



A Multimedia Model For Nanoparticle Fate And Biotic Update In The Environment

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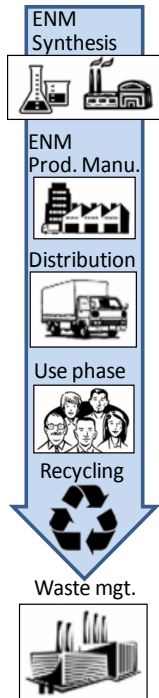
Outline

- Overall aims of NanoFASE
- ENM complexity and environmental fate modelling
- The object-oriented approach
- Conceptualisation
- Nanoparticle forms and states
- Transport and transformations
- Flexibility and futureproofing
- Next steps in NanoFASE

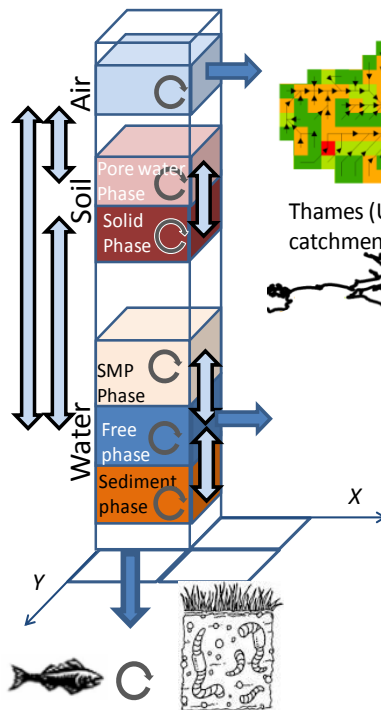
Overall aims of NanoFASE

■ Nanomaterial Fate and Speciation in the Environment

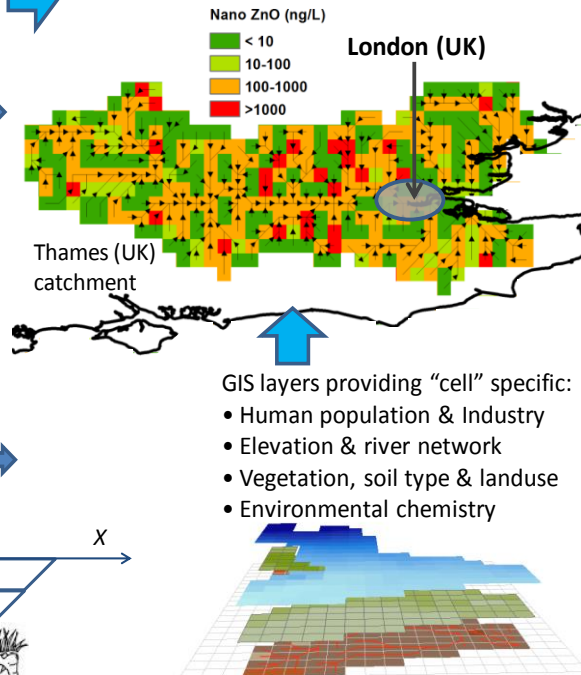
1) ENM enabled
Product value chains
& release pathways



2) Environmental
„cell“
reactors

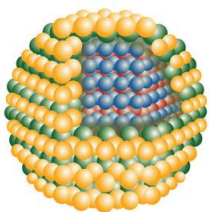


3) Object-oriented multimedia fate models
dynamically connecting “Environmental cells”

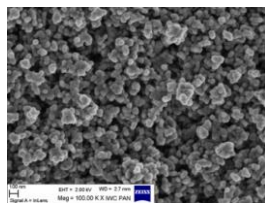


- “Reactors” and relevant ENMs (using the right starting materials at each step)
- Functional fate groups a tool to understand and reduce complexity
- Exposure assessment framework catalogue of models, parameters and methods
- Multimedia fate models – simplified to feed regulatory models (SimpleBox for Nano)

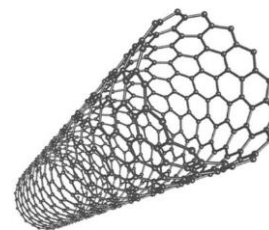
ENM complexity and fate modelling



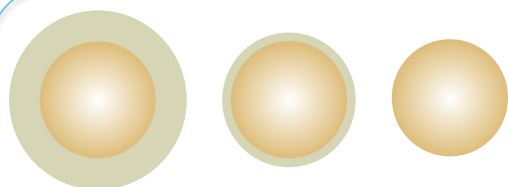
Quantum dots



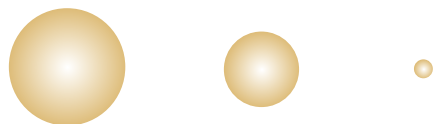
Metal oxides



Carbon nanotubes



Coating loss



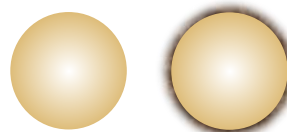
Dissolution



Chemical alteration



Heteroaggregation



Environmental
corona

Form: individual particle composition
(physical & chemical)

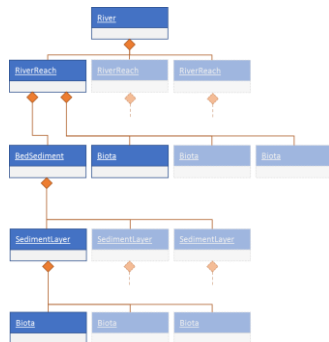
State: of the particle population
e.g. free, homoaggregated,
heteroaggregated

The object-oriented approach

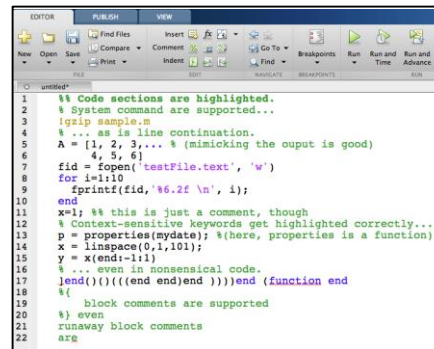
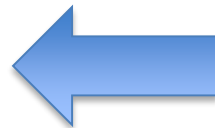
ENVIRONMENT



GEEK
PROGRAMMER



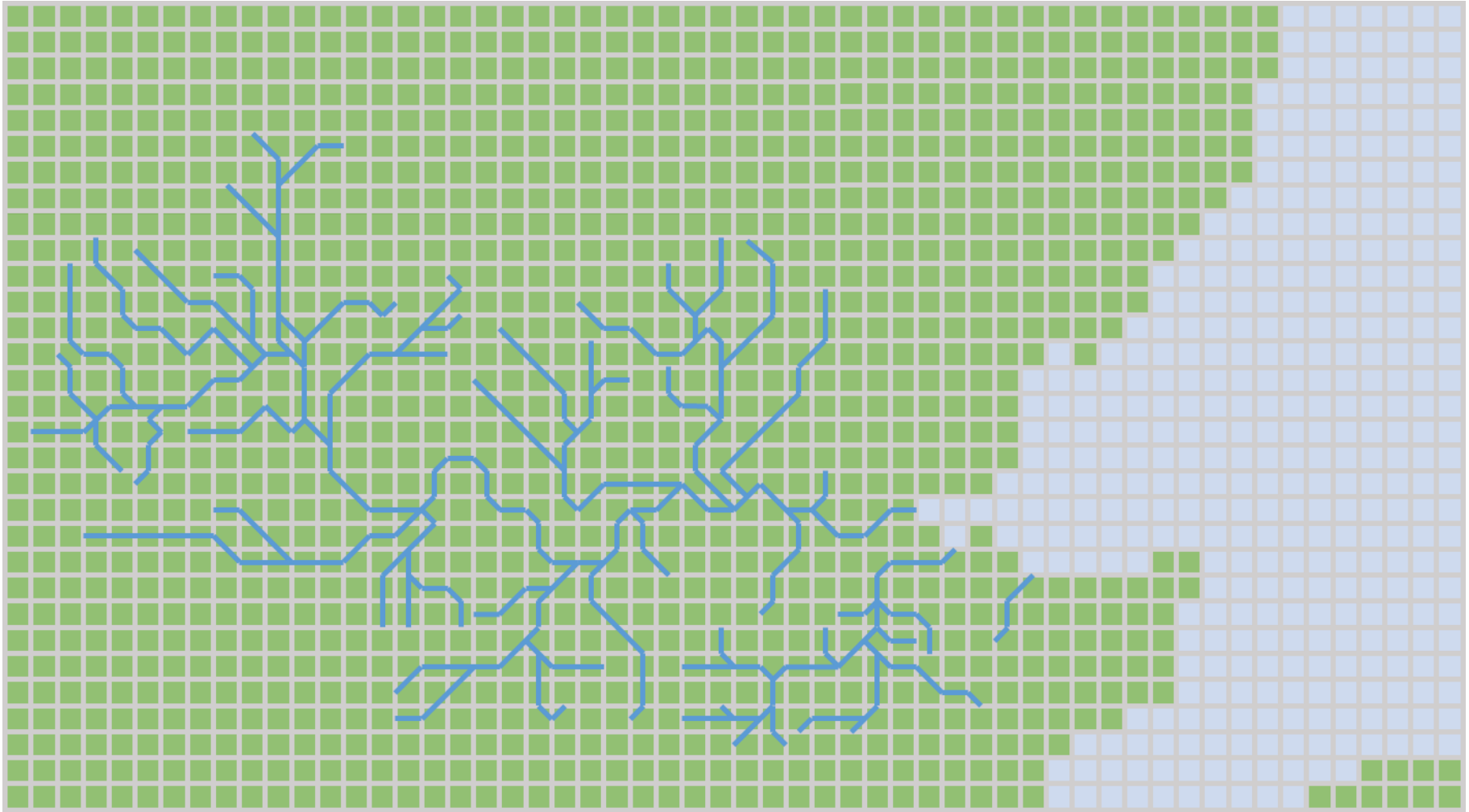
OBJECTS



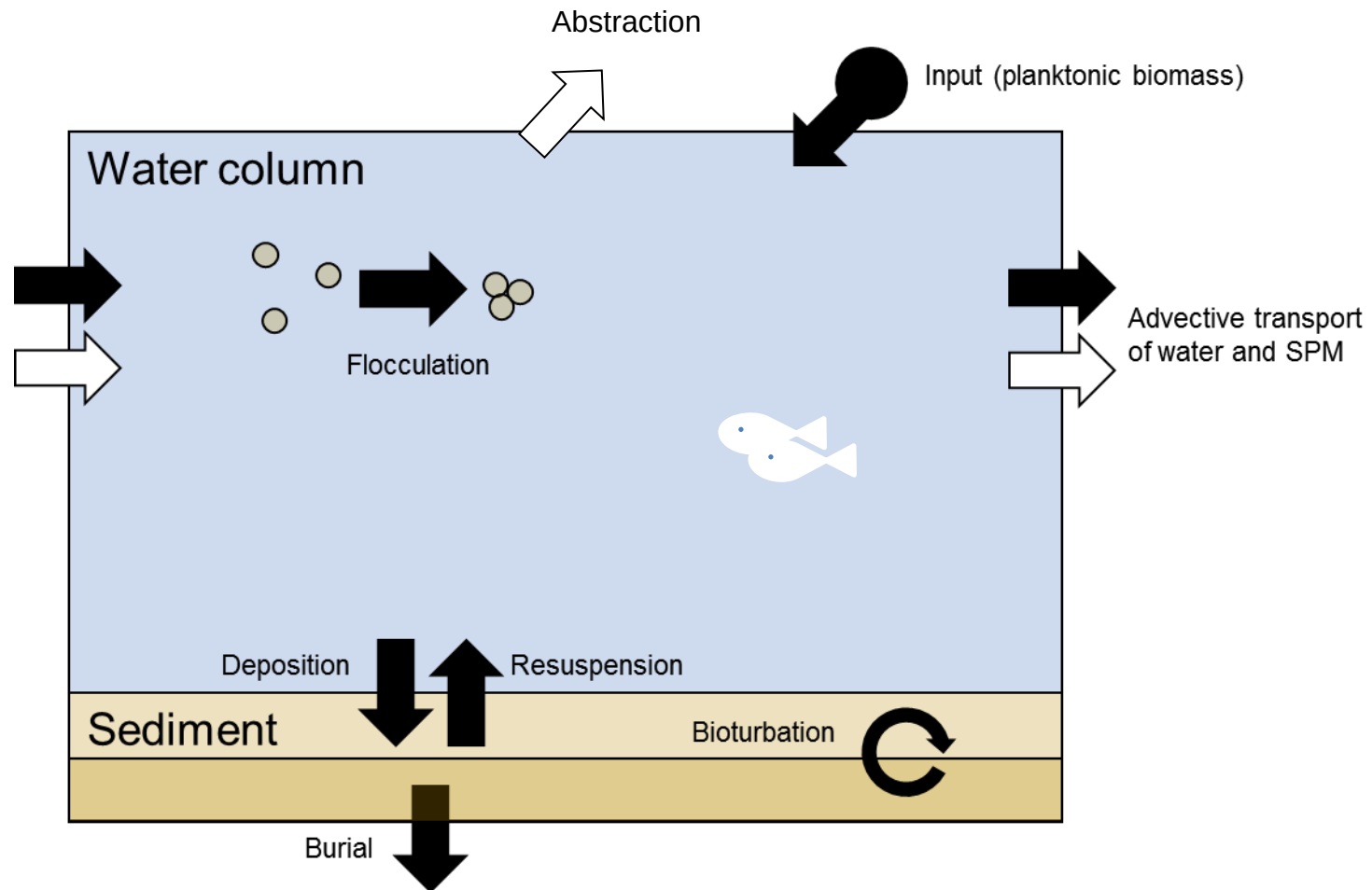
CLASSES



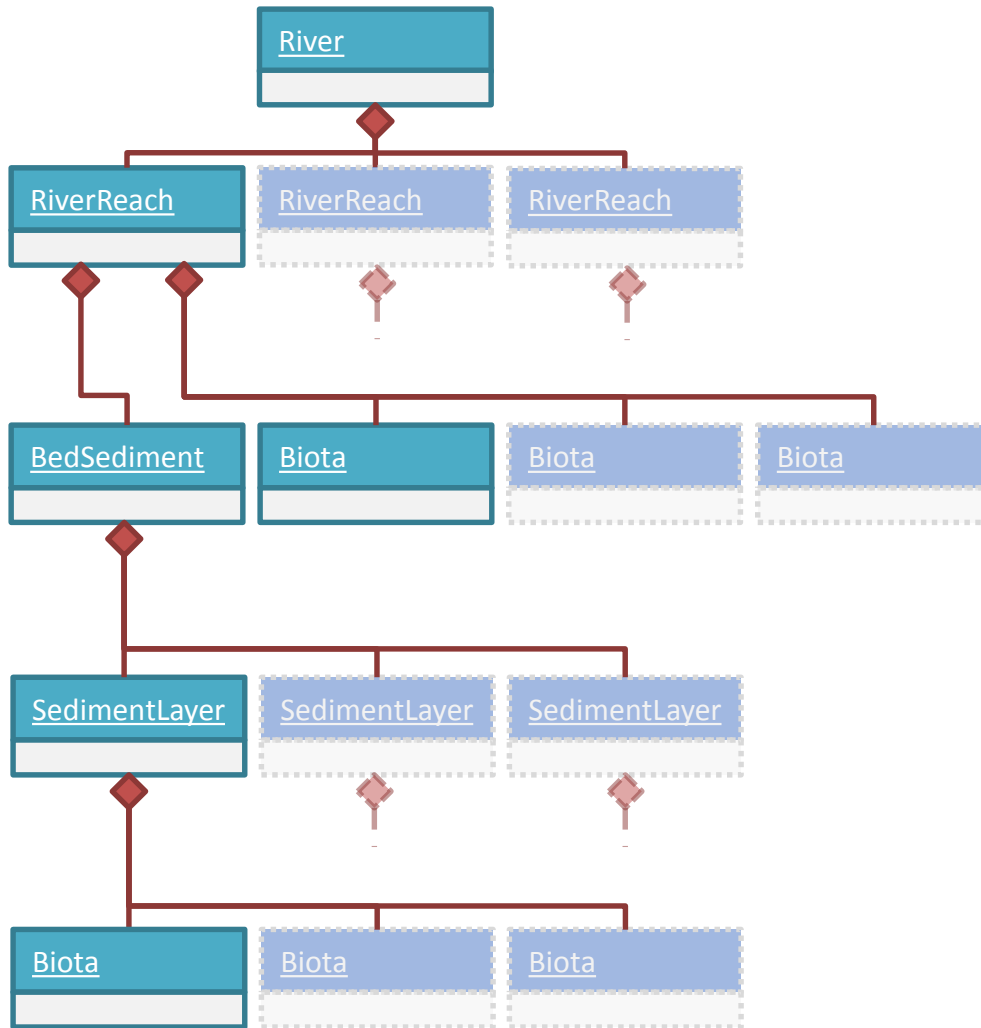
Conceptualisation



Conceptualisation II



Conceptualisation III



 = 'compositional relationship'

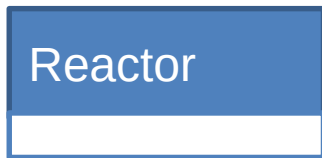
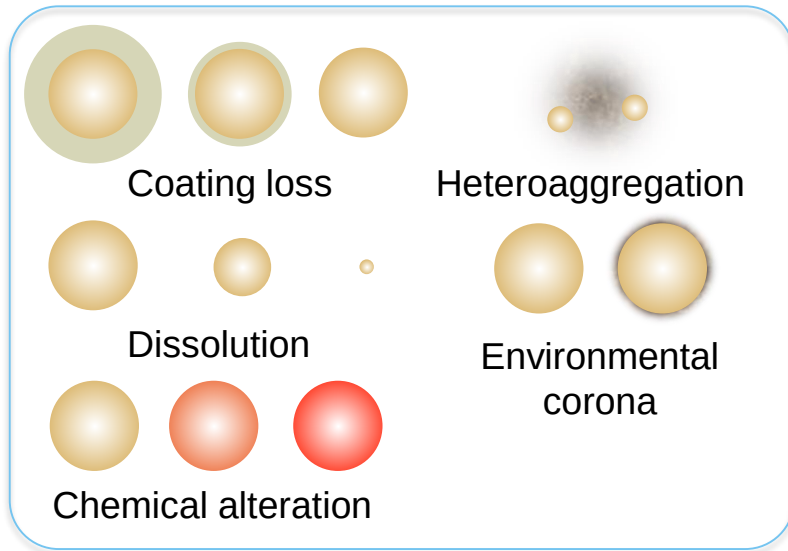
Object is contained within another object.

e.g. river reaches will contain biota

>>>

River object contains one or more Biota objects

Conceptualisation of nanoparticles



Transformations 'wrapped' into
Reactor class

Reactor objects define nanoparticles

EXAMPLE

F1 = free particles

F2 = heteroaggregated

S1 = coated, no corona

S2 = uncoated, no corona

S3 = coated, corona

S4 = uncoated, corona

	S1	S2	S3	S4
F1	C(1,1)	C(2,1)	C(3,1)	C(4,1)
F2	C(1,2)	C(2,2)	C(3,2)	C(4,2)

S1 → S2 : coating lost

S1 → S3 : corona acquired (coating present)

S2 → S3 : corona acquired

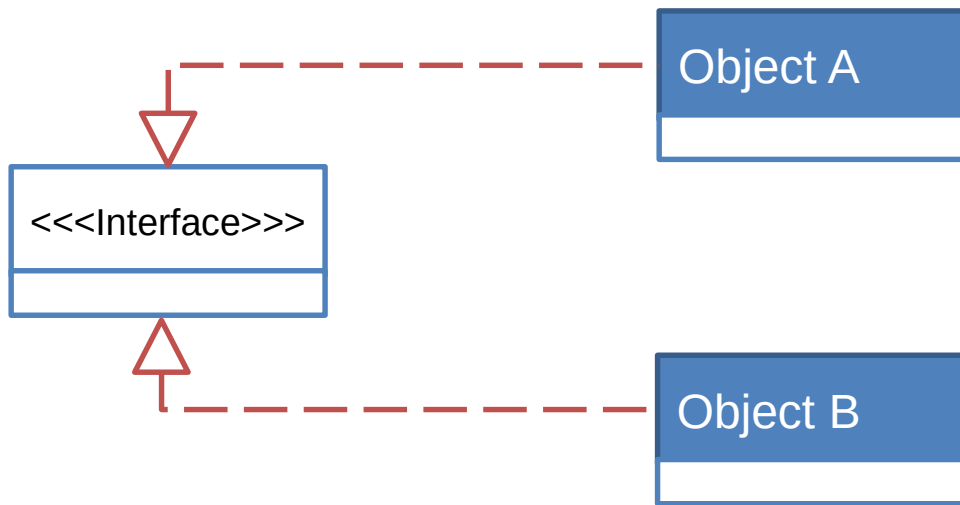
Flexibility and futureproofing

INHERITANCE



SubClass extends BaseClass with new functionality (e.g. extending a Reactor with new transformation types)

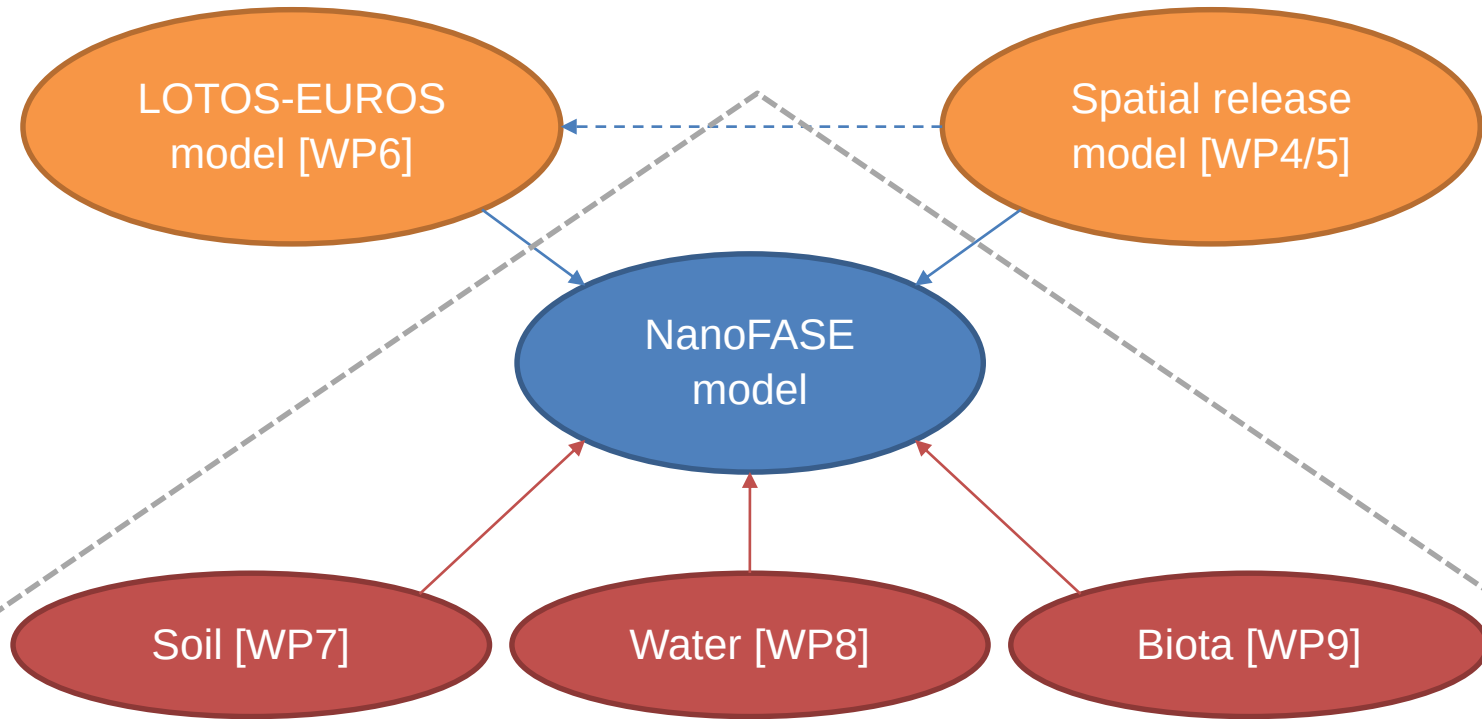
INTERFACING



Interface 'hides' objects – they appear to be the same but are not

e.g. types of waterbody (river, lake) within a grid cell

Interfacing with other models



Next steps in NanoFASE

- Write transport model soil & waters
- ‘Technical’ workpackages: develop & parameterise transformation algorithms
- Integrate algorithms and parameters into transport model (Reactor classes > objects)
- Interfacing of soil-water model with release and atmospheric models



Thank you very much

Any Questions?