GOODE: A GAUSSIAN OFF-THE-SHELF ORDINARY DIFFERENTIAL EQUATION SOLVER

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GOODE: A Gaussian Off-The-Shelf ODE Solver

What are we doing?

Ordinary Differential Equations (ODEs)

$$\frac{d}{dt}y(t) = f(y(t), t)$$

Vector-valued, changes in time

- Important mathematical models
- Broad range of applications

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- Recently ODE (solver) also in ML, e.g.
  - Building blocks in NNets [Chen 2018] Neural ODEs
  - [Grathwohl 2019] FFJORD
  - Accelerate optimization [Zhang 2018]

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ODE approximation! → Error!

Probabilistic Numerical Methods (PNMs)

- Return probability distributions
- Represent numerical approximation error

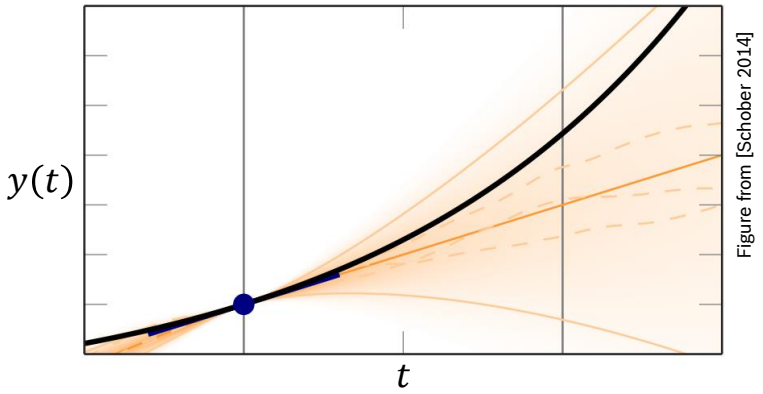

Figure from [Schober 2014]

Be certain about your uncertainty!

GOODE: A Gaussian Off-The-Shelf ODE Solver
More specific!

What is the problem?

Nonlinear two-point
Boundary Value Problem (BVP)

Find $\boldsymbol{y}: [\boldsymbol{a}, \boldsymbol{b}] \rightarrow \mathbb{R}^{\boldsymbol{d}}$ such that

ODE $\quad \boldsymbol{y}'(\boldsymbol{t}) = \boldsymbol{f}(\boldsymbol{y}(\boldsymbol{t}), \boldsymbol{t})$

BC $\quad \boldsymbol{0} = \boldsymbol{g}\big(\boldsymbol{y}(\boldsymbol{a}), \boldsymbol{y}(\boldsymbol{b})\big)$

Standard non-probabilistic solver exist.

But no general-purpose probabilistic solver!

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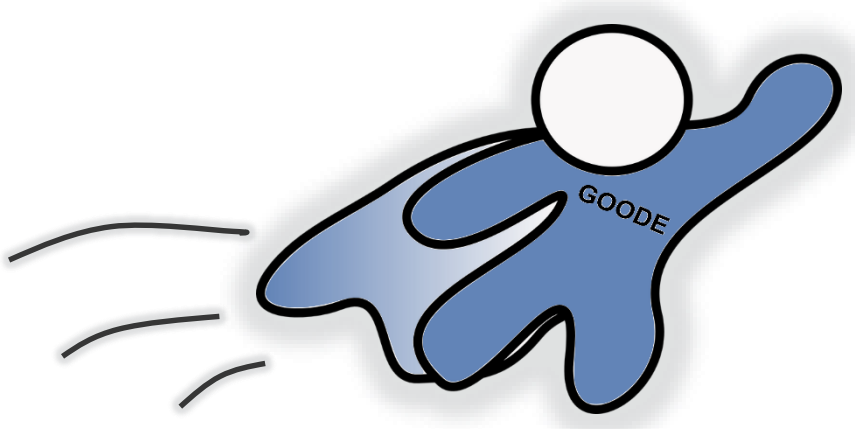

GOODE specs

- Novel functionality: probability distribution over solution space
- Intrinsic error estimation
- Convergence theory exists

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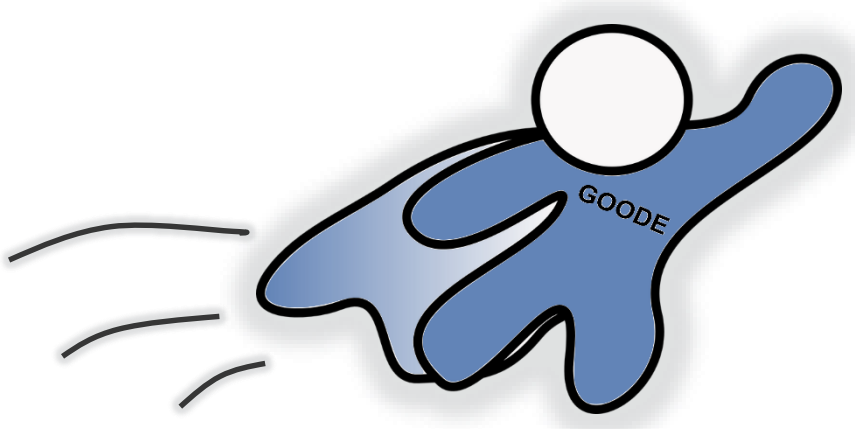

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How does GOODE work?

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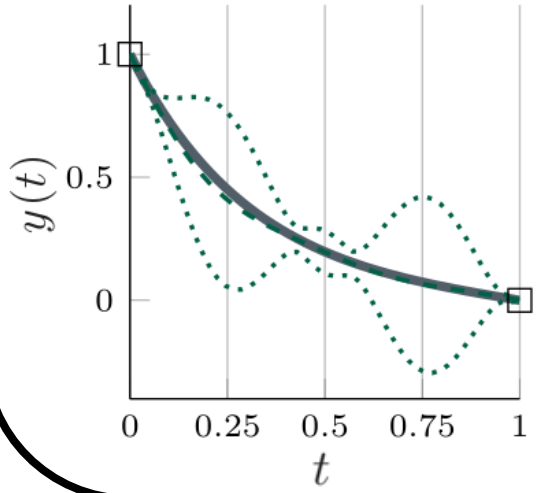
How does GOODE work?

Gaussian Process regression for linear BVP

[Owhadi 2015; 2017], [Cockayne 2016]

$$\left[\frac{d}{dt} - A\right] y(t) = q(t)$$

$$P\big(y(t)\big) = GP(m(t), k(t,t') \otimes V)$$



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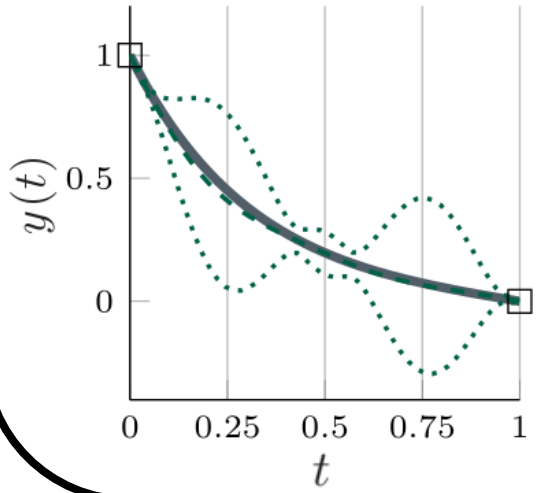
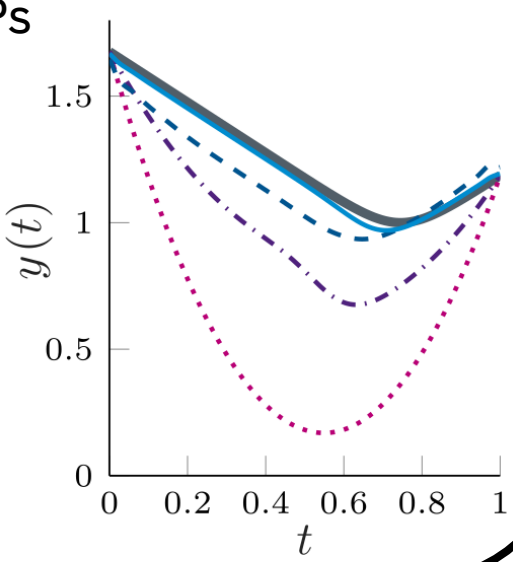


Quasilinearization of nonlinear BVP

[Bellman, Kalaba 1965]

Newton's method in function space

- Series of linear BVPs



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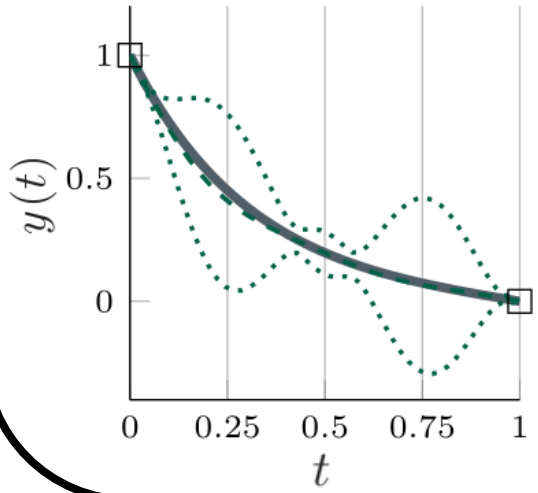

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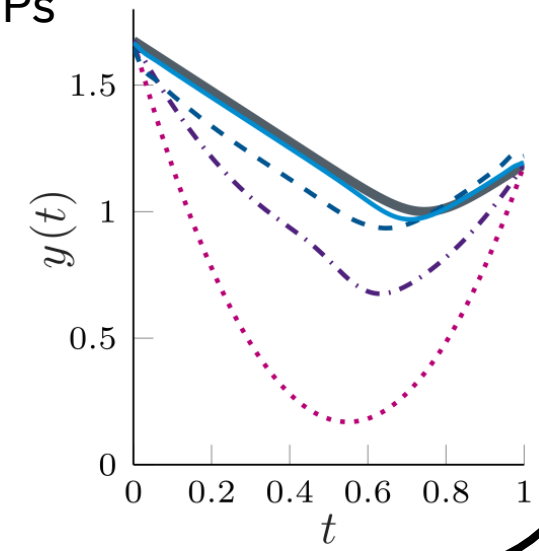

GOODE

Iteratively approximate nonlinear problem

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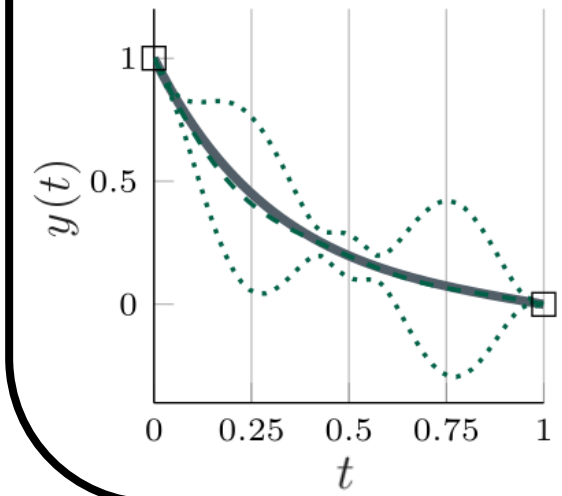

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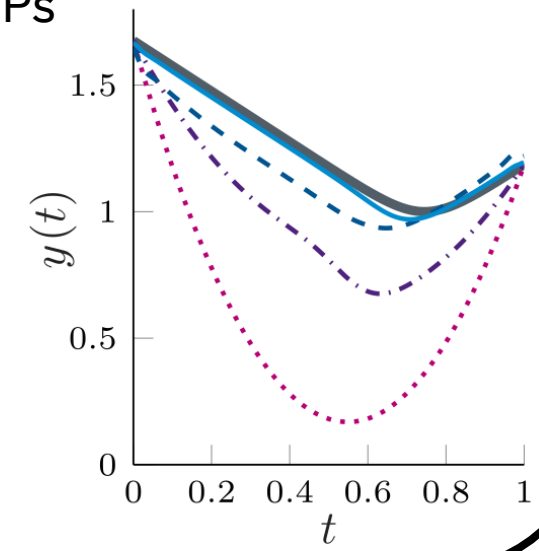

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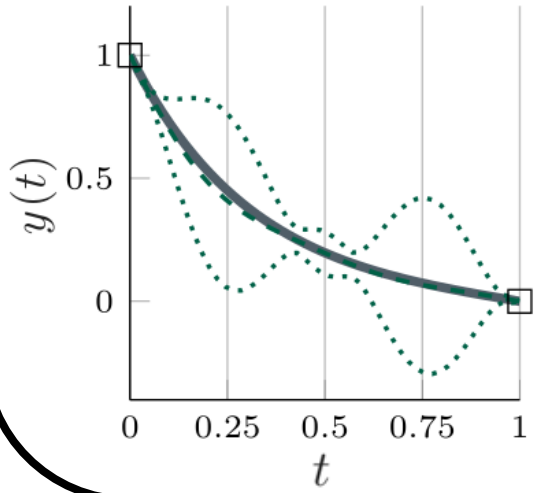

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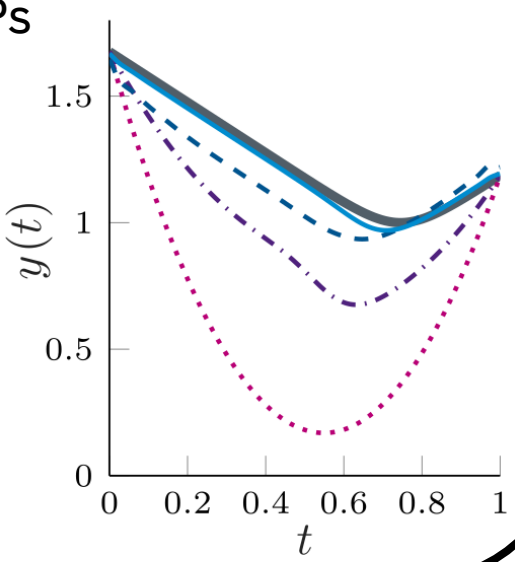

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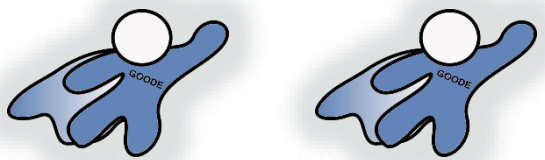

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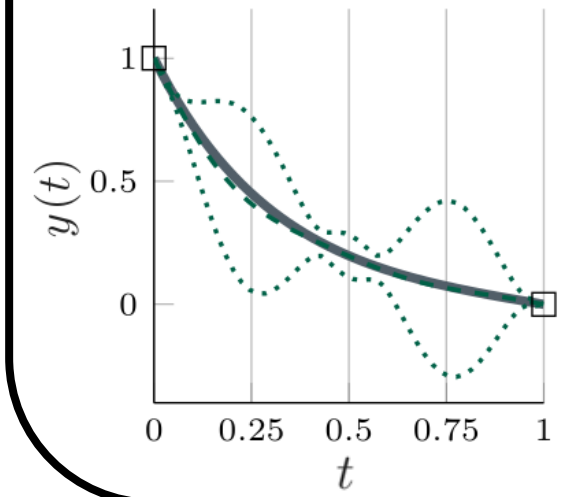

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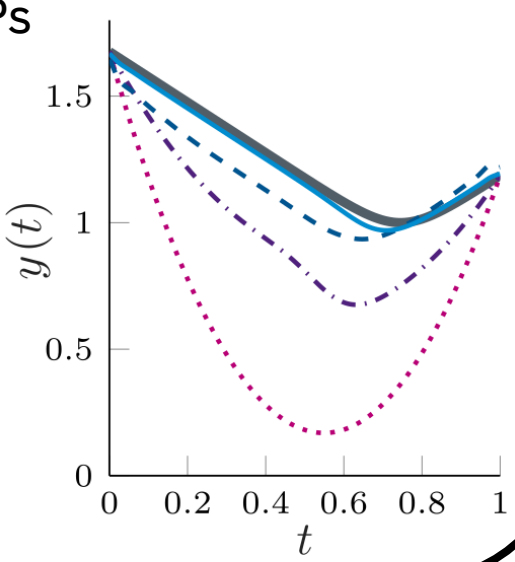

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Iteratively approximate nonlinear problem

Return predictive posterior GP

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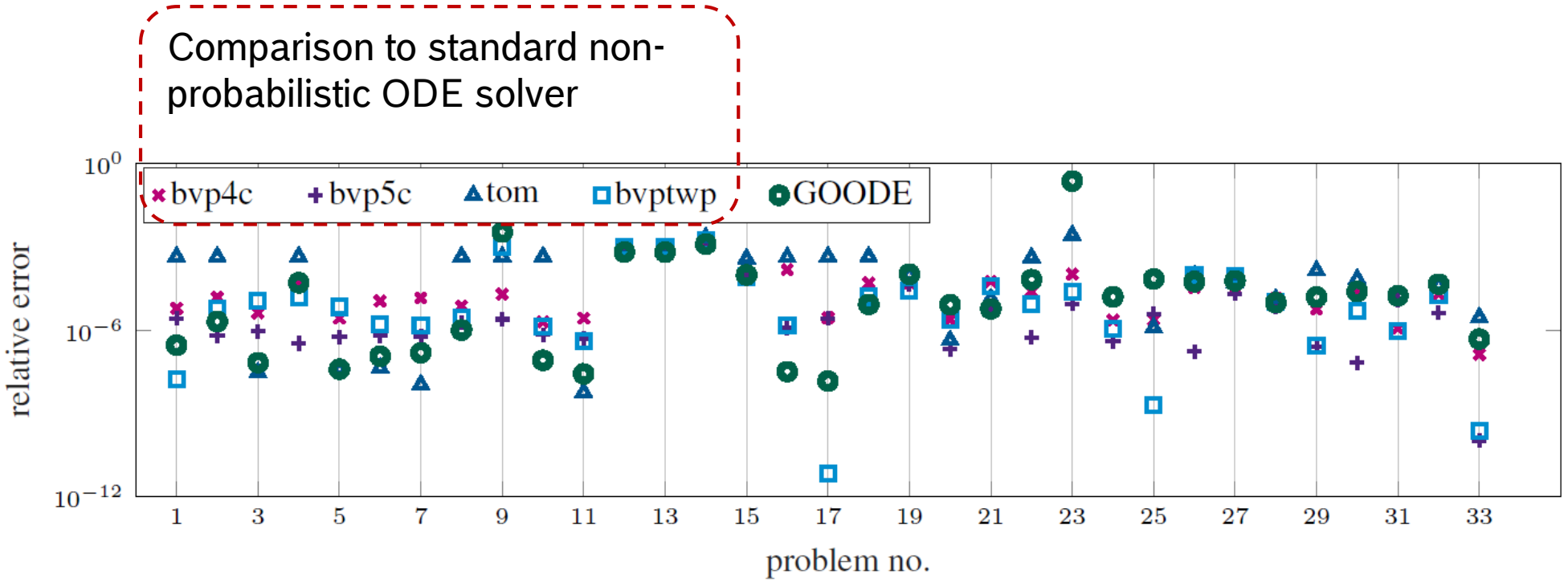
How **good** does GOODE work?



Testset of 33 problems [Mazzia 2014]

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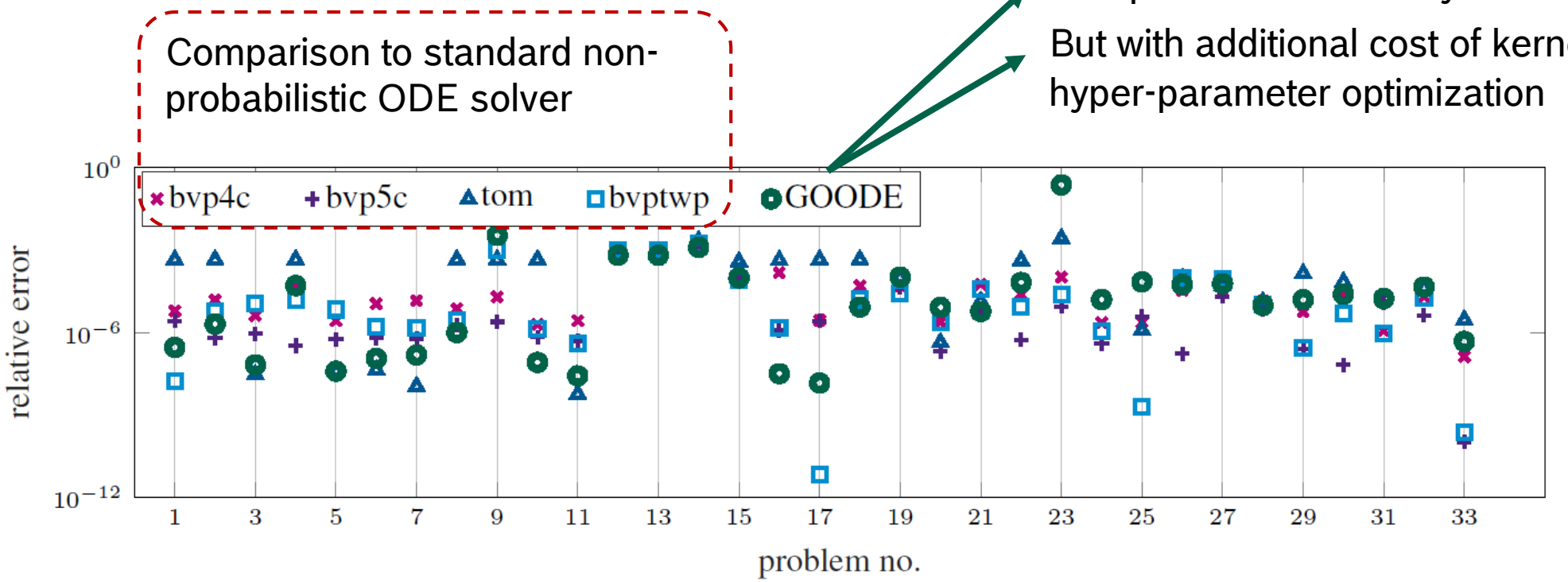
How **good** does GOODE work?

Comparable in accuracy!

But with additional cost of kernel hyper-parameter optimization



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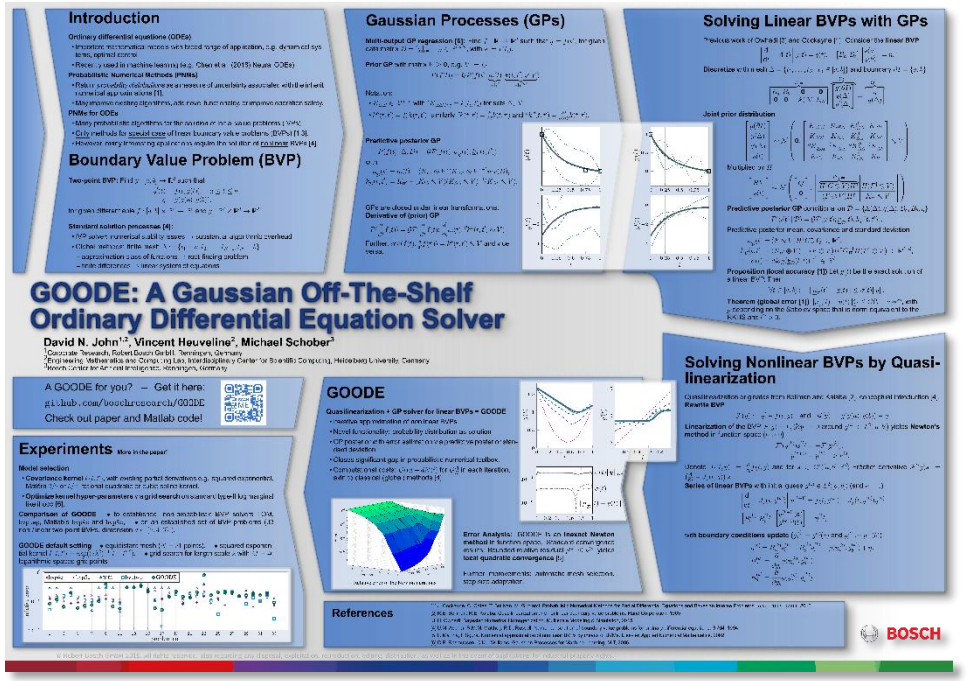
Want to know more?

Matlab code @ github.com/boschresearch/GOODE

Poster #214



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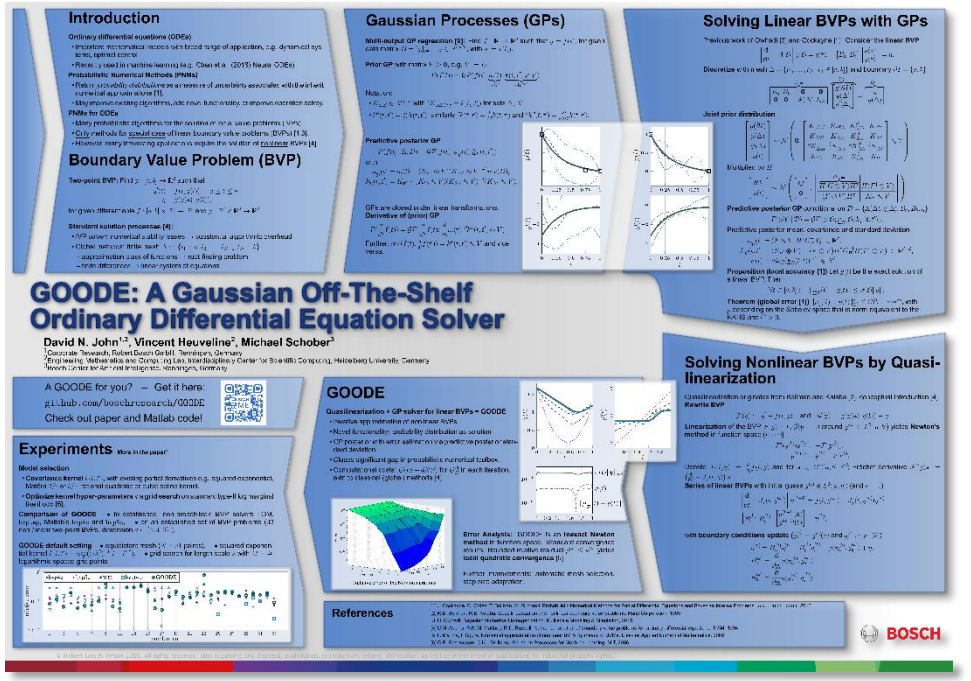

THANK YOU!

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