Foundational Approaches for End-to-end Formal Verification of Computational Physics

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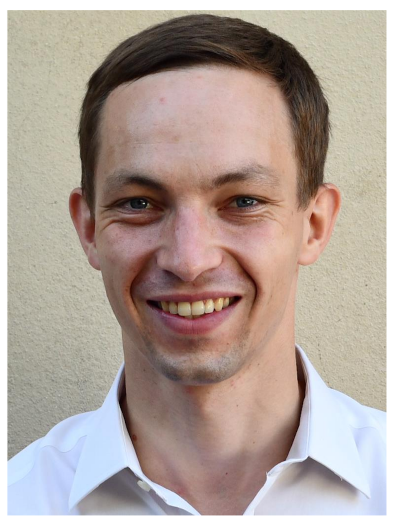
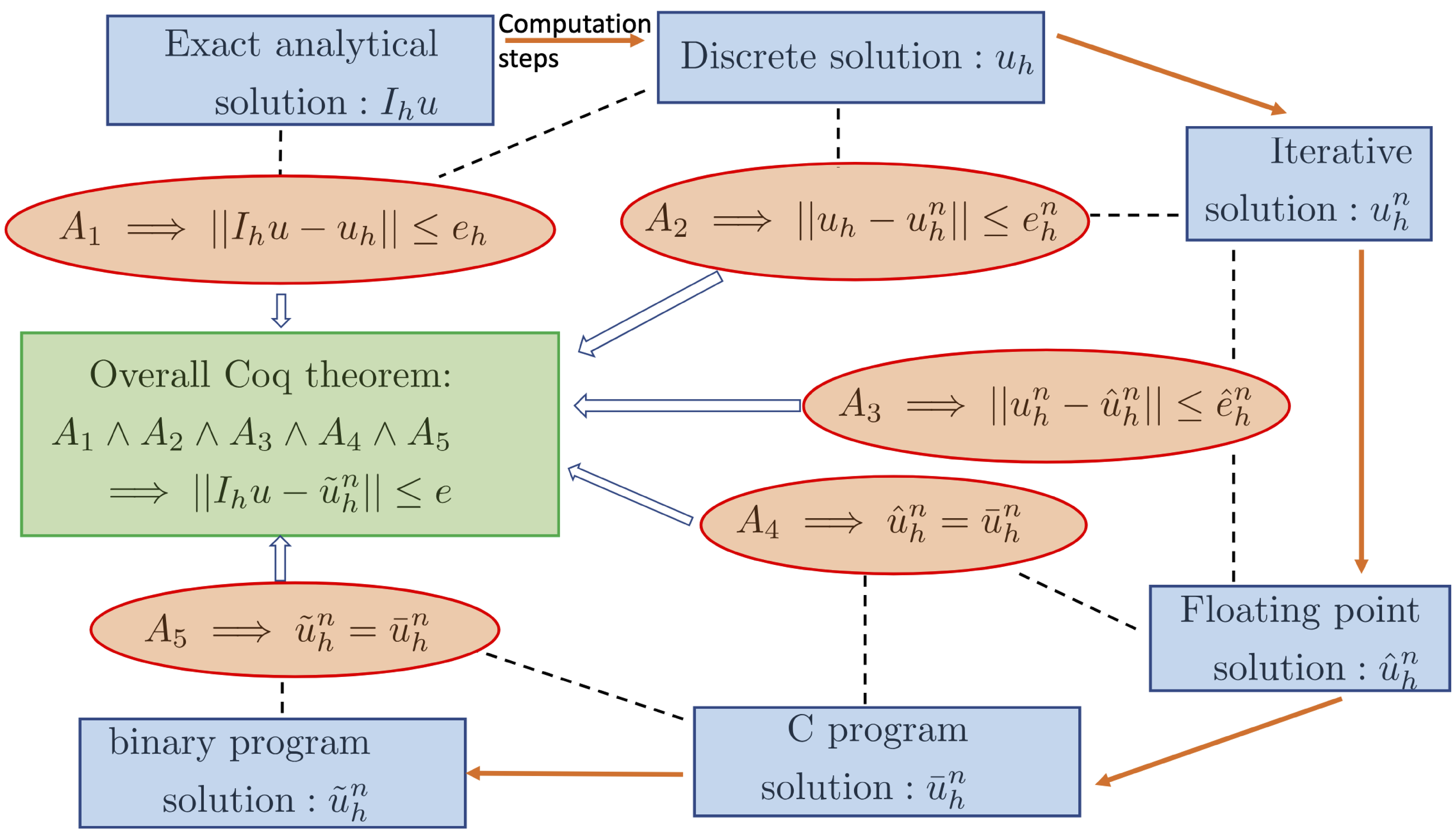
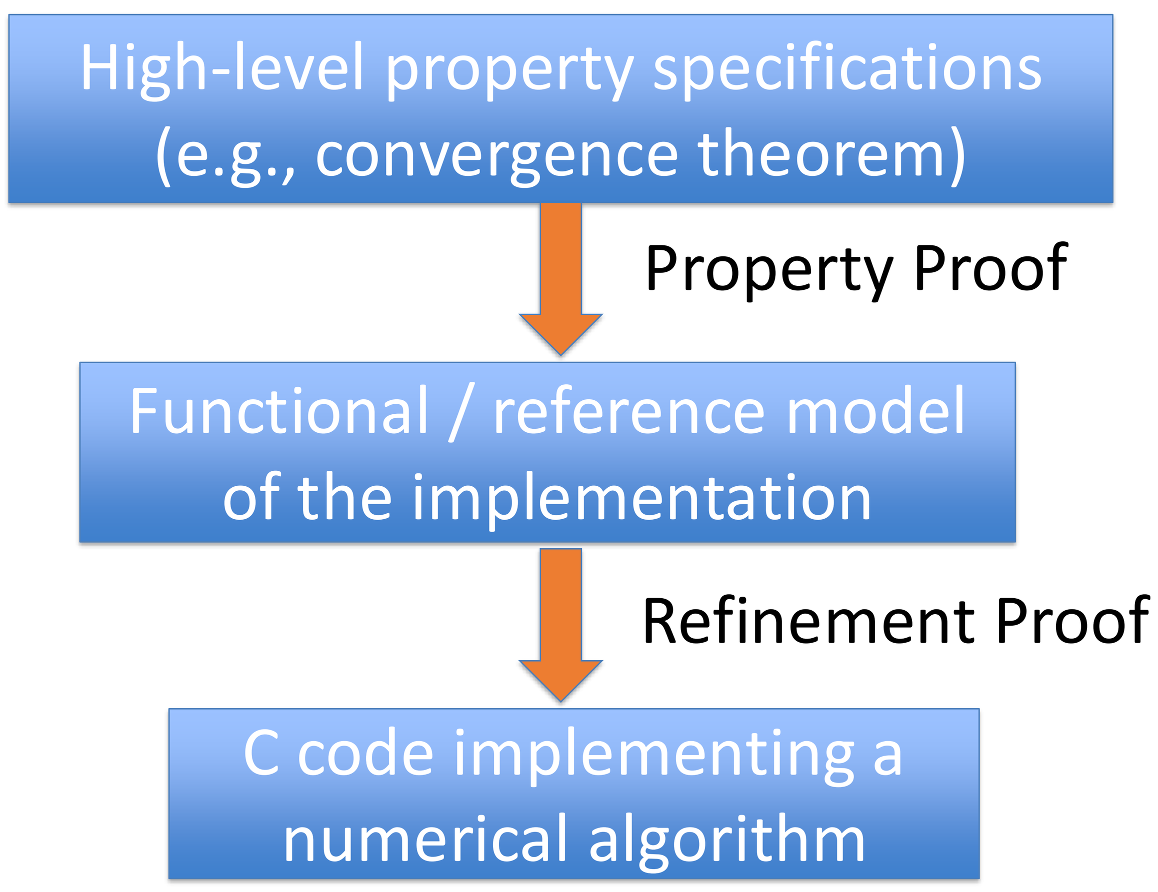
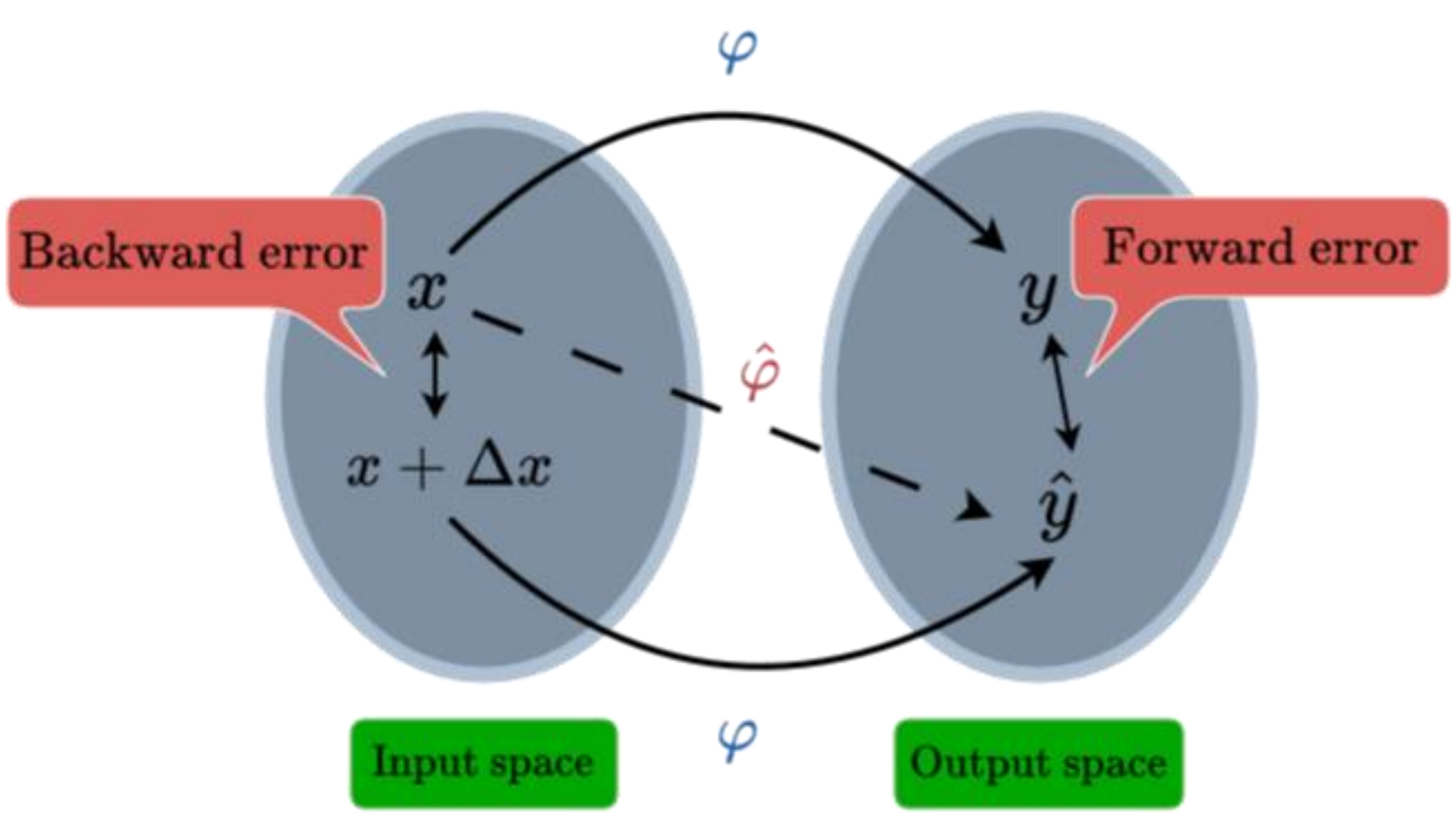


Natural and Physical systems are typically modeled by differential equations, for which obtaining **analytical solutions is often intractable**. As a result, these differential equations are **solved numerically** in a finite computation domain. To have high confidence in the results, we use formal verification techniques:

- **Formal proof in an interactive theorem prover (Coq)** of classical convergence results (Lax theorem) [NFM'21].
- Formal proofs of correctness, accuracy and convergence of an **iterative linear Jacobi solver** [CICM'23, NFM'24], including **precise convergence conditions** and deterministic bounds of accuracy for **floating-point computations**.
- **Tighter probabilistic rounding uncertainty** quantification for computing **dot-products** and solving a **stochastic ODE** with an underlying tri-diagonal linear system in low-precision arithmetic [under review SIAM JSC].







Probabilistic rounding

- The effect of rounding can be modeled as **perturbations to the true function**, which can be bounded probabilistically.
- Modeling relative rounding errors as uniformly distributed i.i.d. variables enables bounding their accumulation via **Bernstein's inequality**, including higher-order error statistics.
- Modeling rounding errors as random variables **accounts for error cancellation**, providing tighter estimates than deterministic analysis.

FMitF scientific impacts

- We provide correctness and accuracy guarantees for computational methods typically used in the **design of embedded systems**.
- Matrix operations with floating-point arithmetic are widely used in **machine learning**. We equip them with formally verified deterministic and probabilistic accuracy bounds.

Broader impacts

- **Mechanically-checked** formal guarantees on numerical computations, such that the computational physicist can set and achieve a **desired level of accuracy**
- Tighter rounding uncertainty quantification enables **more efficient computational resource allocation**, enhancing model accuracy and reliability in predictive applications.
- Strengthen links between theoretical CS and computational science.

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