ABOUT THE UNIVERSITY

• Graduate Program in Engineering:
  • 9,418 MSc Thesis and 3,037 PhD Thesis (from 1963 to 2010)
  • 325 faculty members and 2,800 students (1,200 PhD students) in 12 Departments;
  • Among the best Mechanical Engineering Departments in Brazil
INTERACTION WITH INDUSTRY
INTERACTION WITH INDUSTRY

GE Research Center

Petrobras Research Center
ABOUT OUR TOPICS OF RESEARCH

• Basic and Applied Research in Inverse Problems and Optimization in Heat Transfer, Combustion and Thermal Machines;

• Financed by several Brazilian agencies:

• Partnerships with industry:
ABOUT OUR INFRASTRUCTURE

ASTM/CFR Engines to test fuel quality (Diesel and Otto)

3 AVL Dynos (160 kW, 360 kW and 500 kW) fully equipped with air and fuel conditioning (AVL), gas analyzers (Horiba MEXA 7100 EGR and AVL FTIR) and particulate measurements (AVL Smart Sampler)

Brayton and Rankine test bench

Intel cluster (384 cores)

2 large Marine Engines (MAN Innovator and Wartsila 4L20) fully instrumented with gas and particulate analysers (AVL+Horiba) and Dyno (Horiba) to test heavy fuel and lubricants
BAYESIAN PARTICLE FILTERS?
BAYESIAN PARTICLE FILTERS?
BAYESIAN PARTICLE FILTERS?

- I guess the distribution.
- Solve $\frac{1}{2} \frac{d^2 t}{dt^2} = \nabla^2 t$
- Verify if $T_{\text{measured}} = T_{\text{estimated}}$
- Update the guess
BAYESIAN PARTICLE FILTERS?

Many observers!!

- Different guesses
- Different errors
- Probabilistic distribution
SUMMARY

• State Estimation Problem
• Filtering Problem
• Physical Problems
• Results
• Conclusions
STATE ESTIMATION PROBLEM

State Evolution Model: \[ x_k = f_k(x_{k-1}, v_{k-1}) \]

Observation Model: \[ z_k = h_k(x_k, n_k) \]

\( x \in R^{n_x} = \) state variables to be estimated

\( v \in R^{n_v} = \) state noise

\( z \in R^{n_z} = \) measurements

\( n \in R^{n_n} = \) measurement noise

Subscript \( k = 1, 2, \ldots \), denotes an instant \( t_k \) in a dynamic problem
STATE ESTIMATION PROBLEM

**Definition:** The state estimation problem aims at obtaining information about $x_k$ based on the state evolution model and on the measurements given by the observation model.

$z_{1:k} = \{z_i, i = 1, \ldots, k\}$
The evolution-observation model is based on the following assumptions:

(i) The sequence $x_k$ for $k = 1, 2, \ldots$, is a Markovian process, that is,
$$
\pi(x_k | x_0, x_1, \ldots, x_{k-1}) = \pi(x_k | x_{k-1})
$$

(ii) The sequence $z_k$ for $k = 1, 2, \ldots$, is a Markovian process with respect to the history of $x_k$, that is,
$$
\pi(z_k | x_0, x_1, \ldots, x_k) = \pi(z_k | x_k)
$$

(iii) The sequence $x_k$ depends on the past observations only through its own history, that is,
$$
\pi(x_k | x_{k-1}, z_{i:k-1}) = \pi(x_k | x_{k-1})
$$

\[\text{State Evolution Model:} \quad x_k = f_k(x_{k-1}, v_{k-1})\]

\[\text{Observation Model:} \quad z_k = h_k(x_k, n_k)\]
FILTERING PROBLEM

By assuming that $\pi(x_0 | z_0) = \pi(x_0)$ is available, the posterior probability density $\pi(x_k | z_{1:k})$ is then obtained with Bayesian filters in two steps: prediction and update.

Bayes’ Theorem

$\pi(x_k | z_k) \propto \pi(z_k | x_k) \ast \pi(x_k)$

Posterior $\propto$ likelihood $\ast$ prior

FILTERING PROBLEM: GENERAL ALGORITHM

PREDICTION
Drawn $N$ Particles from a prior density $\pi(x_k|x_{k-1})$

WEIGHTS
Calculate the weight (importance) of each particle $w^i_k$.

UPDATE
Calculate the posterior density $\pi(x_k|z_k)$.

RESAMPLE
If necessary, resample to avoid degeneration.

FILTERING PROBLEM: DIFFERENT ALGORITHMS

Bayes' Theorem

\[ \pi(x_k|z_k) \propto \pi(z_k|x_k) \ast \pi(x_k) \]

Posterior \( \propto \) likelihood \( \ast \) prior

**BASIC IDEA:** Obtain the posterior probability function, based on the weights (prior) of the individual particles (\( \mathcal{W} \) is the normalized weight).

\[ \pi(x_k|z_k) = \sum w_i^k x_i^k \]

Some algorithms use some sort of **resampling** in order to avoid the degeneration of the particles.
FILTERING PROBLEM: DIFFERENT ALGORITHMS

WEIGHTS

SIR: Sampling Importance
Resampling Filter –
"bootstrap filter" (Gordon et al, 1993)

1. Construct the cumulative sum of weights (CSW) by computing
   \[ c_i = c_{i-1} + w_i \]
   for \( i = 1, \ldots, N \), with \( c_0 = 0 \).

2. Let \( i = 1 \) and draw a starting point \( u_1 \) from the uniform
   distribution \( U[0,1/N] \).

3. For \( j = 1, \ldots, N \)
   Move along the CSW by making \( u_j = u_1 + (j-1)/N \).
   While \( u_j > c_i \) make \( i = i + 1 \).
   Assign sample \( x^j_k = x^i_k \).
   Assign weight \( w^j_k = 1/N \).

• It uses the likelihood: \( w^i_k = \pi(z_k | x^i_k) \)
• It uses a resampling strategy based on the cumulative sum of weights.
FILTERING PROBLEM: DIFFERENT ALGORITHMS

WEIGHTS

SIR: Sampling Importance Resampling Filter—“bootstrap filter” (Gordon et al, 1993)

• It uses the likelihood: \( w^i_k = \pi(z_k|x^i_k) \)
• It uses a resampling strategy based on the cumulative sum of weights.

All methods try to calculate the posterior probability \( \pi(x_k|z_k) \)

\[
\begin{align*}
  w^i_k &= w^i_{k-1} \frac{\pi(z_k|x^i_k)}{q(x^i_k|x^i_{k-1}, z_k)} \frac{\pi(x^i_k|x^i_{k-1})}{q(x^i_k|x^i_{k-1}, z_k)} \\
  q(x^i_k|x^i_{k-1}, z_k) &\text{ is the importance or proposal density}
\end{align*}
\]

Under the viewpoint of importance sampling, the SIR filter uses a suboptimal choice of the importance density, based on the transitional prior, which does not take into account the measurements.
FILTERING PROBLEM: DIFFERENT ALGORITHMS

WEIGHTS

ASIR: Auxiliary SIR Filter
(Pitt and Shephard, 1999)

- It generates a sub-set of particles from a prior density \( \pi(x^*_k|x_{k-1}) \) and, after resampling the sub-set of particles, calculate the weight as a ratio of likelihoods (incorporate some information about the measurements into the prior density):

\[
w^i_k = \frac{\pi(z_k|x^i_k)}{\pi(z_k|x^*i_k)}
\]

Under of viewpoint of importance sampling, it tries to approximate an optimal choice of the **importance density**, taking into account the measurements.
**ASIR: Auxiliary Sampling Importance Resampling Filter**

**WEIGHTS**

- It uses the likelihood: $w^i_k = \pi(z_k|x_{i-k})$
- It uses a **resampling** strategy based on the cumulative sum of weights.

- The advantage of ASIR over SIR is that it naturally generates points from the sample at $k-1$, which, conditioned on the current measurement, are most likely to be close to the true state.

- The resampling is based on some point estimate $\mu^i_k$ that characterize $\pi(x_k|x_{i-k-1})$, which can be the mean $\mu^i_k = E[\pi(x_k|x_{i-k-1})]$ or simply a sample of $\pi(x_k|x_{i-k-1})$. If the state evolution model noise is small, $\pi(x_k|x_{i-k-1})$ is generally well characterized by $\mu^i_k$, so that the weights $w^i_k$ are more even and the ASIR algorithm is less sensitive to outliers than the SIR algorithm. On the other hand, if the state evolution model noise is large, the single point estimate $\mu^i_k$ in the state space may not characterize well $\pi(x_k|x_{i-k-1})$ and the ASIR algorithm may not be as effective as the SIR algorithm.
### ASIR: Auxiliary Sampling Importance Resampling Filter

**Step 1**
For $i=1,\ldots,N$ draw new particles $x_k^i$ from the prior density $\pi(x_k|x_{k-1}^i)$ and then calculate some characterization of $x_k^i$ given $x_{k-1}^i$, as for example the mean $\mu_k^i=E[x_k|x_{k-1}^i]$. Then use the likelihood density to calculate the correspondent weights $w_k^i=\pi(z_k|\mu_k^i)w_{k-1}^i$.

**Step 2**
Calculate the total weight $t=\sum_i w_k^i$ and then normalize the particle weights, that is, for $i=1,\ldots,N$ let $w_k^i = \frac{t}{w_k^i}$.

**Step 3**
Resample the particles as follows:
Construct the cumulative sum of weights (CSW) by computing $c_i=c_{i-1}+w_k^i$ for $i=1,\ldots,N$, with $c_0=0$.
Let $i=1$ and draw a starting point $u_1$ from the uniform distribution $U[0,N^{-1}]$.
For $j=1,\ldots,N$
- Move along the CSW by making $u_j=u_1+N^{-1}(j-1)$.
- While $u_j>c_i$ make $i=i+1$.
- Assign sample $x_k^i=x_k^i$.
- Assign sample $w_k^i=N^{-1}$.
- Assign parent $i^j=i$.

**Step 4**
For $j=1,\ldots,N$ draw particles $x_k^j$ from the prior density $\pi(x_k|x_{k-1}^{i^j})$, using the parent $i^j$, and then use the likelihood density to calculate the correspondent weights $w_k^j=\pi(z_k|x_k^j) / \pi(z_k|\mu_k^{i^j})$.

**Step 5**
Calculate the total weight $t=\sum_j w_k^j$ and then normalize the particle weights, that is, for $j=1,\ldots,N$ let $w_k^j = \frac{t}{w_k^j}$.
FILTERING PROBLEM: DIFFERENT ALGORITHMS

WEIGHTS

1. Generate a set of particles \( \theta^i_k \) with \( N(\theta_k|z_{k-1}, \sigma^2_\theta) \), 
   \( i=1\ldots N \).
2. Calculate an auxiliary variable:
   \[ m^i_k = a \theta^i_k + (1-a)\theta_{\text{average}}k, \]
   where \( a \in [0.97, 0.99] \), \( i=1\ldots N \).
3. Generate auxiliary particles \( \theta^{*i}_k \) with \( N(m^i_k, h^2\sigma^2) \),
   where \( h^2=1-a^2 \), \( i=1\ldots N \).
4. Generate two sub-sets of particles from prior densities
   \( \pi(x_k|x_{k-1}, \theta_k) \) and \( \pi(x_k|x_{k-1}, m_k) \)
5. Calculate the weight as the ratio of the likelihoods
   (minimize the variance of the parameter)
   \[ w^i_k = \pi(z_k|x^i_k, \theta^i_k)/\pi(z_k|x^{*i}_k, m^i_k) \]
FILTERING PROBLEM: DIFFERENT ALGORITHMS

WEIGHTS

SMC: Sequential Monte Carlo Samplers
(Del Moral et al, 2006)

- It uses the likelihood: \( w^i_k = \pi(z_k | x^i_k) \)
- It uses a resampling strategy based on the Metropolis-Hasting algorithm.

SMC without likelihoods:
(Sisson and Fran, 2007)

- The likelihood is replaced by a kernel based on the Euclidian distance between the observed and estimated quantities.
- It uses a resampling strategy.
PHYSICAL PROBLEM #1
Heat transfer problem inside a combustion chamber of a SI Engine


\[
\frac{dP}{d\theta} = -\gamma \frac{P}{V} \frac{dV}{d\theta} + (\gamma - 1) \frac{dQ}{d\theta} = Q_{\text{total}} \frac{d}{d\theta} \left\{ 1 - e^{-a\left(\frac{\theta - \theta_0}{\Delta \theta}\right)^{m+1}} \right\} - \frac{dQ_w}{d\theta}
\]

\[Q_w = hA(T - T_{\text{gas}})\]

Results were validated against experimental data of Melo et al (2007).
STATE ESTIMATION PROBLEM

In general:

State Evolution Model: \( x_k = f_k(x_{k-1}, v_{k-1}) \)

Observation Model: \( z_k = h_k(x_k, n_k) \)

In general

\[ z = \{P\} \quad \text{(Measured pressure)} \]

\[ x = \{h, T, P\} \quad \text{(Heat transfer coefficient, temperature and pressure)} \]

STATE ESTIMATION PROBLEM

State evolution model

\[ \frac{dP}{d\theta} = -\gamma \frac{P}{V} \frac{dV}{d\theta} + \frac{(\gamma - 1)}{V} \frac{dQ}{d\theta} \]

\[ \frac{dQ}{d\theta} = Q_{\text{total}} \frac{d}{d\theta} \left\{ 1 - e^{-\left[ -a \left( \theta - \theta_c \right) \Delta\theta \right]^{m+1}} \right\} - \frac{dQ_w}{d\theta} \]

\[ Q_w = hA \left( T - T_{\text{gas}} \right) \]

\[ h_{\text{est}}(t) = h_{\text{est}}(t-\Delta t) + \sigma_h \varepsilon h_{\text{est}}^j(t - \Delta t) \]

Observation model

Simulated measurements

\[ P_{\text{meas}}(t) = P_{\text{exa}}(t) \left( 1 + \sigma_{\text{meas}} \xi \right) \]

\[ h(W/m^2K) = 3.26 B(m)^{-0.2} P(kPa)^{0.8} T(K)^{-0.55} \omega(m/s)^{0.8} \]

For the simulated measurements, we used the Woschni's model.

RESULTS

\[ \sigma_{\text{meas}} = 1\% P_{\text{meas}}, \quad h_{\text{guess}} = N(253, 20) \frac{\text{W}}{\text{m}^2 \cdot ^\circ\text{C}} \]

\[ \sigma_{\text{meas}} = 1\% P_{\text{meas}}, \ h_{\text{guess}} = N(400,400) \text{ W/m}^2\text{oC} \]

RESULTS

\[
\sigma_{\text{meas}} = 1\% P_{\text{meas}}, \quad h_{\text{guess}} = N(400,400) \text{W/m}^2\text{oC}
\]

20,000 particles

96774 Hz (6.5 meas./crank angle)

7444 Hz (0.5 meas./crank angle)

13825 Hz (1.1 meas./crank angle)

Modern data acquisition system can handle more than 100 kHz

RESULTS

\[ h_{\text{guess}} = N(400,400) \text{ W/m}^2\text{oC} \]

96774 Hz (6.5 meas./crank angle)

1,000 particles \( \sigma_{\text{meas}} = 0.1 \text{ bar} \)

5,000 particles \( \sigma_{\text{meas}} = 1\% P_{\text{meas}} \)

Modern data acquisition system can handle more than 100 kHz with accuracy of \( \pm 1\% \) of IMEP or \( \pm 0.1 \text{ bar} \)

5,000 particles \( \sigma_{\text{meas}} = 0.1 \text{ bar} \)

IMEP of current engine is 5.22 bar

CONCLUSIONS

1. The particle filter approach seems to be a promising technique to estimate the heat transfer coefficient in internal combustion engines, which can influence the performance and emissions of these machines.

2. The performance of the filter is excellent, even for initial guesses away from the exact solution.

3. Future works shall compare the performance of other filters, as for example the ASIR (Auxiliary Sampling Importance Resampling) Filter, and also estimate the mass fraction burned together with the heat transfer coefficient.

PHYSICAL PROBLEM #2

Natural convection in a square cavity

\[ q_2(t) ??? \]

\[ T = T_c \]

\[ \frac{\partial (\rho \phi)}{\partial t} + \frac{\partial (u \rho \phi)}{\partial x} + \frac{\partial (v \rho \phi)}{\partial y} = \nabla \cdot (\nabla \phi) + S \]

\[ T = T_h \]

\[ \phi = \begin{bmatrix} 1 \\ u(x, y, t) \\ v(x, y, t) \\ T(x, y, t) \end{bmatrix} \quad \Gamma^\phi = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \mu & 0 & 0 \\ 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & \frac{K}{C_p} \end{bmatrix} \]

\[ S^\phi = \begin{bmatrix} 0 \\ -\frac{\partial P(x, y, t)}{\partial x} \\ -\frac{\partial P(x, y, t)}{\partial y} - \rho g \{1 - \beta [T(x, y, t) - T_{ref}]\} \\ 0 \end{bmatrix} \]

Fluid = air
\[ T_c = 2^\circ C; \quad T_h = 12^\circ C \]
Width=height=0.045841 m
Ra=10^5

STATE ESTIMATION PROBLEM

State Evolution Model:
\[ x_k = f_k(x_{k-1}, v_{k-1}) \]

Observation Model:
\[ z_k = h_k(x_k, n_k) \]

In general
\[ x = \{q_2, u, v, T\} \]

\[ q_2(t) = 1; \]
\[ u(x,y); v(x,y); T(x,y) = 11 \times 11 \text{ volumes each} \]

364 state variables!

\[ z = T \text{ at top and bottom of the cavity} \]
STATE ESTIMATION PROBLEM

Simulated measured temperatures at the top and bottom walls were taken, where an experimental error with standard deviation equals to 1% of the local value of the temperature was used.

State evolution model

\[ u(t) = u(t)[1 + 0.01\epsilon] \]
\[ x_k = x_k + \sigma\epsilon \Rightarrow v(t) = v(t)[1 + 0.01\epsilon] \]
\[ T(t) = T(t)[1 + 0.01\epsilon] \]
\[ q_2(t) = q_2(t - 1) + \sigma_q\epsilon \]

Observation model

Simulated measured temperatures at the top and bottom walls were taken, where an experimental error with standard deviation equals to 1% of the local value of the temperature was used.

## RESULTS

**Test-cases analyzed**

<table>
<thead>
<tr>
<th>Case</th>
<th>Heat flux</th>
<th>Particles</th>
<th>Frequency of measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$q_2(t)=0.01 , t , [W/m^2]$</td>
<td>10</td>
<td>1 Hz</td>
</tr>
<tr>
<td>2</td>
<td>$q_2(t)=5 , W/m^2 , for , t&gt;500s$</td>
<td>100</td>
<td>10 Hz</td>
</tr>
<tr>
<td>3</td>
<td>$q_2(t)=0 , W/m^2 , for , t&lt;500s$</td>
<td>10</td>
<td>10 Hz</td>
</tr>
<tr>
<td>4</td>
<td>$q_2(t)=5 , W/m^2 , for , t&gt;500s$</td>
<td>100</td>
<td>10 Hz</td>
</tr>
</tbody>
</table>

RESULTS – linear profile

<table>
<thead>
<tr>
<th>10 Particles</th>
<th>100 Particles</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1 Hz</strong></td>
<td><strong>1 Hz</strong></td>
</tr>
<tr>
<td><img src="image1" alt="Graph 1 Hz 10 particles" /></td>
<td><img src="image2" alt="Graph 1 Hz 100 particles" /></td>
</tr>
<tr>
<td><strong>10 Hz</strong></td>
<td><strong>10 Hz</strong></td>
</tr>
<tr>
<td><img src="image3" alt="Graph 10 Hz 10 particles" /></td>
<td><img src="image4" alt="Graph 10 Hz 100 particles" /></td>
</tr>
</tbody>
</table>

RESULTS – linear profile

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Real</th>
<th>Estimated</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>10 Particles</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1 Hz</td>
</tr>
<tr>
<td>100</td>
<td><img src="image1" alt="Real" /></td>
<td><img src="image2" alt="10 Hz" /></td>
</tr>
<tr>
<td>500</td>
<td><img src="image6" alt="Real" /></td>
<td><img src="image7" alt="10 Hz" /></td>
</tr>
<tr>
<td>1000</td>
<td><img src="image11" alt="Real" /></td>
<td><img src="image12" alt="10 Hz" /></td>
</tr>
</tbody>
</table>

### RESULTS – linear profile

<table>
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<tr>
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</tr>
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<tbody>
<tr>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>1 Hz</td>
</tr>
<tr>
<td>100</td>
<td><img src="image1" alt="Image" /></td>
<td><img src="image2" alt="Image" /></td>
</tr>
<tr>
<td>500</td>
<td><img src="image7" alt="Image" /></td>
<td><img src="image8" alt="Image" /></td>
</tr>
<tr>
<td>1000</td>
<td><img src="image13" alt="Image" /></td>
<td><img src="image14" alt="Image" /></td>
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</table>

RESULTS – step profile

# RESULTS – step profile

<table>
<thead>
<tr>
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<th>Real</th>
<th>Estimated</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>10 Particles</td>
</tr>
<tr>
<td></td>
<td>1 Hz</td>
<td>10 Hz</td>
</tr>
<tr>
<td>100</td>
<td><img src="image1" alt="Real" /></td>
<td><img src="image2" alt="10 Particles 1 Hz" /></td>
</tr>
<tr>
<td>500</td>
<td><img src="image6" alt="Real" /></td>
<td><img src="image7" alt="10 Particles 1 Hz" /></td>
</tr>
<tr>
<td>1000</td>
<td><img src="image11" alt="Real" /></td>
<td><img src="image12" alt="10 Particles 1 Hz" /></td>
</tr>
</tbody>
</table>

### RESULTS – step profile

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<th>Estimated</th>
</tr>
</thead>
<tbody>
<tr>
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<td></td>
<td>10 Particles</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1 Hz</td>
</tr>
<tr>
<td>100</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
</tr>
<tr>
<td>500</td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
</tr>
<tr>
<td>1000</td>
<td><img src="image9.png" alt="Image" /></td>
<td><img src="image10.png" alt="Image" /></td>
</tr>
</tbody>
</table>

CONCLUSIONS

1. The use of Bayesian Filters to a Natural Convection problem resulted in good estimations for an unknown heat flux;
2. As the frequency of the measurements decreases, the results improve;
3. As the number of particles increase, the results improve as well.

PHYSICAL PROBLEM #3

Transient heat conduction in a semi-infinite medium

\begin{equation}
\frac{\partial^2 \theta(X, \tau)}{\partial X^2} = \frac{\partial \theta(X, \tau)}{\partial \tau}
\end{equation}

\begin{equation}
- \frac{\partial \theta(X, \tau)}{\partial X} = Q(\tau)
\end{equation}

\begin{equation}
\frac{\partial \theta(X, \tau)}{\partial X} + Bi \theta(X, \tau) = 0
\end{equation}

\text{Temperature measured at } X=L/5

STATE ESTIMATION PROBLEM

State Evolution Model:
\[ x_k = f_k(x_{k-1}, v_{k-1}) \]

Observation Model:
\[ z_k = h_k(x_k, n_k) \]

In general

Variable to be estimated (state variable): Heat flux \( Q(\tau) \)
Variable to be observed: Temperature \( \theta(L/5, \tau) \)
Parameter to be estimated (CPSE Filter): Biot number

STATE ESTIMATION PROBLEM

State Evolution Model: 

$$Q_k = f_k(Q_{k-1} | v_{k-1})$$

Random walk model for the heat flux $Q(\tau)$

$$Q_k = Q_{k-1} + \sigma_Q W, \text{ were } W = N[0,1], \sigma_Q = [0.025\% Q(\tau)_{\text{max}}, 0.035\% Q(\tau)_{\text{max}}]$$

In the CPSE filter, $\sigma_{Bi} = 1\%$ of Biot

Observation Model: 

$$\theta_k = h_k(Q_k | n_k)$$

Solution of the Direct Problem by the Finite Difference Method, given the state variable $Q(\tau)$ and the measurements errors with $\sigma = 0.45 \, ^\circ\text{C}$ (5% of the maximum temperature)

RESULTS
Simulated temperatures for the squared and triangular variations of heat flux

Observed values with standard deviation $\sigma=5\%$ of the maximum temperature

### RESULTS:

**Squared heat flux**

<table>
<thead>
<tr>
<th>Filter</th>
<th>Particles</th>
<th>CPU time</th>
<th>RMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>SIR</td>
<td>3000</td>
<td>1.53 min.</td>
<td>0.82</td>
</tr>
<tr>
<td>ASIR</td>
<td>2000</td>
<td>1.46 min.</td>
<td>0.60</td>
</tr>
<tr>
<td>SMC Samplers</td>
<td>100</td>
<td>1.29 min.</td>
<td>0.54</td>
</tr>
<tr>
<td>CPSE</td>
<td>3000</td>
<td>4.50 min.</td>
<td>0.60</td>
</tr>
<tr>
<td>SMC w/o likelihoods</td>
<td>100</td>
<td>0.42 min.</td>
<td>0.35</td>
</tr>
</tbody>
</table>

---

## RESULTS:
### Triangular heat flux

<table>
<thead>
<tr>
<th>Filter</th>
<th>Particles</th>
<th>CPU time</th>
<th>RMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>SIR</td>
<td>5000</td>
<td>3.01 min.</td>
<td>0.59</td>
</tr>
<tr>
<td>ASIR</td>
<td>1000</td>
<td>0.64 min.</td>
<td>0.12</td>
</tr>
<tr>
<td>SMC Samplers</td>
<td>200</td>
<td>4.31 min.</td>
<td>0.34</td>
</tr>
<tr>
<td>CPSE</td>
<td>2000</td>
<td>2.23 min.</td>
<td>0.13</td>
</tr>
<tr>
<td>SMC w/o likelihoods</td>
<td>100</td>
<td>0.18 min.</td>
<td>0.25</td>
</tr>
</tbody>
</table>

CONCLUSIONS

1. The use of Bayesian Filters to a Heat Conduction Problem resulted in good estimations for the heat transfer coefficient.
2. The SIR filter presented the worst results among all methods.
3. The ASIR and the CPSE filters presented the best results.
4. The CPSE filter is capable to estimate a parameter in addition to the state variable, being very useful in engineering problems.

Johannes Purkinje (1787–1869) was a prolific Czech anatomist and physiologist. He established the first Department of Physiology in the world in 1839 in Prussia.

GENERAL DESCRIPTION OF THE PROBLEM

- SA nodes fires at 60-100 bpm – primary pacemaker
- AV junction (surrounds AV node) fires at 40-60 bpm
- Purkinje fibers fire at 15-40 bpm
- In case of failure: SA $\rightarrow$ AV $\rightarrow$ Purkinje

- **P wave** $\rightarrow$ Associated with the SA node. Electrical impulse travels through the right and left atrium to the AV node.
- **PR segment** $\rightarrow$ Necessary as a delay to prevent both atria and ventricles to contract at the same time.
- **QRS complex** $\rightarrow$ Associated with the Purkinje fibers. Electrical activity through the ventricles.
- **ST, T, etc** $\rightarrow$ Repolarization to restore the normal state.

GENERAL DESCRIPTION OF THE PROBLEM

• Action potential ➔ Some types of cells may suffer variations in their electric potential and then return to their equilibrium state.
• Ionic channels ➔ Sodium and potassium.
• Variation in the voltage by chemical control.

GENERAL DESCRIPTION OF THE PROBLEM

- Purkinje fibers
  1. Normal (rest) state
  2. Depolarization
  3. Repolarization
  4. Sodium and potassium pump

Hodgkin and Huxley (1952) proposed a model for the action potential in an axon, in terms of an electric circuit with capacitance and ionic currents. Sodium and potassium ions are the most important in the action potential and are distinguished in terms of their own proper currents, in comparison to the other ions. The model involves a non-linear system of four ordinary differential equations, whose coefficients are given in terms of functions of the applied potential. Although Hodgkin-Huxley's model has been originally proposed for the experimental data involving an axon, it has also been used to model the action potential in heart cells, like Purkinje fibers (Noble, 1962). The objective of this work is to estimate the state variables appearing in the Hodgkin-Huxley’s model applied to the Purkinje fibers.
MATHEMATICAL PROBLEM

- Hodgkin and Huxley’s experiments (1952) with axons conductance of some ions across the cell membrane, like sodium and potassium, varied with changes in the axon's potential. Intracellular electric resistance was neglected.

- Imposed electric current across the cell membrane modeled in terms of capacitive and ionic currents, being the sodium and potassium ions recognized as the most important ones in this process.

- Basic difference between axons and Purkinje fibers in the last ones the potassium flow is governed by both a fast and a slow channel dynamics.

- The imposed electric current is null for the case involving Purkinje fibers because these cells are auto-excitable (Noble, 1962).
MATHEMATICAL PROBLEM


\[
C_m \frac{dV_m}{dt} + G_{Na}(V_m - V_{Na}) + G_{K}(V_m - V_K) = 0
\]

Conductances:

\[
G_{Na} = G_{Na}^{\text{max}} m^3 h + G_{Na,l}
\]

\[
G_{K} = 1.2 \exp\left(-\frac{V_m + 90}{50}\right) + 0.015 \exp\left(\frac{V_m + 90}{60}\right) + 1.2 n^4
\]

\(m\) and \(n\) represent the open fraction, or probability of the channels being open (activation), for sodium and potassium, respectively, while \(h\) is the probability of the channel being closed (inactivation) for the sodium ions.
MATHEMATICAL PROBLEM

Channels opening/closing dynamics
(Hodgkin and Huxley, 1952):
\[
\frac{dm}{dt} = \alpha_m (1 - m) + \beta_m m \quad \frac{dh}{dt} = \alpha_h (1 - h) + \beta_h h
\]
\[
\frac{dn}{dt} = \alpha_n (1 - n) + \beta_n n
\]

Parameters for activation and inactivation
(Noble, 1962):
\[
\alpha_m = -0.1\exp\left[\frac{V_m + 48}{15}\right] - 1
\]
\[
\beta_m = \frac{0.12(V_m + 8)}{\exp\left[\frac{V_m + 8}{5}\right] - 1}
\]
\[
\alpha_h = 0.17\exp\left[-\frac{V_m + 90}{20}\right]
\]
\[
\beta_h = \left[\exp\left(-\frac{V_m + 42}{10}\right) + 1\right]^{-1}
\]
\[
\alpha_n = -\frac{10^{-4}(V_m + 50)}{\exp\left(-\frac{V_m + 50}{10}\right)-1}
\]
\[
\beta_n = 0.002\exp\left[-\frac{V_m + 90}{80}\right]
\]
### MATHEMATICAL PROBLEM

Other parameters:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values</th>
<th>Parameter</th>
<th>Values</th>
<th>Parameter</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_m \left( \mu F \text{ cm}^{-2} \right)$</td>
<td>12</td>
<td>$V_{Na} \left( mV \right)$</td>
<td>40</td>
<td>$G_{Na,l} \left( mS \right)$</td>
<td>0.14</td>
</tr>
<tr>
<td>$G_{Na}^{\text{max}} \left( mS \right)$</td>
<td>400</td>
<td>$V_k \left( mV \right)$</td>
<td>-100</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
STATE ESTIMATION PROBLEM

State Evolution Model:
\[ x_k = f_k(x_{k-1}, v_{k-1}) \]

Observation Model:
\[ z_k = h_k(x_k, n_k) \]

\[ x = \{V_m, m, h, n\} \]

\[ m, h, n \text{ need several parameters} \]

\[ x = \{V_m, m, h, n; C_m, G_{Na}^{max}, G_{Na,l}\} \]

Liu and West Algorithm (based on ASIR)

Cell potential \( V_m \)

---

RESULTS – State Variables

RESULTS – Comparison of Methods

RMS errors and computational times for the SIR algorithm

<table>
<thead>
<tr>
<th>$N_p$</th>
<th>CPU Time (s)</th>
<th>$V_m$ (mV)</th>
<th>$m$</th>
<th>$n$</th>
<th>$h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>3.12</td>
<td>2.8126</td>
<td>0.0945</td>
<td>0.0806</td>
<td>0.0289</td>
</tr>
<tr>
<td>50</td>
<td>7.35</td>
<td>1.6984</td>
<td>0.0889</td>
<td>0.0743</td>
<td>0.0240</td>
</tr>
<tr>
<td>100</td>
<td>15.01</td>
<td>1.5899</td>
<td>0.0884</td>
<td>0.0698</td>
<td>0.0231</td>
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<tr>
<td>500</td>
<td>72.07</td>
<td>1.5811</td>
<td>0.0883</td>
<td>0.0669</td>
<td>0.0221</td>
</tr>
<tr>
<td>1000</td>
<td>140.08</td>
<td>1.5778</td>
<td>0.0882</td>
<td>0.0662</td>
<td>0.0221</td>
</tr>
<tr>
<td>2000</td>
<td>247.73</td>
<td>1.5769</td>
<td>0.0882</td>
<td>0.0662</td>
<td>0.0220</td>
</tr>
</tbody>
</table>

RMS errors and computational times for the ASIR algorithm

<table>
<thead>
<tr>
<th>$N_p$</th>
<th>CPU Time (s)</th>
<th>$V_m$ (mV)</th>
<th>$m$</th>
<th>$n$</th>
<th>$h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>15.91</td>
<td>1.4275</td>
<td>0.0902</td>
<td>0.0757</td>
<td>0.0191</td>
</tr>
<tr>
<td>100</td>
<td>48.00</td>
<td>1.4195</td>
<td>0.0901</td>
<td>0.0732</td>
<td>0.0182</td>
</tr>
<tr>
<td>200</td>
<td>111.03</td>
<td>1.4118</td>
<td>0.0900</td>
<td>0.0711</td>
<td>0.0174</td>
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<tr>
<td>300</td>
<td>205.77</td>
<td>1.4069</td>
<td>0.0900</td>
<td>0.0706</td>
<td>0.0173</td>
</tr>
<tr>
<td>400</td>
<td>332.19</td>
<td>1.4043</td>
<td>0.0900</td>
<td>0.0692</td>
<td>0.0170</td>
</tr>
<tr>
<td>500</td>
<td>485.80</td>
<td>1.4021</td>
<td>0.0900</td>
<td>0.0685</td>
<td>0.0170</td>
</tr>
</tbody>
</table>

## RESULTS – Comparison of Methods

### RMS errors and computational times for the ASIR algorithm

<table>
<thead>
<tr>
<th>( N_p )</th>
<th>CPU Time (s)</th>
<th>( V_m ) (mV)</th>
<th>( m )</th>
<th>( n )</th>
<th>( h )</th>
<th>( C_m ) (( \mu F \text{ cm}^{-2} ))</th>
<th>( G_{Na} ) (mS)</th>
<th>( G_{Na,L} ) (mS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>15.91</td>
<td>1.4275</td>
<td>0.0902</td>
<td>0.0757</td>
<td>0.0191</td>
<td>0.0621</td>
<td>5.2964</td>
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<tr>
<td>100</td>
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<td>7.0376</td>
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</tr>
<tr>
<td>200</td>
<td>111.03</td>
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<td>0.0711</td>
<td>0.0174</td>
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<tr>
<td>300</td>
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<td>0.0706</td>
<td>0.0173</td>
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<td>8.5989</td>
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<tr>
<td>400</td>
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### RMS errors and computational times for Liu and West's algorithm

<table>
<thead>
<tr>
<th>( N_p )</th>
<th>CPU Time (s)</th>
<th>( V_m ) (mV)</th>
<th>( m )</th>
<th>( n )</th>
<th>( h )</th>
<th>( C_m ) (( \mu F \text{ cm}^{-2} ))</th>
<th>( G_{Na} ) (mS)</th>
<th>( G_{Na,L} ) (mS)</th>
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<tbody>
<tr>
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<td>0.0135</td>
<td>0.0782</td>
<td>8.9281</td>
<td>0.0009</td>
</tr>
</tbody>
</table>

CONCLUSIONS

1. The use of Bayesian Filters to state estimation of action potential in Purkinje fibers showed very good results;

2. Although the SIR and the ASIR algorithms are capable of accurately estimating the state variables, we notice that the more general algorithm by Liu and West allows the simultaneous estimation of the state variables and model parameters. Furthermore, such quantities can be estimated with better accuracy than those related to the estimation of only the state variables.

ACKNOWLEDGMENTS
Bayesian Particle Filters 
Applied to Heat Transfer 
and Biomedical Problems

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Thank you for your attention!