Representing Natural Kinds by Spatial Inclusion and Containment

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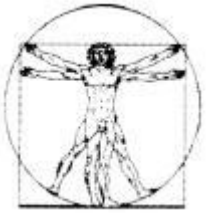
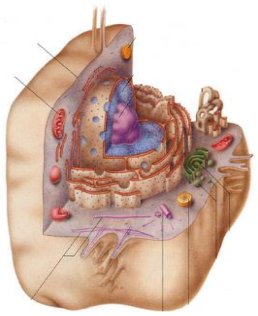
Ontologies of Biological Structure

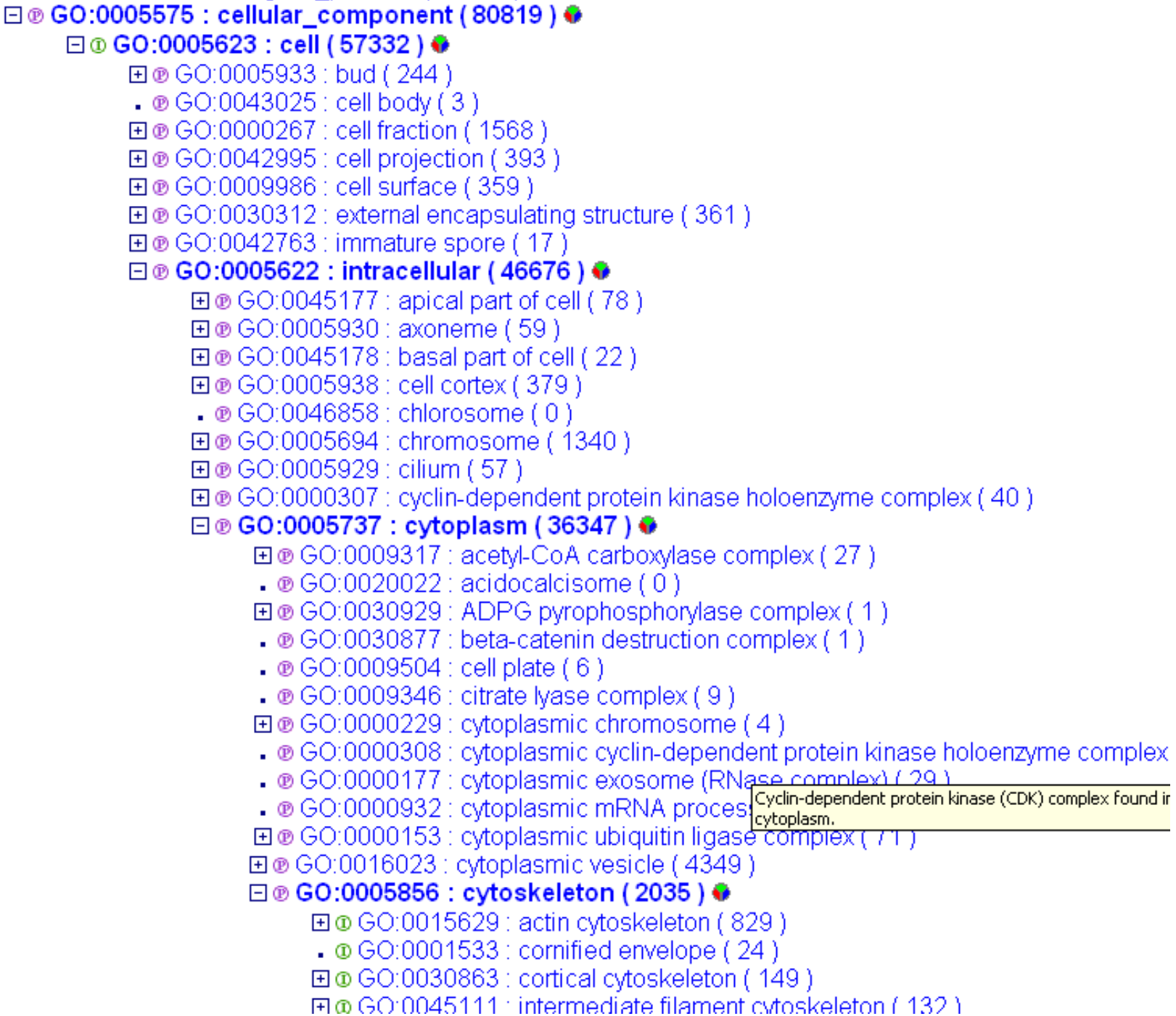
- Representation of Physical Parts of Organisms
- Large terminological repositories in biology exist and grow ...
  - Foundational Model of Anatomy: Human
    sig.biostr.washington.edu/projects/fm/



  - Open Biological Ontologies (OBO): Mouse, Fly, Fish, Worm, Fungi, …
    obo.sourceforge.net

  - Gene Ontology (GO) cellular component: Species independent
    www.geneontology.org/




GO:0005575 : cellular_component (80819)
GO:0005623 : cell (57332)
GO:0005933 : bud (244)
GO:0043025 : cell body (3)
GO:0000267 : cell fraction (1568)
GO:0042995 : cell projection (393)
GO:0009986 : cell surface (359)
GO:0030312 : external encapsulating structure (361)
GO:0042763 : immature spore (17)
GO:0005622 : intracellular (46676)
GO:0045177 : apical part of cell (78)
GO:0005930 : axoneme (59)
GO:0045178 : basal part of cell (22)
GO:0005938 : cell cortex (379)
GO:0046858 : chlorosome (0)
GO:0005694 : chromosome (1340)
GO:0005929 : cilium (57)
GO:0000307 : cyclin-dependent protein kinase holoenzyme complex (40)
GO:0005737 : cytoplasm (36347)
GO:0009317 : acetyl-CoA carboxylase complex (27)
GO:0020022 : acidocalcisome (0)
GO:0030929 : ADPG pyrophosphorylase complex (1)
GO:0030877 : beta-catenin destruction complex (1)
GO:0009504 : cell plate (6)
GO:0009346 : citrate lyase complex (9)
GO:0000229 : cytoplasmic chromosome (4)
GO:0000308 : cytoplasmic cyclin-dependent protein kinase holoenzyme complex
GO:0000177 : cytoplasmic exosome (RNase complex) (29)
GO:0000932 : cytoplasmic mRNA proces
Cyclin-dependent protein kinase (CDK) complex found ir
cytoplasm.
GO:0000153 : cytoplasmic ubiquitin ligase complex (71)
GO:0016023 : cytoplasmic vesicle (4349)
GO:0005856 : cytoskeleton (2035)
GO:0015629 : actin cytoskeleton (829)
GO:0001533 : cornified envelope (24)
GO:0030863 : cortical cytoskeleton (149)
GO:0045111 : intermediate filament cytoskeleton (132)

Canonic Representation of Mereotopological Structure

- *rel* ($Class_1$,$Class_2$) , *e.g.*

  part-of (*CellNucleus, Cell*)

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- Open questions:
  - What is the meaning of mereotopological relations in Biology
  - Class level reading of mereotopological relations, how to interpret ?

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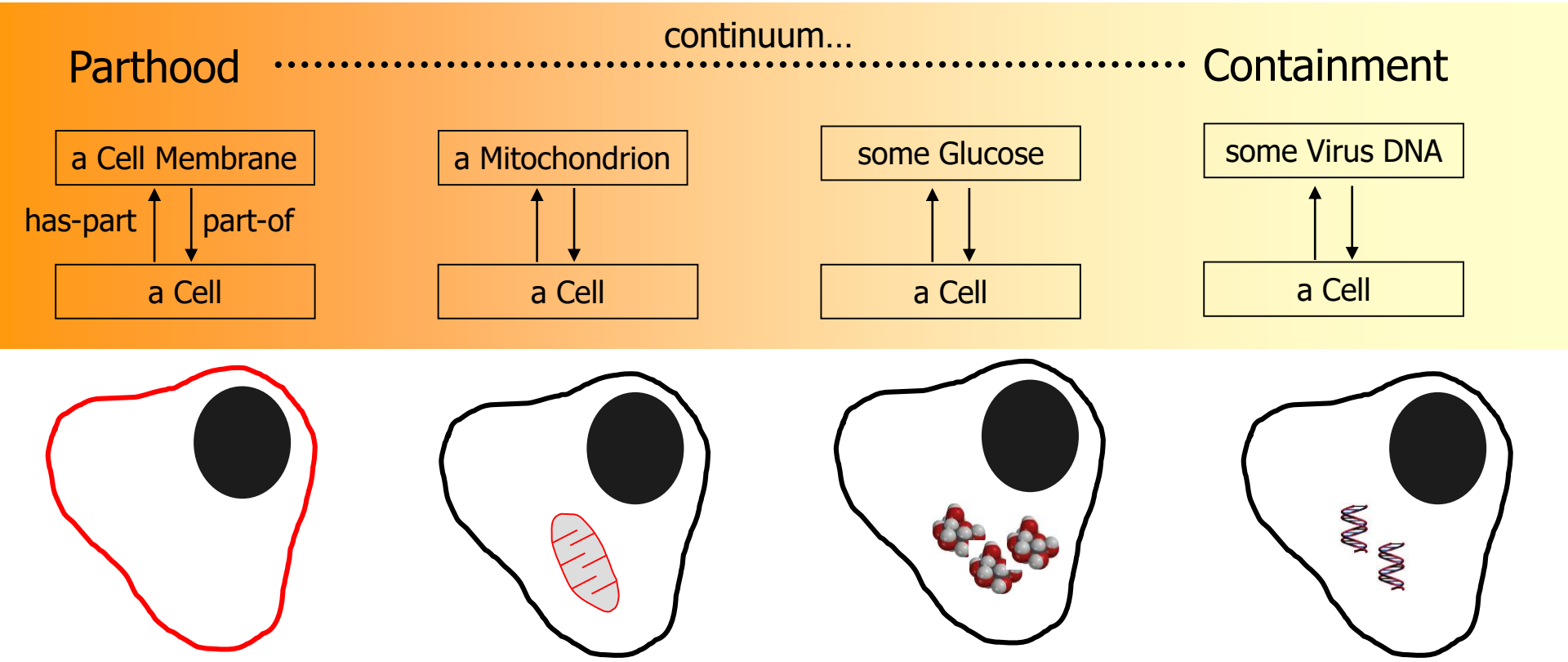
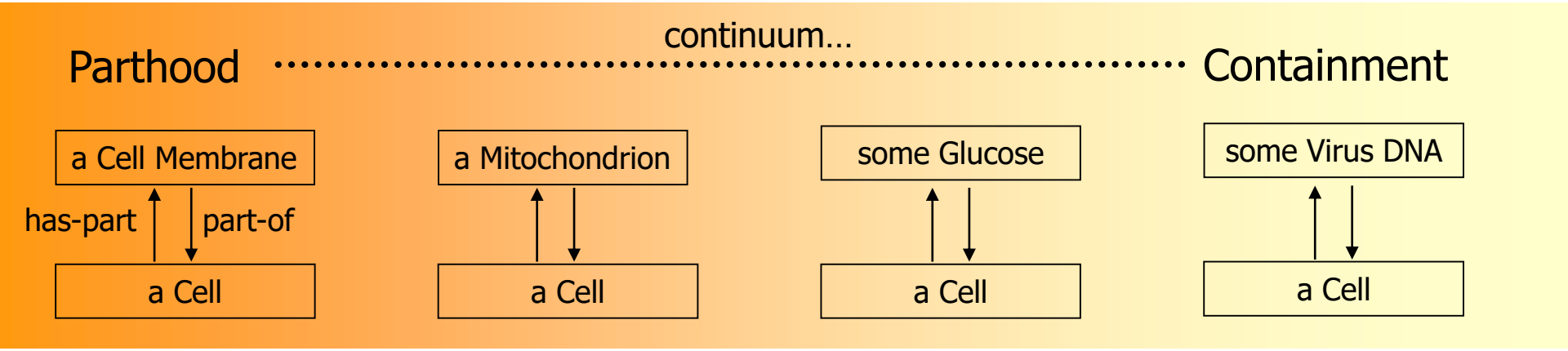
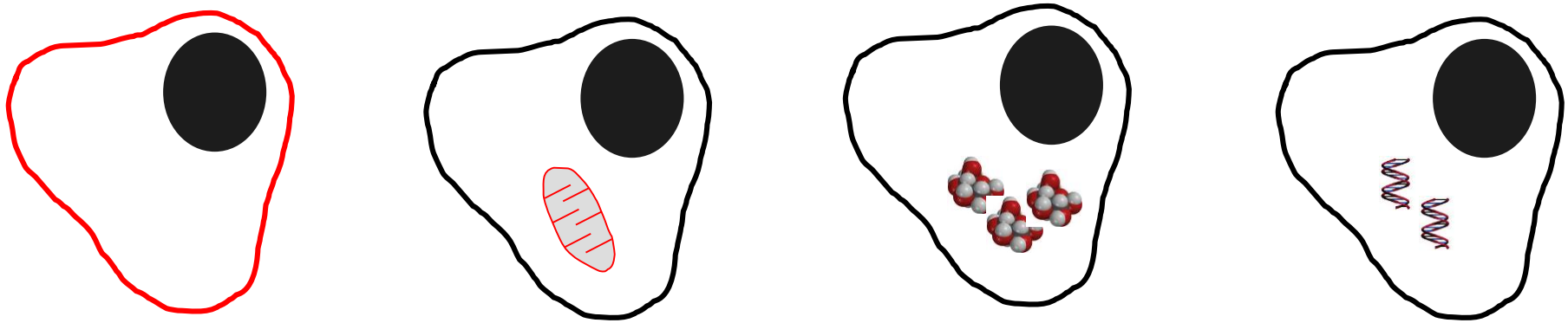
Fuzziness of Mereotopological Relations in Biology



Fuzziness of Mereotopological Relations in Biology





includes / containee-of

has-part / part-of

location-of / has-location

Canonic Representation of Mereotopological Structure

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  part-of (CellNucleus, Cell)
- Open questions:
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Class level reading of mereotopological relations

$R(C_1, C_2)$ expression, e.g. $Includes(Cell, CellNucleus)$

Alternative, conflicting interpretations:

- expresses ontological dependencies
  - "*each* cell includes a cell nucleus" and / or
  - "*each* cell nucleus is included in a cell"
- permits possible relations
  - "a cell *may* include a cell nucleus"
- reject any assertion not sanctioned by a *R(C1 ,C2)* expression:
  - "there is a cell nucleus which included in a protein molecule"

Instance and Class level reading of mereotopological relations (I)

Instance level:

containee-of, *includes:* transitive, reflexive, antisymmetric

$containee\text{-}of(x,y) \leftrightarrow includes(y,x)$

Class level:

- class A is a **specific containee** of class B:

$$SC(A,B) =_{def} \forall x: instance\text{-}of(x, A) \rightarrow \exists y: instance\text{-}of(y, B) \wedge containee\text{-}of(y,x)$$

- class B is a **specific includer** of class A:

$$SI(B,A) =_{def} \forall y: instance\text{-}of(y, B) \rightarrow \exists x: instance\text{-}of(x, A) \wedge includes(y,x)$$

Instance and Class level reading of mereotopological relations (II)

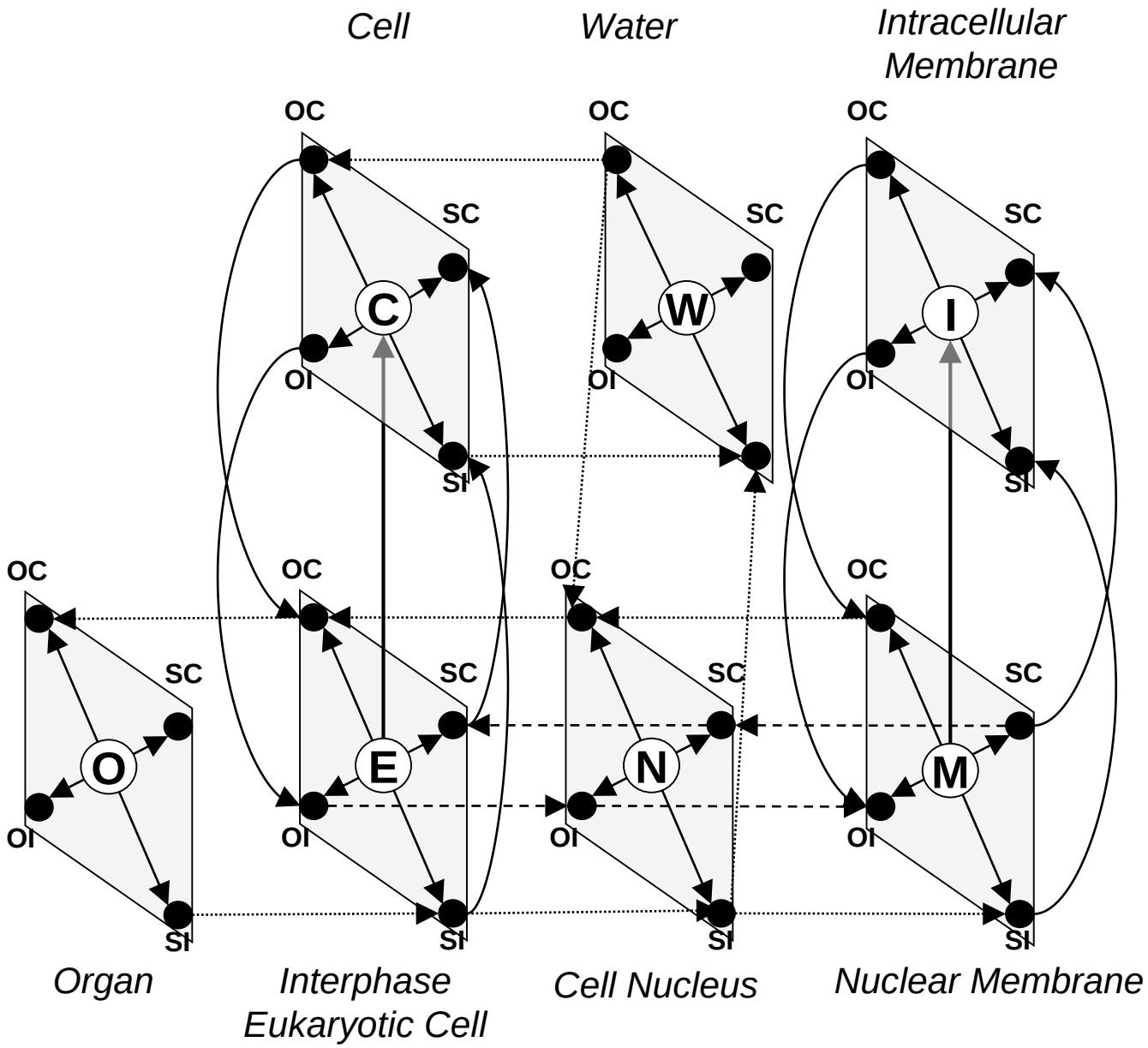
- $SC(A,B)$ is not the inverse of $SI(B,A)$
- class A is an **obligatory containee** of class B
  $OC(A,B) \leftrightarrow_{def} SI(B,A)$
- class B is an **obligatory includer** of class A
  $OI(B,A) \leftrightarrow_{def} SC(A,B)$
- SC, SI, OC, OI: transitive, reflexive, antisymmetric
- SC and SI propagate via $Is\text{-}A$:
  if A is a specific containee (includer) of B, every subclass of A is a specific containee (includer) of B, too
- OC and OI do not propagate via $Is\text{-}A$:
  if A is an obligatory containee (includer) of B, not any subclass of A is an obligatory containee (includer) of B

Arg2 / Arg1	Cell	Neuron	Axon	Cell Membrane	Organ	Cell Nucleus	Heart	Water	Blood	Insulin	Electron
Cell		**Is-A^{-1}**	**OI**	**SI** **OI**	**OC**	**OI**	**OC**	**SI**	**OC**		**SI**
Neuron	**Is-A**		**OI**	**SI**		**SI**		**SI**			**SI**
Axon	**SC**	**SC**						**SI**			**SI**
Cell Membrane	**SC** **OC**	**OC**			**OC**		**OC**		**OC**		**SI**
Organ	**SI**			**SI**		**SI**	**Is-A^{-1}**	**SI**	**SI**	**SI**	**SI**
Cell Nucleus	**SC**	**OC**			**OC**		**OC**	**SI**	**OC**		**SI**
Heart	**SI**			**SI**	**IS-A**	**SI**		**SI**	**SI**	**SI**	**SI**
Water	**OC**	**OC**	**OC**		**OC**	**OC**	**OC**		**OC**		**SI**
Blood	**SI**			**SI**	**OC**	**SI**	**OC**	**SI**		**SI**	**SI**
Insulin					**OC**		**OC**		**OC**		**SI**
Electron	**OC**	**OC**	**OC**	**OC**	**OC**	**OC**	**OC**	**OC**	**OC**	**OC**	

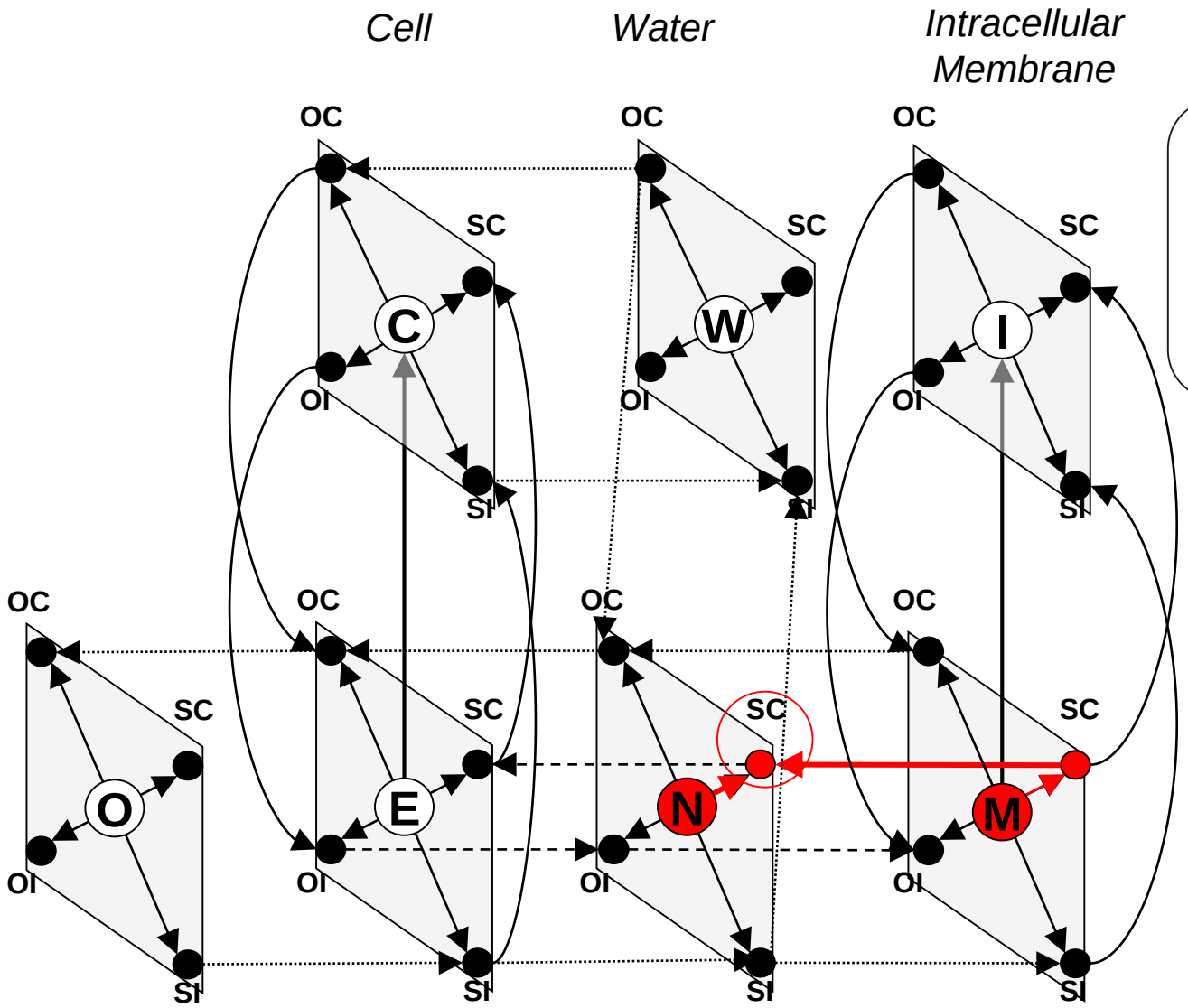
Extended Taxonomies

- Express mereotopological hierarchies as taxonomies
- Purpose: Better performance in large knowledge bases
- Introduction of reificator nodes:
  real classes:
  $Is\text{-}A(A,B_{SC}) =_{def} SC(A,B)$
  $Is\text{-}A(A,B_{SI}) =_{def} SI(A,B)$
  "pseudo classes" (do not capture properties of all instances !):
  $Is\text{-}A(A,B_{OC}) =_{def} OC(A,B)$
  $Is\text{-}A(A,B_{OI}) =_{def} OI(A,B)$
  A must be terminal nodes

Extended Taxonomies

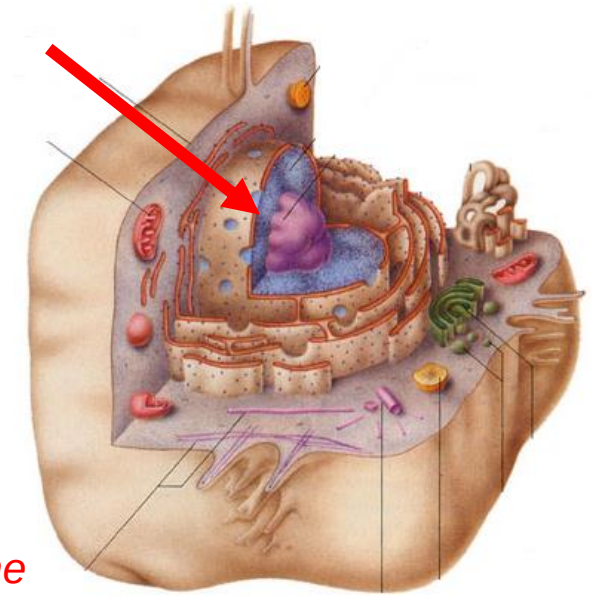


Extended Taxonomies



Specific Containees of Cell Nucleus

Cell Nucleus
Nuclear Membrane



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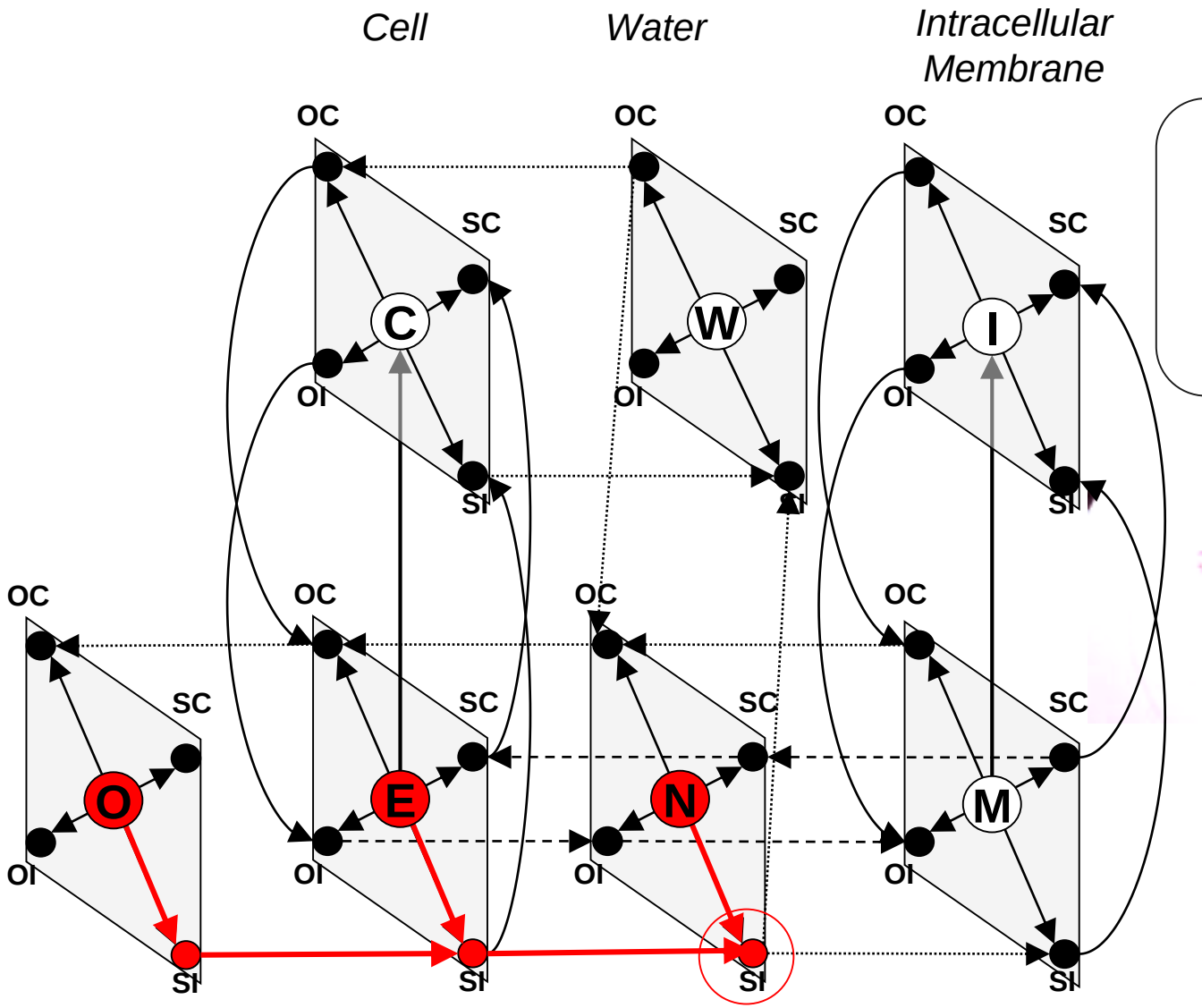
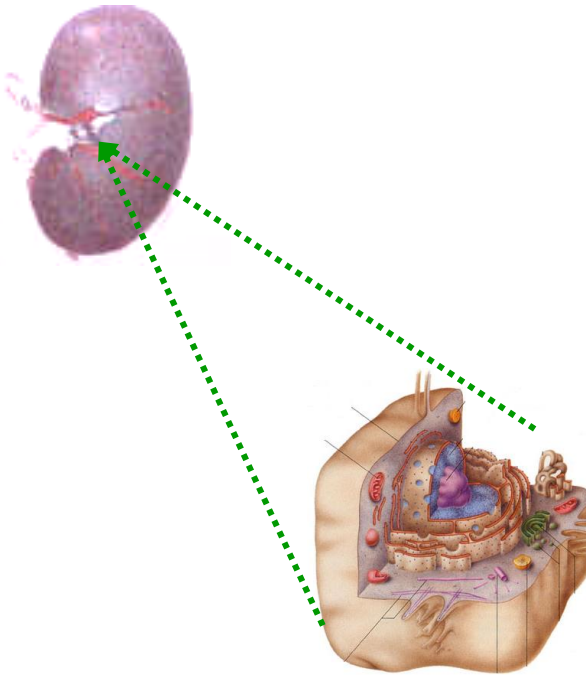
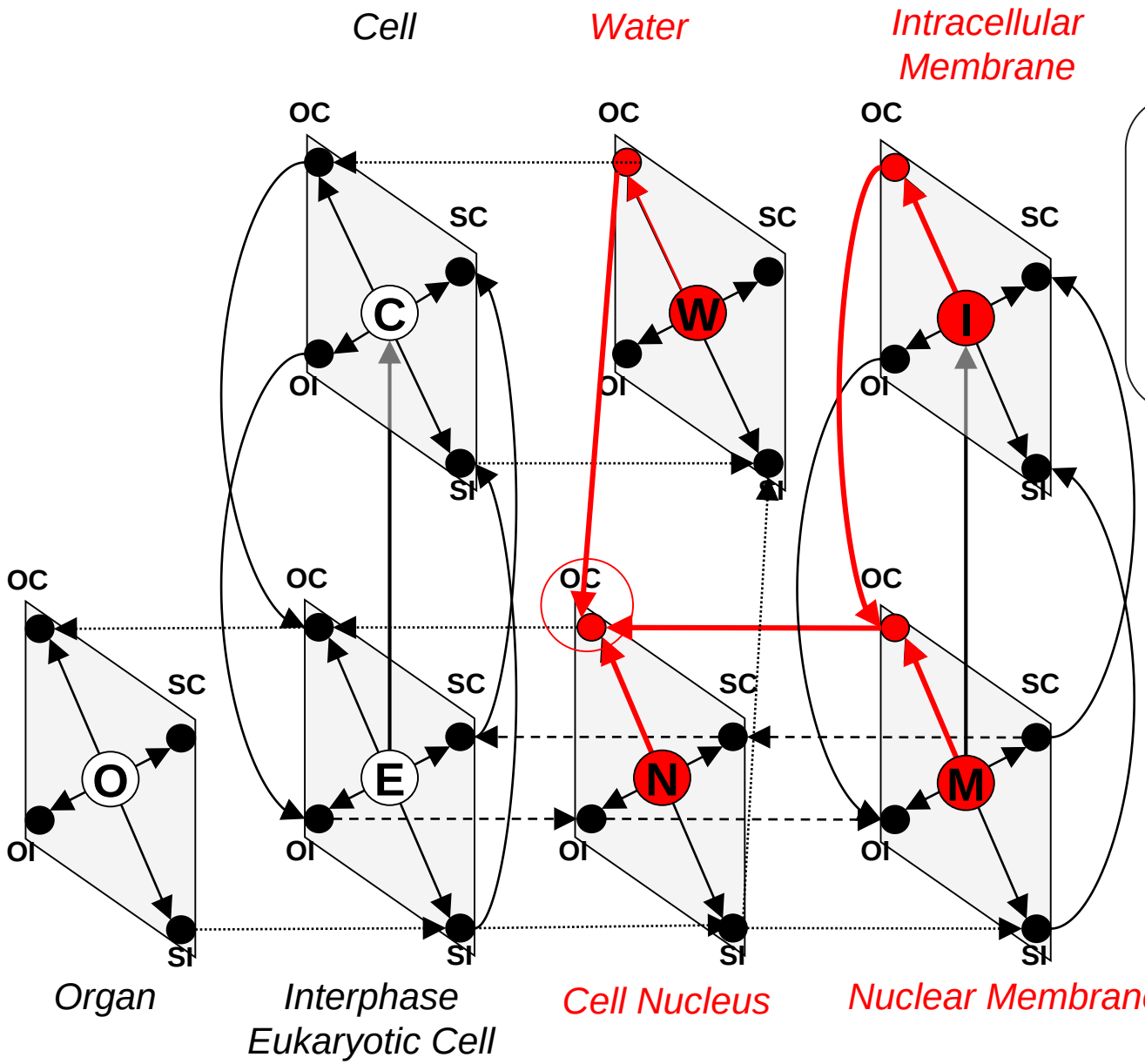


Specific Includers of Cell Nucleus

Interphase Eukaryotic Cell, Tissue, Organ, Blood, Organism (...)

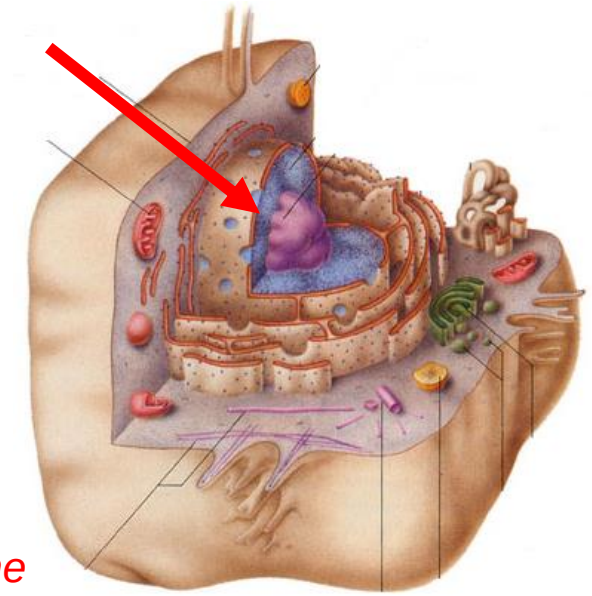


Extended Taxonomies



Obligatory Containees of Cell Nucleus

Cell Nucleus
Nuclear Membrane
Intracellular Membrane
Water



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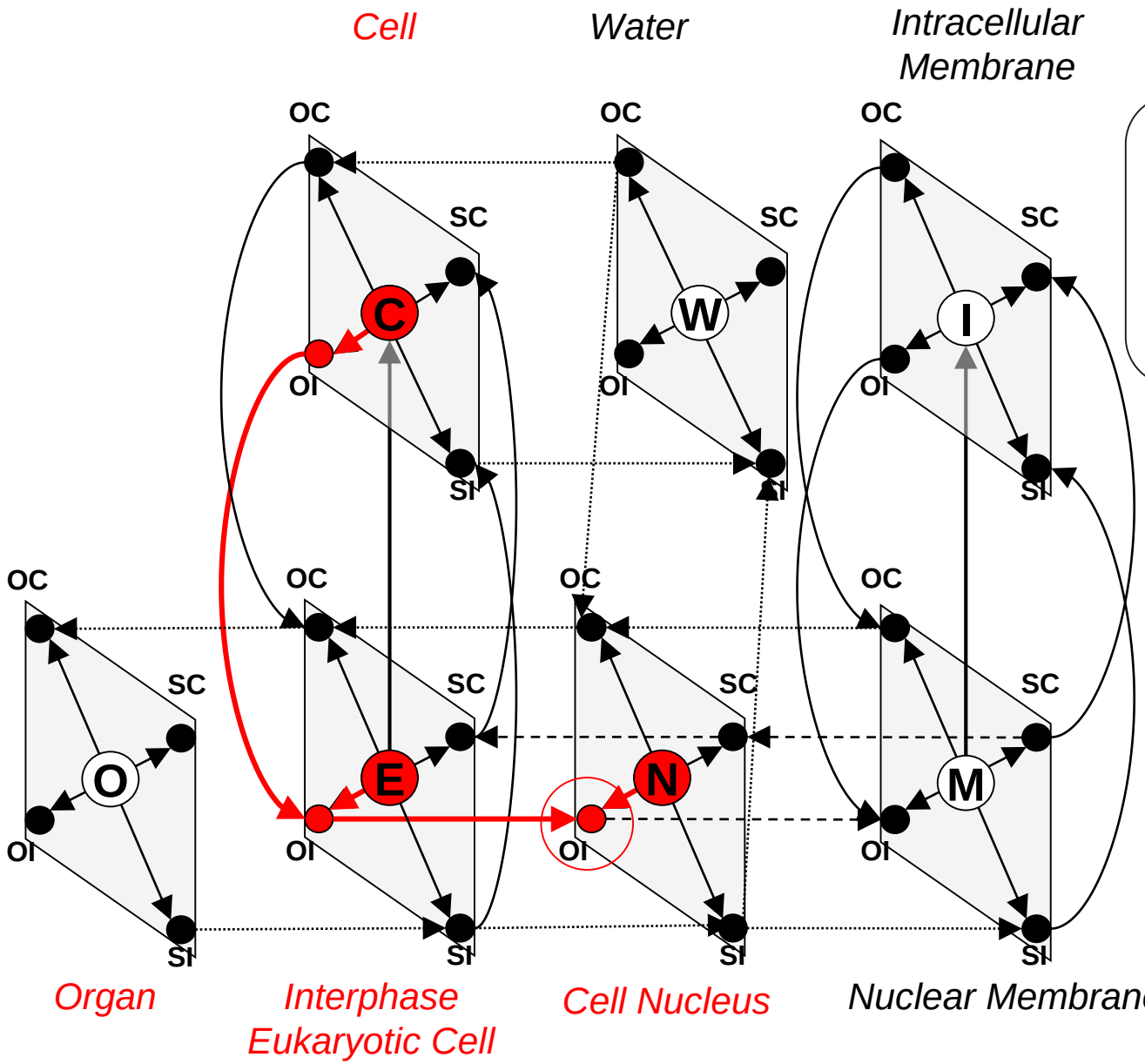
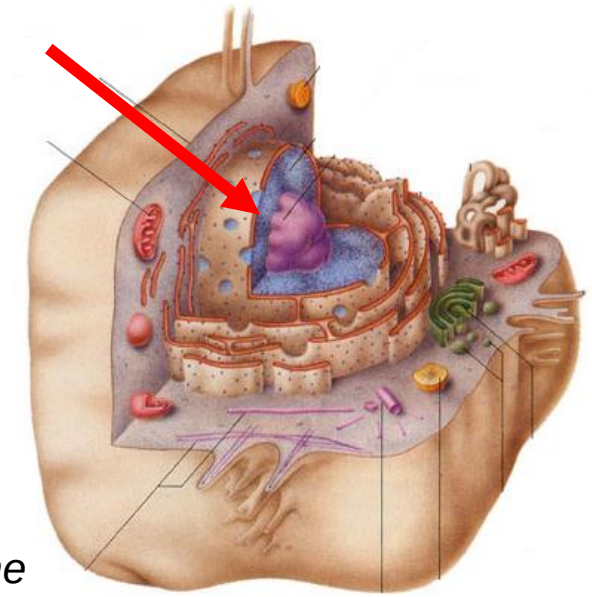


Obligatory Includers of Cell Nucleus

Interphase Eukaryotic Cell, Cell



Conclusion

- Capturing mereotopological basics in biomedical ontologies: Two recommendations:
  - Create consensus by conflating part-whole and locative relations to one base relation (containee-of / includes)
  - Eliminate ambiguity by explicitly introducing class level relations with a precise semantics
- Using extended taxonomies: Improve reasoning in large knowledge bases
- To do: express other mereotopological relations (overlap, disconnectedness) in terms of class-level predicates

www.imbi.uni-freiburg.de/medinf