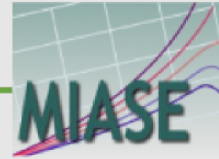
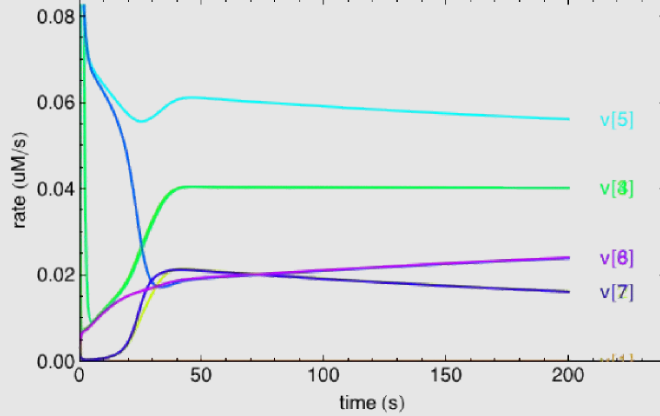


Kinetic Simulation Algorithm Ontology

Dagmar Waltemath, Anna Zhukova,
Nick Juty, Camille Laibe and
Nicolas Le Novère

COMBINE 2011
Heidelberg, 3rd - 7th September





Modeling

Simulation

Numerical Results

- Algorithm used
- Initial set-up



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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
 - tau-leaping method
 - deterministic cellular automata
- algorithm using stochastic rules
 - tau-leaping method

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*subsumption-based
subclassing*



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multiple inheritance

The diagram illustrates multiple inheritance in the KiSAO 1.0 ontology. A central text label 'multiple inheritance' has three blue arrows pointing to the 'tau-leaping method' entries under three different algorithm categories: 'adaptive timesteps', 'discrete variables', and 'stochastic rules'.

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KiSAO 2.0 (OWL)

- deterministic cellular automata
- Bortz-Kalos-Liebowitz method
- tau-leaping method
- algorithm characteristic
 - type of variable
 - type of system behaviour
 - type of progression time step

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KiSAO 2.0 vs 1.0

*more
methods*

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- algorithm characteristic
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 - type of system behaviour
 - type of progression time step
- algorithm parameter

- 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
 - weighted stochastic simulation algorithm
- type of system behaviour
 - stochastic system behaviour
 - deterministic system behaviour
- type of progression time 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

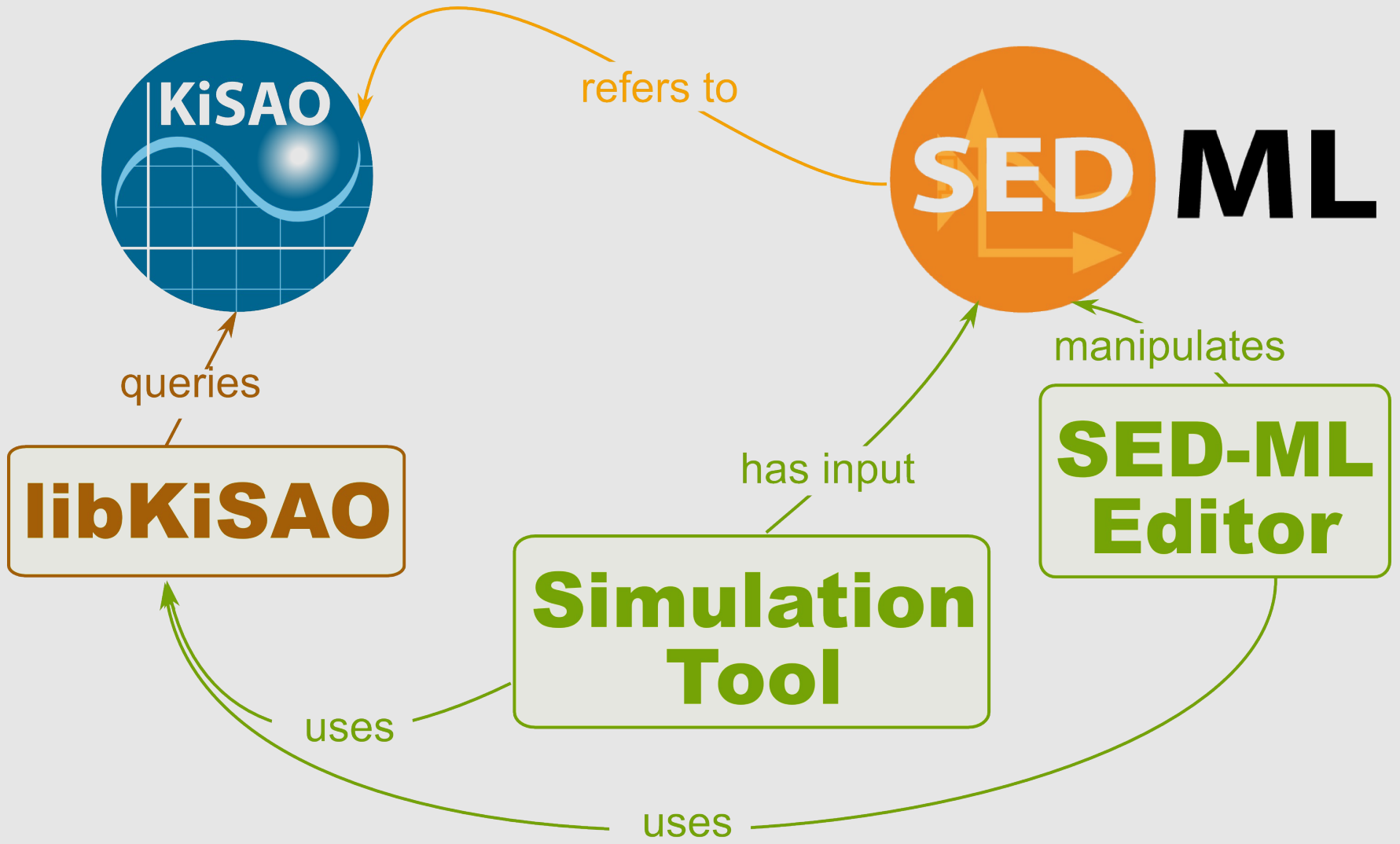
Characteristics

Parameters

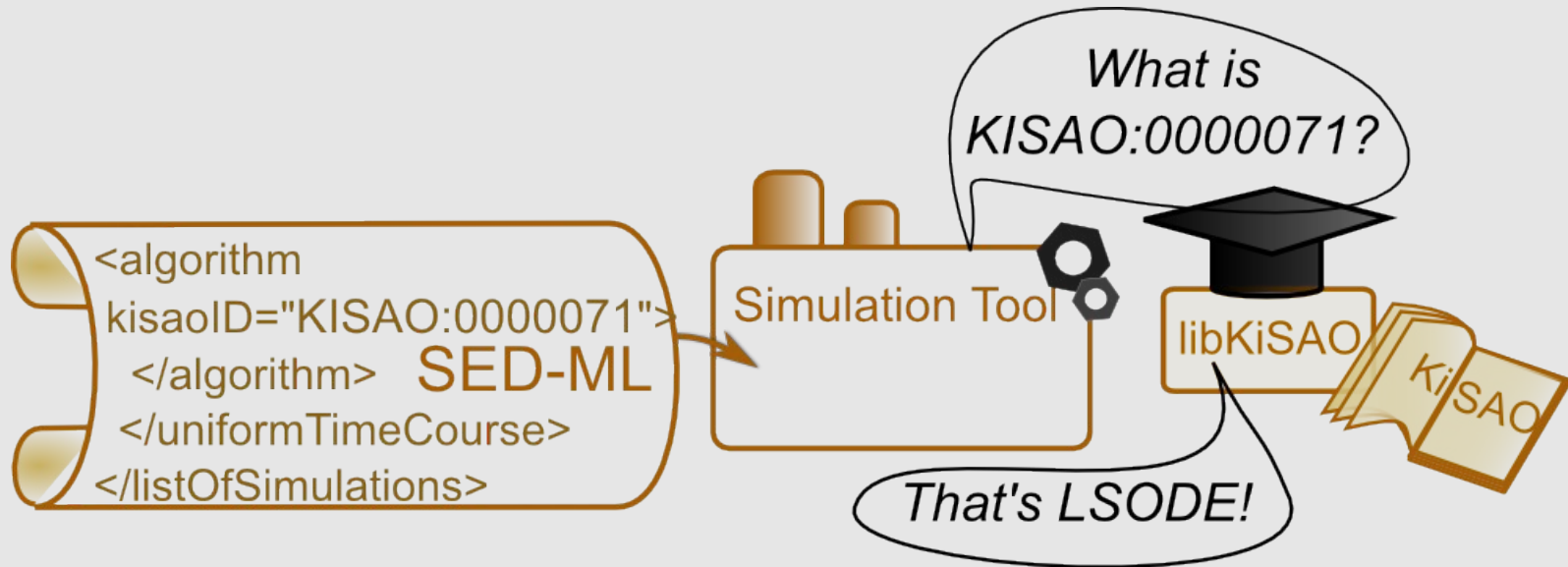
Parameter type

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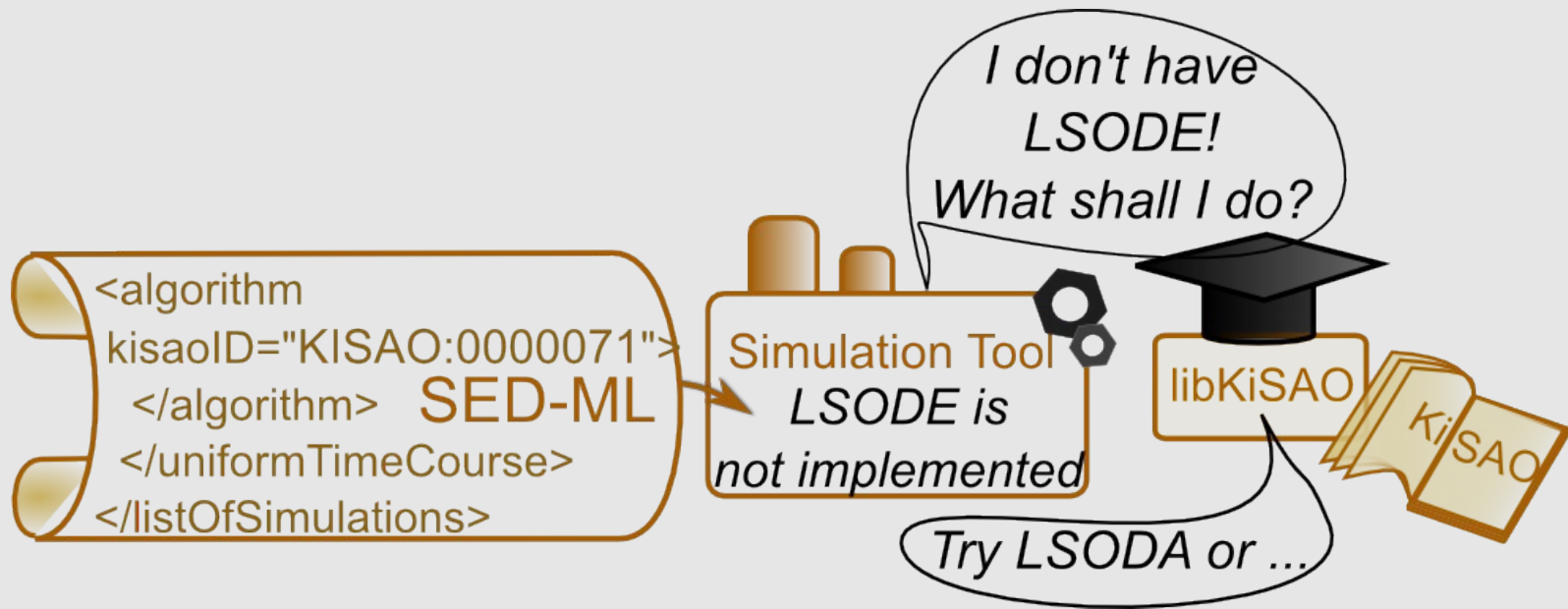
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time into subintervals and "leaps" from one to another, firing all
the reaction events in each subinterval.",
@ rdfs:comment "Gillespie DT. Approximate accelerated
stochastic simulation of chemically reacting systems. The
Journal of Chemical Physics, 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:
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    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
@ rd
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:10.10
SubClassOf:
    error control parameter
    has type some xsd:double
    
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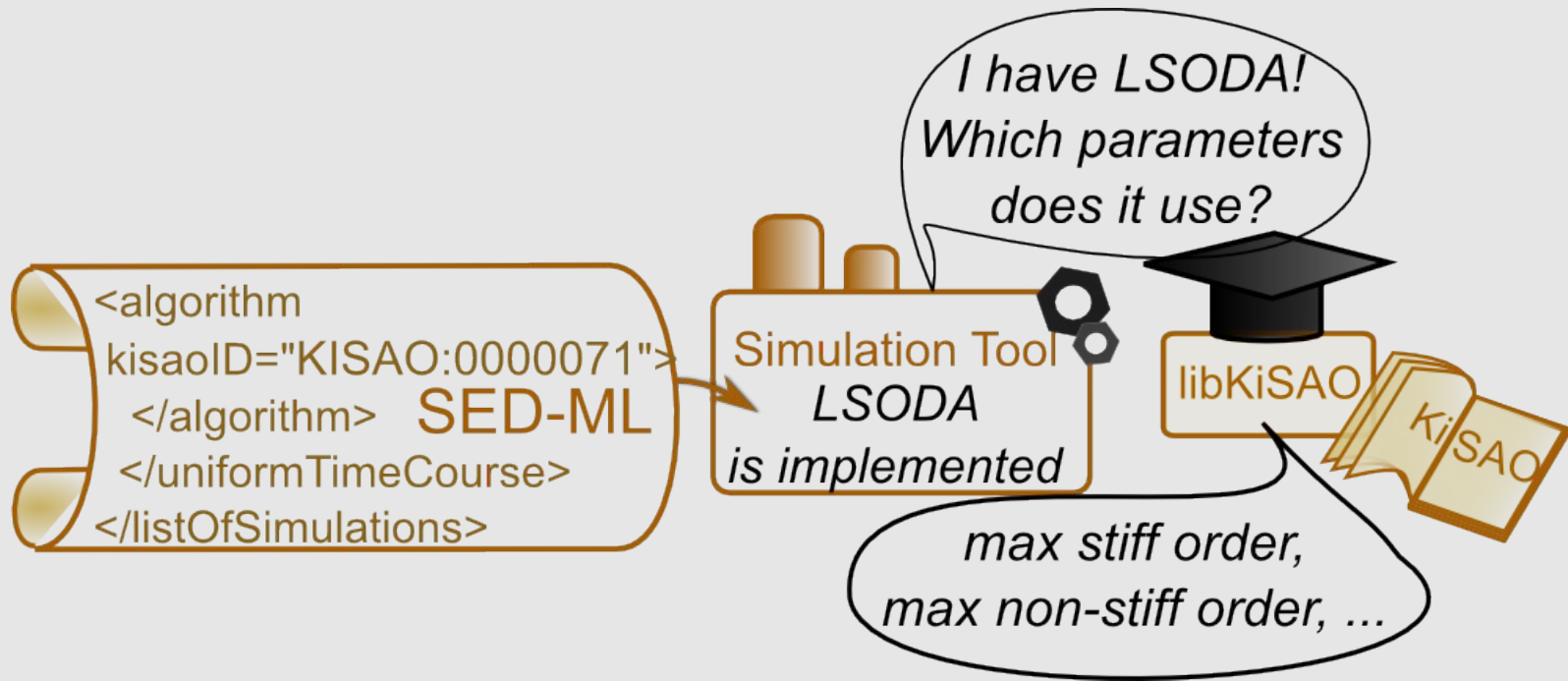
Use Case: libKiSAO and Simulation Tools



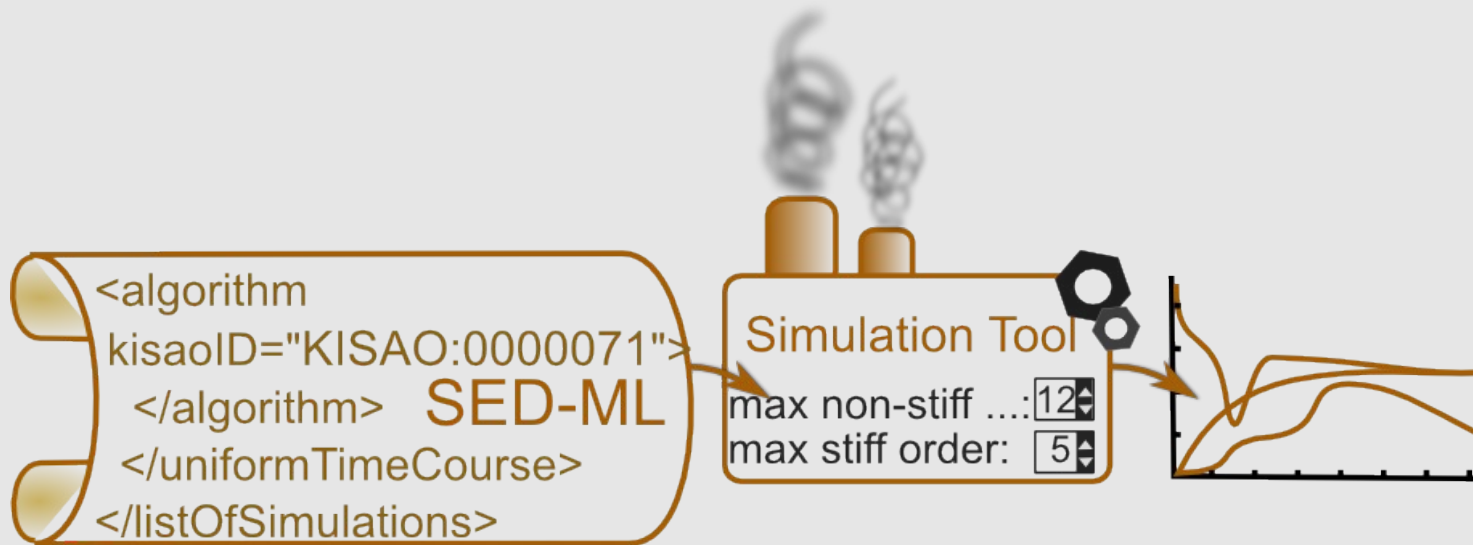
Use Case: libKiSAO and Simulation Tools



Use Case 2: libKiSAO and Simulation Tools



Use Case: libKiSAO and Simulation Tools



Acknowledgments

KiSAO

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Anna Zhukova, Nick Juty,
Camille Laibe,
Nicolas Le Novère

libKiSAO

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Adams, Camille Laibe,
Nicolas Le Novère

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

We would like to thank European Molecular Biology Laboratory and
Marie-Curie BioStar for providing resources to carry out this work.



<http://biomodels.net/kisao>

- ✓ Download
- ✓ libKiSAO
- ✓ Suggest terms
- ✓ Submit bugs

zhutchok@ebi.ac.uk (Anna Zhukova)