Frequency domain estimation of parabolic partial differential equations with spatially varying transport coefficients

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CST Seminar, May 31, 2017

Goal of reasearch

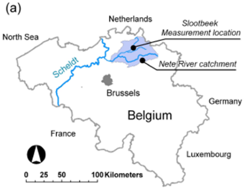
Develop algorithm to determine $D(x)$, $V(x)$, $K(x)$, $P(x)$ to estimate, simulate, and control heat transport:

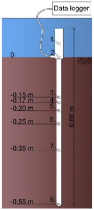
$$\frac{\partial T}{\partial t} = D(x)\frac{\partial^2 T}{\partial x^2} + V(x)\frac{\partial T}{\partial x} + K(x)\,T(x,t) + P(x)\,p(t)$$

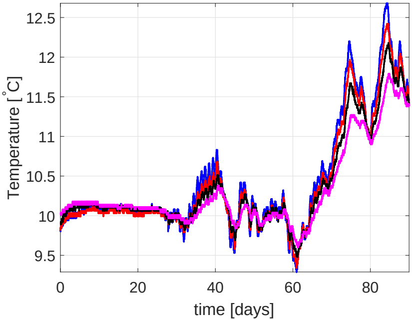
The desired algorithm should be:

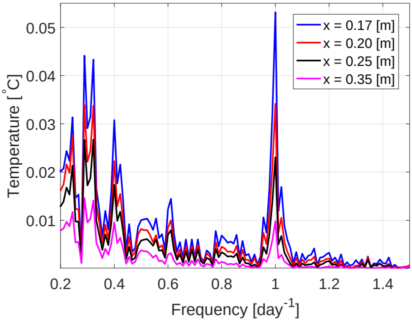
- accurate
- computationally cheap
- flexible in terms of spatial variations of $D(x)$, $V(x)$, $K(x)$, $P(x)$
- robust with respect to initialization

Examples of heat transport (hydrology)

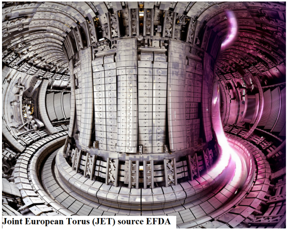




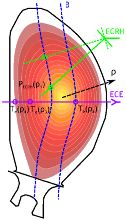


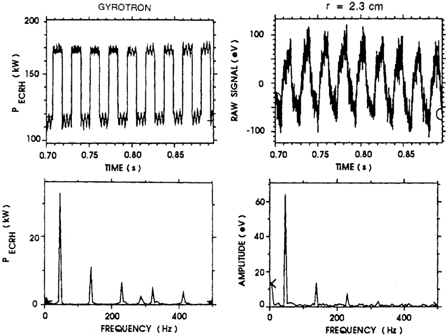


Examples of heat transport (fusion)



Joint European Torus (JET) source EFDA

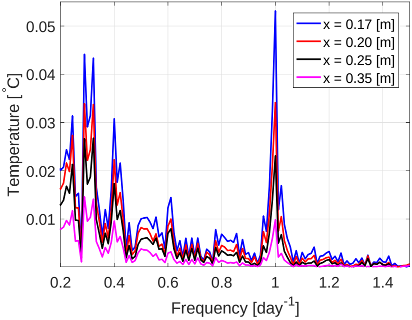


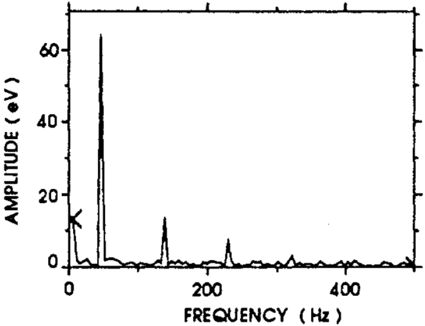


Giannone, Nuclear Fusion 32 (11), 1992

Sparse signals frequency domain

Only few dominant harmonics: exploit sparseness in frequency domain





Generalized transport model

Generalized 1D transport model (note that this also is a generalization for cylindrical geometry)

$$\frac{\partial T}{\partial t} = D(x)\frac{\partial^2 T}{\partial x^2} + V(x)\frac{\partial T}{\partial x} + K(x)\,T(x,t) + P(x)\,p(t)$$

Various possible boundary conditions

Neumann	$\frac{\partial T}{\partial x}(x = x_b) = 0$
Diriclet	$T(x_b, t) = 0$
Boundary measurement	$T(x_b, t) = T_{meas}(x)$

Analytic solution is not an option

$$\frac{\partial T}{\partial t} = D(x)\frac{\partial^2 T}{\partial x^2} + V(x)\frac{\partial T}{\partial x} + K(x)\,T(x,t) + P(x)\,p(t)$$

Analytic solution for

$$D(x) = a_2 x + b_2,\; V(x) = a_1 x + b_1,\; K(x) = a_0 x + b_0,\; P(x) = 0$$

Frequency solution in terms of confluent hypergeometric functions

$$\Theta(\omega, x) = C_1 e^{\frac{\sqrt{D}-a_1}{2a_2}x}\Phi\left(a, b; \frac{x + b_2/a_2}{\lambda}\right) + C_2 e^{\frac{\sqrt{D}-a_1}{2a_2}x}\Psi\left(a, b; \frac{x + b_2/a_2}{\lambda}\right),$$

$$D = a_1^2 - 4a_0 a_2 \qquad a = \tfrac{b_2 k^2 + b_1 k + b_0 - i\omega}{2a_2 k + a_1} \qquad k = \tfrac{\sqrt{D}-a_1}{2a_2}$$

$$b = (a_2 b_1 - a_1 b_2)\,a_2^{-2} \qquad B = b_2 k^2 + b_1 k + b_0 \qquad \lambda = \tfrac{-a_2}{2a_2 k + a_1}$$

Numerical solution necessary!

Finite difference approximation (flexible)

$$\frac{\partial T}{\partial t} = D(x)\frac{\partial^2 T}{\partial x^2} + V(x)\frac{\partial T}{\partial x} + K(x)\,T(x,t) + P(x)\,p(t)$$

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

Gives in state-space form ($D(x_i)$, $V(x_i)$, $K(x_i)$ are diagonal matrices):

$$\frac{\partial \boldsymbol{T}_i}{\partial t} = \underbrace{\left(D(x_i)\,L_D + V(x_i)\,L_V + K(x_i)\,L_K\right)}_{A}\boldsymbol{T}_i + \underbrace{P(x_i)}_{B}\,p(t)$$

Results in tri-diagonal (sparse matrices):

$$L_D = \begin{bmatrix} \ddots & \ddots & & \\ \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \end{bmatrix}, L_V = \begin{bmatrix} & \ddots & & \\ \ddots & & \ddots & \\ & \ddots & & \ddots \\ & & \ddots & \end{bmatrix}, L_K = \begin{bmatrix} \ddots & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \ddots \end{bmatrix}$$

State-space solution

$$\begin{aligned} \frac{\partial T(t,x_i)}{\partial t} &= AT(t,x_i) + B\,p(t) \\ T_{sim} &= CT(x_i),\; C(x_i = x_{meas}) \neq 0 \end{aligned}$$

In the frequency domain gives $\mathcal{F}(T(t,x_i)) = \Theta(\omega,x_i)$

$$G_{sim}(\omega,x_i) = \frac{\Theta_{sim}(\omega,x_i)}{p(\omega)} = C(i\omega I - A)^{-1} B$$

PDE solution has been reduced to solving matrix equality in terms of sparse matrices per frequency.

If the number of frequency lines is limited very fast to solve!

Estimating $D(x)$, $V(x)$, $K(x)$, $P(x)$

Standard least-squares distributed systems cost function

$$V = \int_0^1 \left|G_{meas}(\omega, x) - G_{sim}(\omega, x, D(x), V(x), K(x), P(x))\right|^2 dx$$

Discrete equivalent cost function (w_j weighted LS)

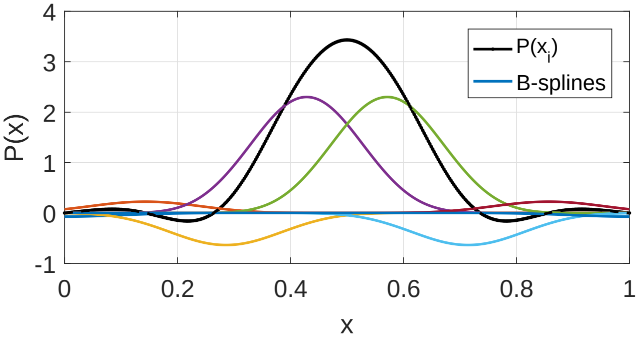
$$V_{LS} = \sum_i^I \sum_j^J \frac{1}{w_i w_j} \left|G_{meas}(\omega_j, x_i) - C\left(i\omega_j I - A\right)^{-1} B\right|^2$$

Problem: finite difference consists of many discretization points (<200) impossible to estimate all $D(x_i)$

General definition of basis-function

$$D(x) = \sum_{k}^{K} B_k(x)\gamma_k \text{ or } D(x_i) = B_D(k, x_i)\gamma(k)$$

Instead of estimating $D(x)$, $V(x)$, $K(x)$ estimate a few γ_k.
Examples: polynomial $D(x) = ax^2 + bx + c$ and B-splines:



Optimization (analytic Jacobian)

Minimize

$$\gamma_{best} = \underset{\gamma=[\gamma_1 \cdots \gamma_K]}{\arg\min} \sum_i^I \sum_j^J \frac{1}{w_i w_j} \left| G_{meas}(\omega_j, x_i) - C\left((i\omega_j I - A)^{-1} B \right) \right|^2$$

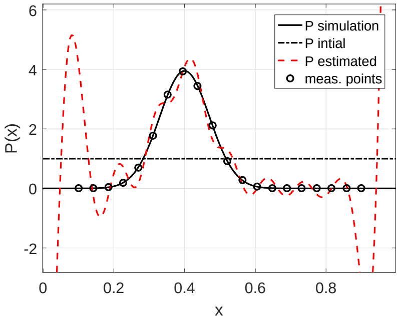
with gradient descent method $0 = \frac{\partial V_{LS}}{\partial \gamma_k}$ using chain-rule and property $\frac{\partial A^{-1}}{\partial \gamma_k} = A^{-1} \frac{\partial A}{\partial \gamma_k} A^{-1}$:

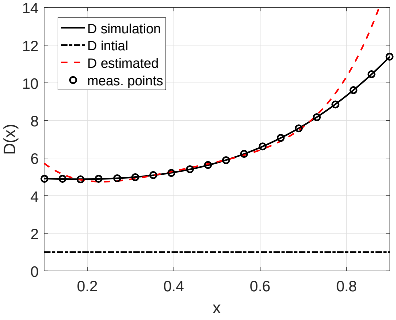
$$C \frac{\partial \left((i\omega I - A)^{-1} B \right)}{\partial \gamma_k} = C(i\omega I - A)^{-1} \left(diag\left(\frac{\partial \gamma}{\partial \gamma_k} B_D \right) L_D \right) (i\omega I - A)^{-1} B$$

Jacobian only (requires currently one additional $C/(i\omega I - A)$) per frequency line.

First: simulation results

1. If exactly the same profiles and discretization is used: solution is exact.
2. Simulation with reduced discretization and discrepancy between real profile and B-spline profile (oscillations):





Conclusion

A code is under development to estimate spatially varying profiles in 1D-PDE in the frequency domain

- Initial results are promising
- At the boundaries still problems
- No noise implemented

Future work

- Problems at the boundary need to be resolved (regularization, estimation of different boundary properties, etc.)
- Inclusion of noise (robustness, validation, MLE)
- Application to experimental data
- Speed can be further increased changing spatial discretization