Uncertainty Quantification for Plasma- and PWI- models

U. von Toussaint, R. Preuss, D. Coster
Max-Planck-Institut für Plasmaphysik, Garching
EURATOM Association

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Overview

- Motivation
- Approaches to Uncertainty Quantification
- Example: Vlasov-Poisson-system
- Sensitivity Analysis
- Emulators: Gaussian Processes
- Example: SOLPS-data
- Challenges

Preliminaries

Two types of uncertainties (lack of knowledge) are to be distinguished:

- Isolatable uncertainties eg.
  - electron mass
  - cross-sections from first principles
  - ...
- non-isolatable uncertainties
  - most non-trivial simulations eg. climate- or plasma-simulation output
  - complex/integrated data analysis

Motivation

Verification, Validation and Uncertainty Quantification in a scientific software/modeling context:

- Simulations provide *approximate* solutions to problems for which we do not know the exact solution.

This leads to three more questions:

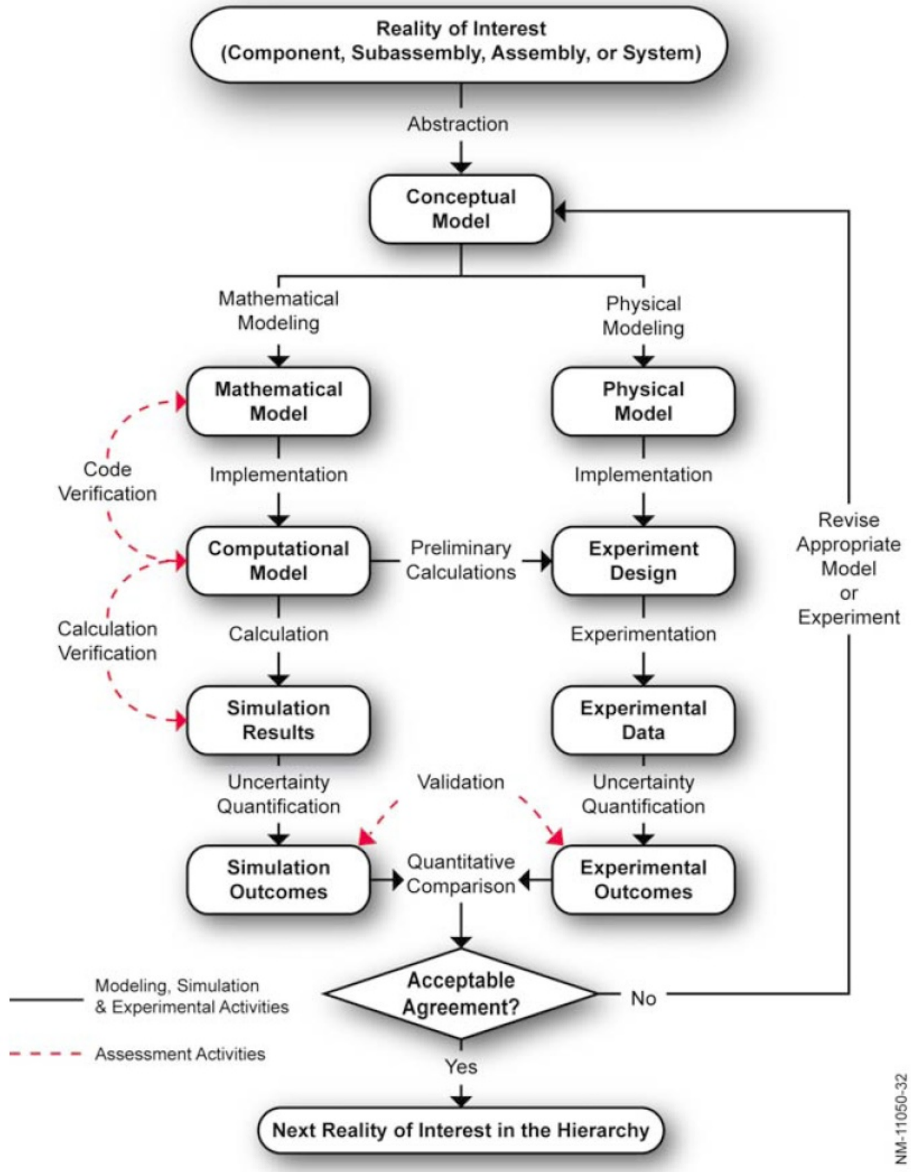
- How good are the approximations?
- How do you test the software?
- '*Predictive*' power?

Motivation

Different Assessment Techniques for Different Sources of Uncertainty or Error

Problem:	Assessment:
• Model(s) not good enough	• Validation
• Numerics not good enough	
• Algorithm is not implemented correctly	• Code verification
• Algorithm is flawed	• Code verification
• Problem definition not good enough	• Uncertainty quantification

Motivation



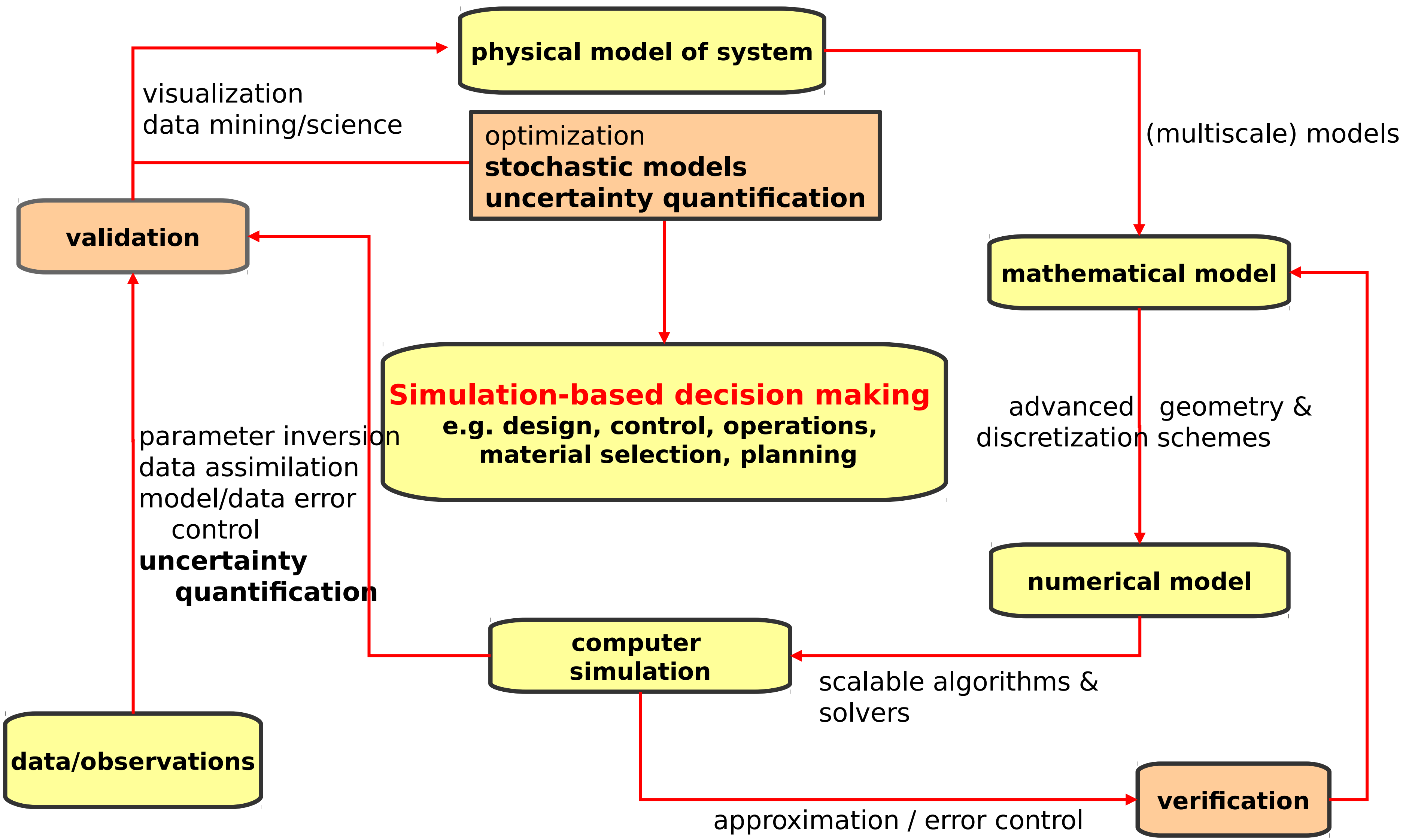
Recognized in many other (engineering) fields

Example:

V&V process flowchart from the ASME Solid Mechanics V&V guide (2006).

May be to simplistic…

Motivation: Design Cycle



Motivation

- **Systematic Uncertainty Quantification in Plasma Physics**

  - Often still at the very beginning (parameter scans)
  - Importance increasingly realized ('shortfall'): V&V&UQ
  - connection with 'surrogate' models

Setting up a reference case based on relevant, non-trivial and well understood system in plasma physics:

Vlasov-Poisson-Model

UQ-Model System: Vlasov-Poisson

- Phase-space distribution function f(x,v) of collisionless plasma:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial x} + \frac{q}{m}(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \cdot \frac{\partial f}{\partial v} = 0$$

$$\begin{aligned} \rho(\boldsymbol{x}, t) &= q \int f(\boldsymbol{x}, \boldsymbol{v}, t) d\boldsymbol{v} \\ \boldsymbol{J}(\boldsymbol{x}, t) &= q \int f(\boldsymbol{x}, \boldsymbol{v}, t) \boldsymbol{v} d\boldsymbol{v} \end{aligned}$$

$$\begin{aligned} \nabla \times \boldsymbol{B} &= \boldsymbol{J} \\ \nabla \times \boldsymbol{E} &= 0 \\ \nabla \cdot \boldsymbol{E} &= \frac{\rho}{\varepsilon_0} \\ \nabla \cdot \boldsymbol{B} &= 0 \end{aligned}$$

$$-\Delta \phi = 1 - \rho(t, \boldsymbol{x}) = 1 - q \int f(t, \boldsymbol{x}, \boldsymbol{v}) \mathrm{d}\boldsymbol{v}$$

$$\boldsymbol{E} = -\nabla \phi \quad .$$

UQ-Model System: Vlasov-Poisson

- Phase-space distribution function f(x,v,t) of collisioness plasma:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial x} + \frac{q}{m}\left(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}\right) \cdot \frac{\partial f}{\partial v} = 0$$

System details:

- 1+1-dimensional (x,v-space)
- Solver: Semi-Lagrangian-solver
- Boundary conditions: periodic
- Negligible **B**-field contributions
- Static ion-background
- External **random** E-field contribution $\mathbf{E_0}$(x)

Effect of the random E-field?

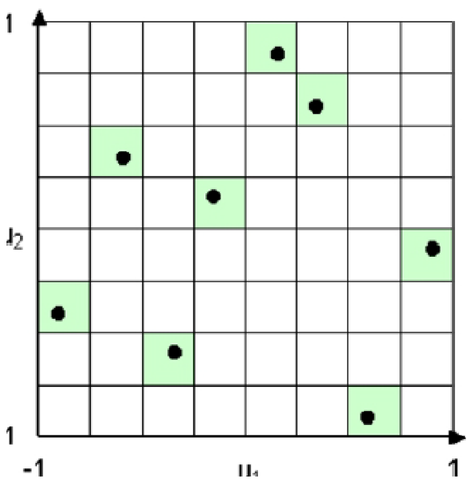
Methods applied in Uncertainty Quantification

- Sampling
- Spectral Expansion
  - Galerkin Approach
  - Stochastic Collocation
  - Discrete Projection
- Surrogate models (eg. Gaussian processes)

➢ Sampling approach

Use random sample S={**x**$^{(i)}$, i=1,…,N}

to compute distribution p(**y**) and moments :



$$\langle y_j \rangle = \frac{1}{N} \sum_{i=1}^{N} M(x^i)_j$$

$$var(y) = \langle y^2 \rangle - \langle y \rangle^2$$

+ higher order terms….

Advantages: - Includes all correlations (→ verification)
- Parallel & straightforward

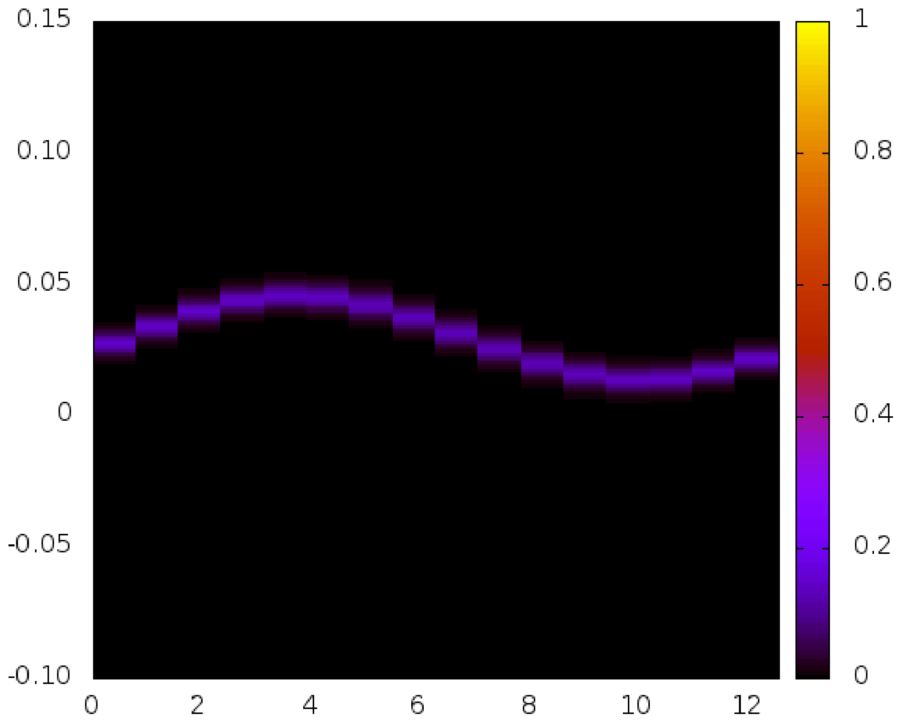
Downside: - sample point density: **curse of dimensions**: $\rho \sim \rho_0^{-Dim}$

Results

➢ Sampling approach

Example: Vlasov-Poisson, random external field $E=E_0+\mathcal{N}(\mu=0,\sigma=0.1E_0)$

t=0.4 s   t=2.8 s



Results

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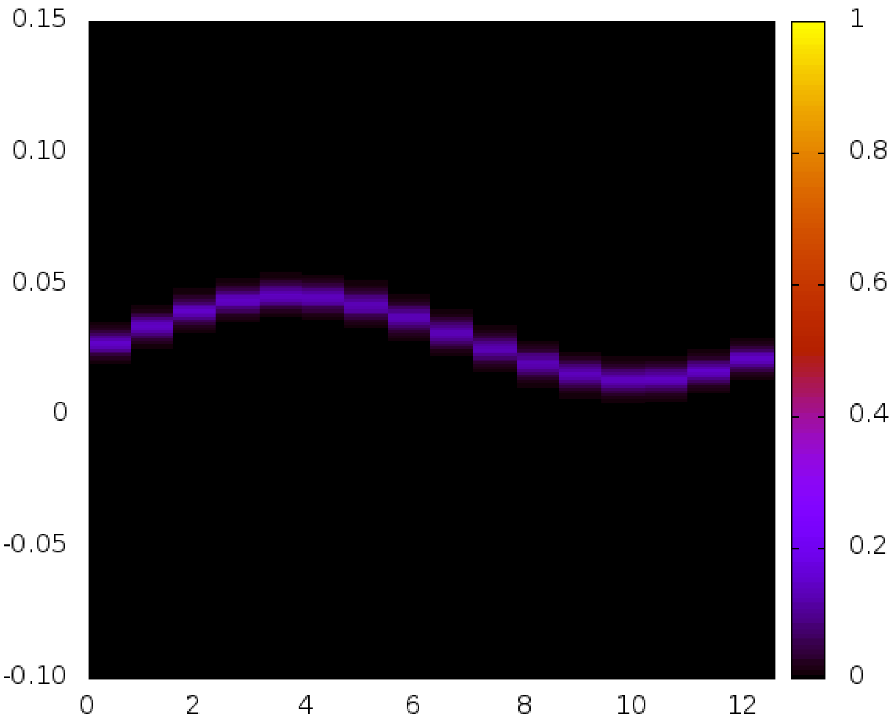
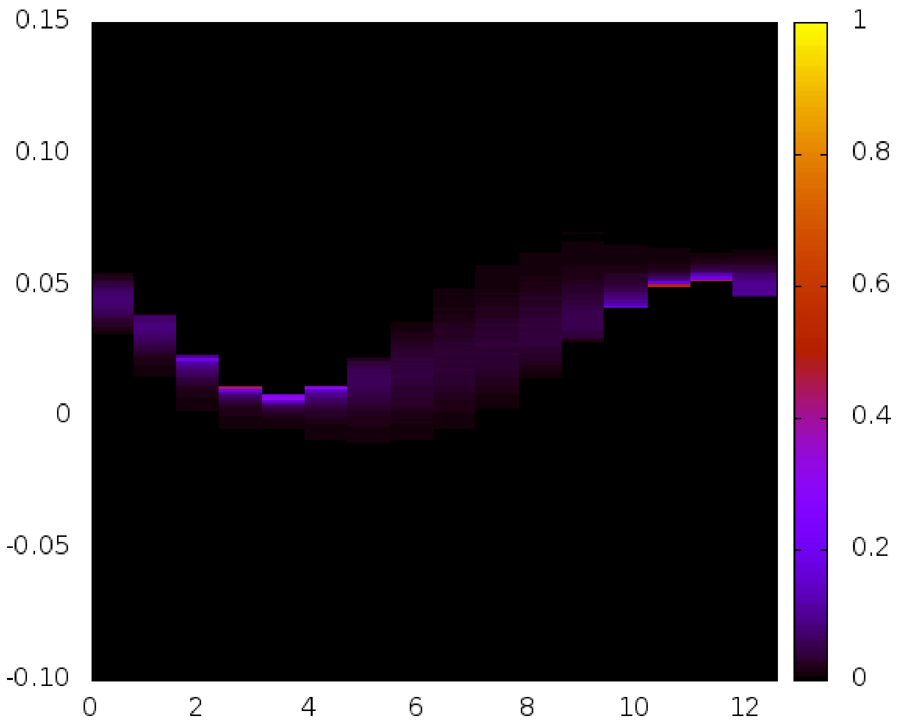


t=2.8 s



➢ Spectral Expansion (Polynomial chaos expansion)

- Consider a computational model $\mathcal{M} : \mathcal{D} \subset \mathbb{R}^M \mapsto \mathbb{R}$ and a probabilistic model for the uncertainty in the input parameters, say $\boldsymbol{X} \sim f_X(\boldsymbol{x}) = \prod_{i=1}^{M} f_{X_i}(x_i)$.

- Assuming that $\mathbb{E}\left[\mathcal{M}(\boldsymbol{X})^2\right] < \infty$ one can represent the random response $Y = \mathcal{M}(\boldsymbol{X})$ in a suitable Hilbert space.

- There exists a countable orthonormal basis $\{\psi_j \,,\, j \in \mathbb{N}\}$ such that :

$$Y = \sum_{j=0}^{\infty} y_j \, \Psi_j(\boldsymbol{X})$$

where :

- y_j : coefficients to be computed (coordinates)
- Ψ_j : basis functions *e.g.* multivariate orthonormal polynomials

Methods in Uncertainty Quantification

- **Spectral Expansion**

Two different approaches:

- **Intrusive methods depend on the formulation and solution of a *stochastic* version of the original model**

- **Nonintrusive methods require multiple solutions of the original (deterministic) model only**

Methods in Uncertainty Quantification

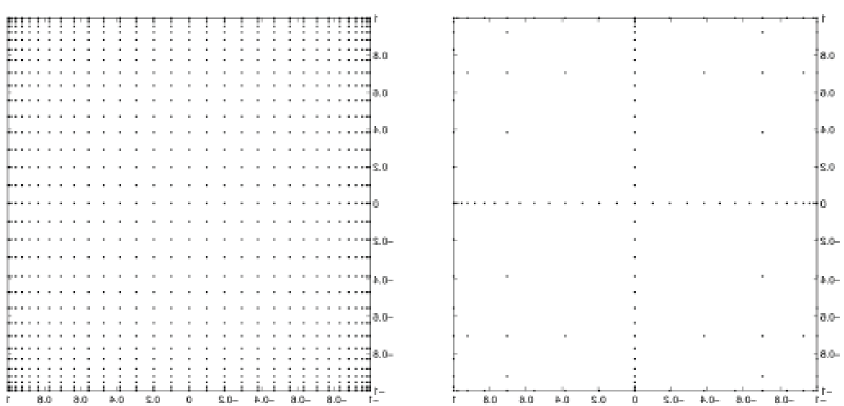
➢ Spectral Expansion – Non-intrusive I

- **Stochastic Collocation**
  - No need to reformulate governing equations (“non-intrusive”)
  - *gPC-based pseudospectral approach:*

Seek $\tilde{Y}_N(\xi) = \sum_{|\boldsymbol{k}|<N} \tilde{a}_k \Psi_k(\xi)$ by computing $a_k = \int Y(\xi)\Psi_k(\xi)\rho(\xi)d\xi$

$$\approx \sum_{j=1}^{Q} Y\left(\xi^{(j)}\right)\Psi_k\left(\xi^{(j)}\right)w^{(j)} \equiv \tilde{a}_k$$

  - Quadrature rule $\left\{\xi^{(j)}, w^{(j)}\right\}_{j=1}^{Q}$ can be sparse (e.g., Smolyak)



➢ Spectral Expansion – Non-intrusive I

➢ Computation of multi-dim integrals:

- exploit structure (Gaussian p(ξ)): Gauss-Hermite quadrature

$$Y(\xi) = \sum_{k=0}^{P} a_k \psi_k(\xi) \quad \text{with} \quad a_k = \frac{\langle Y(\xi), \psi_k(\xi)\rangle}{\langle \psi_k(\xi), \psi_k(\xi)\rangle}$$

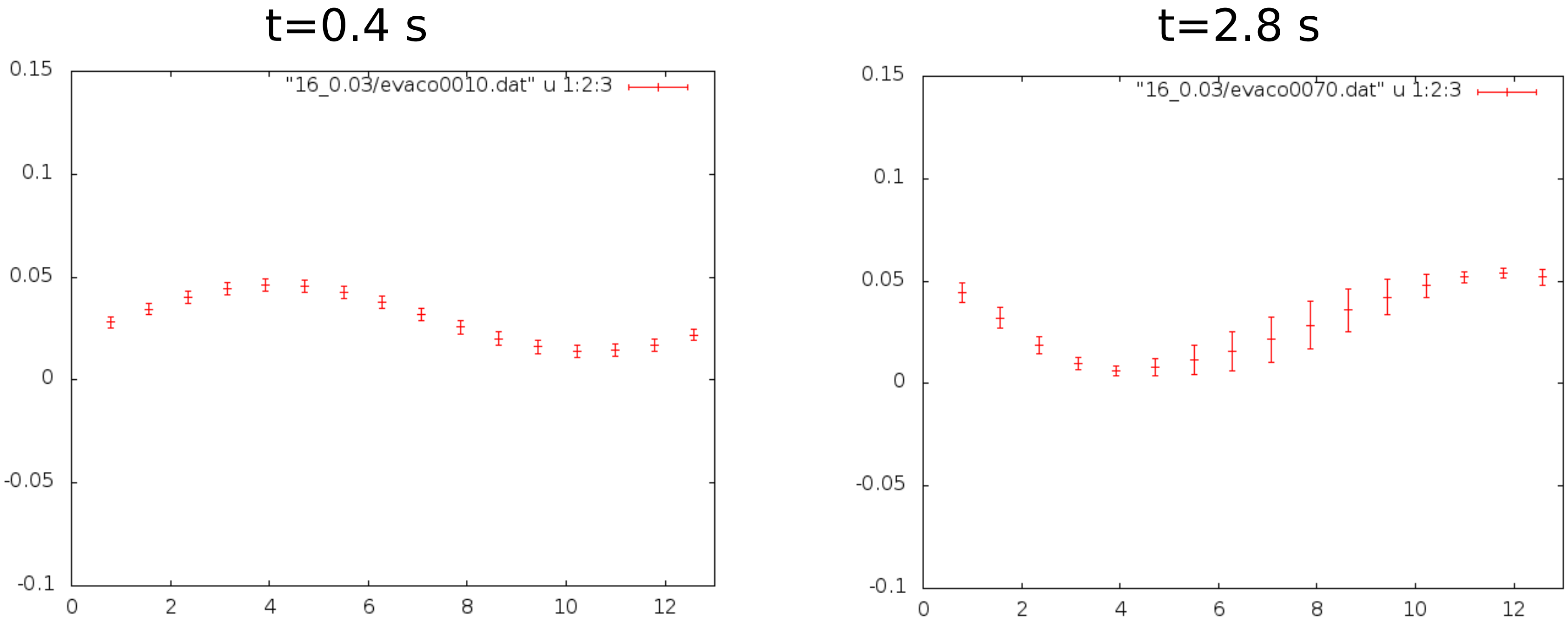
$$\langle h_1(\xi), h_2(\xi)\rangle = \int h_1(\xi) h_2(\xi) p(\xi) \mathrm{d}\xi \overset{\text{G.H.}}{=} \sum_{l=1}^{L} h_1(\xi_l) h_2(\xi_l) w_l$$

➡ Mean <Y>=a_0 and variance σ^2:

$$\sigma_R = \mathcal{E}(R^2) - \mathcal{E}(R)^2 = \sum_{k=1}^{P} a_k^2 \langle \psi_k, \psi_k \rangle = \sum_{k=1}^{P} a_k^2 k!$$

➢ Spectral Expansion – Non-intrusive I

Example: Vlasov-Poisson, random external field $E=E_0+\mathcal{N}(\mu=0,\sigma=0.1E_0)$



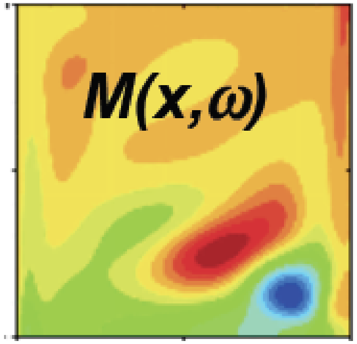
4-th order expansion in excellent agreement with MC in fraction of computing time

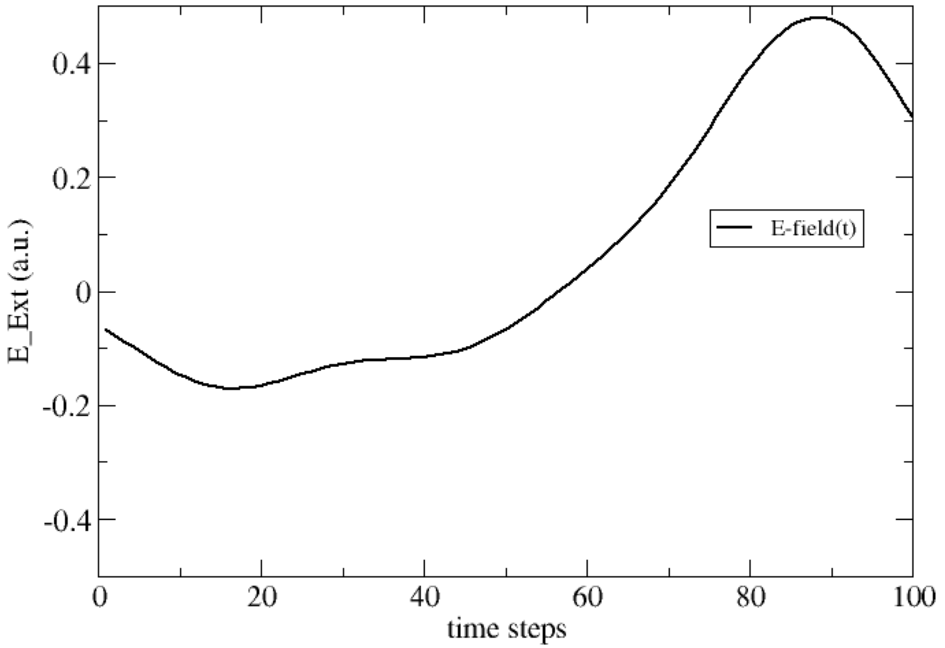
➢ Spectral Expansion – Non-intrusive II

Now: **Random field** M(x,t) instead of random variable(s)

Infinite number of random variables ??

Example: E-field fluctuation





Methods in Uncertainty Quantification

- **Covariance matrix:** correlation length essential:

  ➡ no white noise!

$$C_{ij} = \exp\left\{-\frac{1}{2}\frac{(t_i - t_j)^2}{\lambda^2}\right\}$$

Methods in Uncertainty Quantification

- Let $M \sim GP(\mu, C)$
- Introduce the **Karhunen-Loève expansion** & truncate:

$$M(\boldsymbol{x},\omega) = \mu(\boldsymbol{x}) + \sum_{i=1}^{K} \sqrt{\lambda_i}\, c_i(\omega)\, \phi_i(\boldsymbol{x})$$

  - λ_i and $\phi_i(\boldsymbol{x})$ are eigenvalues/eigenfunctions of $C(\boldsymbol{x}_1,\boldsymbol{x}_2)$

$$\int_D C(\boldsymbol{x}_1,\boldsymbol{x}_2)\phi_i(\boldsymbol{x}_2)\,d\boldsymbol{x}_2 = \lambda_i \phi_i(\boldsymbol{x}_1)$$

  - $c_i \sim N(0,1)$
- Transform the inverse problem **(dim = *K* << *n*)**

$$d = \tilde{G}(\boldsymbol{c}) + \eta$$

- **I) Covariance matrix:**

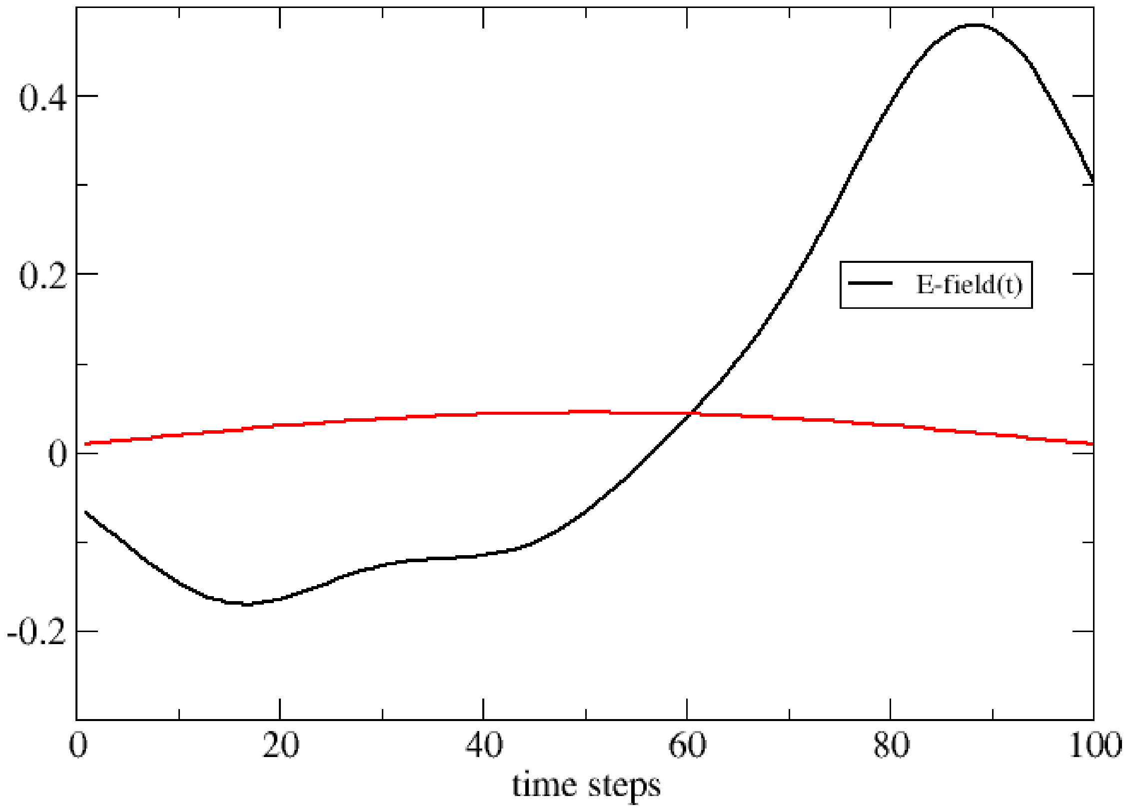
$$C_{ij} = \exp\left\{-\frac{1}{2}\frac{(t_i - t_j)^2}{\lambda^2}\right\}$$

Eigenvectors

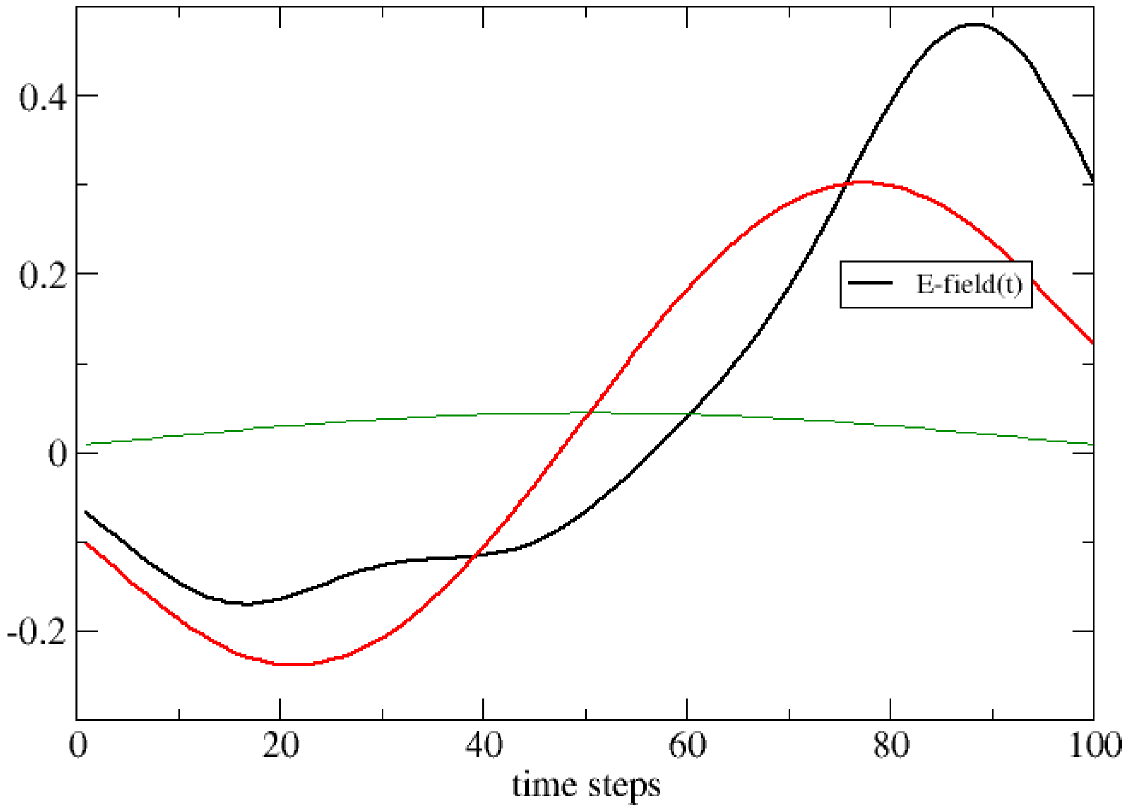
Eigenvalues

Methods in Uncertainty Quantification

➢ **Expansion of random field in KL-representation**



- **Expansion of random field in KL-representation**



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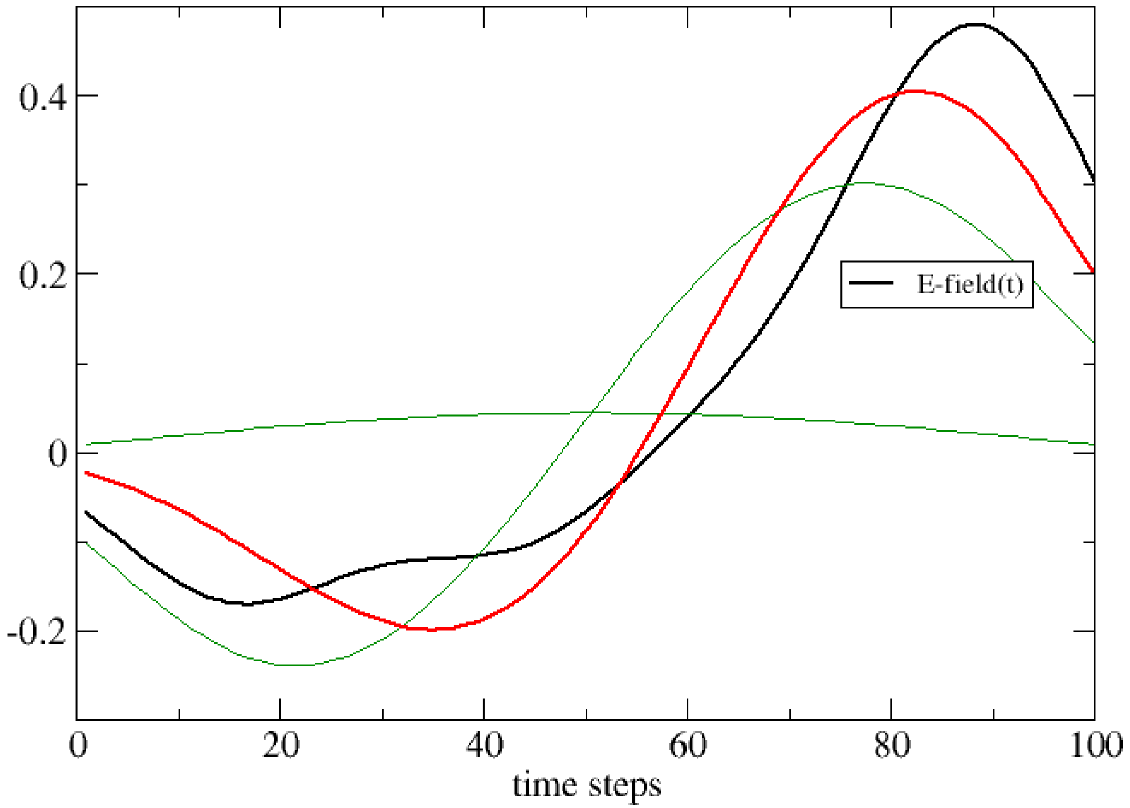

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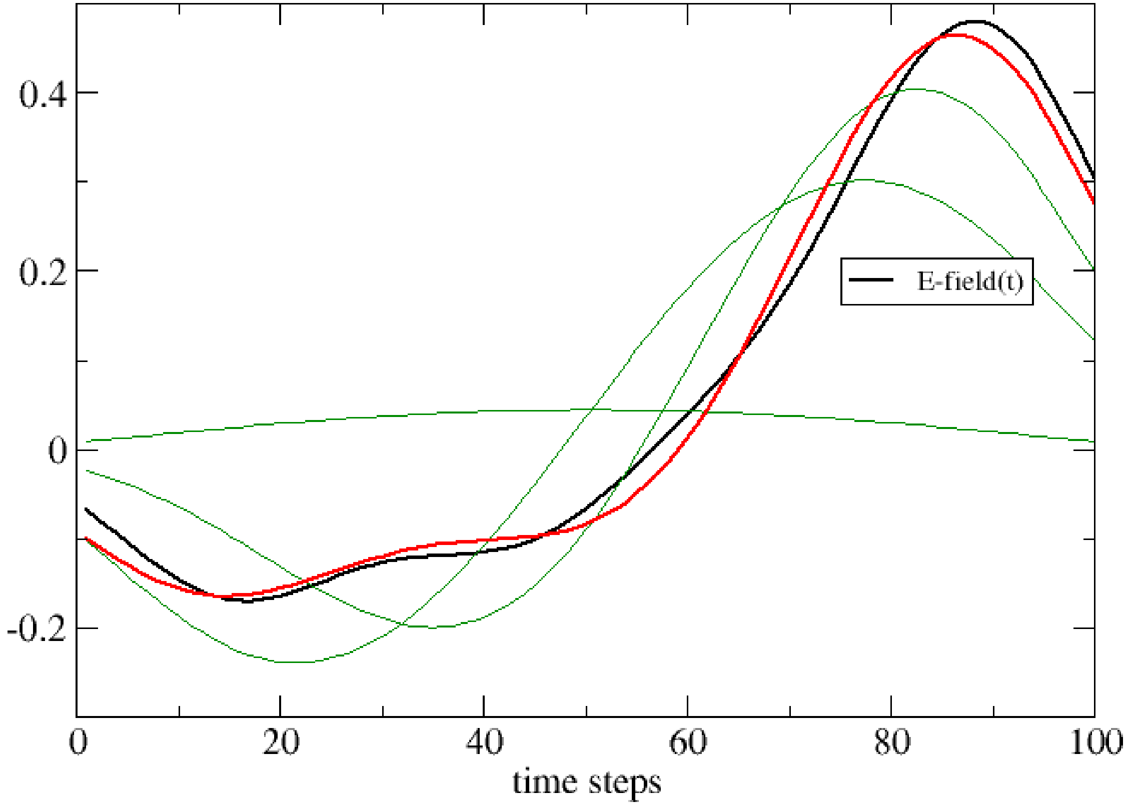

Methods in Uncertainty Quantification

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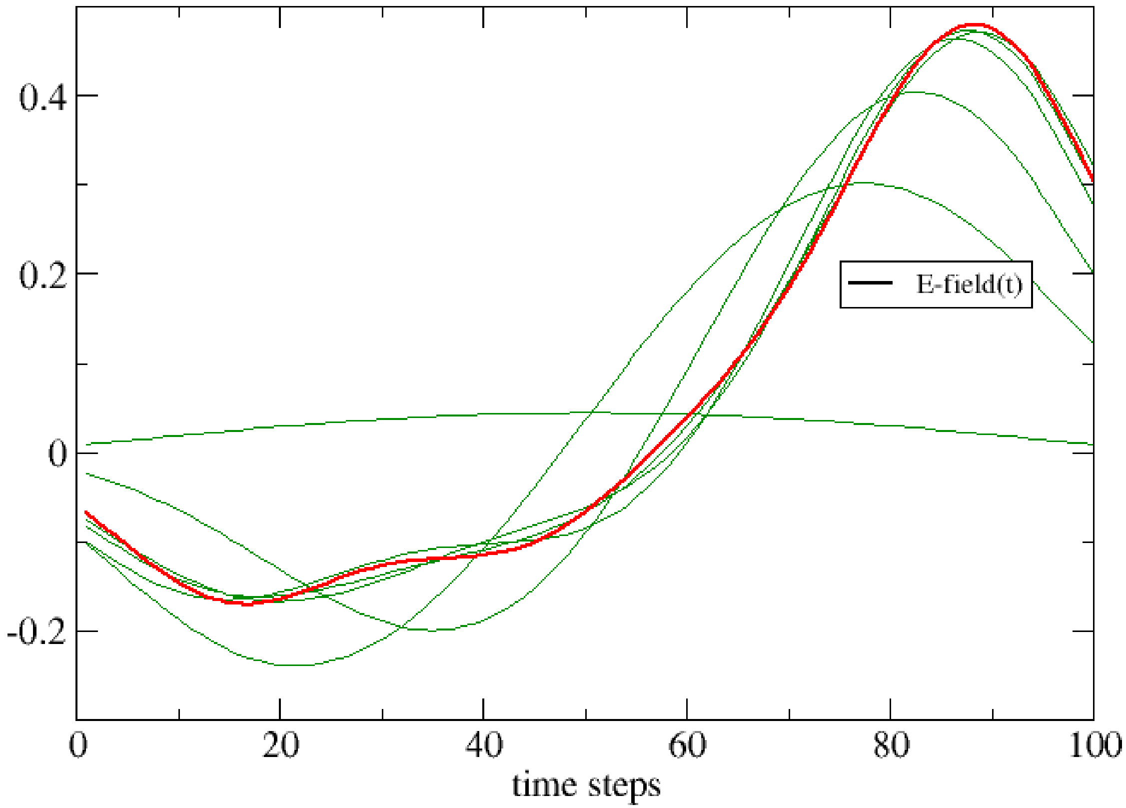
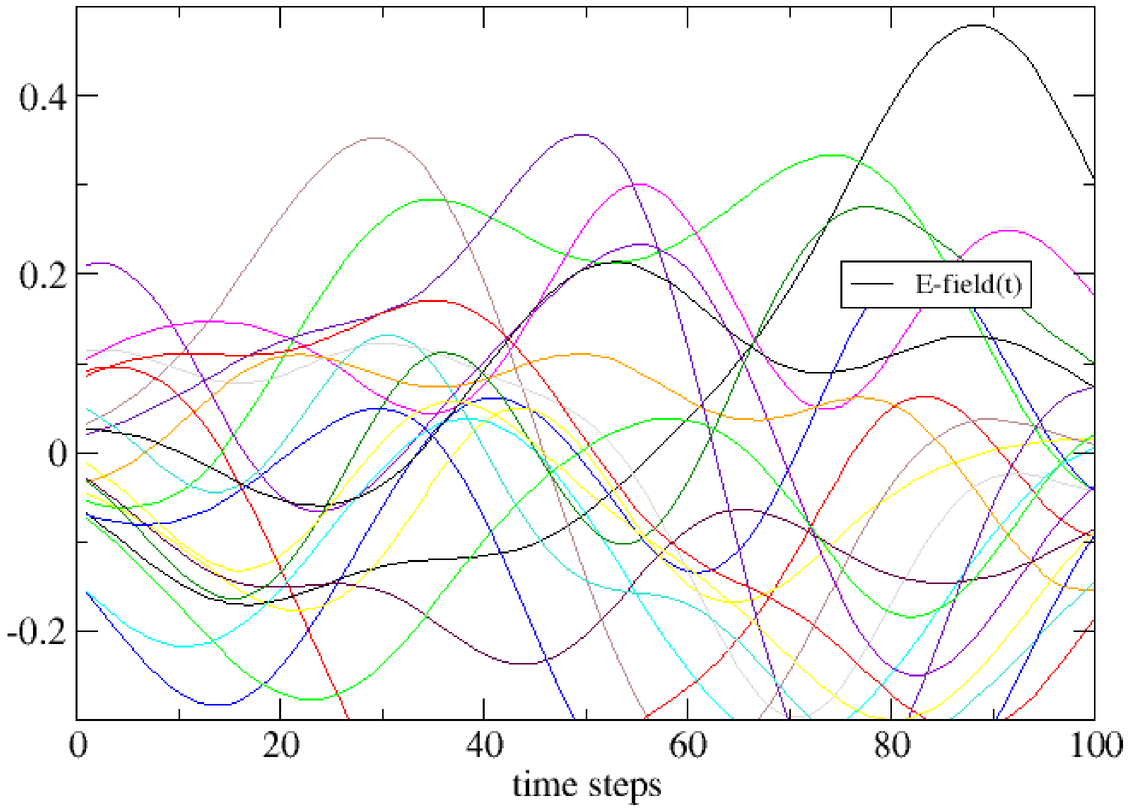


➢ **Random samples of random field in KL-representation**



Result

- Vlasov-Poisson with fluctuating external E-field: Uncertainty?
- Now multivariate Gauss-Hermite integration:

$$a_k = \frac{1}{k!} \int \dots \int \mathrm{d}\xi_1 \dots \mathrm{d}\xi_M \, g(\xi_1, \dots, \xi_M) \psi_k(\xi_1, \dots, \xi_M) p(\xi_1, \dots, \xi_M)$$

j	$\boldsymbol{\alpha}$	$\Psi_{\boldsymbol{\alpha}} \equiv \Psi_j$
0	$[0,0]$	$\Psi_0 = 1$
1	$[1,0]$	$\Psi_1 = \xi_1$
2	$[0,1]$	$\Psi_2 = \xi_2$
3	$[2,0]$	$\Psi_3 = (\xi_1^2 - 1)/\sqrt{2}$
4	$[1,1]$	$\Psi_4 = \xi_1 \xi_2$
5	$[0,2]$	$\Psi_5 = (\xi_2^2 - 1)/\sqrt{2}$
6	$[3,0]$	$\Psi_6 = (\xi_1^3 - 3\xi_1)/\sqrt{6}$
7	$[2,1]$	$\Psi_7 = (\xi_1^2 - 1)\xi_2/\sqrt{2}$
8	$[1,2]$	$\Psi_8 = (\xi_2^2 - 1)\xi_1/\sqrt{2}$
9	$[0,3]$	$\Psi_9 = (\xi_2^3 - 3\xi_2)/\sqrt{6}$

Example: M=2, P=3

$$\tilde{Y} \equiv \mathcal{M}^{\mathrm{PC}}(\xi_1, \xi_2) = a_0 + a_1 \xi_1 + a_2 \xi_2$$
$$+ a_3 (\xi_1^2 - 1)/\sqrt{2} + a_4 \xi_1 \xi_2$$
$$+ a_5 (\xi_2^2 - 1)/\sqrt{2} + a_6 (\xi_1^3 - 3\xi_1)/\sqrt{6}$$
$$+ a_7 (\xi_1^2 - 1)\xi_2/\sqrt{2} + a_8 (\xi_2^2 - 1)\xi_1/\sqrt{2}$$
$$+ a_9 (\xi_2^3 - 3\xi_2)/\sqrt{6}$$

$$N_{\mathrm{int}} = \frac{(M+P)!}{M!P!}$$

Partial variance

- Consider :

$$D_{i_1 \ldots i_s} = \int_{[0,1]^s} \mathcal{M}^2_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s})\, dx_{i_1} \ldots dx_{i_s}$$

- Then :

$$D = \sum_{i=1}^{M} D_i + \sum_{1 \leqslant i < j \leqslant M} D_{ij} + \ldots + D_{12\ldots M}$$

- The Sobol' indices are obtained by normalization :

$$S_{i_1 \ldots i_s} = \frac{D_{i_1 \ldots i_s}}{D}$$

They represent the fraction of the total variance $\mathrm{Var}[Y]$ that can be attributed to each input variable i (S_i) or combinations of variables $\{i_1 \ldots i_s\}$

Sensitivity Assessment: Example

Computational model $Y = \mathcal{M}(X_1, X_2)$

Probabilistic model $X_i \sim \mathcal{N}(\mu_i, \sigma_i) \qquad i = 1, 2$

Isoprobabilistic transform $X_i = \mu_i + \sigma_i \, \xi_i \qquad i = 1, 2$

Chaos degree $p = 3$, *i.e.* $P = 10$ terms

j	$\boldsymbol{\alpha}$	$\Psi_{\boldsymbol{\alpha}} \equiv \Psi_j$
0	[0, 0]	$\Psi_0 = 1$
1	[1, 0]	$\Psi_1 = \xi_1$
2	[0, 1]	$\Psi_2 = \xi_2$
3	[2, 0]	$\Psi_3 = (\xi_1^2 - 1)/\sqrt{2}$
4	[1, 1]	$\Psi_4 = \xi_1 \xi_2$
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9	[0, 3]	$\Psi_9 = (\xi_2^3 - 3\xi_2)/\sqrt{6}$

Variance

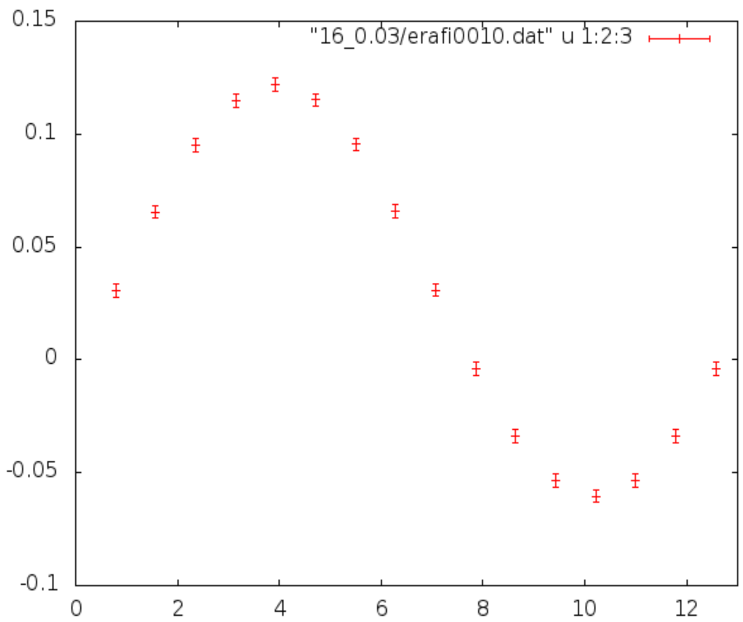
$$D = \sum_{j=1}^{9} a_j^2$$

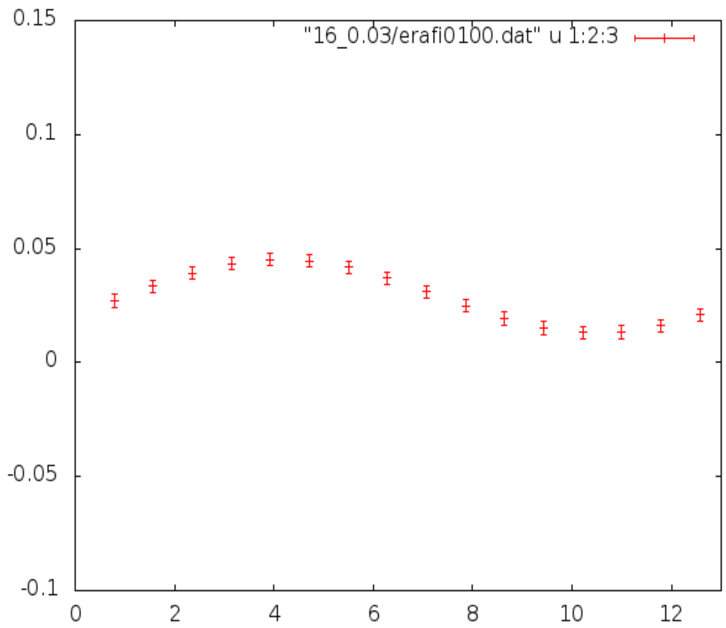
Sobol' indices

$$\begin{aligned} S_1 &= \left(a_1^2 + a_3^2 + a_6^2\right)/D \\ S_2 &= \left(a_2^2 + a_5^2 + a_9^2\right)/D \\ S_{12} &= \left(a_4^2 + a_7^2 + a_8^2\right)/D \end{aligned}$$

Result

- Vlasov-Poisson with fluctuating external E-field: all gentle...
- Initial E-field amplitude more important than E-field variation





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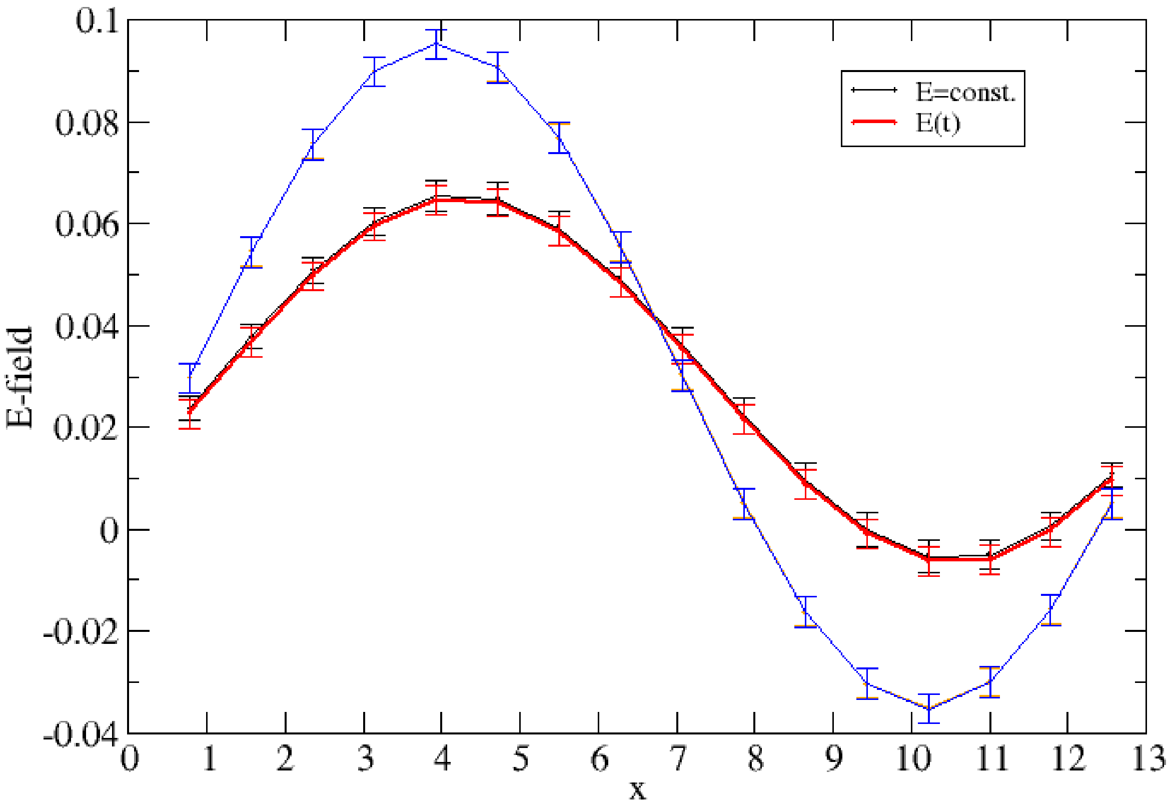


Conclusion I

- **Spectral expansion approach**
  - intrusive methods: best (only?) suited for new codes
  - non-intrusive methods: general purpose approach
    - selection of collocation points
    - sparse methods for larger problems possible
    - influence of input parameter combinations as byproduct: Sobol decomposition
- Proof of principle for 1+1 Vlasov-Poisson Equation
- Validated against MC-approach (and other test cases)
- Some implementations: eg. DAKOTA

- **Best suited for medium number of dimensions (O(10)) and moderately expensive simulators (forward models)**

Emulators

What if conditions for Spectral expansion do *not* hold?

⇨ Use of *emulators* as surrogate for *simulators*

- A simulator is a model of a real process
  - Typically implemented as a computer code
  - Think of it as a function taking inputs x and giving outputs y:
  - **x** → **Code** → **y(x)**
- An emulator is a statistical representation of this function
  - Expressing knowledge/beliefs about what the output will be at any given input(s)
  - Built using prior information and a **training set** of model runs

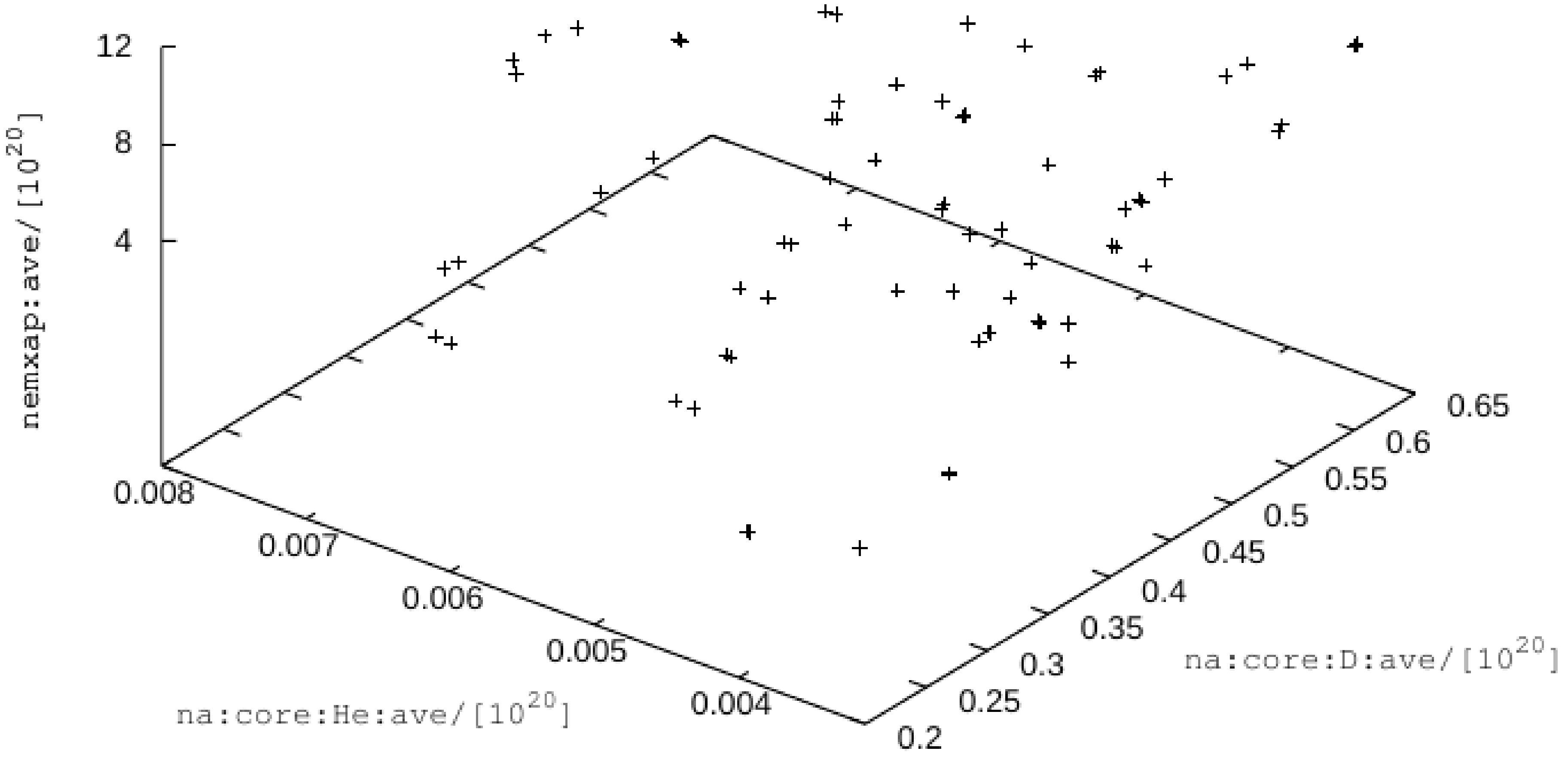
⇨ Focus on *Gaussian Processes*

SOLPS-Application

SOLPS-Data base: - 1500 parameters

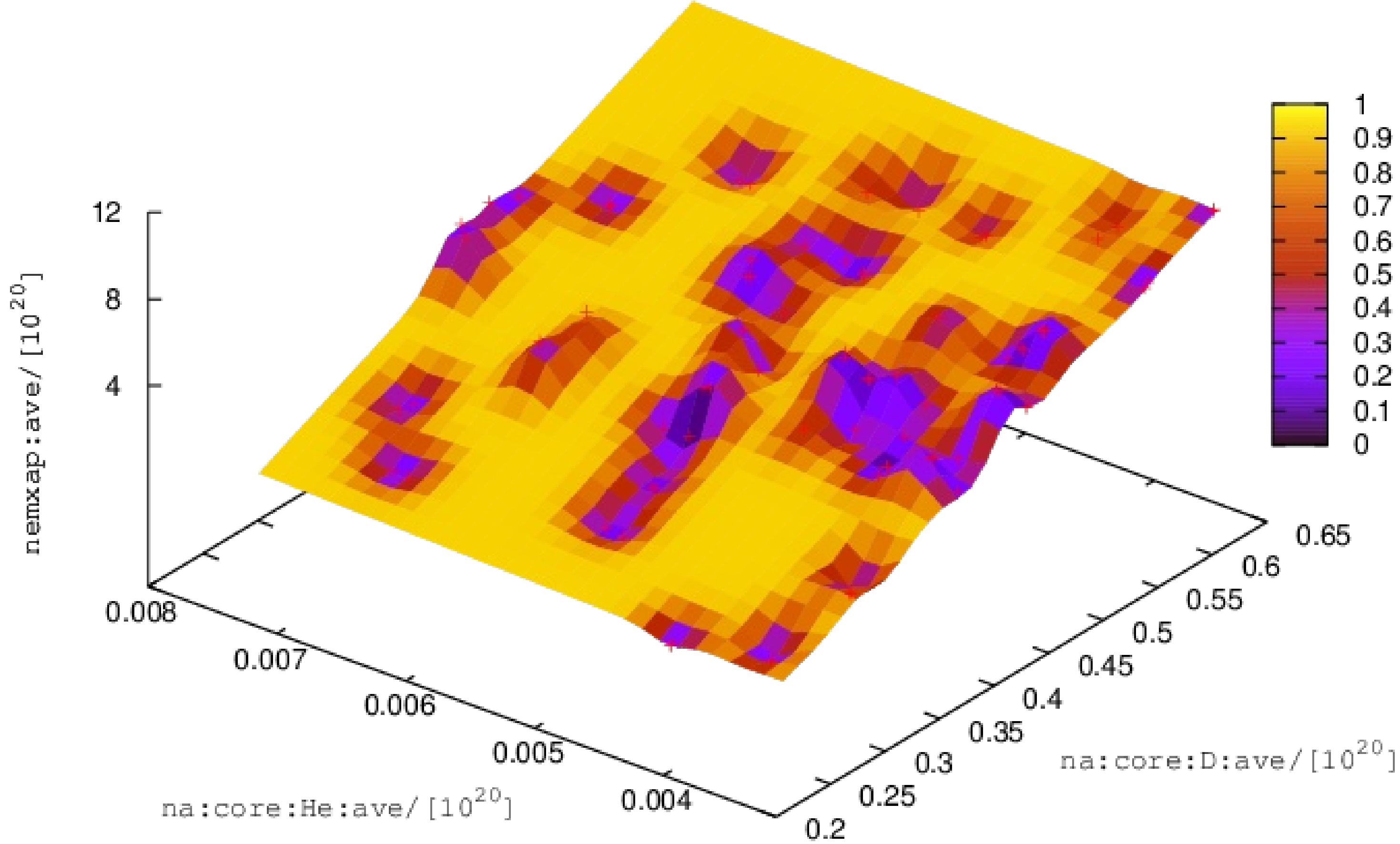
- collected by D. Coster

Idea: exploit for initialization, scans

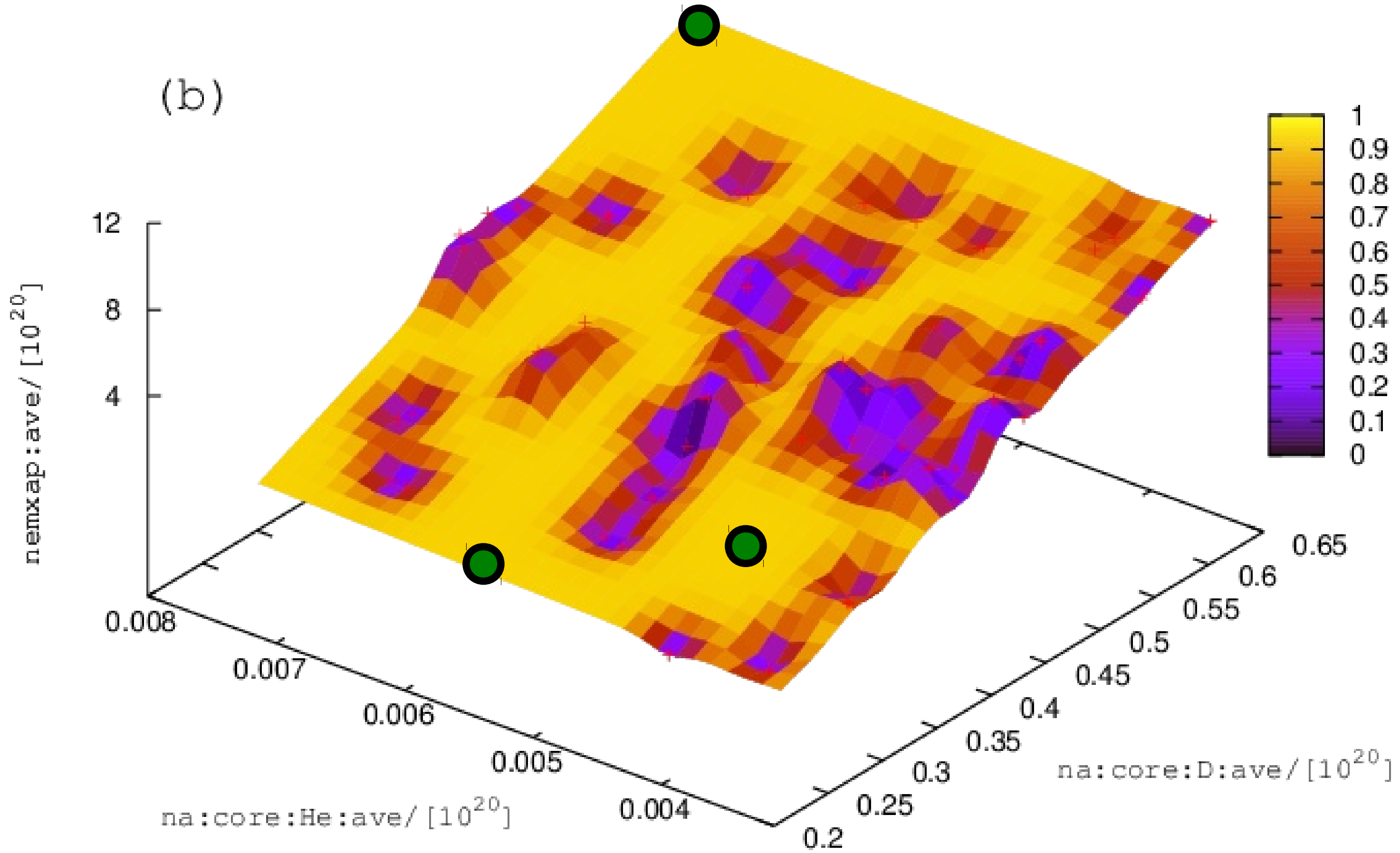


SOLPS-Data

- Result of GP-interpolation
- Color code: normalized variance



Input-space locations with largest information gain:



SOLPS-Application

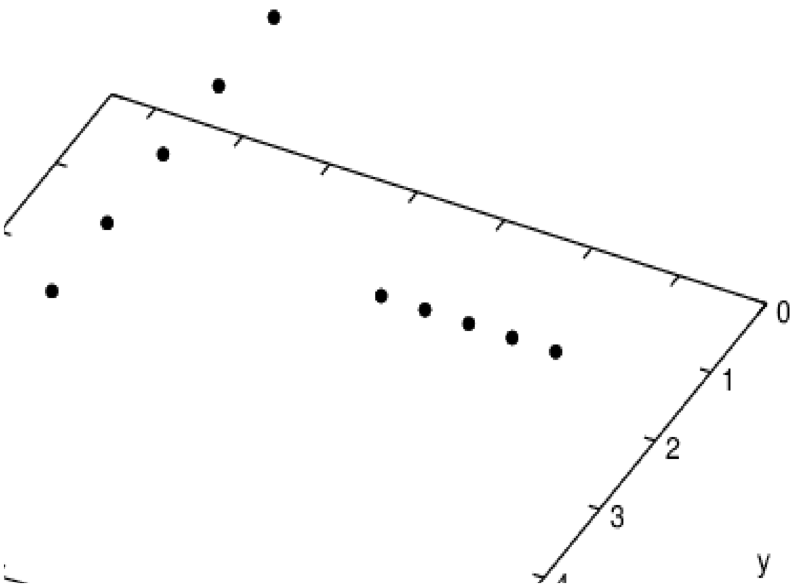
- GP-algorithm established

  - Mid size problems: 1000 data points, ~50 dimensions
  - many areas of application, ie. fitting of MD-potentials to DFT-data

  but...

SOLPS-Application

- Present data base "**insufficient**" …
  - Physic based line-scans (power, density, temperature...)
  - Does not cover space (eg. approx. Latin hypercube)



SOLPS-Application

- GP-algorithm now in routine application
- Present data base **insufficient**

→ Semi-automated data base generation (eg. Bayesian Experimental Design):

- Design Cycle:

  - Determine best location(s) for next simulation(s): Utility
  - Recompute uncertainty estimates
  - Check for design criteria: exit?

SOLPS-Application

- GP-algorithm now in routine application
- Present data base **insufficient**

➡ Semi-automated data base generation (eg. Bayesian Experimental Design):

- Design Cycle:

  - Determine best location(s) for next simulation(s): Utility

  - Recompute uncertainty estimates

  - Check for design criteria: exit?

- Challenges: - adequate coverage of relevant input space
  - code convergence

Gaussian Processes: Challenges

- **Scaling**: N^3 : not yet prohibitive

- **Correlated output**

  - Standard approach: *independent* scalar response variables
    Drawback: Prediction not satisfactory: co-variance

  - Difficulty: design of pos. def. **cross**-correlation matrices

- **Phase transitions**: 'global' scale of covariance matrix

Conclusion II

- Gaussian Processes are powerful tool for high-dimensional interpolation → fast emulators → UQ
- Analytical formulas for mean and variance → exp. Design
- Best suited for scalar output

- Automated experimental design cycle:
  - works on test cases
  - At present: too much human intervention needed for plasma codes
  - Problems appear solvable

- Correlated output: research and tests ongoing

The End

Thank you!

References

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