A few of the ideas I learned from Soto and some applications

Carmen Chicone
chiconeC@missouri.edu
Department of Mathematics
University of Missouri

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Outline

- Mathematical ideas with broad brush, details for another time.
- A few mathematical moments with Soto
  - Libraries
  - Two-dimensional variational equations
  - Fiber contraction
  - Mathematicians and numerics
- Ceramic binder burnout
  - Optimal Control
  - Pseudo Steady State Approximation
- Oscillating Heat Pipes
  - Modeling
  - Hopf, Hopf-Hopf, . . .
  - Smoothed Particle Hydrodynamics (SPH)

Memories

- First meeting: Early 1980s.
- Visits to IMPA; reciprocal visits to Math Department at University of Missouri.
- Repository of Knowledge
  - Love of books and libraries.
  - Late for lunch while browsing stacks in the MU Engineering Library.
- At IMPA: Introduced me to the paper of S. Diliberto, who solved the variational equations for a planar system in geometric quadrature. For a solution $t \mapsto \phi_t(\xi)$ of $\dot{x} = f(x)$,

$$
\begin{aligned}
\dot{W} &= Df(\phi_t(\xi))W, \qquad W(0) = I, \\
W(t)f(\xi) &= f(\phi_t(\xi)), \\
W(t)f^{\perp}(\xi) &= a(t,\xi)f(\phi_t(\xi)) + b(t,\xi)f^{\perp}(\phi_t(\xi)),
\end{aligned}
$$

  where a and b are integrals of $\operatorname{div} f$, $\operatorname{curl} f$, and κ along $t \mapsto \phi_t(\xi)$.

Fiber Contraction Principle

- Lleida Spain, while others enjoyed a grand banquet
- A bundle map $\Gamma : X \times Y \to X \times Y$, for X and Y metric spaces, given by $\Gamma(x, y) \mapsto (\Lambda(x), \Psi(x, y))$, is a fiber contraction if $y \mapsto \Psi(x, y)$ is a contraction for each x and the contraction constants are uniformly bounded above over X.
- Theorem (C. Pugh 60s): If Γ is continuous, the base map Λ has a globally attracting fixed point x_∞, and y_∞ is a fixed point of $y \mapsto \Psi(x_\infty, y)$, then (x_∞, y_∞) is a globally attracting fixed point of Γ.
- Completeness not required.

Application of Fiber Contraction

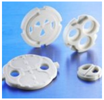
- X is a closed subset of the Banach space $C_b(A, B)$ of bounded continuous functions between two Banach spaces A and B.
- $\Lambda : X \to X$ is a contraction with $\Lambda(\alpha) = \alpha$.
- Is α in $C^1(A, B)$?
- If $\beta \in C^1(A, B)$ and $\Lambda(\beta) \in C^1(A, B)$, then $D\Lambda(\beta) \in Y := C(A, L(A, B))$. Then for $\Phi \in L(A, B)$, there is $\Psi(\beta, \Phi) = D\Lambda(\beta)\Phi$ and bundle map $\Gamma : X \times Y \to X \times Y$ given by $\Gamma(\beta, \Phi) = (\Lambda(\beta), \Psi(\beta, \Phi))$.
- Pick $\alpha_0 \in C^1(A, B)$ and $\Phi_0 := D\alpha_0$, define $(\alpha_{n+1}, \Phi_{n+1}) = \Gamma(\alpha_n, \Phi_n)$ and prove
  (1) Γ is a continuous fiber contraction
  (2) $\Phi_n = D\alpha_n$
  (3) convergence to Fiber Contraction Limit (α, Φ_∞) is uniform.
  Then α is differentiable with derivative Φ_∞.
- Idea applies to smoothness of solutions of ODEs, invariant manifolds, and operator equations. Where else?

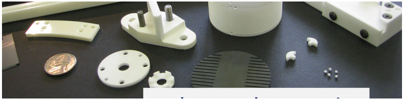
What mathematicians should do and what should be left for applied mathematicians and numerics

- Soto and I were considering a bifurcation problem. He offered a clear vision for mathematical analysis.
  - As usual, he already knew what would be true.
  - Mathematicians should prove a description of all local bifurcations.
  - "Global" bifurcations are generally beyond current understanding; leave them for numerical investigation.
- Basic training and practice: genericity, hyperbolicity, linearization at invariant sets, continuation, and bifurcation.
- This paradigm is being generalized from finite to infinite-dimensional dynamical systems (PDEs).
- Computation is currently dominant in applied mathematics. Correct answers? What about the rest of parameter space?
- What are the useful great challenges in Dynamical Systems?

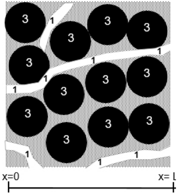
Second Half of Talk, Topic 1: Binder Burnout

- Collaborators (Engineers): Steve Lombardo, David Retzloff
- Aluminum Oxide Ceramic Industrial Parts:





- Binder burnout schematic:



with ceramic (3), polymer binder (grey), gas exhaust pore (1).

Process Problem

- Kiln temperature is raised to burn off the binder.
- Outgassing changes pressure in pores.
- Green body might crack.
- Low temperature means long process time (several days).
- Problem: What is the least time optimal temperature control?
- Common Sense:
  - Determine pressure as function of temperature.
  - Set pressure upper bound.
  - Raise temperature as fast as possible without exceeding bound.
- Currently no practical way to incorporate sensors.
- Modeling problem is open-ended: more complete physics (usually) implies new optimal temperature protocol.

Modeling

- Binder ϵ_2, gas density ρ, and temperature T model:

$$
\begin{aligned}
(\epsilon_2)_t &= -A\exp\left(\frac{-E}{RT(t)}\right)\epsilon_2, \\
(\epsilon\rho)_t &= \frac{\kappa RT(t)}{\mu}\nabla\cdot(\rho\nabla\rho) + \frac{\rho_2}{M}A\exp\left(\frac{-E}{RT(t)}\right)\epsilon_2, \\
\epsilon+\epsilon_2 &= 1-\epsilon_3\,\text{(a constant)}, \\
RT(t)\rho(x,t) &= P_0,\ \ x\in\partial\Omega\,\text{(essential boundary condition)}
\end{aligned}
$$

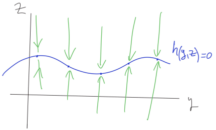
- $\rho\nabla\rho$ (not $\nabla\rho$) makes PDE a porous medium equation.
- Dynamic pressure $(x,t)\mapsto RT(t)\rho(x,t)$ is constrained.
- Set $\delta>0$. Given admissible T, evolve until $\epsilon_2(t_f)\le\delta$.
- Problem: Find T that minimizes functional $T\mapsto t_f$.
- We worked on and solved this problem: Proved OC exists and developed viable algorithm to find it.

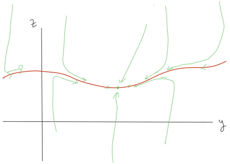
Optimal Control (OC)

- Binder burnout is TOC problem with state and control constraints.
- Maximize $\Lambda(q,u) := \int_{t_i}^{t_f} L(q,u,t)\,dt$ subject to $\dot{q} = f(q,u,t)$ with q specified at t_i or t_f and possibly other constraints.
- Classical calculus of variations when $\dot{q} = u$.
- Calculus of variations view of OC culminates in Pontryagin's Maximum Principle:
- Define control Hamiltonian:
  $H(q,u,p,t) := \langle p, f(q,u,t)\rangle - L(q,u,t)$
  for admissible control $u(t) \in \mathcal{A}$. The optimal state q^* and costate p^* satisfy Hamilton's equations: $\dot{q} = H_p,\ \dot{p} = -H_q$ and
  $$H(q^*(t), u^*(t), p^*(t), t) := \max_{u(t)\in\mathcal{A}} H(q^*(t), u, p^*(t), t).$$
- For linear ODE almost complete understanding; for nonlinear ODE or PDE not so much! BVPs are important.

Pseudo Steady State Approximation PSSA or Quasi Steady State Approximation (QSSA)

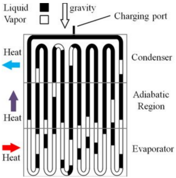
- Rate equations in biochemistry model might be
$$\dot{y} = g(y,z), \quad \dot{z} = H(y,z)$$
- During measurement z (usually intermediate reactant concentration) changes slowly. Maybe $\dot{z} = \epsilon h(x,y)$ and $0 < |\epsilon| \ll 1$.
- In principle, you know what to do:

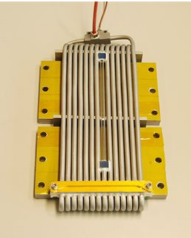




- In chemistry this is called the PSSA.
- $(\epsilon_2)_s = -a\exp(-\frac{\gamma}{\Gamma(s)})\epsilon_2$,
$(\epsilon\eta)_s = \Gamma(s)q(\epsilon)(\epsilon\eta(\epsilon\eta)_\xi)_\xi + c\exp(-\frac{\gamma}{\Gamma(s)})\epsilon_2$.
- Maybe $(\epsilon\eta)_s \approx 0$, then PSSA for PDE.

Oscillating Heat Pipe: Z.C. Feng, S. Lombardo, D. Retzloff





- Device for heat transport with no moving mechanical parts.
- Two-phase flow (liquid and vapor) in a narrow serpentine tube through a hot and cold zone.
- Evaporation, condensation, and vapor pressure cause the motion.
- Ideal: Efficient heat transfer from hot to cold zone.
- Current main application: cooling of electronic equipment

Oscillating Heat Pipe: Startup Problem

- Configuration space is a circle.
- $$\gamma_i \ddot{\theta}_i + \nu \gamma_i \dot{\theta}_i = \frac{\phi_i}{\beta_i} - \frac{\phi_{i+1}}{\beta_{i+1}},$$
  $$\dot{\phi}_i = \mathrm{ev}(\theta_{i-1} + \gamma_{i-1}) + \mathrm{ev}(\theta_i), \quad i = 1, 2, \ldots, n, \ i + n \equiv i.$$
- θ is clockwise left-end meniscus position of liquid slug and ϕ/β is pressure.
- ev is nonlinear evaporation function; its parameters involve the difference of hot and cold zone temperatures and wall temperatures along the OHP.
- All liquid in cold zone, cold zone filled, and zero velocities at menisci corresponds to equilibrium of ODE system.

Results

- Proposition: There is a function of temperature σ (evaporation rate) such that at $\sigma = \nu$ a bifurcation occurs; Linearization at equilibrium has only negative, zero, and pure imaginary eigenvalues.
- Theorem: For $n = 2$, a supercritical nondegenerate Hopf bifurcation occurs. Because of zero eigenvalues, reduction to center manifold was required to apply Hopf's theorem and compute the stability index.
- For case $n = 3$ at least some cases of Hopf-Hopf are required. In general, multiple pairs of complex conjugate eigenvalues cross the imaginary axis. Exactly what happens is an open problem.
- As usual in applied mathematics, the system has special features. Maybe unknown full Hopf-Hopf bifurcation is not needed. But, this is an open question.

OHP operation

- The startup model is not viable for OHP dynamics; fluid slugs may merge and boiling may create new slugs.
- Multiphysics modeling is possible; perhaps a partially phenomenological model will reveal correct qualitative behavior.
- Smoothed Particle Hydrodynamics (SPH) might be a viable methodology.

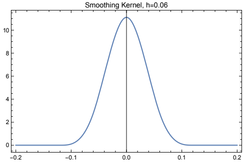
SPH (Monaghan, Gingold, Lucy *circa* 1977

- Imagine a flow of particles, perhaps embedded in a gas or liquid and their dual nature:
  - particles of the substance
  - interpolation points
- Multiphysics modeling is possible; but, perhaps a partially phenomenological model will reveal correct qualitative behavior.
- Smoothed Particle Hydrodynamics (SPH) might be a viable methodology.

SPH

- Fundamental Continuum Lagrangian: $\mathcal{L} = \int \rho(\frac{1}{2}v \cdot v - u(\rho, S))\, dV$.
- Discretize: $dV_j = m_i/\rho_i$ and suppose entropy is constant (?) along particle trajectories. $L = \sum_{j=1}^{N} m_j(\frac{1}{2}v_j \cdot v_j - U(\rho_j))$
- Equations of motion: $\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q}$ are discrete version of Euler's equations. Conservation laws are automatically satisfied.
- $m_j \dot{v}_j = \frac{\partial U}{\partial \rho}\frac{\partial \rho}{\partial x}$.
- From 1st Law of Thermodynamics $dU = Tds - pd\mathcal{V}$.
- With volume viewed as inverse density, $dU = Tds - pd(\frac{1}{\rho}) = Tds + \frac{p}{\rho^2}d\rho$.
- So, formally at least, $\frac{\partial U}{\partial \rho} = \frac{p}{\rho^2}$.

SPH



- Now SPH: For a positive and normalized smoothing kernel w, the SPH bridge between discrete and continuous is $\rho(x) = \sum_{j=1}^{N} m_j w(x - x_j, h)$.
- It leads to the foundational model: $\dot{x}_i = v_i$, $\dot{v}_i = -\sum_{\substack{j=1 \\ j\neq i}}^{N} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) w'(x_j - x_i)\frac{x_j - x_i}{|x_j - x_i|} + \frac{f_i}{\rho_i}$, which is closed by an equation of state $p = g(\rho)$.
- Two phase flow can (with difficulty) be implemented using two different particle masses. What motion is predicted?
- Toy examples with special features where a dynamical system analysis can be done might be insightful. Does SPH always agree with Euler? What happens when parameters are changed?

In Memorium

Many cast about in love, work, and play as time passes too quickly. Few find true love, create enduring work, and have a positive and lasting influence on their community. We honor one of the outstanding few today. Thank you Soto.

Optimal Control History

- Wonderful Article: H. Sussmann and J. Willems *300 Years of Optimal Control*, IEEE, 1997
- Main takeaway: Hamilton wrote down the wrong Hamiltonian
- Hamilton said $\dot{p} = \frac{\partial L}{\partial \dot{q}}(q, \dot{q}, t)$ and $H(q, p, t) = \langle q, \dot{q} \rangle - L(p, \dot{q}, t)$

Pontryagin's maximum principle

The main result on necessary conditions for time optimal control is of course the Pontryagin Maximum Principle (PMP). It is usually stated for the classic problem where the dynamic is $\dot{x} = f(x, u)$ with initial state $x(0) = x_0 \in \mathbb{R}^k$ and a payoff function

$$G(u) = \int_0^\tau g(x(t), u(t))\, dt$$

where g is some running payoff function and τ is defined to be the first time the state reaches some preassigned surface $\mathcal{S}$. The (free time, fixed endpoint) problem is to find u^* that maximizes the payoff. Here the control theory Hamiltonian is defined by

$$H(x, p, \upsilon) = \langle f(x, \upsilon), p \rangle + g(x, \upsilon).$$

The PMP states that if u^* is the control policy that maximizes the payoff and x^* is the corresponding solution of the dynamical system, then there is a function $p^* : [0, \tau^*] \to \mathbb{R}^k$ (called the co-state)

Maximum Principle

such that

$$\dot{x}^* = H_p(x^*, p^*, u^*),$$
$$\dot{p}^* = -H_x(x^*, p^*, u^*),$$

the boundary conditions for x are satisfied (that is, the initial data and the final point on $\mathcal{S}$), the maximum principle holds

$$0 = H(x^*(t), p^*(t), u^*(t)) = \max_{\upsilon \in U} H(x^*(t), p^*(t), \upsilon), \quad 0 \leq t \leq \tau^*,$$

and the transversality condition holds: final costate $p(\tau*)$ is orthogonal to the surface $\mathcal{S}$.
For time-optimal control (TOC) the running payoff is given by $g(x, \upsilon) = -1$.

Maximum Principle

The maximum principle for optimal control problems with state constraints is complicated by the nature of the constraints. In case the constraint is in the form of a simple inequality, say $g(x(t)) \leq 0$, the formulation takes a simple form. As in the usual context for Lagrange multipliers when a constraint is present, suppose that x happens to lie in the boundary of the constraint set for some portion of the time interval on which it is defined; that is, $g(x(t)) = 0$ for some time interval. Then, of course,

$$\nabla g(x(t))\dot{x}(t) = 0.$$

Maximum Principle

Let $c : \mathbb{R}^k \times \mathbb{R}^k \to \mathbb{R}$ be the function defined by $c(x,u) = \nabla\langle g(x), f(x,u)\rangle$. As before, suppose that u^* and x^* are the optimal control and corresponding state trajectory. If x^* is not in the boundary of the constraint, then the usual maximum principle applies. If x^* is in the boundary on some interval of time, then there is a co-state p^* and a function $\lambda^* : \mathbb{R} \to \mathbb{R}$ defined on this interval such that the dynamical system associated with the problem is solved by x^* and u^*, the co-state solves

$$\dot{p}^* = -H_x(x^*, p^*, u^*) + \lambda c_x(x^*, u^*)$$

and

$$H(x^*(t), p^*(t), u^*(t)) = \max_{\upsilon \in U}\{H(x^*(t), p^*(t), \upsilon) : c(x^*(t), \upsilon)\} = 0.$$

Of course, λ is akin to a Lagrange multiplier and the constraint also constrains the admissible controls.