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Particle approach to inverse problems via gradient-based optimization

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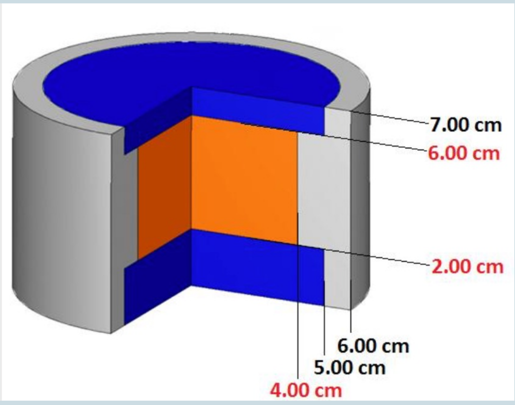
Develop uncertainty quantification capability for Monte-Carlo particle approaches to non-linear inverse problems

- ***Such a capability is non-existent*** within particle-based models for Brownian dynamics, radiation transport, low-density fluids and plasmas.
- ***Our approach is to reuse*** the existing particle trajectories to estimate sensitivities (gradients) of quantities of interest (expectations).
- ***Why can we do this?***

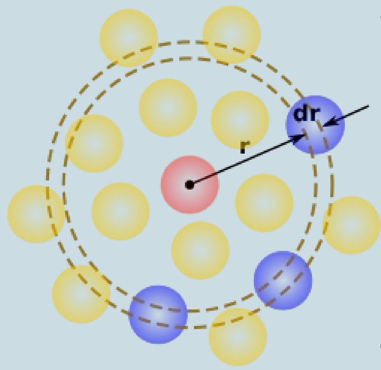
$$\begin{array}{ccc} \mathbb{E}[f(X_t)] & \longleftrightarrow & \frac{1}{n}\sum f(X_t) \\ \big\downarrow \text{ Stochastic calculus of variations, statistical theory} & & \big\downarrow \text{ Physically based Monte-Carlo relationship to a partial differential and integral equation} \\ \frac{d}{d\theta}\mathbb{E}[f(X_t)] = \mathbb{E}[f(X_t)Y_t] & \overset{?}{\longleftrightarrow} & \frac{d}{d\theta}\frac{1}{n}\sum f(X_t) \end{array}$$

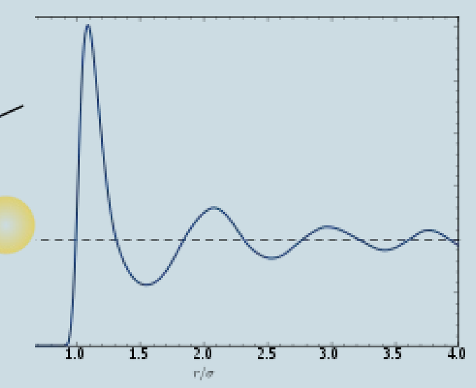


Inverse Problem: given radiation leakage on the top and bottom, infer the location of the uranium

Reuse existing sample averages to estimate sensitivities (gradients)

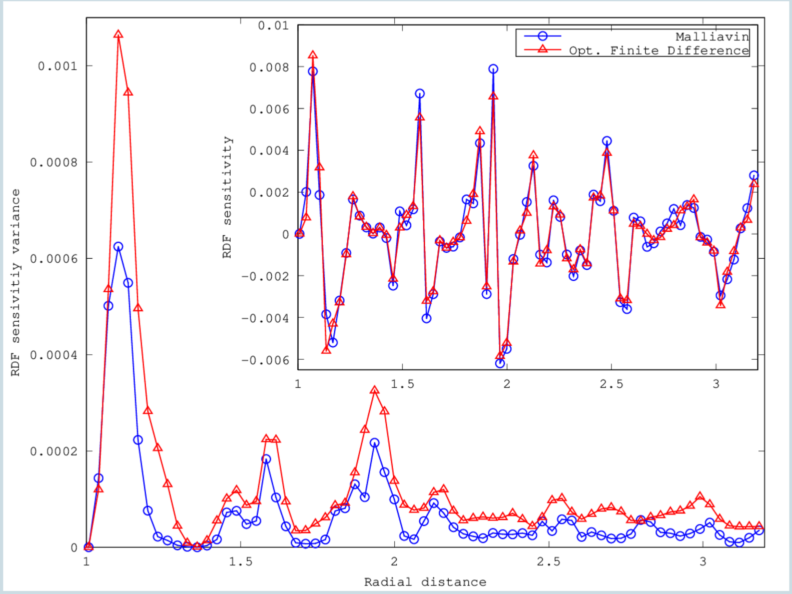
- Exploit tools in stochastic calculus of variations (i.e. Malliavin Calculus) to weight existing sample average estimators to approximate the sensitivities (gradients).
  - Our inspiration came from studying the quantitative financial literature





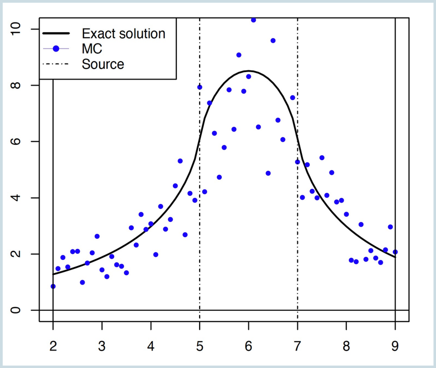
- Significant computational savings over a finite difference approach that requires at least twice as many Monte-Carlo simulations and fine tunning.
- Example: Sensitivity of the radial distribution function under a Lennard-Jones potential to the attraction parameter

$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

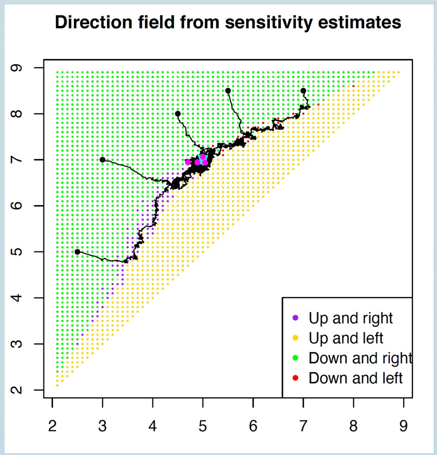


Model inverse problem of radiation leakage

- Given radiation leakage on the top and bottom, infer the location of the uranium for a two-dimensional slice
- Approximate the uranium location by minimizing a nonlinear least-squares functional.
- The particle trajectories can be reused to solve an inverse problem via a Bayesian or frequentist techniques.
- No need for a deterministic approach, e.g., Boltzmann equation.



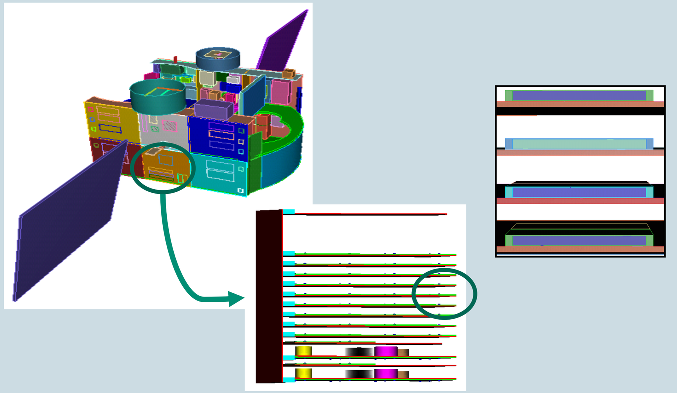
Monte-Carlo approximation to the particle expectation (which satisfies the Boltzmann equation)

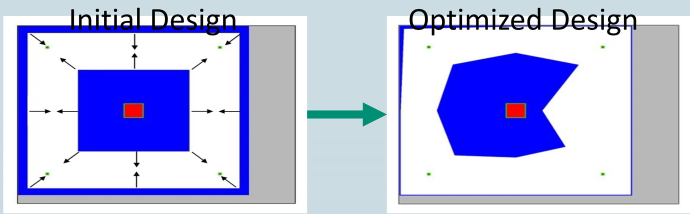


Noisy gradient method—step in the direction of Monte-Carlo sensitivities approximated by reusing the above Monte-Carlo samples.

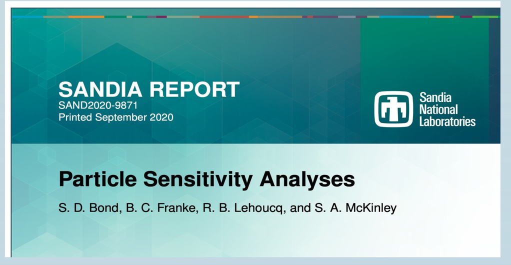
Impact

- Deployment of a non-existent capability in mission codes for radiation transport, low-density fluids and plasmas.
- Go beyond forward simulation: inverse problems, design-based optimization, rigorous verification.
- Uncertainty quantification for the inverse problem, e.g., confidence or credible intervals
- Big Picture: there is a lot of information available in the sampled particle trajectories beyond what's currently used





Satellite shielding: Protect electronics packaging from radiation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