Developing efficient and transparent groundwater modeling workflows to aid with decision support

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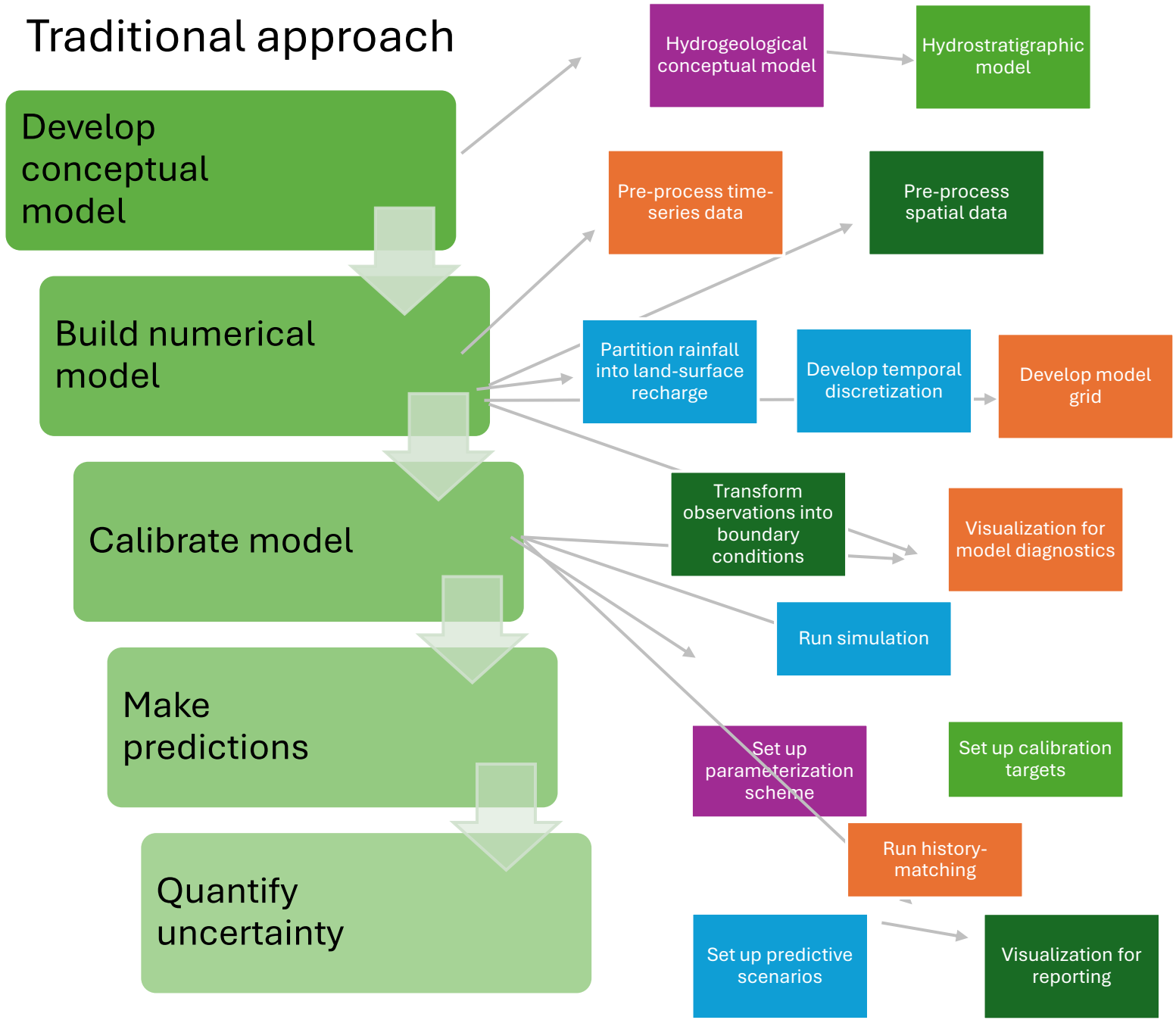
Groundwater modelling workflow

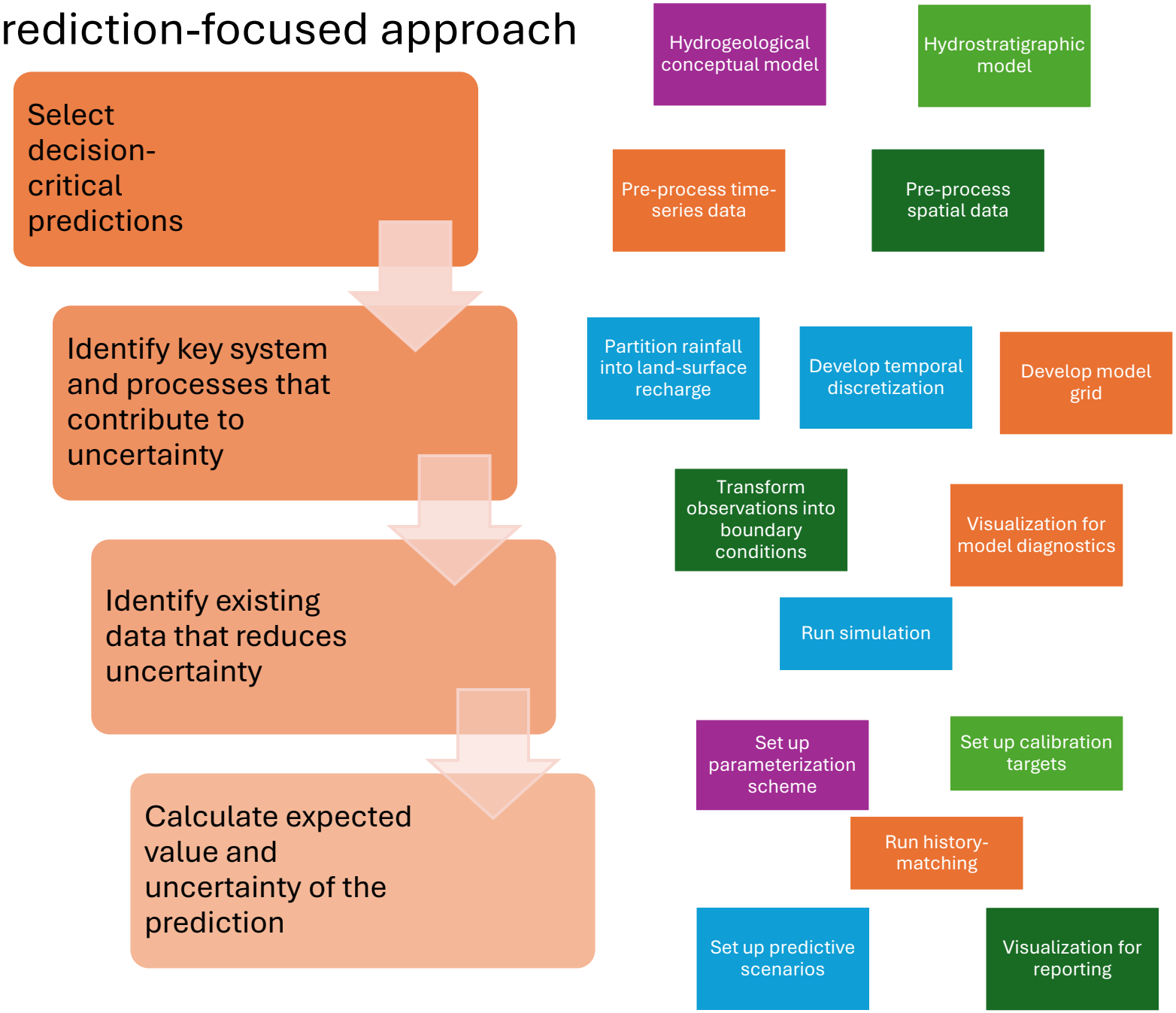
Doherty & Moore, 2020.
Groundwater 58(3)



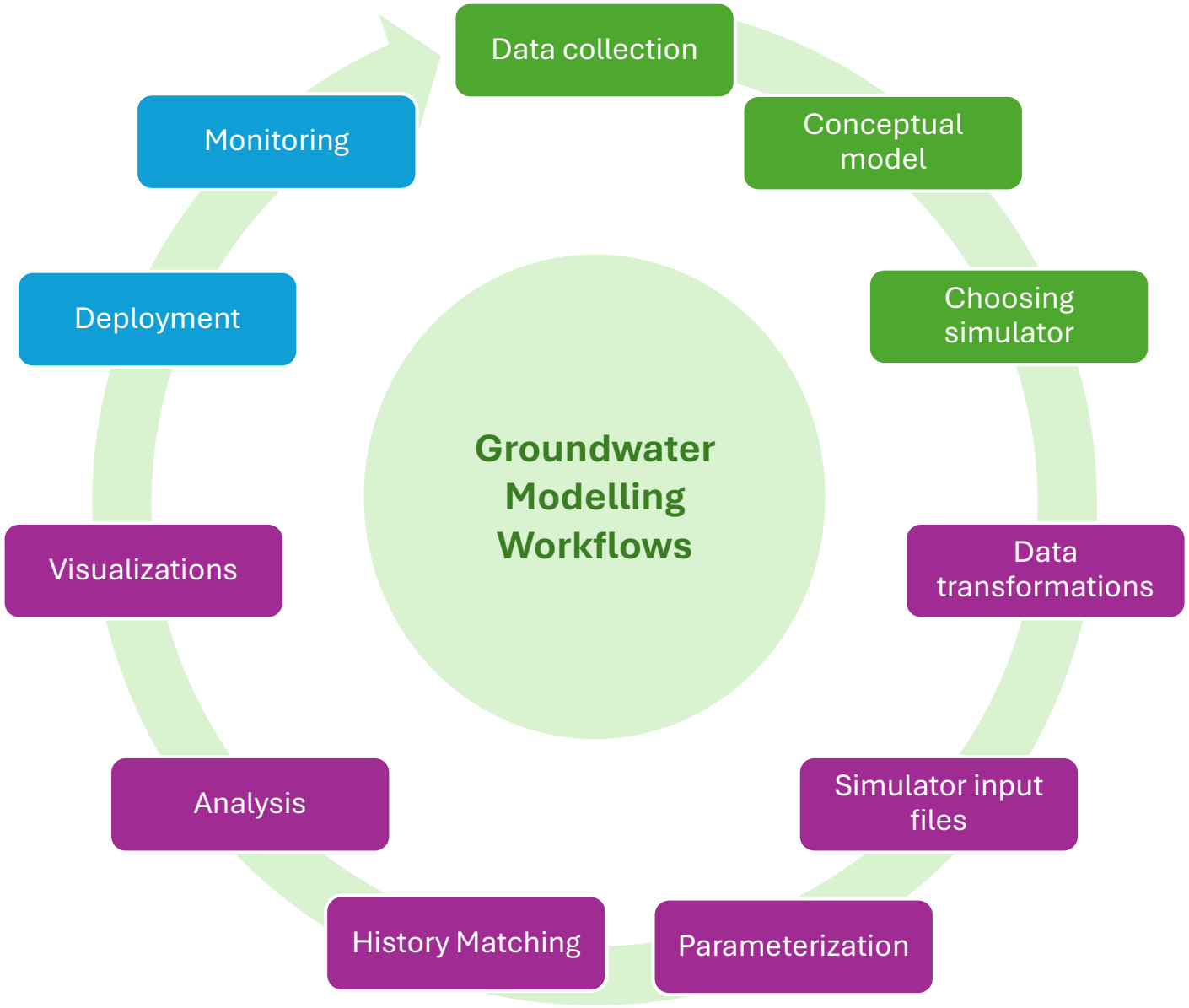
Decision Support Modelling

Doherty & Moore, 2020.
Groundwater 58(3)

Prediction-focused approach



Fully scripted modelling workflows



Fully scripted modelling workflows

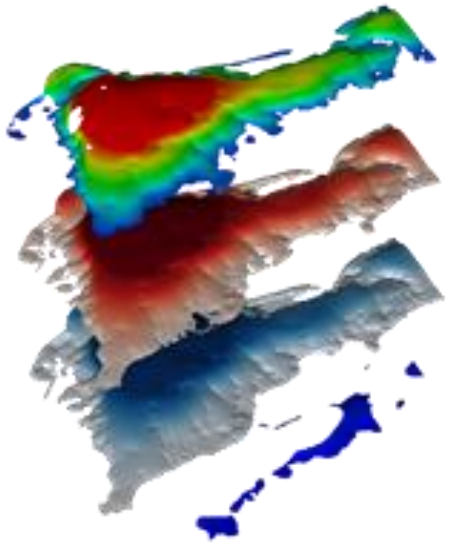
Findable	• Do we know where the model is?
Accessible	• Is the model in a format that can be easily accessed?
Interoperable	• Can the model be used by other people? • Do the model outputs work with other project aspects?
Reusable / reproducible	• Can we reproduce the model? • Can we reuse components of the model for other purposes?

Fully scripted modelling workflows
Development tools

- Flexible programming languages for data processing and wrapping everything together (e.g., python)
- Version control in code repositories to keep track of scripts
- Developer platforms for interacting with repositories and collaborating across organisations
- Integrated Development Editors (IDEs) to facilitate code development

Fully scripted modelling workflows
Simulation and data processing tools

- Spatial libraries for geospatial data processing (GeoPandas, Shapely)
- Time-series processing (Pandas, Pastas)
- Simulator and support libraries such as FloPy and or MODFLOW-SETUP
- GUI support (Groundwater Vistas, FEFLOW)



Example: Hutt Aquifer Model

Hutt Aquifer Model
Modelling objectives

Planning

- Wellfield replacement strategy
- Water resource management
- Monitoring system design

Operations

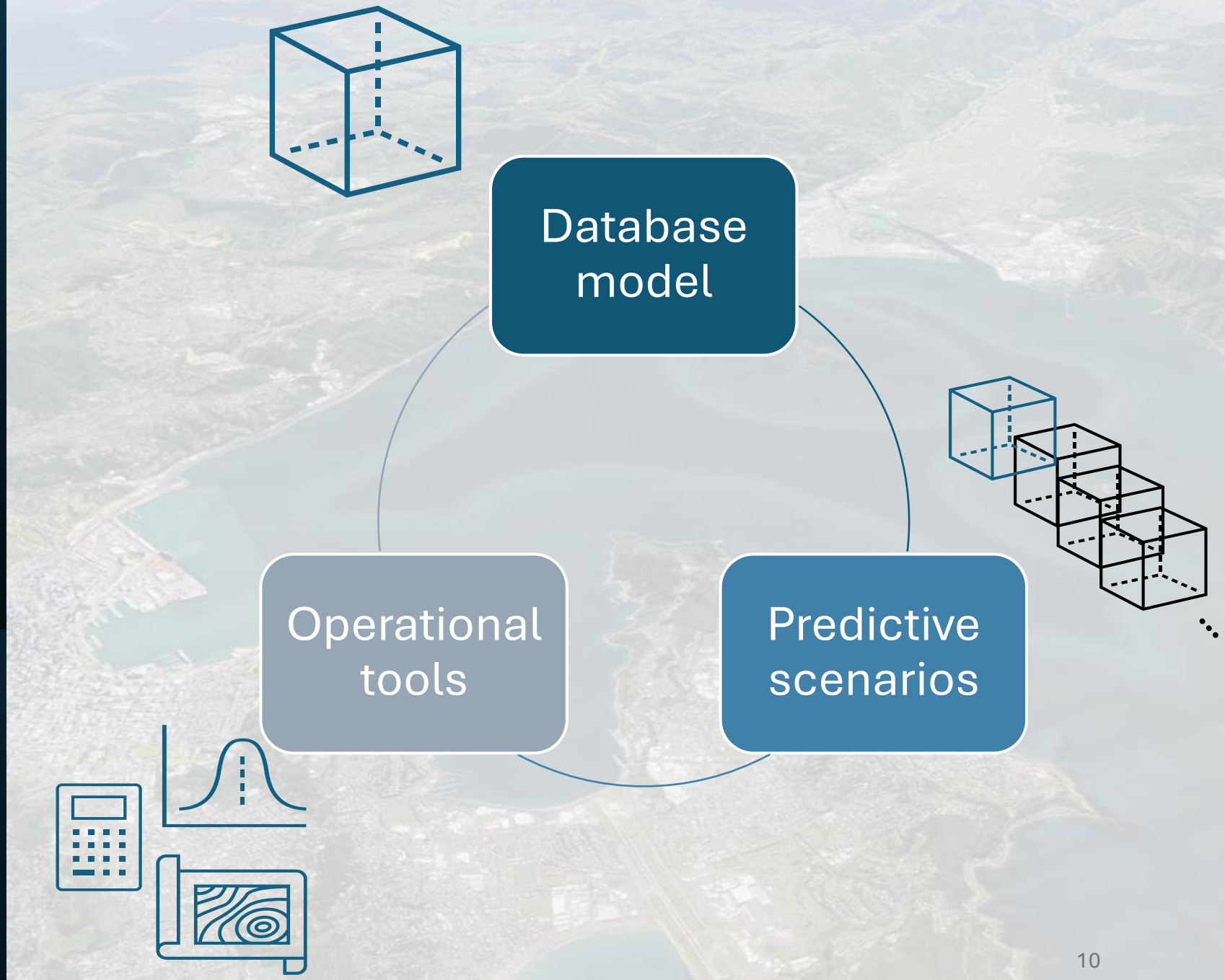
- Yield forecasting and optimisation
- Contamination response
- Aquifer management

Uncertainty with respect to:

- Geological conceptual model
- Permitting requirements
- Asset replacement strategy

Scripted modelling approach

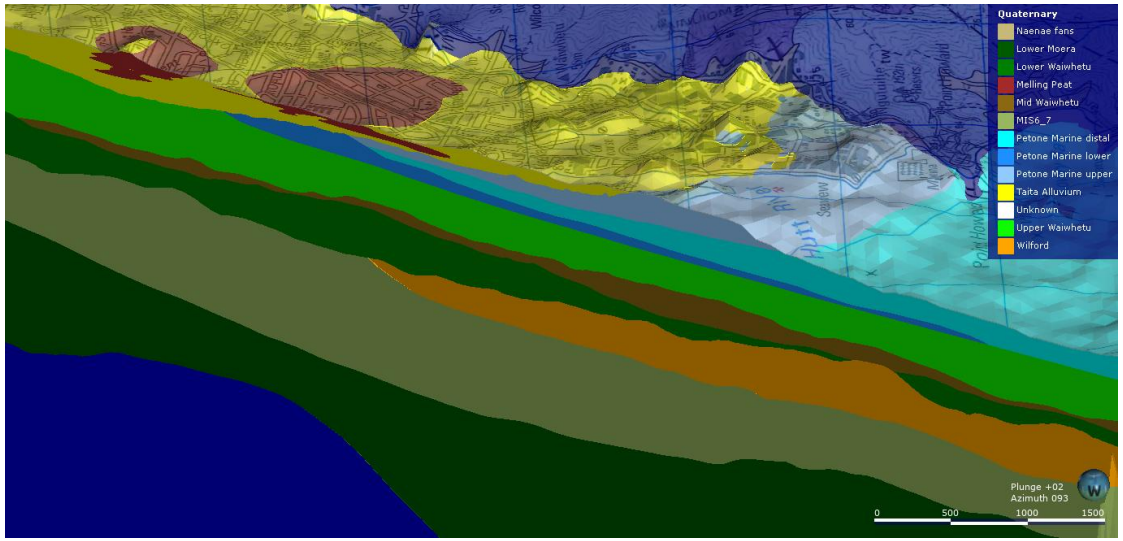
Example: Hutt Aquifer Model

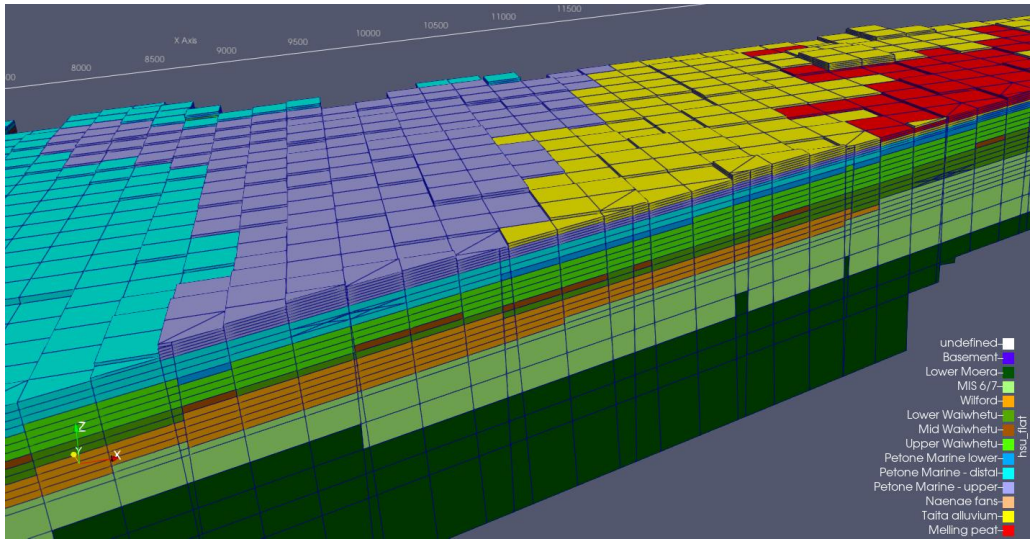


Hutt Aquifer Model
Modelling components

- Leapfrog hydrostratigraphic model
- Boundary conditions derived from climate data and an existing surface water model
- Simulation with MODFLOW 6
- History-matching using PEST_HP, incorporating PLPROC
- Uncertainty analysis with PEST-IES
- Reporting and interactive visualization with Plotly

Hutt Aquifer Model
Hydrostratigraphic model

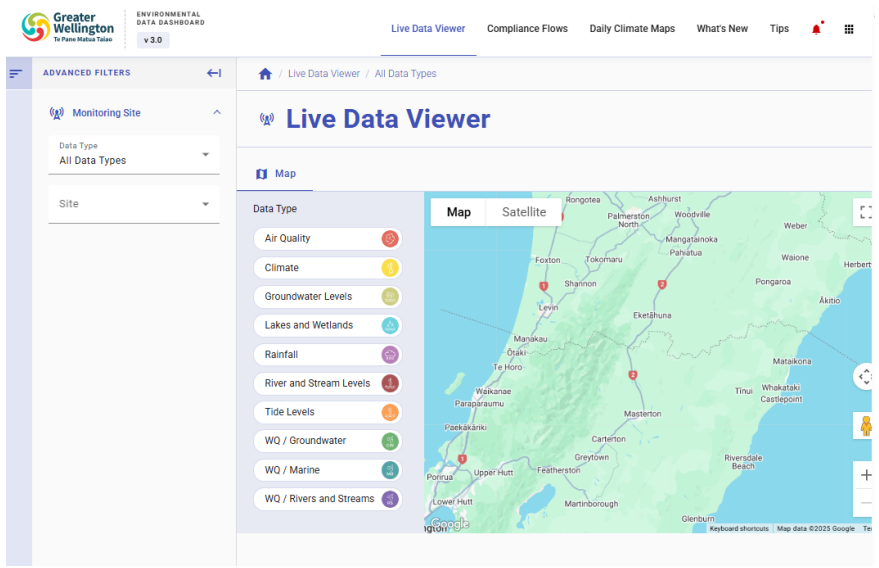


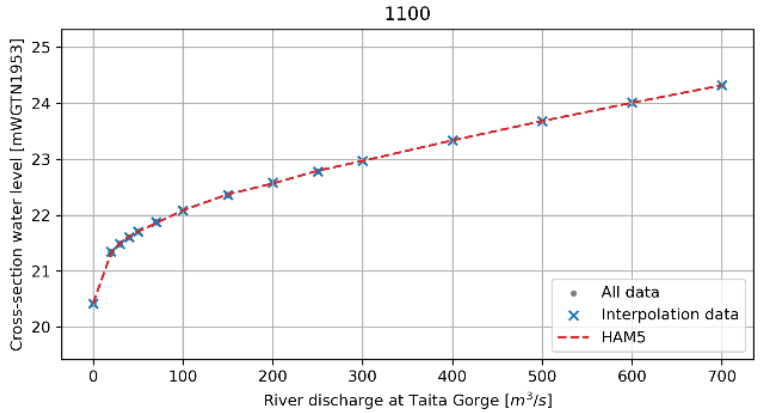


- Evaluation of hydrostratigraphy to the model grid
- Flexibility to account for uncertainty in the geological model

Hutt Aquifer Model
Boundary conditions

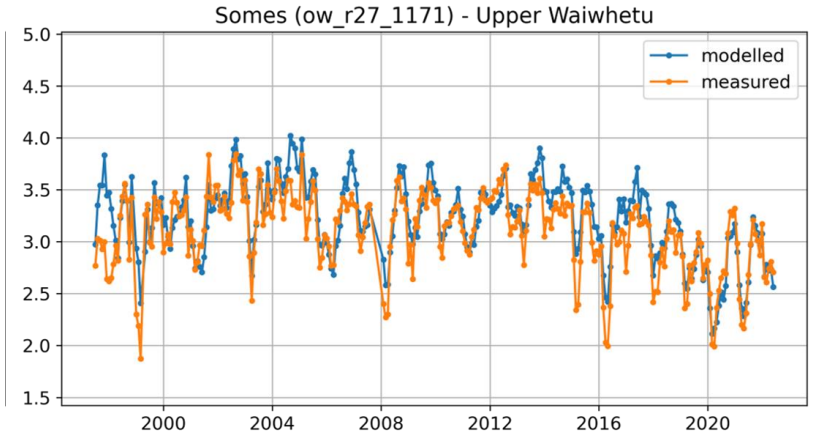
- Observations downloaded via Application Programming Interface
  - Climate
  - Groundwater levels
  - River flows
- Pumping provided by water supplier
- Land-surface recharge calculated using python functions
- River boundaries derived from existing surface water model

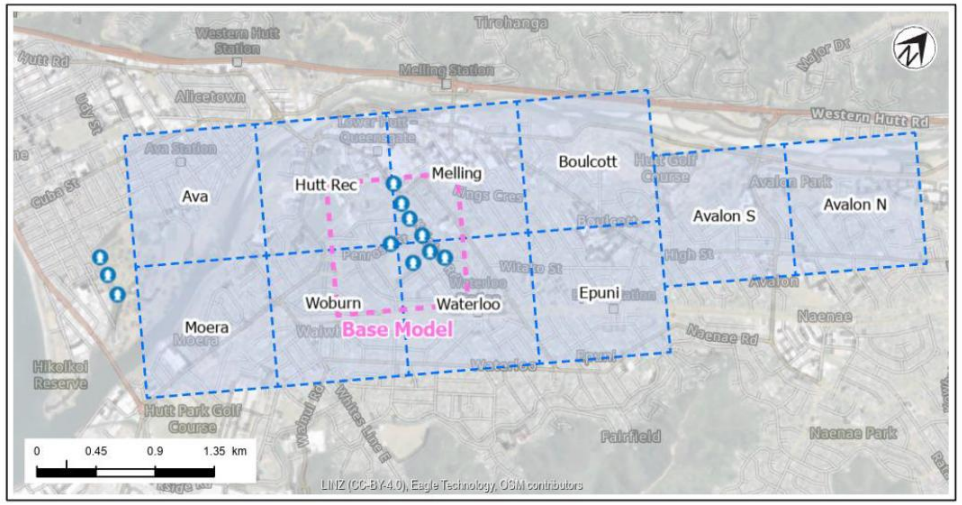




Hutt Aquifer Model
Model results

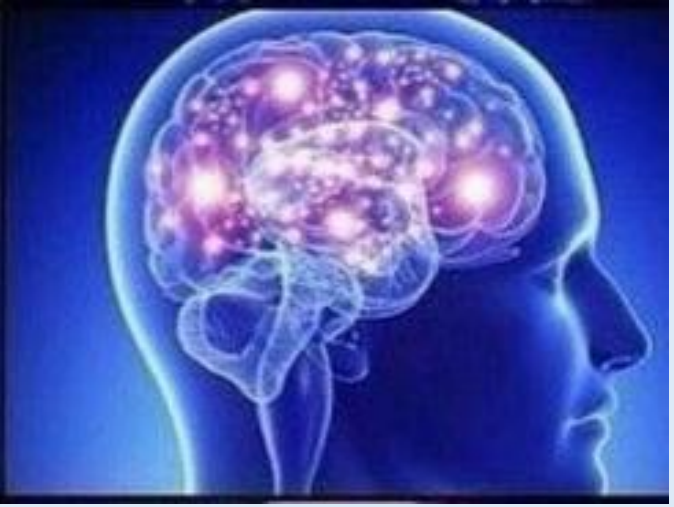
- Approach supported iterative history-matching parameterization schemes as well as predictive scenario analysis
- Flexible temporal and spatial discretization for local-scale issues possible



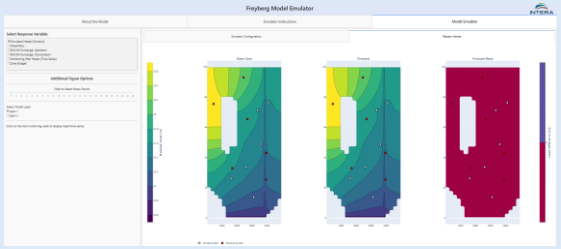


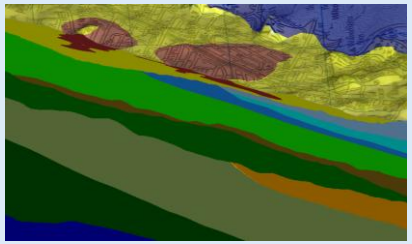
Hutt Aquifer Model
Lessons learned

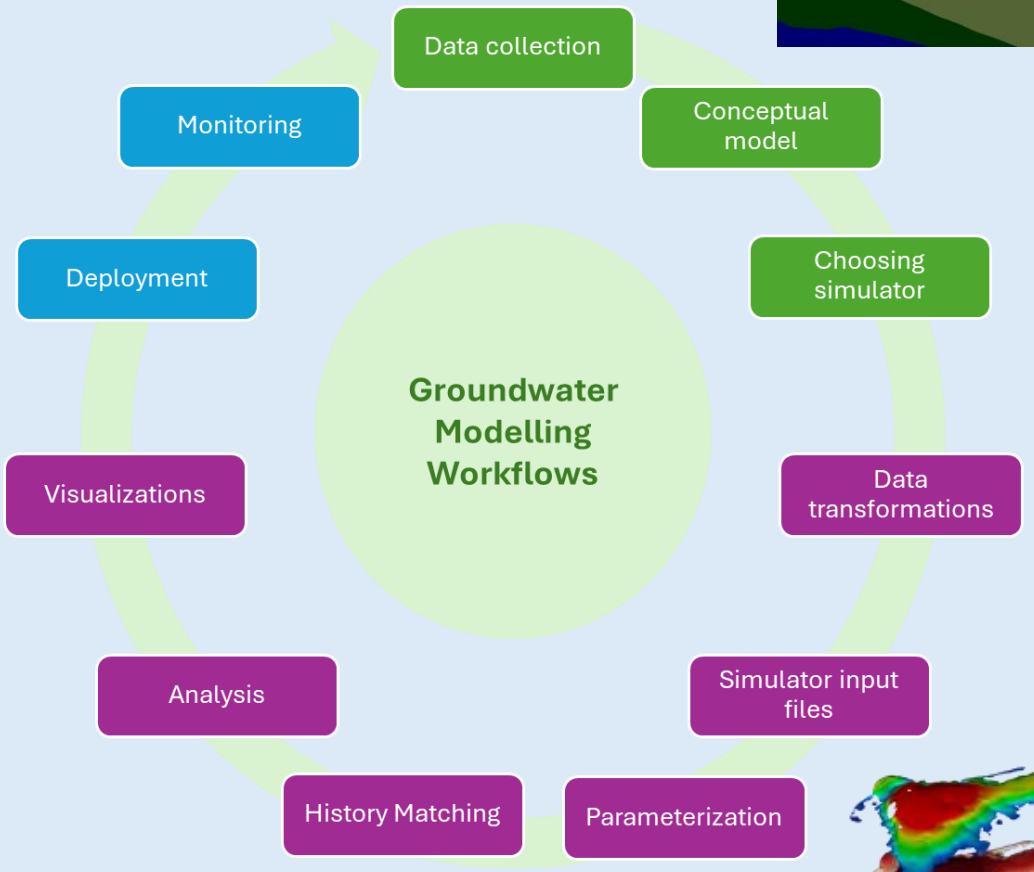
- Engage early with end users and stakeholders to determine predictions of interest and model uses
- Version control can save your bacon
- Set up your diagnostic visualizations early to avoid surprises
- Configuration files (e.g., toml, yaml) can be helpful to track simulation setups
- Setting up a computational environment cannot be neglected (e.g., python virtual environments, Docker containerization)

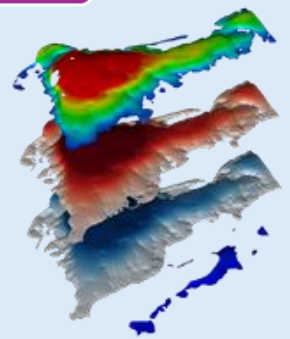


Groundwater modelling workflows



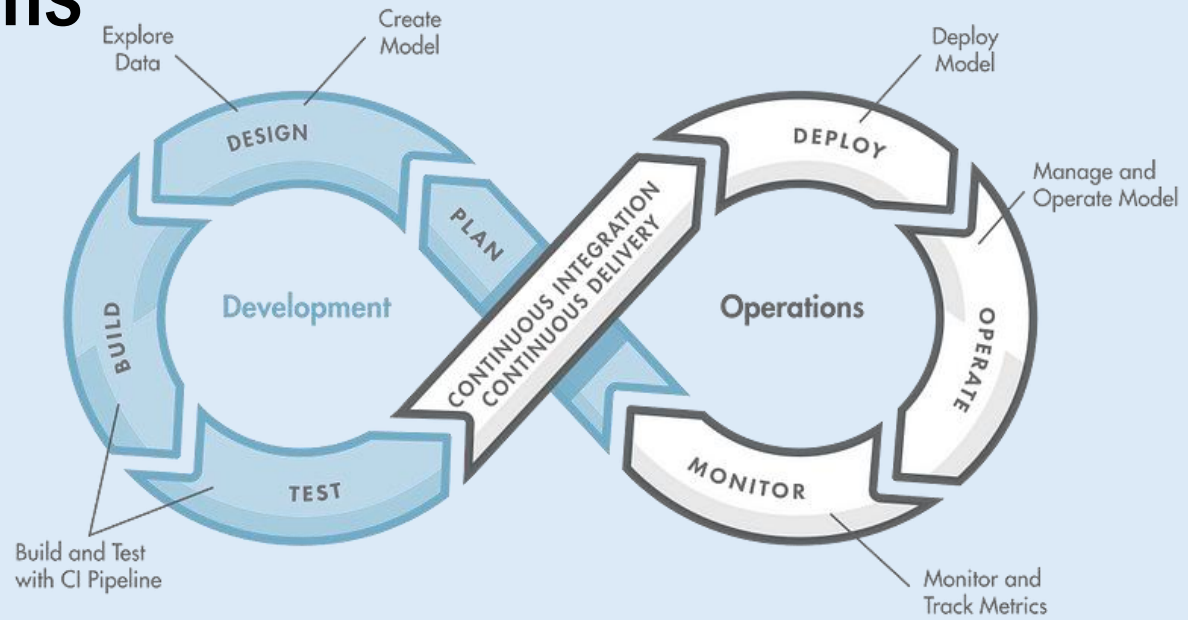






Groundwater modelling workflows

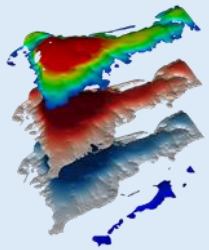
Machine Learning Operations

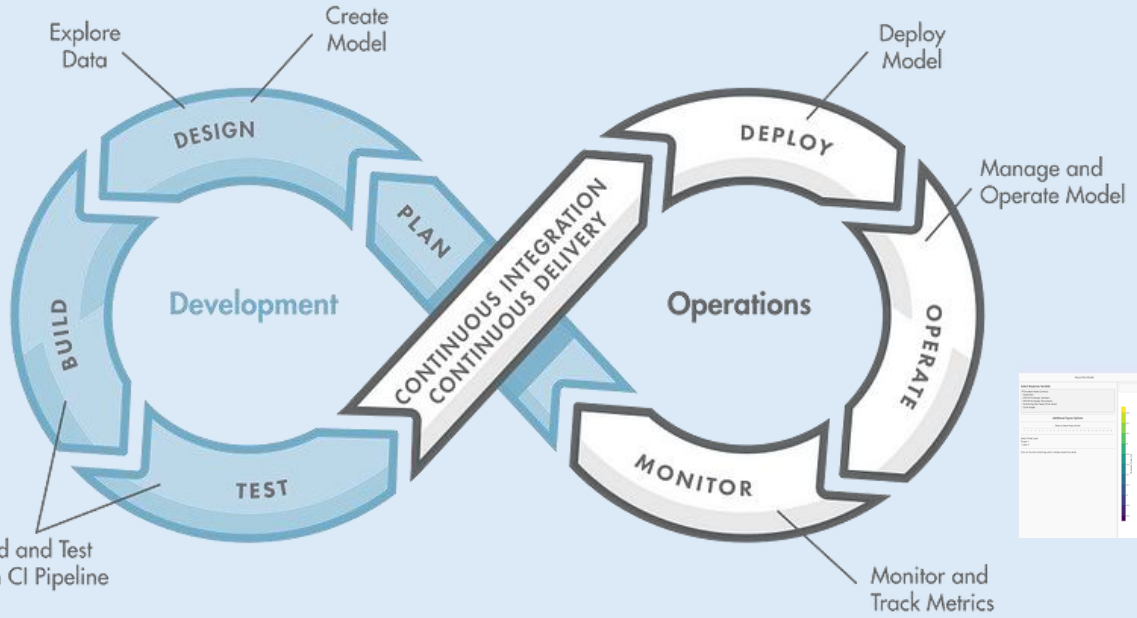


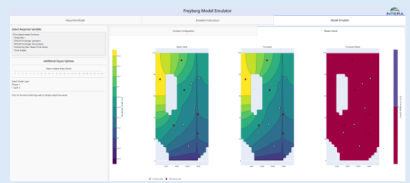
MLOps - MATLAB & Simulink

Groundwater modelling workflows

Machine learning operations







Decision Support Operations

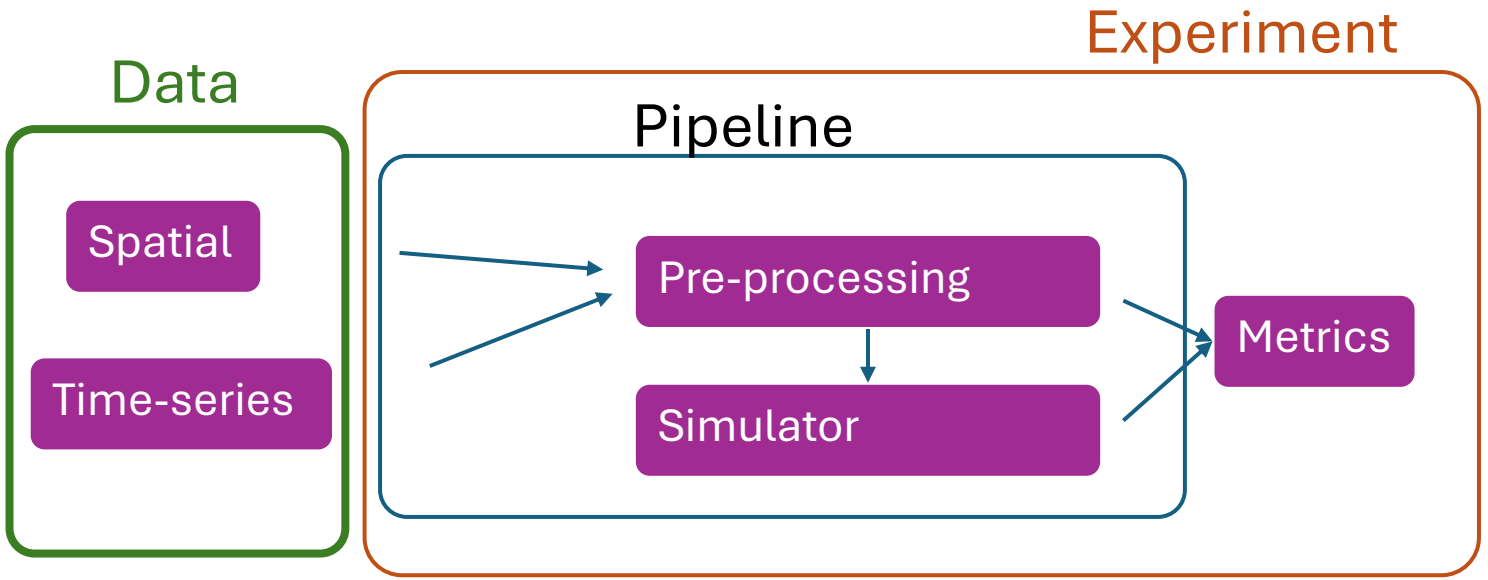
The opportunities of DSOps

- Cool new words to use!
- Explicit definition and versioning of data, pipelines and metrics
- Tracking of experiments and models
- Test-driven development – model review built in
- Link predictions to models and subsequent uses
- Ubiquity of data science and machine learning tools to assist

DSOps in practice

Prediction 1

Experiment 1: Simulator setup



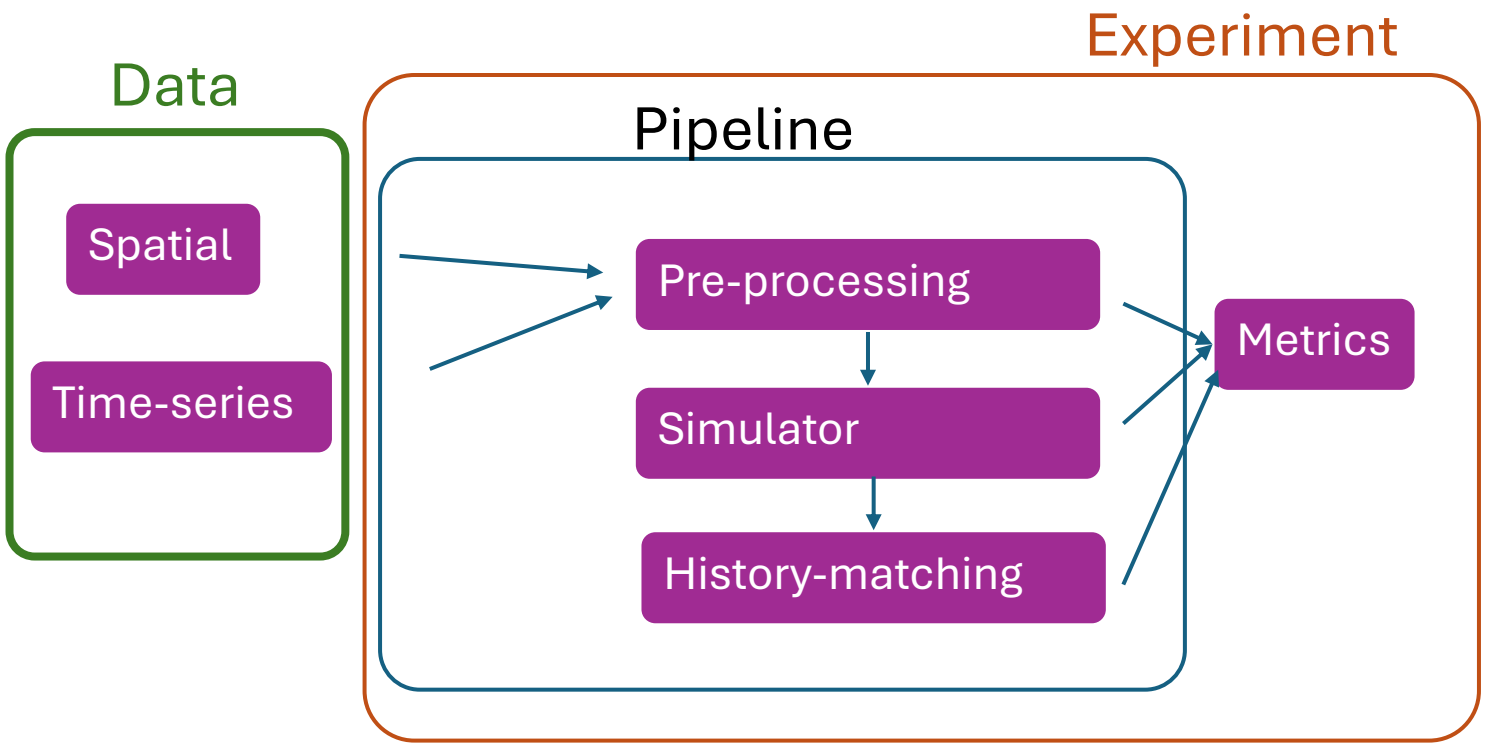
DSOps in practice

Prediction 1

Experiment 1: Simulator setup → Experiment 2: Add history-matching → Experiment 3: Change parameterization scheme → Experiment 4: Predictive simulation

Prediction 2

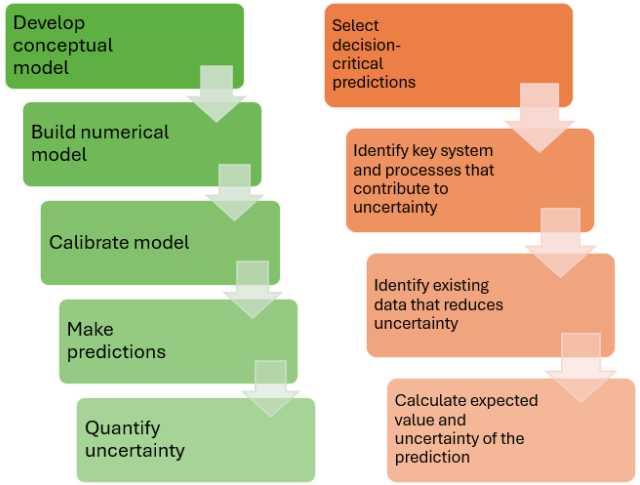
Experiment 5: Predictive simulation



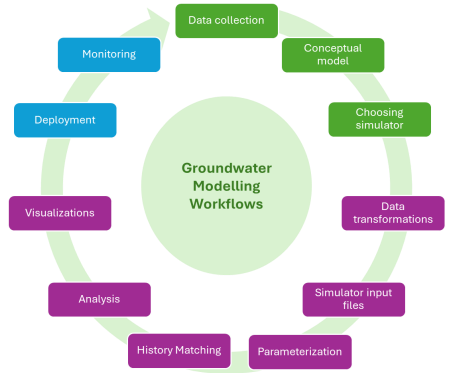
Summary

Developing efficient and transparent groundwater modeling workflows to aid with decision support

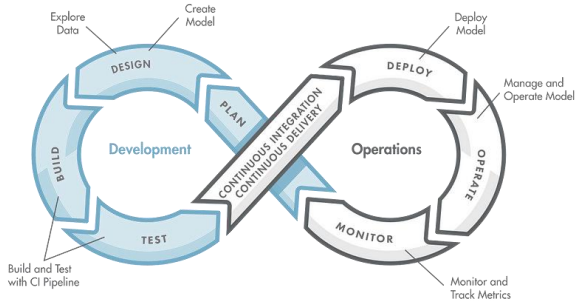
INTERA



Prediction-focussed modelling requires efficient and transparent workflow approaches



Scripted groundwater modelling workflows successfully applied to the Hutt Aquifer, New Zealand



Existing and emerging data science approaches can assist with modelling decision support workflows (DSOps)

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GNS SCIENCE TE PŪ AO

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