BIASlab
Bayesian Intelligent Autonomous Systems lab

CASIMIR INSTITUTE FUTURE CHIPS AND HIGH-TECH SYSTEMS

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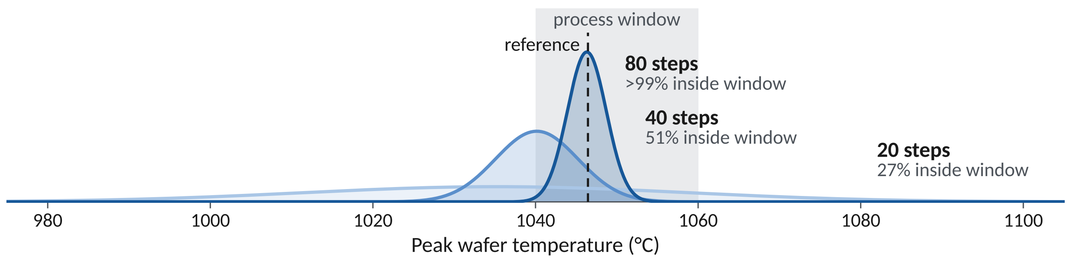
Probabilistic numerics for semiconductor manufacturing

COMPUTATION WITH ERROR ESTIMATES, TO KNOW WHEN TO STOP AND WHERE TO ACT

COMPUTATION AS AN INFERENCE PROBLEM

Lithography scanners, process tools and chip-design flows run on numerical solvers. They solve linear systems, integrate differential equations and optimise designs, often under tight time budgets.

Classical solvers typically return only a number and ignore the error caused by discretisation and early stopping. Probabilistic numerics treats computation itself as an inference problem. A probabilistic solver produces a probability distribution over the unknown quantity, quantifying uncertainty about the estimate. Performing more computation concentrates the distribution, decreasing uncertainty.

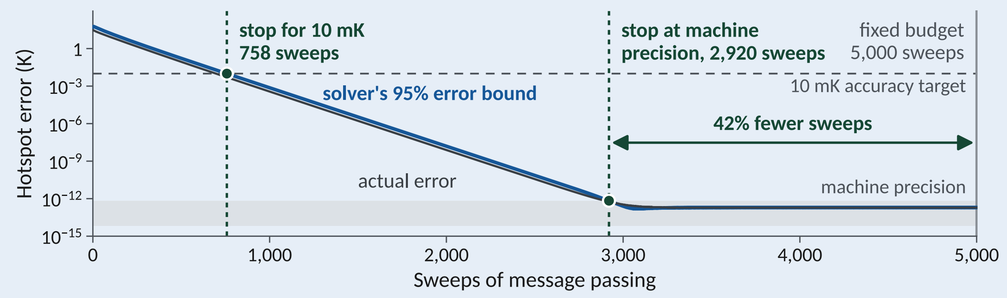


Posterior distribution over the peak wafer temperature in a rapid thermal anneal, from a probabilistic ODE solver with 20, 40 and 80 steps.

KNOW WHEN TO STOP

Probabilistic solvers track their own error through quantified uncertainty. Iterations can stop as soon as the estimated error is small enough for the task.

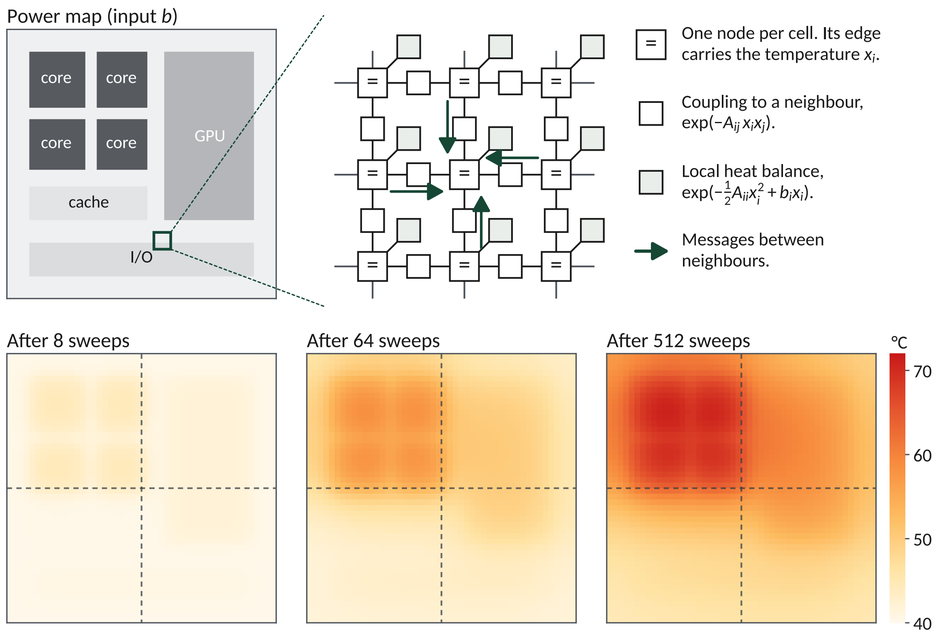
On the die example below it stops after 758 sweeps for 10 mK, or after 2,920 at machine precision, instead of a fixed budget of 5,000.



Gaussian belief propagation on the die example. Error bound from a probabilistic iterative method (Cockayne et al., 2021), calibrated on the solver's own iterates. The actual error is unknown in practice.

LINEAR SOLVERS AS MESSAGE PASSING

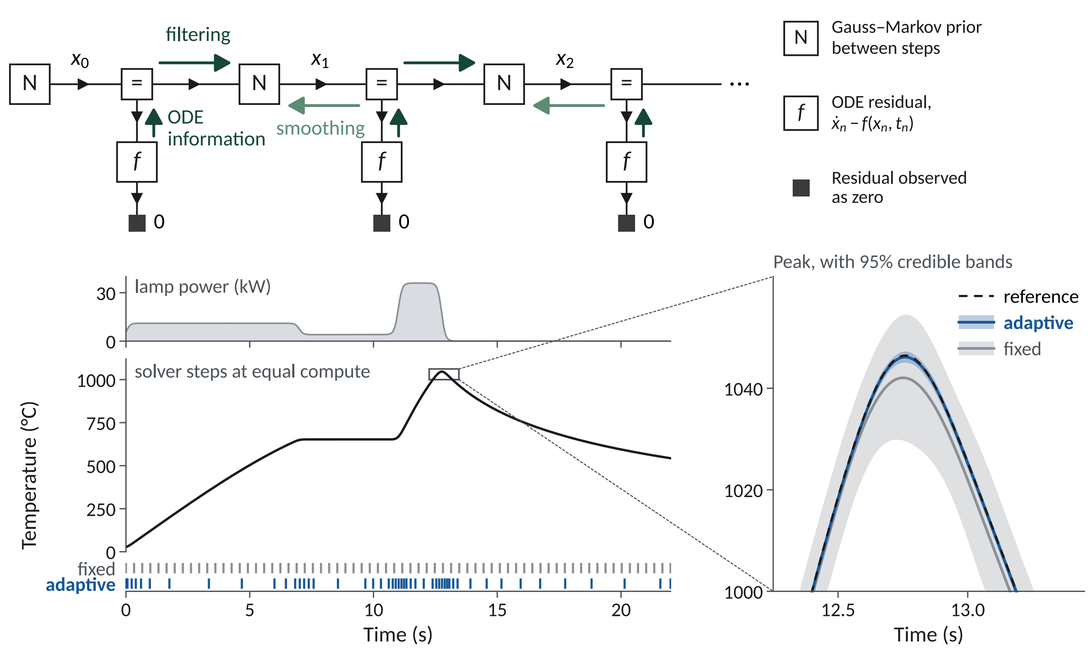
For a symmetric positive-definite matrix A, the solution of $Ax = b$ is the mean of the Gaussian $p(x) \propto \exp(-\tfrac{1}{2}\, x^{\mathsf{T}}Ax + b^{\mathsf{T}}x)$. Each unknown becomes a node in a factor graph and each nonzero entry of A a local factor. Gaussian belief propagation solves the system by passing messages between neighbours. Every node holds a Gaussian belief, so uncertainty comes as a by-product.



Steady-state temperature of an example 12 × 12 mm die (48 × 48 cells, 45 W). Each sweep moves information one cell further. Dashed lines split the die over four devices that exchange messages only across their borders.

PROBABILISTIC ODE SOLVERS AS MESSAGE PASSING

A probabilistic ODE solver puts a Gauss–Markov prior on the trajectory and conditions it on the differential equation at every step. Filtering and smoothing are forward and backward messages on a chain. The solver uses its own error estimate to choose the step size, so it spends steps where the dynamics change quickly.



Wafer temperature in an example spike anneal, $C\,\mathrm{d}T/\mathrm{d}t = P(t) - \varepsilon\sigma A(T^4 - T_w^4)$. At equal compute (67 evaluations), adaptive steps cut the maximum error from 4.5 K to 0.4 K. Both 95% bands cover the reference.

WHY MESSAGE PASSING ON FACTOR GRAPHS

MODULAR

Solvers are built from reusable factors. Swap a prior, a physics model or a solver block without rewriting the rest.

DISTRIBUTED

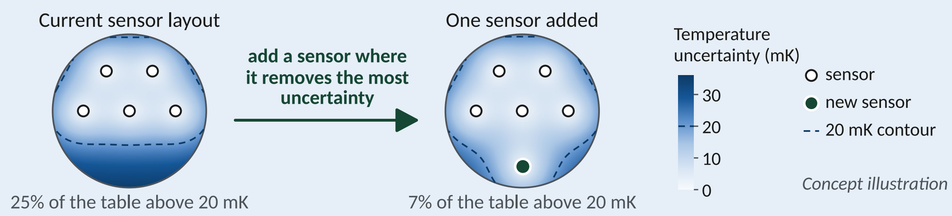
Messages are local. A large solve can be split over cores, GPUs or devices that only exchange messages along their borders.

UNCERTAINTY QUANTIFICATION

Numerical uncertainty flows through the graph into estimation, control and decisions.

USE CASE · SENSOR PLACEMENT

A probabilistic thermal model shows where a wafer table's temperature is least certain. One sensor placed there shrinks the area above 20 mK from 25% to 7%.



LOOKING FOR INDUSTRY PARTNERS

Do you run simulation-heavy or compute-constrained workflows? We would like to test these methods on real problems. Think of thermal models of wafers, reticles and dies, process simulation, inverse problems in metrology or real-time models for control.

Contact Wouter Kouw, w.m.kouw@tue.nl

Scan for our ProbNum 2026 tutorial on linear solvers by message passing.

rxinfer

Bagaev & de Vries (2023). Reactive message passing for scalable Bayesian inference. *Scientific Programming.*
Bosch, Hennig & Tronarp (2021). Calibrated adaptive probabilistic ODE solvers. *AISTATS.*
Cockayne, Ipsen, Oates & Reid (2021). Probabilistic iterative methods for linear systems. *JMLR.*
Hennig, Osborne & Kersting (2022). Probabilistic numerics: computation as machine learning. *Cambridge University Press.*
Shental et al. (2008). Gaussian belief propagation solver for systems of linear equations. *IEEE ISIT.*
Tronarp et al. (2019). Probabilistic solutions to ordinary differential equations as nonlinear Bayesian filtering. *Statistics and Computing.*