Dr.-Ing. Thomas Reimann, Prof. Dr. Rudolf Liedl

General Strategies with numeric modeling

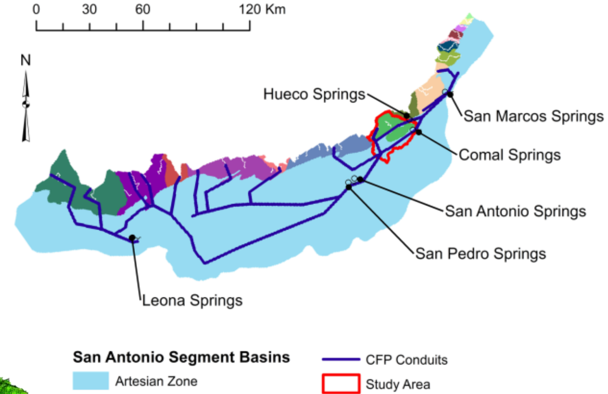
Some insights and examples for complex settings

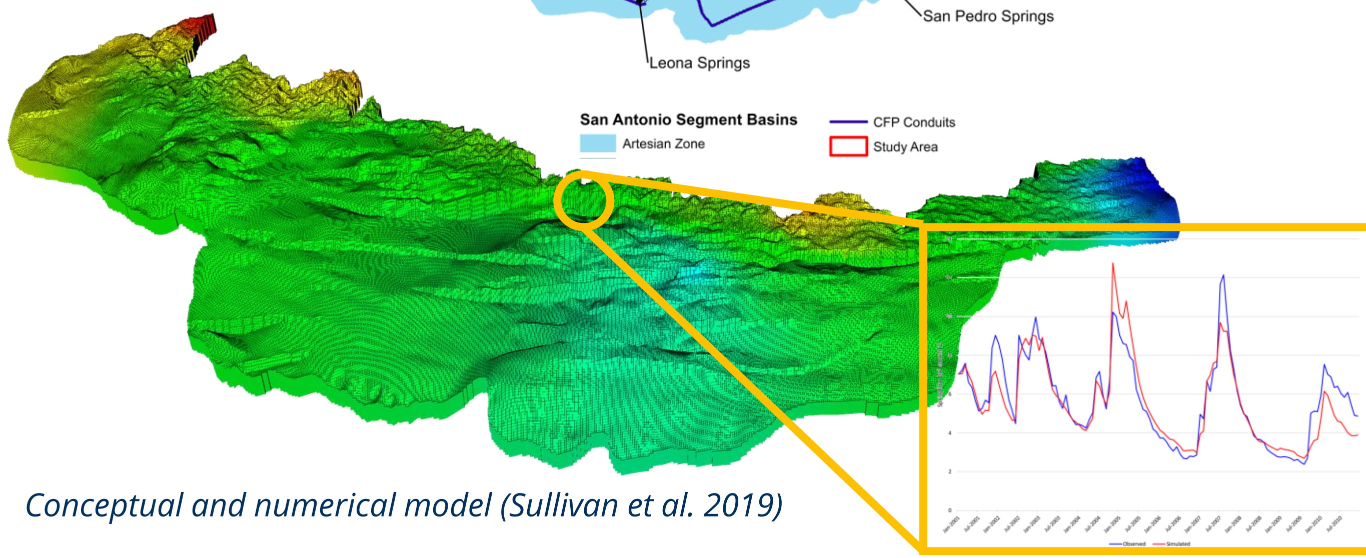
Praha, March 4th, 2019

Investigation and Management of complex systems

Edwards Aquifer (Texas, US) = initial example for motivation

- very productive and important aquifer
- provides drinking water for > 2 million people, agriculture, and industry
- complex karstic system





Comal spring (karst outlet)

Conceptual and numerical model (Sullivan et al. 2019)

The model helps to predict and manage this water resource

Content
of the presentation

- <u>**General workflow**</u>
- Examples:
  - Lez catchment (France)
  - Sheshpeer spring (Iran)
- Conclusion and Outlook

General workflow
Numerical groundwater modeling

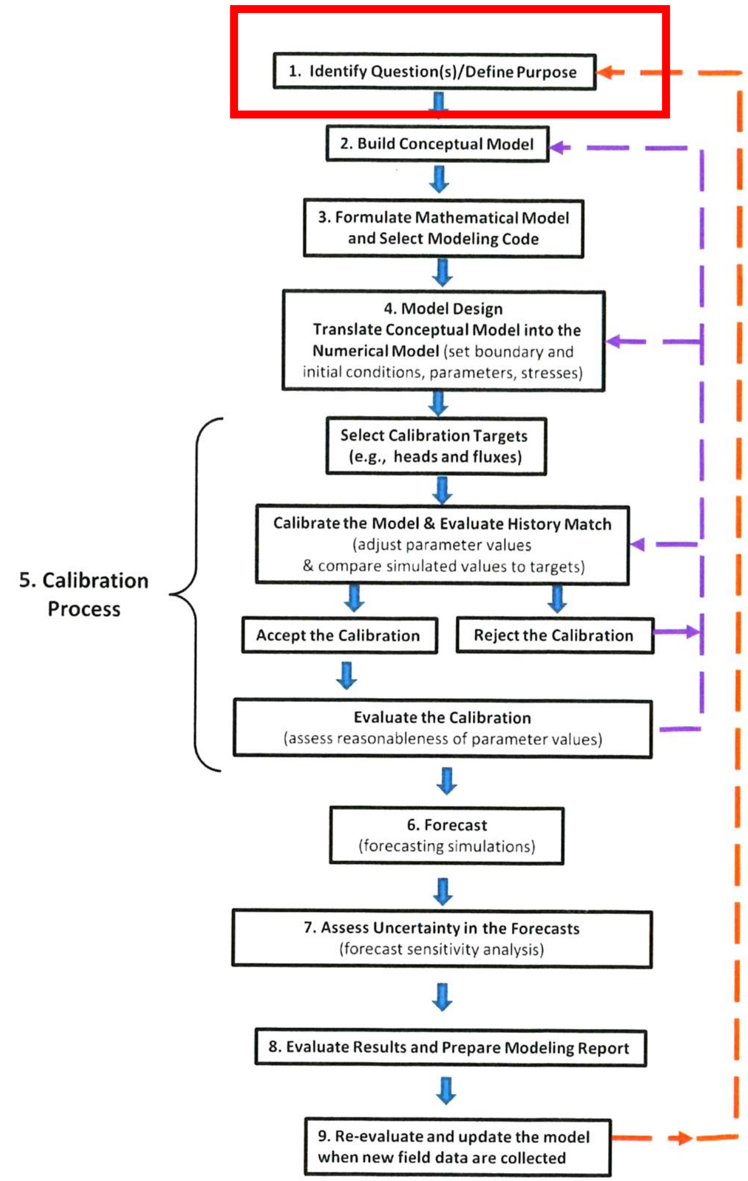
General workflow
1) Question / Purpose

Starting point for modeling:

Question / Purpose

Typical purposes

- prediction
- parameter identification
- system understanding
- analysis / interpretation



Scheme from Anderson et al. 2015

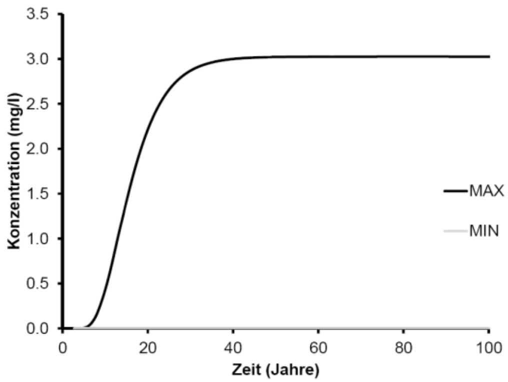
General workflow
1) Question / Purpose

Starting point for modeling:

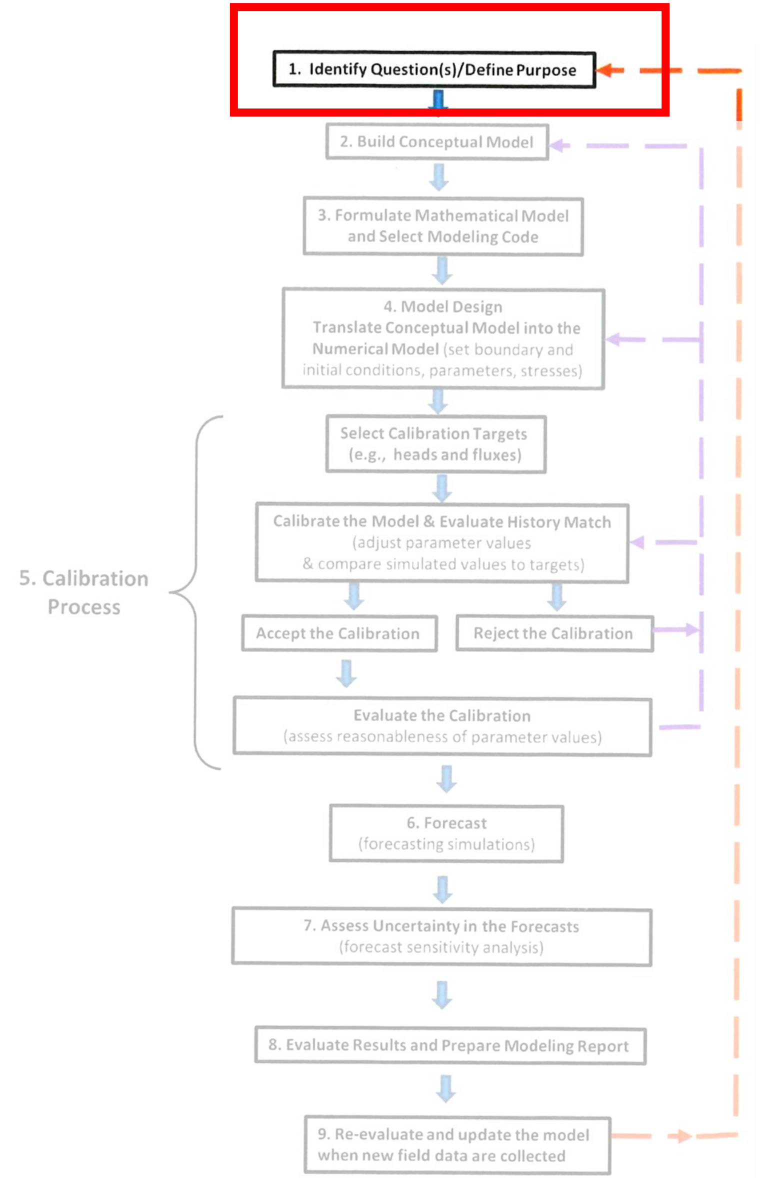
Question / Purpose

Typical purposes

- <u>**prediction**</u>
- parameter identification
- system understanding
- analysis / interpretation



Predicition of solute concentration downstream from a contamination



Scheme from Anderson et al. 2015

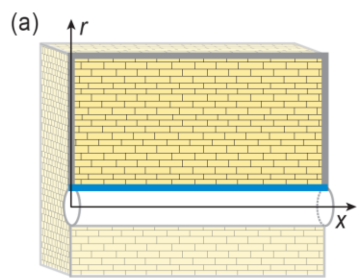
General workflow
1) Question / Purpose

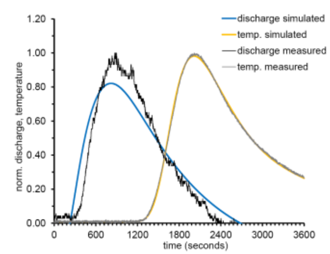
Starting point for modeling:

Question / Purpose

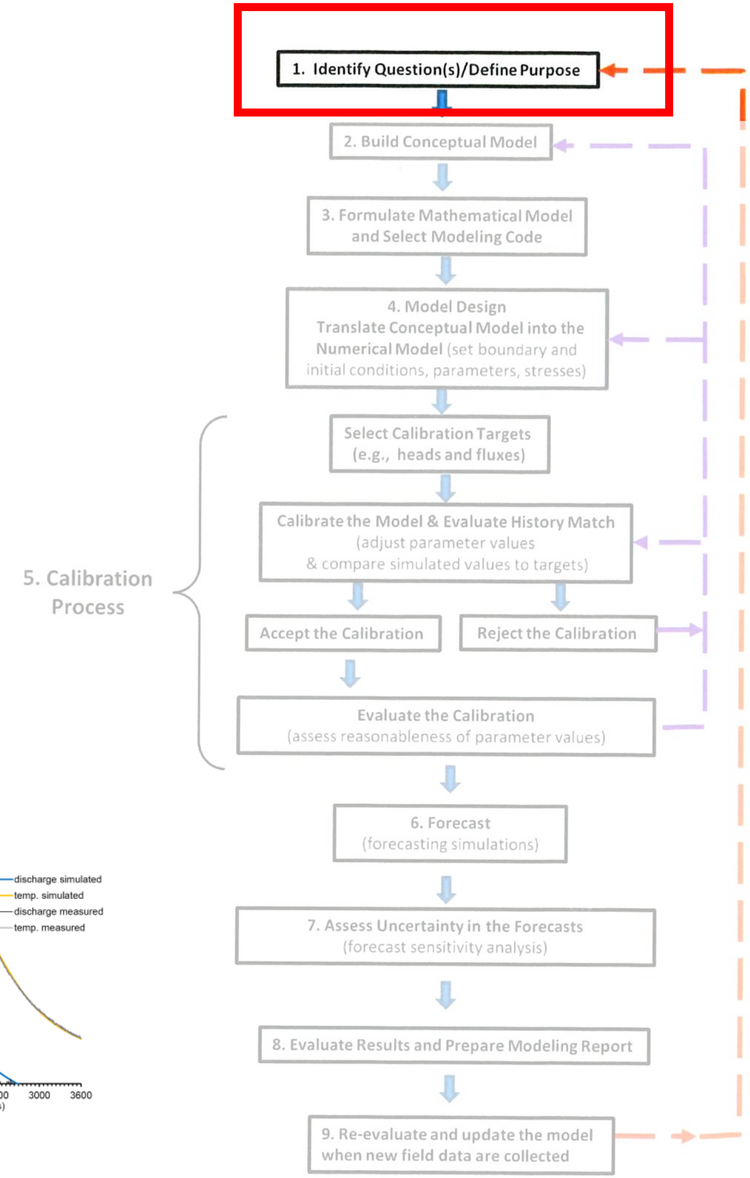
Typical purposes

- prediction
- **parameter identification**
- system understanding
- analysis / interpretation





Inverse parametrization with tracer testing at a karst system (Freiheit Spring, USA)



Scheme from Anderson et al. 2015

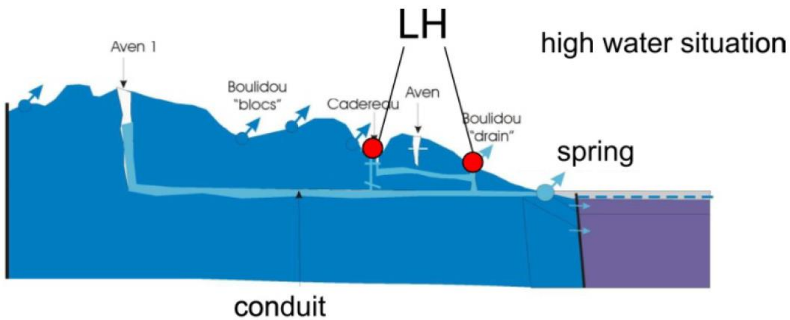
General workflow
1) Question / Purpose

Starting point for modeling:

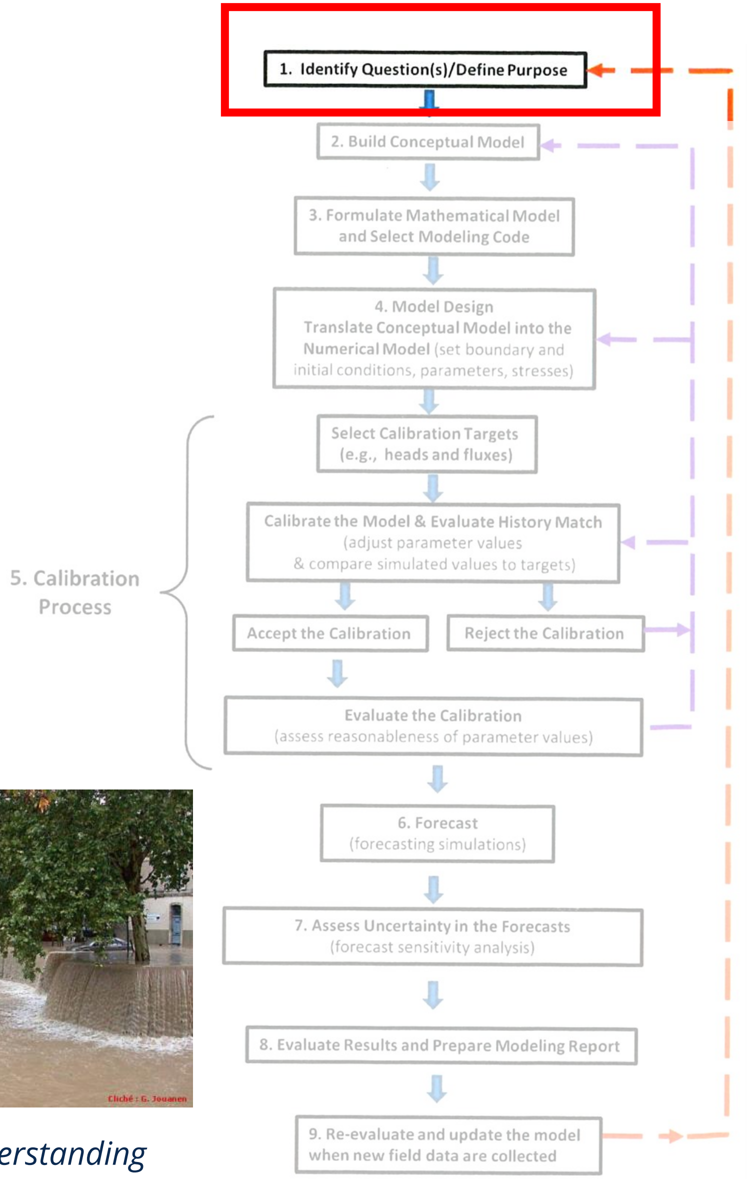
Question / Purpose

Typical purposes

- prediction
- parameter identification
- **system understanding**
- analysis / interpretation



Simulation of a karst system in Nimes (France); the model supports the understanding of the system behavior (overflow springs; Figure: J.-C. Maréchal and photo: G. Jouanen)



Scheme from Anderson et al. 2015

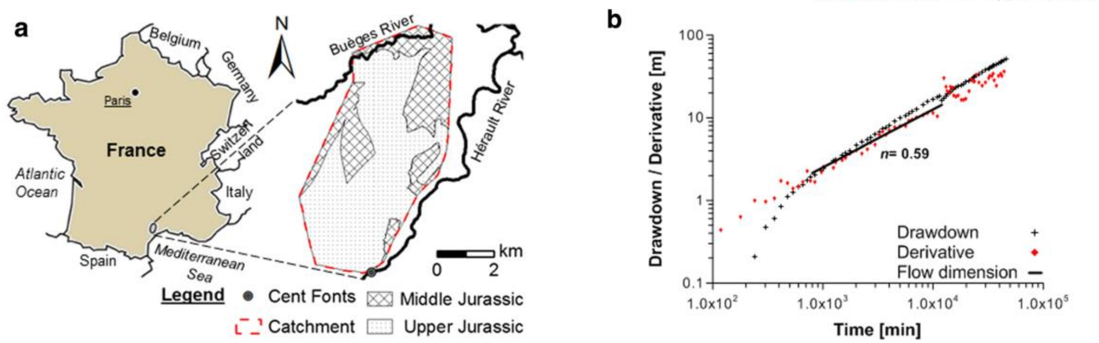
General workflow
1) Question / Purpose

Starting point for modeling:

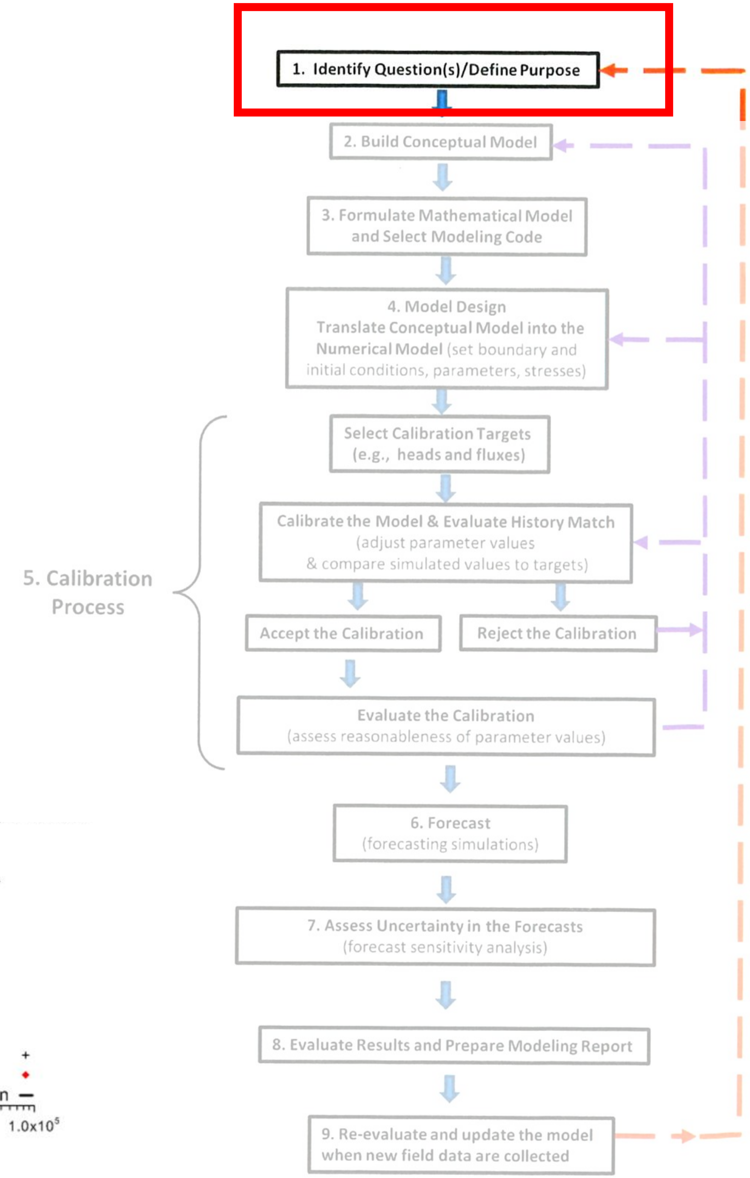
Question / Purpose

Typical purposes

- prediction
- parameter identification
- system understanding
- **analysis / interpretation**



Interpretation of hydraulic tests (e.g. pumping tests; Figures from Giese et al. 2017)



Scheme from Anderson et al. 2015

General workflow
2) Conceptual Model

Very important step

- qualitative system behavior (structure, boundaries)
- interpretation of (current) knowledge
- also: depict current uncertainty
- *further (suggested) reading: Bredehoeft 2005*

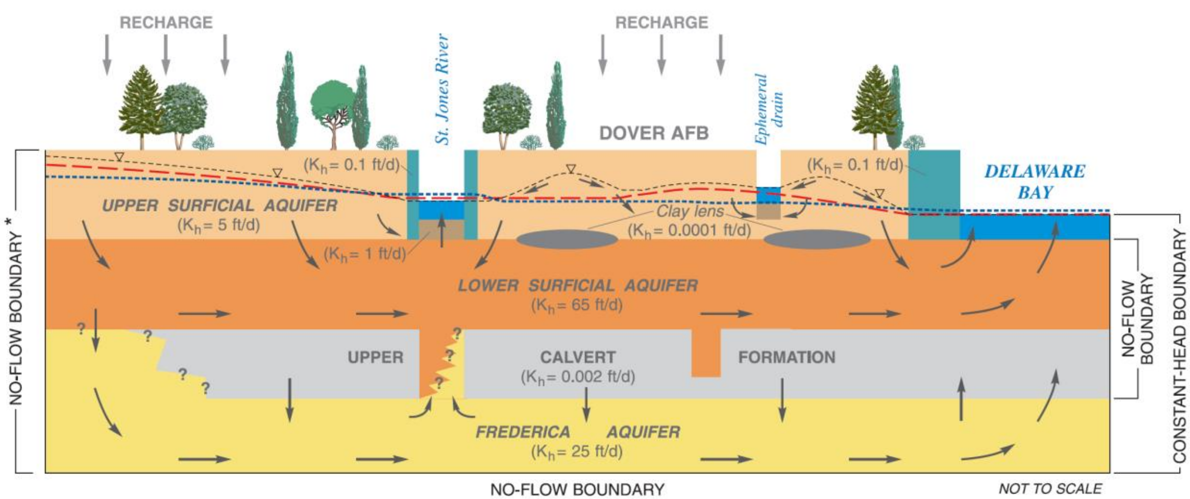
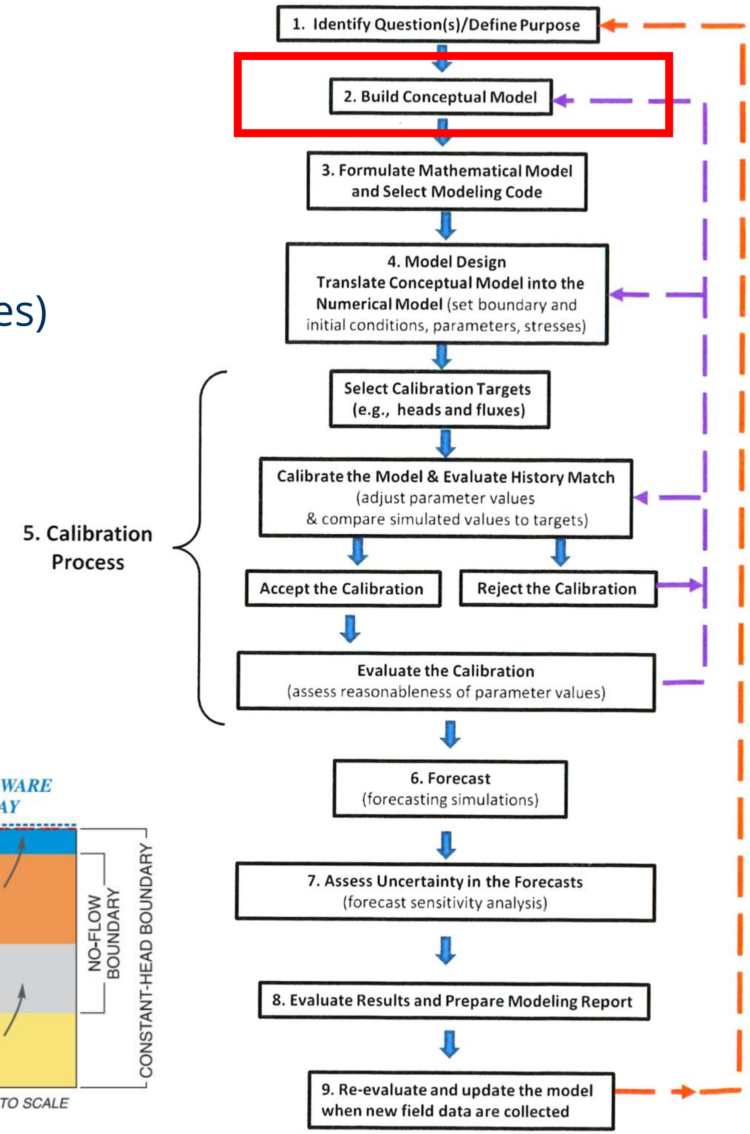


Figure: Example of a conceptual model (USGS WRIR 99-4224)

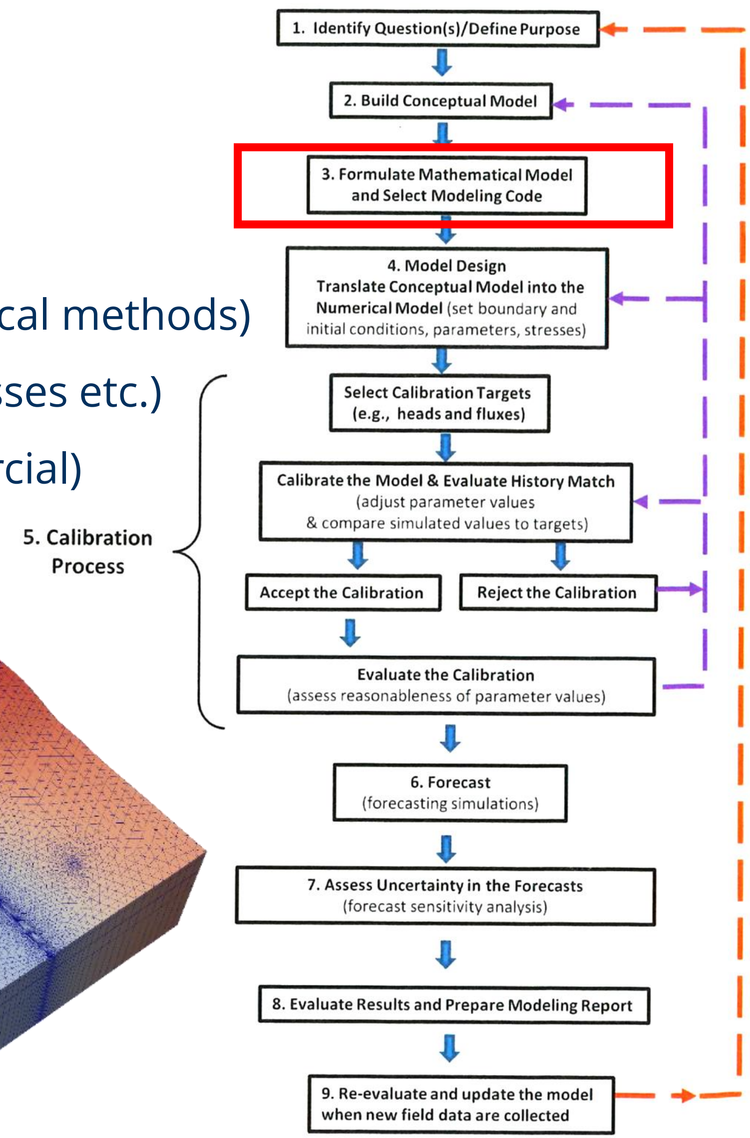


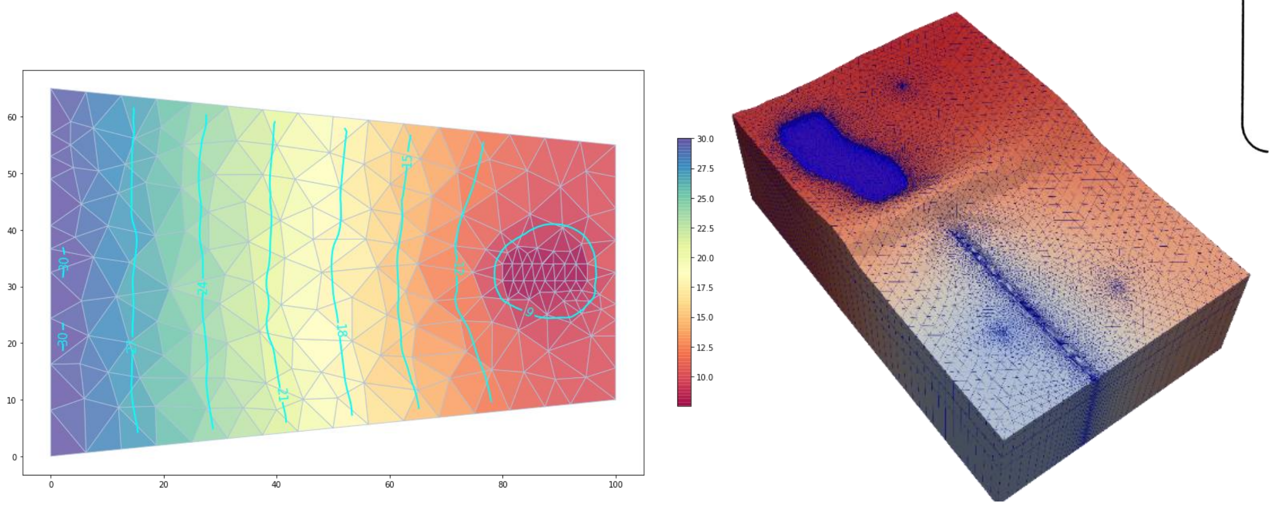
Scheme from Anderson et al. 2015

General workflow
3) Mathematical Model

Quantitative Solution

- Various approaches possible (analytical / numerical methods)
- Intended to reflect the conceptual model (processes etc.)
- Wide range of software available (free & commercial)





Figures: Examples of numerical models (based on MODFLOW6)

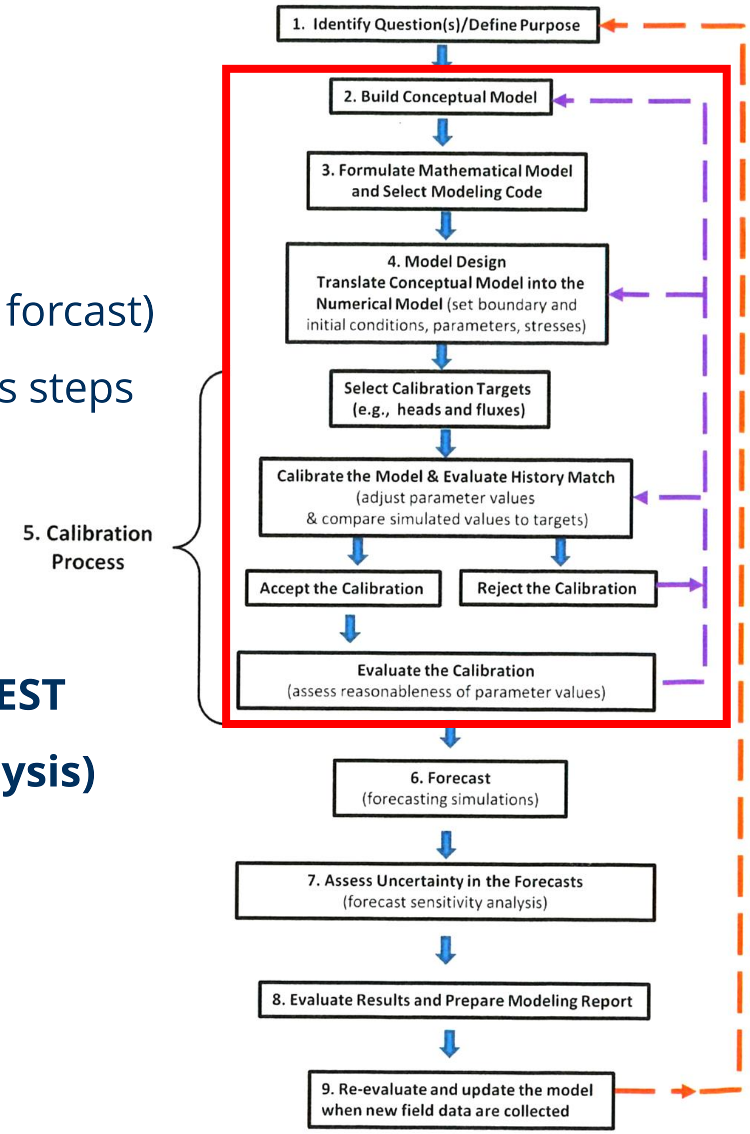
Scheme from Anderson et al. 2015

General workflow
Subsequent steps

Calibration, Sensitivity and Uncertainty analysis

- Depending on the initial question / purpose (e.g. forcast)
- Iterative process with a feedback loop to previous steps

→ **Advanced methods for further analysis like PEST (e.g. automatic calibration & uncertainty analysis)**



Scheme from Anderson et al. 2015

Content
of the presentation

- General workflow
- **Examples:**
  - **Lez catchment (France)**
  - Sheshpeer spring (Iran)
- Conclusion and Outlook

Example

Lez karst spring (France)

Modification of conceptual model

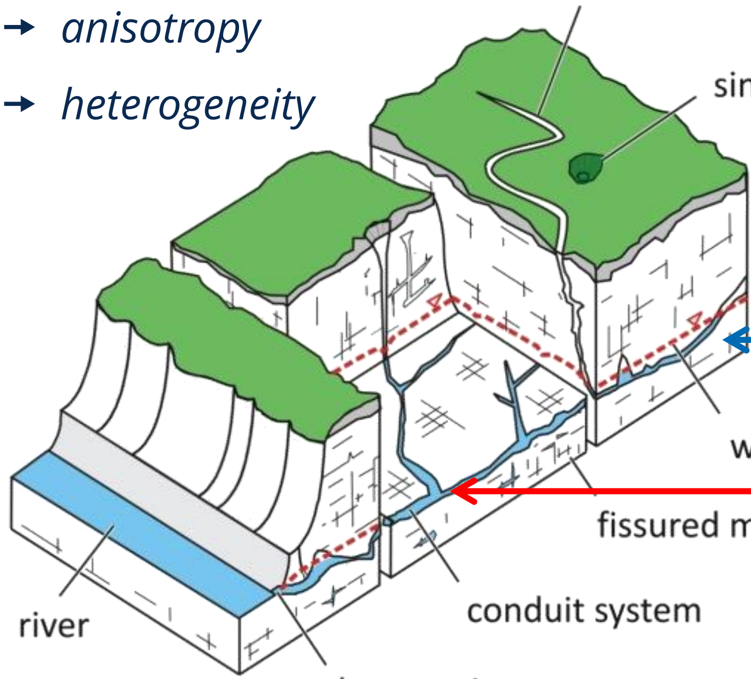
Example: Lez karst spring
Evaluation of large scale pumping

Conceptualization of karstic systems

very distinctive

→ *anisotropy*

→ *heterogeneity*



(from Geyer 2008)

Fractured porous rock matrix:

- low conductivity/large storage
- linear flow (**laminar**)

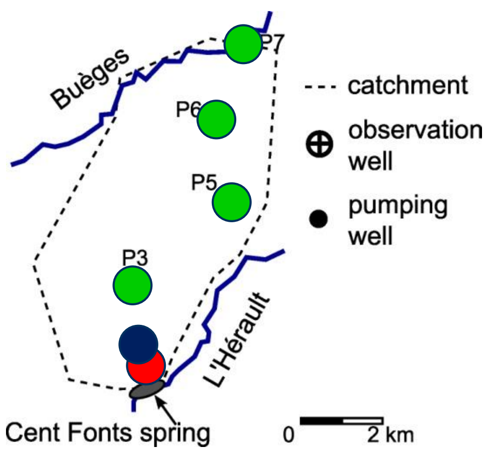
Karst conduits:

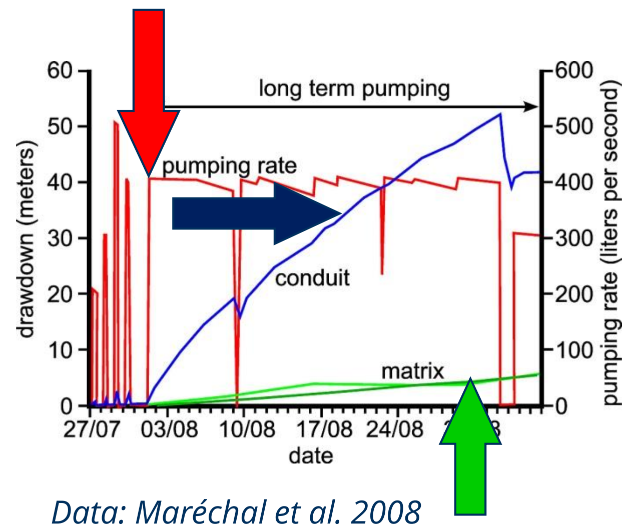
- large conductivity/low storage
- linear/nonlinear flow (**turbulent**)

Example: Lez karst spring
Evaluation of large scale pumping

Karst characterization with artificial signals (high-capacity pumping)

- Lez aquifer (near Montpellier, South of France)
- high capacity pumping test was conducted to investigate the system (cost ~ 14 Mio. €)





Data: Maréchal et al. 2008

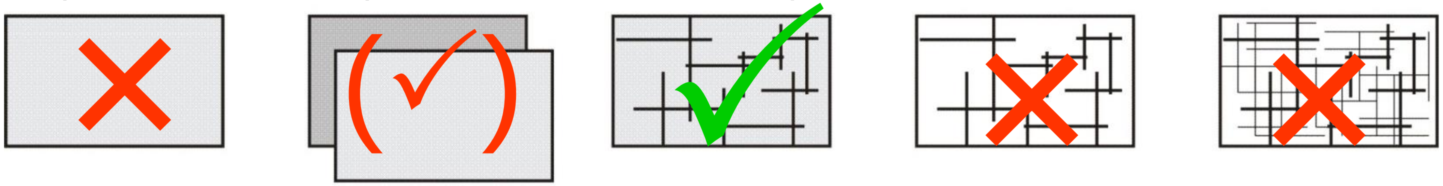
- pumping well
- conduit head observation
- matrix head observation

→ **temporal and spatial system reaction**

Example: Lez karst spring
Evaluation of large scale pumping

Approaches for mathematical models to account for karstic systems

SCPE	DCPE	HM *	DSFS	DMFS
Single Continuum Porous Equivalent	Double Continuum Porous Equivalent	Hybrid Model (Discrete Conduit – Continuum)	Discete Single Fracture Set	Discete Multiple Fracture Set



Deterministic Approach → Stochastic Approach

small — Investigation Effort → high

high ← Practical Applicability — small

limited — Capability to Simulate Heterogeneities → good

** considers turbulent flow in discrete karst conduits that interact with a laminar matrix continuum)*

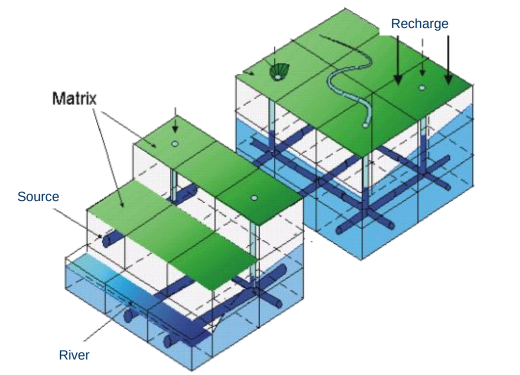
(from Teutsch and Sauter 1991)

Example: Lez karst spring
Evaluation of large scale pumping

Discrete Conduit – Continuum numerical model (Hybrid Modell Approach)

<u>Matrix</u>

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)\pm W = S_S\frac{\partial h}{\partial t}$$



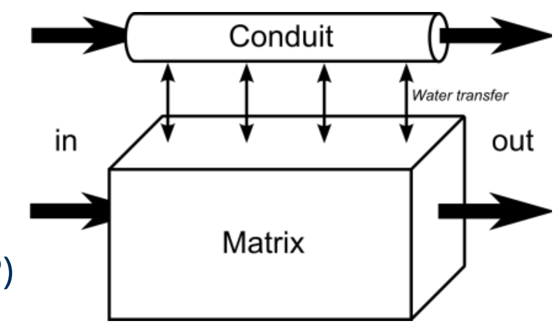
Karst aquifer scheme (Bauer 2002)

<u>Conduit system</u>

laminar $$v = -\frac{d^2\,g}{32\,\nu}I$$ *Hagen Poiseuille*

turbulent $$v = 2log\left(\frac{k_c}{3.71d}+\frac{2.51\nu}{d\sqrt{2gdI}}\right)\sqrt{2gdI}$$ *Colebrook-White*

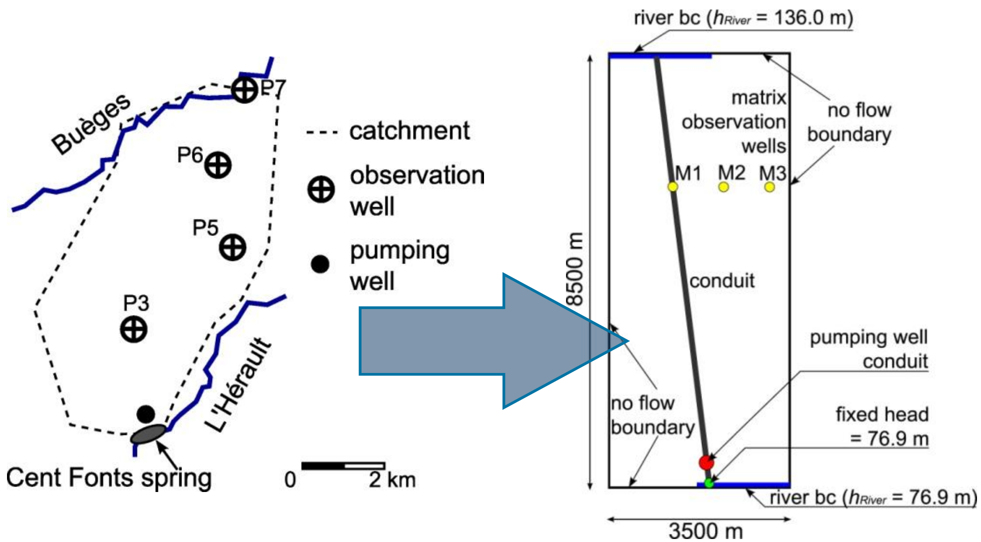
<u>Transfer</u> $$Q_{ex} = \alpha_{ex}(h_c - h_m)$$



Freely available software: MODFLOW-2005 Conduit Flow Process (CFP)

Example: Lez karst spring
Evaluation of large scale pumping

Conceptual model ➝ Idealized numerical model



some available data (e.g. Maréchal et al. 2008)

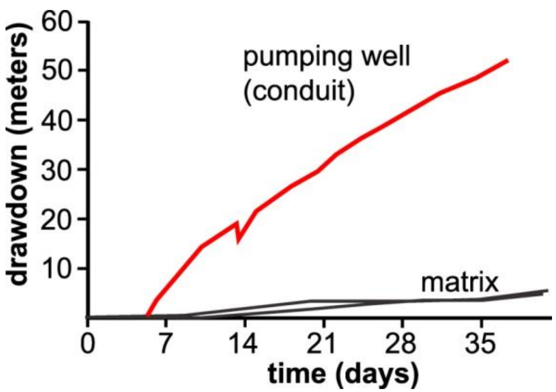
- main conduit diameter ~ 3.5 m
- Transmissivity T_{matrix} 1.6E-5 m^2/s
- Storage S_{matrix} 0.007
- Buèges river loses ~ 0.015 m^3/s
- Hérault inflow during pumping ~ 0.030 m^3/s
- and more …

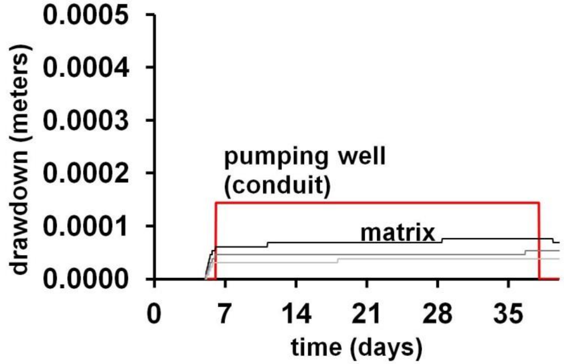
Example: Lez karst spring
Evaluation of large scale pumping

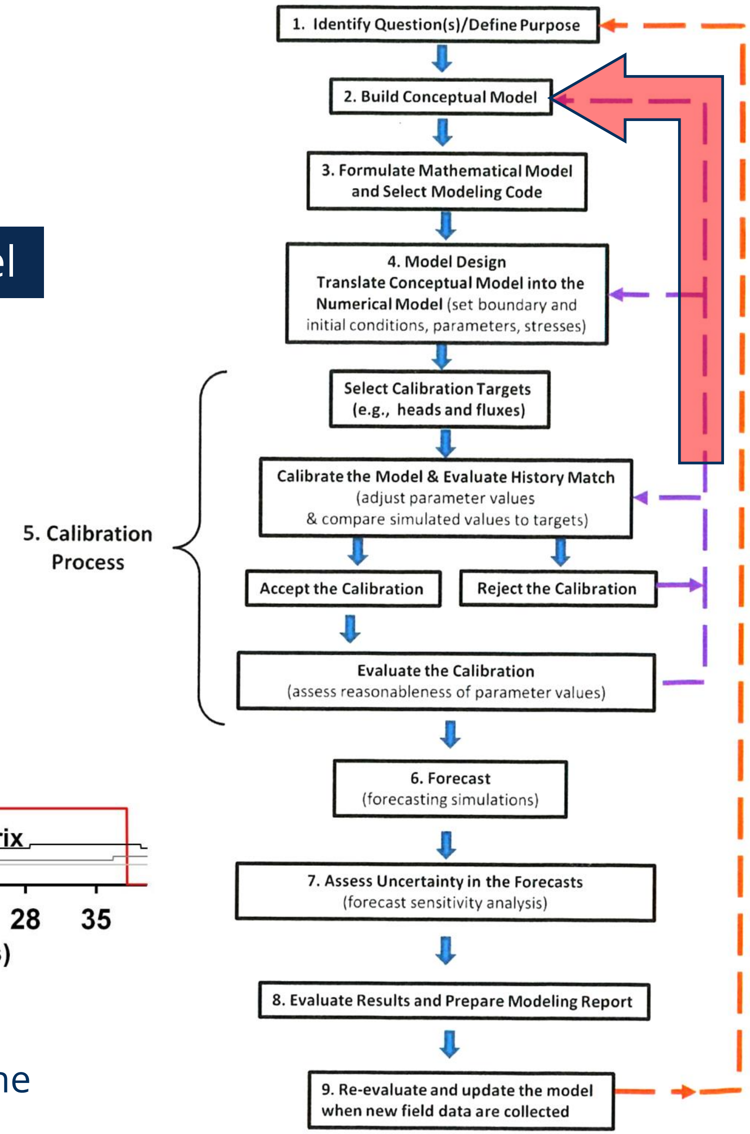
Calibration results with the initial numerical model

Initial results

observed *simulated*







→ necessary revision of the conceptual model to reflect the driving processes because the initial model lack some processes

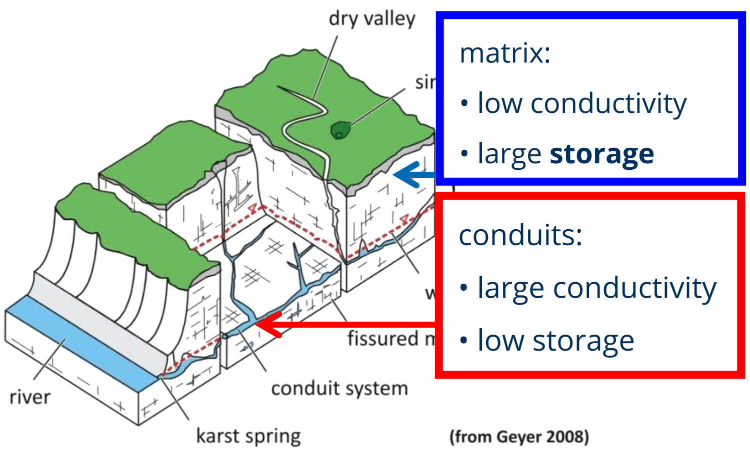
Scheme from Anderson et al. 2015

Example: Lez karst spring
Evaluation of large scale pumping

Enhancement of the mathematical model – consideration of an additional process

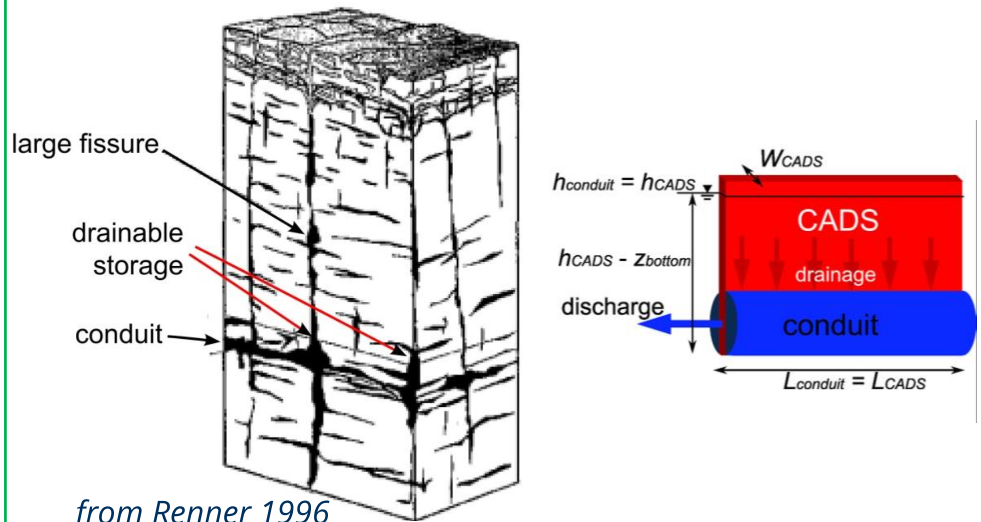
- existing model: **storage** mainly provided by the **matrix**, no storage from the conduit system
- updated model: additional (fast reacting) storage associated with conduits (e.g. large fractures, caves)

Existing model



(from Geyer 2008)

Updated model



from Renner 1996

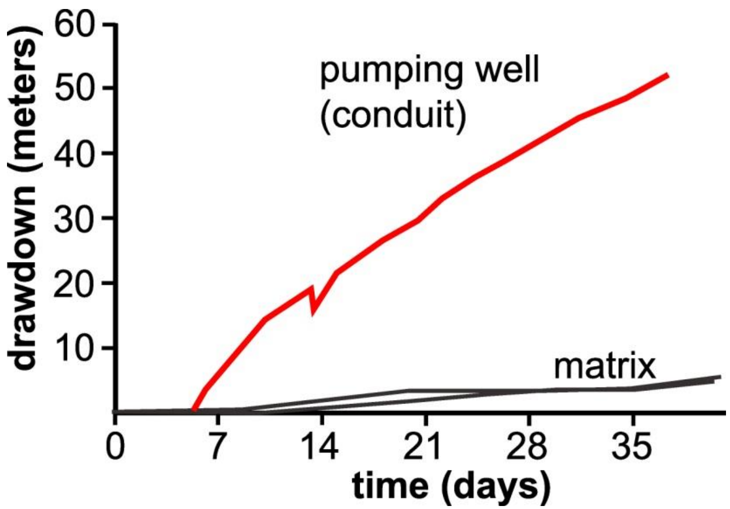
→ **Addition of drainable storage to conduits as already depicted in the concept of Renner 1996**

Example: Lez karst spring
Evaluation of large scale pumping

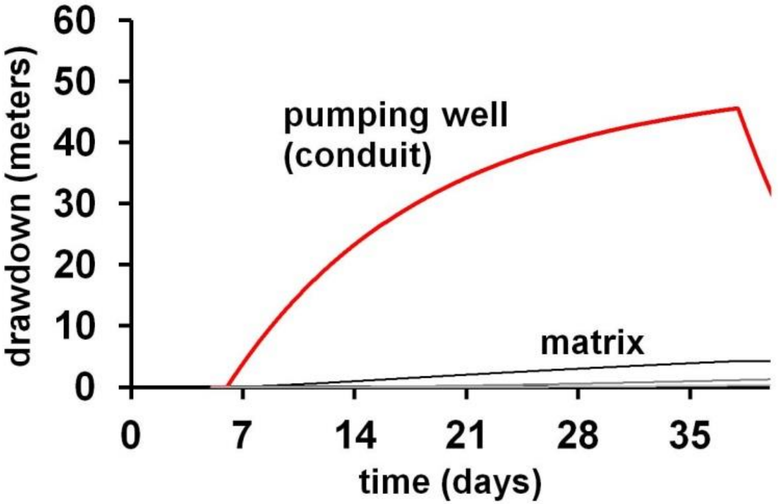
Calibration results with the enhanced numerical model

Preliminary results

observed



simulated



→ the (enhanced) numerical model can reflect the processes (ready for a refined calibration)

Content
of the presentation

- General workflow
- **Examples:**
  - Lez catchment (France)
  - **Sheshpeer spring (Iran)**
- Conclusion and Outlook

Sheshper spring Iran

Multi-criteria-optimization

Example: Sheshpeer spring
Karst characterization with multiple signals

Example: Sheshpeer Catchment, Iran

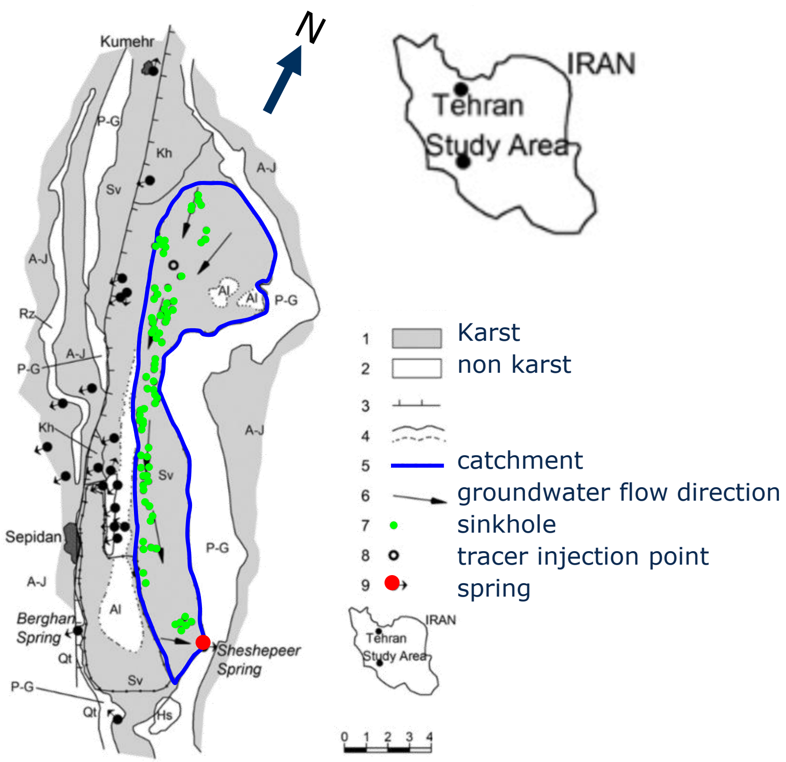
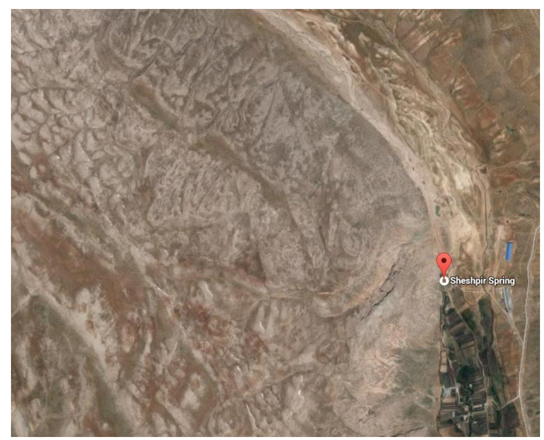


Figure from Raeisi 2010



from Google maps

Content
of the presentation

- General workflow
- Examples:
  - Lez catchment (France)
  - Sheshpeer spring (Iran)
- **<u>Conclusion and Outlook</u>**

General strategies with numeric modeling

Conclusion and Outlook

General strategies with numeric modeling
Conclusion and Outlook

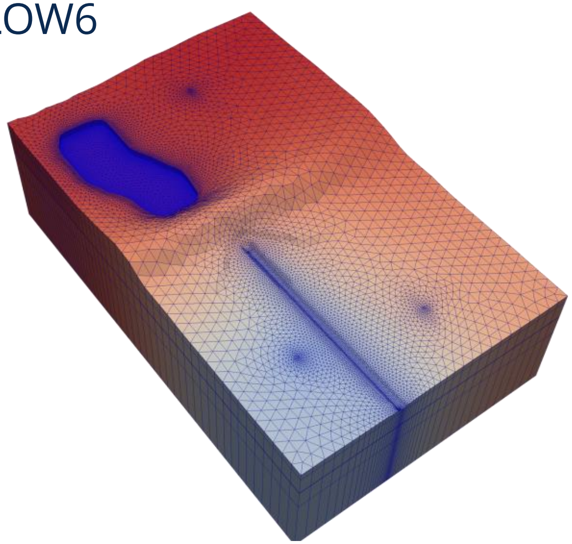
Development trends

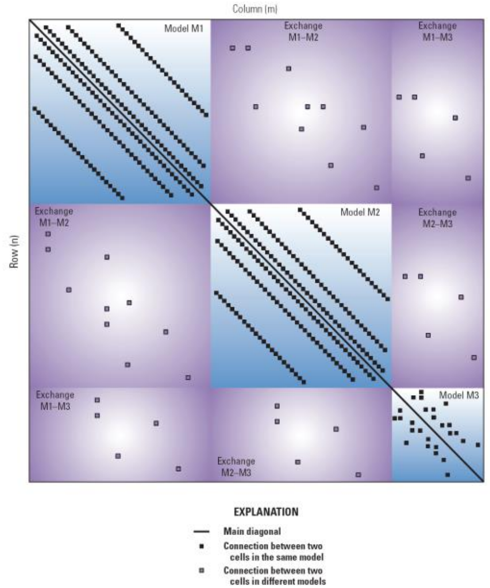
- Increasing computing power
- Increasing connection and networking
- Data: Improved access and increasing amount

General strategies with numeric modeling
Conclusion and Outlook

Development of the numerical flow model MODFLOW (open source & state of the art)

- MODFLOW6





MODFLOW6: flexible finite-volume discretization and flexible coupling of several models

(figures from MODFLOW6 documentation)

➔ flexible spatial discretization (control finite volume)

➔ coupling of several models (one solution matrix for several models)

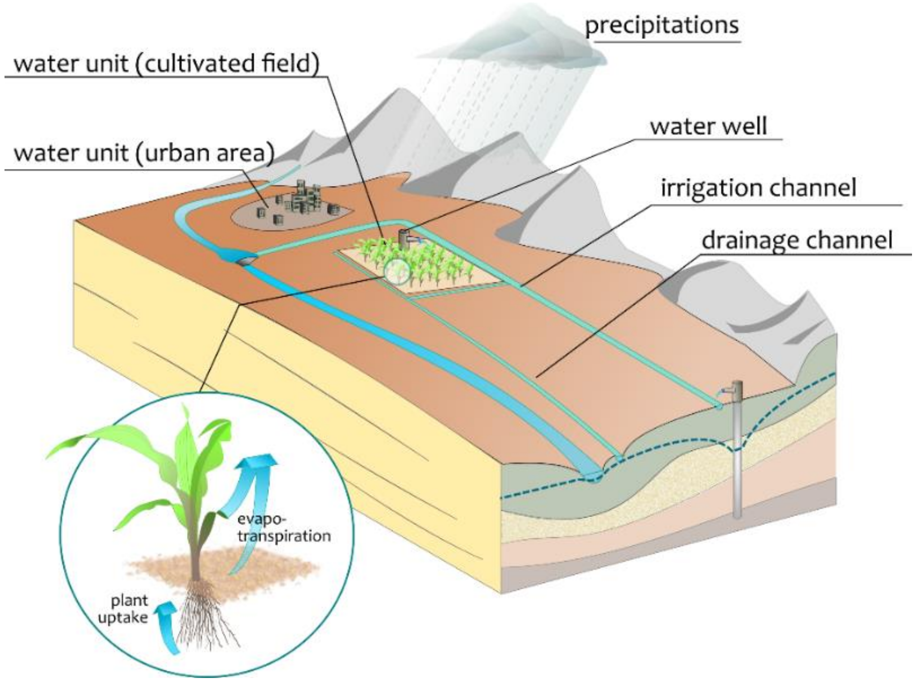
General strategies with numeric modeling
Conclusion and Outlook

Development of the numerical flow model MODFLOW (open source & state of the art)

- MODFLOW6
- MODFLOW One-Water-Hydrologic-Modell (OWHM2)

➜ reflects the overall hydrologic cycle

➜ several processes (agriculture, unsaturated zone, streams etc.)



MODFLOW-OWHM: integrated hydrologic model

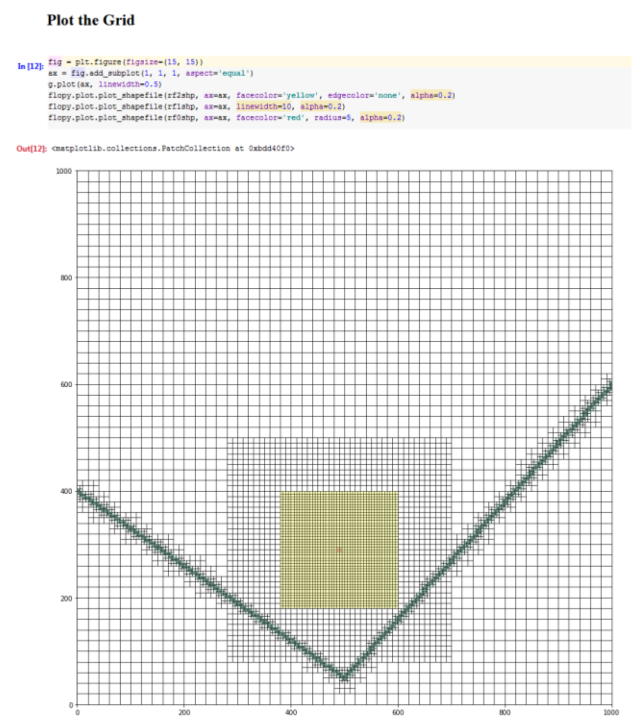
General strategies with numeric modeling
Conclusion and Outlook

Development of the numerical flow model MODFLOW (open source & state of the art)

- MODFLOW6
- MODFLOW One-Water-Hydrologic-Modell (OWHM2)

Development of Pre- and Postprocessing

- Script based (Python, FloPy)



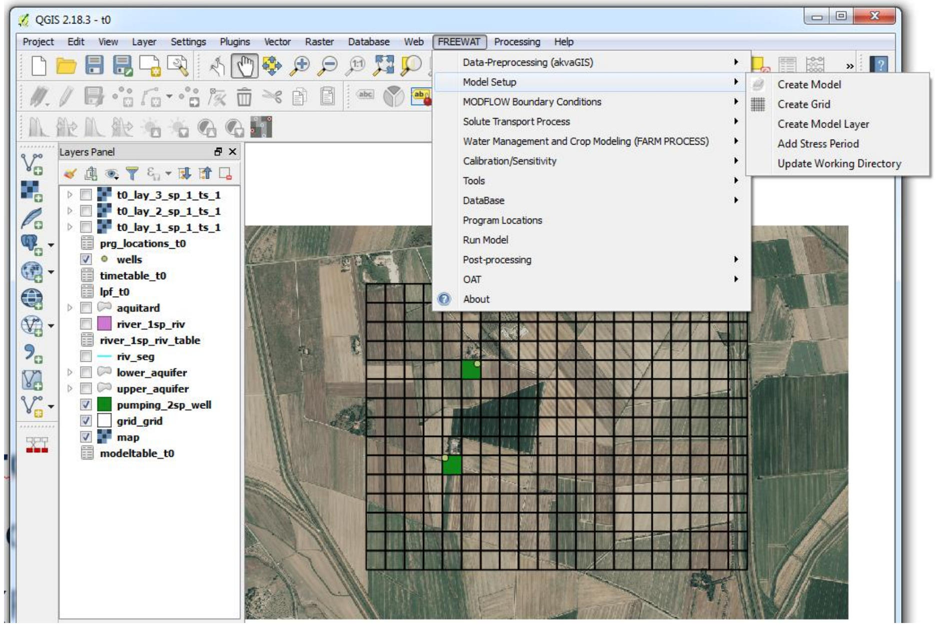
General strategies with numeric modeling
Conclusion and Outlook

Development of the numerical flow model MODFLOW (open source & state of the art)

- MODFLOW6
- MODFLOW One-Water-Hydrologic-Modell (OWHM2)

Development of Pre- and Postprocessing

- Script based (Python, FloPy)
- Integration in GIS (QGIS; FREEWAT)



References and some further readings

- Sullivan, T. P., Gao, Y., Reimann, T.: Nitrate Transport in a Karst Aquifer: Numerical Model Development and Source Evaluation. Journal of Hydrology, https://doi.org/10.1016/j.jhydrol.2019.03.078.
- Giese, M., Reimann, T., Bailly-Comte, V., Maréchal, J.-C., Sauter, M., & Geyer, T.: Turbulent and laminar flow in karst conduits under unsteady flow conditions: Interpretation of pumping tests by discrete conduit-continuum modeling. Water Resources Research, 54, 1918–1933, https://doi.org/10.1002/2017WR020658.
- Giese, M., Reimann, T., Liedl, R., Maréchal, J.-C., Sauter, M.: Application of the flow dimension concept for numerical drawdown data analyses in mixed-flow karst systems. Hydrogeol J. 25: 799. https://doi.org/10.1007/s10040-016-1523-7.
- Reimann, T., Giese, M., Geyer, T., Liedl, R., Maréchal, J.C., and Shoemaker, W.B.: Representation of water abstraction from a karst conduit with numerical discrete-continuum models, Hydrol. Earth Syst. Sci., 18, 227-241, doi: 10.5194/hess-18-227-2014.
- Langevin, Christian D.; Hughes, Joseph D.; Banta, Edward R.; Niswonger, R. G.; Panday, Sorab; Provost Alden M. (2017): Documentation for the MODFLOW 6 Groundwater Flow Model. United States Geological Survey USGS. Reston, Virginia, USA (US Geological Survey Techniques and Methods, TM6-A55).
- Anderson, Mary P.; Woessner, William W.; Hunt, Randall J. (2015): Applied groundwater modeling. Simulation of flow and advective transport. Second Edition. Amsterdam: Elsevier.
- Bredehoeft, John (2005): The conceptualization model problem? Surprise. In: Hydrogeol J 13 (1), S. 37–46. DOI: 10.1007/s10040-004-0430-5.

Further information and contact: Thomas.Reimann@tu-dresden.de