National Aeronautics and
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Uncertainty Quantification for Science and Engineering Applications

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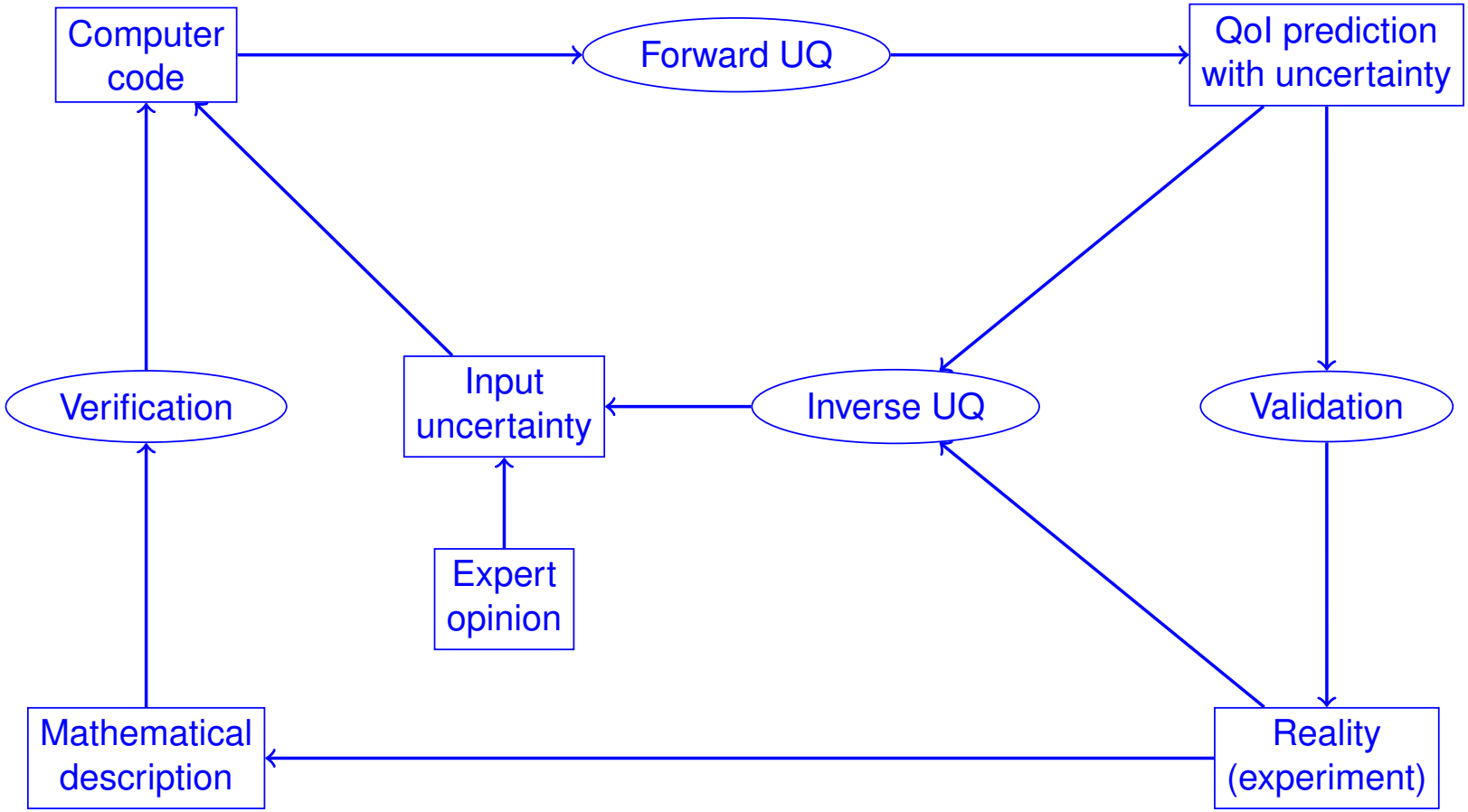
Outline

- Introduction
- What is Uncertainty Quantification (UQ)?
- Various definitions
- UQ for remote sensing observing systems
- Engineering viewpoint
- Science viewpoint
- Simulation-based UQ (time permitting)
- Discussion

What is UQ?

- Like “Statistics” vs. “statistics”.
- Uncertainty Quantification is an emerging meta-discipline
  - theory from Math and Statistics, and generally relies on probability
  - practice is like that of Statistics: depends on application
  - effective implementation depends on intimate knowledge of domain
- “uncertainty quantification” is any activity that delivers a number and declares it to represent “uncertainty” in the English-language sense.

What is UQ?



Adapted from Wu et al, (2018). DOI: 10.1016/j.nucengdes.2018.06.004.

Some definitions

Ralph Smith:

> *The synergy between statistics, applied mathematics and domain sciences required to quantify uncertainties in inputs and QoI when models are too computationally complex to permit sole reliance on sampling-based methods.*

Some definitions

National Research Council:

> *The process of quantifying uncertainties associatied with model calculations of true, physical QoIs, with the goals of accounting for all sources of uncertainty and quantifying the contributions of specific sources to the overall uncertainty.*

From *Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Validation, Verifiction, and Uncertainty Quantification* (2012).

Some definitions

- Focus on output of deterministic models.
- Began with engineering applications.
- Forward propagation of known variability in inputs through the model.
- What if input uncertainties are not known? $\longrightarrow$ inverse UQ.
- What if the model itself isn't perfect? $\longrightarrow$ model discrepancy.
- If brute force Monte Carlo isn't feasible for forward propagation,
  - Polynomial chaos
  - Response surface methodology + design of experiments + emulators
  - Sensitivity analysis?

Some definitions

Me:

Determination of the sampling distribution of the model (as an estimator), and its relationship to the true value of the QoI.

Determination of the joint distribution of the model's estimate and the true value of the QoI.

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Remote sensing observing systems

True state | Forward function | Noiseless radiance | Instrument | Observation | Retrieval | State estimate

Retrieval is an inference problem: estimate X when you only get to see Y.

F_0 = nature's true forward function; B_0 = other true quantities.

F_1 = forward model used in retrieval, R; B_1 = other retrieval inputs.

ϵ = instrument measurement error.

. . . = other retrieval algorithm inputs.

Remote sensing observing systems

What is the computational model here?

True state	Forward function	Noiseless radiance	Instru-ment	Obser-vation	Retrieval	State estimate

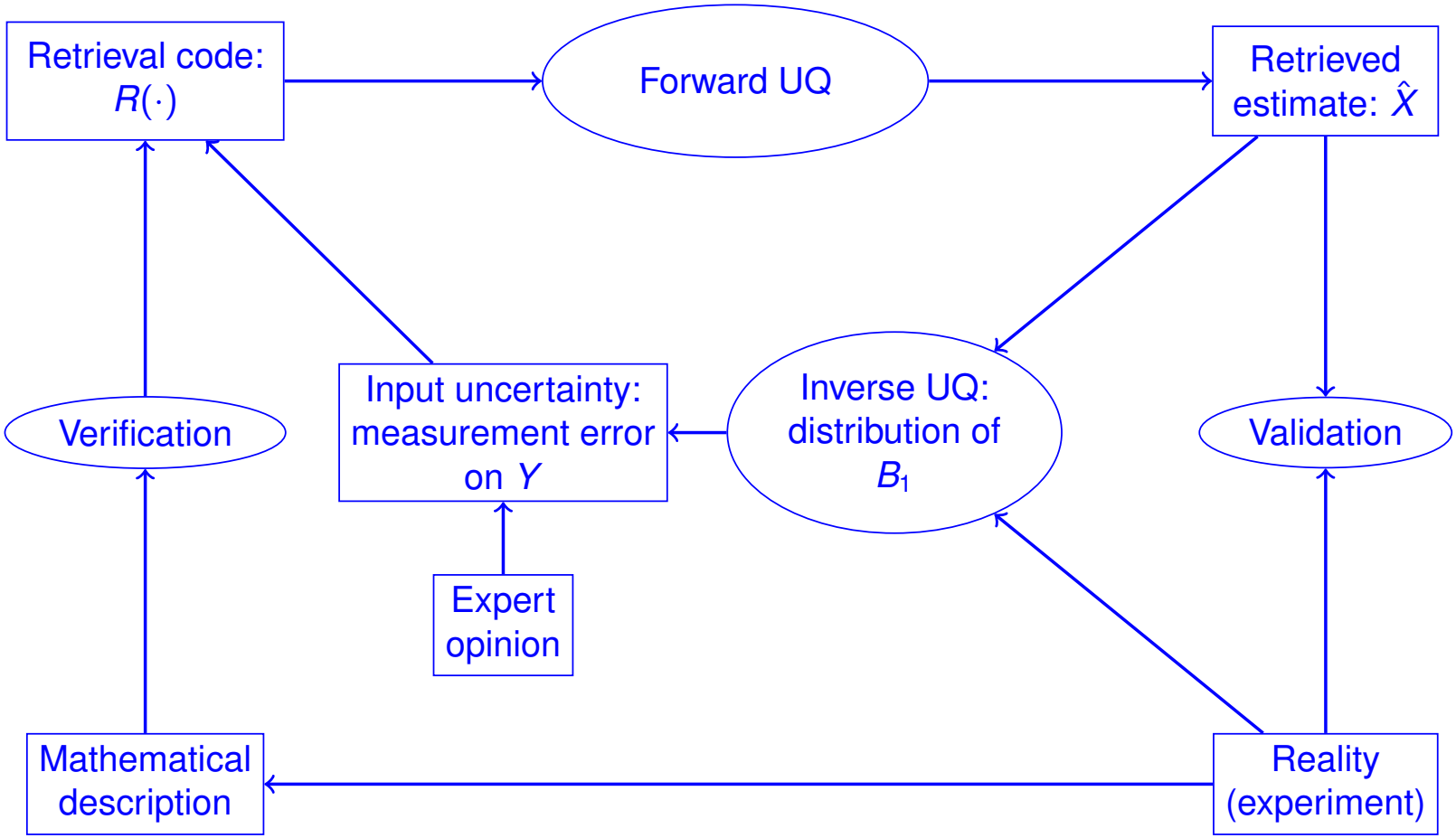
$$X \longrightarrow \boxed{F_0(\cdot, B_0)} \longrightarrow \mathcal{Y}_0 \longrightarrow \boxed{\mathcal{Y}_0 + \epsilon} \longrightarrow Y \longrightarrow \boxed{R(\cdot, F_1, B_1 \ldots)} \longrightarrow \hat{X}$$

Or,

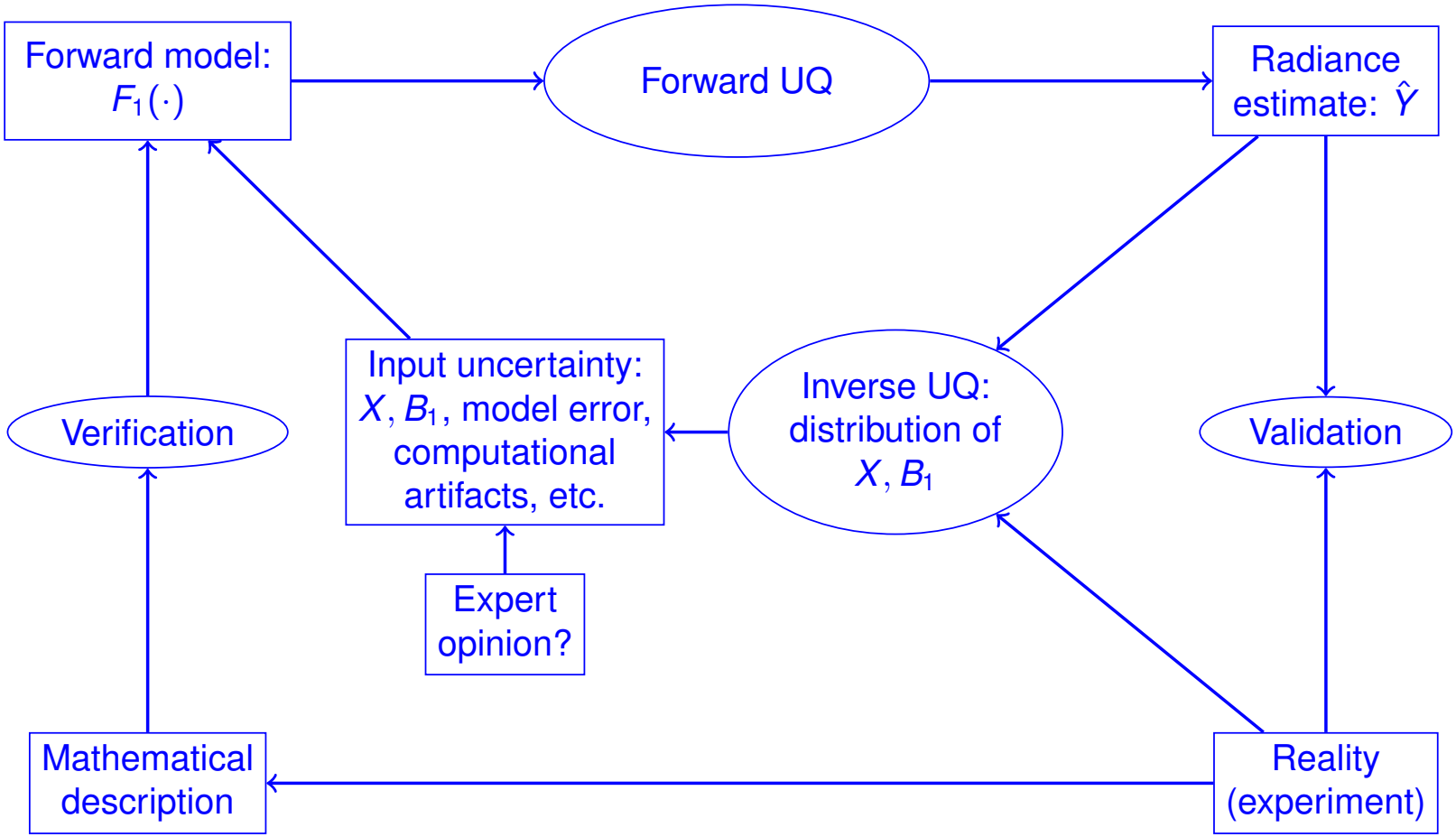
True state	Forward function	Noiseless radiance	Instru-ment	Obser-vation	Retrieval	State estimate

$$X \longrightarrow \boxed{F_0(\cdot, B_0)} \longrightarrow \mathcal{Y}_0 \longrightarrow \boxed{\mathcal{Y}_0 + \epsilon} \longrightarrow Y \longrightarrow \boxed{R(\cdot, F_1, B_1 \ldots)} \longrightarrow \hat{X}$$

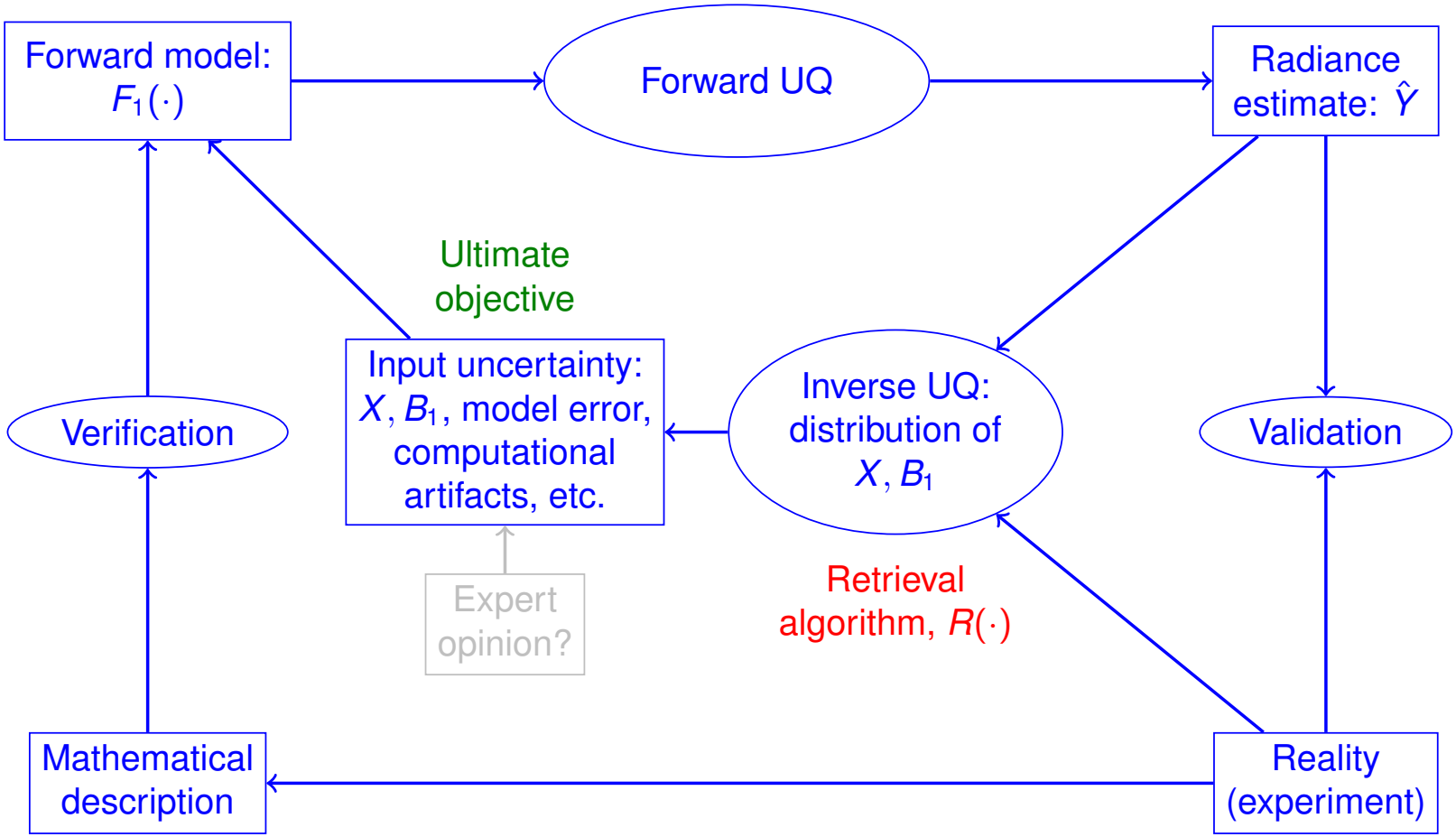
Engineering view



Science view



Science view



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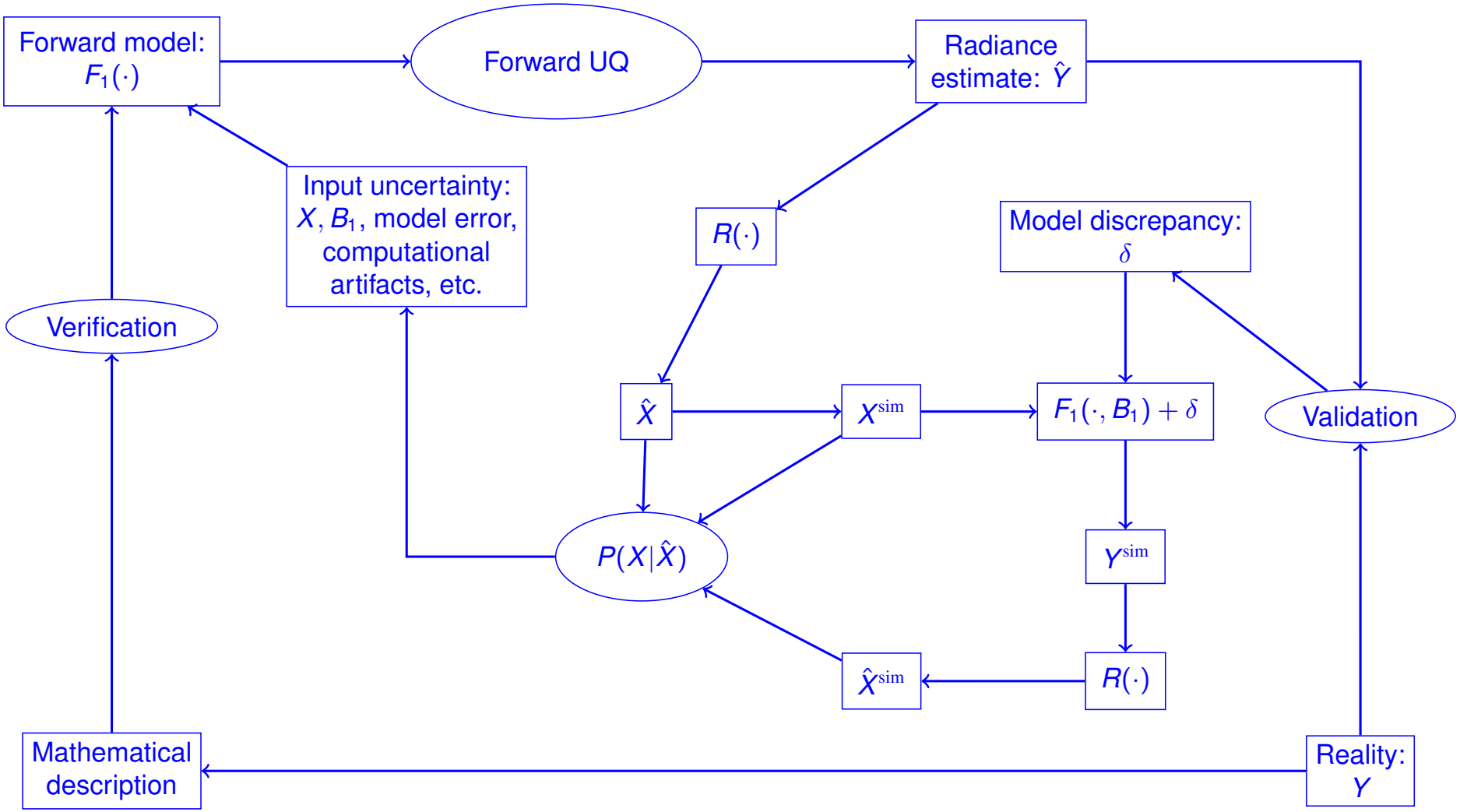
Simulation-based UQ for science



Discussion

- UQ for engineering problems is (relatively) well constrained
  - physical models better-known
  - processes are more circumscribed
- UQ for science is harder
  - physical models are in flux (UQ is *part* of the development process)
  - more unknowns
  - unknown unknowns
  - coupled models are exponentially more complex
- UQ for retrievals: is it engineering or science? Both?