Notes for specification of SBGN

Edinburgh group proposal

Requirements

- Tolerance to diversity of target audience
- Tolerance to incomplete knowledge
- Prevent emergence and dissemination of wrong information (malfunction)
  - Do not make drawer speculate about unknown mechanism or draw more details than known
  - Clear visualisation validated/not validated data
- Represent combinatorial complexity

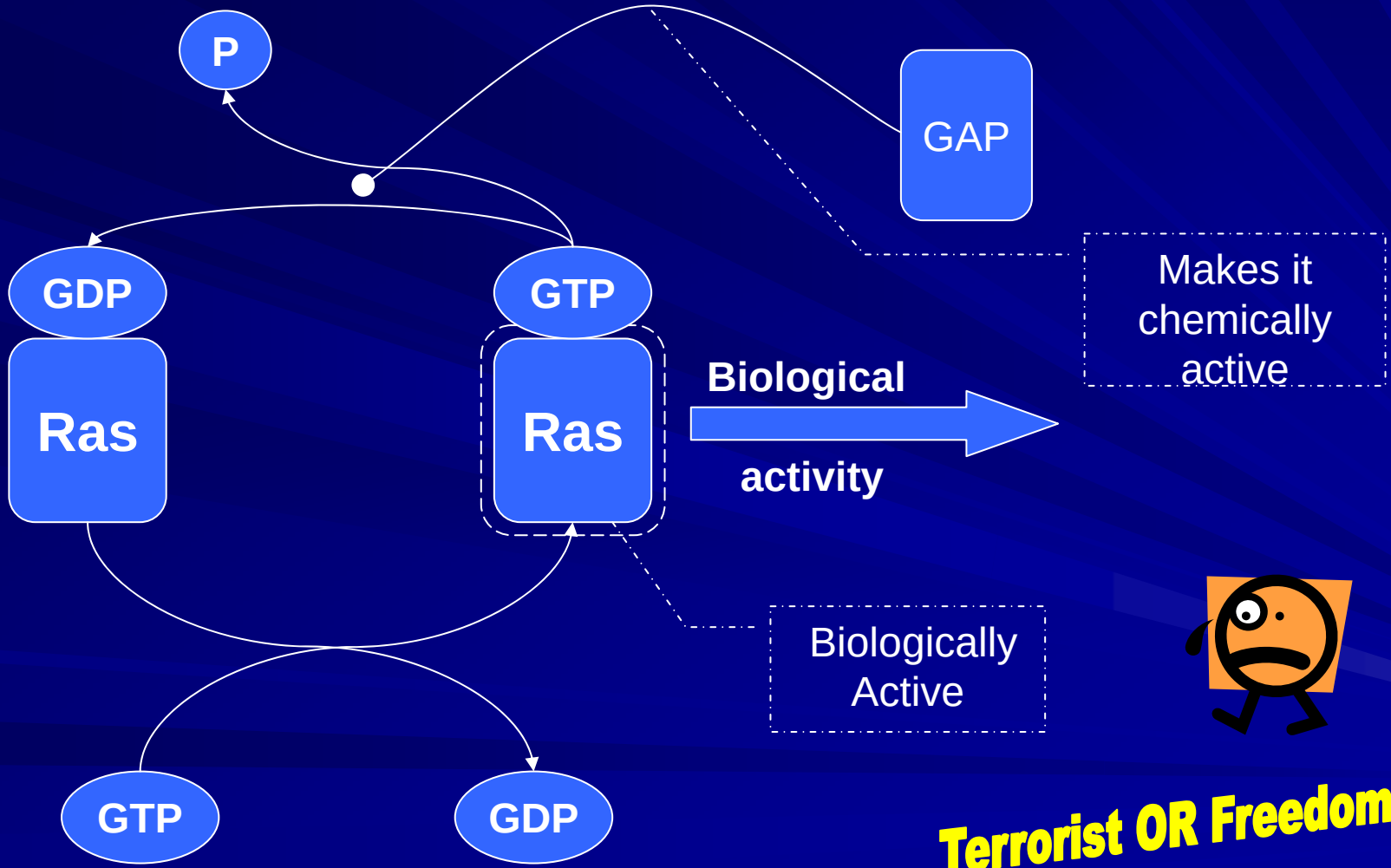
Focal point

- Development of object model for SBGN
- Development of clear set of rules for:
  - reading SBGN
  - mapping ER to PD notations
  - export SBGN to other formats
- Development of validator for SBGN diagrams

Object model

- Should be small, non-redundant
- To emphasise specific role of the element (kinase, receptor, scaffold) could be used stereotypes
- To show that extra information about element (is/is not) available could be used decorators
- Should avoid or highly restrict usage of ambiguous elements

Activation ambiguity



Terrorist OR Freedom fighter

Isoforms/Generics

- At different level of knowledge should be a way to refer from isoform to generic
- Helps to deal with combinatorial problems
- When generic is used it should be way to state:
  - I don’t know which particular form required
  - I know that Specific forms are required
  - I know that Any form is sufficient

Isoforms/Generics

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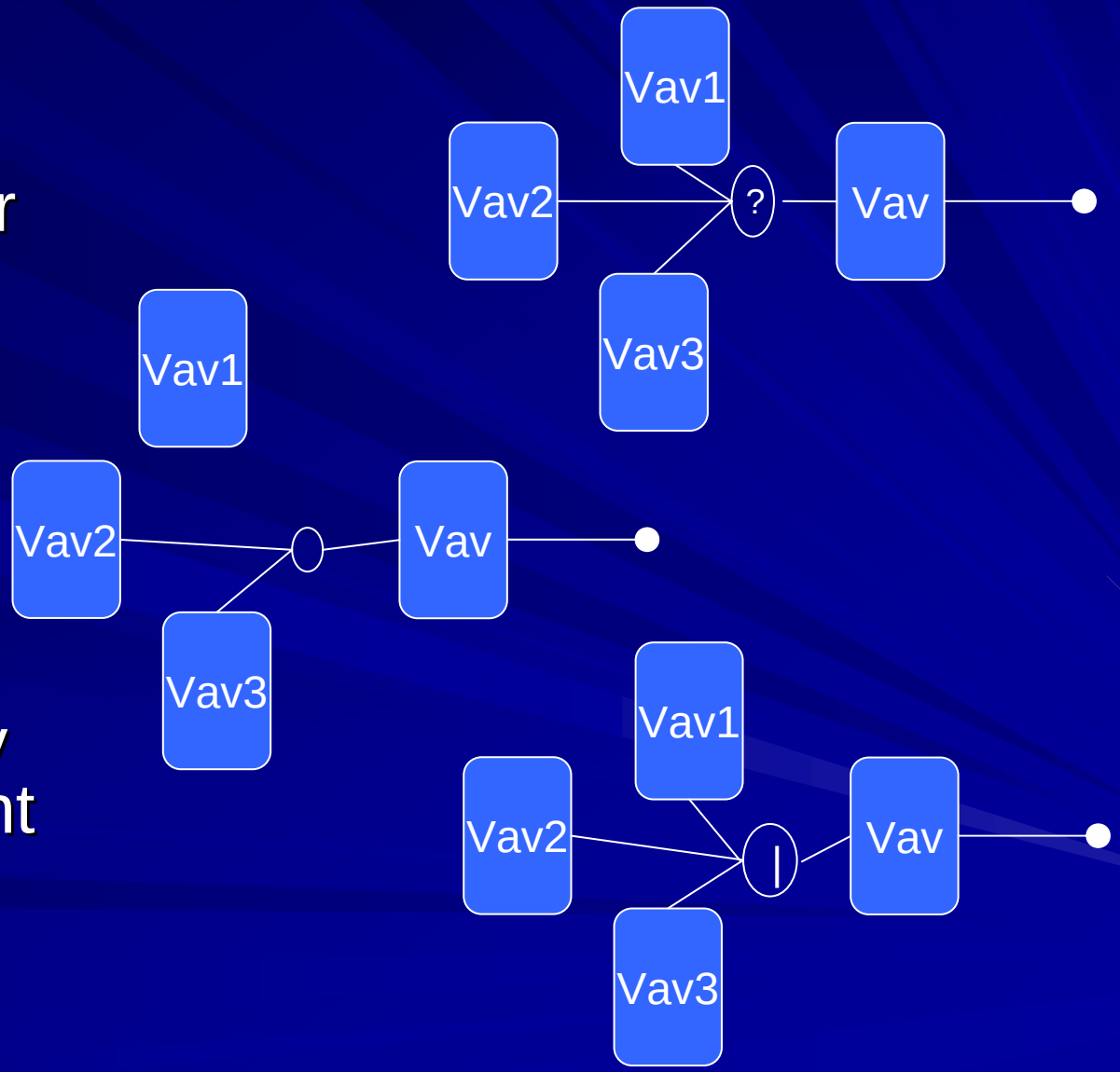
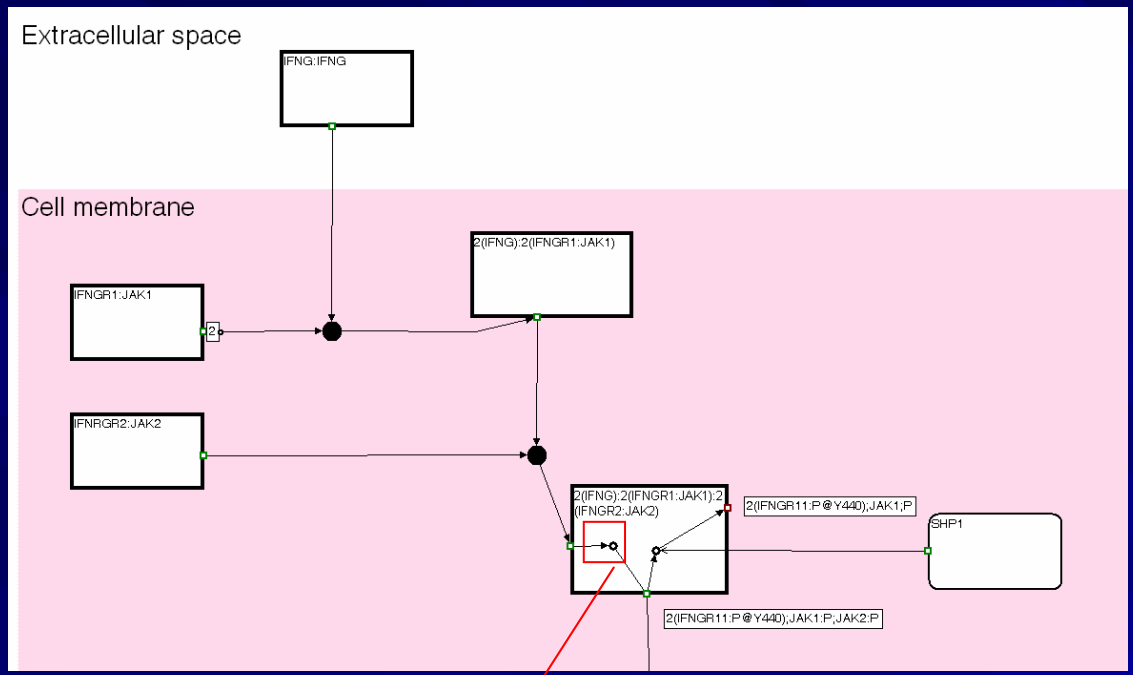
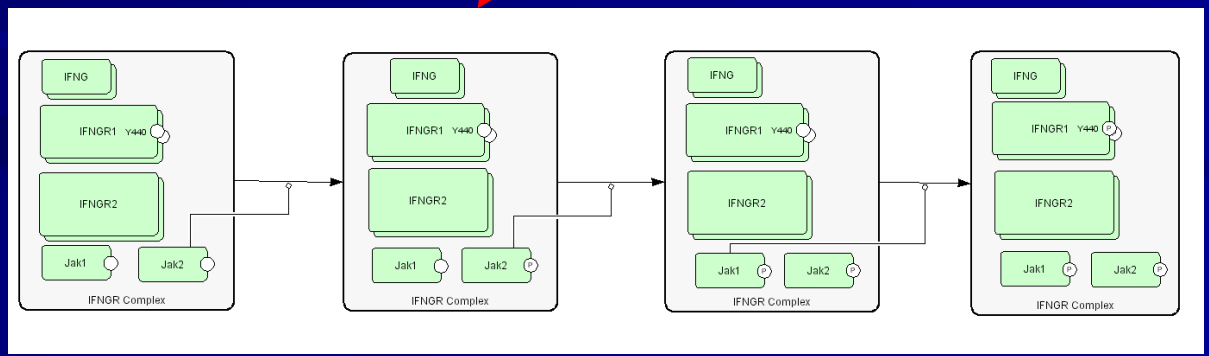


Granular hierarchy





- Different level of detalisation.
- Different level of available knowledge

Granular hierarchy

- To represent
  - global system organisation,
  - subtle biochemical details and mechanisms
  - structural information
- Create set of interlinked diagrams/pictures with different level of detalisation.
- Should be clear visual indication that more detailed information available/not available
- Should be referencing mechanism

Granular hierarchy

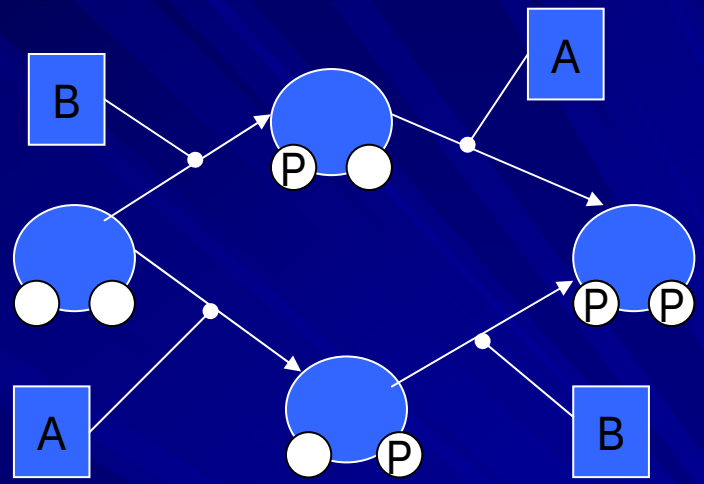
- Modularity
  - Easy to incorporate new data
- Reusability
  - Easy to extend existing models and reuse common pathways
- Decoupling
- Easy verification and update

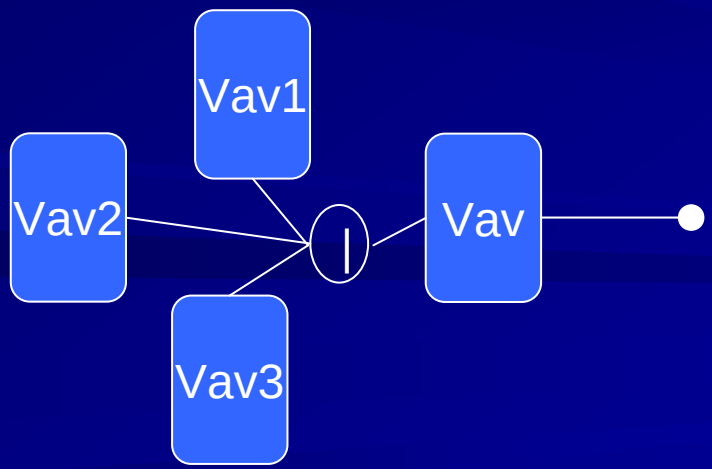
Logical representation

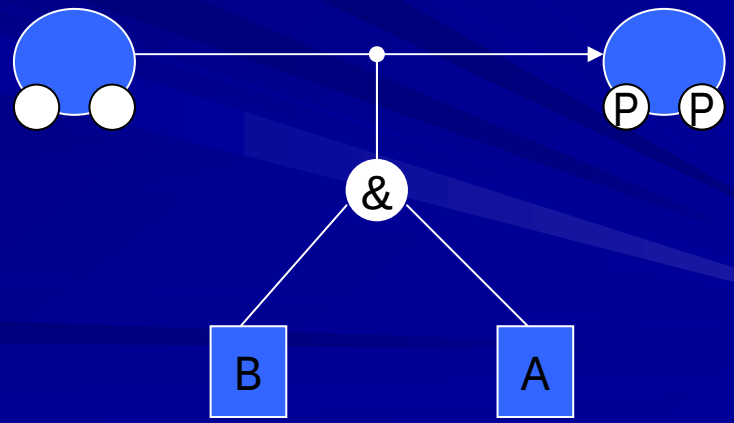
- Clearly indicate absence of detailed mechanism information
- Concise
- Could help with incomplete information
- Could help with combinatorial explosion
- Could help with Generic/Isoform relation resolution

Logical representation

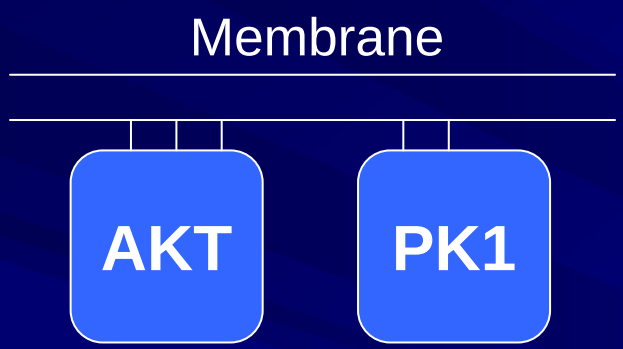
- Representation of unknown information
- Combinatorial complexity
- Generic/specific relation







Noncompartmental localisation



“recruited to” membrane

- Scaffold related translocation
- Could be unknown mechanism
- Could be represented as compartment in SBML but semantically different

Issues

- Connection to existing metabolic reconstructions
- Transcription regulation
- Translation regulation (splicing, iRNA)
- Hierarchy
- Combinatorial explosion
- Isoforms/Generics
- Non-compartmental localisation (recruited by)

Acknowledgments

- CSB
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