The 28th Inverse Days in Kuopio December 12–16 2022

on the occasion of 60th birthday of Professor Jari Kaipio

Registration

- **Early bird: September 30**
- **Final: October 30.**

https://sites.uef.fi/inversedays2022

Recovery from modelling errors in non-stationary inverse problems

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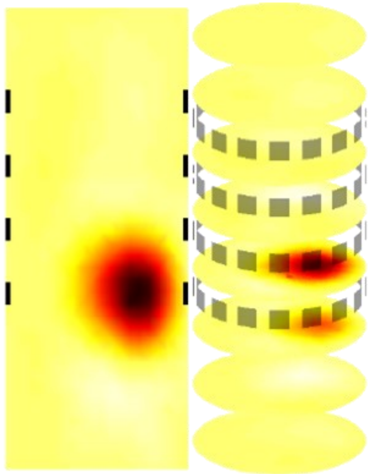
ACCC CLEAN AIR. SAFE CLIMATE.

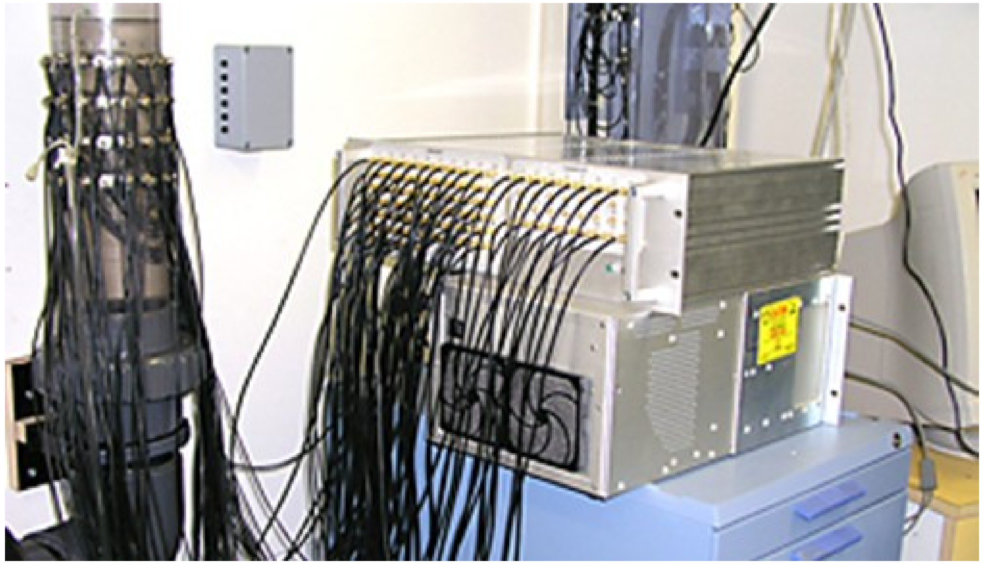
CENTRES OF EXCELLENCE IN RESEARCH

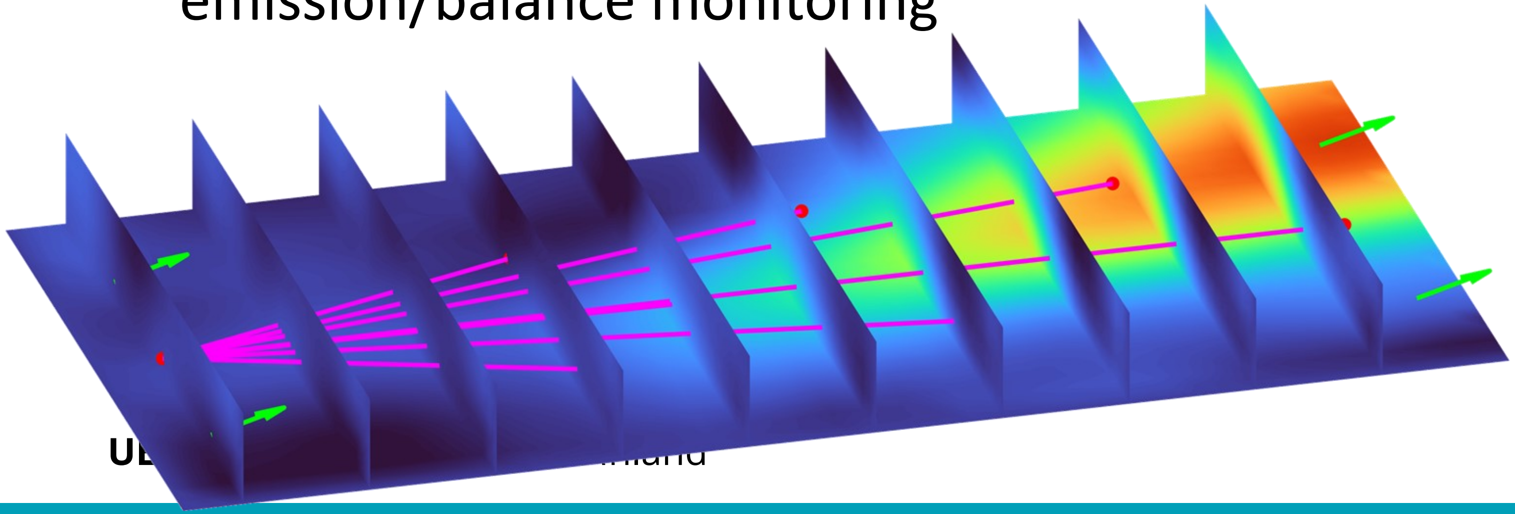
Finnish Centre of Excellence in Inverse Modelling and Imaging

Outline

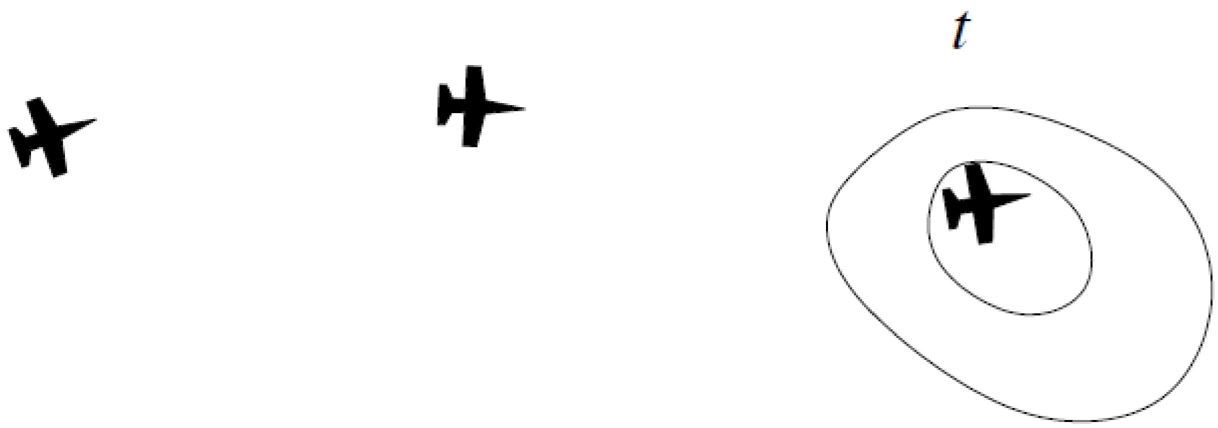
- Non-stationary inverse problems & state estimation
- Convection-diffusion problems
- Bayesian approximation error method in non-stationary inversion
- Application 1: Industrial process tomography
- Application 2: Greenhouse gas emission/balance monitoring





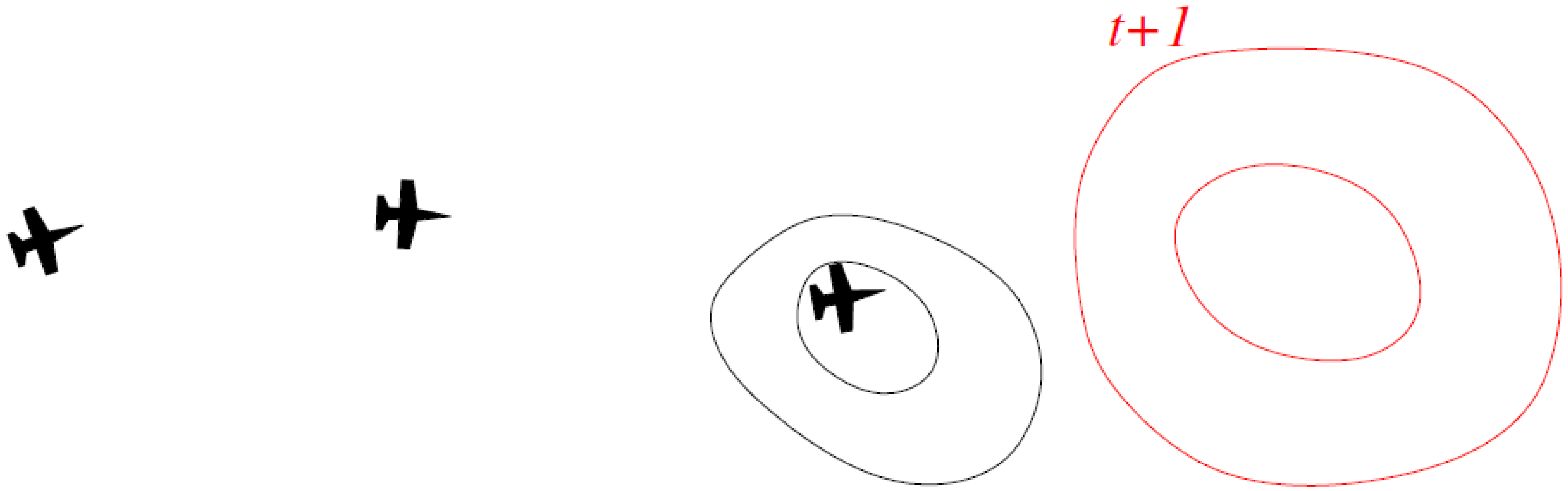


Bayesian State estimation



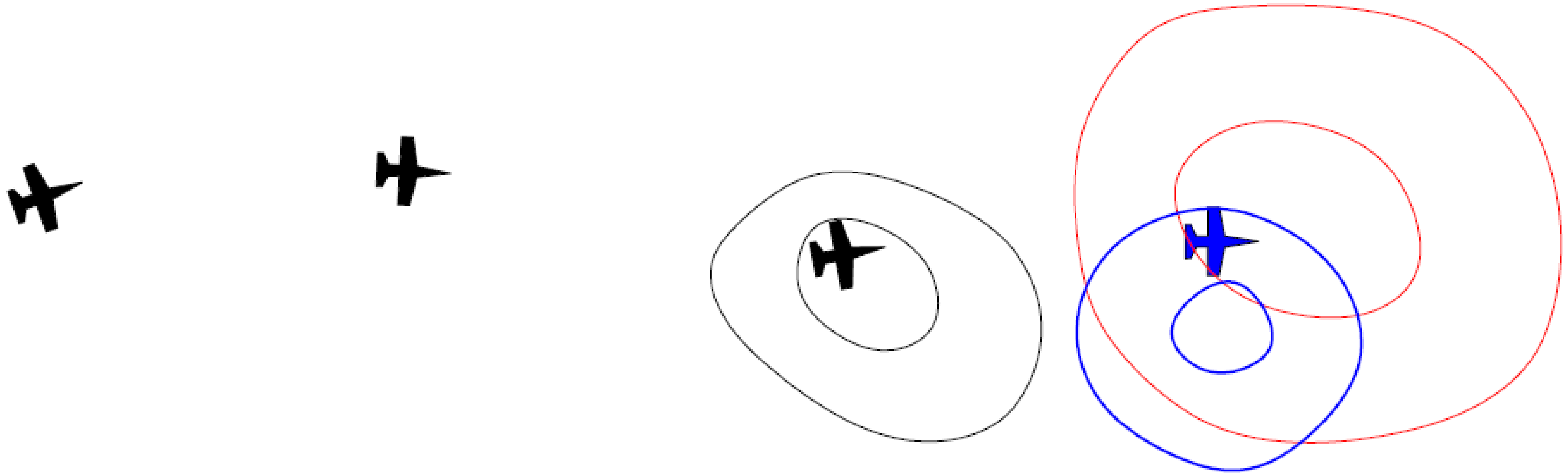
(Posterior) estimate at time t

Bayesian State estimation



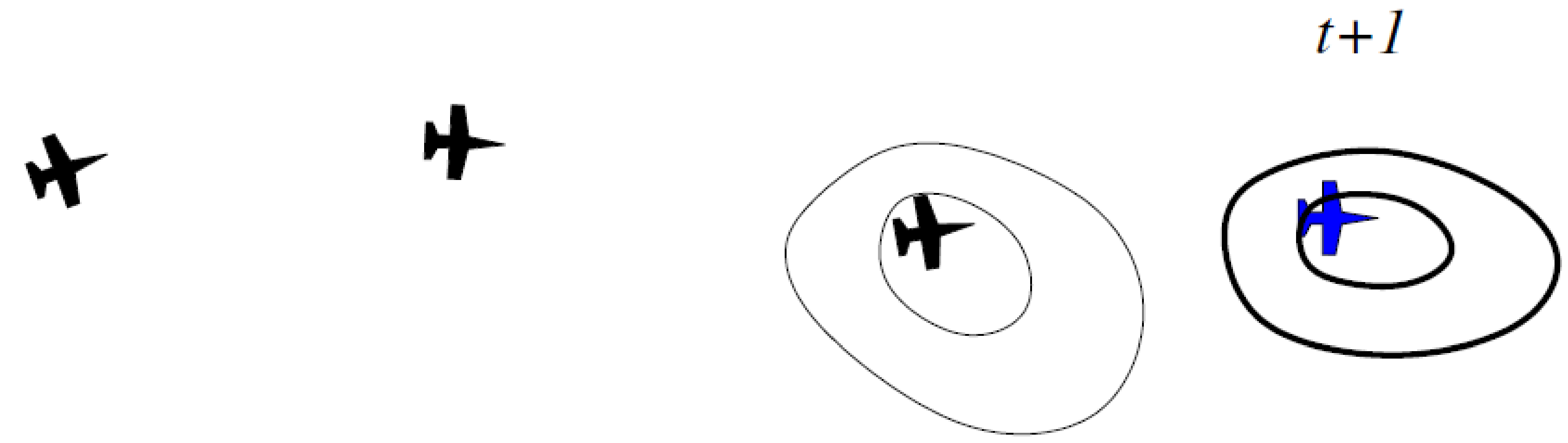
Prediction for time t+1

Bayesian State estimation



Observation at time t+1: likelihood

Bayesian State estimation



Posterior at time t+1 =
prediction x likelihood

Bayesian state estimation

- The state-space system

$$\theta_{t+1} = f_\theta(\theta_t) + \bar{w}_{t+1} \quad \longleftarrow \text{(Evolution model)}$$

$$y_t = H_\theta(\theta_t) + v_t. \quad \longleftarrow \text{(Observation model)}$$

- State estimation problem(s):
  - Given a sequence of measurements $y_1,\ldots,y_k$, form the conditional probability density of θ_t

$$p(\theta_t \mid y_1,\ldots,y_k) \approx N(\theta_{t|k}, \Gamma_{t|k})$$

(If we make Gaussian approximations)

  - If: $k < t$: Prediction
    $k = t$: Filtering
    $k > t$: smoothing

Bayesian state estimation

Extended Kalman filter (EKF)

For $t = 1,\ldots,T$

Prediction

$$\theta_{t+1|t} = f_\theta(\theta_{t|t}) + \bar{w}_{t+1}$$

$$\Gamma_{t+1|t} = J_{f_\theta}(\theta_{t|t})\Gamma_{t|t}J_{f_\theta}(\theta_{t|t})^T + \Gamma_{\bar{w}_{t+1}}$$

$$K_{t+1} = \Gamma_{t+1|t}J_{H_\theta}(\theta_{t+1|t})^T (J_{H_\theta}(\theta_{t+1|t})\Gamma_{t+1|t} \cdot J_{H_\theta}(\theta_{t+1|t})^T + \Gamma_{v_{t+1}})^{-1}$$

Measurement update

$$\theta_{t+1|t+1} = \theta_{t+1|t} + K_{t+1}(y_{t+1} - H_\theta(\theta_{t+1|t}))$$

$$\Gamma_{t+1|t+1} = \Gamma_{t+1|t}(I - J_{H_\theta}(\theta_{t+1|t})^T K_{t+1}^T).$$

...and Kalman smoother

For $t = T\text{-}1,\ldots,1$

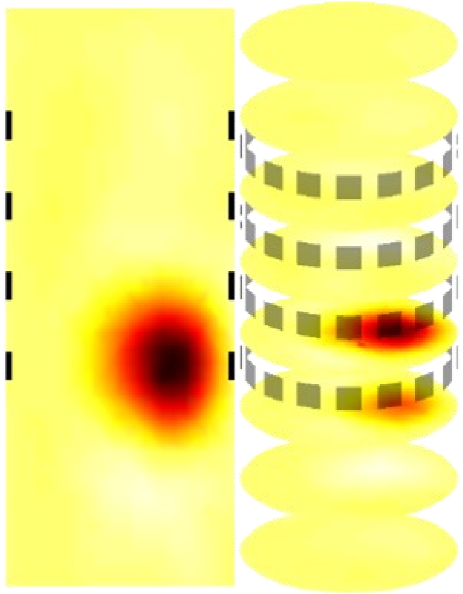
$$\begin{aligned} G_t &= \Gamma_{t|t}F_{t+1}^T\Gamma_{t+1|t}^{-1} \\ \theta_{t|T} &= \theta_{t|t} + G_t(\theta_{t+1|T} - \theta_{t+1|t}) \\ \Gamma_{t|N} &= \Gamma_{t|t} + G_t(\Gamma_{t+1|T} - \Gamma_{t+1|t})G_t^T \end{aligned}$$

Backward recursion

Convection-diffusion (inverse) problems

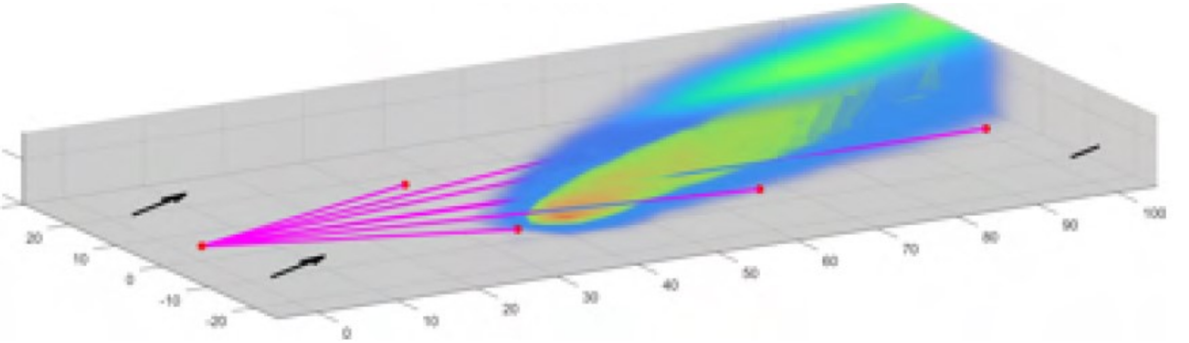
1. Industrial process tomography
   - Measurements: Electrical impedance tomography
   - Evolution model: convection-diffusion eq.

$$\frac{\partial c}{\partial t} = \underbrace{-\bar{v} \cdot \nabla c}_{\text{Convection}} + \underbrace{\nabla \cdot (\kappa \nabla c)}_{\text{Diffusion}}$$



2. Greenhouse gas emission monitoring
   - Measurements: Laser dispersion spectroscopy (& tomography)
   - Evolution model: convection-diffusion eq.

$$\frac{\partial c}{\partial t} = \underbrace{-\bar{v} \cdot \nabla c}_{\text{Convection}} + \underbrace{\nabla \cdot (\kappa \nabla c)}_{\text{Diffusion}} + \underbrace{S}_{\text{Gas emission rate}}$$



Evolution: convection-diffusion model

- Convection diffusion model

$$\frac{\partial c}{\partial t} = -\bar{v} \cdot \nabla c + \nabla \cdot \kappa \nabla c$$

- FE-approximation & stochastic modeling of uncertainties$\Rightarrow$

$$c_{t+1} = F_t(\bar{v}) c_t + s_t(\bar{v}) + w_t(\bar{v}),$$

Electrical impedance tomography

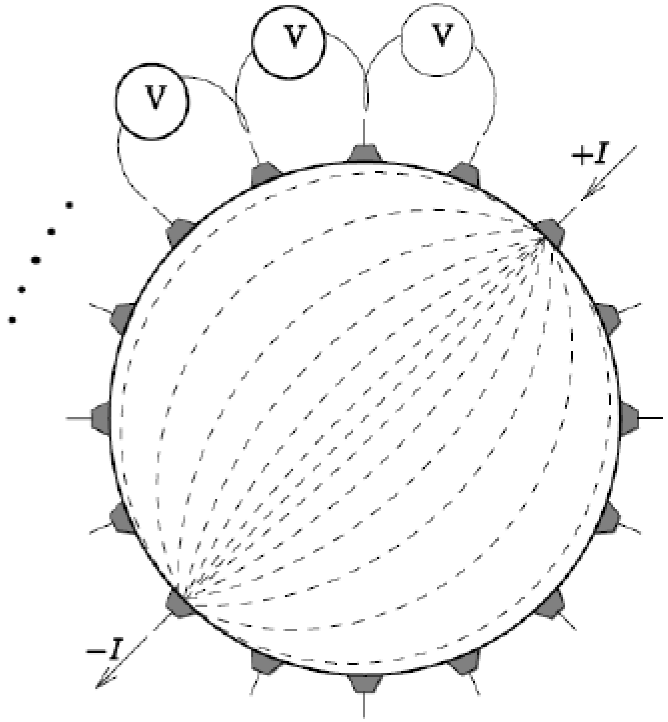
The complete electrode model

$$\nabla \cdot (\sigma \nabla u) = 0, \quad \bar{r} \in \Omega$$

$$u + z_\ell \sigma \frac{\partial u}{\partial \nu} = U^{(\ell)}, \quad \bar{r} \in e_\ell, \; \ell = 1, 2, \dots, L$$

$$\int_{e_\ell} \sigma \frac{\partial u}{\partial \nu} \mathrm{d}S = I^{(\ell)}, \quad \ell = 1, 2, \dots, L$$

$$\sigma \frac{\partial u}{\partial \nu} = 0, \quad \bar{r} \in \partial\Omega \setminus \cup_{\ell=1}^{L} e_\ell$$



Electrical impedance tomography

- FE-approximation & stochastic modeling of uncertainties$\Rightarrow$

$$V_t = R_t(\sigma_t) + \epsilon_t + n_t,$$

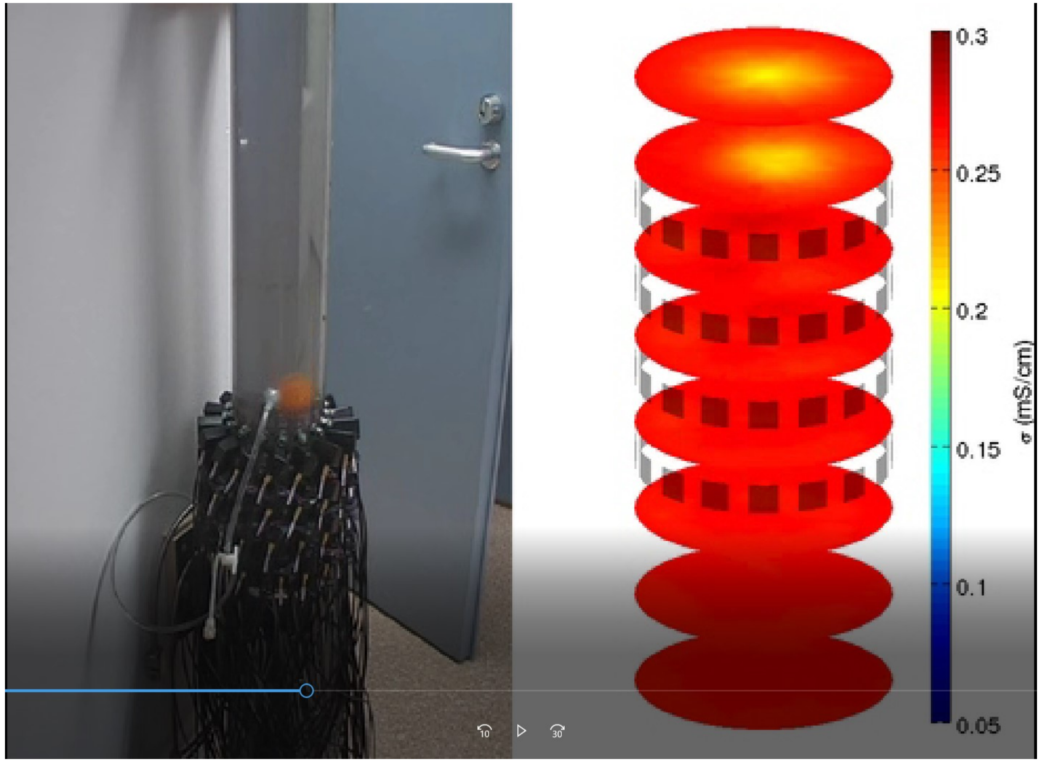
- Model between concentration c and conductivity σ

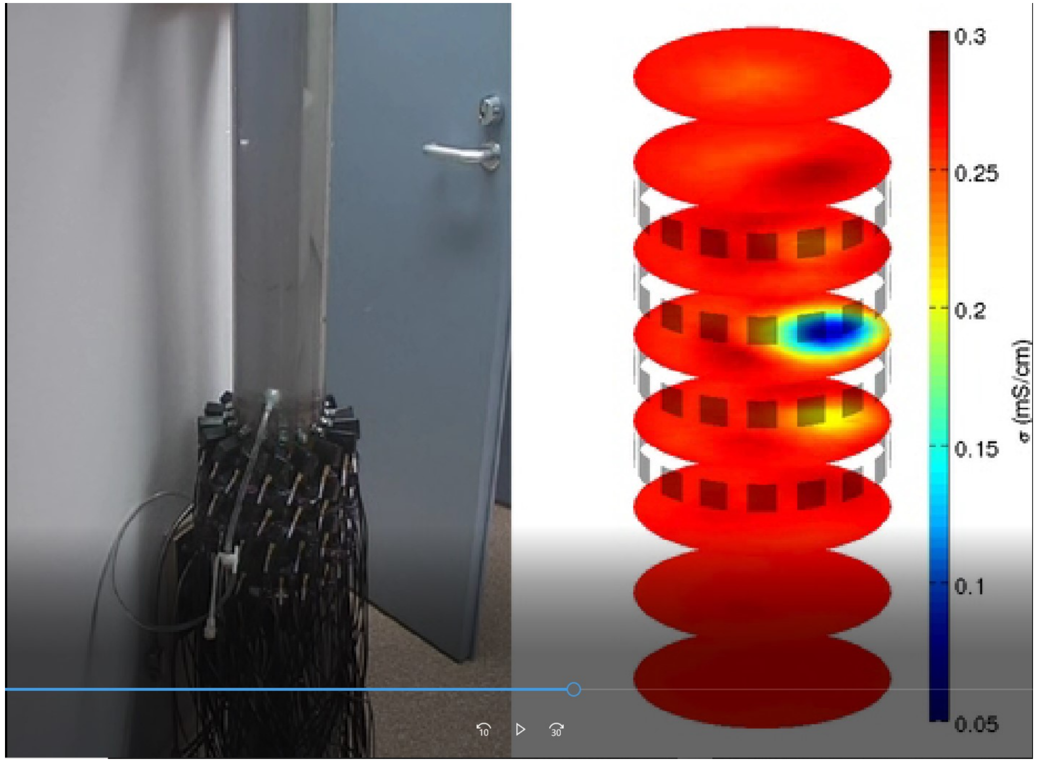
$$\sigma(c) = \Lambda_0 - \lambda c^{3/2}$$

- Observation model

$$\begin{aligned} V_t &= R_t(\sigma(c_t)) + \epsilon_t + n_t \\ &= U_t(c_t) + \epsilon_t + n_t \end{aligned}$$

Electrical impedance tomography: State estimation





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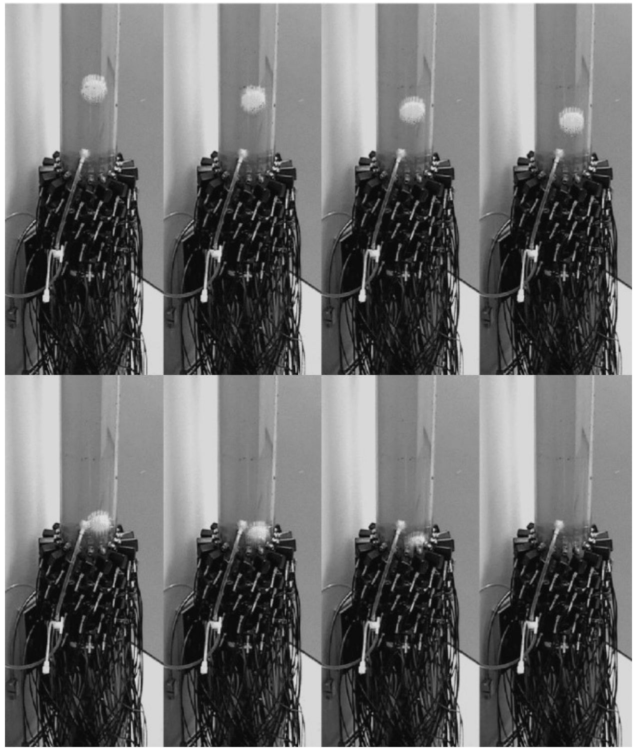
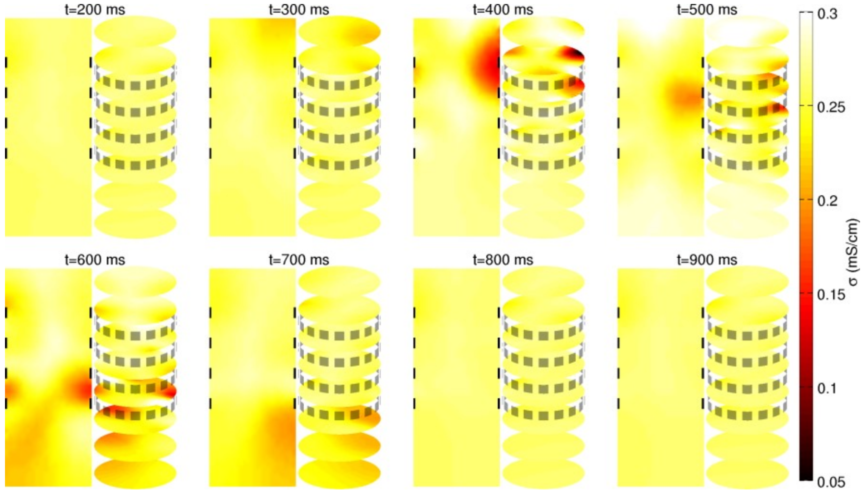
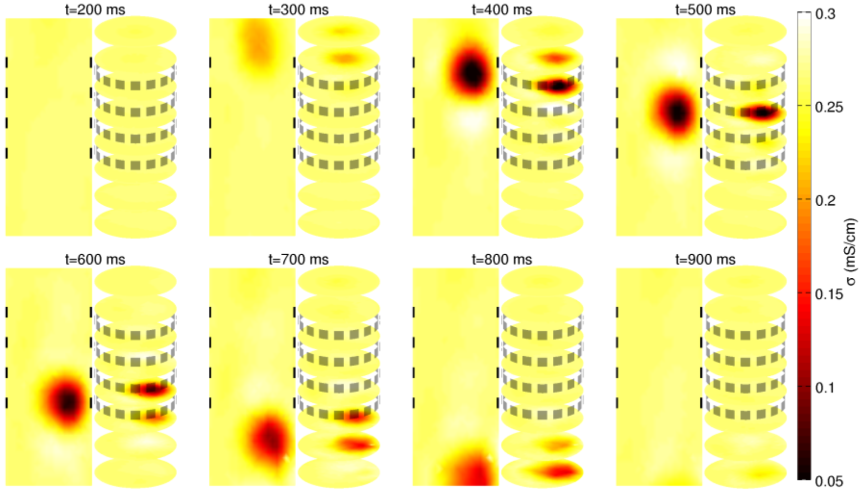
Stationary reconstructions vs. state estimates



(Lipponen et al 2011)



Stationary MAP estimate, smoothness prior



State estimates

Notes

- No need for spatial prior information or regularization – the evolution model carries temporal prior information of the target
- Modeling errors & uncertainties were accounted for (discretization, truncation of the computational domain and unknown contact impedances)
- Stationary approximation for the velocity field

State estimate without and with accounting for the modeling errors

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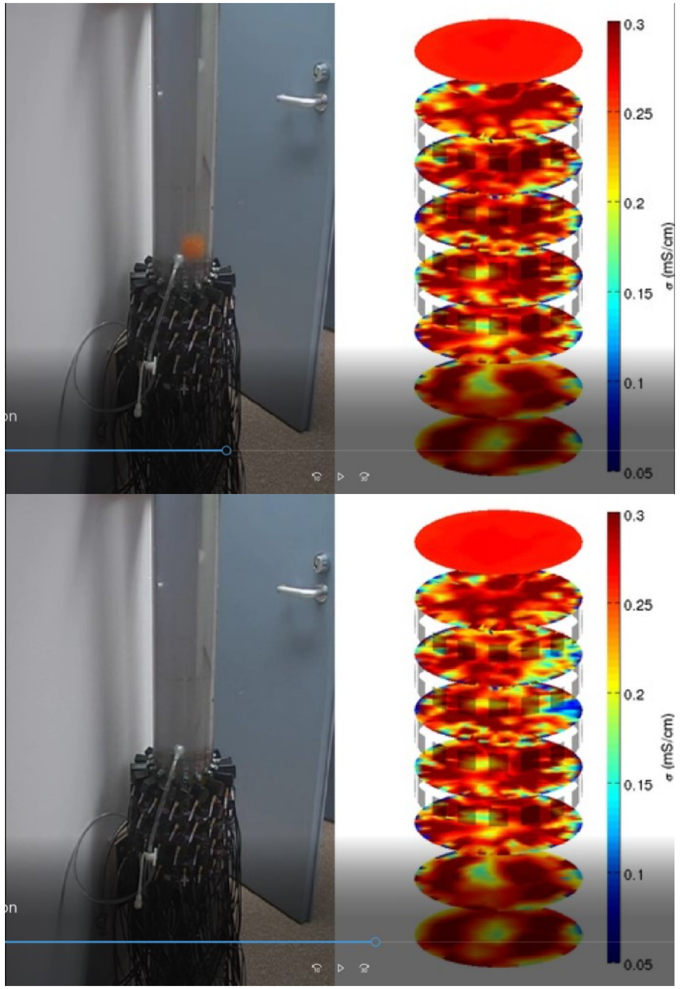
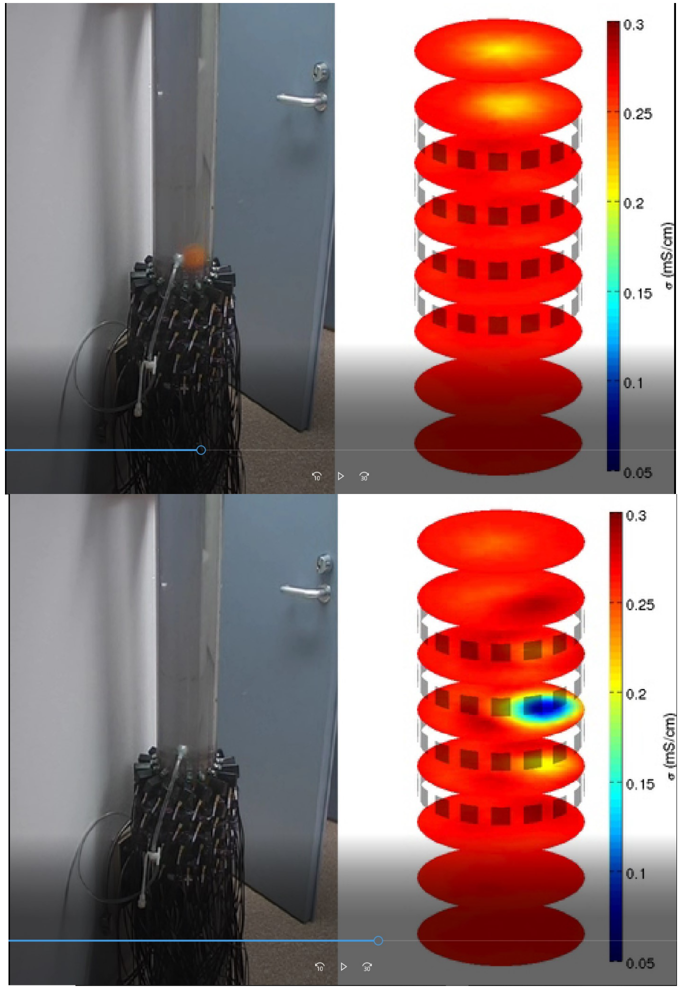
Without accounting for the modeling errors





With accounting for the modeling errors

(Lipponen et al 2011)

Modeling of uncertainties

- Uncertainties and inaccuracies in the observation model
  - Unknown contact impedances
  - Discretization error
  - Truncation of the computational domain
- Uncertainties and inaccuracies in the evolution model
  - Unknown velocity field $\bar{v}(\bar{r}, t)$
  - Unknown input concentration $c_{\mathrm{in}}(\bar{r}, t)$
  - Discretization error
- Statistical modeling of uncertainties and unknowns, approximation error method

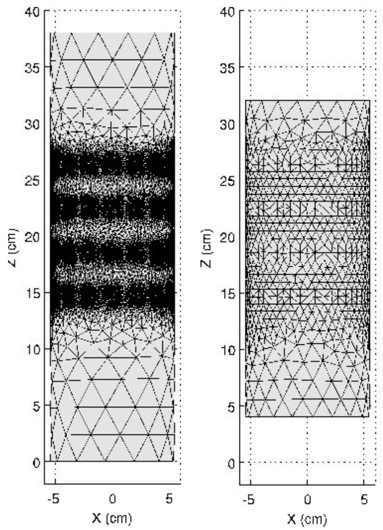
Uncertainties of the observation model

- **Accurate observation model** (known contact impedances z_ℓ, negligible discretization & domain truncation errors)

$$V_t = U_t(c_t) + n_t$$

- **Approximate/reduced order observation model** (approximate contact impedances, sparse mesh, etc.)

$$V_t \approx U_t^{\mathrm{r}}(c_t) + n_t$$



- Write the observation equation in the form

$$\begin{aligned} V_t &= U_t(c_t) + U_t^{\mathrm{r}}(c_t^{\mathrm{r}}) - U_t^{\mathrm{r}}(c_t^{\mathrm{r}}) + n_t \\ &= U_t^{\mathrm{r}}(c_t^{\mathrm{r}}) + \epsilon_t + n_t \end{aligned}$$

  where

$$\epsilon_t = U_t(c_t) - U_t^{\mathrm{r}}(c_t^{\mathrm{r}}) = U_t(c_t) - U_t^{\mathrm{r}}(h(c_t))$$

  is the approximation error

- Approximate the statistics of ϵ_t by Monte Carlo simulations

- The prior model for the concentration is the convection-diffusion model $\Rightarrow$ the samples of c_t are taken from same evolution as that used for constructing the error model for the evolution equation.

Uncertainties of the evolution model

- **Accurate evolution model** corresponding to known $\bar{v}(\bar{r},t)$, $c_{\text{in}}(\bar{r},t)$, dense FE-mesh $\mathcal{M}$:

$$c_{t+1} = F_t c_t + s_t$$

- **Approximate/reduced order evolution model** corresponding to temporal means of $\bar{v}(\bar{r},t)$, $c_{\text{in}}(\bar{r},t)$ and sparse FE-mesh $\mathcal{M}_{\text{r}}$:

$$c^{\text{r}}_{t+1} = F c^{\text{r}}_t + s$$

- Denote interpolation mapping between the dense FE-mesh $\mathcal{M}$ and the sparse mesh $\mathcal{M}_{\text{r}}$ by h

- Write c^{r}_{t+1} in the form

$$\begin{aligned} c^{\text{r}}_{t+1} &= h(c_{t+1}) = h(F_{t+1}c_t + s_{t+1}) \\ &= h(F_{t+1}c_t + s_{t+1}) + Fc^{\text{r}}_t + s - Fc^{\text{r}}_t - s \\ &= Fc^{\text{r}}_t + s + w_t \end{aligned}$$

- where w_t is the approximation error

$$w_t = h(F_{t+1}c_t + s_{t+1}) - Fc^{\text{r}}_t - s$$

- Approximation error method: approximate second order statistics of w_t based on simulation:
  - Run a long sample evolution of c_t based on Navier-Stokes flow model and time-varying input concentration
  - Approximate w_t as a (discrete-time) Gaussian stochastic process
  - Compute $E\{w_t\}$ and Γ_{w_t} as ergodic averages

State estimation problem

- Approximate / reduced order state space representation

$$\begin{aligned} c_{t+1} &= Fc_t + s + w_t \\ V_t &= U_t^{\mathrm{r}}(c_t) + \epsilon_t + n_t \end{aligned}$$

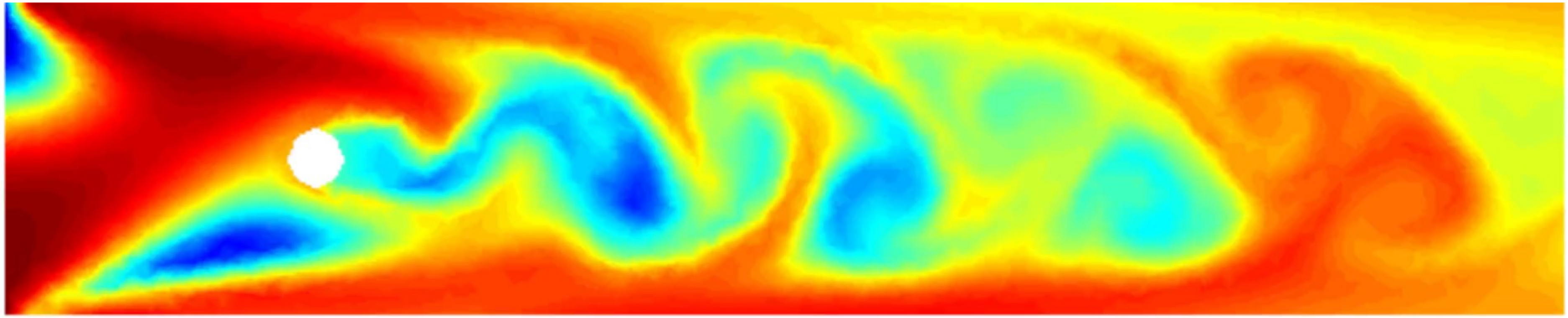
- *Maximum a posteriori* estimate

$$c_{t|t} = \arg\max_{c_t} \pi(c_t | V_1, \ldots, V_t)$$

corresponding to approximate state space representation with error models

- Extended Kalman filter

Process tomography: recovery from uncertainties of the velocity field



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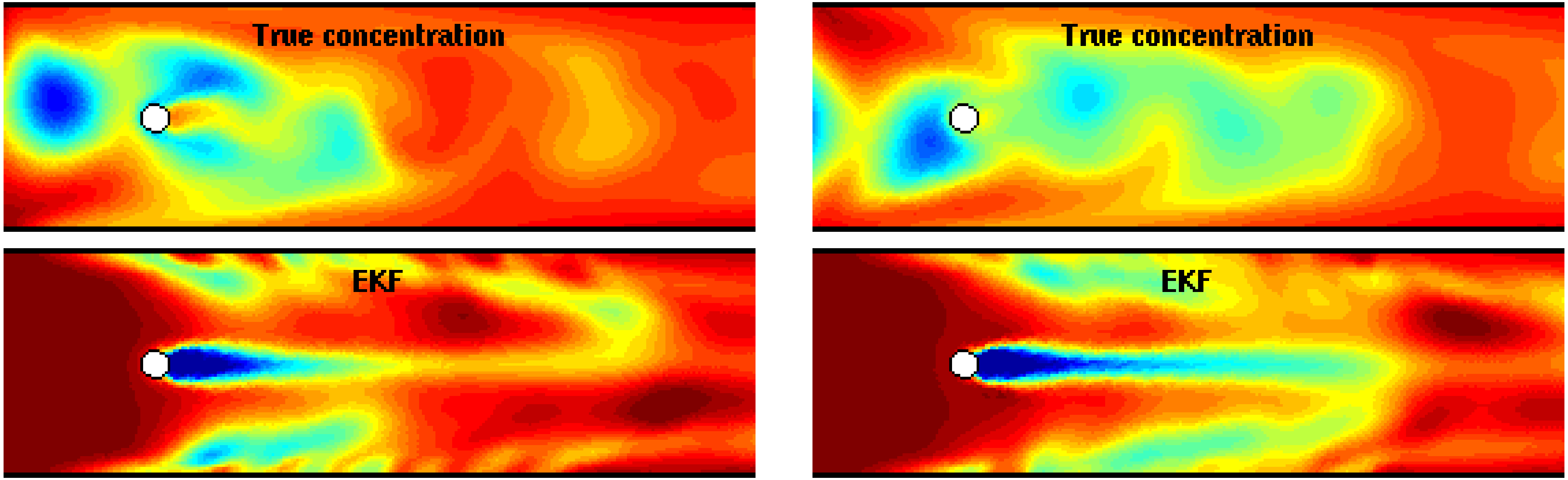
- Unknown and non-stationary velocity field $\bar{v}(\bar{r}, t)$ and input concentration $c_{\text{in}}(\bar{r}, t)$
- Use temporal average of $\bar{v}(\bar{r}, t)$ and $c_{\text{in}}(\bar{r}, t)$ in the convection-diffusion model
- Write a statistical model for the error induced by the use of time averaged approximations of $\bar{v}(\bar{r}, t)$ and $c_{\text{in}}(\bar{r}, t)$

Stationary flow approximation, no error models included



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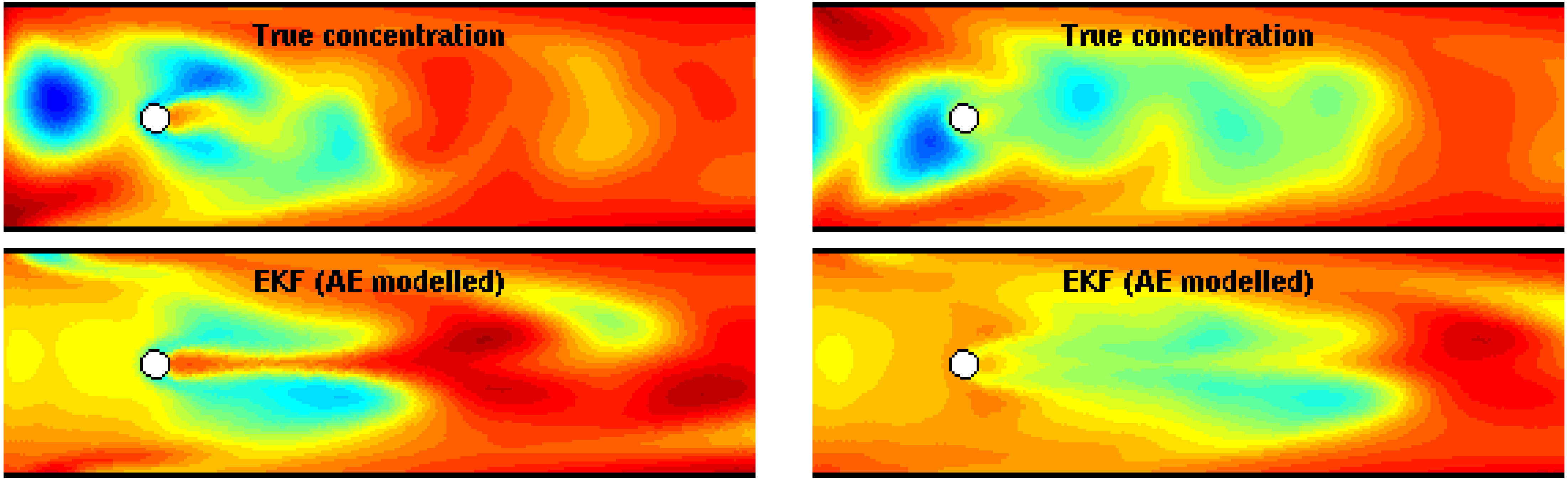
Approximation error modeling approach



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Dual estimation of concentration and velocity

- Navier-Stokes equations

$$\rho\frac{\partial\bar{v}}{\partial t} + \rho\bar{v}\cdot\nabla\bar{v} - \mu\Delta\bar{v} + \nabla p = \rho\bar{f}$$
$$\nabla\cdot\bar{v} = 0$$

- Reduced order Navier-Stokes model (based on principal component analysis): small dimensional approximation:

$$\bar{v} \approx \bar{v}_0 + \Sigma_{i=1}^{N_\beta}\beta_i(t)\bar{v}_i$$

- Reduced order FE-approximation $\Rightarrow$

$$\beta_{t+1} = h(\beta_t) + \psi_t$$

- Evolution model

$$\underbrace{\begin{pmatrix}\beta_{t+1}\\ c_{t+1}\end{pmatrix}}_{\theta_{t+1}} = \underbrace{\begin{pmatrix}h(\beta_t)\\ F_t(\beta_t)c_t + s_t(\beta_t)\end{pmatrix}}_{f_t(\theta_t)} + \underbrace{\begin{pmatrix}\psi_t\\ w_t(\beta_t)\end{pmatrix}}_{\omega_t}$$

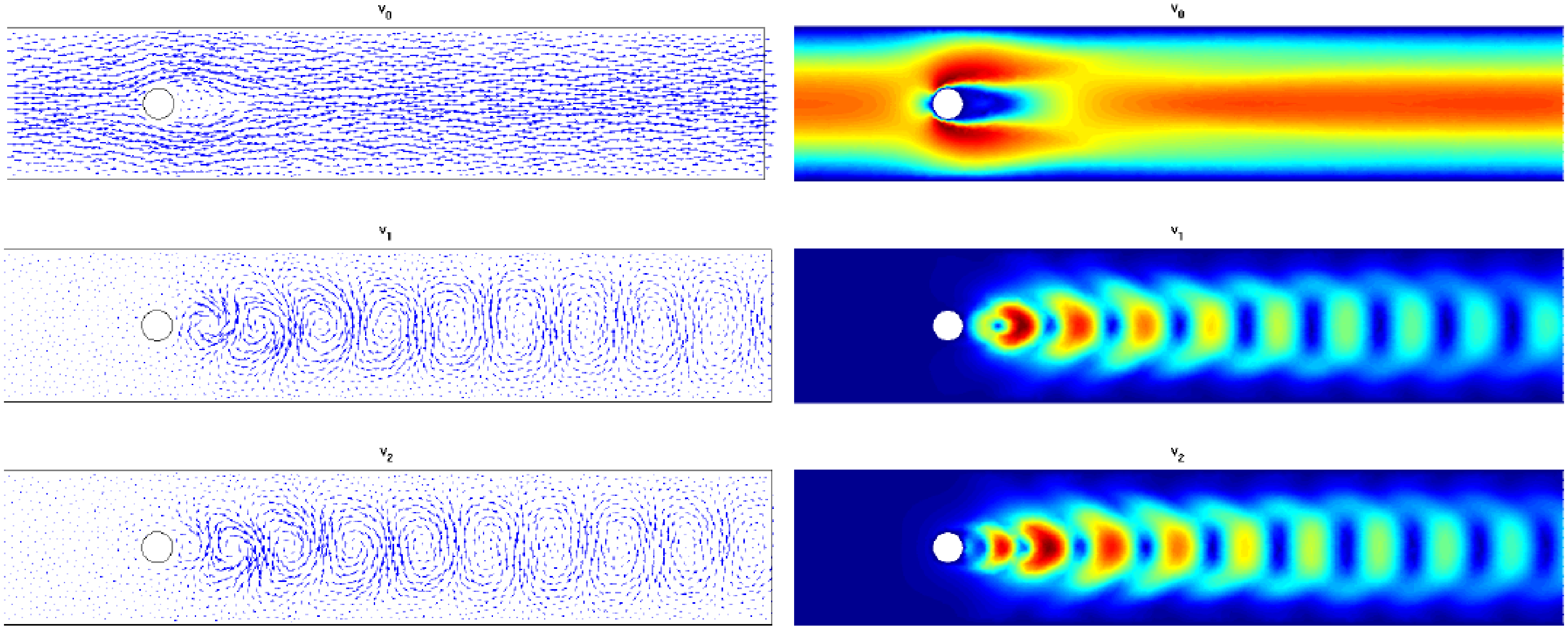
- Observation model

$$\begin{aligned} V_t &= U_t(c_t) + n_t \\ &= U_t^*(\theta_t) + n_t \end{aligned}$$

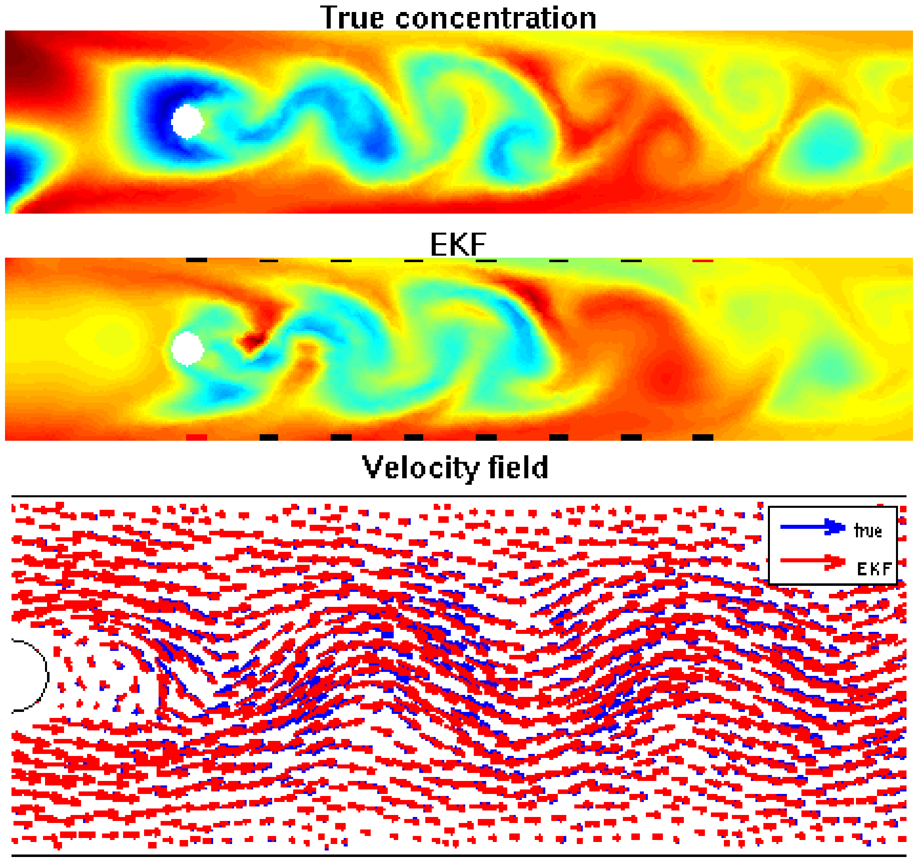
- Filtering problem: Write the posterior density

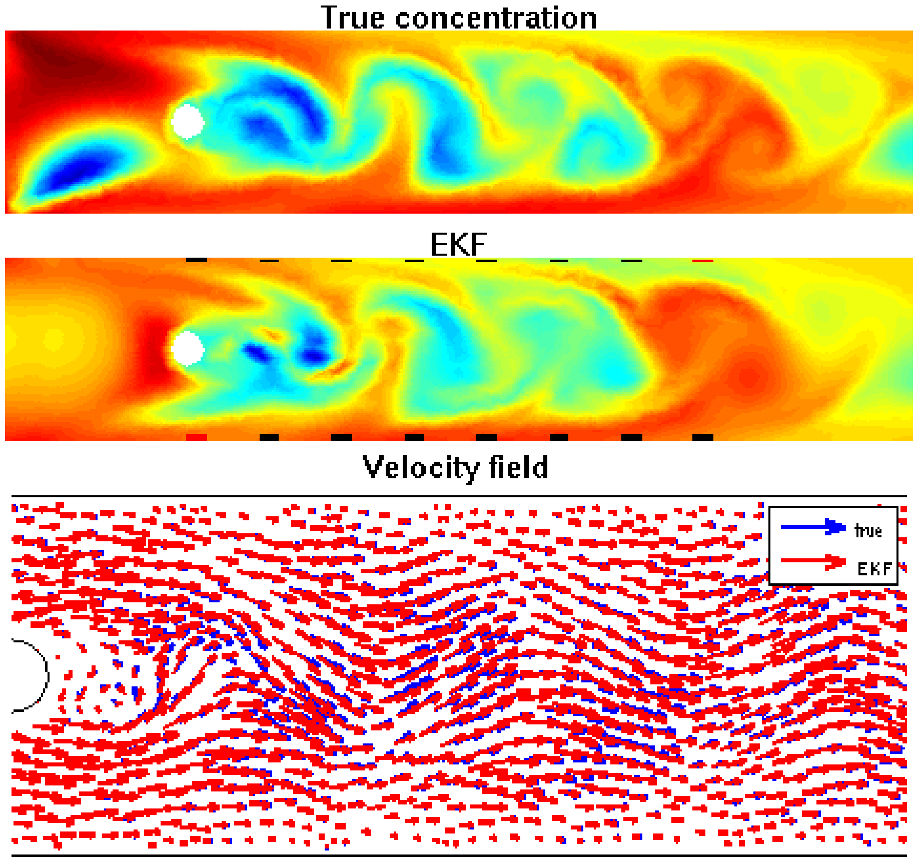
$$\pi(\theta_t|V_1,\ldots,V_t)$$

Dual estimation – basis functions for the velocity



Dual estimation of concentration and velocity





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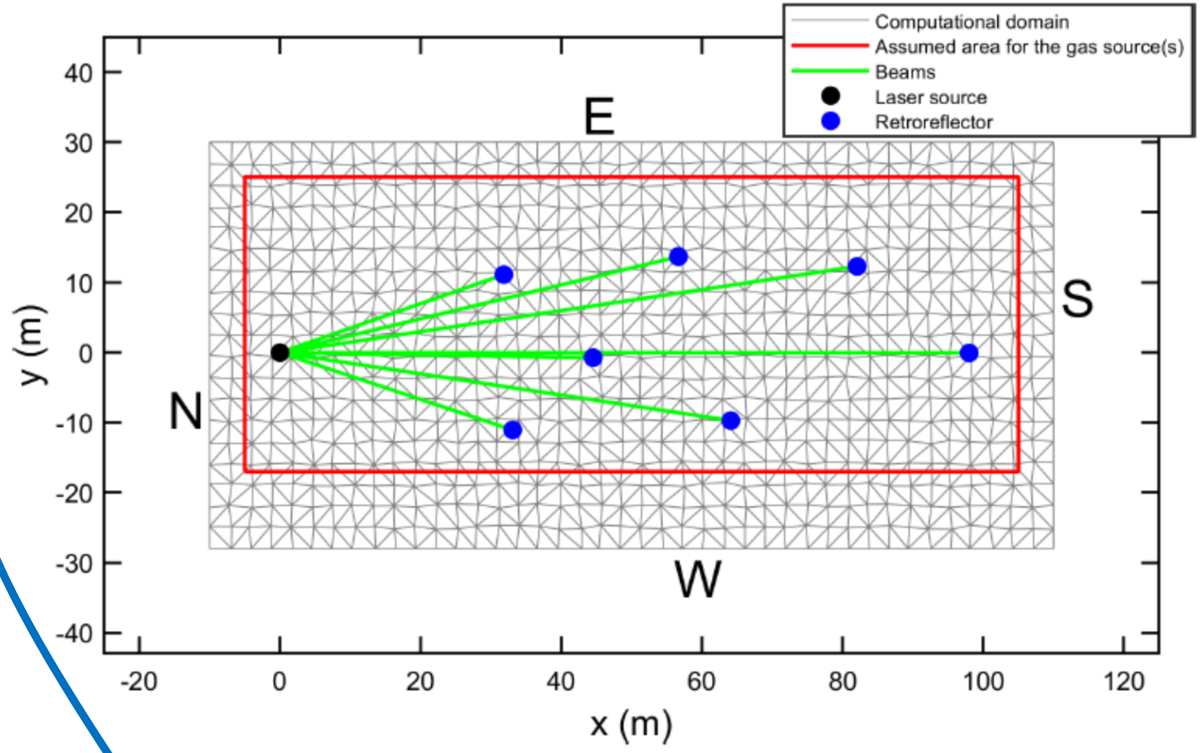
Gas emission monitoring

- Measurement system produced by MIRICO Ltd
- Application: Monitoring of greenhouse gas emissions (carbon dioxide, methane, etc)

Estimation problem

- Sequential measurements (*t = 0,…,T*)
  - Laser dispersion measurements y_t -> line-integrals of concentration *c(x,t)*
  - Wind velocity (speed and direction) $\bar{v}(x,t)$
- State estimation problem
  - Estimate the (spatially and temporally varying) concentration *c(x,t)* and the gas emission rate *S(x,t)*
  - *Bayesian state estimation, based on*
    - *Measurement model* (line-integrals)
    - *Evolution model (convection-diffusion equation)*
  - Kalman filtering/smoothing

Limited angle tomography problem …



+ Currently, we measure wind velocity only in a single point…

Evolution model: convection-diffusion equation

- Convection-diffusion equation

- **Unknowns** in the model
  c(x,t) and *S(x,t)*

$$\frac{\partial c}{\partial t} = \underbrace{-\bar{v} \cdot \nabla c}_{\text{Convection}} + \underbrace{\nabla \cdot (\kappa \nabla c)}_{\text{Diffusion}} + \underbrace{S}_{\text{Gas emission rate}}$$

- Stochastic modelling of c_t and a_t (discrete counterparts of *c(x,t)* and *S(x,t)*)

$$c_{t+1} = F_t c_t + s_{t+1} + \tilde{s}(a_t) + w_{t+1}$$

(FEM approximation of the CD model)

$$a_{t+1} = A_0 a_t + A_1 a_{t-1} + v_{t+1}$$

(2nd order Markov model promoting spatial and temporal smoothness)

Evolution model

- Augmented state variable:

$$\theta_t = \begin{bmatrix} c_t \\ a_t \\ a_{t-1} \end{bmatrix}$$

We also make another reparametrization to implement positivity constraints for c_t and a_t but let's skip them here…

- Evolution model in terms of this state variable

$$\begin{bmatrix} c_{t+1} \\ a_{t+1} \\ a_t \end{bmatrix} = \begin{bmatrix} F_t & T_t & \mathbf{0} \\ \mathbf{0} & A_0 & A_1 \\ \mathbf{0} & I & \mathbf{0} \end{bmatrix} \begin{bmatrix} c_t \\ a_t \\ a_{t-1} \end{bmatrix} + \begin{bmatrix} s_{t+1} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} w_{t+1} \\ v_{t+1} \\ \mathbf{0} \end{bmatrix}$$

$$\Longrightarrow \quad \theta_{t+1} = \bar{F}\theta_t + \bar{s}_{t+1} + \bar{w}_{t+1}$$

Observation model

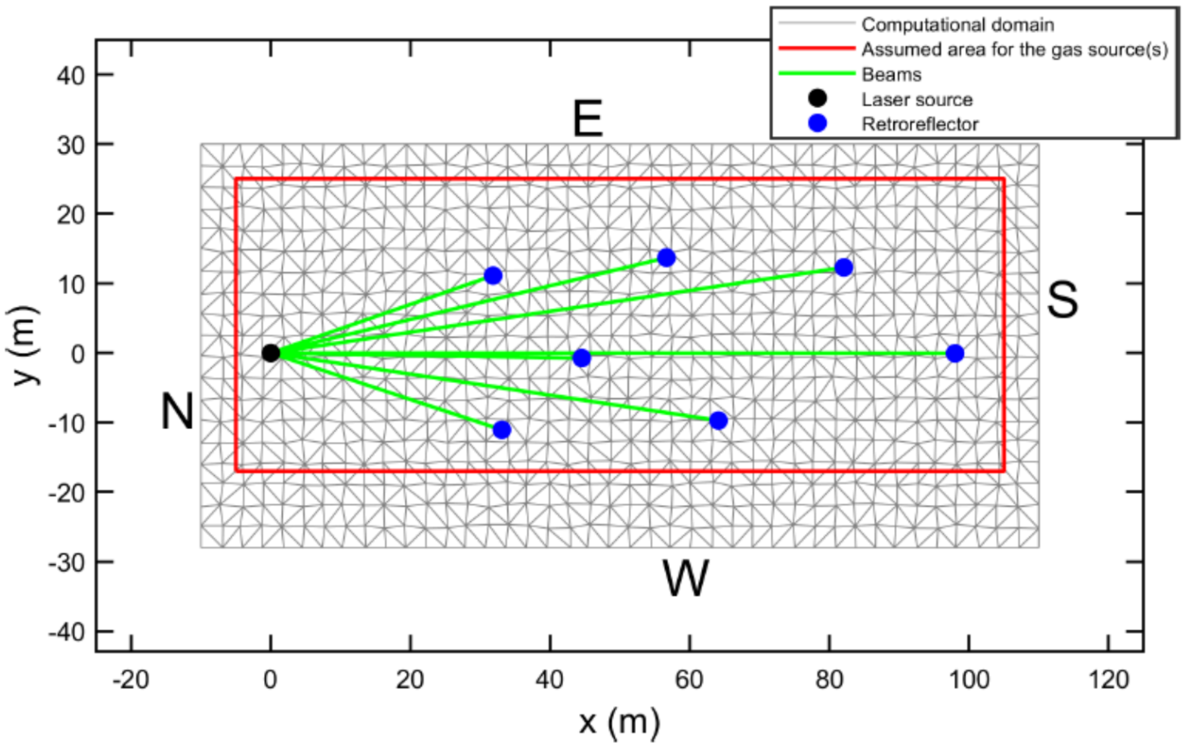
$$\theta_t = \begin{bmatrix} c_t \\ a_t \\ a_{t-1} \end{bmatrix}$$

- Observations y_t: line-integrals of $c(x,t)$

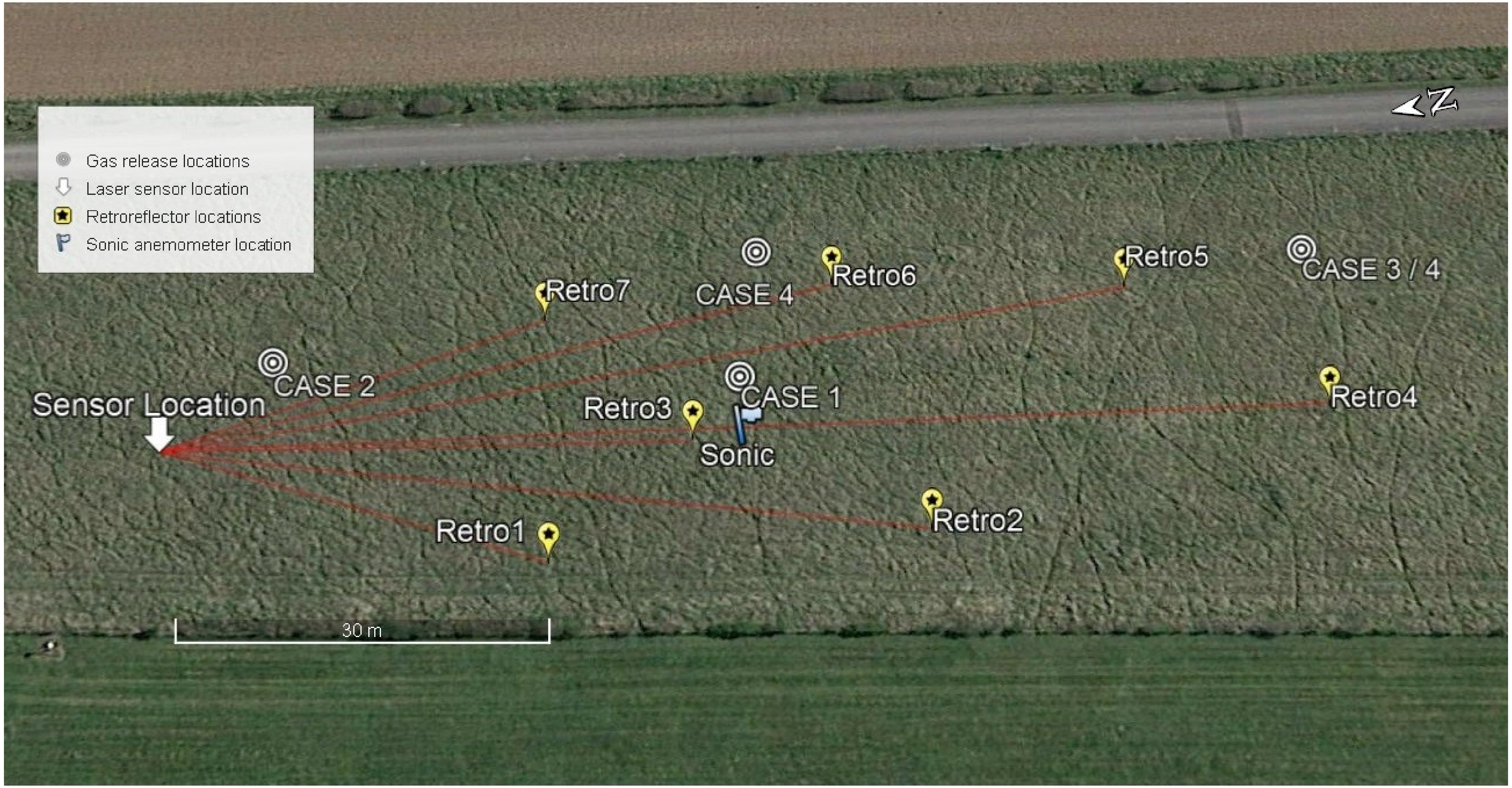
$$y_t = Hc_t + v_t$$

$$= H \cdot \begin{bmatrix} I & 0 & 0 \end{bmatrix} \cdot \theta_t + v_t$$

$$= H_\theta(\theta_t) + v_t$$

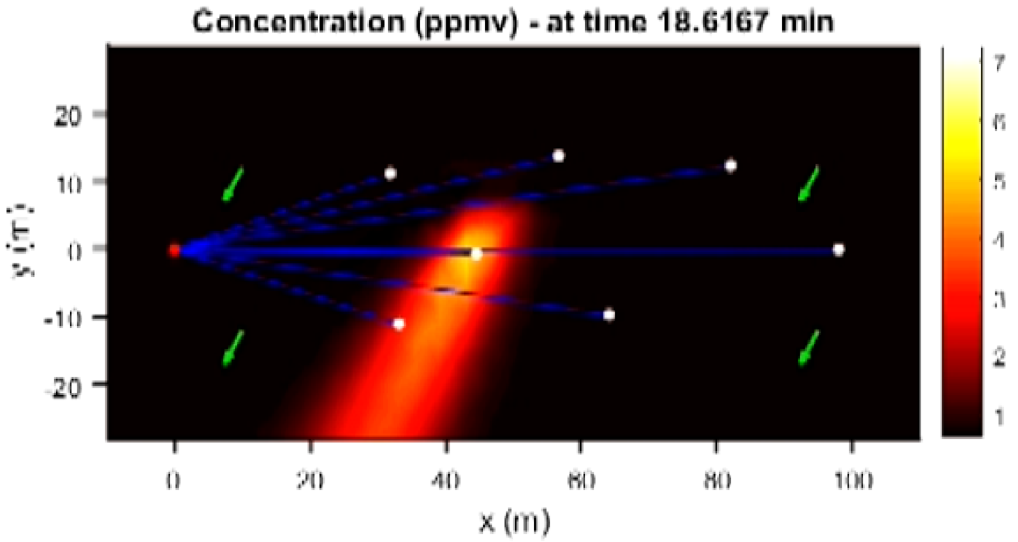


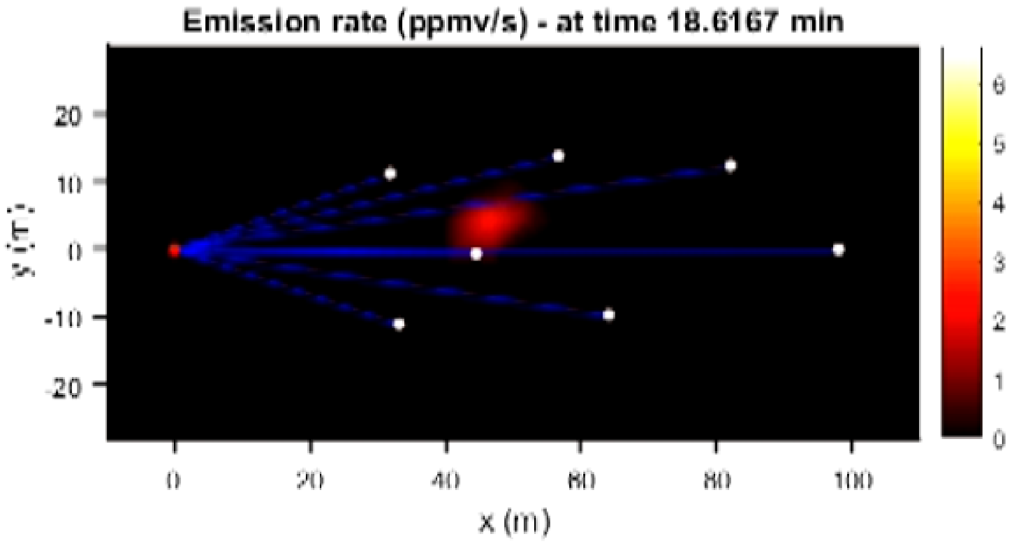
Field test, experimental setup



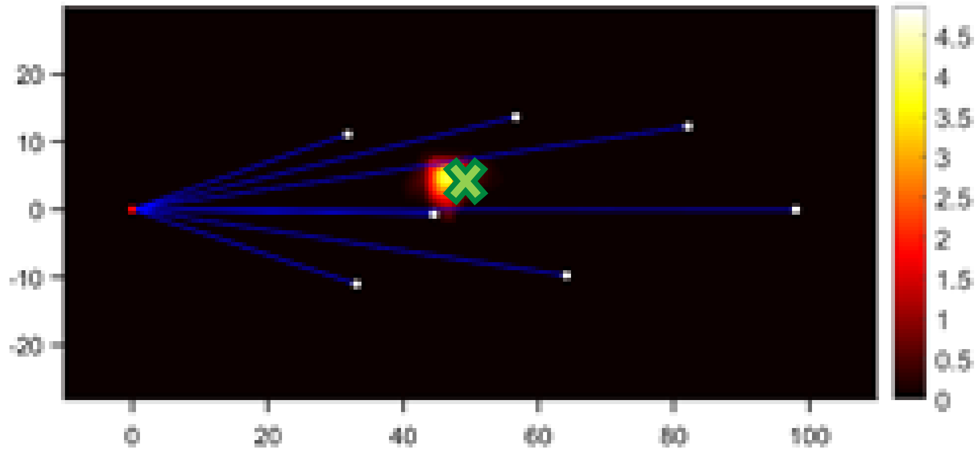
State estimation, example

(Animation removed from the pdf-version, snapshots only)

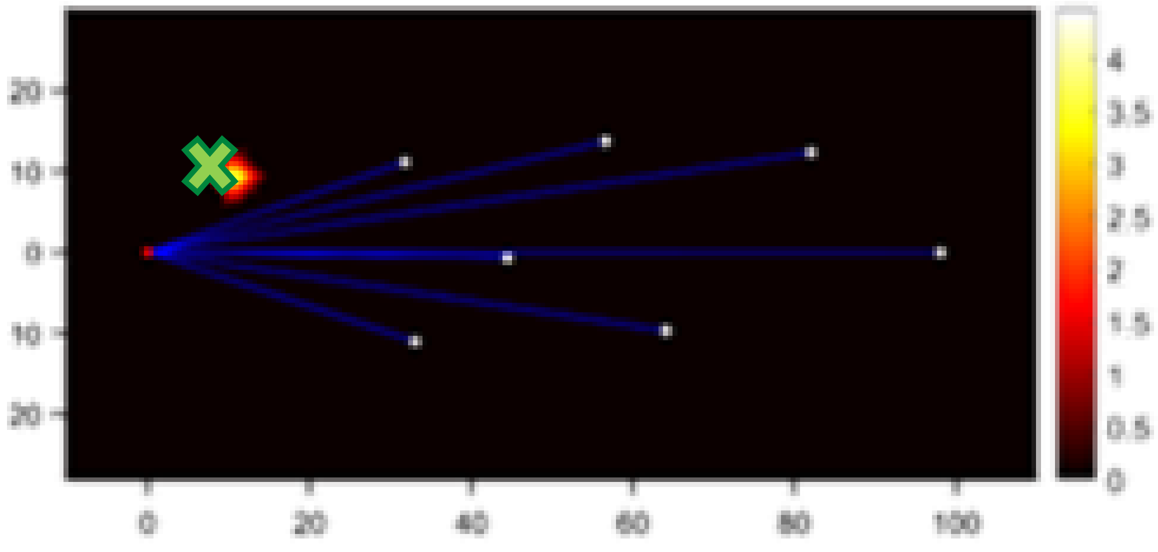


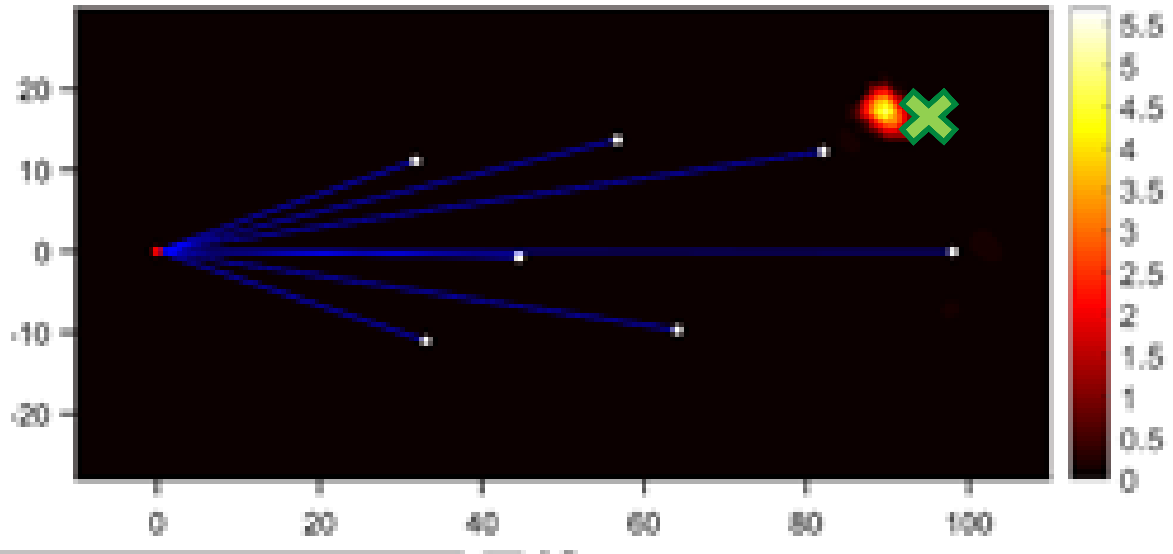


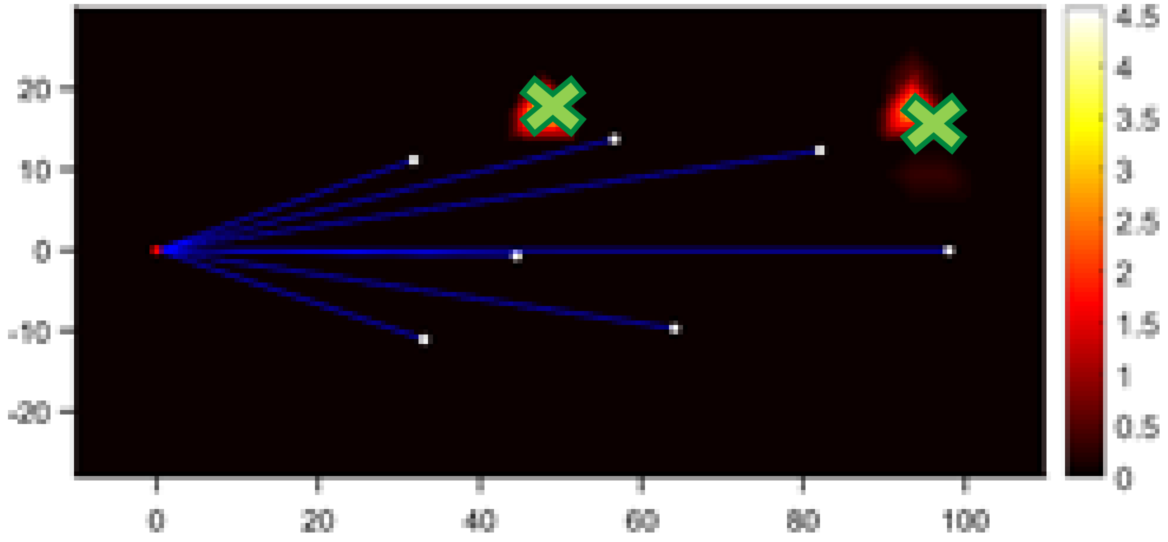
- Weighted temporal average of the emission rate
- True source location?



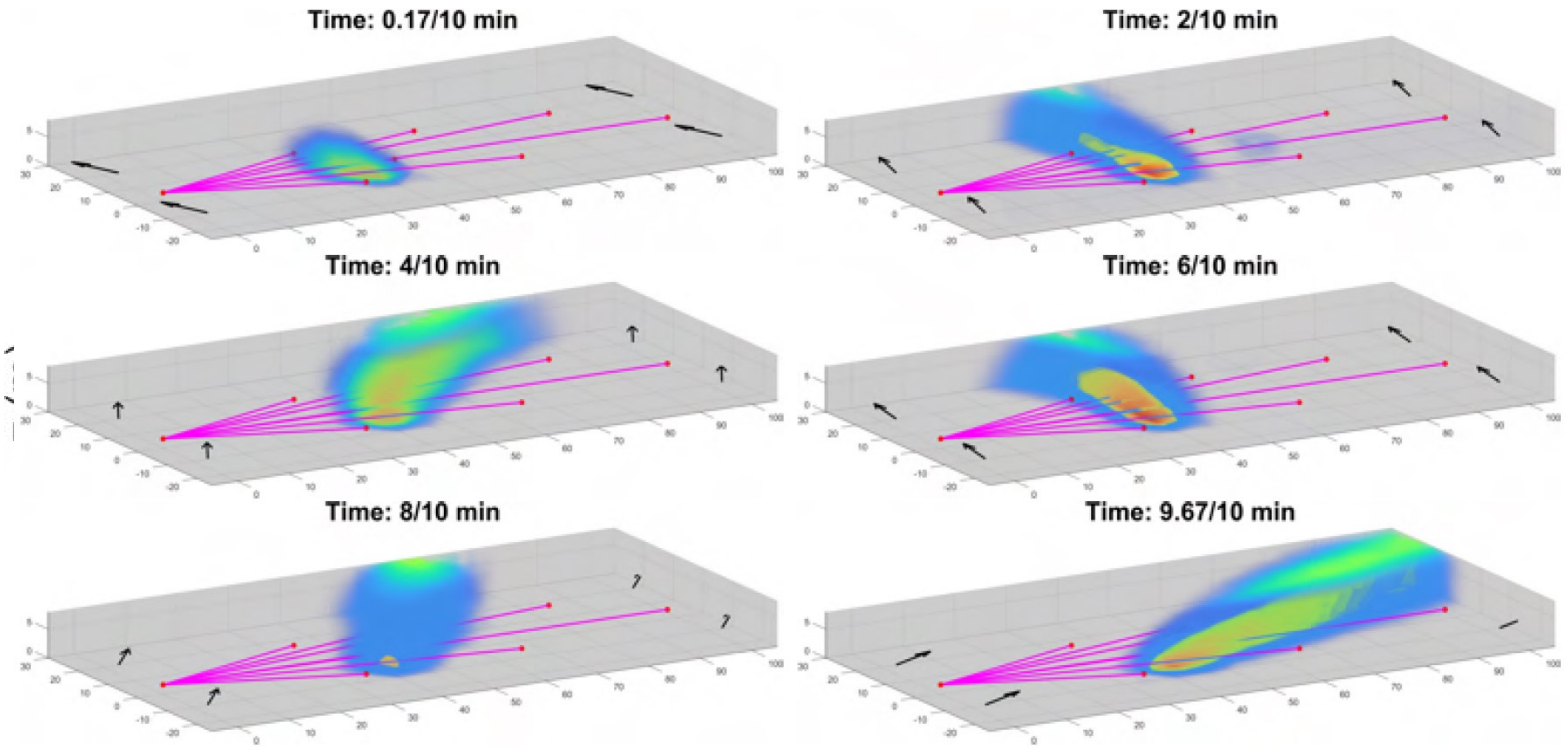
More test cases





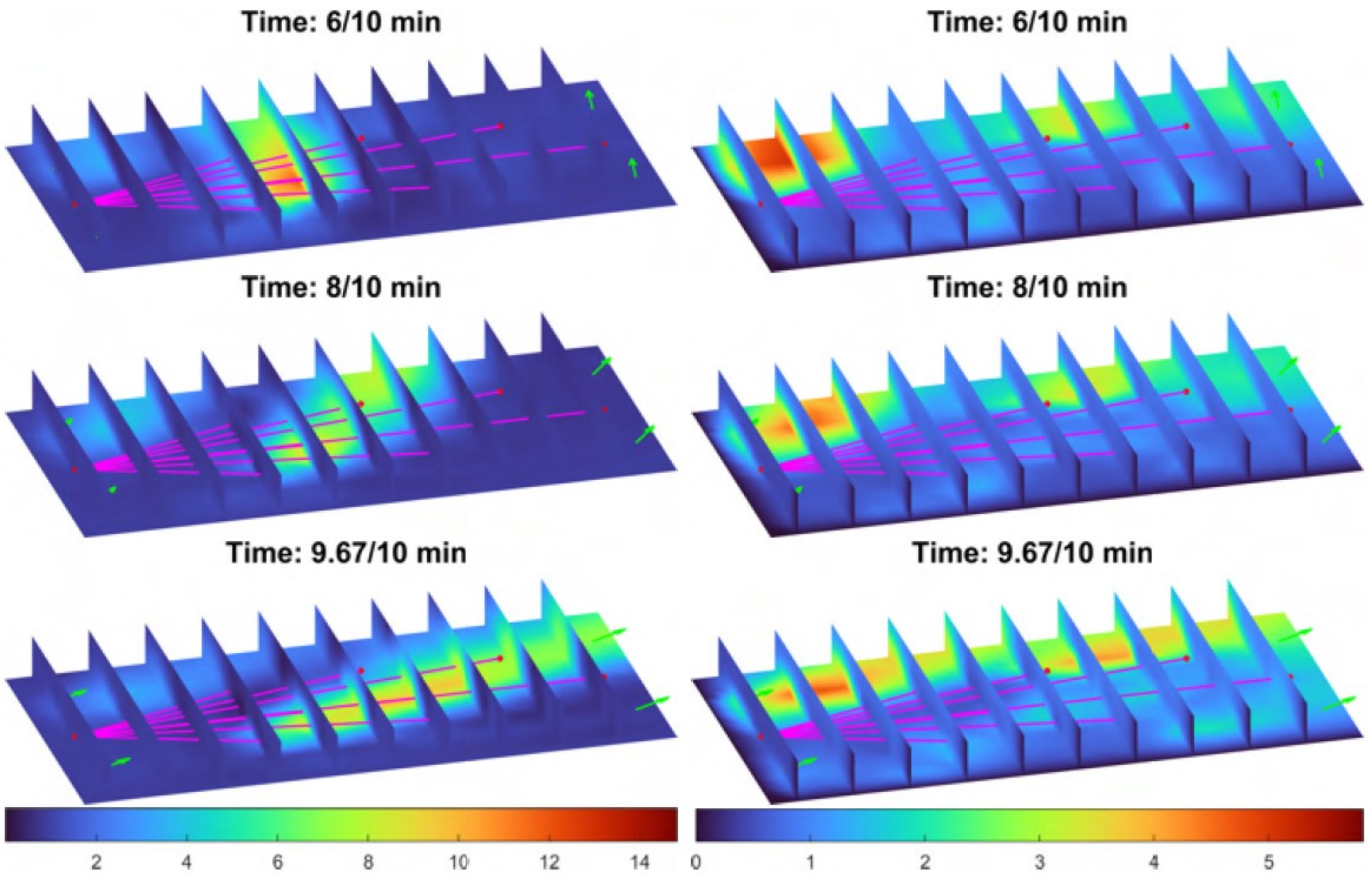


3D modeling



Time: 0.17/10 min
Time: 2/10 min
Time: 4/10 min
Time: 6/10 min
Time: 8/10 min
Time: 9.67/10 min

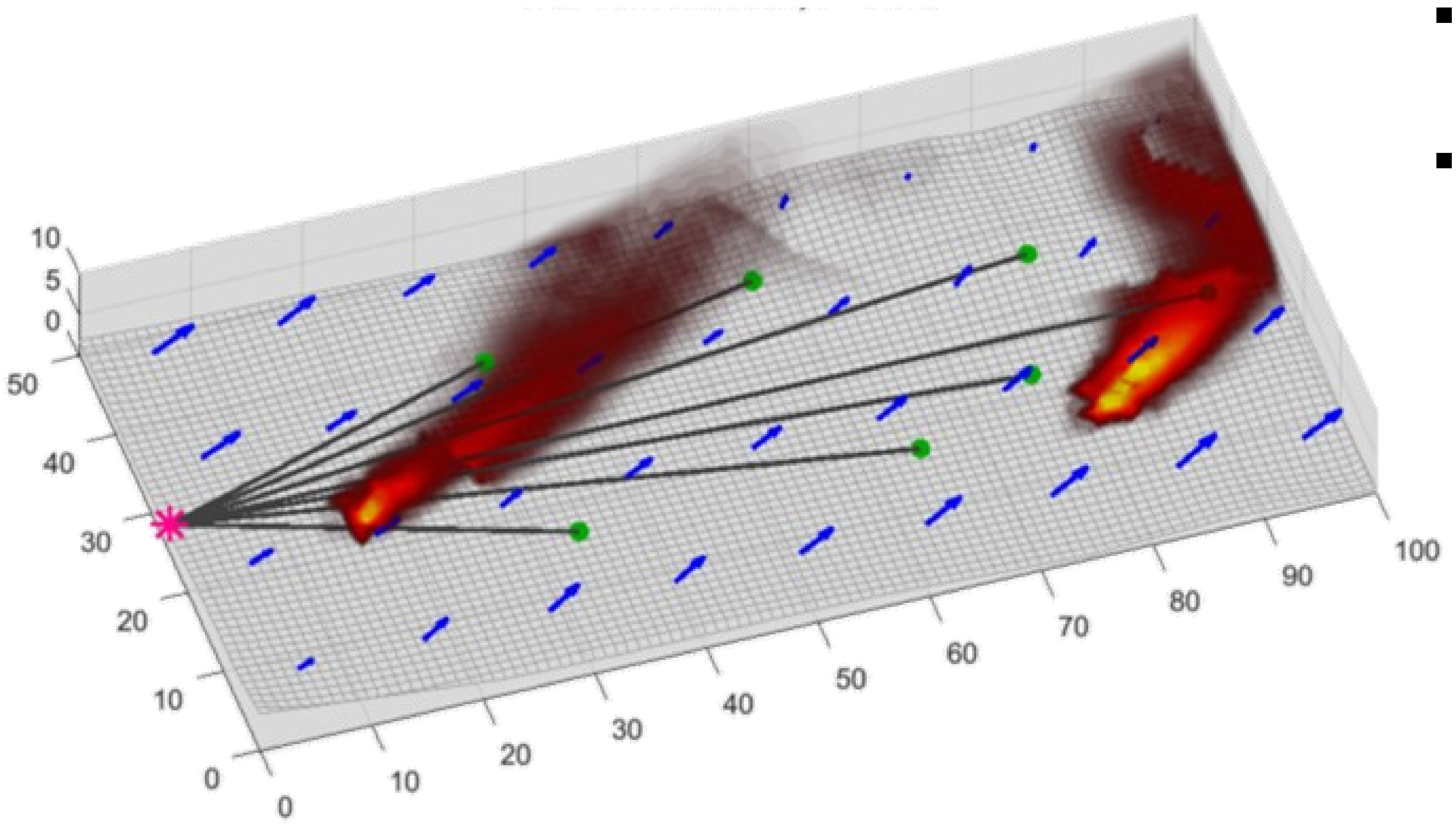
3D reconstruction & uncertainty quantification



- Left column: reconstructed 3D concentration.
- Right column 95 % credibility interval width.

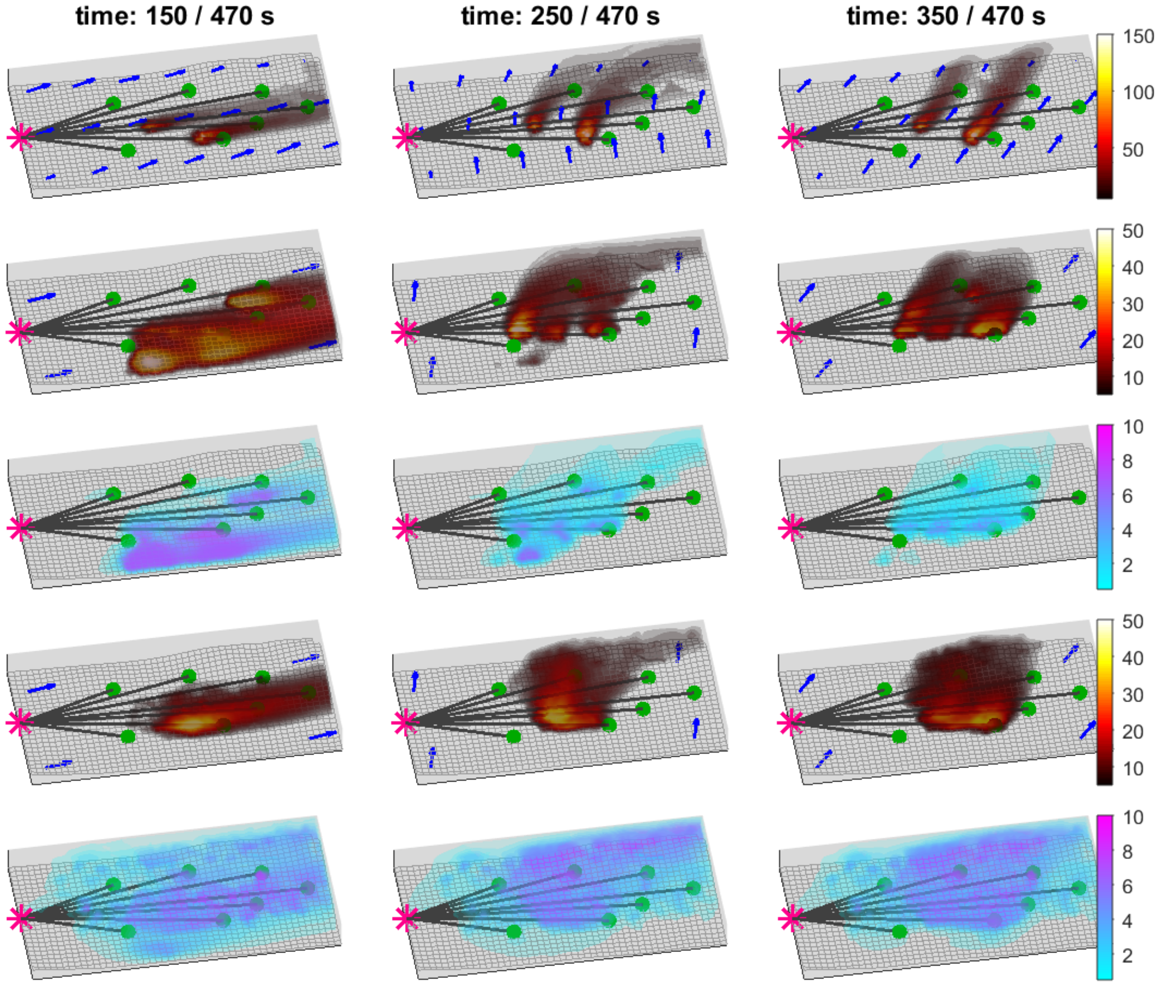
(Elias Vänskä, MSc thesis, UEF, 2022)

Modeling errors

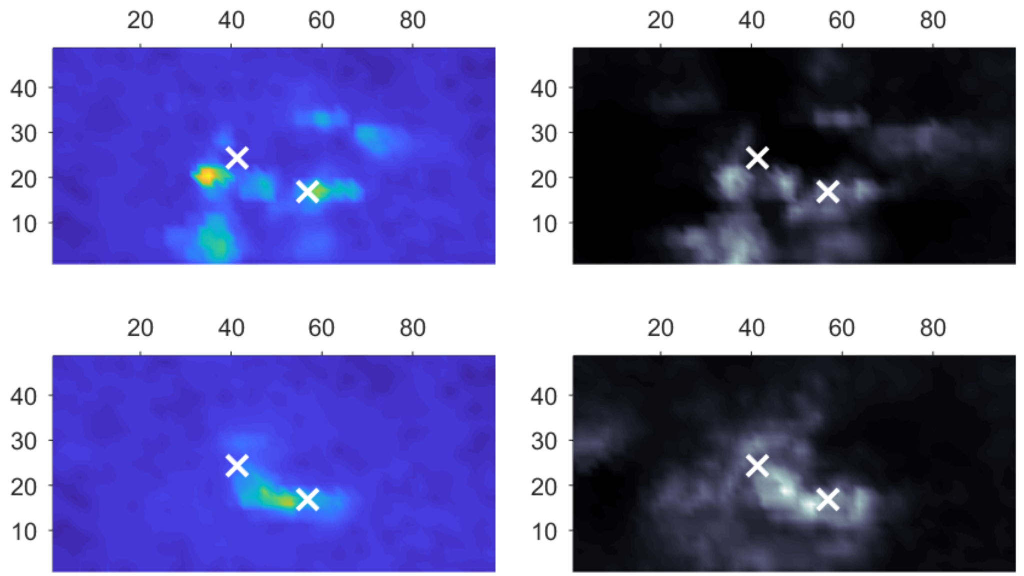


- Uncertainties in the wind field
- Approximation of the evolution using a single-gas model (CD model)

Effect of uncertainty in the wind field



True concentration, conventional estimate and its 95% credible interval width, error enhanced estimate and its 95% credible inteval width.



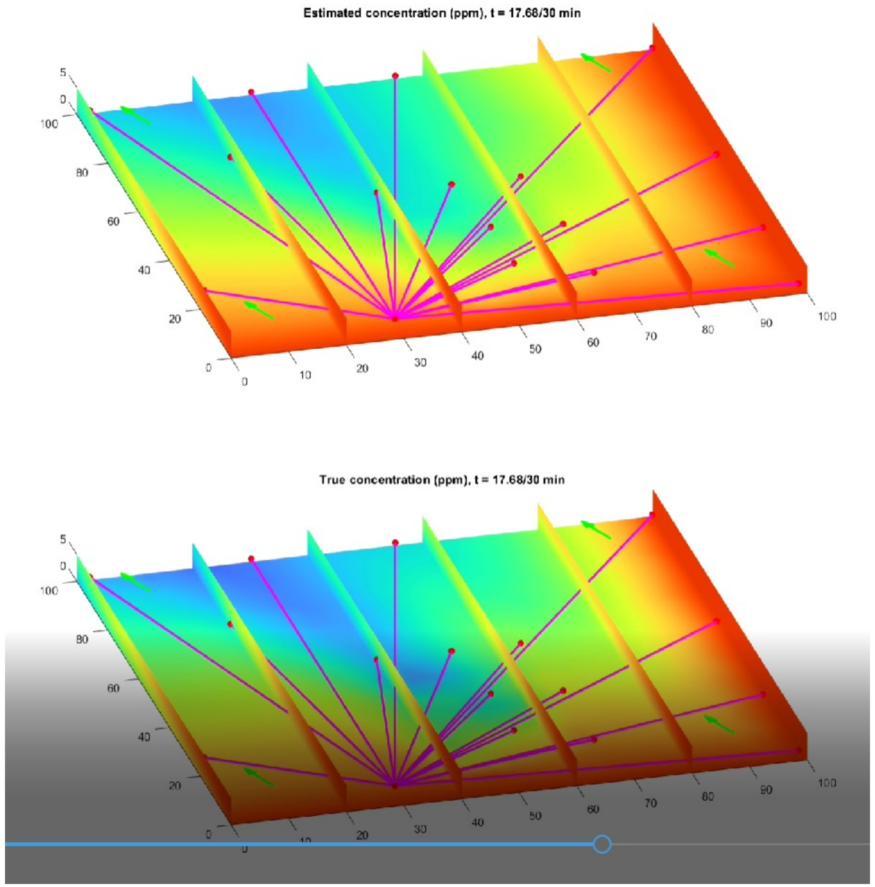
Time-average emission rates (left column) and corresponding 95% credible interval widths (right column). Conventional and error enhanced estimate

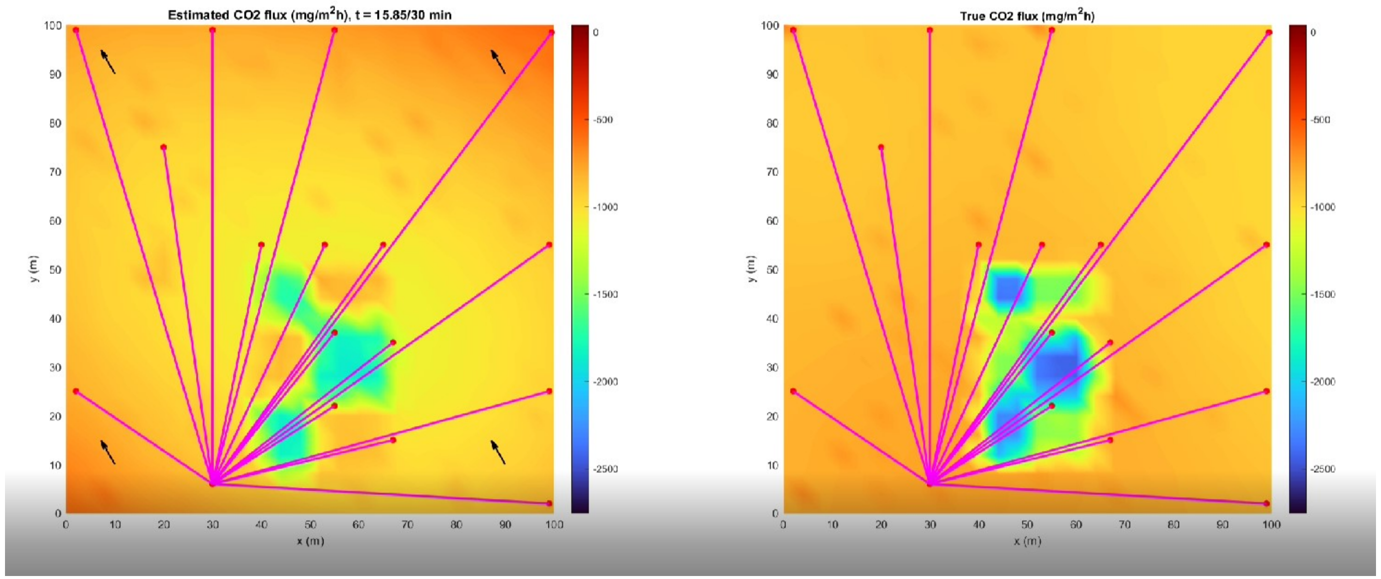
(Outi Kurri, MSc thesis, UEF, 2022)

New application: Monitoring effects of farming management on the greenhouse gas balance in agriculture

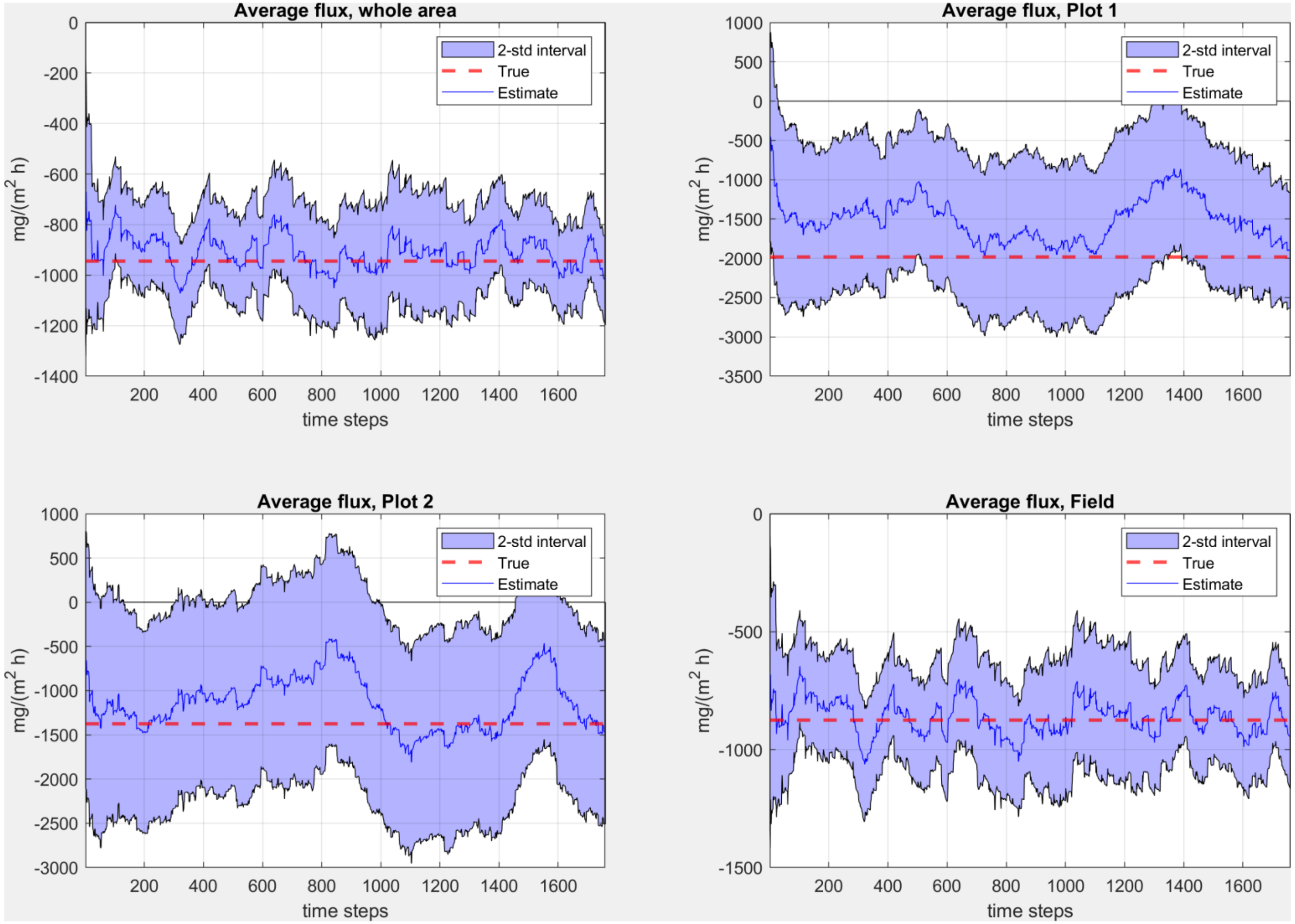
Diffuse source case (numerical simulation)

(Animations removed from the pdf-version, snapshots only)





Diffuse source case (numerical simulation)



Summary

- Convection-diffusion problems
- Sequential measurements
- Bayesian state estimation
- Application 1: Process tomography
- Application 2: Greenhouse gas emission/balance monitoring
- Approximation error modeling
- Uncertainty quantification

References

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[3] A. Lipponen, A. Seppänen, J.P. Kaipio: Reduced order estimation of nonstationary flows with electrical impedance tomography, *Inverse Problems*, 26: 074010 (20pp), 2010.

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