Discrete Mechanics Optimal Control
And Model Predictive Control for
Process Industry
Applications of Numerical Geometric Methods in
Dynamics and Control

Jerrold E. Marsden Memorial Activities

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PROCESS CONTROL PROBLEM

- Moving arm actuator/sensing

MOVING ACTUATOR

- Process Industry: Welding, Drying of mat boards, Steel processing
Multiphysics Process Model

- Model dynamics:
  - Rigid body dynamics
    - inertial & damping properties
    - control constraints
  - Reaction-diffusion model (distributed parameter system)
    - optimal state evolution
    - input/state/output constraints

- Optimal Control formulation & Constraints
  - Discrete mechanics and optimal control (DMOC)
  - Modal model predictive control (MMPC)
OPTIMAL CONTROL PROBLEM
MODEL DYNAMICS

- Mechanical system: rigid body dynamics
  - Inertial, dissipative and elastic forces
    \[ M\ddot{q}(t) + C\dot{q}(t) + kq(t) = f(t) \]

- Reaction-diffusion system
  \[ \frac{\partial x}{\partial t} = \kappa \frac{\partial^2 x}{\partial \zeta^2} + \eta x + b(q(t))u(t), \quad 0 \leq \zeta \leq l \]

- Limited actuator capacity induces input constraints
- Performance considerations induce state constraints
  \[ u_{\text{min}} \leq u(t) \leq u_{\text{max}} \]
  \[ x_{\text{min}} \leq \int_0^l \delta(\zeta_c - \zeta)x(\zeta,t)d\zeta \leq x_{\text{max}} \]
OPTIMAL CONTROL FORMULATION

“compute the actuator force $f(t)$ over a given finite time interval $T$ which brings the system to a desired state while minimizing a user-specified cost function combining the energy required for heating/cooling injected by the actuator as well as the actuator control effort, subject to the dynamics of the catalytic rod and the actuator as well as to temperature and input injection constraints”

$$\min_{u(t), f(t)} \int_0^T \left( \|y(t)\|_Q + \|u(t)\|_R + \|f(t)\| \right) dt$$

$$M\ddot{q}(t) + C\dot{q}(t) + kq(t) = f(t)$$

$$\frac{\partial x}{\partial t} = \kappa \frac{\partial^2 x}{\partial \zeta^2} + \eta x + b(q(t))u(t)$$

$$y(t) = Cx(t)$$

$$u_{\text{min}} \leq u(t) \leq u_{\text{max}}$$

$$x_{\text{min}} \leq \int_0^l \delta(\zeta_c - \zeta)x(\zeta, t)d\zeta \leq x_{\text{max}}$$
CONTROL OF DISSIPATIVE SYSTEMS

  - Lyapunov based and optimal controller synthesis
  - Optimal principles: Pontryagin
  - Constrained optimization

- Recent results:
  - Discrete Mechanics & variational integrators (Marsden & West, 2001)
    - Numerical stability and accuracy
    - Energy preserving and/or momentum preserving schemes

- Standard approach: (Balas, 1979; Ray, 1981; Curtain, 1995; Biegler, 2003)
  - Derivation of ODE models using spatial discretization method
  - Control design using methods for ODEs
CONTROLLER SYNTHESIS

- Discrete mechanics and optimal control (DMOC)
  - Variational integrators
  - Langrange-d’Alembert principle
  - Preservation of properties (momentum, energy)
  - Numerical stability and accuracy
  - Holonomic and nonholonomic constraints

- Model modal predictive control (MMPC)
  - Dissipative parabolic PDEs
  - Discrete methodology
  - Optimality & input/state/output constraints

DMOC and MPC Model-based Controller Synthesis
Discrete Mechanics and Optimal Control

- Mechanical system
  - “Find a trajectory \( q : [0, T] \rightarrow Q \) which minimizes”
  
  \[
  J(q, f) = \int_{0}^{T} \Theta(q(t), f(t))dt
  \]

  subjected to \( M\ddot{q}(t) + C\dot{q}(t) + kq(t) = f(t) \)

  \( \Theta = \frac{1}{2} ||f(t)|| \) or \( \Theta = 1 \) (time)

- Lagrange-d’Alembert variational principle

  \[
  \delta \int_{0}^{T} L(q, \dot{q})dt + \int_{0}^{T} f \cdot \delta q = 0 \rightarrow \partial_t \partial_q L - \partial_q L = f
  \]
Discrete Mechanics and Optimal Control

Discrete Lagrange-d’Alembert principle

- Discretization of variational principle directly:

\[
\delta \int_0^T L(q, \dot{q}) \, dt + \int_0^T f \cdot \delta q = 0
\]

\[
\delta \sum_{k=0}^{N_d-1} L(q_{k+\alpha}, \frac{q_{k+1} - q_k}{h}) + \sum_{k=0}^{N_d-1} f_{k+\alpha} \cdot \delta q_{k+\alpha} = 0
\]

- Discrete Lagrange-d’Alembert variational principle

\[
D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) + f_d^+(q_{k-1}, q_k) + f_d^-(q_k, q_{k+1}) = 0
\]
Example: Simple dynamics in potential field

Falling rigid body

- System’s Lagrangian
  - Kinetic energy: \( E_k(q) = \frac{1}{2} m \dot{q}^2 \)
  - Potential energy: \( E_p(q) = gmq = mV(q) \)
  - Lagrangian
    \[
    L(q, \dot{q}) = E_k(\dot{q}) - E_p(q)
    \]
  - Euler-Lagrange
    \[
    \frac{\partial L}{\partial q} - \frac{d}{dt} \left[ \frac{\partial L}{\partial \dot{q}} \right] = -mg - \frac{d}{dt}(m\dot{q}) = 0
    \]

or define discrete Lagrangian

\[
L_d(q_k, q_{k+1}) = hL(q_k + \frac{1}{2}, \frac{q_{k+1} - q_k}{h})
\]

and discrete analog

\[
D_2L_d(q_{k-1}, q_k) + D_1L_d(q_k, q_{k+1}) = 0
\]

which yields discrete analog to \(-mg = \frac{d}{dt}(m\dot{q})\)

\[
m \frac{q_{k+1} - 2q_k + q_{k-1}}{h^2} = -m \frac{1}{2} \left( \nabla V(q_k - \frac{1}{2}) + \nabla V(q_k + \frac{1}{2}) \right)
\]
**DMOC:** \( M\ddot{q}(t) + C\dot{q}(t) + kq(t) = f(t) \)

- Lagrangian of the system \( L(q, v) = \frac{1}{2} (v^T Mv - q^T Kq) \)
  
  \[ v_k = \frac{q_{k+1} - q_k}{h} \]

  \[ f_d = f(t) - Cv \]

\[ M\frac{v_0 - v(0)}{h} - (1 - \alpha)Kq_0 = (1 - \alpha)(f_\alpha - Cv_0), \]

\[ M\frac{v_k - v_{k-1}}{h} - (1 - \alpha)Kq_{k+\alpha} - \alpha Kq_{k-1+\alpha} \]

\[ = (1 - \alpha)(f_{k+\alpha} - Cv_k) + \alpha(f_{k-1+\alpha} - Cv_{k-1}), \]

\[ M\frac{v(T) - v_{N_d-1}}{h} - \alpha Kq_N = \alpha(f_{N_d-1+\alpha} - Cv_{N_d-1}) \]

for \( k = 1, \ldots, N_d - 1 \). It becomes as \( Aq = C \) system of equations
**DMOC:** \( M\ddot{q}(t) + C\dot{q}(t) + kq(t) = f(t) \)

Parameters: \( L = 10, \; K = 2/L, \; M = 10/L^2, \; C = 10^{-3}/L. \)
LINEAR PARABOLIC PDE

- PDE description:

\[
\frac{\partial x}{\partial t} = -b \frac{\partial^2 x}{\partial \zeta^2} + \alpha x + b(q(t))u(t)
\]

\[
y = \int_0^1 Cx(\zeta, t)d\zeta
\]

- Boundary conditions:

\[
\frac{\partial x}{\partial \zeta}(0, t) = 0, \quad \frac{\partial x}{\partial \zeta}(1, t) = 0
\]

- Input and state constraints:

\[
u^{\text{min}} \leq u(t) \leq u^{\text{max}}
\]

\[
\chi^{\text{min}} \leq \int_0^1 r(\zeta)x(\zeta, t)d\zeta \leq \chi^{\text{max}}
\]

- Typography:
  - \(x(\zeta, t)\) : state variable
  - \(\zeta \in [0, 1]\) : spatial coordinate
  - \(\alpha\) : constant
  - \(\bar{b}\) : diffusion coefficient
INFINITE–DIMENSIONAL SYSTEM FORMULATION

- Infinite dimensional Hilbert space: \( \mathcal{H}([0, 1]; \mathbb{R}) \)
- State function: \( x(t) = x(\zeta, t), x(t) \in \mathcal{H} \)

Operator \( A: A\phi = \bar{b} \frac{d^2 \phi}{d\zeta^2} + \alpha \phi; \) Input operator:
\( B(t)u = b(q(t))u \)
\( \mathcal{D}(A) = \{ \phi(\zeta) \in L_2(0, 1) : \phi(\zeta), \frac{d\phi(\zeta)}{d\zeta} \text{ are abs. cont.}, \ A\phi \in L_2(0, 1), \phi'(0) = 0 = \phi'(1) \} \)

- Representation in \( \mathcal{H} \):
\[
\dot{x}(t) = Ax(t) + B(t)u(t), \ x(0) = x_0 \\
u_{\text{min}} \leq u(t) \leq u_{\text{max}} \\
\chi_{\text{min}} \leq (r, x(t)) \leq \chi_{\text{max}}
\]

- Eigenvalue problem: \( A\phi_j = \lambda_j \phi_j \)
MODEL PREDICTIVE CONTROL
(Muske & Rawlings, AIChE J., 1993)

- LTI description:
  \[
  x_s(k + 1) = \tilde{A}_s x_s(k) + \tilde{B}_s u(k) \\
  y(k) = \tilde{C}_s x_s(k)
  \]

- Regulator is the solution of the infinite horizon open-loop quadratic problem
  \[
  \Phi(k) = \sum_{i=1}^{\infty} x_s(k + i|k)'\tilde{C}_s' Q \tilde{C}_s x_s(k + i|k) + u(k + i|k)' R u(k + i|k)
  \]
  where \( Q = Q' \geq 0, R = R' > 0 \)

- Finite-horizon optimal control:
  \[
  \min_{u(k|k), \ldots, u(k+N-1|k)} \{ \Phi(x_s(k), u(\cdot)) | u(\cdot) \in \mathcal{U}, x_s(k) \in \mathcal{V} \}
  \]

- Finite set of available control input vectors
  \[
  \{u[k] : u(t) = u(k\Delta), \forall \ t \in [k\Delta, (k+1)\Delta] \} 
  \]
MODAL MODEL PREDICTIVE CONTROL

- **Performance index:**

$$\min_u \Phi(x(k), u(k)) = \min_u \sum_{i=0}^{N-1} \left[ x_s(k+i|k)\tilde{C}^T_s Q \tilde{C}_s x_s(k+i|k) + u(k+i|k)' Ru(k+i|k) \right] + x_s(k+N|k)' Q_p x_s(k+N|k)$$

- $[u(k|k), \ldots, u(k+N-1|k)]$ is the minimizer of QP problem:

$$J(k) = \min_{u(k|k), \ldots, u(k+N-1|k)} \Phi(k) + \epsilon^T(k) Q \epsilon(k)$$

$$u^{\min} \leq u(k+i|k) \leq u^{\max}$$

$$G z(k+i|k) \leq g + \epsilon(k) \quad i = 0, 1, \ldots, N$$

- **Stability properties**

- **Set of initial conditions, $\Omega$**

$$\Omega = \Omega(\tilde{A}_s, \tilde{B}_s, U, V, N, Q, R)$$

- **Initially and successively feasible**
\[
\begin{align*}
\min_u \sum_{i=0}^{N-1} & \left[ x_s(t + i|t) \tilde{C}_{sj}^T Q \tilde{C}_{sj} x_s(t + i|t) + u(t + i|t) \tilde{R} u(t + i|t) \right] + \\
+ x_s(t + N|t) & \tilde{Q}_{pj} x_s(t + N|t) + \min_{q_0 : N_d, f_0 : N_d} \sum_{k=0}^{N_d-1} \Theta_d(q_k + \alpha, f_k + \alpha) \\
& x_s(i + 1|t) = \tilde{A}_s x_s(i|t) + \tilde{B}_s(q_k) u(i|t) \\
& x_f(i + 1|t) = \tilde{A}_f x_f(i) + \tilde{B}_f(q_k) u(i|t) \\
& u^\text{min} \leq u(i|t) \leq u^\text{max} \\
& \tilde{S}_{sw} x_s(i|t) \leq x_w^\text{max} - \tilde{S}_{sf} x_f(i|t) \\
& -\tilde{S}_{sw} x_s(i|t) \leq -x_w^\text{min} + \tilde{S}_{sf} x_f(i|t) \\
x_{us}(N) = 0, \quad i = 0, 1, \ldots, N - 1 \\
M^{v_0 - v(0)}_h - (1 - \alpha) K q_0 = (1 - \alpha) (u_\alpha - C v_0) \\
M^{v_k - v_{k-1}}_h - (1 - \alpha) K q_{k+\alpha} - \alpha K q_{k-1+\alpha} = (1 - \alpha) (u_{k+\alpha} - C v_k) + \alpha (u_{k-1+\alpha} - C v_{k-1}) \\
M^{v(T) - v_{N_d-1}}_h - \alpha K q_{N_d} = \alpha (u_{N_d-1+\alpha} - C v_{N_d-1}), \quad k = 1, \ldots, N_d - 1 \\
q_0 = q(0), \quad q_{N_d} = q(T), \quad v(0) = 0, \quad v(T) = 0
\end{align*}
\]
DMOC & MMPC

Actuator arm activation policy algorithm

1. At the time instance $t$ and the given position of actuator $p_j$ and for all $m_a$-prespecified actuator positions, $p_j = [p_1, p_2, \cdots, p_{m_a}]$, a standard linear predictive control program constructed. A DMOC problem is constructed as it is given in for all possible combinations of actuator positions,

2. At the time instance $t$, a quadratic constrained predictive control programs for MPC and DMOC is solved and among the possible actuator moves choose the one that minimizes the cost functional given by:

$$p^* = \arg \min_{p_i} [J(x(t), k, u(\cdot), p_i) + J_{dmoc}(q(k), \dot{q}(k), f(k), p_i, p_j)]$$

3. If the smallest cost implies $p_j \neq p^*$, move arm to $p^*$ and solve the family of the model predictive control programs which are parameterized by the $q(t)$ evolution for each instance of actuator transition from $p_j$ to $p^*$ and applied MPC input as the arm moves in time at each $q_k$

4. Repeat step (1)
DMOC & MMPC
Stabilization of the state of the parabolic PDE by moving actuator
DMOC & MMPC
Moving actuator evolution

$q(t)$ actuator position

$t$
DMOC & MMPC
Closed loop system
DMOC & MMPC

Constrained input evolution
SUMMARY

- DMOC and MMPC of rigid body dynamics and linear parabolic PDE distributed process system

Optimal stabilization in the presence of input constraints

- Methodology for stabilization of PDEs by predictive control techniques under the presence of state/input constraints

- Discrete mechanics and optimal control
  - Order reduction using modal decomposition
  - Model predictive optimization framework
  - Low-order modal model predictive controller designs that achieve:
    - PDE stabilization
    - Control constraints satisfaction

- Thank you Jerry for your encouragement in efforts to bring Discrete Mechanics and Process Control closer