Modelling with Partial Differential Equations in Metrology

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255th PTB. Seminar / Workshop of EURAMET Focus Group Math & IT
• Partial Differential Equations (PDEs)
• Inverse Methods in PDEs: Scatterometry
• Multiscale Methods: Homogenization, Averaging
• Flow Simulations
I. Partial Differential Equations (PDEs)

- **diffusion eq., heat eq.**
  \[ \partial_t u = D \Delta u \]

- **phase transitions: Ginzburg-Landau eq.**
  \[ \partial_t u = -\frac{\partial V(u)}{\partial u} + \gamma \Delta u = \varepsilon u - \alpha |u|^2 u + \gamma \Delta u \]

- **phase separation, thin films: Cahn-Hilliard type eq.**
  \[ \partial_t u = \nabla \cdot \left( M(u) \nabla \left( \frac{\partial V(u)}{\partial u} - K \Delta u \right) \right) \]

- **electromagnetic fields: Maxwell eqs., Helmholtz eq.**
  \[ \Delta u(x, y, z, t) - k^2(x, y, z) \cdot u(x, y, z, t) = 0 \]

- **hydrodynamics: Navier-Stokes eqs.**
PDEs in Metrology

Applied mathematics:
- Analytical methods, perturbation theory
- Numerics, discretization schemes – FEM, FD, FV etc.
- Multiscale systems: homogenization, averaging

Metrology:
- PDEs as measurement models
- PDEs as quantitative models
- PDEs & inverse problems
- Uncertainty evaluation
II. Inverse Problem - Scatterometry

Periodic scattering geometry given by parameters $P_i$

Forward problem:
Plane waves $\rightarrow$ Geometry $(P_i) \Rightarrow$ Scattering efficiencies $E_i$

Inverse problem:
Scattering efficiencies $E_i \rightarrow$ Geometry $(P_i)$

Cooperation with WIAS Berlin (DIPOG-Software), AMTC Dresden
Mathematical Model Scatterometry

Helmholtz-equation

\[ \Delta u(x, y) = k(x, y)^2 u(x, y) \]

with

\[ k(x, y) = \omega \sqrt{\mu_0 \varepsilon(x, y)} \]

+ boundary conditions

2D: geometry

Lithography mask
Solution of the Inverse Problem

Compare simulated scattering efficiencies $E_m(h)$ with measurement data ->
Reconstruction: Minimization of functional $\Phi$

$$\Phi(E_m(h)) = \sum_{m \in M} \omega_m \left| E_m(h) - E_m^{\text{meas}} \right|^2$$

-> profile parameters $h$ characterize profile

Test with simulated data:
Succesful reconstruction

Failed reconstruction
(too few input data)

EUV-Scatterometry at PTB

EUV(13nm)-Reflectometer (PTB, Berlin)

Details of setup, model -> talk by M. A. Henn
Optimal Simulation Results vs. Measured Data

Deviations simulated vs. measured efficiencies: 10 – 15 %
Measurement noise: < 3 %

**Systematic errors are important!**
- Substrate model, roughness, incomplete information.....
  -> model errors
  *T. Germer et al. SPIE Proc. 2009*
  *H. Groß et al. Meas. Sci. Tech. 2009*

Propagation of uncertainties in simulations:
- Monte Carlo method, covariance approach
- uncertainties in range < 5 nm (< 2 %)

Improved treatment of random & systematic errors needed
  -> *Talk by M. A. Henn*
• Determination of parameters in PDEs: coefficients, simple geometry from data
• Computationally expensive
• Applications:
  - Heat conduction (see L. Wright talk)
  - Scatterometry (see M. A. Henn talk)
• Outlook: Statistical inverse problems, uncertainty evaluation
III. PDEs and Multiscale Systems

• Multiscale temporal and/or spatial dynamics

• Homogenization (averaging in space):
  Heterogeneous reaction-diffusion systems

• Simulation of fluid flows:
  Turbulence modelling (averaging in time)
Electrical Excitation in the Heart

Compare: surface electrograms, propagation velocities, electro- & magnetocardiograms
Heart Modelling: Bidomain Equations

Coupled continua

$\phi = \phi_i - \phi_e \quad \frac{\partial n}{\partial t} = g(\phi, \bar{n})$

10^{10} Cells

coupled parabolic & elliptic PDEs for intra- and extracellular potentials $\phi_i$, $\phi_e$ and ionic channel dynamics $\bar{n}$

monodomain approximation: reaction-diffusion equations

$-\nabla(\sigma_e \nabla \phi_e) = \chi(C_m \frac{\partial \phi}{\partial t} + \frac{1}{R_m} f(\phi, \bar{n}))$

$\nabla(\sigma_i \nabla \phi_i) = \chi(C_m \frac{\partial \phi}{\partial t} + \frac{1}{R_m} f(\phi, \bar{n}))$
Heterogeneous Reaction-Diffusion Systems

- Model equations
  \[ \partial_t c = \nabla \cdot (D(r) \nabla c) + R(c, r) \]
- \(D(r), R(r)\) describe heterogeneities (scale \(l_{\text{het}}\))
- Effective models: homogeneity on scale \(\lambda \gg l_{\text{het}}\)

Homogenization

Detailed model → Effective model
• Model equations with heterogeneous reaction and diffusion

\[ \partial_t c = \nabla \cdot (D(r) \nabla c) + R(c, r) \]

• Averaging, coarse-graining:

\[ \partial_t \langle c \rangle = \langle \nabla \cdot (D(r) \nabla c) \rangle + \langle R(c, r) \rangle \]

• Homogenization

\[ \partial_t \langle c \rangle = \nabla \cdot (D_e \nabla \langle c \rangle) + R_e \left( \langle c \rangle \right) \]

• Goal: Analytical expressions of effective diffusion constants and reaction rates
Example: Random Binary Medium

- Binary media: two phases with fractions $\phi$, $1-\phi$
- Diffusion and reaction of both phases: $D_1$, $R_1$ and $D_2$, $R_2$

\[
0 = \frac{D_1 - D_e}{D_1 + (d-1)D_e} \cdot (1-\phi) + \frac{D_2 - D_e}{D_2 + (d-1)D_e} \cdot \phi
\]  

\[
R_e(\langle c \rangle) = R_1(\langle c \rangle) \cdot (1-\phi) + R_2(\langle c \rangle) \cdot \phi
\]

- Validation by simulation of heterogeneous media
IV. Simulating Fluid Dynamics

- Goal: Supplement/replace experiments
- Quantitative modelling of reference experiments
- Application: Explosion protection, flow measurements

Experiment: free jet (helium in air)  
non-stationary simulation (CFX software package)
Navier-Stokes Equation & Averaging

\[
\frac{\partial u}{\partial t} + (u \, \text{grad}\, u) + \text{grad}\, p = \nu \Delta u + f \quad \text{velocity field}
\]

\[
\text{div}\, u = 0
\]

Averaging of velocity fields, e. g. :

\[
U = \lim_{T \to \infty} \frac{1}{T} \int_{0}^{T} u(x, t) dt \quad \text{(RANS)}
\]

\[
U(t) = \frac{1}{\Delta T} \int_{t-\Delta t/2}^{t+\Delta t/2} u(x, \tau) d\tau, \quad \text{(URANS)}
\]

+ closure relations
Comparison of Turbulence Models

Averaged Navier-Stokes equations
Degree of averaging

Comparison Velocity Profiles

Comparison Experiment – Simulation

propagation velocity o. k., but profile widths disagree

Summary: Multiscale Models

Homogenization and averaging necessary to reduce computational costs

Simulation of detailed models for validation of averaged models

Applications:
- Flow: hydrodynamics & heat transfer
- Explosion protection: hydrodynamics & chemistry
- Electromagnetic fields
Conclusion

- PDEs as quantitative models in metrology
- Inverse problems & PDEs
- Effective PDE descriptions in multiscale systems
- Uncertainty in PDE models:
  Monte-Carlo methods, statistical approach
Questions?

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