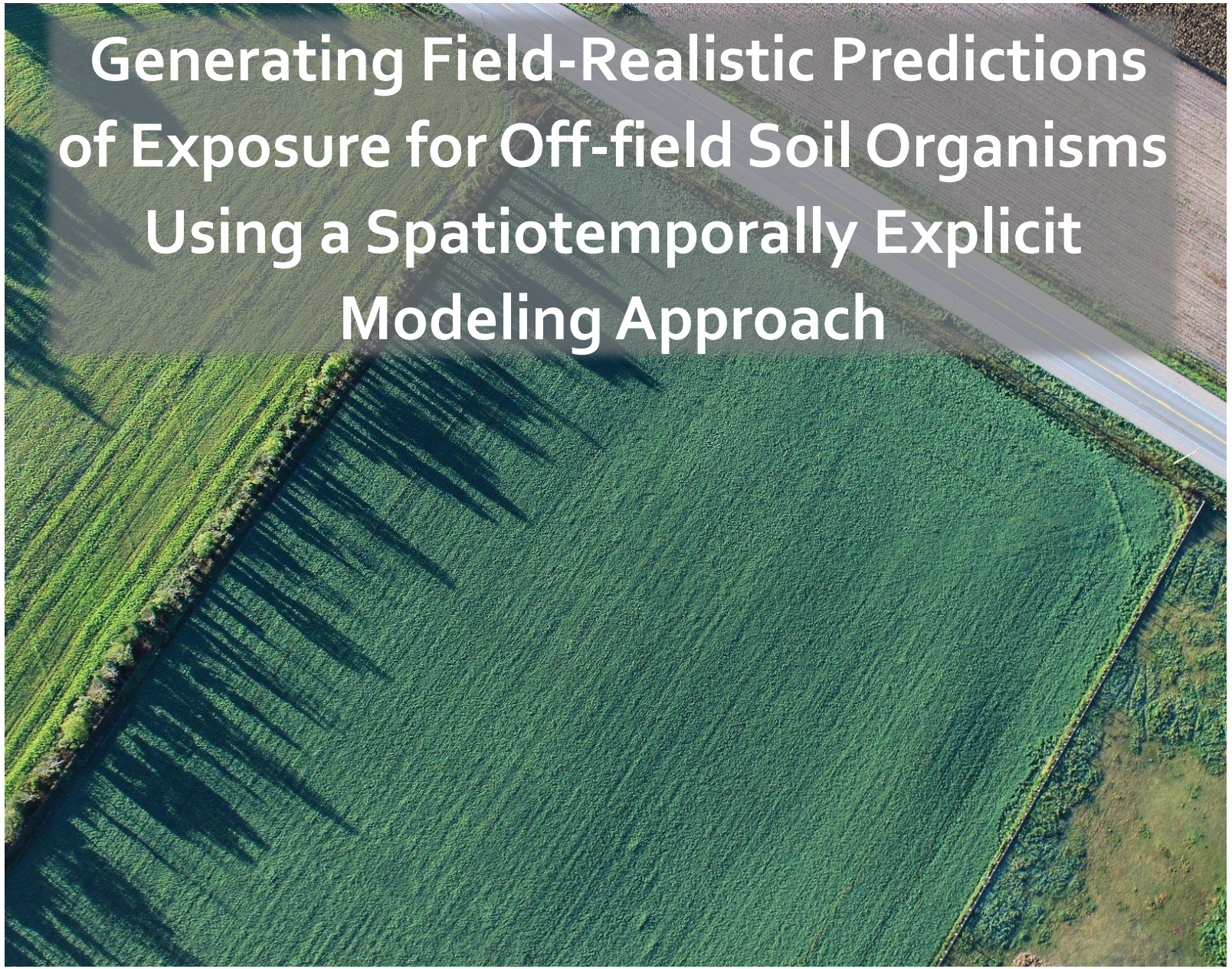
Generating Field-Realistic Predictions of Exposure for Off-field Soil Organisms Using a Spatiotemporally Explicit Modeling Approach



SETAC Europe 2025

"Innovation for Tomorrow: Progress in Safe and Sustainable Concepts"

Session: 3.03.C - Measuring, Modelling and Monitoring the Environmental Behaviour and Exposure of Pesticides

May, 2025

Christopher Holmes, Thorsten Schad, Sascha Bub, Gregor Ernst, Julian Heinrich

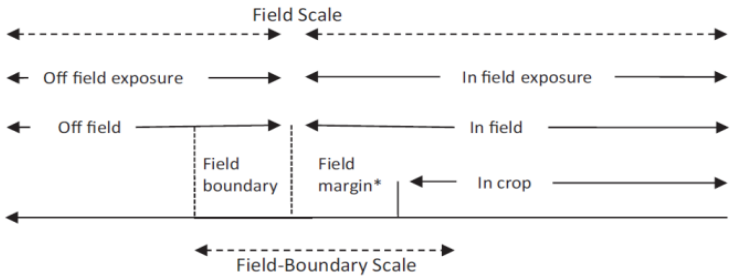
APPLIED ANALYSIS SOLUTIONS LLC

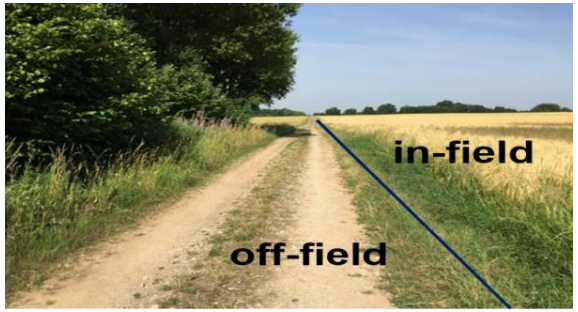
BAYER

Introduction

- The **European Food Safety Authority** (EFSA) released a **scientific opinion** "*addressing the state of the science on **risk assessment of plant protection products for in-soil organisms***" in which **spray-drift** and **runoff** are identified as potential exposure routes of **off-field soil organisms**
- **'off-field'** refers to **areas outside the agricultural field** boundaries
- **EFSA outlined a first approach to estimate off-field soil exposure**, designed closely to the FOCUS surface water model approach

The conservative nature of the approach and the **necessity for model and scenario development**, is indicated in EFSA





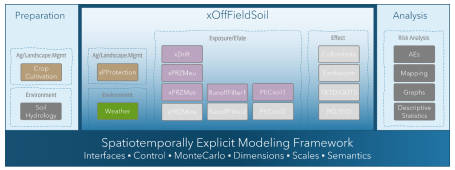
Study Goals - xOffFieldSoil

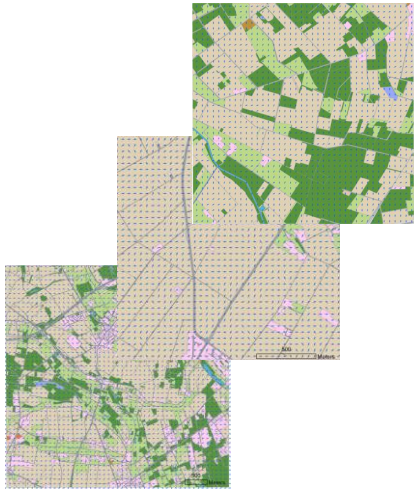
Develop (open source)

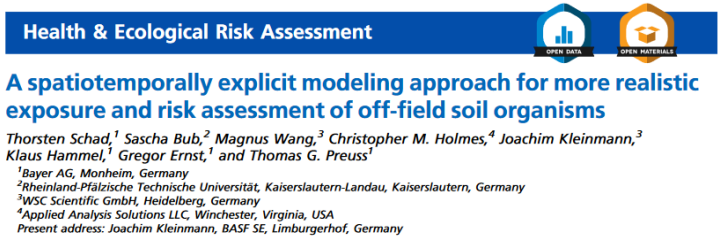
1. a **model approach** to appropriately combine off-field soil exposure due to runoff & drift,
2. **scenarios** based on real-world conditions
3. a **case study** to gain insights into off-field soil exposure and risk, including **mitigation**

to

- **inform the scientific discussion** on design of off-field soil exposure, effect and risk characterization approaches in a **tiered RA scheme**
- support the **development of Assessment Endpoints**, e.g., spatiotemporal percentiles of off-field exposure
- identify effective **risk mitigation options**






Health & Ecological Risk Assessment

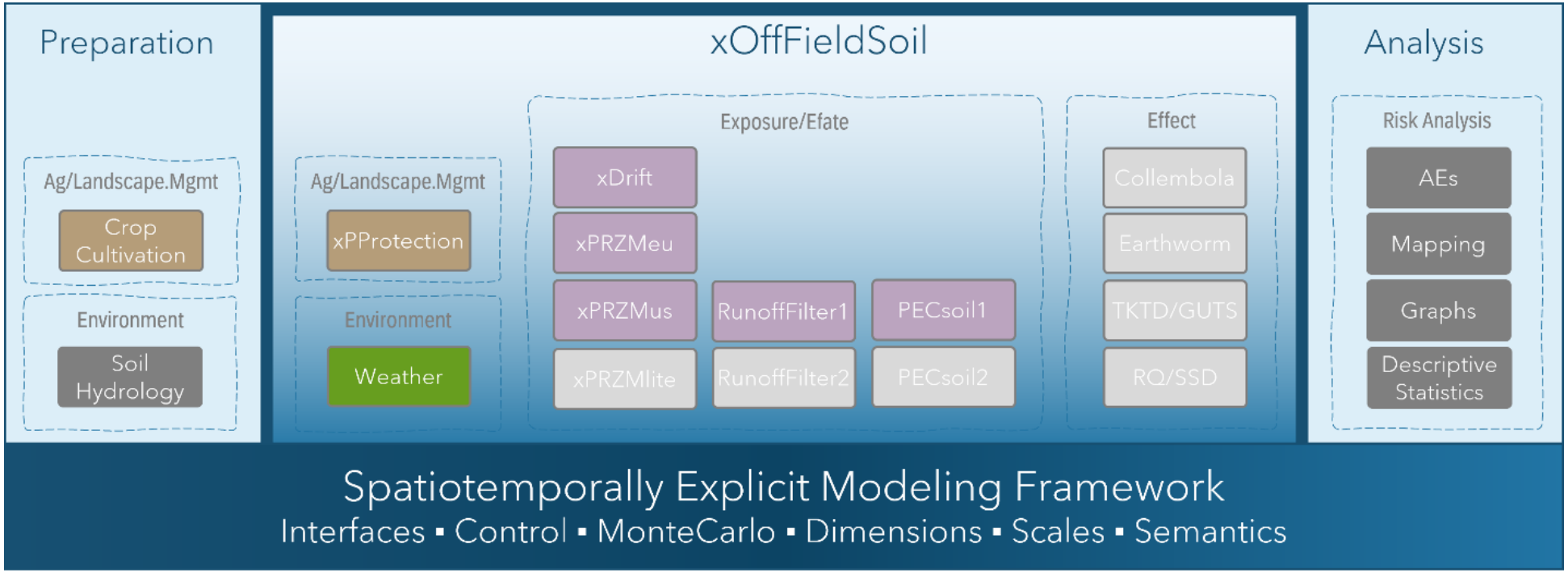
A spatiotemporally explicit modeling approach for more realistic exposure and risk assessment of off-field soil organisms

Thorsten Schad,[1] Sascha Bub,[2] Magnus Wang,[3] Christopher M. Holmes,[4] Joachim Kleinmann,[3] Klaus Hammel,[1] Gregor Ernst,[1] and Thomas G. Preuss[1]

[1]Bayer AG, Monheim, Germany
[2]Rheinland-Pfälzische Technische Universität, Kaiserslautern-Landau, Kaiserslautern, Germany
[3]WSC Scientific GmbH, Heidelberg, Germany
[4]Applied Analysis Solutions LLC, Winchester, Virginia, USA
Present address: Joachim Kleinmann, BASF SE, Limburgerhof, Germany

Open Access publication in IEAM https://doi.org/10.1002/ieam.4798
Github: https://github.com/xlandscape/xOffFieldSoilRisk

xOffFieldSoil Model

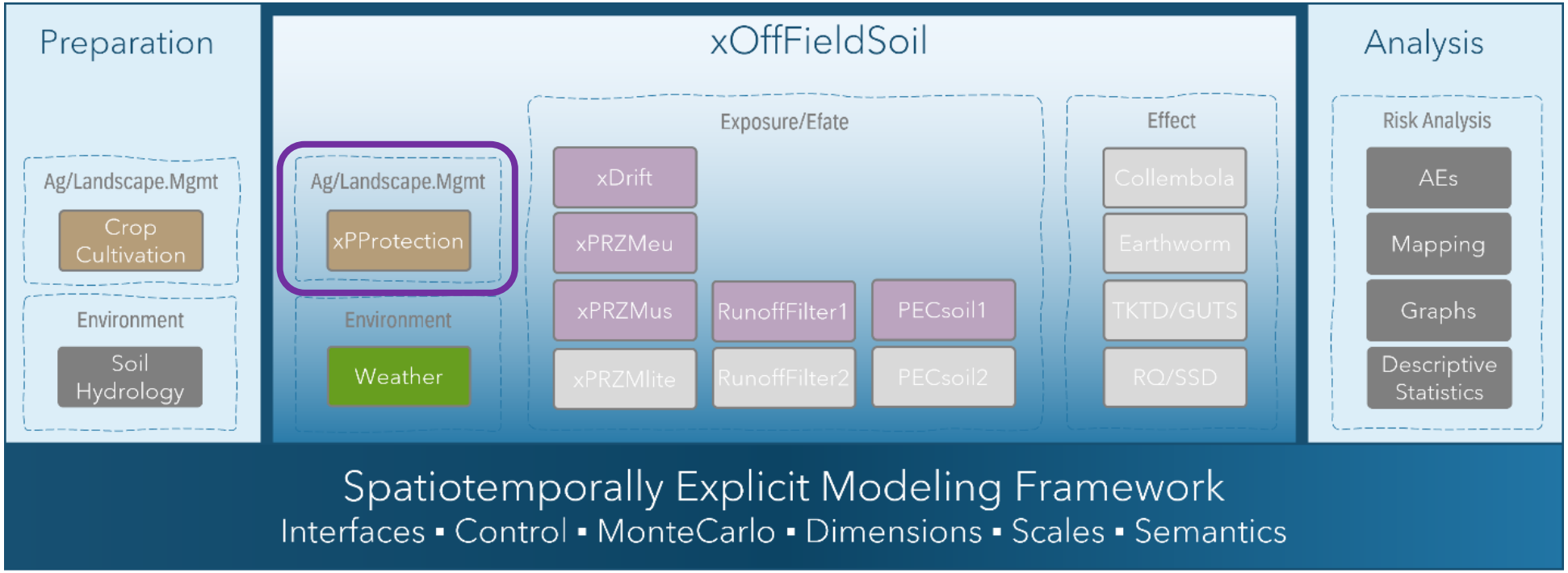


Derived from the **xLandscape Framework**, a **modular toolbox** to

- build **landscape models**, for spatiotemporally explicit simulations
- enable the **integration of existing models** (e.g., PRZM, xDrift) as **components**
- build **endpoints** that link to the attributes, risk dimensions and scales in **Specific Protection Goals**

https://github.com/xlandscape

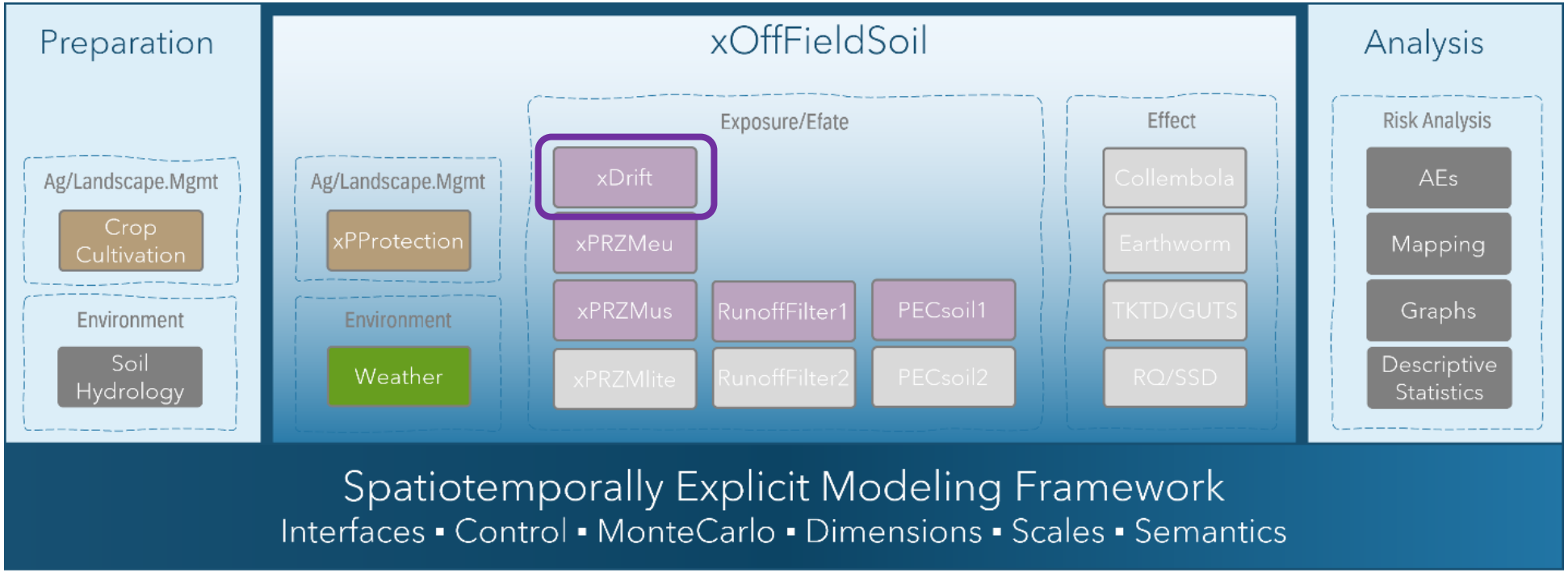
xOffFieldSoil Components – Plant Protection Product Use



- ***xPProtection*** simulates the variability of **applications** of a single PPP to a single crop type
- A **simplified version** of the ***CropProtection*** *component (open source)* →*Poster Monday 204*
- Applications are defined by use rates, application time windows and using probability distribution functions (PDF)

https://xlandscape.github.io/xCropProtectionDemo/
https://github.com/xlandscape/xCropProtectionDemo

xOffFieldSoil Components – Spray-Drift Deposition



- ***xSprayDrift*** simulates the **variability of spray-drift depositions** along the field edge as observed in drift trials (Rautmann 2001)
- Published and open source:


SoftwareX 12 (2020) 100610

Contents lists available at ScienceDirect

SoftwareX

journal homepage: www.elsevier.com/locate/softx

Original software publication

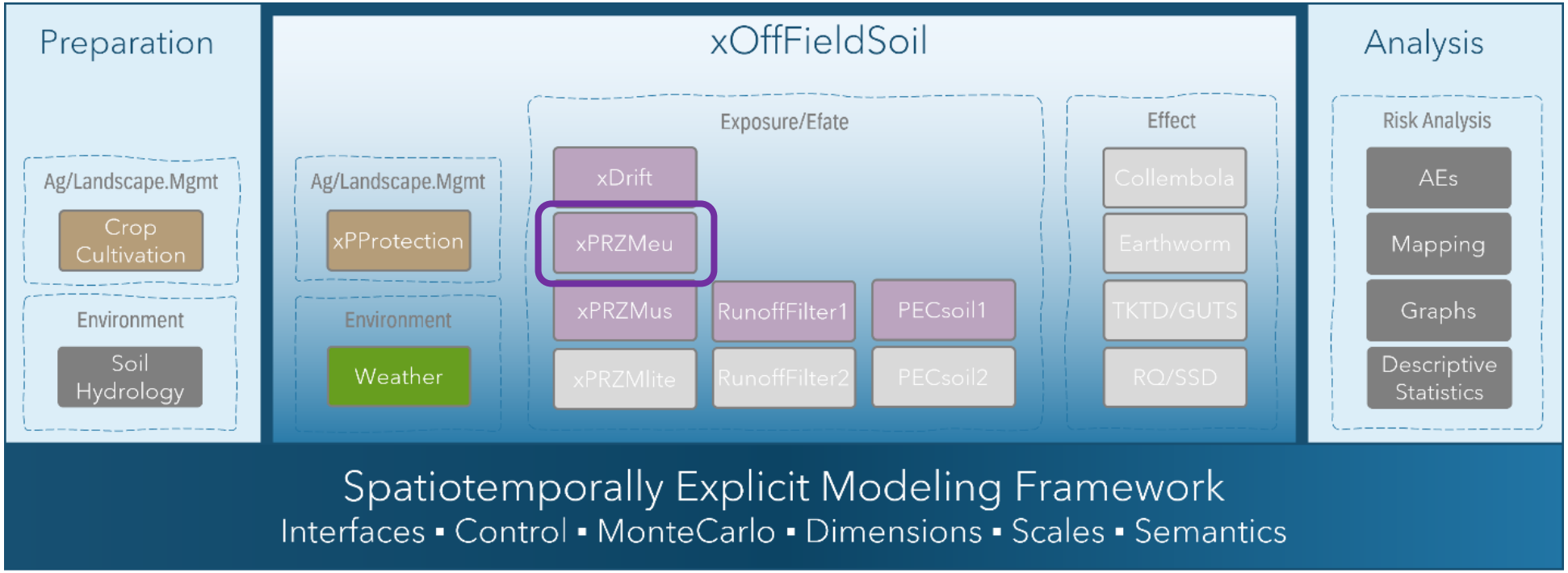
XDrift—An R package to simulate spatially explicit pesticide spray-drift exposure of non-target-species habitats at landscape scales

Sascha Bub [a,*], Thorsten Schad [b], Zhenglei Gao [b]

[a] Institute for Environmental Sciences, University of Koblenz-Landau, D-76829 Landau, Germany
[b] Bayer AG, Alfred-Nobel-Str. 50, 40789 Monheim, Germany

https://github.com/xlandscape/XSprayDrift-Component

xOffFieldSoil Components – Runoff

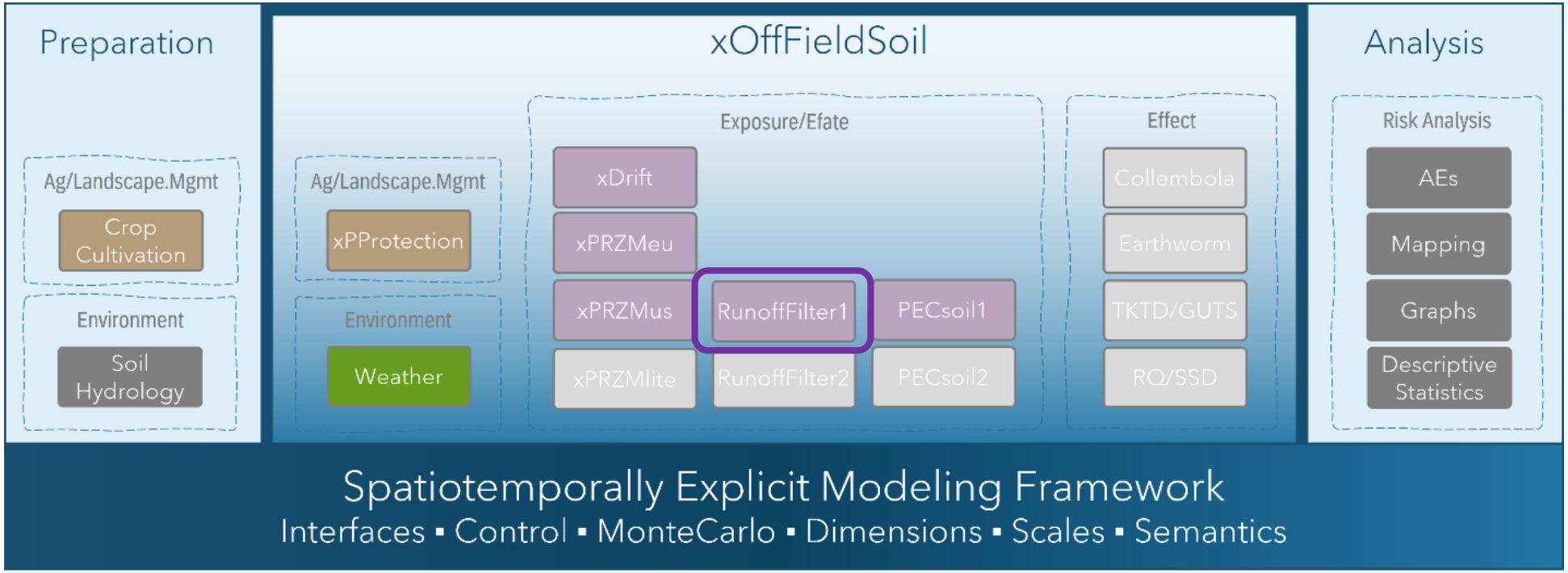


- Due to **regulatory context**, **initially** the **FOCUSsw** model **PRZM** was used. Parameterization:

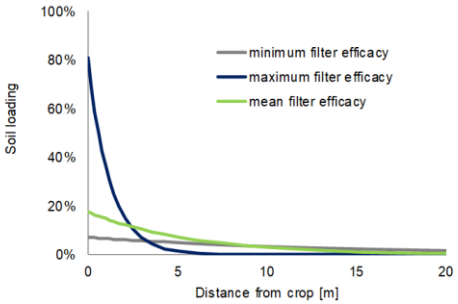
  PPP application, efate of the substance, soil and weather data input, utilizing local env. conditions
- Three sub-processes: soil surface hydrology, runoff on fields, runoff filtering in off-field
- **alternative runoff models** are in a testing phase

https://github.com/xlandscape/RunOffPrzm-Component

xOffFieldSoil Components – Runoff Filtering

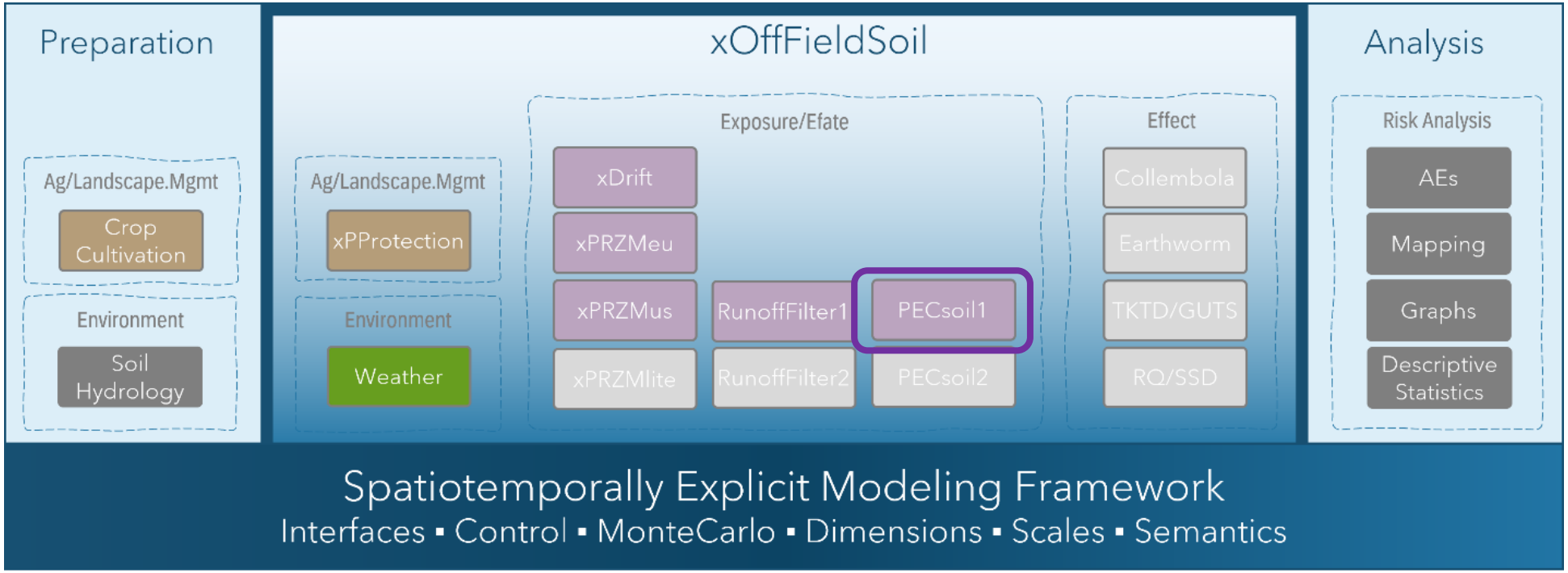


- **Runoff filtering** causes local runoff exposure. **Two alternative components**:
  - i. **Filter function**, based on FOCUS (2007) filter efficacy values for pesticides
  - ii. **VFSMOD** (Vegetative Filter Strip Modeling System) (https://abe.ufl.edu/faculty/carpena/vfsmod/index.shtml)



https://github.com/xlandscape/RunOffPrzm-Component

xOffFieldSoil Components – Soil Concentrations



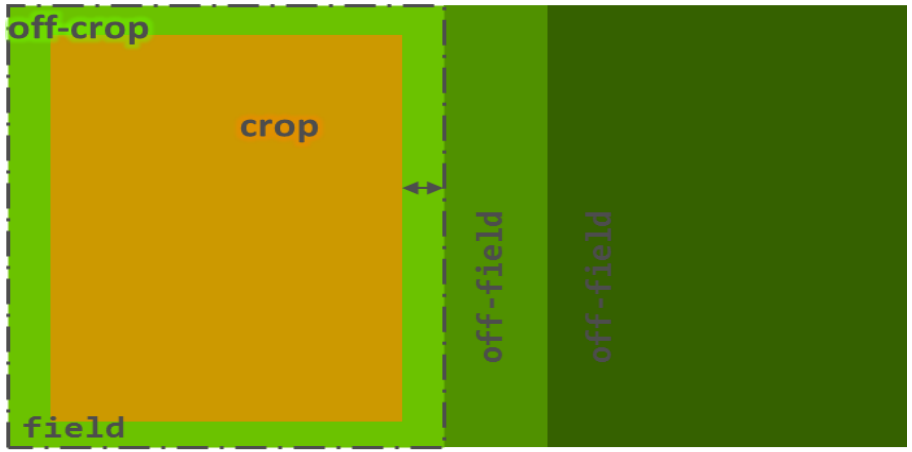
- **Initially, a simple PECsoil component** calculates exposure of soil dwelling organisms (PECsoil) from the combined spray-drift and runoff deposited mass
  (assuming a soil depth of 5 cm and a dry bulk density of 1.5 kg/L, and first-order degradation)
- **Alternative PECsoil components using PRZM and PEARL** are currently in a testing phase

https://github.com/xlandscape/xxx

Scenarios

Schematic Scenarios (edge-of-field)

- Single field and an off-field area (parameterized as a small strip or patch)
- Simplicity → important to understand and verify complex system behavior

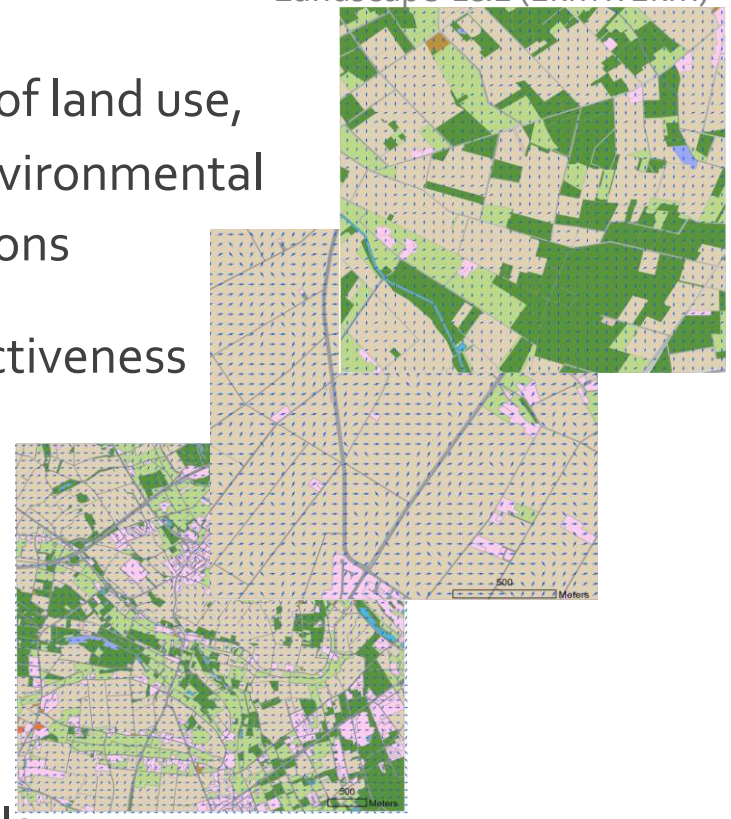


Schematic scenario (100m x 100m)

Landscape Scenarios

- Realistic variability of land use, landscape structure, environmental and agricultural conditions
- Risk mitigation effectiveness
- Reality
  →Address population, community and biodiversity attributes, of Specific Protection Goals

Landscape-1&2 (2km x 2km)



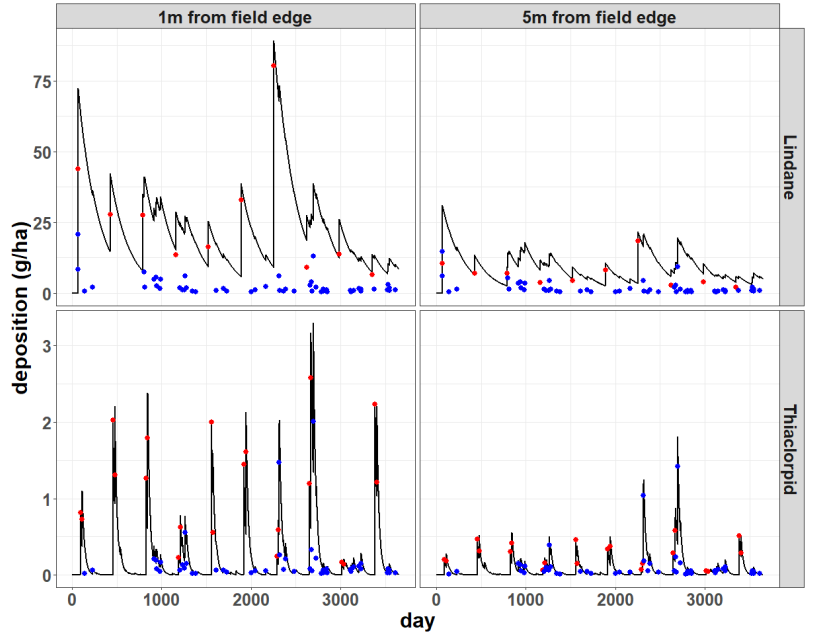
Landscape-3 (5km x 5km)

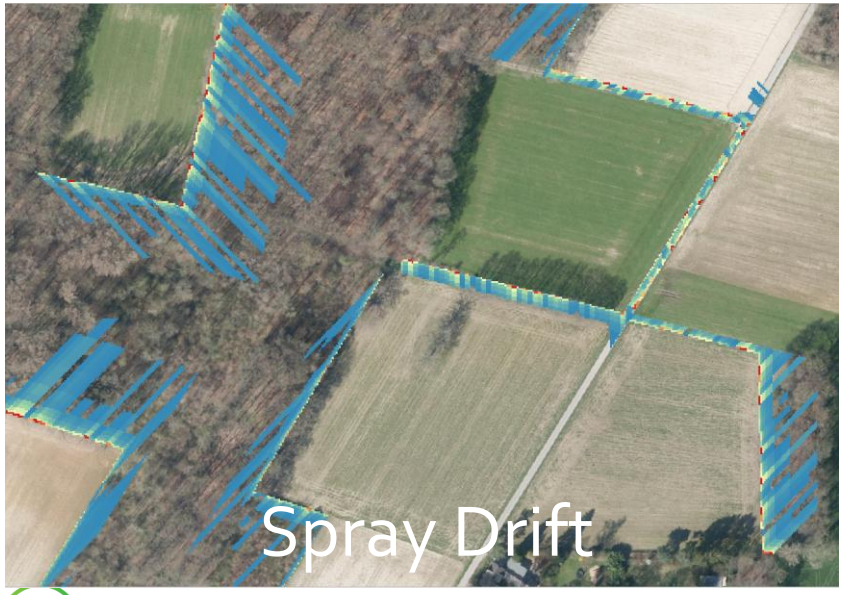
https://github.com/xlandscape/Scenario-NRW1
https://github.com/xlandscape/Scenario-NRW2
https://github.com/xlandscape/Scenario-NRW3

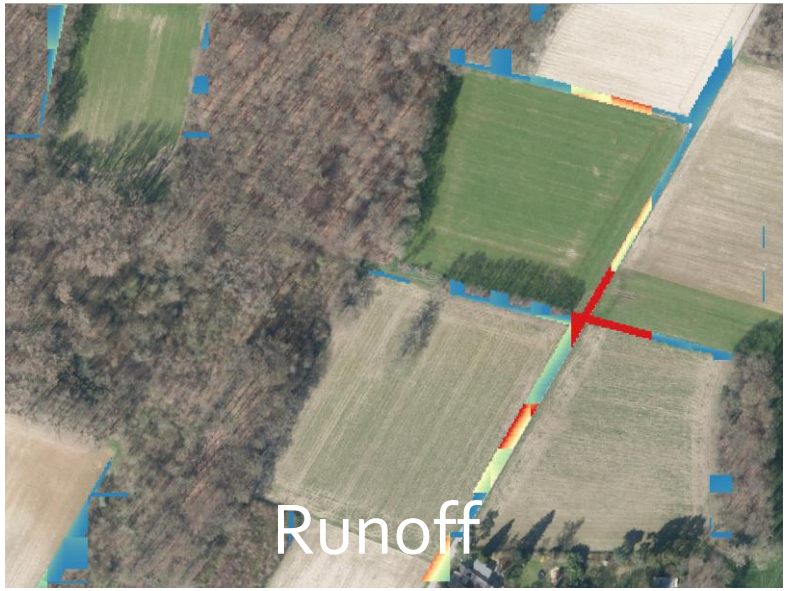
Variability of Exposure in Space and Time

Case study: **Lindane** and **Thiacloprid** (of different DT50, Koc)

- **Variability**: application, wind direction, drift deposition, precipitation
- **PECsoil for grid cells** of **1 m²** (*x*) with a **1-day** time step (*t*)
- **Mitigation options**: in-crop-buffer, in-field-margin, drift reduction







Local (1 m2) maximum PECsoil over a 10-year experiment using 30 Monte Carlo simulations (max PECsoil for illustration only)

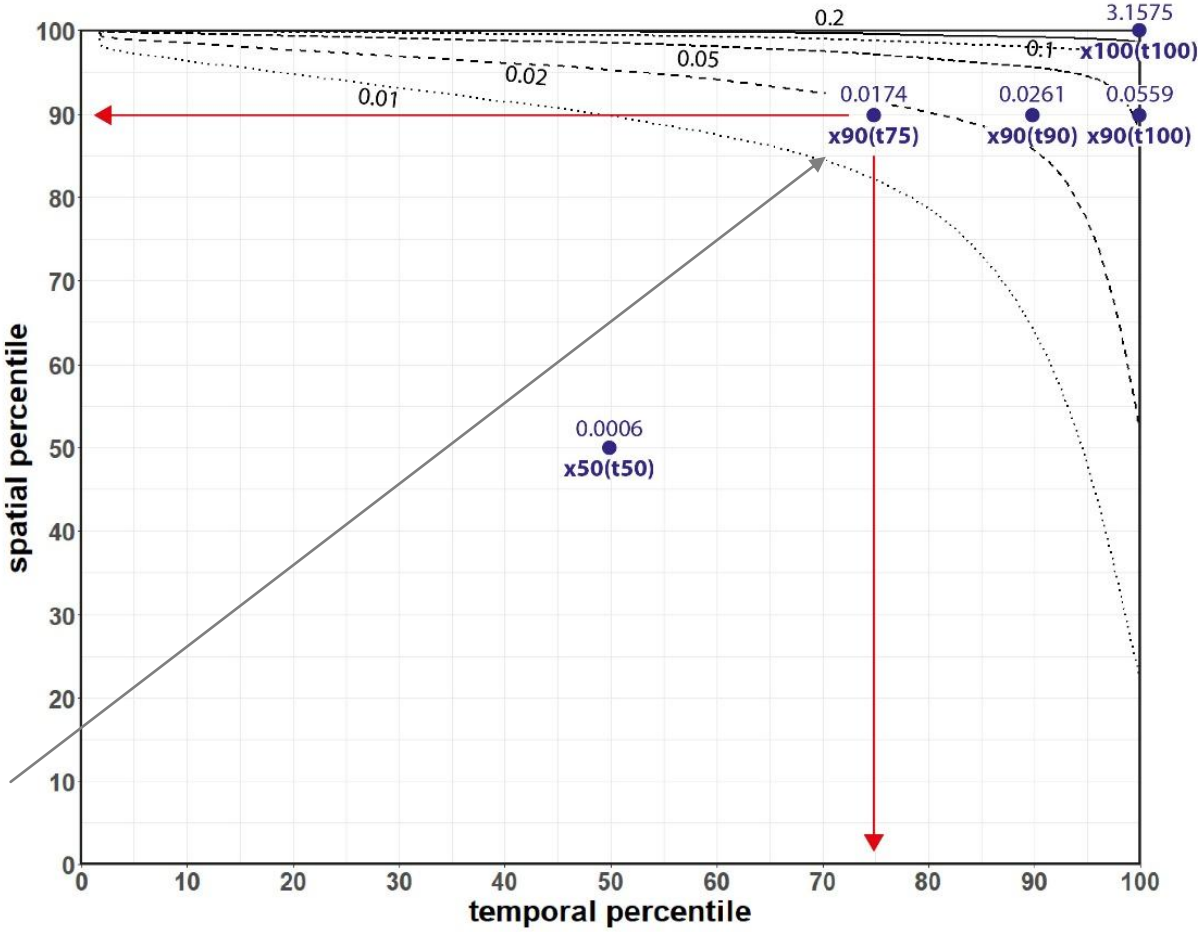
Develop Risk Endpoints from Spatiotemporal Variability

Stepwise calculation of percentiles

along the temporal and spatial dimensions:

1. A **temporal percentile** is calculated over the full simulation period for each local off-field grid cell (1 m²). E.g.,
   PECsoil(*x*(*t*75)) represents the spatial distribution of the 75th %ile PECsoil over time
2. A **spatial percentile** is calculated from these single values across 1 m² grid cells
3. A **PECsoil(*x*90(*t*75))** represents the 90th spatial percentile of the local 75th %iles over time. E.g.,

   in 75% of time, 90% of off-field soil grids will have an exposure <0.0174 mg/kg



Conclusions & Outlook

- **Initial approach** to assess exposure/risk of off-field soil organisms due to spray-drift and runoff
  - **Flexible** and able to operate at any desired spatial and temporal resolution
  - **Adaptable** to use alternative exposure models and analysis routines
  - **Risk mitigation** options can be utilized
  - **Scalable** to run local and large real-world scenarios
- Spatiotemporally explicit **raw output transparently** aggregated into exposure values to **build meaningful Assessment Endpoints for regulatory Risk Assessment**

Outlook

- Discussion in the **regulatory scientific community**
- Employ alternative exposure models. Integrate soil organism **effect models** (e.g., earth worm)

THANK YOU

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[2]Rheinland-Pfälzische Technische Universität, Kaiserslautern-Landau, Kaiserslautern, Germany
[3]WSC Scientific GmbH, Heidelberg, Germany
[4]Applied Analysis Solutions LLC, Winchester, Virginia, USA
Present address: Joachim Kleinmann, BASF SE, Limburgerhof, Germany

IEAM article: https://doi.org/10.1002/ieam.4798

xOffFieldSoil has been published on GitHub: https://github.com/xlandscape/xOffFieldSoilRisk

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Contact: sascha.bub@rptu.de, tschadwork@gmail.com, chrisholmes@appliedanalysis.solutions