Automated Bayesian Inference for PDE-constrained Inverse Problems

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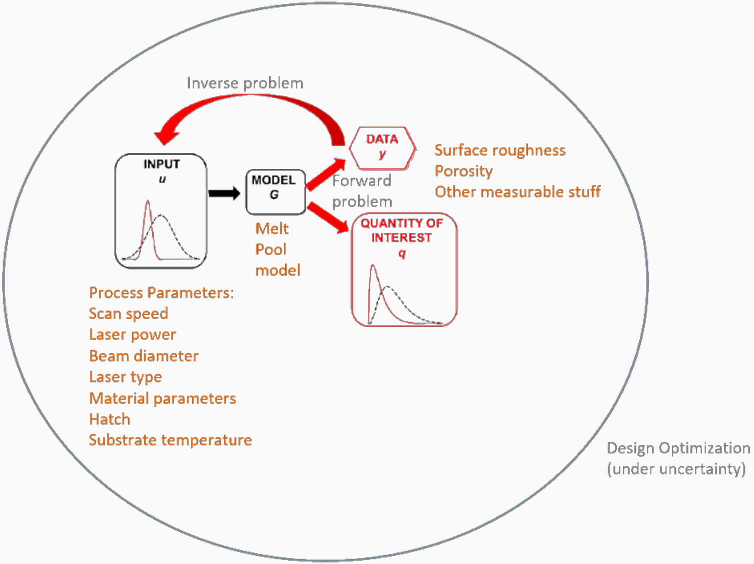
Model + Simulation + Data



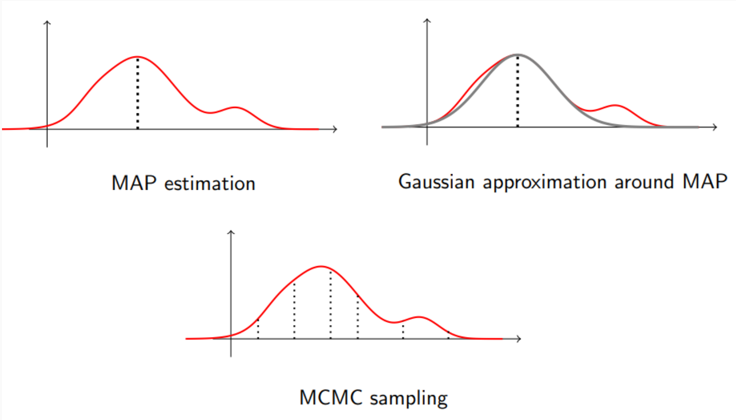
Bayesian inference summary

A generative physical model: $\boldsymbol{X} \sim \mathcal{F}_\theta$, being $\mathcal{F}_\theta$ a PDE system

$$F(\boldsymbol{X}; \boldsymbol{\theta}) = 0$$

Having observed some data $\boldsymbol{y}$ define a likelihood $p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta})$ and combine with a prior distribution $p(\boldsymbol{\theta})$ to obtain the posterior

$$p(\boldsymbol{\theta}|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta})p(\boldsymbol{\theta})\, d\boldsymbol{\theta}}$$



Approximate methods: MCMC (lots of variants), Variational method (lots of variants), Laplace approximation, neural nets, sparse grid, etc.

Bayesian inference challenges and opportunities

Because of ...

high-dimensionality of the target we need to utilize *derivative* information

repeated PDE solution we need to utilize the resources efficiently, use advanced solvers

not everyone can do this we need to lower the barriers of skills needed by providing the tools

My PhD Components

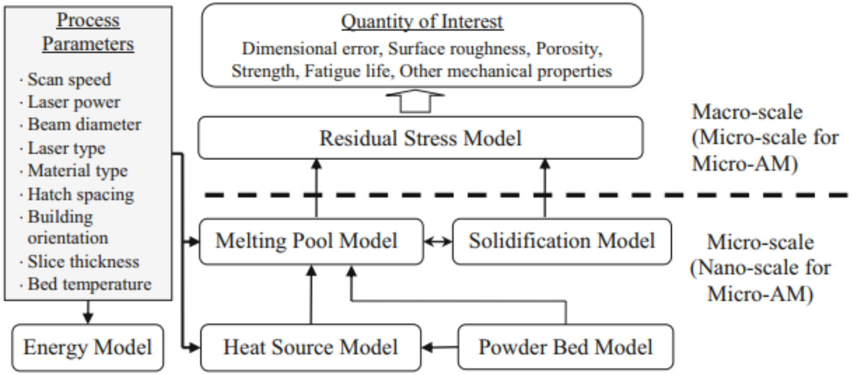
- Automatic differentiation for PDE systems
  Automated generation of adjoint problems and efficient integration of the adjoint solution into AD framework
- Bayesian analysis for inverse problems
  Assessing prediction reliability and accuracy guarantees
- Case studies
  Focus on Additive Manufacturing
  Large-scale multiphysics simulations
- Software development

Additive Manufacturing

Model	Methods	Inputs	Outputs
Heat source	· Gaussian distribution for horizontal intensity · Direct measurement · Trajectory tracking of photons · Monte Carlo simulation (MCS)	· Material type · Powder distribution · Beam diameter · Laser power · Powder shape · Thermal diffusivity · Scan speed	· Absorbed energy · Absorption coefficients of materials · Vertical absorption distribution
Powder bed	· Raindrop model · Discrete element method (DEM) · Nonlinear Hertzian contact model	· Sliding friction coefficient · Rolling friction coefficient · Young's modulus · Radius distribution · Hamaker constant · Damping coefficient · Restitution coefficient	· Packing density · Radial distribution function (RDF) · Porosity of the powder bed
Melting pool	· Thermal model for melting · Lattice Boltzmann (LB) approach (2D and 3D) · Extended LB approach · Computational fluid dynamics (CFD) by including heat transfer, melting, and Marangoni force	· Scan speed · Laser power · Particle radial distribution · Absorption coefficient · Melting temperature · Thermal diffusivity · Layer thickness · Beam diameter	· Melt pool width · Melt pool shape · Diffusion efficiency · Cross-sectional area · Length-to-depth ratio · Porosity and layer bonding defects · Thermal boundary conditions · Surface roughness
Solidification	· Microscopic cellular automaton (CA) coupled with Macroscopic finite element (FE) approach · Phase field (PF) approach	· Cooling rate · Thermal history · Material properties	· Grain size · Thermo-mechanical properties of materials · Metallurgical properties
Residual stress	· Couple finite volume (FV) with FE approach · Thermal-mechanical FE models	· Thermal boundary condition · Mechanical boundary condition · Material properties	· Residual stress · Shrinkage · Deformation · Fatigue life

Adapted from Zhen Hu, 2017

Additive Manufacturing



Source: Zhen Hu, 2017