

# The Kinetic Simulation Algorithm Ontology (KiSAO)

A Proposal for the Classification of Simulation  
Algorithms in Systems Biology

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# Motivation

“The aim of MIASE is to provide all the information necessary to link a model to a set of numerical results, in order to reproduce the latter.”

In line with the development of MIASE, one requirement was to be able to unambiguously reference simulation algorithms.

KiSAO:

- One of the parameters of MIASE
- Collection and classification of kinetic simulation algorithms used in Systems Biology

# KiSAO – Characteristics

- model characteristic
  - type of variable used
    - discrete variable
    - continuous variable
  - spatial resolution characteristic
    - spatial description
    - non-spatial description
- numerical kinetic characteristic
  - systems behaviour
    - deterministic behaviour
    - stochastic behaviour
  - time steps used
    - fixed timestep
    - adaptive timestep

# KiSAO – Characteristics

- Algorithms are classified according to the different characteristics
- Covered algorithms are, for example, Gillespie variations, StochSim, Euler methods, Runge-Kutta, Tau-Leaping, Cellular Automata
- Additional information provided for each algorithm:
  - KiSAO ID
  - Name + Synonyms
  - Definition
  - Reference paper
  - Short description of the algorithm (or publication abstract)

# KiSAO - Implementation

- Implemented in the OBO format using Obo-Edit



[Term] id: KiSAO:0000022

name: **next-subvolume method**

def: "Elf J, Ehrenberg M. Spontaneous [..]" doi:10.1049/sb\.:2004502

comment: The next-subvolume method [NSM] is [...]

exact\_synonym: "Elf algorithm" []

exact\_synonym: "NSM" []

is\_a: KiSAO:0000095 ! sub-volume stochastic reaction-diffusion algorithm


relationship: hasProperty KiSAO:0000004 ! spatial description ...

# KiSAO – Screenshot


The screenshot displays the OBO-Edit interface for the kisao.obo ontology. The main window shows a class hierarchy under 'Classes'. The selected class is 'Ordinary Differential Equation Solver for Stiff or Non-Stiff Systems', which is highlighted in blue. This class has several 'is\_a' relationships and 'hasProperty' relationships. The 'is\_a' relationships include 'Ordinary Differential Equation Solver for Stiff or Non-Stiff Systems', 'LSODIS', 'Livermore solver for ordinary differential equations, implicit', 'Livermore solver for ordinary differential equations with automatic method switching and root finding', 'Livermore solver for ordinary differential equations for stiff systems', 'Livermore solver for ordinary differential equations', 'Deterministic behaviour', 'Stochastic behaviour', and 'Type of timesteps used'. The 'hasProperty' relationships include 'Parallel Code Value ODE solver', 'Partial differential equation method', 'Runge-Kutta based method', 'Bortz-Kalos-Liebowitz method', 'Gillespie derived stochastic simulation method', 'Multi-state agent-based simulation method', 'Smoluchowski equation based method', 'StochSim nearest-neighbour algorithm', 'Code Value ODE solver', 'Deterministic cellular automata update algorithm', 'Euler backward method', 'Euler forward method', and 'Livermore solver'. The right-hand panel shows the 'Search & Filter' section with 'Parent Plugin' selected. Below this, there are 'Term filter' and 'Advanced Options' sections. The 'Term filter' section is empty. The 'Advanced Options' section has radio buttons for 'Ignore obsoletes', 'Search all' (selected), and 'Search children of selection'. Below this, the 'ID' is 'KISAO:0000089', the 'Namespace' is 'kisao', and the 'Name' is 'Ordinary Differential Equation Solver for Stiff or Non-Stiff Systems'. The 'Definition' section is active, showing the text: 'Petzold LR, Hindmarsh, AC. LSODAR: Livermore solver of ordinary differential equations with automatic method switching and root finding, Computing and Mathematics Research Division, 1-316 Lawrence Livermore National Laboratory (1987)'. The bottom-left corner of the interface shows a legend for 'Relations' (a plus sign in a square) and 'Obsolete' (a square with a diagonal line).


# KiSAO – Screenshot (Additional Information)

Search & Filter Parent Plugin

Term filter  Advanced Options

Term filter

 Search

 Filter

Ignore obsoletes  Search all  Search children of selection  Search ontology of selection

ID KiSAO:0000029

Namespace **kisao**

Name Gillespie's direct method

Definition \* Comment \* Cross Products

Definition

Gillespie DT. Exact stochastic simulation of coupled chemical reactions. Journal of Physical Chemistry, Vol. 81, No. 25. (1977), pp. 2340-2361.

Dbxrefs

dk:100CT2007

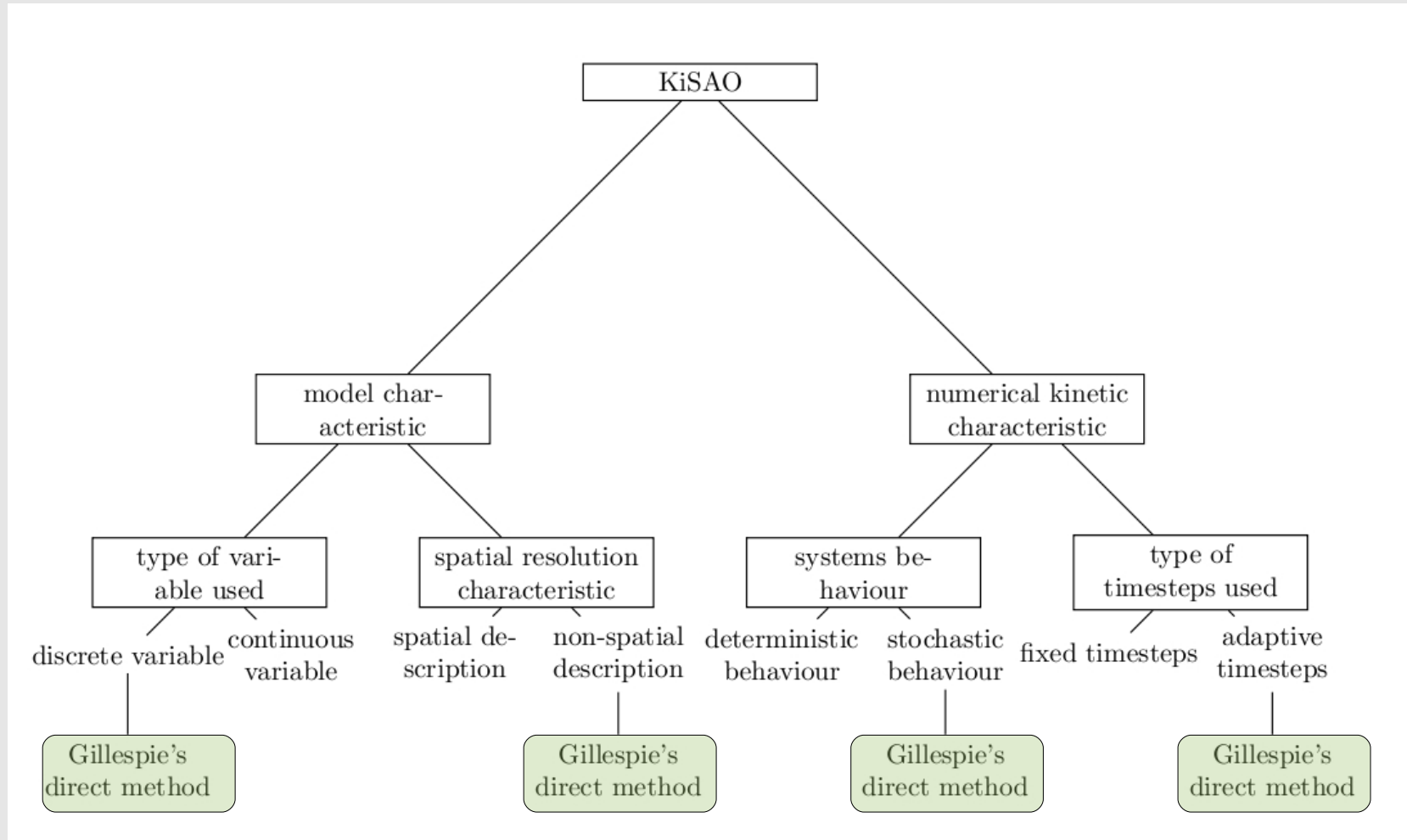
Edit

Dbxrefs Synonyms \* Categories

DM	Synonym text
SSA	SSA
stochastic simulation algorithm	Synonym scope
	Exact Synonym
	Synonym type
	<no synonym category>
	DbXrefs
	Edit

Add Del

# KiSAO – Sample Classification: Gillespie's direct method



# KiSAO – State of the Art

- KiSAO V0.1.0 published as a first draft (December 2007)

## Online Ressources:

- <http://sourceforge.net/projects/miase>
- <http://www.ebi.ac.uk/compneur-srv/miase>

## What can you do?

- check classification of algorithms you know/work with/implemented in your tool, add knowledge ...
- [lenov@ebi.ac.uk](mailto:lenov@ebi.ac.uk)
- [dagmar@ebi.ac.uk](mailto:dagmar@ebi.ac.uk)