# Bayesian Estimation of Thermal Conductivity in Polymethyl Methacrylate

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Ongoing work with

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- Valerio Mussi (Politecnico di Milano)

## OUTLINE OF THE TALK

- Origin of the work
- Statement of the problem and aim of the work
- Past related works
- Experiment
- Heat equation
- Results
- Work ahead

# ORIGIN OF THE WORK

- Hiring of Ettore (Ph.D. in Bioengineering) in November 2011
- Start of my cooperation with Ettore
- Previous work with Sara on Bayesian analysis of SDE applied to predator-prey systems
- My involvement in SAMSI programme on *Uncertainty Quantification*, where Bayesian methods were widely presented in association with PDE (inverse problems)
- $\Rightarrow$ Bayesian analysis of parameter(s) in the heat equation
- Mixed team: Ettore (Engineer), Fabrizio (Bayesian statistician), Sara (Applied probabilist) and Valerio (Experimental engineer)

# STATEMENT OF THE PROBLEM

- Thermal processes adopted in many industrial applications, with components heated or cooled to obtain a desired behavior

- Knowledge of thermal properties of a body, especially thermal conductivity, important in many applications (e.g., thermal insulation or thermal exchanger dimensioning)

- Information on thermal properties not always known $\Rightarrow$ needs for estimation
  - polymers: range of thermal conductivity known, but not actual value
  - metals: thermal conductivity tabulated for pure metals but unknown, in general, for alloys

- ISO (International Organization for Standardization) standards propose different methods for measuring the thermal conductivity, which require complex and expensive experimental layouts, while other simpler but accurate methods are not widespread

- ISO standards take into account only marginally uncertainty of measurement and estimation procedure

# AIM OF THE WORK

- Bayesian (and frequentist) estimation procedure coupled with simple experimental layout to estimate thermal conductivity of a homogeneous body and to reproduce the entire temperature profile evolution over time by means of the determination of latent temperature data

- Measurement of temperature evolution over time in a limited number of (internal and surface) points

- Estimation of evolution of temperatures in latent points where no measurement is taken

- Estimation of thermal conductivity (MLE, posterior mean and posterior distribution)

# PAST: PREDATOR-PREY (LOTKA-VOLTERRA)

$$\begin{cases} dx_t = \left[ r x_t G\left(x_t\right) - y_t F\left(x_t, y_t; q\right) \right] dt & x(0) = x_0 \\ dy_t = \left[ c y_t F\left(x_t, y_t; q\right) - u y_t \right] dt & y(0) = y_0 \end{cases}$$

- $x_t$ ($y_t$) normalised biomass of prey (predator)
- $r$ = specific growth rate of the prey
- $c$ = specific production rate of the predator
- $u$ = specific loss rate of predator
- $q$ = efficiency of the predation process
- $G(x)$ = prey growth in absence of predators
  ($G(x) = 1 - x$ to penalize overcrowding)
- $F(x, y; q)$ = **functional response** of predator to prey abundance ($F(x, y; q) = qx$)

# PAST: PREDATOR-PREY (LOTKA-VOLTERRA)

- Functional response $q$ subject to noise and dependent on time
  $\Rightarrow q_t = q_0 + \sigma \xi_t$

- Introduction of two Wiener processes to model demographic and environmental stochasticities
  (the first acting on $x_t y_t$ and the second on $x_t$ and $y_t$ separately)

- Introduction of an adhoc, continuously differentiable and Lipschitz function to keep $x_t$ and $y_t$ in $[0, 1]$

$$\begin{cases} dx_t &= [r x_t(1 - x_t) - q_0 x_t y_t]\chi(x_t)dt - \sigma x_t y_t \chi(x_t) dw_t^{(1)} + \varepsilon x_t \chi(x_t) dw_t^{(2)} \\ dy_t &= [c q_0 x_t y_t - u y_t]\chi(y_t)dt + c\sigma x_t y_t \chi(y_t) dw_t^{(1)} + \eta y_t \chi(y_t) dw_t^{(2)} \end{cases}$$

# EULER-MARUYAMA APPROXIMATION

- SDE: $dX_t = \mu(t, X_t)dt + \beta(t, X_t)dW_t$
- In general, SDE solved by numerical method (see Kloeden and Platen, 1999)
  - Interest in solving the SDE in $[0, T]$
  - Consider $0 = t_0 < t_1 < \ldots < t_n = T$
    (e.g. equispaced: $t_i - t_{i-1} = T/n, i = 1, \ldots, n$)
  - $\Rightarrow$ Euler-Maruyama approximation given by the Markov chain $\{X_t\}$, with

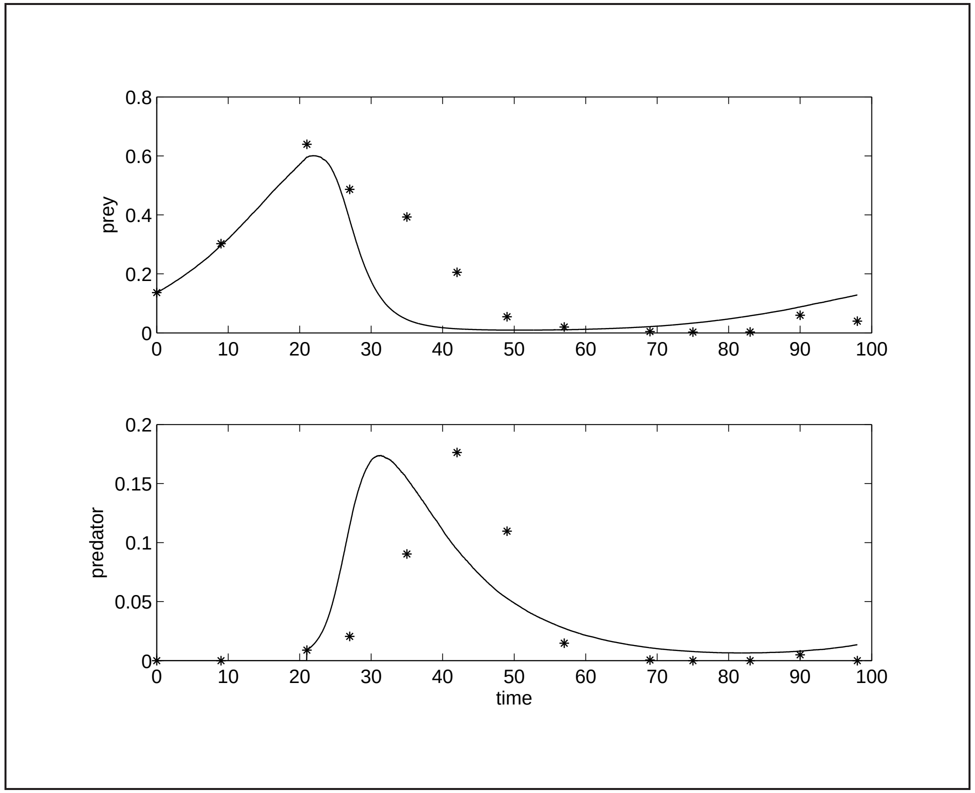
    $$X_{t_i} = X_{t_{i-1}} + \mu\left(t_{i-1}, X_{t_{i-1}}\right)\Delta_i + \beta\left(t_{i-1}, X_{t_i}\right)\left(W_{t_{i+1}} - W_{t_i}\right),$$

    for $i = 1, \ldots, n$ and $\Delta_i = t_i - t_{i-1}$
  - $\Delta W_i = W_{t_i} - W_{t_{i-1}}$ independent $\mathcal{N}(0, \Delta_i)$

# PAST: PREDATOR-PREY (LOTKA-VOLTERRA)

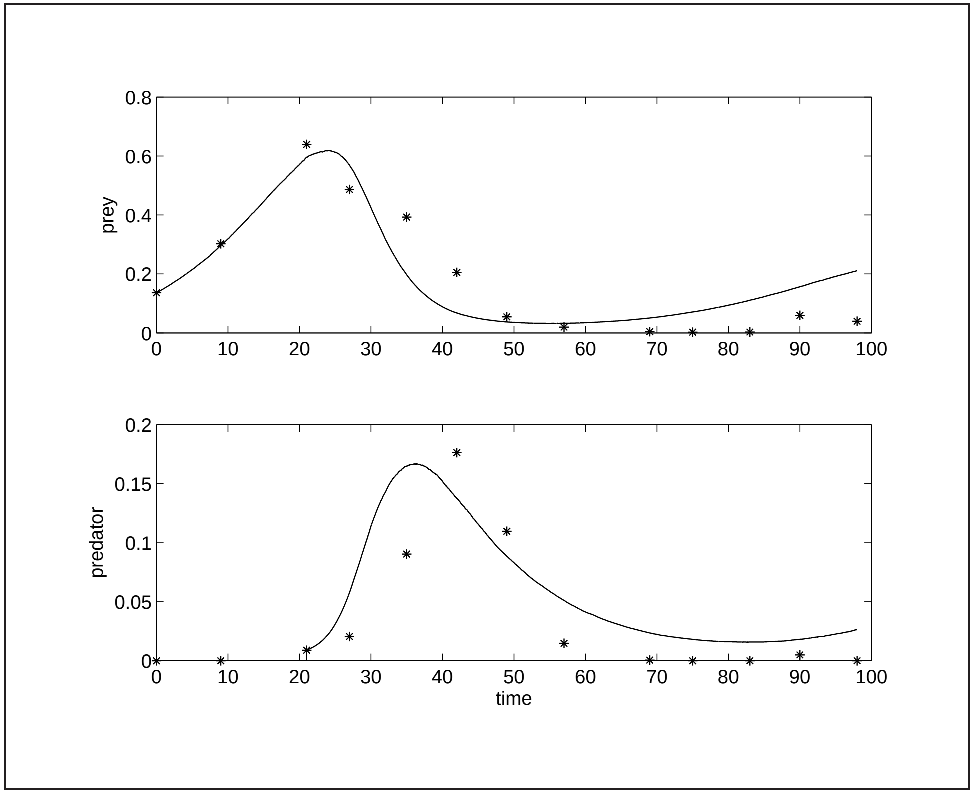
- Euler-Maruyama approximation good for *small* intervals; o.w. there are biases
- Introduction of latent data between actual ones
  - improvement in the use of Euler-Maruyama approximation
  - errors due to use of unobserved data
  - $\Rightarrow$ need to find a proper balance between sources of error and an *optimal* number of latent data
- Latent data treated as *parameters* in Bayesian estimation through MCMC
  - generation of latent data (all together, one at the time, random number, etc.)
  - optimal choice of number of latent data (rule of thumb: visual inspection, sensitivity, spread of estimates, etc.)

# PREDATOR-PREY DYNAMICS (MLE)




Continuous line: mean of 1000 trajectories of prey and predator for $q_0 = 2.6218$. Asterisks: field observations

# PREDATOR-PREY DYNAMICS (BAYES - LATENT DATA)



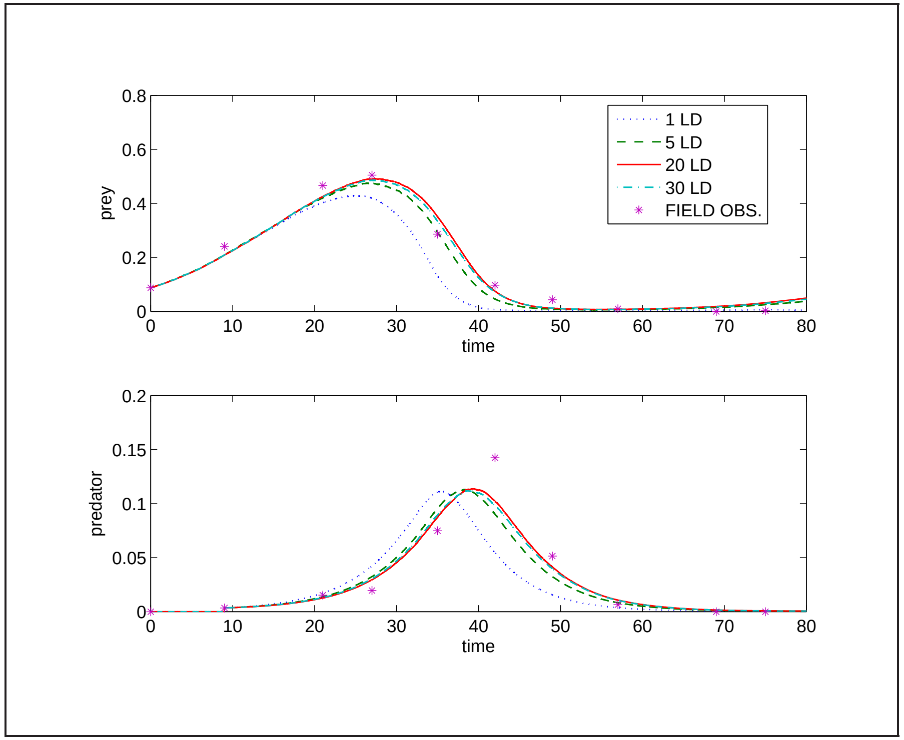

MCMC estimate with 7 latent data between two observations. Continuous line: mean of 1000 trajectories of prey and predator for $q_0 = 1.8008$. Asterisks: field observations

# PAST: PREDATOR-PREY (IVLEV MODEL)

$$\begin{cases} dx_t = \left[rx_t(1-x_t) - by_t\left(1-e^{-q_0 x_t}\right)\right]dt + b\sigma y_t e^{-x_t} dw_t^{(1)} + \varepsilon x_t dw_t^{(2)} \\ dy_t = y_t\left[b'\left(1-e^{-q_0 x_t}\right) - u\right]dt - b'\sigma y_t e^{-x_t} dw_t^{(1)} + \eta y_t dw_t^{(2)} \end{cases}$$

- Initial conditions: $(x(0), y(0)) = (x_0, y_0)$
- $x_t$ and $y_t$: biomass of prey and predator at time $t$ per habitat unit (plant) normalised w.r.t. prey carrying capacity per habitat unit
- $r$: maximum specific growth rate of the prey
- $b$: maximum specific predation rate
- $b'$: maximum specific predator production rate
- $u$: specific predator loss rate due to natural mortality
- $q_0$: measure of the efficiency of the predation process

# IVLEV MODEL: FORECASTS FOR DATA IN A FIELD




Prey and predator biomass as function of time, for different values of latent data. Trajectories as mean over 100 simulations and 50 values of $q_0$, $\sigma$, $\varepsilon$ and $\eta$ from posterior distributions. Asterisks denote field data

# ISO NORMATIVE

- Normative ISO 22007 (Plastics – Determination of thermal conductivity and thermal diffusivity) as reference for estimation of thermal conductivity in polymers

- ISO 22007 describes some methods for estimation of thermal conductivity and thermal diffusivity, including results of tests conducted in parallel in different laboratories

- Methods divided into
  - *steady-state* methods, where a specimen of simple geometry, in contact with a heat source and temperature sensors, is maintained at a given temperature to obtain the coefficients based on the supplied heat
  - *temperature-transient* methods, where temperature, recorded by sensors, changes over time and coefficients are determined considering specimen geometry and boundary conditions

# ISO NORMATIVE

- Transient methods proposed for estimation of thermal conductivity
  - *hot-wire*, where a wire heater is placed in a specimen or between two specimens. Temperature measured over time, once the heater is turned on, either by the wire itself or by a thermocouple placed close to the wire
  - *line-source*, where a line source is located at the specimen center, with both kept at a constant initial temperature. During measurement, a known amount of heat produced by the line source results in a heat wave radially propagating into the specimen
  - *plane-heat-source*, using thin, plane, electrically insulated resistive element as both heat source and temperature sensor, bringing it into thermal contact with two halves of the specimen. Thermal conductivity measured from resistance increase over time, when supplying constant electrical power to the sensor
- Proposed approach as a temperature-transient method, differing from normative
  - temperature measured in more than one point, and not just a single point close to the heat source
  - statistical approach for estimating thermal conductivity and its uncertainty

# EXPERIMENT

- Identification, search and purchase of material
- Search of a laboratory with interest in the experiment, proper oven and instruments, and willing to do for free
- Planning of the experiment (insulation, thermocouples, experimental conditions like initial conditions, heating and cooling, repeated trials)
- Thermocouples calibrated at another laboratory (free, for friendship)
- Actual experiment in laboratory with data acquisition from repeated trials
- Check of data for quality and consistency

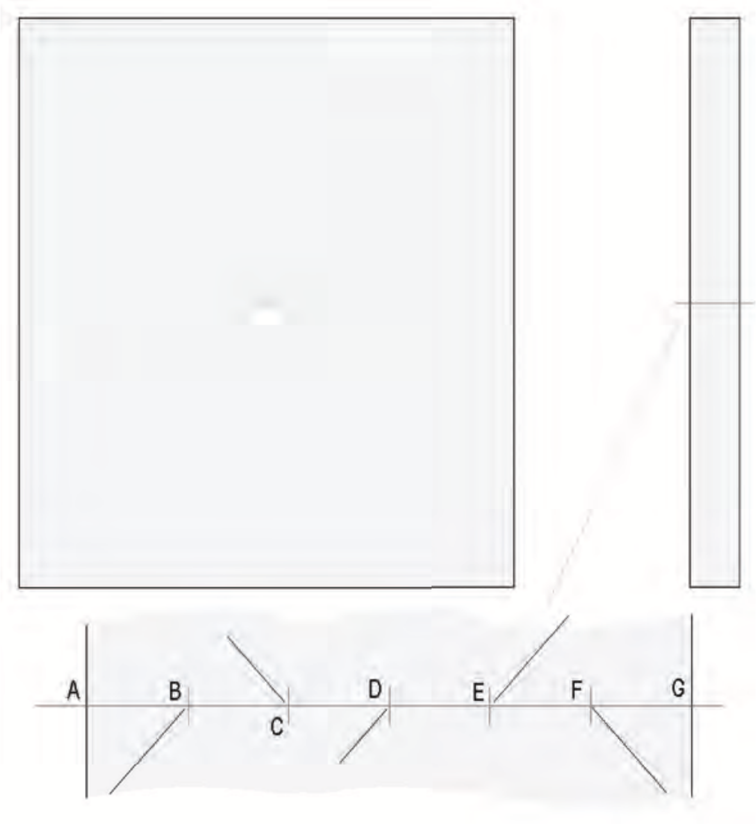
# EXPERIMENT

- Bayesian approach suitable for estimation of thermal conductivity of polymers
  - prior knowledge given by range of variability of the thermal conductivity assigned to each polymer family
  - specific value within the range usually unknown and dependent on other variables such as molecular weight, crystal structure and temperature values at which test is performed
- Choice of polymethyl methacrylate (PMMA) (known also as plexiglas)
  - family of polymers considered in ISO standards
  - used in many applications, from low cost objects, furniture and building to more complex applications like bone cement used for the insertion of prostheses
- Plate of PMMA with square faces (side of 20 cm) and thickness of 15 cm
- Homogeneous and isotropic material to apply heat equation
- Specimen externally heated and cooled in forced convection so no internal thermal power generation is present (affecting term in heat equation)

# EXPERIMENT

- Seven thermocouples installed in the center of the square section and lateral rectangular faces covered with thermal insulator to guarantee unidirectionality of heat flow and avoid border effects
- Two thermocouples placed on surface of square faces and five internally
- Thermocouples placed on a line at 2.5 cm one from the other
- Internal thermocouples positioned in the specimen by piercing the plate and refilling with new polymer (the polymerization reaction took place in the holes in order to restore the material continuity)
- Diameter of holes kept as small as possible and re-polymerization reaction carefully conducted to avoid alterations due to possible discontinuity of the material
- Superficial thermocouples positioned to obtain initial surface conditions

# EXPERIMENT




Positioning of thermocouples A, B, C, D, E, F e G and holes for positioning of internal thermocouples

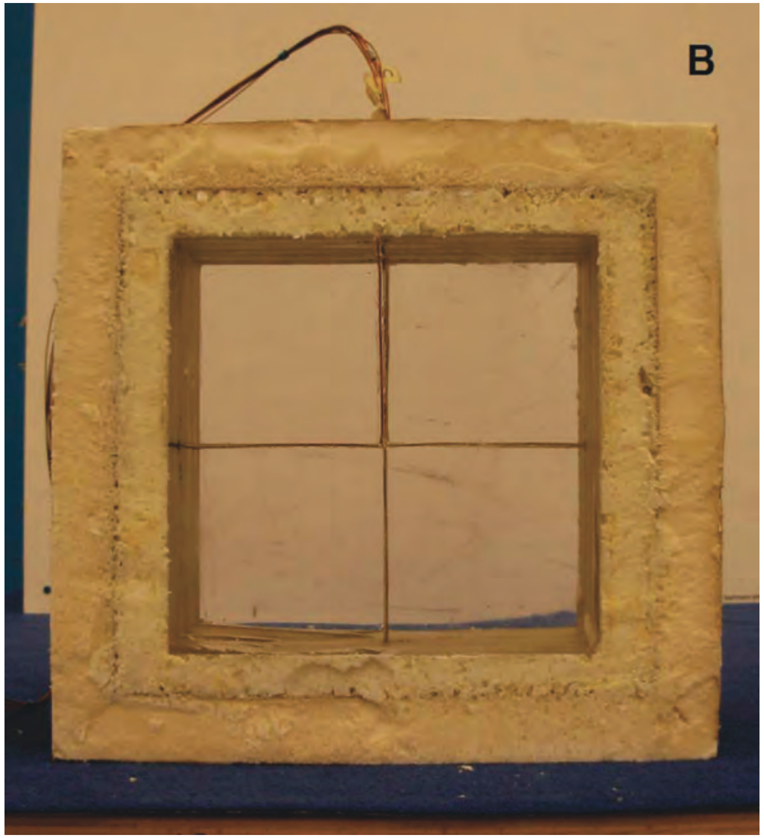
# EXPERIMENT

PMMA being drilled to get holes for thermocouples

# EXPERIMENT

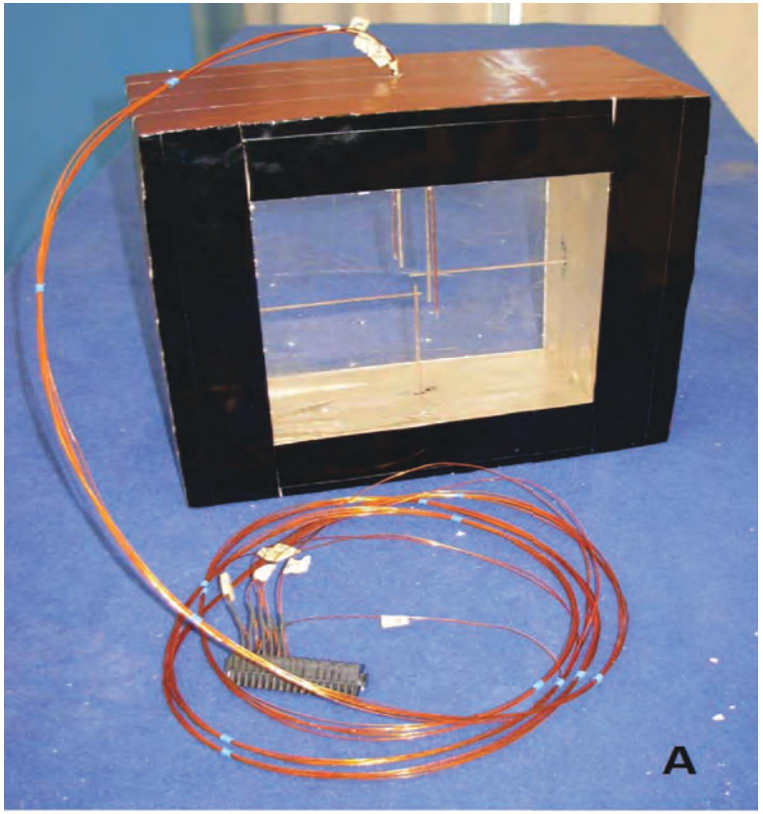
PMMA after drilling with holes for thermocouples

# EXPERIMENT




PMMA plate with with thermocouples in the center

# EXPERIMENT

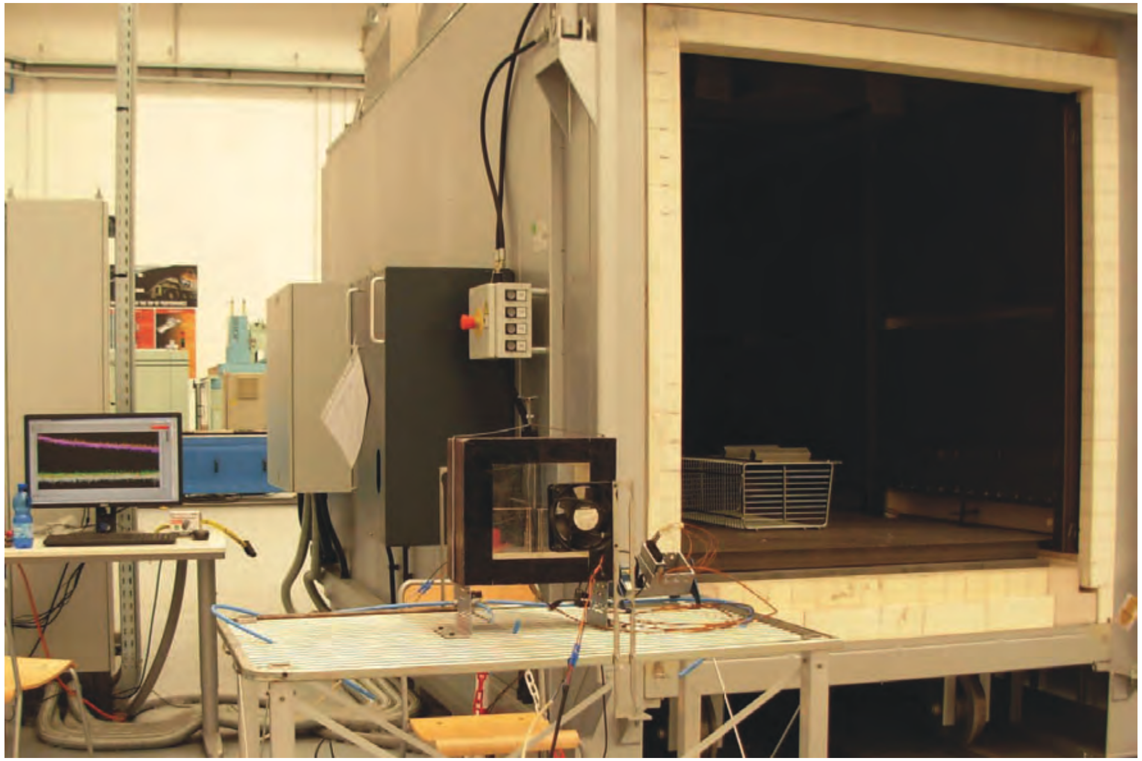



PMMA plate equipped with thermocouples, with cables ready for interface with conditioning circuit and lateral thermal insulator

# EXPERIMENT

- Cycle of heating and cooling given to the specimen
  - specimen starts at homogeneous ambient temperature of about 25$^o$C, heated in oven in forced ventilation until it reaches homogeneous temperature of about 88-90$^o$C
  - specimen taken out from oven and cooled until it reaches a quite homogeneous ambient temperature. Cooling process carried out in forced convection, placing two fans in front of the square faces, and maintaining the laboratory temperature as constant as possible
- Forced convection adopted for two main reasons
  - finer control of temperature values along with the process, with more regular and homogeneous temperature profiles at the specimen surfaces
  - associated with higher convection coefficients, resulting into more rapid heat exchanges between specimen and air and, consequently, lower times to reach the final temperature of the heating or cooling process
- Minimum and maximum temperatures chosen to get quite constant thermal conductivity (ISO 22007), unlike for lower or higher temperatures

# EXPERIMENTAL LAYOUT



PMMA with one fan (other behind PMMA), with oven inlet on the right and PC for data acquisition on the left. PMMA with handling tool, to insert and extract from oven without direct contact with operator

# HEAT EQUATION

Temperature evolution in a body described by

$$\rho c \frac{\partial T(x,y,z,t)}{\partial t} - \lambda \nabla^2 T(x,y,z,t) = \dot{q}(x,y,z,t)$$

- $t$: time, expressed in $[s]$
- $x$, $y$ and $z$: spatial coordinates, expressed in $[m]$
- $T(x,y,z,t)$: temperature, expressed in $[K]$
- $\dot{q}(x,y,z,t)$: internal thermal power generation (i.e. derivative of generated heat w.r.t. time), in $[\frac{W}{m^3}]$
- $\rho$: density of the material, expressed in $[\frac{kg}{m^3}]$
- $c$: specific heat of the material (amount of heat required to change its temperature by a given amount), expressed in $[\frac{J}{kgK}]$
- $\lambda$: **thermal conductivity** of the material, expressed in $[\frac{W}{mK}]$

# HEAT EQUATION

$$\rho c \frac{\partial T\left(x,y,z,t\right)}{\partial t} - \lambda \nabla^2 T\left(x,y,z,t\right) = \dot{q}\left(x,y,z,t\right)$$

The formulation refers to a homogeneous material

$\Rightarrow$ physical properties (i.e., $\rho$, $c$ and $\lambda$)

- uniform in space
- constant over time
- constant over variation of other quantities (e.g., the temperature)

# HEAT EQUATION

Unidirectional heat flow

$$\rho c \frac{\partial T(x,t)}{\partial t} - \lambda \frac{\partial^2 T(x,t)}{\partial x^2} = \dot{q}(x,t)$$

Plate with thickness $L$

- Coordinate $x$ varies from $x = 0$ to $x = L$
- Time $t$ evolves from $t = 0$ until $t = t_f$

Two Dirichlet conditions and one initial condition:

$$\begin{cases} T(0,t) = g_a(t) & t \in [0, t_f] \\ T(L,t) = g_b(t) & t \in [0, t_f] \\ T(x,0) = T_0(x) & x \in [0, L] \end{cases}$$

# HEAT EQUATION - INVERSE PROBLEM

- Compute the heat flux $q(x, y, z, t)$ on part of the boundary given appropriate boundary conditions on the remaining boundary and temperature measurements at some points within the domain

- $q(\cdot)$ approximated by basis expansion and parameters estimated with
  - deterministic procedures (e.g. least squares)
  - stochastic methods (e.g. Bayesian with priors on parameters)

# DISCRETIZATION AND STOCHASTICITY

Statistical estimation $\Rightarrow$ tractable likelihood

- spatial discretization for coordinate $x$
- introduction of stochastic coefficients
- further discretization in time $t$
- Euler-Maruyama approach

# SPATIAL DISCRETIZATION

- $(N+2)$ equispaced points $\{x_0, \ldots, x_{N+1}\}$ in $[0, L]$
  - $x_i = ih, i = 0, \ldots, N+1$
  - $h = \frac{L}{N+1}$
  - Choice of $h$ discussed later
- Corresponding temperature values: $T_i(t) = T(x_i, t), i = 0, \ldots, N+1$

Finite differences for second derivative of temperature w.r.t. $x$

$$\frac{\partial^2 T(x,t)}{\partial x^2} = \frac{\frac{T_{i+1}(t) - T_i(t)}{h} - \frac{T_i(t) - T_{i-1}(t)}{h}}{h} = \frac{T_{i+1}(t) - 2T_i(t) + T_{i-1}(t)}{h^2}$$

# SPATIAL DISCRETIZATION

Heat equation split into system of $N$ equations, one for each $T_i(t)$, $i = 1, \ldots, N$

$$\rho c \frac{dT_i(t)}{dt} - \lambda \frac{T_{i+1}(t) - 2T_i(t) + T_{i-1}(t)}{h^2} = \dot{q}(x_i, t)$$

The $N$ differential equations rewritten in a vectorial form:

$$\frac{d\mathbf{T}(t)}{dt} = \lambda \mathbf{L}(\mathbf{T}(t)) + \dot{\mathbf{q}}(t)$$

# SPATIAL DISCRETIZATION

$$\frac{d\mathbf{T}(t)}{dt} = \lambda \mathbf{L}(\mathbf{T}(t)) + \dot{\mathbf{q}}(t)$$

$$\mathbf{T}(t) = [T_1(t) \cdots T_i(t) \cdots T_N(t)]^T \qquad \mathbf{L}(\mathbf{T}(t)) = \mathbf{A}\mathbf{T}(t) + \mathbf{b}(t)$$

$$\mathbf{A} = -\frac{1}{\rho c h^2} \begin{bmatrix} 2 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ \vdots & & & & & \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & \cdots & 0 & -1 & 2 \end{bmatrix} \qquad \mathbf{b}(t) = \frac{1}{\rho c h^2} \begin{bmatrix} g_a(t) \\ 0 \\ \vdots \\ 0 \\ g_b(t) \end{bmatrix}$$

$$\dot{\mathbf{q}}(t) = \frac{1}{\rho c} [\dot{q}(x_1, t) \cdots \dot{q}(x_i, t) \cdots \dot{q}(x_N, t)]^T$$

Temperatures $T_0(t)$ and $T_{N+1}(t)$ not described by a differential equation, but associated to Dirichlet conditions

$$\begin{cases} T_0(t) = g_a(t) \\ T_{N+1}(t) = g_b(t) \end{cases}$$

# STOCHASTIC COEFFICIENTS

Thermal conductivity $\lambda$ subject to small variation over time and space

- $\lambda = \lambda_0 + \eta\xi_{it}$

- $\lambda_0$ *true* value to be estimated

- Independent Gaussian white noises $\xi_{it}$, function of both space $i$ and time $t$

- positive $\eta$

# STOCHASTIC COEFFICIENTS

$$\frac{d\mathbf{T}(t)}{dt} = \lambda_0 \mathbf{L}(\mathbf{T}(t)) + \dot{\mathbf{q}}(t) + \eta \,\mathbf{diag}_{\mathbf{L}(\mathbf{T}(t))} \mathbf{\Xi}_1$$

$$\mathbf{\Xi}_1 = \begin{bmatrix} \xi_{1t} \\ \vdots \\ \xi_{it} \\ \vdots \\ \xi_{Nt} \end{bmatrix} \qquad \mathbf{diag}_{\mathbf{L}(\mathbf{T}(t))} = \begin{bmatrix} L_1(\mathbf{T}(t)) & 0 & 0 \\ \vdots & & \\ 0 & L_i(\mathbf{T}(t)) & 0 \\ \vdots & & \\ 0 & 0 & L_N(\mathbf{T}(t)) \end{bmatrix}$$

Multiplying by $dt \Rightarrow \xi_{it} dt$ Wiener process, denoted $d\omega_{it}^{(1)}$

$$d\mathbf{T}(t) = [\lambda_0 \mathbf{L}(\mathbf{T}(t)) + \dot{\mathbf{q}}(t)]\, dt + \eta \,\mathbf{diag}_{\mathbf{L}(\mathbf{T}(t))} \mathbf{dW}_1$$

$$\mathbf{dW_1} = \left[ d\omega_{1t}^{(1)} \cdots d\omega_{it}^{(1)} \cdots d\omega_{Nt}^{(1)} \right]^T$$

# STOCHASTIC COEFFICIENTS

Measurement errors in recording temperature

- introduction of second Wiener process $\varepsilon T_i(t)\, d\omega_{it}^{(2)}$
- error assumed additive and proportional to $T_i(t)$
- errors are assumed independent
- no measurement errors related to surface points in $x = 0$ and $x = L$ because of no differential equation for corresponding points $i = 0$ and $i = N + 1$

$$d\mathbf{T}(t) = [\lambda_0 \mathbf{L}(\mathbf{T}(t)) + \dot{\mathbf{q}}(t)]\, dt + \eta\, \mathbf{diag}_{\mathbf{L}(\mathbf{T}(t))} \mathbf{dW}_1 + \varepsilon\, \mathbf{diag}_{\mathbf{T}(t)} \mathbf{dW}_2$$

$$\mathbf{dW_2} = \begin{bmatrix} d\omega_{1t}^{(2)} \\ \vdots \\ d\omega_{it}^{(2)} \\ \vdots \\ d\omega_{Nt}^{(2)} \end{bmatrix} \qquad \mathbf{diag}_{\mathbf{T}(t)} = \begin{bmatrix} T_1(t) & 0 & 0 \\ \vdots & & \\ 0 & T_i(t) & 0 \\ \vdots & & \\ 0 & 0 & T_N(t) \end{bmatrix}$$

# TEMPORAL DISCRETIZATION

- Time $t$ considered at discrete values, $j$, separated by $\mathbf{\Delta}_j$
- Temperature at time $j = 0$ given by initial condition $T_0(x)$, while the temperature evolves for $j > 0$
- Temperature $T_i(t)$ discretized into values $T_{i,j}$ and, consequently, vector $\mathbf{T}(t)$ discretized into $\mathbf{T}_j$

Finite-difference equation:

$$\mathbf{T}_j = \mathbf{T}_{j-1} + \left[\lambda_0 \mathbf{L}(\mathbf{T}_{j-1}) + \dot{\mathbf{q}}_{j-1}\right] \mathbf{\Delta}_j + \eta \, \mathbf{diag}_{\mathbf{L}(\mathbf{T}_{j-1})} \mathbf{\Delta W}_1 + \varepsilon \, \mathbf{diag}_{\mathbf{T}_{j-1}} \mathbf{\Delta W}_2$$

- $\mathbf{L}(\mathbf{T}_{j-1}) = \mathbf{A}\mathbf{T}_{j-1} + \mathbf{b}_{j-1}$
- coherent modifications for $\mathbf{diag}_{\mathbf{L}(\mathbf{T}_{j-1})}$ and $\mathbf{diag}_{\mathbf{T}_{j-1}}$
- $\mathbf{b}_{j-1}$ obtained considering the corresponding time instant from $g_a(t)$ and $g_b(t)$

# TEMPORAL DISCRETIZATION

- Introduction of a finite difference scheme could cause stability problems when the errors made at one step of the calculation would increase in the next steps

- Von Neumann stability criterion used to check stability of finite difference schemes applied to linear partial differential equations

- For one-dimensional heat equation Von Neumann stability criterion imposes

$$0 \leq \frac{\lambda}{\rho c} \frac{\Delta_j}{h^2} \leq \frac{1}{2}$$

- Condition fulfilled in our case
  - temporal discretization $\Delta_j$ highly dense with respect to spatial discretization (continuous analogical signal acquired, then sampled with a high frequency)
  - large value of $h$ used because of few points acquired in the specimen

# LIKELIHOOD FUNCTION

- Likelihood $f\left(\widehat{\mathbf{T}}|\lambda_0\right) = \prod_{j=1}^{m} f\left(\mathbf{T}_j|\mathbf{T}_{j-1},\lambda_0\right)$ for $\widehat{\mathbf{T}}$, set of observations $\mathbf{T}_j$

- Finite-difference equation

$$\mathbf{T}_j = \mathbf{T}_{j-1} + \left[\lambda_0 \mathbf{L}\left(\mathbf{T}_{j-1}\right) + \dot{\mathbf{q}}_{j-1}\right]\Delta_j + \eta \mathbf{diag}_{\mathbf{L}(\mathbf{T}_{j-1})}\boldsymbol{\Delta}\mathbf{W}_1 + \varepsilon \mathbf{diag}_{\mathbf{T}_{j-1}}\boldsymbol{\Delta}\mathbf{W}_2$$

$\Rightarrow \mathbf{T}_j|\mathbf{T}_{j-1},\lambda_0 \sim \mathcal{MVN}\left(\mu_j\left(\mathbf{T}_{j-1}\lambda_0\right); \boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)\right)$ with

$$\mu_j\left(\mathbf{T}_{j-1},\lambda_0\right) = \mathbf{T}_{j-1} + \left[\lambda_0 \mathbf{L}\left(\mathbf{T}_{j-1}\right) + \dot{\mathbf{q}}_{j-1}\right]\Delta_j$$

$$\begin{aligned}\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right) &= \left[\eta^2 \mathbf{diag}_{\mathbf{L}(\mathbf{T}_{j-1})}\mathbf{diag}^T_{\mathbf{L}(\mathbf{T}_{j-1})} + \varepsilon^2 \mathbf{diag}_{\mathbf{T}_{j-1}}\mathbf{diag}^T_{\mathbf{T}_{j-1}}\right]\Delta_j \\ &= \left[\eta^2 \mathbf{diag}^2_{\mathbf{L}(\mathbf{T}_{j-1})} + \varepsilon^2 \mathbf{diag}^2_{\mathbf{T}_{j-1}}\right]\Delta_j\end{aligned}$$

- 

$$\begin{aligned}f\left(\mathbf{T}_j|\mathbf{T}_{j-1},\lambda_0\right) &= (2\pi)^{-\frac{N}{2}}\left|\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)\right|^{-\frac{1}{2}} \\ &= \exp\left\{-\frac{1}{2}\left[\mathbf{T}_j - \mu_j\left(\mathbf{T}_{j-1},\lambda_0\right)\right]^T \boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)^{-1}\left[\mathbf{T}_j - \mu_j\left(\mathbf{T}_{j-1},\lambda_0\right)\right]\right\}\end{aligned}$$

- Inverse of $\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)$ easily computed since diagonal matrix

# LIKELIHOOD FUNCTION

$$f\left(\widehat{\mathbf{T}}|\lambda_0\right) = \prod_{j=1}^{m} f\left(\mathbf{T}_j|\mathbf{T}_{j-1},\lambda_0\right) = \prod_{j=1}^{m} (2\pi)^{-\frac{N}{2}} \left|\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)\right|^{-\frac{1}{2}}$$
$$\exp\left\{-\frac{1}{2}\sum_{j=1}^{m}\left(\left[\mathbf{T}_j-\mu_j\left(\mathbf{T}_{j-1},\lambda_0\right)\right]^T \boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)^{-1}\left[\mathbf{T}_j-\mu_j\left(\mathbf{T}_{j-1},\lambda_0\right)\right]\right)\right\}$$

Summation in exponential term of likelihood written as function of $\lambda_0$: $\dfrac{\left(\lambda_0-\lambda_0^l\right)^2}{\sigma_l^2}$ with

$$\lambda_0^l = \frac{\sum_{j=1}^{m}\Delta_j\left[\begin{array}{c}\left(\mathbf{T}_j-\mathbf{T}_{j-1}-\dot{\mathbf{q}}_{j-1}\boldsymbol{\Delta}_j\right)^T\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)^{-1}\mathbf{L}\left(\mathbf{T}_{j-1}\right)\\ +\mathbf{L}\left(\mathbf{T}_{j-1}\right)^T\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)^{-1}\left(\mathbf{T}_j-\mathbf{T}_{j-1}-\dot{\mathbf{q}}_{j-1}\boldsymbol{\Delta}_j\right)\end{array}\right]}{2\sum_{j=1}^{m}\boldsymbol{\Delta}_j^2\left[\mathbf{L}\left(\mathbf{T}_{j-1}\right)^T\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)^{-1}\mathbf{L}\left(\mathbf{T}_{j-1}\right)\right]}$$

$$\sigma_l^2 = \left\{\sum_{j=1}^{m}\boldsymbol{\Delta}_j^2\left[\mathbf{L}\left(\mathbf{T}_{j-1}\right)^T\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)^{-1}\mathbf{L}\left(\mathbf{T}_{j-1}\right)\right]\right\}^{-1}$$

# MLE ESTIMATION

Loglikelihood

$$\begin{aligned}\mathcal{L}\left(\lambda_0, \widehat{\mathbf{T}}\right) &= \log\left[f\left(\widehat{\mathbf{T}}|\lambda_0\right)\right] \\ &= \log\left\{\prod_{j=1}^{m}(2\pi)^{-\frac{N}{2}}\left|\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)\right|^{-\frac{1}{2}}\right\} - \frac{1}{2}\frac{\left(\lambda_0-\lambda_0^l\right)^2}{\sigma_l^2}\end{aligned}$$

$$\begin{aligned}\Rightarrow \text{MLE } \widehat{\lambda} &= \lambda_0^l \\ &= \frac{\sum_{j=1}^{m}\Delta_j\left[\begin{array}{c}\left(\mathbf{T}_j-\mathbf{T}_{j-1}-\dot{\mathbf{q}}_{j-1}\boldsymbol{\Delta}_j\right)^T\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)^{-1}\mathbf{L}\left(\mathbf{T}_{j-1}\right)\\+\mathbf{L}\left(\mathbf{T}_{j-1}\right)^T\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)^{-1}\left(\mathbf{T}_j-\mathbf{T}_{j-1}-\dot{\mathbf{q}}_{j-1}\boldsymbol{\Delta}_j\right)\end{array}\right]}{2\sum_{j=1}^{m}\Delta_j^2\left[\mathbf{L}\left(\mathbf{T}_{j-1}\right)^T\boldsymbol{\Sigma}_j\left(\mathbf{T}_{j-1}\right)^{-1}\mathbf{L}\left(\mathbf{T}_{j-1}\right)\right]}\end{aligned}$$

# BAYESIAN ESTIMATION: PRIOR CHOICE

Many choices, dictated by mathematical convenience or physical properties

- Gaussian prior $\Rightarrow$ Gaussian posterior

  $$\lambda_0 \sim N\left(\lambda_0^p, \sigma_p^2\right) \Rightarrow \lambda_0|\widehat{\mathbf{T}} \sim N\left(\frac{\lambda_0^p \sigma_l^2 + \lambda_0^l \sigma_p^2}{\sigma_l^2 + \sigma_p^2}, \frac{\sigma_l^2 \sigma_p^2}{\sigma_l^2 + \sigma_p^2}\right)$$

- Improper prior $\Rightarrow$ Gaussian posterior

  $$\pi(\lambda_0) \propto c \Rightarrow \lambda_0|\widehat{\mathbf{T}} \sim N\left(\lambda_0^l, \sigma_l^2\right)$$

- Improper prior, positive values $\Rightarrow$ truncated Gaussian posterior

  $$\pi(\lambda_0) \propto c I_{(0,\infty)}(\lambda_0) \Rightarrow \pi(\lambda_0 \widehat{\mathbf{T}}) = \frac{e^{-\frac{1}{2\sigma_l^2}(\lambda_0 - \lambda_0^l)^2}}{\sqrt{2\pi\sigma_l^2}\left[1 - \Phi\left(-\frac{\lambda_0^l}{\sigma_l}\right)\right]} I_{(0,\infty)}(\lambda_0)$$

# BAYESIAN ESTIMATION: PRIOR CHOICE

- Uniform distribution on interval $\Rightarrow$ truncated Gaussian posterior

- Truncated Gaussian prior $\Rightarrow$ truncated Gaussian posterior

prior $\pi(\lambda_0) = \dfrac{e^{-\frac{1}{2\tilde{\sigma}_p^2}\left(\lambda_0 - \tilde{\lambda}_0^p\right)^2}}{\sqrt{2\pi\tilde{\sigma}_p^2}\left[1 - \Phi\left(-\frac{\tilde{\lambda}_0^p}{\tilde{\sigma}_p}\right)\right]} I_{(0,\infty)}(\lambda_0)$

posterior $\pi(\lambda_0|\widehat{\mathbf{T}}) = \dfrac{e^{-\frac{1}{2\tilde{\sigma}_P^2}\left(\lambda_0 - \tilde{\lambda}_0^P\right)^2}}{\sqrt{2\pi\tilde{\sigma}_P^2}\left[1 - \Phi\left(-\frac{\tilde{\lambda}_0^P}{\tilde{\sigma}_P}\right)\right]} I_{(0,\infty)}(\lambda_0)$, with

$\tilde{\lambda}_0^P = \dfrac{\tilde{\lambda}_0^p \sigma_l^2 + \lambda_0^l \tilde{\sigma}_p^2}{\sigma_l^2 + \tilde{\sigma}_p^2}$ and $\tilde{\sigma}_p^2 = \dfrac{\sigma_l^2 \tilde{\sigma}_p^2}{\sigma_l^2 + \tilde{\sigma}_p^2}$

- Gamma prior $\Rightarrow$ posterior with MCMC

# (BAD) GENERATION OF LATENT TEMPERATURES

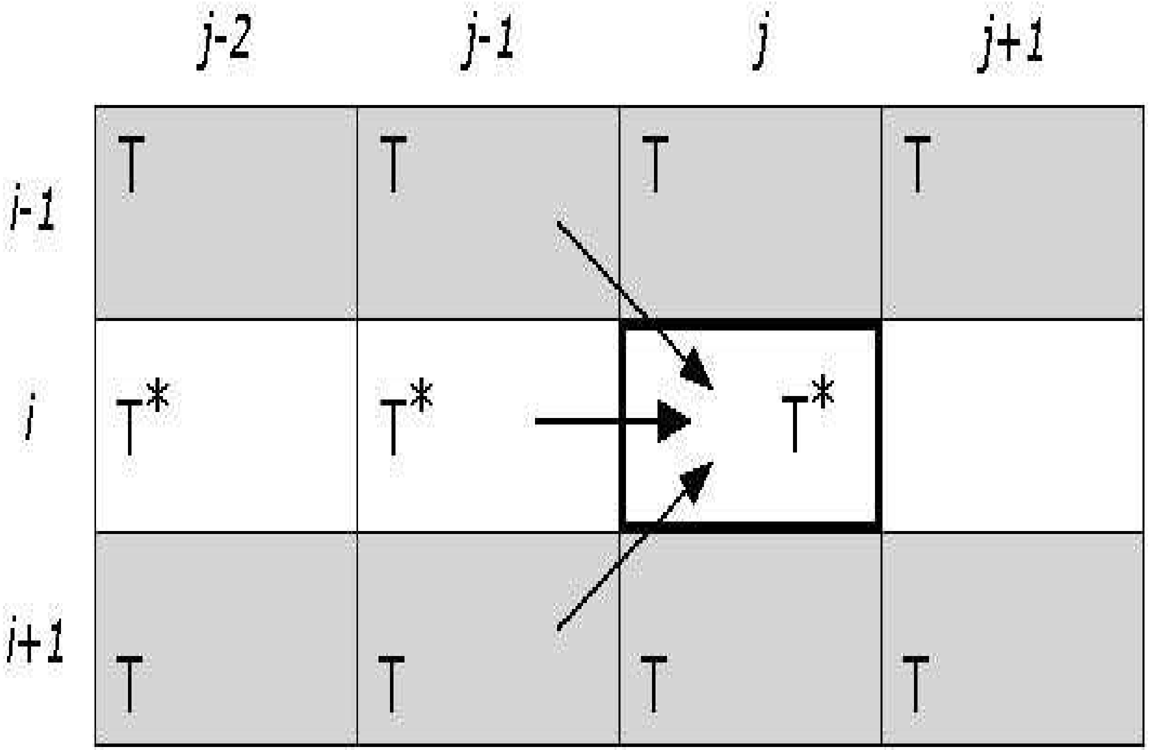
- Latent values $T^*$ introduced in new internal points $x$ where temperature is not acquired, at the same time instants $j$ of the acquired temperatures $\widehat{T}$

- Iterative procedure
  - set initial values of $\lambda_0$ and temperatures at time $t = 0$ in new internal points $x$
  - draw $T^*$ recursively, based on $\lambda_0$, $\widehat{T}$
  - get posterior distribution and mean of $\lambda_0$ from uniform prior distribution and likelihood depending on current values of $\widehat{T}$ and $T^*$
  - compute the average of the posterior means of $\lambda_0$ after a *sufficient* number of iterations

# (BAD) GENERATION OF LATENT TEMPERATURES

- $\mathbf{T}_j$ vector of both acquired and latent data
- $T^*_{i,j}$ denotes components of $\mathbf{T}_j$ with latent temperature
- Introduction of latent temperature $T^*_{i,j}$ between two points with acquired temperature $\Rightarrow \mathbf{T}_j = \left[\cdots T_{i-1,j} T^*_{i,j} T_{i+1,j} \cdots\right]^T$
- Generation of latent temperatures **very critical**

# (BAD) GENERATION OF LATENT TEMPERATURES




Latent value $T^*_{i,j}$ generated based on three values at the previous time instant $j-1$: two acquired values ($T_{i-1,j-1}$; $T_{i+1,j-1}$) and a generated one ($T^*_{i,j-1}$)

# (BAD) GENERATION OF LATENT TEMPERATURES

- Proposal value $T^p_{i,j}$ for temperature $T^*_{i,j}$ generated from finite-difference equation $\mathbf{T}_j = \mathbf{T}_{j-1} + \left[\lambda_0 \mathbf{L}\left(\mathbf{T}_{j-1}\right) + \dot{\mathbf{q}}_{j-1}\right] \Delta_j + \eta \mathbf{diag}_{\mathbf{L}(\mathbf{T}_{j-1})} \mathbf{\Delta W}_1 + \varepsilon \mathbf{diag}_{\mathbf{T}_{j-1}} \mathbf{\Delta W}_2$, i.e.

$$\begin{aligned} T^p_{i,j} &= T^*_{i,j-1} + \frac{\lambda_0 \Delta_j}{\rho c h^2} \left(T_{i-1,j-1} - 2T^*_{i,j-1} + T_{i+1,j-1}\right) + \\ &\quad + \frac{\eta}{\rho c h^2} \left(T_{i-1,j-1} - 2T^*_{i,j-1} + T_{i+1,j-1}\right) \sqrt{\Delta_j} Z_1 + \varepsilon T_{i,j-1} \sqrt{\Delta_j} Z_2 \end{aligned}$$

  - $Z_1$ and $Z_2$ independent draws from standard Gaussian distribution
  - discretization step $h$ properly dimensioned considering actual distance between generated and acquired points

- Proposed value $T^p_{i,j}$ checked for consistency w.r.t. other acquired points

- If accepted, $T^*_{i,j} = T^p_{i,j}$ taken as the latent value; o.w. previous $T^*_{i,j}$ kept

- For the first iteration, $T^*_{i,0} = \frac{1}{2}\left(T_{i-1,0} + T_{i+1,0}\right)$, i.e. average of neighboring acquired temperatures at same time instant 0 ($\Rightarrow$ no influence on likelihood)

# (BAD) GENERATION OF LATENT TEMPERATURES

- Proposed point $T^p_{i,j}$ checked to avoid irregular temperature profiles, like going up and down in neighboring points
  - underestimation of thermal conductivity
    - amplification of irregularities in drawing $T^p_{i,j}$ because of term $T_{i-1,j-1} - 2T^*_{i,j-1} + T_{i+1,j-1}$
    - changes of slope would decrease the numerator of $\lambda^l_0$
  - against physical laws

- Various attempts to generate points
  - as seen before, based on 3 points at previous time
  - full time series at each point $x$
  - None of them fully satisfactory

- Extension to more than one latent vector generated between two acquired points

## (BETTER?) GENERATION OF LATENT TEMPERATURES

- Latent values $\mathbf{T}^*$ introduced in new internal points $x$ where temperature is not acquired, at the same time instants $j$ of the acquired temperatures $\mathbf{T}$

- In a Bayesian framework $\mathbf{T}^*$ treated as parameters

- At each step of MCMC algorithm
  - draw $\lambda_0$ from distribution depending on $\mathbf{T}$, $\mathbf{T}^*$ and past values of $\lambda_0$ (possibly with acceptance/rejection sampling)
  - draw $\mathbf{T}^*$ from distribution depending on $\lambda_0$, $\mathbf{T}$ and past values of $\mathbf{T}^*$ (with acceptance/rejection sampling)

# (BETTER?) GENERATION OF LATENT TEMPERATURES

- For each time instant $j$: vector $\mathbf{Y}_j$ denotes both acquired $\mathbf{T}_j$ and generated $\mathbf{T}_j^*$
- Matrix of all temperatures, up to final time $t_f$: $\mathbf{Y} = \left[\mathbf{Y}_1\ \mathbf{Y}_2\ \ldots\ \ldots\ \mathbf{Y}_{t_f}\right]$
- Introduce latent $T_{i,j}^*$ in the middle between two points with acquired temperatures $T_{i-1,j}$ and $T_{i+1,j}$
- $\Rightarrow \mathbf{Y}_j = \left[\cdots T_{i-1,j} T_{i,j}^* T_{i+1,j} \cdots\right]^T$
- MCMC (currently under implementation)
  - Conditional on $\lambda_0$ exactly known or not, depending on the choice of the prior
  - Conditional on $\mathbf{T}^*$ known apart from a constant

# (BETTER?) GENERATION OF LATENT TEMPERATURES

- $\pi\left(\mathbf{T}_j^{*(n)}|\mathbf{Y}_{j-1}^{(n)}, \mathbf{Y}_{j+1}^{(n-1)}, \mathbf{T}_j, \lambda_0\right) \propto \pi\left(\mathbf{Y}_{j+1}^{(n-1)}|\mathbf{Y}_j^{(n-1)}, \lambda_0\right) \pi\left(\mathbf{Y}_j^{(n-1)}|\mathbf{Y}_{j-1}^{(n)}, \lambda_0\right)$
  - $\pi\left(\mathbf{Y}_{j+1}|\mathbf{Y}_j, \lambda_0\right) = \mathcal{N}\left(\mathbf{Y}_j + [\lambda_0 \mathbf{L}(\mathbf{Y}_j) + \dot{\mathbf{q}}_j]\,\Delta, \left[\eta^2 \mathbf{diag}^2_{\mathbf{L}(\mathbf{T}_j)} + \varepsilon^2 \mathbf{diag}^2_{\mathbf{T}_j}\right]\Delta\right)$
  - $\pi\left(\mathbf{Y}_j|\mathbf{Y}_{j-1}, \lambda_0\right) = \mathcal{N}\left(\mathbf{Y}_{j-1} + [\lambda_0 \mathbf{L}(\mathbf{Y}_{j-1}) + \dot{\mathbf{q}}_{j-1}]\,\Delta, \left[\eta^2 \mathbf{diag}^2_{\mathbf{L}(\mathbf{T}_{j-1})} + \varepsilon^2 \mathbf{diag}^2_{\mathbf{T}_{j-1}}\right]\Delta\right)$

- Gaussian proposal distribution for $T^*_{i,j}|\ldots : \mathcal{N}\left(\mu_{prop_{i,j}} \sigma^2_{prop_{i,j}}\right)$
  - $\mu_{prop_{i,j}} = \dfrac{T_{i+1,j} + T_{i-1,j}}{2} - \left[\dfrac{T_{i+1,j-1} + T_{i-1,j-1}}{2} - T_{i,j-1}\right]$
    (mean of nearby points corrected by *bias* at previous time)
  - $\sigma^2_{prop_{i,j}} = \frac{1}{2}\left[\frac{\eta^2}{\rho^2 c^2 h^4}\left(T_{i-1,j-1} - 2T^*_{i,j-1} + T_{i+1,j-1}\right)^2 + \varepsilon^2 T^2_{i,j-1}\right]\Delta$
    (half variance of Euler-Maruyama for $\mathbf{Y}_j$ conditioned on the past)

- *Usual* acceptance probability

# KNOWLEDGE ABOUT PHYSICAL PARAMETERS

- Fixed values of density $\rho$ and specific heat $c$ and range for thermal conductivity $\lambda_0$
- Choice of density $\rho$
  - range, but not a unique value, available in literature for PMMA
  - stochastic model on $\rho$ as well?
  - sample of material extracted during processing, and $\rho$ as ratio of weight and volume $\Rightarrow 1185 \frac{kg}{m^3}$ (in the range found in literature)
- Choice of specific heat $c$ of PMMA
  - Unique value, 1466 $\frac{J}{kgK}$, from literature (e.g. MIT material property database and MATBASE)

# KNOWLEDGE ABOUT PHYSICAL PARAMETERS

Ranges on thermal conductivity $\lambda_0$ of PMMA family available in literature

| **Reported value** | **Value in** $\left[\frac{W}{mK}\right]$ | **Reference** |
|---|---|---|
| 0.167-0.25 $\left[\frac{W}{mK}\right]$ | 0.167-0.25 | MIT material property db |
| 0.167-0.25 $\left[\frac{W}{mK}\right]$ | 0.167-0.25 | MATBASE |
| 0.17-0.19 $\left[\frac{W}{mK}\right]$ | 0.17-0.19 | TU DELFT |
| 0.1922 - 0.1986 $\left[\frac{W}{mK}\right]$ | 0.1922 - 0.1986 | Assael et al. |
| 0.21 (with reference 0.20-0.24) $\left[\frac{W}{mK}\right]$ | 0.21 | Hu et al |
| 4.0-6.0 $10^{-4}$ $\left[\frac{cal/s}{cmK}\right]$ | 0.167-0.25 | maropolymeronline |
| 0.0012 $\left[\frac{cal/s}{cmK}\right]$ | 0.502 | hybridsnow |

- Range equal to 0.167-0.25 $\frac{W}{mK}$ is considered, based on two worldwide used polymer databases (first two rows of table)
- Results obtained in the ISO normative (ISO 22007) reflect this range

# KNOWLEDGE ABOUT PHYSICAL PARAMETERS

Knowledge of range on $\lambda_0$ reflected in the choice of the prior distribution

- Noninformative proper prior $\Rightarrow$ uniform on $[0.167, 0.25]$
- Gaussian distribution $\mathcal{N}(\lambda_0^p, \sigma_p^2)$
  - suppose $[0.167, 0.25]$ to be given $0.997$ prior probability
  - $\Rightarrow \lambda_0^p = 0.2085 \qquad \sigma_p^2 = 1.914 \cdot 10^{-4}$
- Gamma prior with $0.997$ prior probability to $[0.167, 0.25]$

# KNOWLEDGE ABOUT PHYSICAL PARAMETERS

- Critical choice of errors $\eta$ (related to coefficient stochasticity) and $\varepsilon$ (related to temperature measurement)

- Regarding $\eta$, results available in the ISO normative (ISO 22007) show a maximum error of 10%
  $\Rightarrow$ we take 10% of the mean value of the assumed range $[0.167, 0.25]$, i.e. $\eta = 0.02085\frac{W}{mK}$, as upper limit

- Errors when using thermocouples should not exceed the 0.75% of the measurement, so $\varepsilon = 0.0075\frac{1}{s}$ is taken as upper limit ($\epsilon T_{i,j} < 0.0075 * 100 = 0.75$)

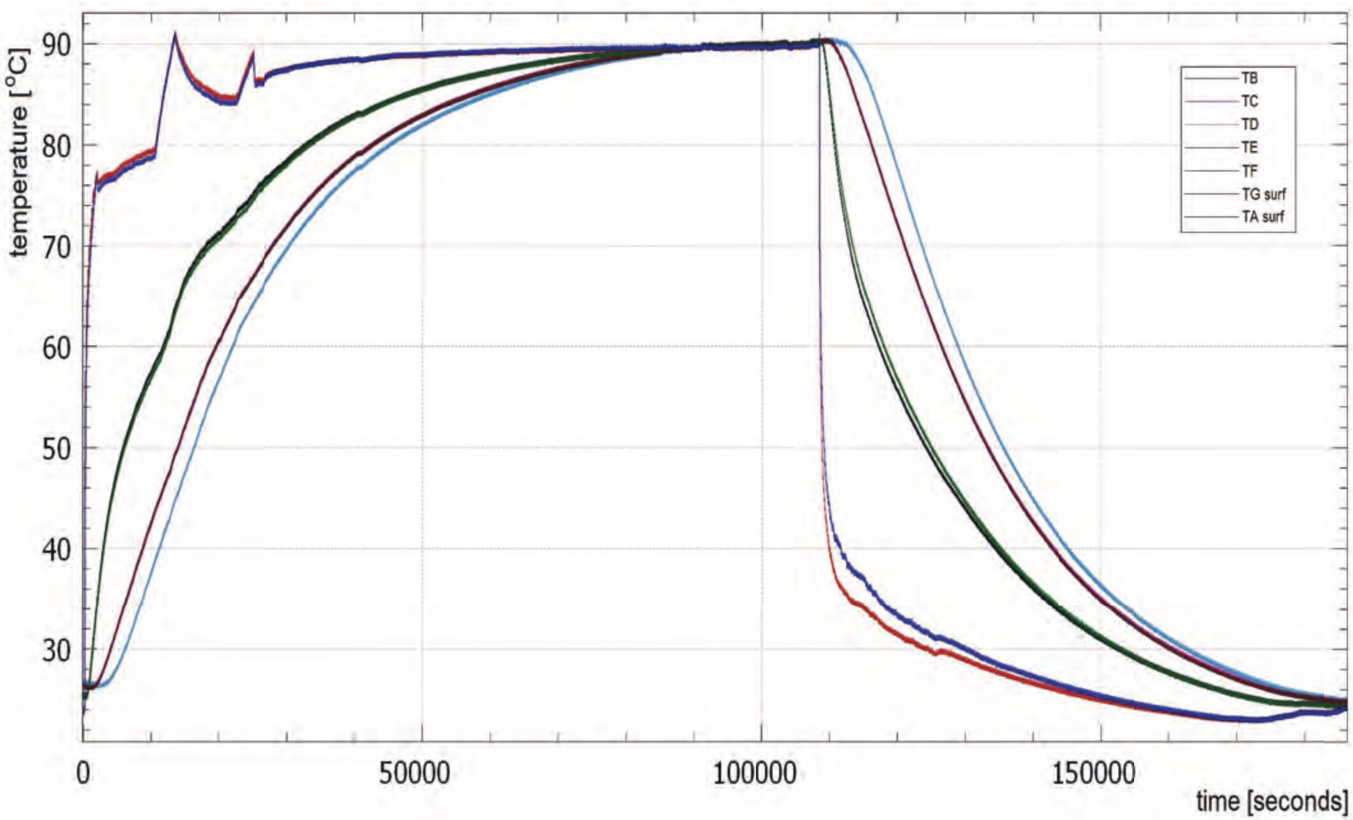
- In our experiments we took $\eta = 10^{-3}\frac{W}{mK}$ and $\varepsilon = 10^{-3}\frac{1}{s}$

- Need to calibrate those values

## ACQUIRED DATA

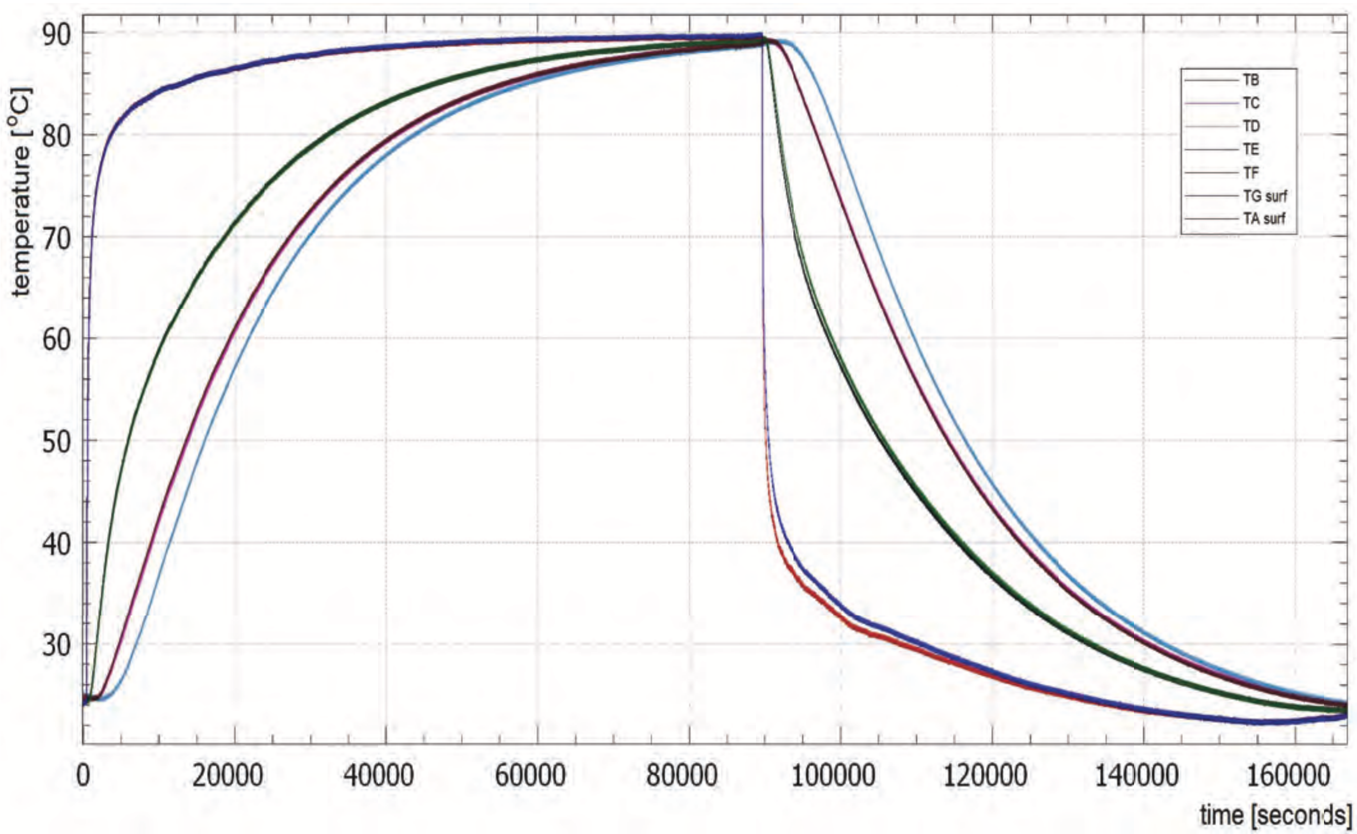
- Experiment repeated three times
- Each experiment lasted about 40 hours
- Detailed temperature trends reported in next slides
- In some cases, oscillations found in the superficial temperatures, due to sudden regulatory mechanisms of the oven control
- Oscillation confined to specimen surface and thermal conductivity not affected by them, being no problem for the experiment
- Regular trends are found over time, with reduced electrical and environment noises
- For those reason, no signal treatment required before applying the proposed methodology (e.g., moving average)

# TEMPERATURE TRENDS



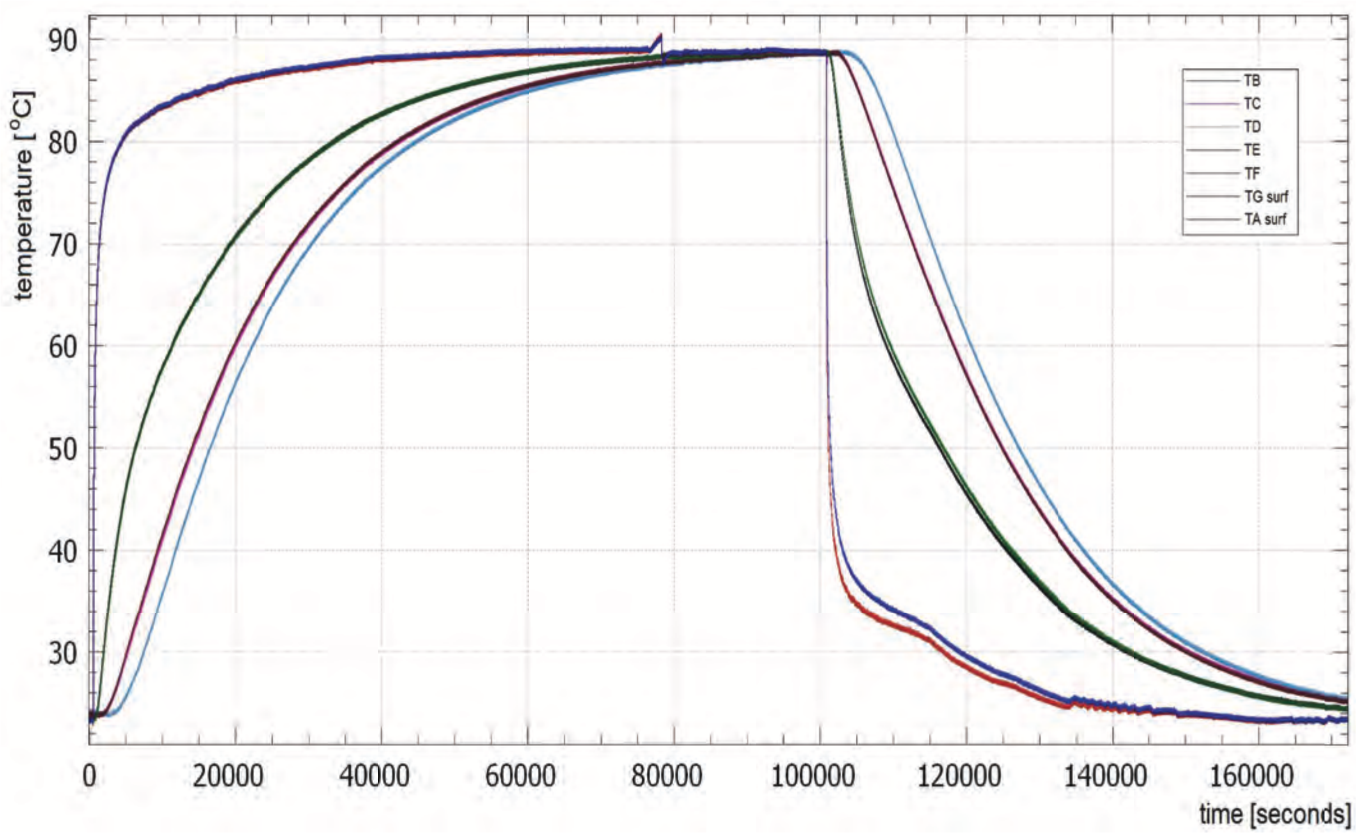

Temperature trends acquired in the first repetition

# TEMPERATURE TRENDS




Temperature trends acquired in the second repetition

# TEMPERATURE TRENDS




Temperature trends acquired in the third repetition

# SIMULATED DATA

- A period of one hour (second hour of heating phase) extracted from second experimental dataset, since the superficial temperatures do not show alterations

- Initial values at beginning of the hour and superficial temperatures in points A and G are taken from the experimental dataset as boundary and Dirichlet conditions, while the internal points are generated considering an imposed thermal conductivity $\lambda_{0gen}$

- Points are generated according to the heat equation (and discretizations)

$$\begin{aligned} T_{i,j} &= T_{i,j-1} + \frac{\lambda_{0gen}\Delta_j}{\rho c h^2}\left(T_{i-1,j-1} - 2T_{i,j-1} + T_{i+1,j-1}\right) + \\ &+ \frac{\eta}{\rho c h^2}\left(T_{i-1,j-1} - 2T^*_{i,j-1} + T_{i+1,j-1}\right)\sqrt{\Delta_j}Z_1 + \varepsilon T_{i,j-1}\sqrt{\Delta_j}Z_2 \end{aligned}$$

- Generation independently repeated 30 times and values averaged among them

- Iterative approach (with improper uniform prior) applied to this simulated dataset

- Validation performed with $\lambda_{0gen}$ = 0.1 $\frac{W}{mK}$, $\lambda_{0gen}$ = 0.2 $\frac{W}{mK}$ and $\lambda_{0gen}$ = 0.3 $\frac{W}{mK}$

# SIMULATED DATA

- Dataset generation procedure repeated 1000 times for each $\lambda_{0gen}$
- Estimates of $\lambda_{0gen}$ given by averaging posterior means over 1000 repetitions
- $\lambda_{0gen}$ estimated pretty well (despite of some variability in Gaussian posterior distribution, as given by $\mathbf{E}\left[\sigma_l^2\right]$, i.e. averaging $\sigma_l^2$)
- Very similar outcomes in repetitions because of small $\mathbf{SD}\left[\lambda_0^l\right]$

| | $\lambda_{0gen}$ **0.1** $\frac{W}{mK}$ | $\lambda_{0gen}$ **0.2** $\frac{W}{mK}$ | $\lambda_{0gen}$ **0.3** $\frac{W}{mK}$ |
|---|---|---|---|
| $\mathbf{E}\left[\lambda_0^l\right]$ | 0.1031 | 0.2052 | 0.3046 |
| $\mathbf{SD}\left[\lambda_0^l\right]$ | 0.0153 | 0.0298 | 0.0169 |
| $\mathbf{E}\left[\sigma_l^2\right]$ | $4.34\ 10^{-4}$ | $6.03\ 10^{-4}$ | $7.72\ 10^{-4}$ |
| $\mathbf{SD}\left[\sigma_l^2\right]$ | $8.58\ 10^{-6}$ | $1.07\ 10^{-5}$ | $1.04\ 10^{-5}$ |

# REAL DATA

- Three experiments separately analyzed, with different subsets: one hour during heating, one hour during cooling, and entire dataset from beginning of heating phase to end of cooling one
- High variability among subsets in estimation, some variability among experiment, despite the same specimen
- Estimates,with no latent data, are far from thermal conductivity range of PMMA, $[0.176, 0.25]$
- Need for (proper) Bayesian approach, latent data generation (maybe a good one)

| | | **Heating phase** | **Cooling phase** | **Entire dataset** |
|---|---|---|---|---|
| **First experiment** | $\lambda_0^l$ | 0.7804 | 0.4133 | 1.3898 |
| | $\sigma_l^2$ | $5.89\ 10^{-4}$ | $7.99\ 10^{-4}$ | $4.81\ 10^{-5}$ |
| **Second experiment** | $\lambda_0^l$ | 0.6809 | 2.0480 | 1.2835 |
| | $\sigma_l^2$ | $4.39\ 10^{-4}$ | $2.39\ 10^{-3}$ | $4.32\ 10^{-5}$ |
| **Third experiment** | $\lambda_0^l$ | 0.7042 | 0.7402 | 1.1660 |
| | $\sigma_l^2$ | $4.14\ 10^{-4}$ | $1.12\ 10^{-3}$ | $4.16\ 10^{-5}$ |

# WORK AHEAD

- A proper Bayesian analysis
  - prior choice
  - efficient method to generate latent data
  - optimal number of latent data
  - estimation of thermal conductivity
- Stochasticity for density $\rho$
- Estimation of quantities related to heating and cooling process, e.g. time required for all points of specimen to go above or below a given temperature
- Inference on process at different, but comparable, initial and final temperature
- Heat equation in $\Re^3$

# WORK AHEAD

A more *classical* approach

- Observed temperatures $T_{i,j}$ at point $i$ and time $j$, $i = 1, N$, $j = 1, m$
- Parameter $\theta$ drawn from prior $\pi(\theta)$
- Numerical solution of PDE $\Rightarrow \widehat{T}_{i,j}(\theta)$
- Likelihood $L(\theta)$ from $T_{i,j} = \widehat{T}_{i,j}(\theta) + \sigma\epsilon_{i,j}$
- $\epsilon_{i,j}$: independent? Markov random fields? Gaussian?
- Posterior distribution of $\theta$: Metropolis-Hastings? Evaluated on a grid?
- Estimation at unobserved points?