Presented at the COMSOL Conference 2009 Milan

Linear LS Parameter Estimation of Nonlinear Distribute Finite Element Models

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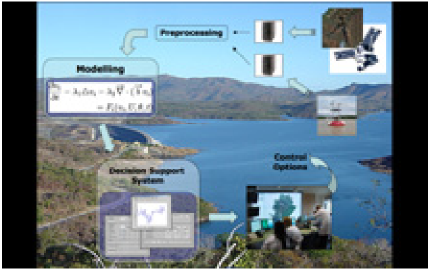
COMSOL Conference 2009. Milan, Italy.

Motivations

Modeling, management and control of aquatic ecosystems
(lakes, large basins, coastal zones, etc.)



- Modeling space and time dynamics of biological and chemical species
- Forecast the future evolution of the systems
- Derive the critical components of the systems

Goal

The main goal of this work concerns the development of

a new direct parameter identification procedure for a class of nonlinear reaction-diffusion equations

Outline

- The model
- Fem discretization
- Parameter identification procedure
- Use of COMSOL Multiphysics
- Simulation results

The Model

Nonlinear reaction-diffusion model

$$\frac{\partial u}{\partial t} - \nabla \cdot (\sigma \nabla u) = F(\theta, u) \quad \text{in } \Omega, \tag{1}$$

where σ is the diffusivity coefficient and $F(\theta, u) = \sum_m^{N_d} \theta_m u^m$.
Subject to suitable initial conditions and Neumann boundary conditions:

$$n \cdot (\sigma \nabla u) = 0 \quad \text{on } \partial\Omega, \tag{2}$$

We suppose that $\Theta = [\sigma, \theta_1, \ldots, \theta_{N_d}]$ is an unknown vector to be estimated.
The parameter estimation procedure is based on the finite element discretization of this model.

FEM discretization

Weak statement of the problem:

$$\left(\frac{\partial v}{\partial t}, w\right)_\Omega - \left(\nabla\left(\sigma \nabla v\right), w\right)_\Omega - (F, w)_\Omega = 0, \tag{3}$$

where $(\cdot,\cdot)_\Omega$ is the usual $L^2(\Omega)$ inner product:

$$(f, g)_\Omega = \int_\Omega f(x)g(x)d\Omega, \quad \forall f, g \in L^2(\Omega). \tag{4}$$

Applying the divergence theorem and using (2) we obtain:

$$\left(\frac{\partial v}{\partial t}, w\right)_\Omega + (\sigma \nabla v, \nabla w)_\Omega - (F, w)_\Omega = 0. \tag{5}$$

FEM discretization

Let V_h be a finite dimensional subspace of $H^1(\Omega)$ spanned by the functions $\left\{\phi_{h1}, \ldots, \phi_{hN_p}\right\}$. Specifically, we consider $\phi_{hi}, i = 1, \ldots, N_p$ as a piecewise polynomials of degree 2 on a quasi uniform triangulation ρ_h of Ω with size h.
We look for a finite element approximation v_h to the solution v of the weak formulation (5) as a linear combination of the finite element basis functions $\phi_i(x)$ with time-dependent coefficients $U_i(t)$, namely:

$$v_h(t, x) = \sum_{i=1}^{N_p} U_i(t)\phi_i(x). \tag{6}$$

FEM discretization

Finite element discretization:

$$L(U) = A\dot{U} + \left(\sigma B - \sum_{m=1}^{N_d} \theta_m M_m(U)\right) U = 0, \tag{7}$$

where $U = \{U_i\}_{i=1}^{N_p}$ and

$$\begin{cases} A = (a_{i,j})_{i,j=1}^{N_p}, a_{i,j} = (\phi_i, \phi_j)_\Omega, \\ B = (b_{i,j})_{i,j=1}^{N_p}, b_{i,j} = (\nabla\phi_i, \nabla\phi_j)_\Omega, \\ M_m(U) = (\mu_{i,j}^m)_{i,j=1}^{N_p}, \\ \mu_{i,j}^m = \int_\Omega \phi_i \left(\sum_{k=1}^{N_d} U_k\phi_k\right)^{m-1} \phi_j d\Omega. \end{cases}$$

This equation will be used for applying the parameter estimation procedure.

Parameter Estimation

The parameter identification procedure is based on the minimization of a cost function, representing the spatial mean square error between simulated and experimental data:

$$\widehat{\Theta} = \arg\min_{\Theta} J(\Theta, \widehat{U}, \bar{U}), \tag{8}$$

where $\bar{U}$ is the vector of real measurements that are assumed to be collected at each time instant in each nodal point of the finite element domain and $\widehat{U}$ is the vector of the model simulation.

Parameter Estimation

Recall equation 7:

$$L(U) = A\dot{U} + \left(\sigma B - \sum_{m=1}^{N_d} \theta_m M_m(U)\right) U = 0,$$

Integrating the equation over a time interval $\Delta_t = [t_i, t_{i+1}]$, gives

$$\frac{U(t_{i+1}) - U(t_i)}{\Delta_t} = \tag{9}$$

$$= A^{-1} \int_{t_i}^{t_{i+1}} \left(-\sigma B + \sum_{i=1}^{N_d} \theta_i M_i(U(t_i))\right) U(t_i) d\tau.$$

Parameter Estimation

Considering Equation (9) for $i = 1, \dots, T-1$, we obtain a linear system of equations in the variable $\Theta := (\sigma, \theta_1, \dots, \theta_{N_d})'$ of the form

$$Y = W\,\Theta, \tag{10}$$

where

$$Y = \left(\frac{U(t_{i+1}) - U(t_i)}{\Delta_t}\right)_{i=1,\dots T-1} \tag{11}$$

and

$$W = \Big(-A^{-1}B \int_{t_i}^{t_{i+1}} U,$$

$$\int_{t_i}^{t_{i+1}} A^{-1} M_1(U(t_i))U(t_i)d\tau, \dots, \tag{12}$$

$$\int_{t_i}^{t_{i+1}} A^{-1} M_{N_d}(U(t_i))U(t_i)d\tau\Big)_{i=1,\dots T-1}.$$

Parameter Estimation

If we replace U by the measurements $\bar{U}$, and approximate the integrals in (9) by numerical quadrature, equation (10) becomes

$$Y \;=\; \widetilde{W}\,\Theta \;+\; e, \tag{13}$$

where e is an error caused by noise and numerical quadrature, and $\widetilde{W}$ is the approximate value of W.
We can now compute a least squares estimate of Θ in (13) as:

$$\Theta_{LS} = (\widetilde{W}'\;\widetilde{W})^{-1}\;\widetilde{W}'Y. \tag{14}$$

This method can be easily implemented in Comsol Multiphysics.

Use of COMSOL Multiphysics

Recall equation 7:

$$L(U) = A\dot{U} + \left(\sigma B - \sum_{m=1}^{N_d} \theta_m M_m(U)\right) U = 0,$$

The Comsol Multiphysics linearization of this finite element model, used in the Newton iteration, is:

$$D(\dot{U} - \dot{U}_0) + K(U - U_0) = L(U_0), \tag{15}$$

where $D = -\partial L/\partial \dot{U}$ and $K = -\partial L/\partial U$ are the mass and the stiffness matrices, respectively.
Computing these matrices for our system leads to:

$$\begin{aligned} D &= -\partial L/\partial \dot{U} = -A, \\ K &= -\partial L/\partial U = -\sigma B + \textstyle\sum_{m=1}^{N_d} \theta_m m M_m(U). \end{aligned} \tag{16}$$

Use of COMSOL Multiphysics

$$D = -\partial L/\partial \dot{U} = -A,$$
$$K = -\partial L/\partial U = -\sigma B + \sum_{m=1}^{N_d} \theta_m m M_m(U).$$

Note that, for different values of $\Theta := (\sigma, \theta_1, \ldots, \theta_{N_d})'$, we are able to obtain different matrices Ks. In particular, we have:

$$\begin{cases} K = B, & \text{for} \quad \Theta = (-1, 0, \ldots, 0)' \\ K = M_m(U), & \text{for} \quad \Theta(m+1) = \frac{1}{m}, \end{cases} \tag{17}$$

with $m = 1, \ldots, N_d$.
This fact allows us to easily compute the approximation $\widetilde{W}$ of W in (14) by the Comsol Multiphysics command *assemble*.

Use of COMSOL Multiphysics

```
fem.Theta(1)=-1;
[A,B] = assemble(fem,'Out',{'D' 'K'})

for t = 1 : T
for m = 1 : Nd
fem.Theta = 0;
fem.Theta(m+1) = 1/m;
Mm(m) = assemble(fem,'Out',{'K'},'U',UM(t));
end
end
```

where UM(t) is the vector of real measurements at time t.

The model parameters can now be easily computed by equation (14).

Simulation Results

In order to numerically validate the results, we suppose that the spatio-temporal dynamics is described by the following nonlinear logistic equation describing the distribution of a population in a domain.:

$$\frac{\partial u}{\partial t} - \nabla \cdot (\sigma \nabla u) = ru\left(1 - \frac{u}{k}\right) \quad \text{in } \Omega. \tag{18}$$

For the parameter identification problem, we set $\Theta = (\sigma, r, r/k)$.

Simulation Results

The vector of real measurements $\bar{U}$ is obtained by simulating the model in a domain $\Omega = (10 \times 10)$ with the following parameter values:

Par.	Value
σ	1e-2
r	1e-1
k	10

and a mesh consisting of 841 nodal points.

Simulation Results

We test the parameter estimation procedure by using different initial conditions and mesh dimension. In particular, we use meshes consisting of and 81, 121 and 256 nodal points and the following initial conditions:

$$u(x, y, 0) = x \tag{19a}$$

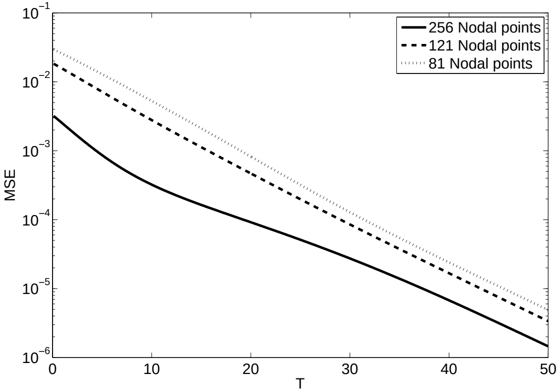
$$u(x, y, 0) = sin\left(\frac{\pi}{2}x\right) + a, \tag{19b}$$

where a is a positive parameter introduced to avoid negative values in the initial state.

The fitting performance is evalueted in terms of the spatial mean square error between measurements $\bar{U}$ and simulated data $\widehat{U}$:

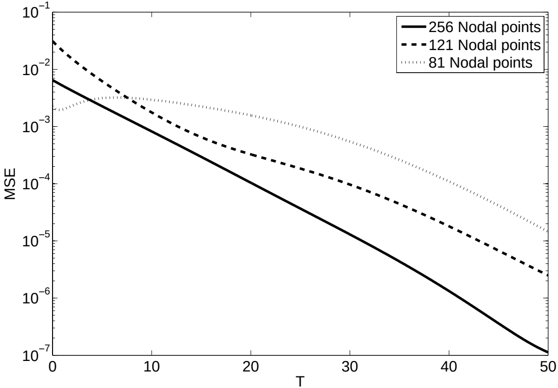
$$\text{MSE(t)} = \frac{1}{N_p}\sum_{i=1}^{N_p}\left(\frac{\bar{U}(i,t) - \widehat{U}(\Theta_{LS}, i, t)}{\bar{U}(i,t)}\right)^2. \tag{20}$$

Simulation Results ($u(x, y, 0) = x$)



Par.	Nominal	$N_p = 81$	$N_p = 121$	$N_p = 256$
σ	1e-2	1.055e-2	0.998e-2	0.967e-2
r	1e-1	0.983e-1	0.989e-1	0.995e-1
k	10	9.999	9.999	9.998

Simulation Results ($u(x, y, 0) = sin\left(\frac{\pi}{2}x\right) + a$)



Par.	Nominal	$N_p = 81$	$N_p = 121$	$N_p = 256$
σ	1e-2	0.875e-2	0.934e-2	0.986e-2
r	1e-1	0.999e-1	0.995e-1	0.999e-1
k	10	9.990	9.996	9.996

Conclusion

- The problem of estimating the parameter of a class of nonlinear reaction-diffusion equations is presented.
- After a finite element discretization of the model, a linear least square method is applied to the resultant system of ordinary differential equations in order to retrieve the parameter values.
- The use of Comsol Multiphysics command *assemble* plays a crucial role in finding the fem matrices.
- The identification procedures are performed by considering two different initial conditions and three mesh dimensions.
- The fitting performances of the estimated models are presented and evaluated in terms of the spatial mean square error.

Future work will concern parameter sensitivity analysis with respect to different initial conditions and mesh dimension. Furthermore, a comparison with nonlinear methods will be considered.