# Semi-intrusive uncertainty quantification for reliable simulations

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17 February 2020

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# Credibility of computational models

**Credibility**
the willingness of persons
to base decisions on information
obtained from the model.[1]

repeat | same experiment same lab

replicate | same experiment different lab

test

reproduce | same experiment different set up

reuse | different experiment some of same

Drummond C Replicability is not Reproducibility: Nor is it Good Science, online
Peng RD, Reproducible Research in Computational Science *Science 2 Dec 2011:* 1226-1227.

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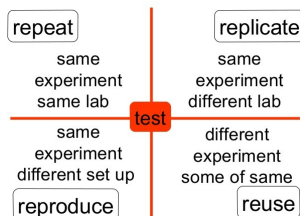[1]  Lee W Schruben. "Establishing the credibility of simulations". In: *Simulation* 34.3 (1980), pp. 101–105.

[2]  Lealem Mulugeta et al. "Credibility, replicability, and reproducibility in simulation for biomedicine and clinical applications in neuroscience". In: *Frontiers in neuroinformatics* 12 (2018), p. 18.
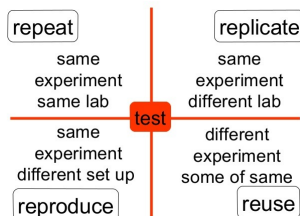
# Credibility of computational models

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**Reproducibility**
the ability of a simulation to be copied
by others to provide a simulation
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| repeat | | replicate |
|---|---|---|
| same experiment same lab | test | same experiment different lab |
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| reproduce | | reuse |

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# Credibility of computational models



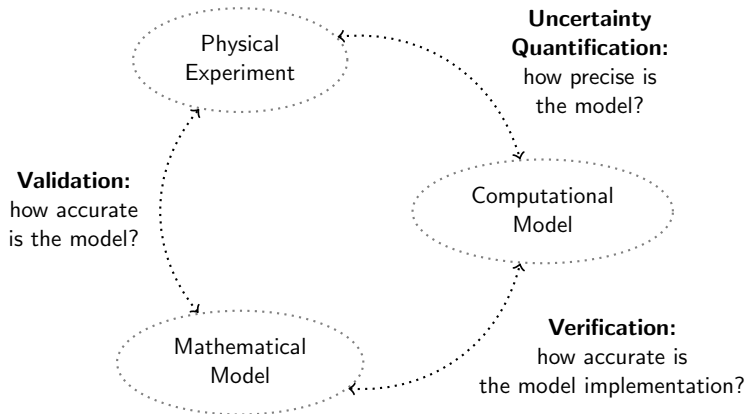**Credibility**
the willingness of persons
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**Reproducibility**
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**Reliability**
the ability of the model to produce accurate and precise results.

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# VVUQ as parts of the reliability assessment



**Uncertainty Quantification:** how precise is the model?

Physical Experiment

**Validation:** how accurate is the model?

Computational Model

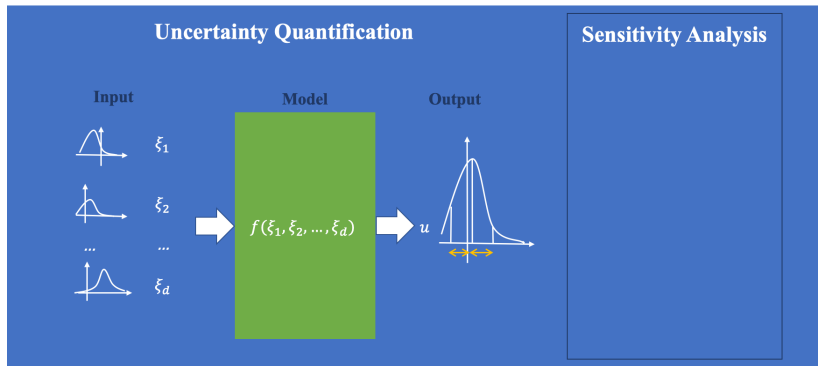Mathematical Model

**Verification:** how accurate is the model implementation?

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Uncertainty Quantification (UQ) is a scientific field, which supports decision making using computational models that involve uncertainties.
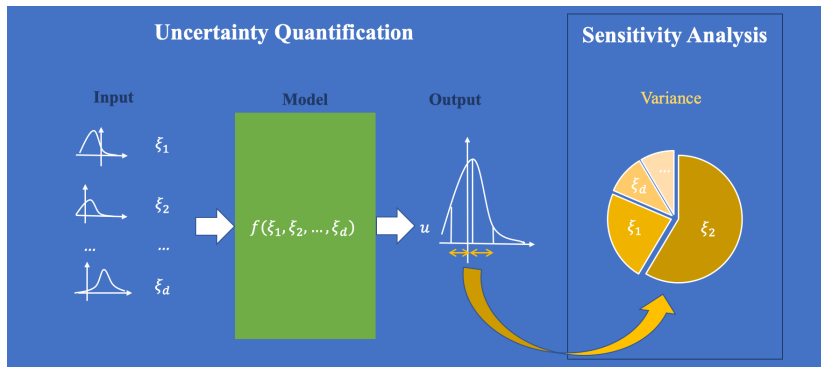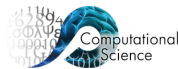
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# Scale separation map[3]
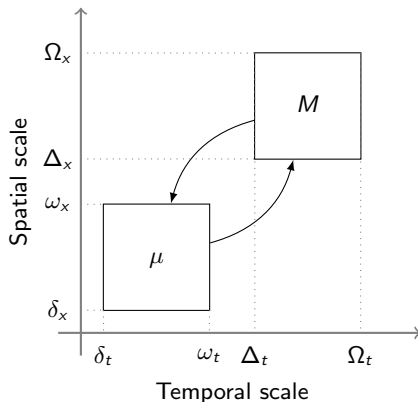
[3] Alfons G Hoekstra et al. "Towards a complex automata framework for multi-scale modeling: Formalism and the scale separation map". In: *International Conference on Computational Science*. Springer. 2007, pp. 922–930.

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[4] A Nikishova et al. "Semi-intrusive multiscale metamodelling uncertainty quantification with application to a model of in-stent restenosis". In: *Philosophical Transactions of the Royal Society A* 377.2142 (2019), p. 20180154.
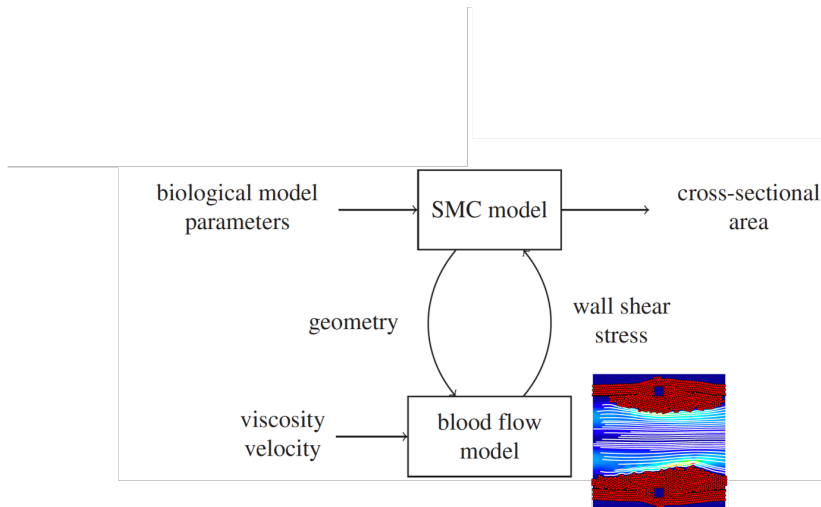
# Non-intrusive vs semi-intrusive metamodeling methods
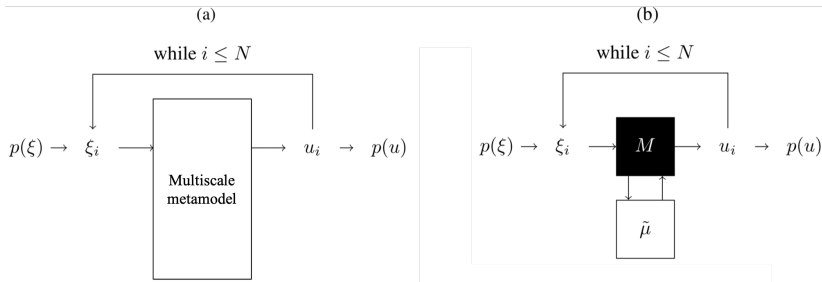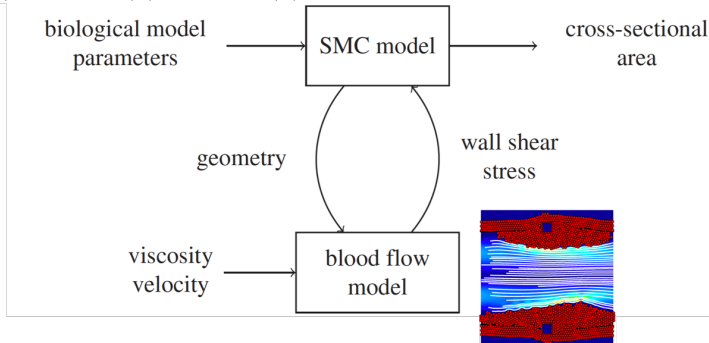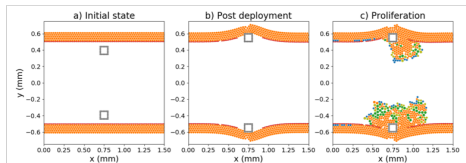
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# 2D multiscale model of in-stent restenosis
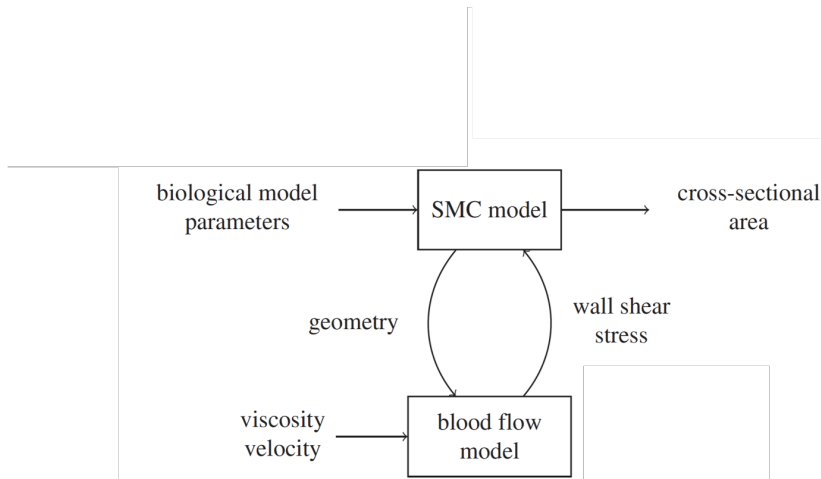
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# 2D multiscale model of in-stent restenosis

UQ methods:

- **Non-intrusive quasi-Monte Carlo (QMC)**
  - reference solution
  - 1024 samples
  - ∼90 minutes per sample



- **Non-intrusive metamodeling (NIM)**
  - 128 training samples
  - training takes ∼5 minutes
  - ∼7 times speed up



- **Semi-intrusive metamodeling (SIUQ)**
  - 4 training samples
  - ∼15 minutes per sample
  - ∼7 times speed up

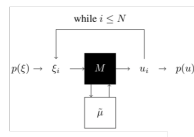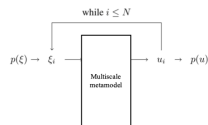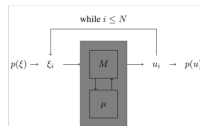# Table of Contents

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# Conclusions

- Multiscale models provide advantages in UQ
    - Better control, since physics is preserved;
    - More accurate metamodeling;
    - Analysis of computationally cheap single-scale models.[5]

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[5] Anna Nikishova, Giovanni E Comi, and Alfons G Hoekstra. "Sensitivity analysis based dimension reduction of multiscale models". In: *Mathematics and Computers in Simulation* 170 (2020), pp. 205–220.

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Thank you!

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