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Published in:
Proceedings of the 20th IFAC World Congress, IFAC'2017

DOI:
10.1016/j.ifacol.2017.08.2454

Published: 01/01/2017

Please cite the original version:
https://doi.org/10.1016/j.ifacol.2017.08.2454
Explicit Boundary Controls for Finite Diffusion Process

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Abstract: Three types of boundary controls are considered: proportional control, feed-forward control and integrated-by-past-values control. They stabilise the diffusion process exponentially at the desired reference on the controlled boundary. The process is actuated through the Neumann boundary while on other boundaries it is given with the Dirichlet data and, in higher dimensions, also with the homogeneous Neumann boundary condition. Two systems, deterministic and stochastic are compared as an ideal and real description of a physical system. Disturbance in the stochastic system is originated by a white noise on the controlled boundary. Physically this noise represents different types of uncertainties like a side-reaction mass-flux and other uncertainties that are not part of a deterministic model. At first the proportional control is analysed on the deterministic system and then it is represented in the feedback integrated past controls form, and lastly the developed controls are modified as a version of stochastic control that applied on the stochastic system, which boundary is disturbed with an unmeasured noise. The regulation error that emerges in the stochastic system control is analysed and prove to be a zero-mean, bounded-variance Gaussian variable that is correlated spatially and temporarily. The process control is demonstrated on an electrodeposition process example.

1. Introduction

The purpose of the paper is to propose and analyse exact controls motivated by applications in electrochemistry of batteries (Tenno and Nefedov, 2014), electroplating (Tenno and Pohjoranta 2014; Pohjoranta and Tenno, 2014) and other oxidation processes where diffusion mass transfer is important and controlled to prevent the ion depletion of the electrolyte or other simpler mass transfer processes like in control of the desalination plant (Nguyen and Tenno, 2017). This paper proves that these controls are stabilizing controls. The proportional feedback control is represented in two equivalent forms as the feed-forward control and integrated-by-past-values control that is more practical as the latter control do not require measurements on the boundary. This control is the right feedback form for a deterministic system and for a stochastic system if the control is modified for the noisy boundary. In applications, the stochastic system emerges from the model uncertainty. For example, from the surface chemistry of real processes that is understood incompletely (Newman et al., 2004). Any model that deals with surface chemistry includes, to some extent, uncertainties. Consequently, a stochastic model should be considered that deals with uncertainties in the form of unmeasured noises. The stochastic model, if applied, should stabilise a process even if a real mass flux that depends on side reactions is modeled as a noise on the boundary that cannot be observed or controlled precisely. The mass flux on average must be controlled on the bases of a stochastic model. This creates a regulation error in the subdomain interior and on the boundary as a difference between the stochastic process and the deterministic process. This paper proves that the regulation error on the boundary has zero mean and bounded variance and is a Gaussian random variable that is strongly correlated temporarily. This error enters the subdomain where it induces a secondary regulation error that is bounded, correlated spatially and temporarily. This proves that in PDEs control slower damping of the regulation error takes place, which is a different property from ODE systems.

2. The problem statement

In this section, a stochastic diffusion process is considered that is controlled through the noisy Neumann boundary with the proportional control and integrated-by-past-values control. The latter control applied afterwards on the stochastic and mean value processes.

The problem statement. Let \( t \in [0, \infty) \), \( L > 0 \) and \( \Omega \) be a bounded subdomain in \( \mathbb{R}^d \) that is a \( d \)-dimensional hypercube \( \Omega = (0, L)^d \). The boundaries of the cube are divided into three sets: \( \Gamma_D \), \( \Gamma_N \), and \( \Gamma_0 \) such that their union is the natural subdomain boundary \( \Gamma_D \cup \Gamma_N \cup \Gamma_0 = \partial \Omega \) without overlapping of boundaries: \( \Gamma_D \cap \Gamma_N = 0 \), \( \Gamma_D \cap \Gamma_0 = 0 \), and \( \Gamma_N \cap \Gamma_0 = 0 \).

In \( Q = \Omega \times [0, \infty) \), diffusion process (1) with constant diffusivity \( D > 0 \) is considered.

\[
c_t = D \Delta c \quad \text{in } Q
\]  (1)

In (1), \( c_t \) is the time derivative and \( \Delta c \) is the Laplacian of \( c \). The process \( c(t, x) \) is set initially on a constant level \( c(0, x) = c_b \) in \( \Omega \). Equation (1) satisfies the mixed boundary
conditions: the Dirichlet condition \( c = c_b \) on boundary \( \Gamma_D \) and the Neumann conditions on other boundaries \( \Gamma_N \) and \( \Gamma_0 \).

The control \( u(t) \) acts through the Neumann boundary \( \Gamma_N \).

\[
-D\nabla c \cdot n = u(t, \omega) + \sigma \dot{W}(t) \quad \text{on} \quad \Gamma_N \times [0, \infty) \tag{2}
\]

In (2), \( \nabla c \) is the gradient of \( c \). The symmetry (or insulation) condition is assumed on other boundaries of \( \Gamma_0 \) (i.e., in between \( \Gamma_D \) and \( \Gamma_N \)).

\[
-D\nabla c \cdot n = 0 \quad \text{on} \quad \Gamma_0 \times [0, \infty) \tag{3}
\]

In (2) and (3), \( n \) denotes the normal to the controlled boundary \( \Gamma_N \) and insulating boundary \( \Gamma_0 \) correspondingly. The controlled boundary \( \Gamma_N \) is a noisy boundary modelled with a generalised white noise \( \dot{W}(t) \) that gains its exact meaning in a weak-form representation through Ito’s integral, where it appears as a finite dimensional Wiener process \( W(t) \) in \( \mathbb{R}^n \), \( m \geq d \). This noise is applied point-wise along the boundary \( \Gamma_N \). The coordinates \( W_i(t) \) of Wiener process \( W(t) \) are given in a canonical probability space \( (\Omega, F, P) \) that is a fixed space once and for ever. \( W(t) \) is a standard Wiener process with variance \( \mathbb{E}[W_i(t)^2] = t \). In (2), \( \sigma \) is the diagonal \( d \times m \) matrix that stands for the variance of noise intensity; \( \omega \) is the outcome of the sampled space \( \Omega \) where all the noise dependent stochastic processes are defined.

This noise on the boundary represents ignored physical processes, like unmodelled secondary or surface reactions in electroplating or some other unmeasured in practice process that must be supressed with an effective control (yet to be found).

This system is assumed to be observed on the Dirichlet boundary \( \Gamma_D \) as the constant \( c_b \) and on the noisy boundary \( \Gamma_N \) as the stochastic control \( u(t, \omega) \) in combination with noise; the noise \( \sigma \dot{W}(t) \) cannot be measured. In (2), a stochastic control \( u(t, \omega) + \sigma \dot{W}(t) \) is applied in a way how real system (1)-(3) it senses. We designate this control with the shorthand \( u_c(t) \) of (4).

\[
\dot{u}_c(t) = u(t, \omega) + \sigma \dot{W}(t) \tag{4}
\]

The system (1)-(3) without boundary noise coincides with the system for mean value process \( \mathbb{E}c = m \) that satisfies (5)

\[
m_c = D\Delta m \quad \text{in} \quad Q \tag{5}
\]

and \( m(0, x) = c_b \) in \( \Omega \). For \( \mathbb{E}u(t, \omega) = u(t) \), this system (5) is deterministic in the subdomain and on all boundaries.

\[
m = c_b \quad \text{on} \quad \Gamma_D \times [0, \infty) \tag{6}
\]

\[
-D\nabla m \cdot n = u(t) \quad \text{on} \quad \Gamma_N \times [0, \infty) \tag{7}
\]

\[
-D\nabla m \cdot n = 0 \quad \text{on} \quad \Gamma_0 \times [0, \infty) \tag{8}
\]

We analyse two specific controls motivated by applications in electrochemistry. These are the proportional control

\[
u(t) = -K_p \left(m(t, 0) - c_d\right) \tag{9}\]

and integrated-by-past-values control

\[
u(t) = -K_p \left(c_b - c_d\right) - \int_{\tau}^{t} \frac{u(r)}{\sqrt{\pi(t - \tau)}} D \left(1 + 2 \sum_{n=1}^{\infty} (-1)^n e^{-\frac{u^2}{(t - \tau)n}}\right) d\tau \tag{10}\]

In (9) and (10), \( K_p \) is the control gain, \( K_p > 0 \) and \( c_d \) is the control reference.

In stochastic realisation, the former control (10) is modified as a stochastic version of integrated control (11) over the past noisy values of controls \( u(t) = u_c(t, \omega), 0 \leq \tau \leq t \)

\[
u(t, \omega) = -K_p \left(c_b - c_d\right) - \int_{\tau}^{t} \frac{u_c(r, \omega)}{\sqrt{\pi(t - \tau)}} D \left(1 + 2 \sum_{n=1}^{\infty} (-1)^n e^{-\frac{u^2}{(t - \tau)n}}\right) d\tau \tag{11}\]

Section 3 states that these controls (9), (10) and (11) stabilize the deterministic process (5)-(8) on the boundary \( m(t, 0) \) at the desired reference \( c_d \) and that the regulation error \( c(t, 0) - m(t, 0) \) of the stochastic process (1)-(4) is unbiased, bounded variance, and Gaussian. The regulation error is correlated temporarily.

The reduced control problem. In dependence on the desired results, two approaches can be applied. The first one is to extend the problem with complex geometry of the subdomain where the process lives and with the functional space noises on the boundary and in the subdomain. In this statement the general theory (Da Prato and Zabczyk, 1992; 1993) provides tools for qualitative analysis. The second approach is to diminish the problem to the case where exact solution of the problem (control law) can be obtained. In control practice, one is more interested in exact results than in qualitative results provided by the general theory for systems with complex geometry and with the functional space noises. In order to have exact analytical results (control law) the problem will be restricted next to the scalar case \( d = 1 \) and then some more comments will be given later for extension of the results to other simple cases \( d > 1 \) (e.g., 2D rectangle or 3D cube) that do not require new ideas of extension.

3. The main results

Theorem 1 and Corollaries 1.1-4 apply to the deterministic system (5)-(8) actuated on the boundary (7) with control (9).
The analytic solution (12)-(14) of the system, the feedforward control law (16) and the steady-state regulation error (18) are given below. The static regulation error is eliminated afterwards with control (19).

Theorem 1 For proportional control (9), the solution of the system (5)-(8) in the subdomain \( Q = (0, L) \times [0, \infty) \) and on the boundaries is given as the function (12)-(14).

\[
m(t, x) = \frac{c_D D + c_p K_p x}{D + K_p L} + \frac{c_D K_p x}{D + K_p L} + \sum_{n=1}^{\infty} \left( \frac{2c_D D K_p}{L K_p^2 + K_p D + \lambda_n^2 LD^2} \right) e^{-\lambda_n^2 t} + \lambda_n \sin \left( \lambda_n x \right) + \lambda_n D K_p \cos \left( \lambda_n x \right), \quad n = 1, 2, \ldots.
\]

\( \lambda_n \) is the eigenvalue that satisfies the transcendental equation (13) for every \( n = 1, 2, \ldots \).

\[
D \lambda_n^2 + K_p \tan \left( \lambda_n L \right) = 0
\]

\( c_o \) is the shorthand of \( c_o - c_d \), and \( Y_n(x) \) is the set of orthogonal functions (14) in the interval \( (0, L) \).

\[Y_n(x) = \sin \left( \lambda_n x \right) + \lambda_n D K_p \cos \left( \lambda_n x \right), \quad n = 1, 2, \ldots \quad (14)\]

Corollary 1.1 Solution of the system (5)-(8) on the controlled boundary, reads:

\[
m(t, 0) = \frac{c_D D + c_p K_p L}{D + K_p L} + \sum_{n=1}^{\infty} \left( \frac{2c_D D K_p}{L K_p^2 + K_p D + \lambda_n^2 LD^2} \right) e^{-\lambda_n^2 t} + \lambda_n \sin \left( \lambda_n x \right) + \lambda_n D K_p \cos \left( \lambda_n x \right), \quad n = 1, 2, \ldots.
\]

Corollary 1.2 The proportional control (9) expressed in the form of feed-forward control that does not depend on measurements on the boundary, reads:

\[
u(t) = -\frac{c_D K_p D}{D + K_p L} + \sum_{n=1}^{\infty} \left( \frac{2c_D D K_p^2}{L K_p^2 + K_p D + \lambda_n^2 LD^2} \right) e^{-\lambda_n^2 t} + \lambda_n \sin \left( \lambda_n x \right) + \lambda_n D K_p \cos \left( \lambda_n x \right).
\]

Corollary 1.3 The steady-state solution of the system (5)-(8) on the controlled boundary, reads:

\[
m_s = \lim_{t \to \infty} m(t, 0) = \frac{c_D D + c_p K_p L}{D + K_p L}.
\]

The proportional control (9) has a static regulation error \( c_d^0 > 0 \) in the steady-state condition:

\[
m_s - c_d = \frac{D}{D + K_p L} c_d^0 = c_d^0.
\]

If \( D < K_p L \) the static regulation error is small \( c_d^0 \approx 0 \) and can be ignored in practice; otherwise the control reference \( c_d \) in (9) should be set lower at \( c_s - c_d^0 \) to compensate for the static control error. Alternatively, this error can be eliminated with an additional integral part to the proportional control law (9). However, such integration of (9) is unnecessary in this case of known and constant static regulation error \( c_d^0 \). A simple formula (19) can be applied for elimination of the regulation error.

\[
u(t) = -K_p \left( m(t, 0) - c_d + c_d^0 \right)
\]

This elimination \( m(t, 0) \to m_s - c_d^0 = c_d \) is a straightforward conclusion from (17) and (18).

Corollary 1.4 The control (19) is an exponentially stabilising control \( (m(t, 0) \to c_d) \). The steady-state level of control equals to the strictly negative constant (20).

\[
\lim_{t \to \infty} u(t) = -K_p c_d^0
\]

This limit (20) is a direct consequence from (16).

Theorem 2 below gives general solution to the system (5)-(8) with arbitrary control \( u(t) \in L^2 \left( [0, \infty), R^1 \right) \). This solution applied in composition of the proportional control law (9) yields control (10) that does not depend on the process values on the boundary recalled briefly as the past control.

Theorem 2 For any \( u(t) \in L^2 \left( [0, \infty), R^1 \right) \), the solution of the system (5)-(8) on the boundary, reads:

\[
m(t, 0) = c_o + \int_0^t \frac{u(\tau)}{\sqrt{\pi(t-\tau)}} \left( 1 + 2 \sum_{n=1}^{\infty} (-1)^n e^{-n^2 \tau^2} \right) d\tau.
\]

Corollary 2.1 Representation of the proportional control (9) in the form of past control, reads:

\[
u(t) = -K_p c_o - K_p \int_0^t \frac{u(\tau)}{\sqrt{\pi(t-\tau)}} \left( 1 + 2 \sum_{n=1}^{\infty} (-1)^n e^{-n^2 \tau^2} \right) d\tau.
\]

Comparison of controls. Technically, these three controls (9), (10) and (16) are identical actuators represented in different versions as the feedback proportional control (9), past control (10), and as the feed-forward control (16). They are asymptotically stabilizing controls if the lower reference \( c_d - c_d^0 \) is aimed (as in (19)) that eliminates the static regulation error (18).

Stochastic control. These controls, in combination with a boundary noise, can be applied for actuation of the stochastic system (1)-(3). However, only the past control (10) is applicable law to the stochastic system. The proportional control (23) that might be thought effective depends on the measured process \( c(t, 0) \) on the boundary and, therefore, cannot be applied in practice.
In electrodeposition \( c(t, 0) \) represents the concentration of species in close vicinity to the boundary that cannot be measured online by any means in the chemical engineering applications. Also, there is no help of control (16) that represents the same deterministic control as (9) in another feed-forward form. As a model-based control it tolerates uncertainties poorly. In contrast to other controls, the past control (10) depends on the past measurements of control variables (4) that are available and can be applied in actuation of the stochastic system (1)-(3). In electrodeposition, these control variables represent electric current that is simple to measure on electrodes. Hence (10) can be applied in practice, and if applied in combination with boundary noise, it is a stochastic control \( u_i(t, \omega) \) that generates a stochastic process

\[
  c(t, 0, \omega) = c_0 + \int_0^t u_i(\tau, \omega) \frac{1}{\sqrt{\pi}} \frac{1}{D} \left( 1 + 2 \sum_{n=1}^{\infty} (-1)^n e^{-\frac{|\tau-k|^2}{D}} \right) d\tau , \quad (24)
\]

which obviously deviates from the mean-value process \( m(t, 0) \) that coincides only the noise-free system.

**Reference system.** If one takes the noise-free system (5)-(8) as a reference for comparison with the stochastic system (1)-(3), then obviously the stochastic controls \( u_i(t, \omega) \) create a regulation error (residual) in the subdomain

\[
  \varepsilon(t, x) = c(t, x) - m(t, x) \quad (25)
\]

and on the controlled boundary (\( \Gamma_N \), where \( x = 0 \))

\[
  \varepsilon(t, 0) = c(t, 0) - m(t, 0) . \quad (26)
\]

The regulation error on this boundary can be characterized as an asymptotically stationary process with zero mean and bounded variance. More precisely, there is no systematic drift \( \mathbf{M} \varepsilon(t, 0) = 0 \) of the regulation error on the controlled boundary. However, the regulation errors are strongly correlated in time i.e., for a relatively long delay \( k > 0 \), the autocovariance \( \gamma(t) = \mathbf{M} \varepsilon(t, 0) \varepsilon(t-k, 0) \) is still not zero. These statements are summarized in Theorem 3.

**Theorem 3** The stochastic boundary control of (4) and (11) induces a regulation error in the stochastic system (1)-(3) with respect to the deterministic system (5)-(7), (10). This error on the controlled boundary is Gaussian variable \( \mathcal{N}(0, \gamma(t)) \); its mean is zero and the covariance function depends on time \( t > k \) (non-stationary process) and delay \( k \geq 0 \) as the function of (27).

\[
  \gamma(t) = \int_0^{t-k} \frac{\sigma^2}{\pi(t-\tau+k)} \left( 1 + 2 \sum_{n=1}^{\infty} (-1)^n e^{-\frac{|\tau-k|^2}{D}} \right)^2 d\tau \quad (27)
\]

**Discussion.** The deterministic problem (5)-(8) with the boundary control (9) is classical. The new feature of the current paper is observation that the boundary control can be represented as the feed-forward control (16) through analytical solution of the closed-loop system. This solution found in whole subdomain depends on the eigenvalues that are roots of the transcendental equation (13). Novelty of the solution (12) and boundary controls (16) is their dependence on a specific transcendental equation (13) that comes from our non-homogeneous mixed type Dirichlet-Robin boundary data. Moreover, the proportional control (9) can be represented as the feedback control (10) through the analytical solution of controlled system. This solution found at first for an arbitrary control and then for the specific control in the form of the convolution integral that depends on the past controls and therefore is suitable for feedback control application. Although the solution in whole subdomain is impossible to find on the boundary it was found in this paper using the Efron’s theorem that allows finding the inverse Laplace transform. Without these key features the closed-loop system properties and feedback control properties presented in this paper were not possible. For instance, this would be unclear whether the proposed controls are exponentially stabilising controls.

The stochastic problem (1)-(3) is not classical either, because of the type of noise and analysis applied in this paper. Generally, a noise on the boundary (and in the subdomain) is a cylindrical Wiener process and the trace-class properties of noise are shown that allow to prove the existence, uniqueness and regularity properties of solution (Da Prato and Zabczyk, 1992; 1993). Our noise on the boundary is finite dimensional and in the 1D case it is just a scalar noise, however enters in the whole subdomain and makes the process random everywhere. If we apply a model-based control like the feed-forward control (16), feedback control (10) or dependent on noisy past measurements stochastic control (11), then the controlled process is still stochastic and deviates from the mean-value process. This deviation is characterised statistically for the control (16) and this is proved that there are no systematic deviations, i.e. the regulation error is with zero mean, and it has bounded variance and is Gaussian. The regulation error on the boundary is auto-correlated.
4. Numerical example

The former theoretical results are in sensible agreement with the simulation results computed on a copper electrodeposition process controlled with electric current on the cathode boundary. Parameters of the process and applied controls are specified in Table 1.

Table 1. List of parameters.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$</td>
<td>$4 \times 10^{-10}$</td>
<td>m$^2$/s</td>
</tr>
<tr>
<td>$L$</td>
<td>$4 \times 10^{-5}$</td>
<td>m</td>
</tr>
<tr>
<td>$K_p$</td>
<td>$1 \times 10^{-4}$</td>
<td>m/s</td>
</tr>
<tr>
<td>$c_d$</td>
<td>100</td>
<td>mol/m$^3$</td>
</tr>
<tr>
<td>$c_b$</td>
<td>860</td>
<td>mol/m$^3$</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>0.025</td>
<td>mol/m$^3$/s</td>
</tr>
</tbody>
</table>

The proportional control (9) and integrated past control (10) are identical controls in Figure 1 while the stochastic control (11) deviates from the former controls in the value of unmodelled side reactions simulated with a white noise that represents induced random flux on the boundary.

The current density $i(t)$ shown in Figure 1 is proportional $i(t) = z F u(t)$ to the mass flux $u(t)$ discussed in the paper. Here $z$ is the electron number 2 of Cu(II) species and $F$ is the Faraday’s constant 96,485 As/mol.

These three controls are exponentially stabilizing controls. The proportional control (9) and past control (10) bring the corresponding deterministic processes $m(t,0)$ that represents concentration of the species at the boundary to the desired reference $c_d$; also the stochastic control (4), (11) brings the stochastic process $c(t,0)$ to the neighbourhood of the same reference $c_d$. In the stochastic case, there is a certain regulation error (26) on the controlled boundary. The regulation error is unbiased or, in other words, its systematic component is zero if compared with the deterministic processes in Figure 2.

![Figure 1](image1.png)

Figure 1. The proportional control (9) and integrated past control (10) are identical (overlapping curves). The stochastic control (4), (11) deviates from the former controls in the value of its current noise and integrated past noises.

![Figure 2](image2.png)

Figure 2. The deterministic and stochastic processes controlled to the reference with past (10), proportional (9) and stochastic (11) controls.

The regulation error on the boundary (26) enters deeply into the subdomain, where it represents the difference (25) between the stochastic (1)-(3) and deterministic (5)-(8) systems. This error is exposed in multiple realisations of the stochastic process in Figure 3 as the residuals between two systems (Tenn, 2014).

![Figure 3](image3.png)

Figure 3. The regulation error penetration deep in the diffusion layer (subdomain interior).

The regulation error on the boundary is characterised with the autocovariance function (27). This function $\gamma_k(t)$ is depicted in Figure 4 as the standard deviation $\gamma_k^{1/2}(t)$ for six delays $k = 0, 1.25, 0.25, 0.5, 1, 2$ sec. The autocovariance changes in time from zero to a certain steady-state level that is a bounded level that depends on the delay. The time-dependence of autocovariance reveals that the regulation error is a nonstationary process.

![Figure 4](image4.png)
Figure 4. Standard deviation of the regulation error on the boundary depends on time and delay ($k=0$ top and $k=2$ bottom curve).

Similar dependence for autocorrelation $r_k(t) = \gamma_k(t) / \gamma_0(\infty)$ is depicted in Figure 5.

Beyond some initial period (say, $t > 1$ sec) the regulation error is close to stationary process; its autocorrelation function $r_k(t)$ is almost time-invariant and convergent in Figure 6. At large delay this rate of convergence is relatively slow. The autocovariance function is positive, which indicates that after a positive (negative) deviation from the mean follows a second positive (negative) smaller deviation and so on; frequent jump between positive and negative values of the regulation errors is unexpected.

Remark. In simulation, the way of data sampling and selection of the initial period has a certain effect on the estimation results in Figure 6. In a small scale this effect observed as the deviation between the curves comes from a limited number of realisations (2500) used for statistical analysis in construction of the curves; in larger scale, it comes from the fact that the initial period (1 second) was selected shorter than needed for complete elimination of the time dependence in Figure 6.

5. Conclusions

The analysed boundary controls are shown to be stabilising controls. It is realised that the past controls can be applied for stochastic process control without knowledge of the process on the boundary; only the past control values are required. In electrodeposition, they represent mass flux on the boundary expressed through the electric current that passes through the system. The regulation error of the stochastic system on the boundary is shown to be an unbiased, bounded variance, temporarily correlated, Gaussian random variable.

Literature


