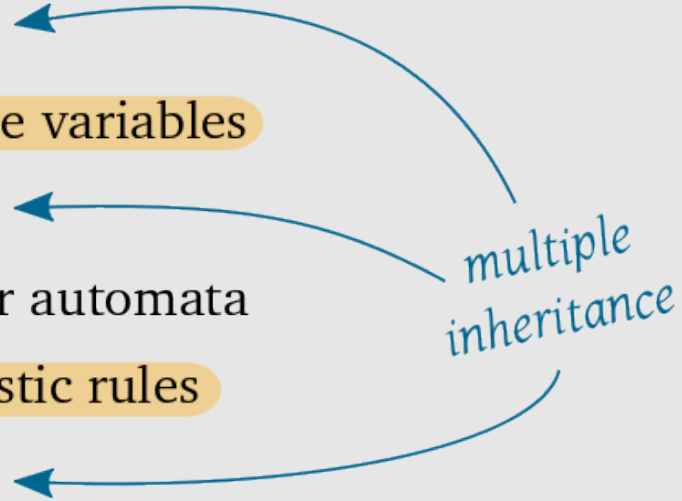

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  - type of variable
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more methods

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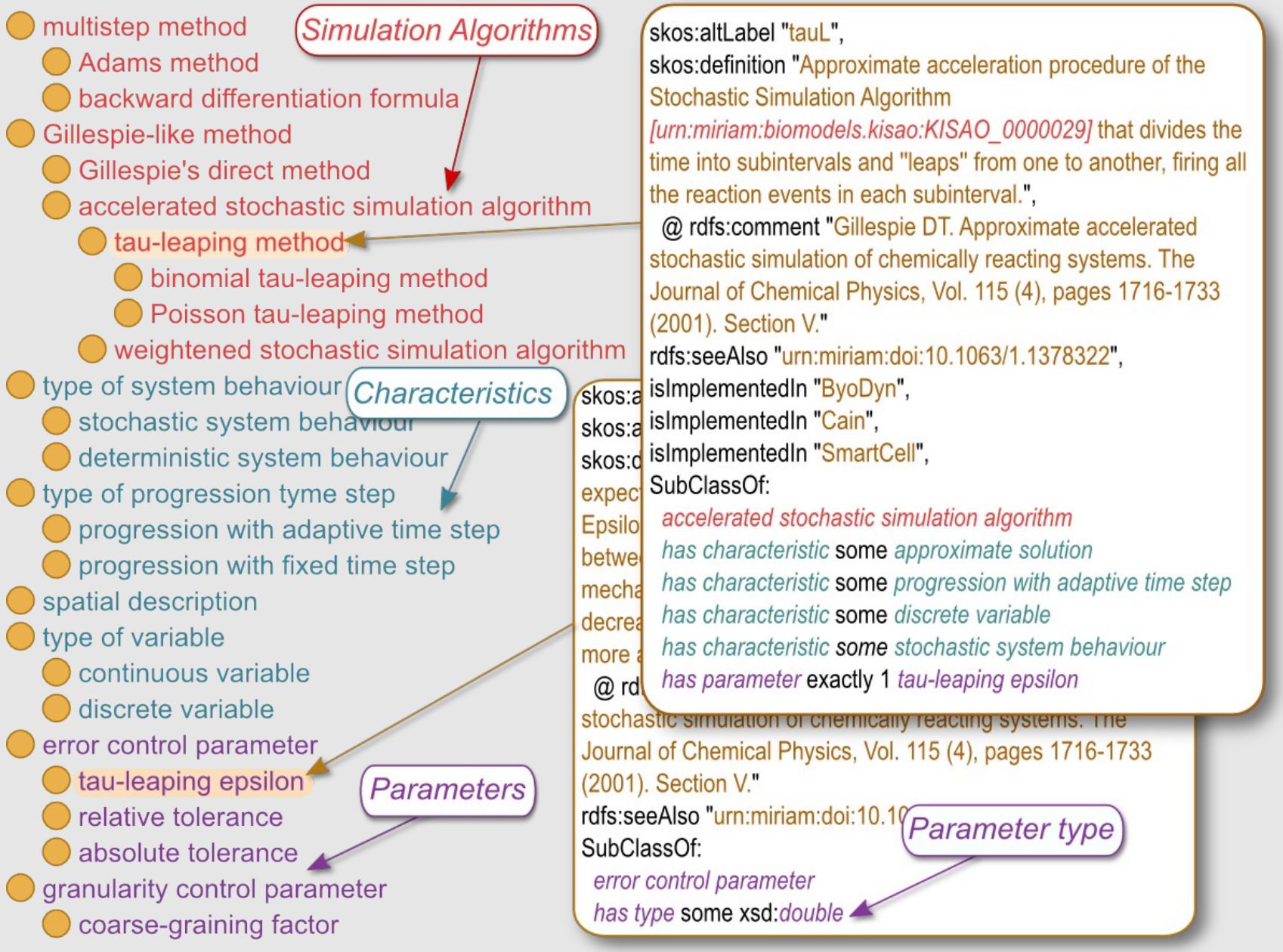
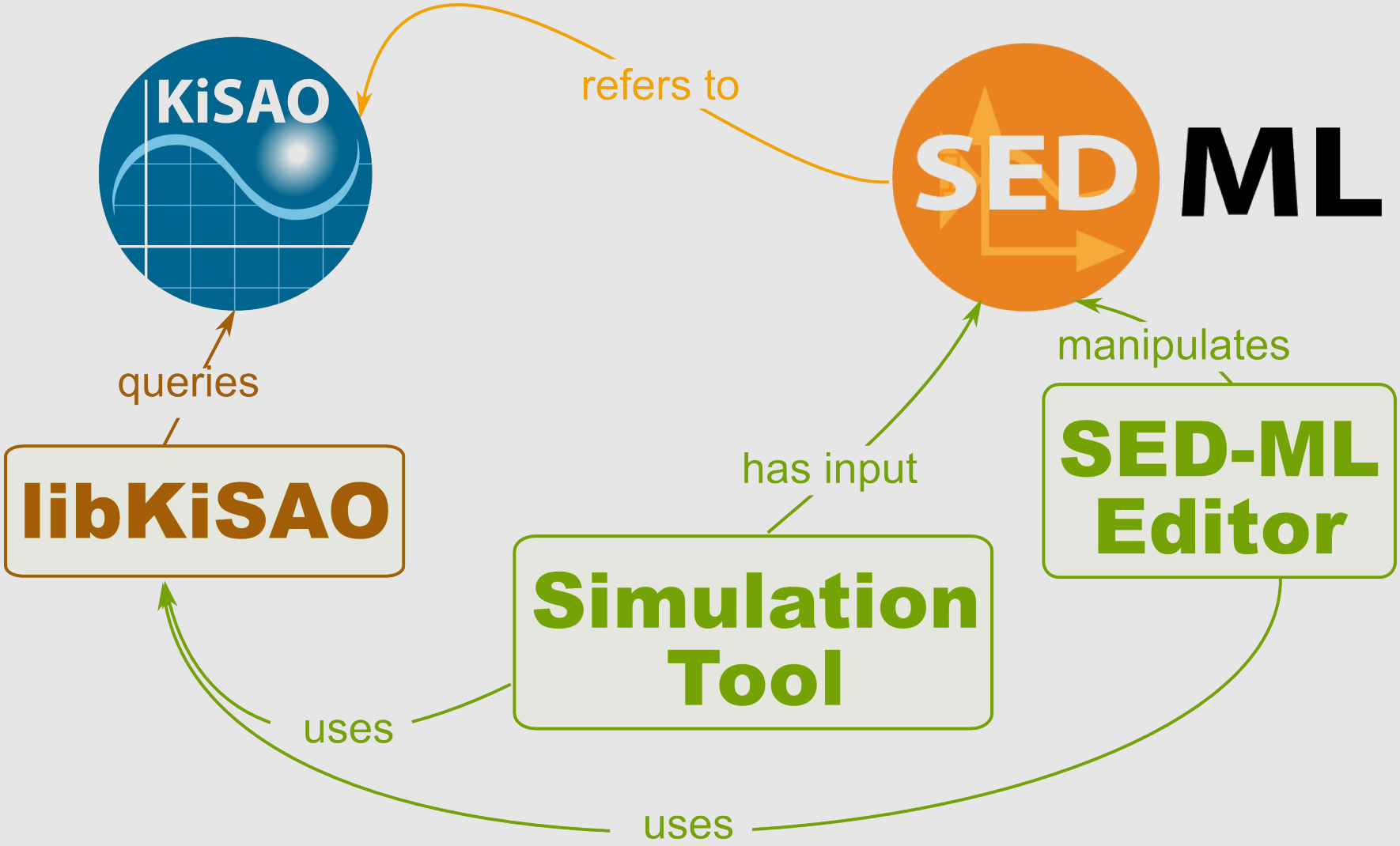
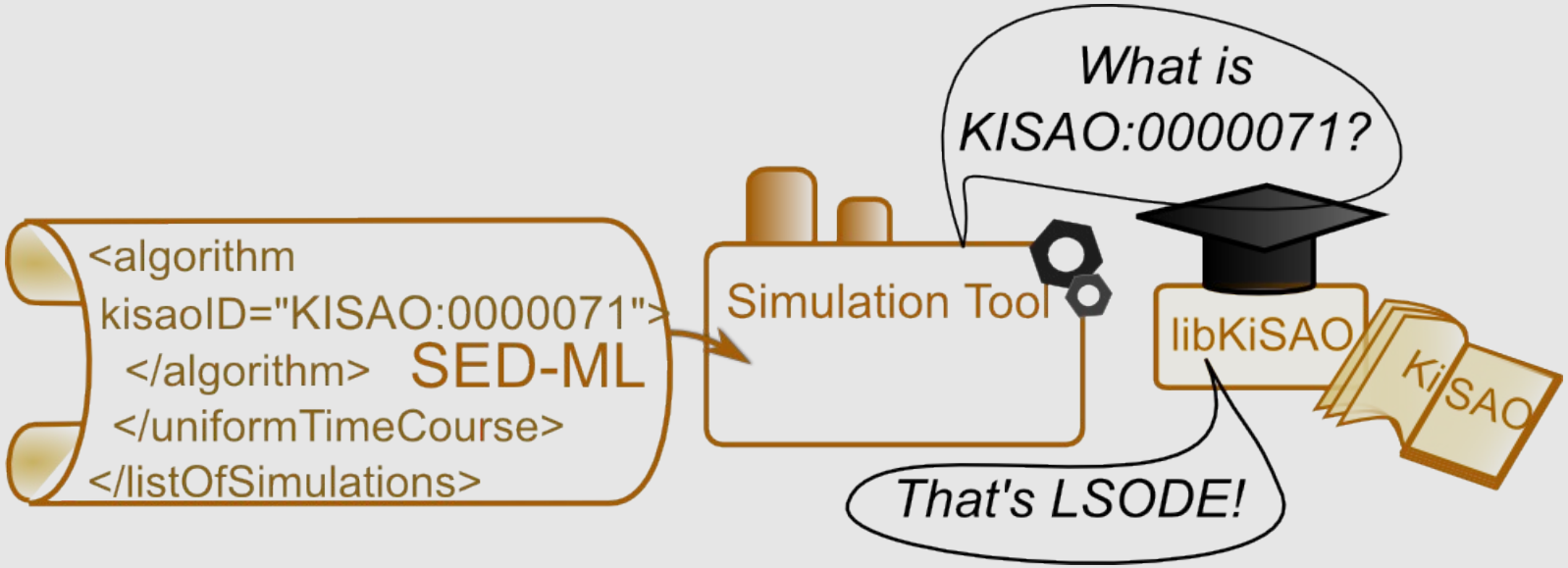

multistep method
Adams method
backward differentiation formula
Gillespie-like method
Gillespie's direct method
accelerated stochastic simulation algorithm
tau-leaping method
binomial tau-leaping method
Poisson tau-leaping method
weightened stochastic simulation algorithm
type of system behaviour
stochastic system behaviour
deterministic system behaviour
type of progression tyme step
progression with adaptive time step
progression with fixed time step
spatial description
type of variable
continuous variable
discrete variable
error control parameter
tau-leaping epsilon
relative tolerance
absolute tolerance
granularity control parameter
coarse-graining factor
Simulation Algorithms
Characteristics
Parameters
Parameter type
skos:altLabel "tauL",
skos:definition "Approximate acceleration procedure of the Stochastic Simulation Algorithm [urn:miriam:biomodels.kisao:KISAO_0000029] that divides the time into subintervals and "leaps" from one to another, firing all the reaction events in each subinterval.",
@ rdfs:comment "Gillespie DT. Approximate accelerated stochastic simulation of chemically reacting systems. The Journal of Chemical Physics, Vol. 115 (4), pages 1716-1733 (2001). Section V."
rdfs:seeAlso "urn:miriam:doi:10.1063/1.1378322",
isImplementedIn "ByoDyn",
isImplementedIn "Cain",
isImplementedIn "SmartCell",
SubClassOf:
accelerated stochastic simulation algorithm
has characteristic some approximate solution
has characteristic some progression with adaptive time step
has characteristic some discrete variable
has characteristic some stochastic system behaviour
has parameter exactly 1 tau-leaping epsilon
Journal of Chemical Physics, Vol. 115 (4), pages 1716-1733
(2001). Section V."
SubClassOf:
error control parameter
has type some xsd:double


KiSAO
refers to
SED ML
queries
manipulates
libKiSAO
has input
SED-ML Editor
Simulation Tool
uses
uses

Use Case: libKiSAO and Simulation Tools



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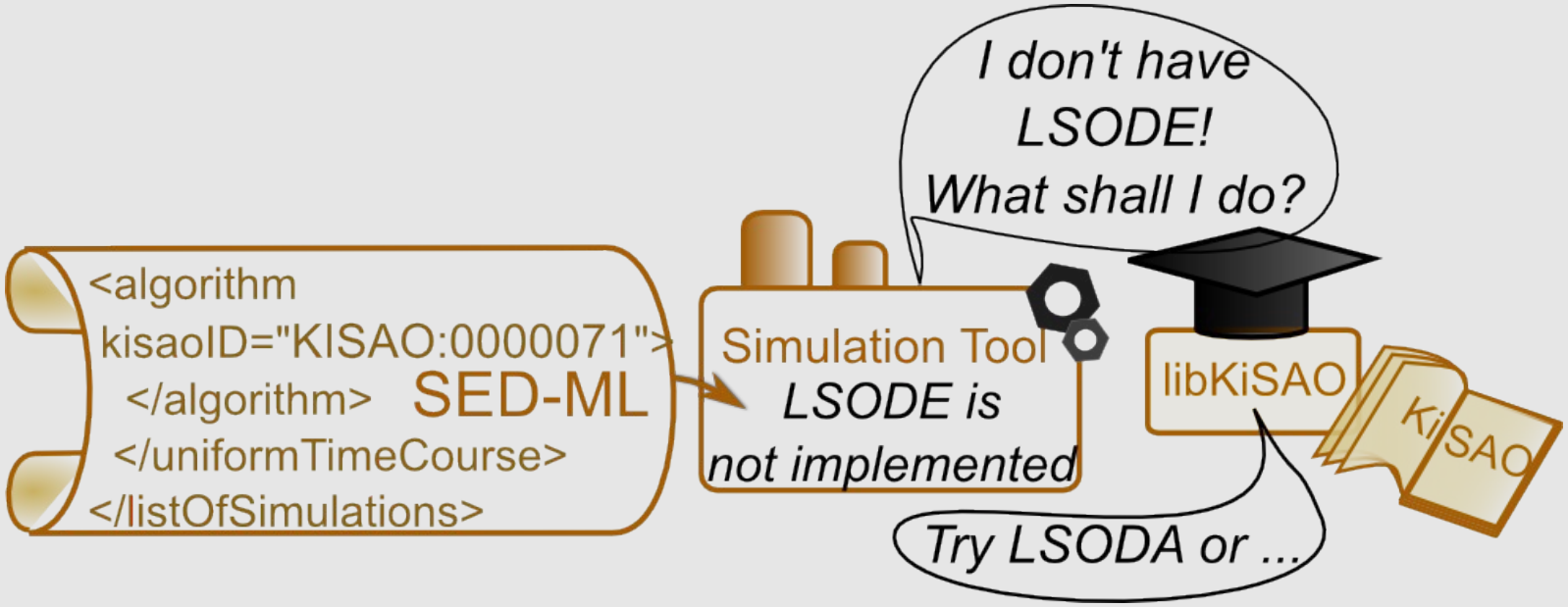
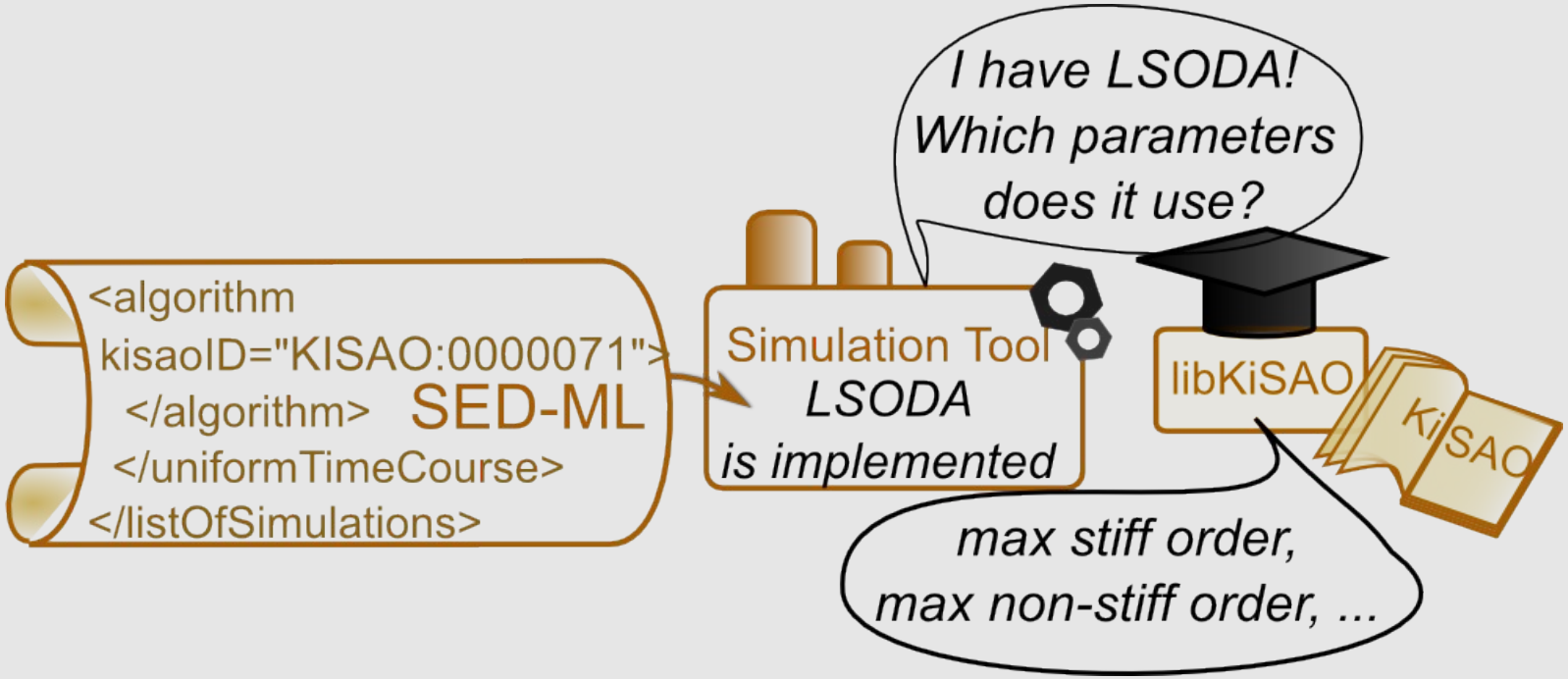


Use Case 2: libKiSAO and Simulation Tools



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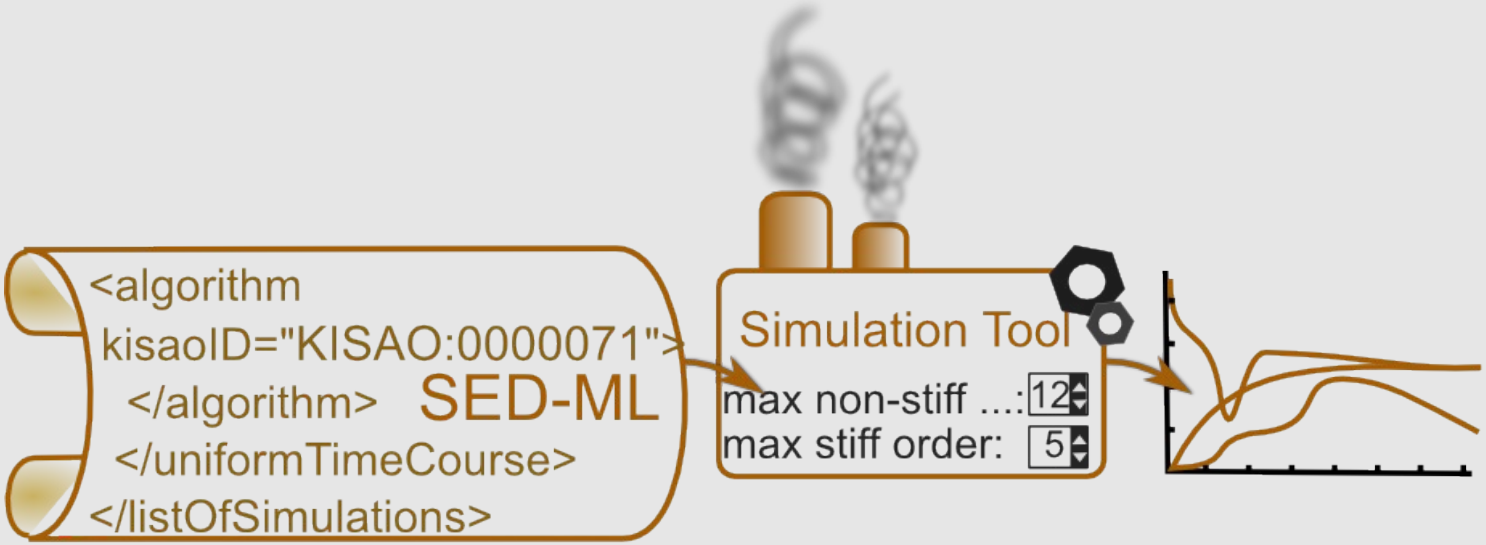

Acknowledgments

KiSAO

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libKiSAO

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The community of SED-ML for their contributions and their comments.

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http://biomodels.net/kisao

- Download
- libKiSAO
- Suggest terms
- Submit bugs

zhutchok@ebi.ac.uk (Anna Zhukova)