Frequency Domain Estimation of Spatially Varying Parameters in Heat and Mass Transport

Amritam Das*, Siep Weiland*, Matthijs van Berkel**

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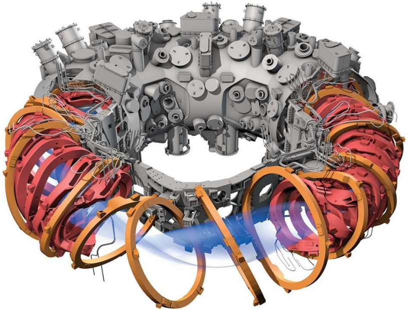
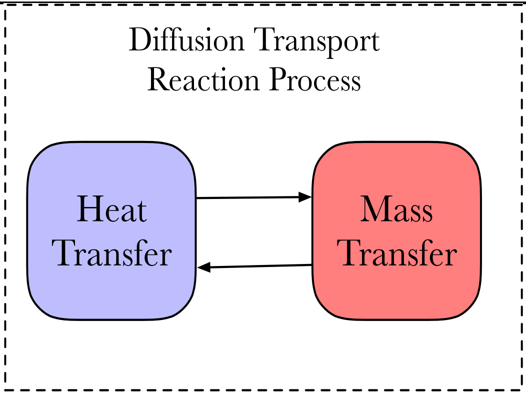
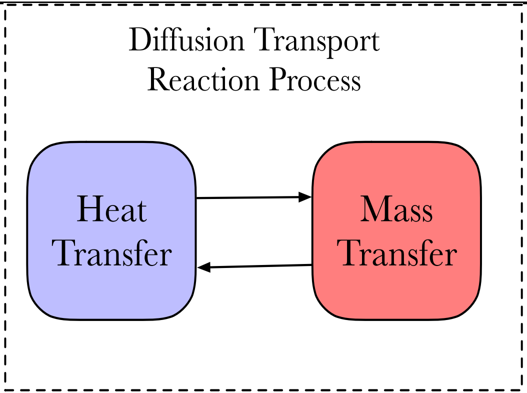


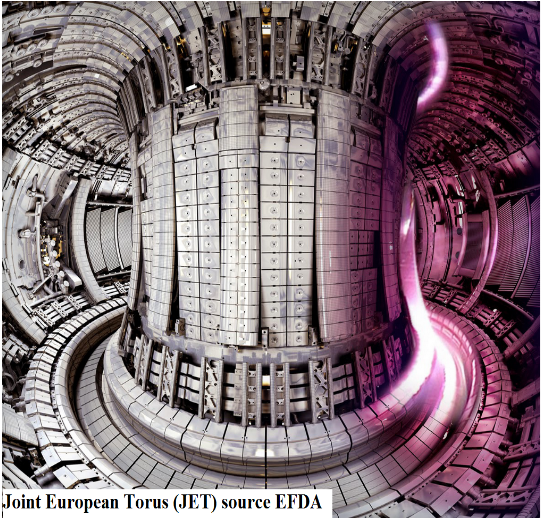

Diffusion Transport
Reaction Process
Heat
Transfer
Mass
Transfer



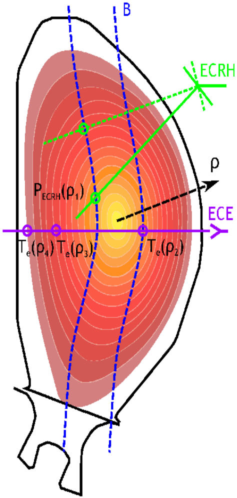
Model Class: Diffusion-Transport-Reaction Equation

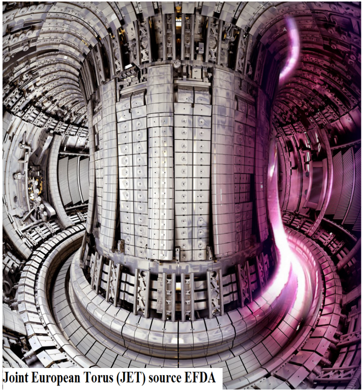
$$E(x)\frac{\partial z(x,t)}{\partial t} = D(x)\frac{\partial^2 z(x,t)}{\partial x^2} + U(x)\frac{\partial z(x,t)}{\partial x} + K(x)z(x,t) + P(x)u(t),$$

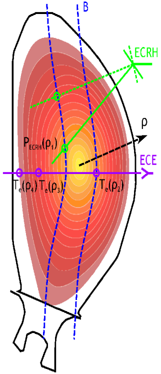
with suitable boundary conditions

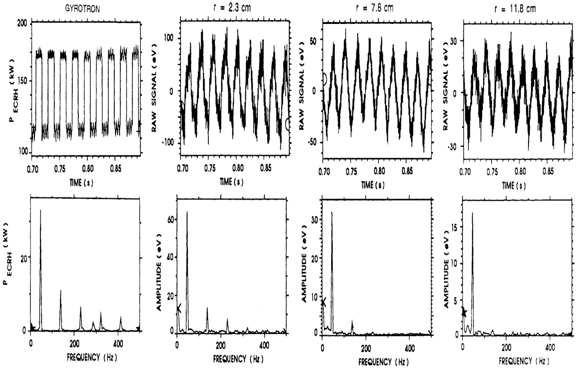


Joint European Torus (JET) source EFDA



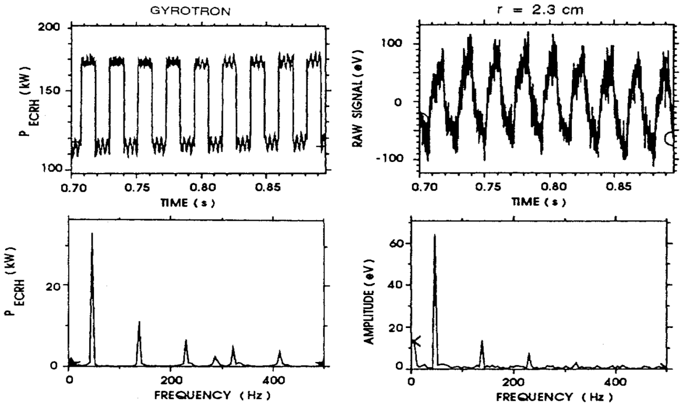






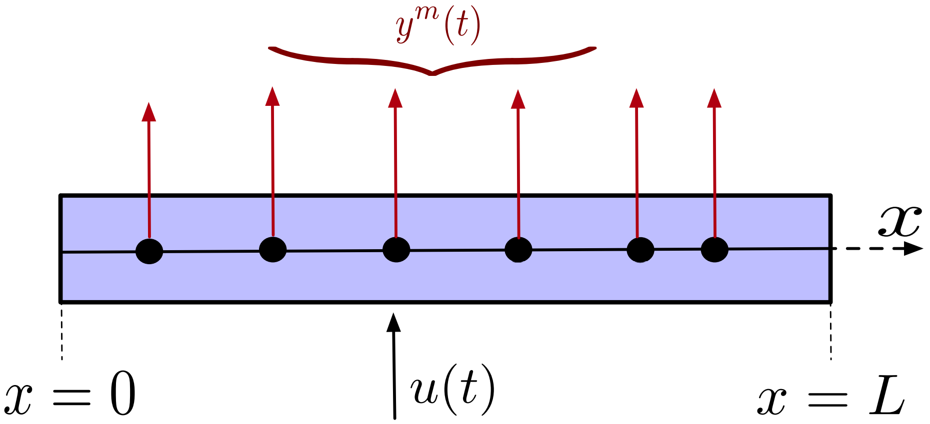
Giannone, Nuclear Fusion 32 (11), 1992

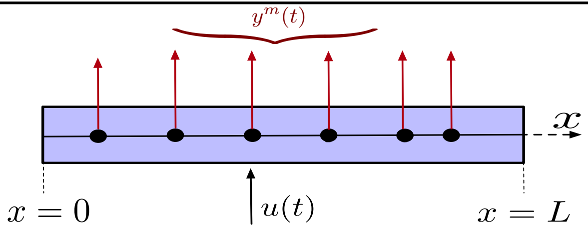
Sparsity in Frequency Domain



Giannone, Nuclear Fusion 32 (11), 1992

Few number of harmonics in frequency domain!


$y^m(t)$
x
$x = 0$
$u(t)$
$x = L$

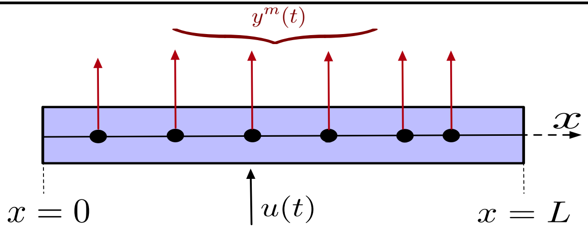


Estimating $E(x), D(x), U(x), K(x), P(x)$

$$E(x)\frac{\partial z(x,t)}{\partial t} = D(x)\frac{\partial^2 z(x,t)}{\partial x^2} + U(x)\frac{\partial z(x,t)}{\partial x} + K(x)z(x,t) + P(x)u(t),$$

- Input $u(t)$
- Point-wise outputs $y^m(t) := z(x^1,t), \cdots, z(x^M,t)$
- Unknown/free boundary conditions

Data-Driven Estimation of Physical Parameters



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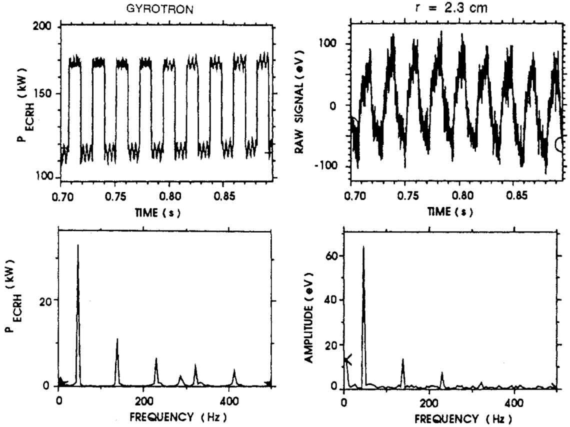
- Unknown/free boundary conditions

Estimation in time domain is at large solved

Alternative Approach: Estimation in Frequency Domain

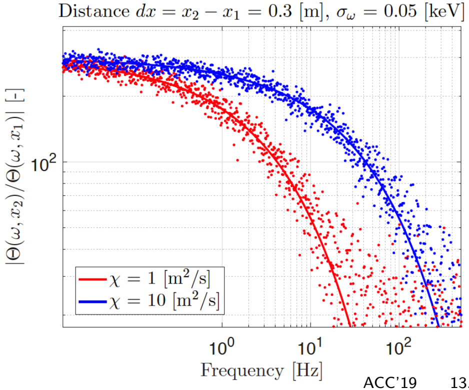
Practical Advantages of Frequency Domain

- Input signal and output data has same frequency (**important for experiment design**)
- Characterization and suppression of noise (**noise model can be incorporated in identification**)



Giannone, Nuclear Fusion 32 (11), 1992

$$\frac{\partial T_e(x,t)}{\partial t} = \chi \frac{\partial^2 T_e(x,t)}{\partial x^2} + P_{\text{ech}}(x,t)$$



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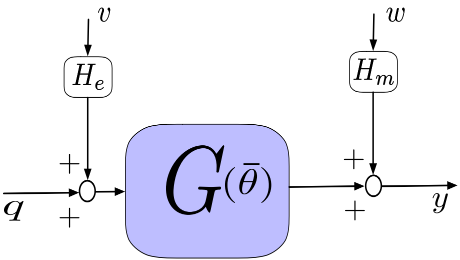


Output Covariance, for frequency points $(\omega_\ell, \ell = 1, \cdots, L)$

$$\sigma_y^2\left(\omega_\ell, \bar{\theta}\right) = \sigma_w^2 \left|H_m(\omega_\ell)\right|^2 + \sigma_v^2 \left|G(\omega_\ell, \bar{\theta})\right|^2 \left|H_e(\omega_\ell)\right|^2 + \sigma_q^2 \left|G(\omega_\ell, \bar{\theta})\right|^2$$

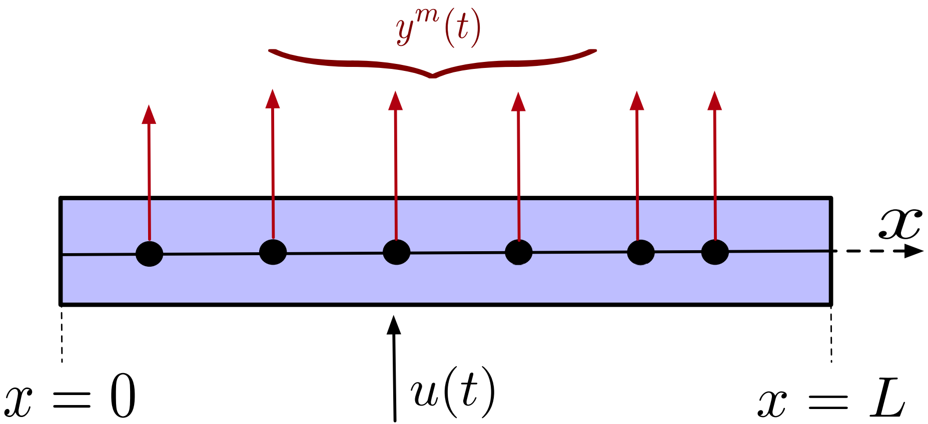
$$\bar{\theta} := \text{col}(E, D, U, K, P)$$

Estimation in frequency domain

Estimation in frequency domain

Steps:

1. Find the transfer function from the applied inputs to the sensed outputs
2. Establish an output-error criterion (measured output-modeled output)
3. Minimize the error in least square sense to determine the unknown parameters



$y^m(t)$
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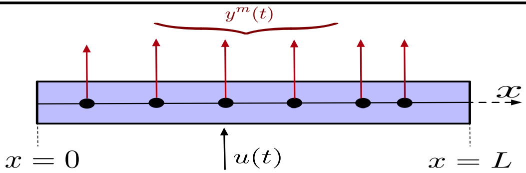


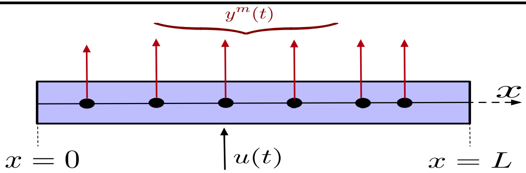
PDE: $E(x)\frac{\partial z(x,t)}{\partial t} = D(x)\frac{\partial^2 z(x,t)}{\partial x^2} + U(x)\frac{\partial z(x,t)}{\partial x} + K(x)z(x,t) + P(x)u(t)$

Applied Input: $u(\omega_\ell), \ell \in \{1, \cdots, L\}$ can be either sinusoids/block waves

Measured Output: $y^m(\omega_\ell) = z(x^1, \omega_\ell), \cdots, z(x^M, \omega_\ell), \quad \ell \in \{1, \cdots, L\}$

Estimation Problem: $\min_{\bar{\theta} := \text{col}(E,D,U,K,P)} \sum_{\ell=1}^{L} \int_{\mathbb{X}^M} |\ y^m(\omega_\ell) - H(\omega_\ell, x, \bar{\theta})\ q(\omega_\ell)\ |^2 \, \mathrm{d}x$

Frequency Domain Estimation- Attempt 1



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Computing $H(\omega_\ell, x, \bar{\theta})$ for arbitrary boundary conditions and parameter profile is hard!

A) Numerical Discretization of PDEs

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Use finite difference

$$\frac{\partial z}{\partial x} \approx \frac{-z\left(x_{i-1}\right)+z\left(x_{i+1}\right)}{2 \cdot \Delta x} \qquad \Downarrow \qquad \frac{\partial^2 z}{\partial x^2} \approx \frac{z\left(x_{i-1}\right)-2z\left(x_i\right)+z\left(x_{i+1}\right)}{(\Delta x)^2}$$

State-space model in terms of unknown sparse matrices $\bar{E}, \bar{D}, \bar{U}, \bar{K}, \bar{P}$. Size depends on mesh-grid

$$\bar{E}\frac{\mathrm{d}\boldsymbol{z}}{\mathrm{d}t} = \left(\bar{D}L_D + \bar{U}L_U + \bar{K}L_K\right)\boldsymbol{z} + \bar{P}u(t)$$

$$L_D = \begin{bmatrix} \ddots & \ddots & & \\ \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \end{bmatrix}, L_U = \begin{bmatrix} & \ddots & & \\ \ddots & & \ddots & \\ & \ddots & & \ddots \\ & & \ddots & \end{bmatrix}, L_K = \begin{bmatrix} \ddots & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \ddots \end{bmatrix}, \bar{E}, \bar{P} = \begin{bmatrix} \ddots & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \ddots \end{bmatrix}$$

Frequency Domain Estimation Using Numerical Approximation

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A) Numerical Discretization of PDEs

Use finite difference

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For large discretization points difficult to estimate $\bar{E}, \bar{D}, \bar{U}, \bar{K}, \bar{P}$

B) Parametrizing spatially varying profile

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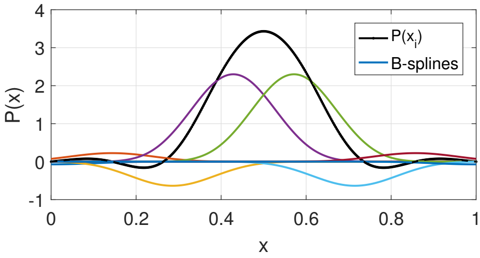
We use orthonormal basis functions

$$\gamma(x) \approx \sum_{r=1}^{R} B_r(x)\theta_r$$

$$E(\bar{\theta})\dot{\boldsymbol{z}} = A(\bar{\theta})\boldsymbol{z} + P(\bar{\theta})u$$

Example: monomials, B-splines etc.



Sparse, Affine parametrization

$$E(\bar{\theta}) = \sum_{r=1}^{R} \theta_r^E L_r^E$$

$$A(\bar{\theta}) = \sum_{r=1}^{R} \left[\theta_r^D L_r^D + \theta_r^U L_r^U + \theta_r^K L_r^K\right]$$

$$P(\bar{\theta}) = \sum_{r=1}^{R} \theta_r^P \bar{P}_r$$

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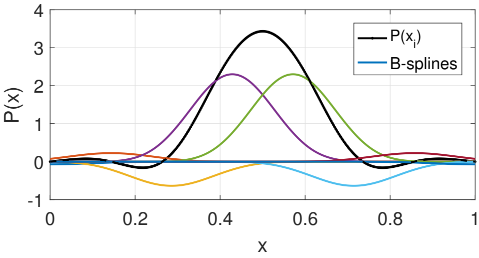

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Number of parameters to be estimated depends on R

C) Boundary conditions are replaced by measurements

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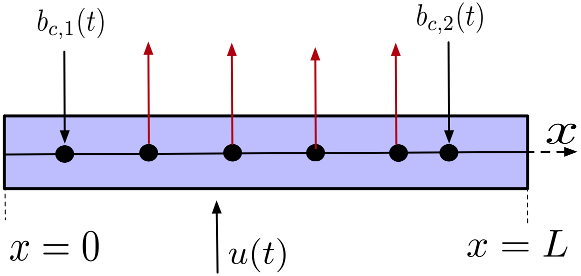
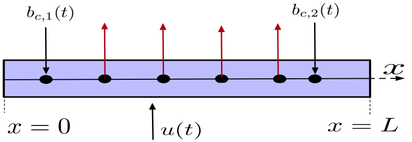


Input vector $q(t)$ consists of $q(t) = \text{col}(u(t), b_{c,1}(t), b_{c,2}(t))$

$b_{c,1}(t), b_{c,2}(t)$ are the real-time measurement about information at (close to) boundary



Inputs: $q(\omega_\ell) = \text{col}\big(u(\omega_\ell), b_{c,1}(\omega_\ell), b_{c,2}(\omega_\ell)\big), \qquad \ell \in \{1, \cdots, L\}$

Finite Difference Discretization of PDEs:

$$\begin{aligned} E(\bar{\theta})\dot{\boldsymbol{z}} &= A(\bar{\theta})\boldsymbol{z} + B(\bar{\theta})q \\ y_m &= C^m \boldsymbol{z} \end{aligned}$$

Estimation Problem:

$$\min_{\bar{\theta}} \sum_{\ell=1}^{L} \sum_{m=2}^{M-1} \frac{1}{w^m w_\ell} \left| y^m(\omega_\ell) - \underbrace{C^m \left[j\omega_\ell E(\bar{\theta}) - A(\bar{\theta}) \right]^{-1} B(\bar{\theta})}_{G^m(\omega_\ell, \bar{\theta})} q(\omega_\ell) \right|^2$$

The sparse and affine structures of $E(\bar{\theta}), A(\bar{\theta})$ play important role

Least Square Estimation Using Levenberg-Marquardt Algorithm

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- **Optimization Problem:**

$$\min_{\bar{\theta}} V(\bar{\theta})$$

$$V(\bar{\theta}) := \sum_{\ell=1}^{L} \sum_{m=2}^{M-1} \frac{1}{w^m w_\ell} \mid y^m(\omega_\ell) \ - G^m(\omega_\ell, \bar{\theta}) \ q(\omega_\ell) \mid^2$$

- **Descent direction:** Combination of Gauss-Newton and Gradient-Descent Method

$$(J_k^* J_k + \lambda_i I) h_{\mathsf{lm},i} = J_k^* V(\bar{\theta}_k)$$

Analytic computation of the Jacobian (J_k)

- Exploiting sparsity of the matrices, we can speed-up the optimization
- Using the Jacobian, we can calculate the uncertainty in the estimation

Uncertainty measure: $\mathsf{Cov}\,(\theta_k) \approx \mathrm{Re}\,(2J_k^* J_k)^{-1}$

Results: Using Real Data from Nuclear Fusion Experiments

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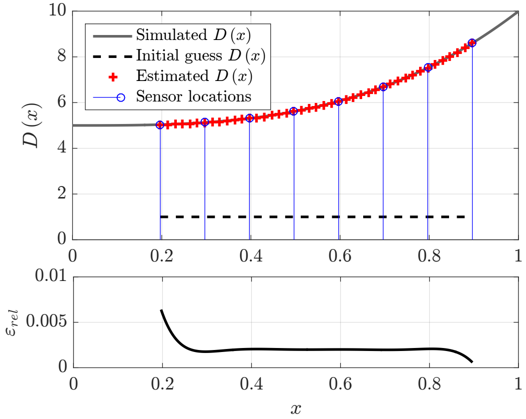
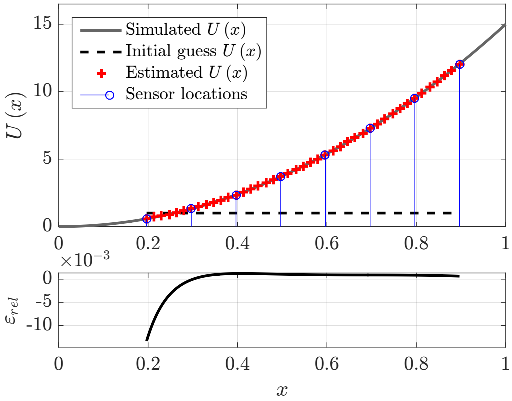
Input: Block waves with 4 harmonics





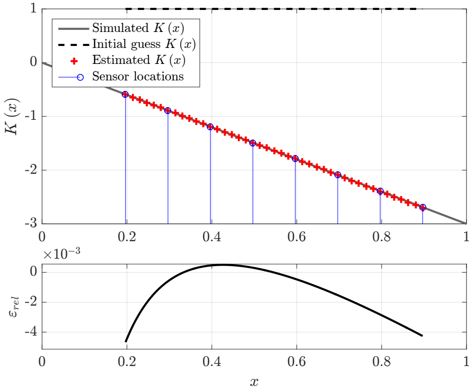
Actual Profile:

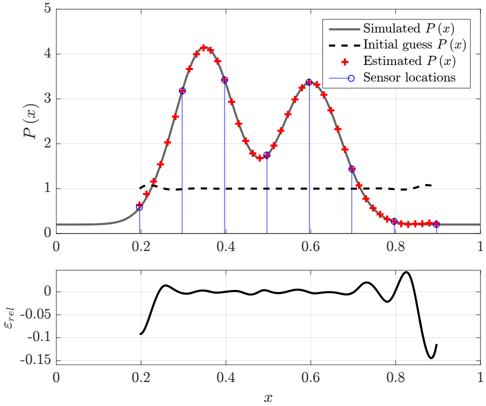
$$D^{\text{real}}(x) = 5x^3 - 0.005x + 5$$

Actual Profile:

$$U^{\text{real}}(x) = 15x^2 - 0.005$$

Input: Block waves with 4 harmonics





Actual Profile:

$$K^{\text{real}}(x) = -3x$$

Actual Profile:

$$P^{\text{real}}(x) = 0.2 + \frac{7}{\sqrt{\pi}} \mathrm{e}^{\frac{-(x-0.35)^2}{(0.1)^2}} + \frac{5.6}{\sqrt{\pi}} \mathrm{e}^{\frac{-(x-0.6)^2}{(0.1)^2}}$$

Excitation Signal: Design of Perturbative Experiments

We are using periodic signals

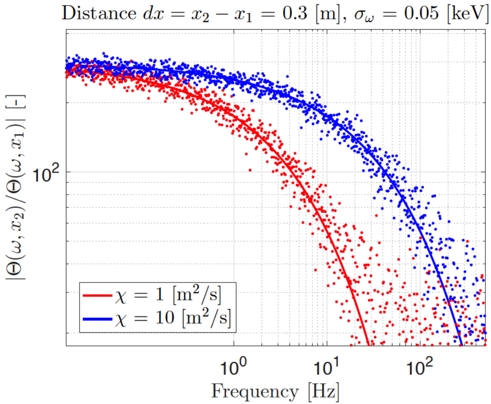
We are using periodic signals

$$\frac{\partial T_e(x,t)}{\partial t} = \chi \frac{\partial^2 T_e(x,t)}{\partial x^2} + P_{\text{ech}}(x,t),$$

$$P_{\text{ech}}(x,t) = p(t)\frac{1}{\sigma_w\sqrt{\pi}}\exp\left(-\frac{(x-x_{\text{dep}})^2}{\sigma_w^2}\right).$$

Transfer Function:

$$G(\omega,\kappa) = \frac{\Theta(\omega,x_2)}{\Theta(\omega,x_1)} = \exp\left(-\sqrt{\frac{i\omega}{\chi}}\Delta x\right)$$



Optimal Experiment Design: A Brief Idea

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Use Fisher Information Matrix $F(\theta_0) = \mathbb{E}\left[\left(\frac{\partial \textbf{ln}(f_z)}{\partial\theta}\right)^\top \left(\frac{\partial \textbf{ln}(f_z)}{\partial\theta}\right)\right] |_{\theta=\theta_0}$

Optimal Experiment Design: A Brief Idea

Use Fisher Information Matrix $F(\theta_0) = \mathbb{E}\left[\left(\frac{\partial \ln(f_z)}{\partial \theta}\right)^\top \left(\frac{\partial \ln(f_z)}{\partial \theta}\right)\right]\Big|_{\theta=\theta_0}$

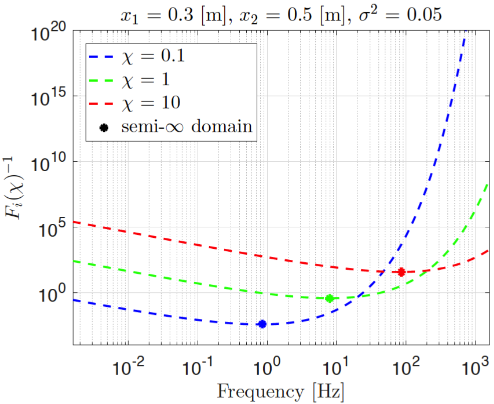
For one frequency:

$$F(\kappa) = \frac{\Delta x^2}{2\sigma^2\chi^3} \exp\left(-\sqrt{\frac{2\omega}{\chi}}\Delta x\right) \mid \Theta(\omega, x_1) \mid^2$$

Upper bound on Modulation Frequency:

$$\omega_{\textbf{opt}} = \frac{2\chi}{(\Delta x)^2}$$

* M. van Berkel et.al (2018): "A systematic approach to optimize excitations for perturbative transport experiment"



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Exploiting System Identification Tools for Data-Driven Parameter Estimation in PDEs

Conclusion

- Basis functions are used to parametrize unknown profile on a discretized domain.
- The non-linear least square method uses analytically computed Jacobian.
- The unknown boundary conditions are handled by data.

Future work

- Handling noisy data for the estimation (Maximum Likelihood Estimation with correlated noise)
- Use data find a suitable a basis function (Gaussian regression).
- Optimal sensor location (minimizing estimation sensitivity with respect to sensor location).

Thank You!