

A Multi-Scale Agent-based Distributed Simulation Framework for Groundwater Pollution Management

Susanne I Schmidt

Cristian Piciooreanu

Bart Craenen

Rae Mackay

Jan-Ulrich Kreft

Georgios Theodoropoulos

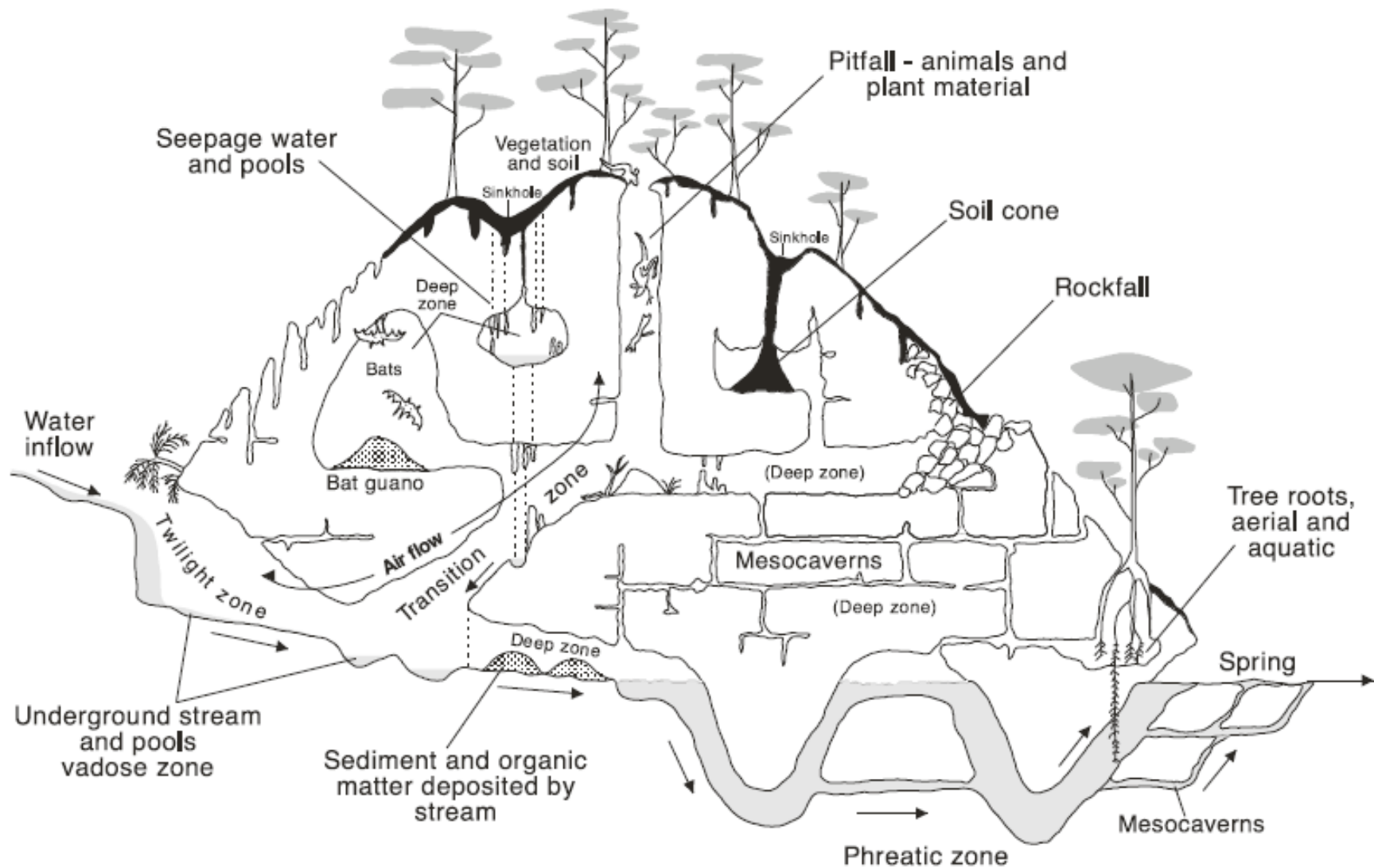


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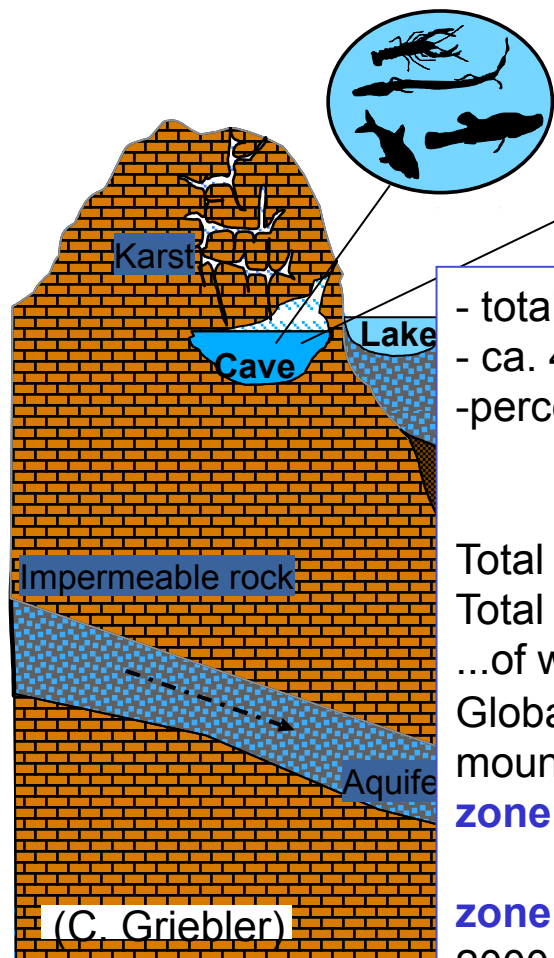
Outline

- Groundwater ecosystem
- Managing groundwater contamination
- A new framework



*Schematic drawing:
W.F. Humphreys*

Ecosystem groundwater



(C. Griebler)

- total groundwater volume takes up 2 % of the total earth water
- ca. 40 % of groundwater is fresh
- percentage of the total liquid earth freshwater: 94 %

	Value	Unit
Total earth water	1,400,000,000	km ³
Total groundwater volume	23,400,000	km ³
...of which fresh	10,530,000	km ³
Global hydrogeological zone 1 , mountainous, 100 m deep	3,600,000	km ³
zone 2 , alluvial, 200 m deep	6,200,000	km ³

zone 3, below zones 1 and 2, reduced water exchange; down to 2000 m of depth; comprising at least three quarters of the total groundwater volume; largely non-renewable; no fauna

The groundwater ecosystem

- like dark matter
- old
- relatively homogeneous
- scarce – water crisis
- porous, i.e. water flows through the pores among sand, silt and gravel
- flow dependent on permeability, affected by pore sizes and connectivities, and the hydraulic gradient
- oligotrophic (offers little to sustain life)
- increasingly threatened by pollution

The groundwater ecosystem

- Groundwater is habitat to a plethora of organisms
 - bacteria
 - archaea
 - fungi
 - unicellular animals (protozoa)
 - multicellular animals such as worms and crustacea (metazoa)
- The ecosystem is characterized by three major constraints:
 - confined spaces
 - limited supplies of electron acceptors, e.g. oxygen, and
 - limited supply of electron donors (mostly carbon/energy sources).
- These limitations lead to low densities as well as low activities of groundwater organisms unless contaminations increase the supply of carbon/energy sources.
- Knowledge about the groundwater animals and microbes is scarce: hardly know who is where let alone what they do and how active they are
 - The microbial community consists mainly of species well-known from other habitats, that are characterized by a flexible metabolism (e.g. long periods of dormancy).
 - The animal species are mainly endemic (only occur in groundwater of a particular region) and are highly adapted to this extreme environment by having a slow metabolism, longevity, low reproduction rate, as well as low mobility rates



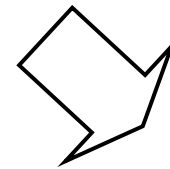
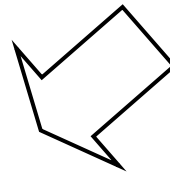
Fauna

animals

highly adapted to environment
(high number of endemics)



Stream fauna
eyes, pigmented



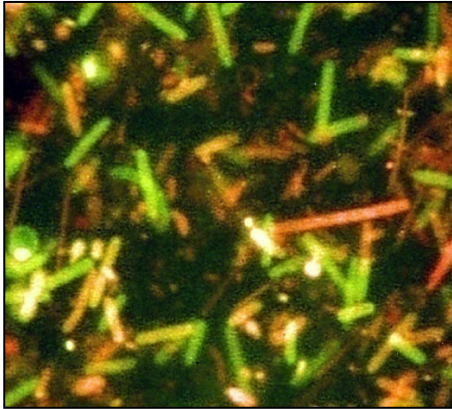
Stygofauna =
groundwater fauna
*blind, no pigments,
often elongate*

**groundwater fauna
displays a different
metabolism**

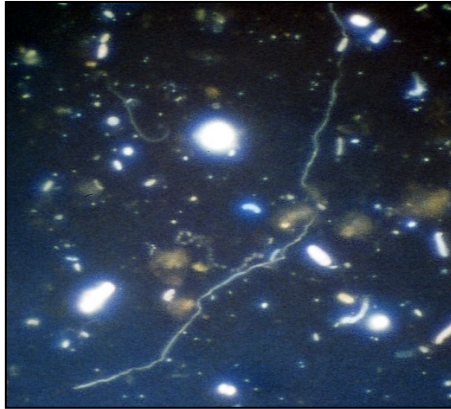


Microbial community

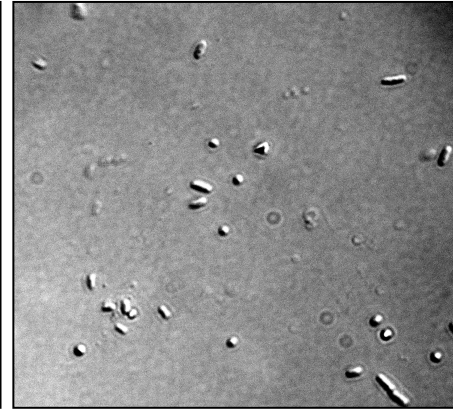
Bacteria – Bacteria abundances and size ranges in comparison



Lake



Organically
contaminated
groundwater aquifer



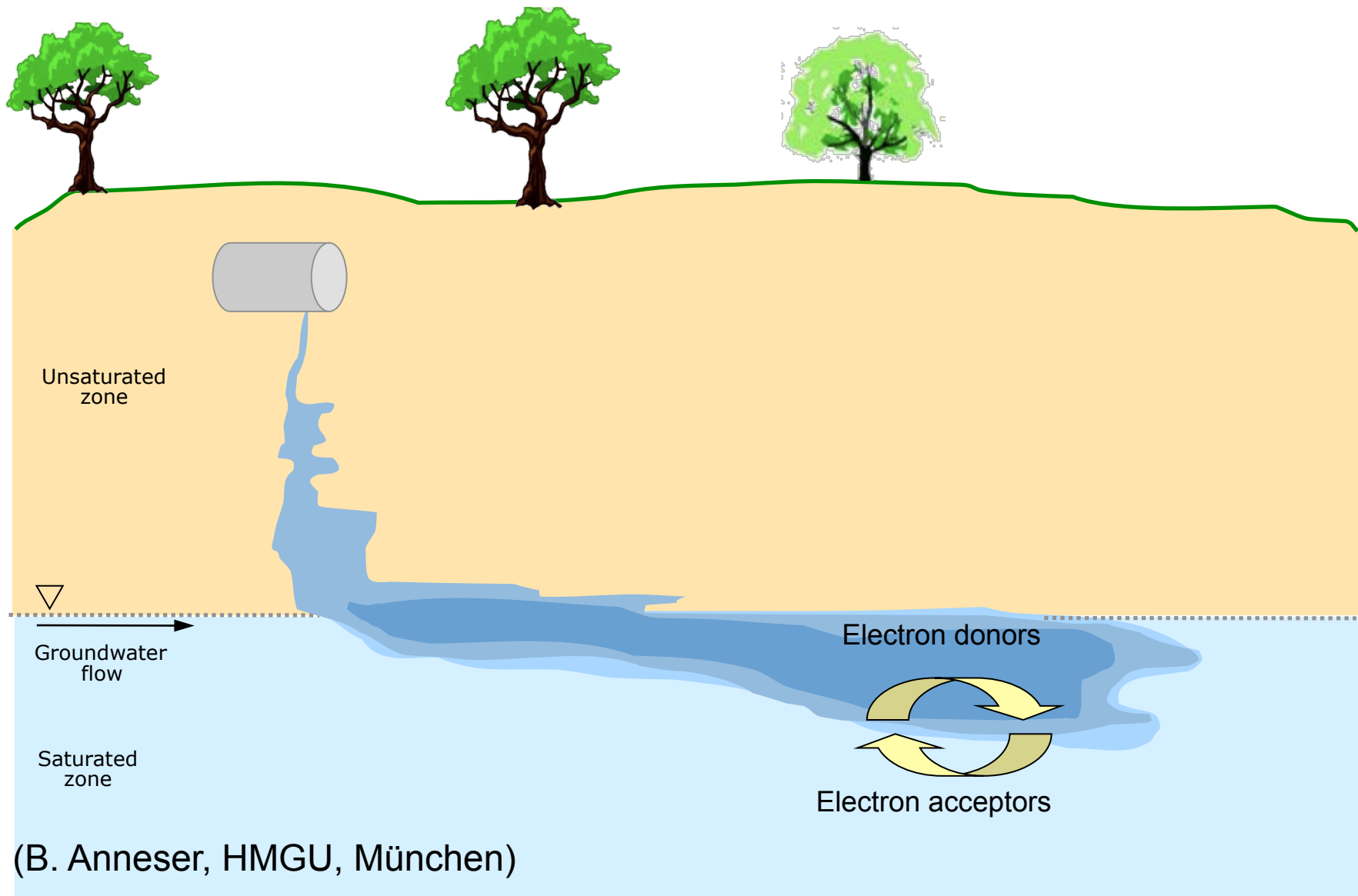
Pristine (=natural)
groundwater aquifer

What do we (think we) know about this community?

- 1-3% of the particle surface is covered with cells
- 10% of the cells live planktonic (*free-swimming*)
- cells in the biofilm are more active than planktonic cells
- composition of sessile cells is more diverse than that of the planktonic cells
- composition of the biofilms dependent on environment

Photos: Christian Griebler und Kathrin Euringer, GSF - Institute for Groundwater Ecology, München

Groundwater contamination



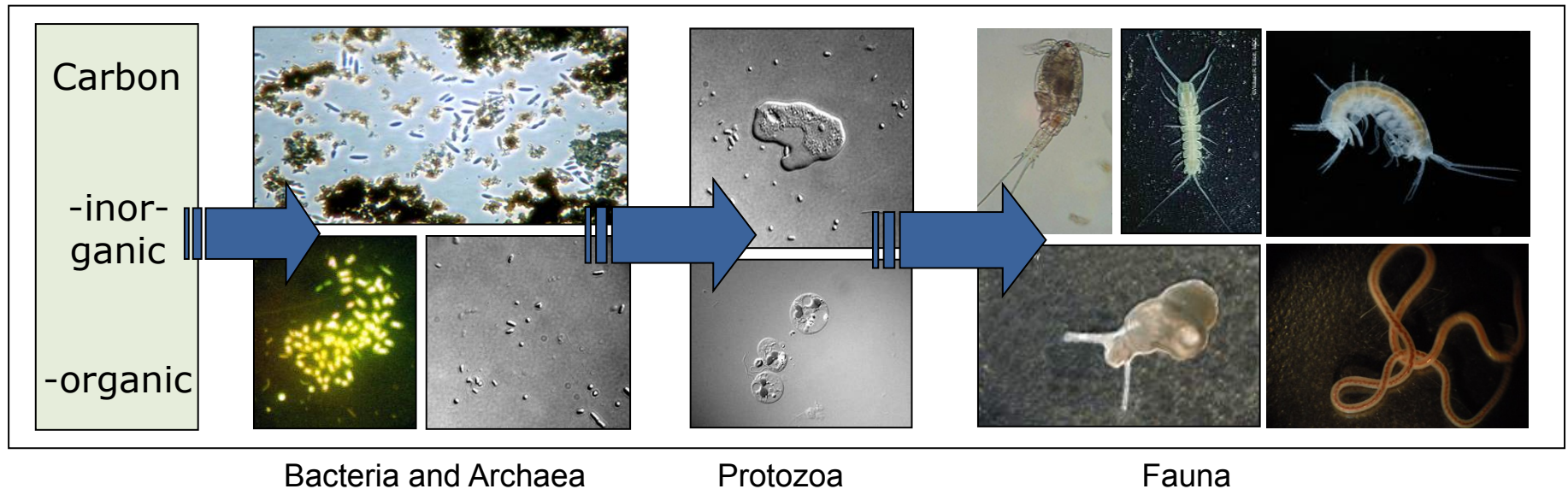
Groundwater contamination

- In 1997, the EC-funded Concerted Action CARACAS identified 750,000 contaminated sites across Europe.
- Can also result in surface water pollution and threaten drinking water production.
- EU Groundwater Directive and the European Water Framework Directive
- Contaminations will only be degraded over very long time spans
- Remediation seeks to speed up the rate of degradation.

Groundwater contamination management

- Remediation techniques include:
 - physical/chemical measures
 - placement of permeable and reactive material, where the reaction leads to less harmful substances
 - thermal remediation technologies use heat to mobilize contaminants so they can be extracted from the ground
 - chemical oxidation is based on injecting aggressive reagents into the contamination to trigger or enhance degradation reactions
 - biological measures (biodegradation): Almost all pollutants can be degraded by some microorganisms at least under some conditions: a very slow process
 - biostimulation: stimulating native microorganisms by adding nutrients, oxygen, or other electron acceptors
 - providing supplementary pre-grown microorganisms to the contaminated site to augment naturally occurring microorganisms (a process called bioaugmentation)
- Using predictive models to evaluate potential bioremediation strategies in order to identify optimal strategies is the basis for future successful groundwater management and remediation strategies.

Biodegradation



Conceptual simplified food web model for groundwater in dependence on carbon

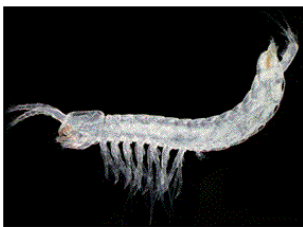
Photos: C. Proctor, R. Wagner, D. Selesi, C. Griebler, K. Euringer

Groundwater contamination management

- Existing groundwater models are mainly mathematical
 - restricted to simulate the transport and degradation of contaminants on the scale of whole contaminated field sites by averaging out the effect of spatial heterogeneity on the availability of the pollutant to the degrading organisms.
 - tend to rely on fitting to data rather than being predictive
 - less suited to incorporate spatial variability and non-linear kinetics and feedbacks.
 - Difficult to validate (time and cost)
- Generally, when the response to environmental conditions is not linear, and these conditions vary in time and space, the average of the response to these varying conditions will differ from the response to the average condition

Groundwater contamination management

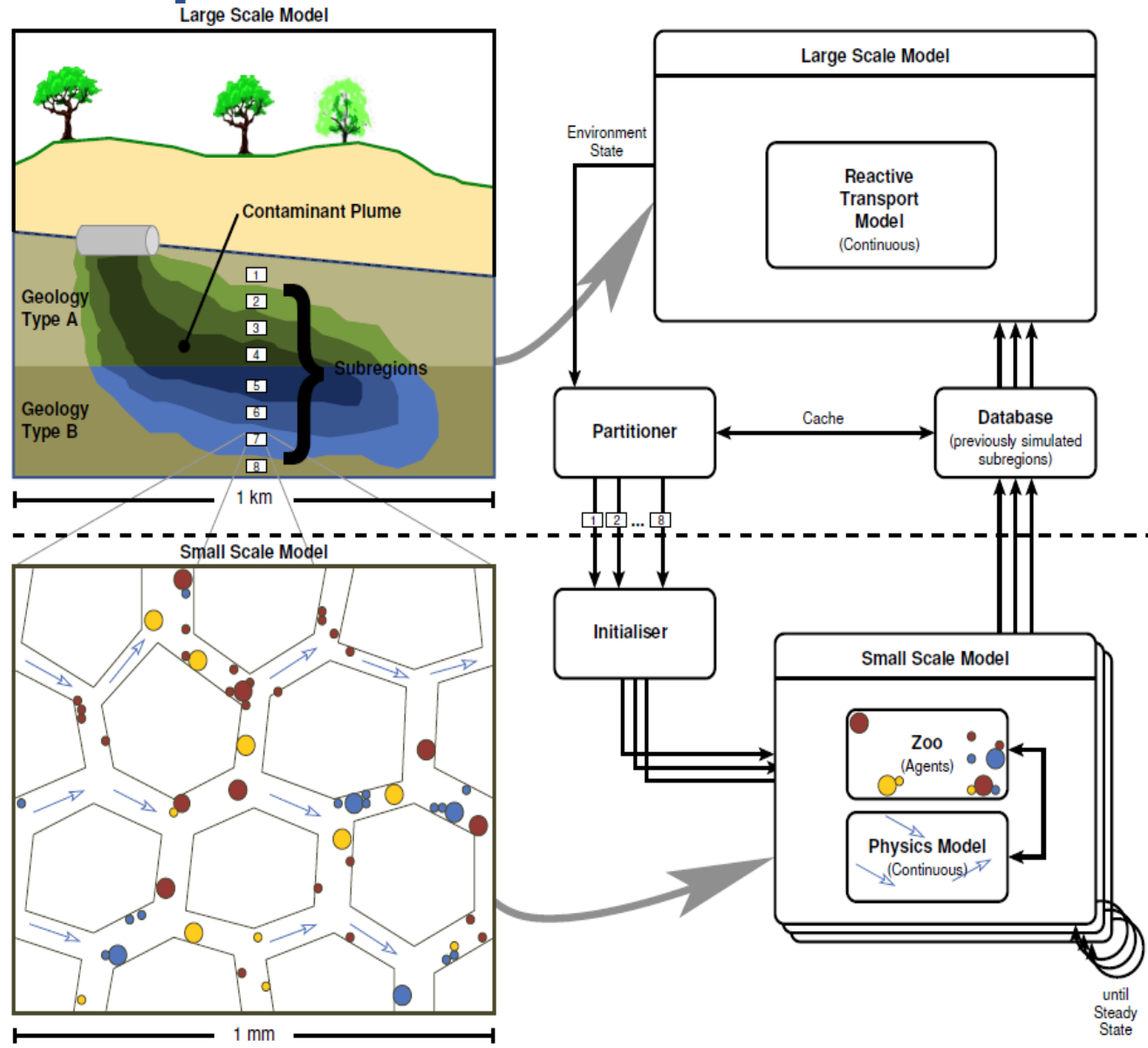
- Allowing for patchiness on the microscale is crucial for robust prediction of contaminant degradation rates under various management scenarios
 - the microbes are grazed on (eaten) by larger organisms, e.g. protozoa. There is a large body of work on "grazing increases productivity" in protozoan ecology that suggests that grazing could enhance degradation rates
 - biomass is mostly attached to surfaces in clusters of cells originating from growth and cell division of a single 'founder' cell, leading to a heterogeneous distribution of cells on the surfaces.
 - locally high biomass density leads to high rates of substrate consumption resulting in low substrate concentrations locally
- This pore-scale heterogeneity of biomass distribution and behaviour can be captured through the utilisation of agent-based modelling



The Proposed Framework

- The proposed framework supports the dynamic partitioning of the site-scale domain into subregions: geology, flow regime, carbon/energy and electron donor concentrations
- It integrates:
 - macroscale (mean field PDE model for contaminated site, scale 100 m up to several km) reactive transport simulation of an aquifer (groundwater body) simulates the flow and degradation of a contaminant plume through various types of porous media,
 - an ensemble of small scale agent-based models
- Instead of evaluating differential equations to obtain the derivatives (reaction rates, velocities, etc.) to step the PDE solver forward, small scale agent-based simulations (corresponding to subregions) are launched, initialized to correspond to the current local state of the PDE model, that will return the 'derivatives' to the PDE solver.
- At the macroscale, contaminant and electron acceptor and degrader distributions can converge/diverge and/or move into different porous medium conditions, which are fed back into the small scale dynamics.
- A database of microscale simulation inputs and outputs prevents unnecessary duplication and can be used for interpolation, thus improving efficiency.

The Proposed Framework



Microscale Parameters

- distribution and transport of contaminants, substrates, and organisms in the pores of the aquifer, and also larger scale heterogeneity, e.g. different geological strata with different pore sizes, different flow rates, and carbon/energy source and electron acceptor concentrations.
- zoo of agents:
 - various metabolic types of species relevant for the degradation of the contaminant of interest (guilds)
 - Generation times in groundwater are not very well known, but are thought to range from 10 days to several years

Summary

- Groundwater is vital as our societies increasingly rely on it as a source of drinking water. At the same time the rate of new groundwater contaminations outpaces the rate of remediation.
- Experimentally, sampling of groundwater is particularly challenging and the typically slow changes require monitoring for quite long periods; as a result data are and will remain very scarce.
- Simulation has therefore a crucial role to play in this realm.
- Our proposed framework
 - is a novel way of describing phenomena in groundwater that vary in time and space and over multiple scales
 - avoids the problems inherent with the traditional large scale averaging of non-linear microscale behaviour and should provide far greater predictive capability
- Lots of unknown parameters
- Parallelisation issues