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# Uncertainty quantification, inverse problems and timescale acceleration in atomic simulation

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**Abstract**

Recent years have seen an explosion in the use of data-driven tools in atomic simulation, following broader trends across computational science. Current efforts have focused on interpolating some approximate electronic structure method; I will discuss how these same tools can be used to quantify model form uncertainties[1], learn from experimental data sources[2], harness adjoint methods familiar to e.g. FEM[3] and provide new strategies to extend simulation timescales[4]. Applications specific to fusion materials science and transferability to general modelling objectives will be discussed.

[1] T.D. Swinburne and D. Perez, Mach. Learn.: Sci. Technol., (2025)
[2] T.D. Swinburne, C. Lapointe, C. Marinica, Nat. Comm. (2026) & NeurIPS AI4Mat (2025)
[3] I. Maliyov, P. Grigorev, T.D. Swinburne, NPJ Computational Materials (2025)
[4] T.D. Swinburne, Phys. Rev. Lett (2023)

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