Future Perspectives on Control of Parabolic PDEs with Moving Boundaries

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DPS Online Seminar, June 8th, 2021, Virtual

Outline

1. Stefan problem: Thermal phase change model of parabolic PDE with a moving boundary

2. Other Stefan-type systems in chemical and biological models

3. Open problems of parabolic PDEs with moving boundaries

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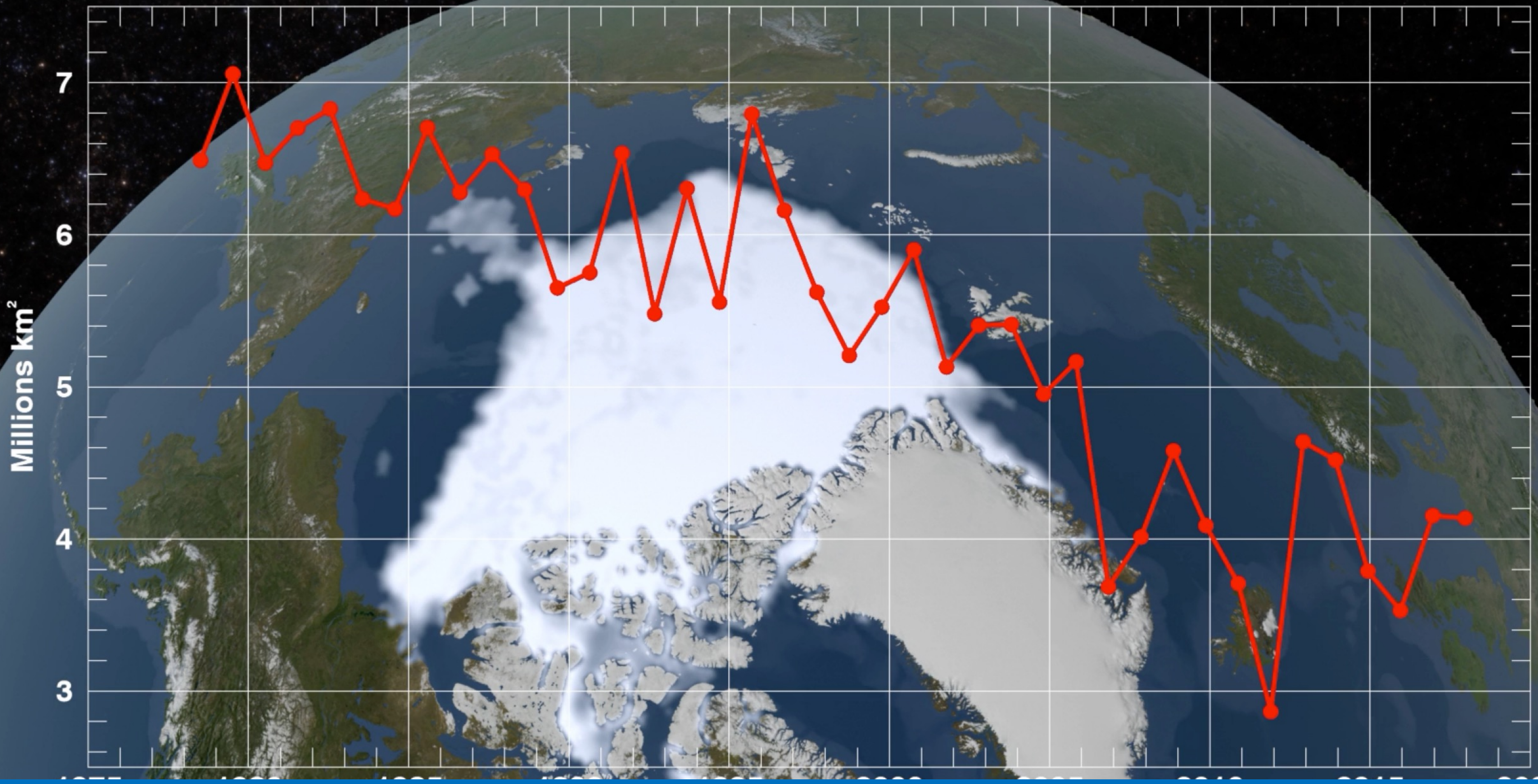
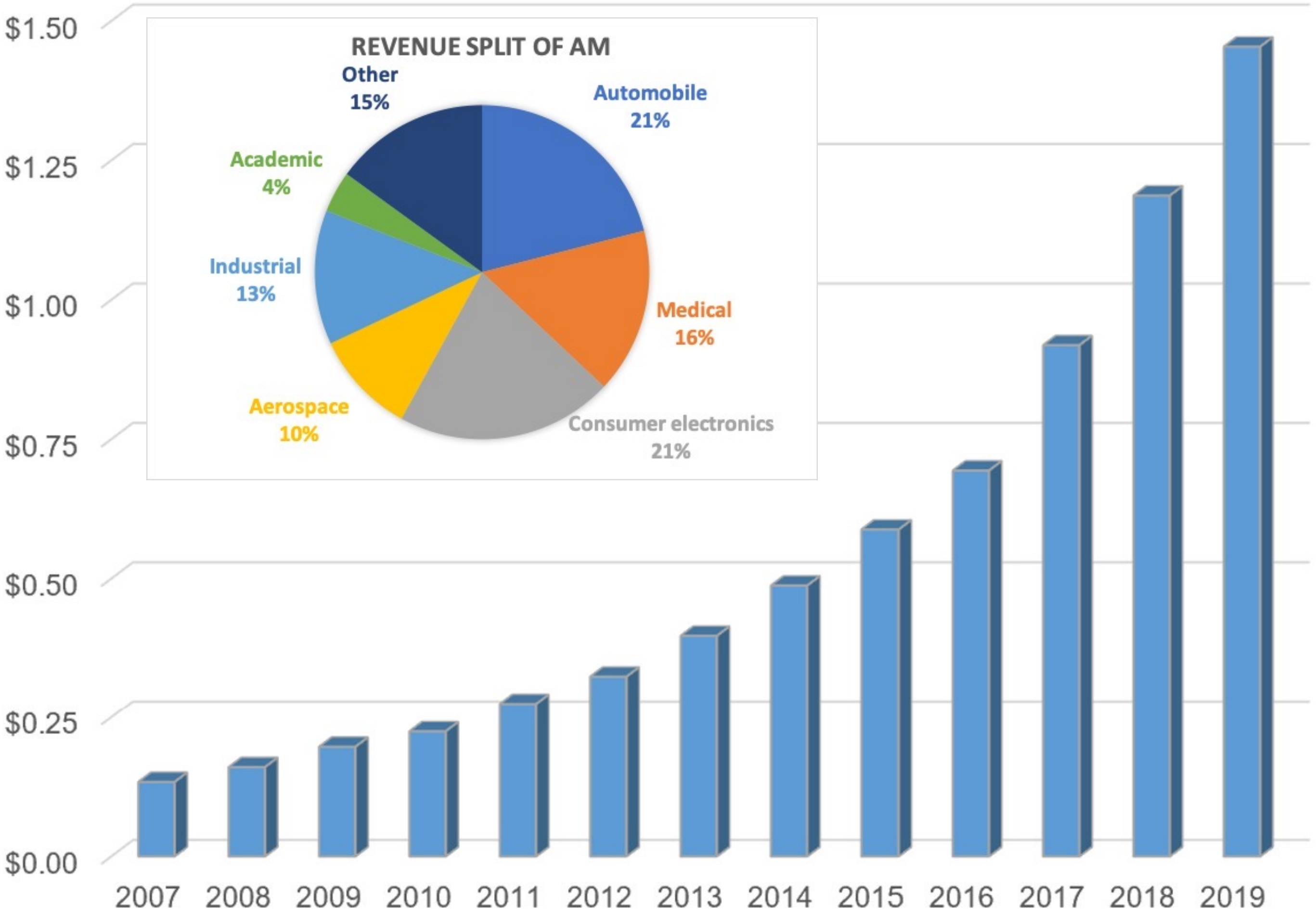
Annual Arctic Sea Ice Minimum Area

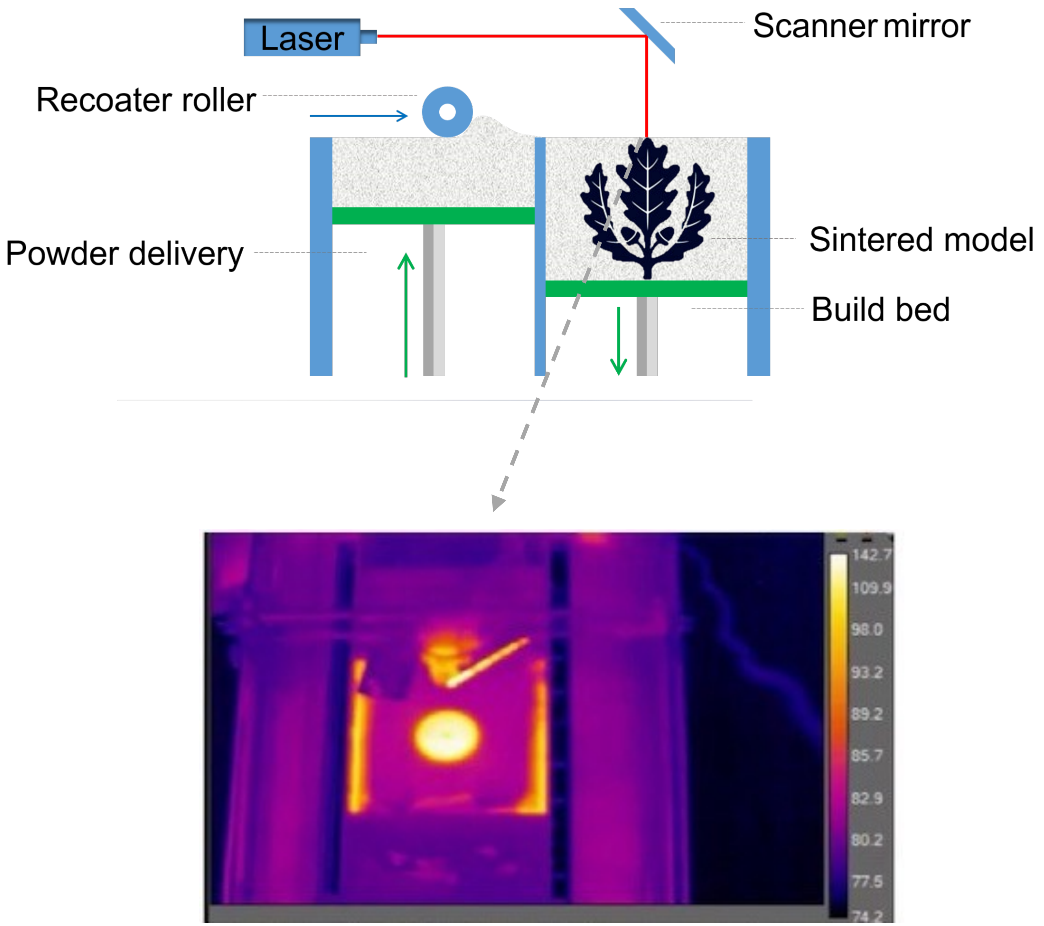


Recent study reports that Arctic will see **<u>“ice-free" summer by 2050</u>**, deduced from majority of simulation models [D. Norz, et al, 2020].

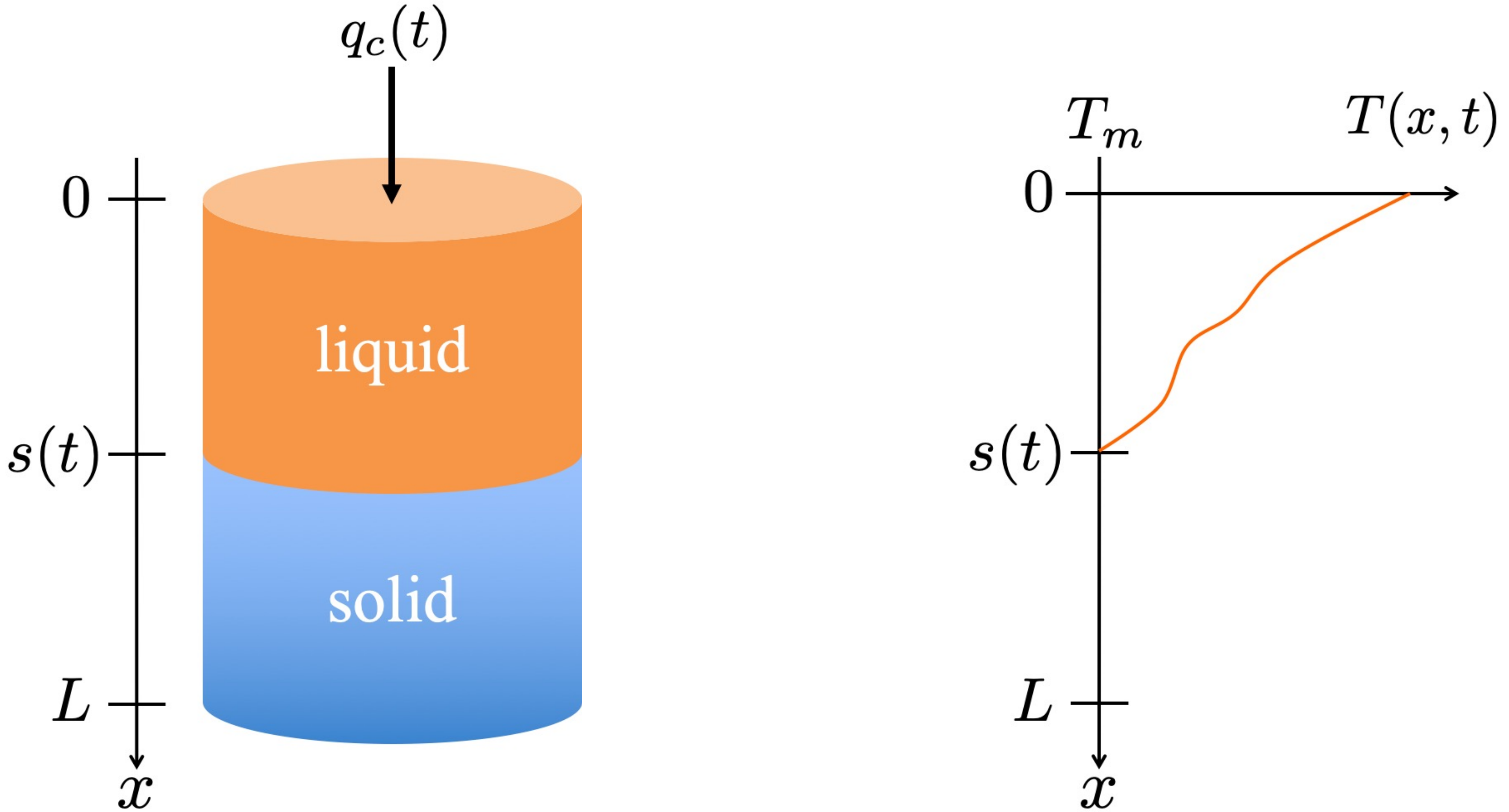
Growth of Additive Manufacturing, a.k.a. 3D-printing



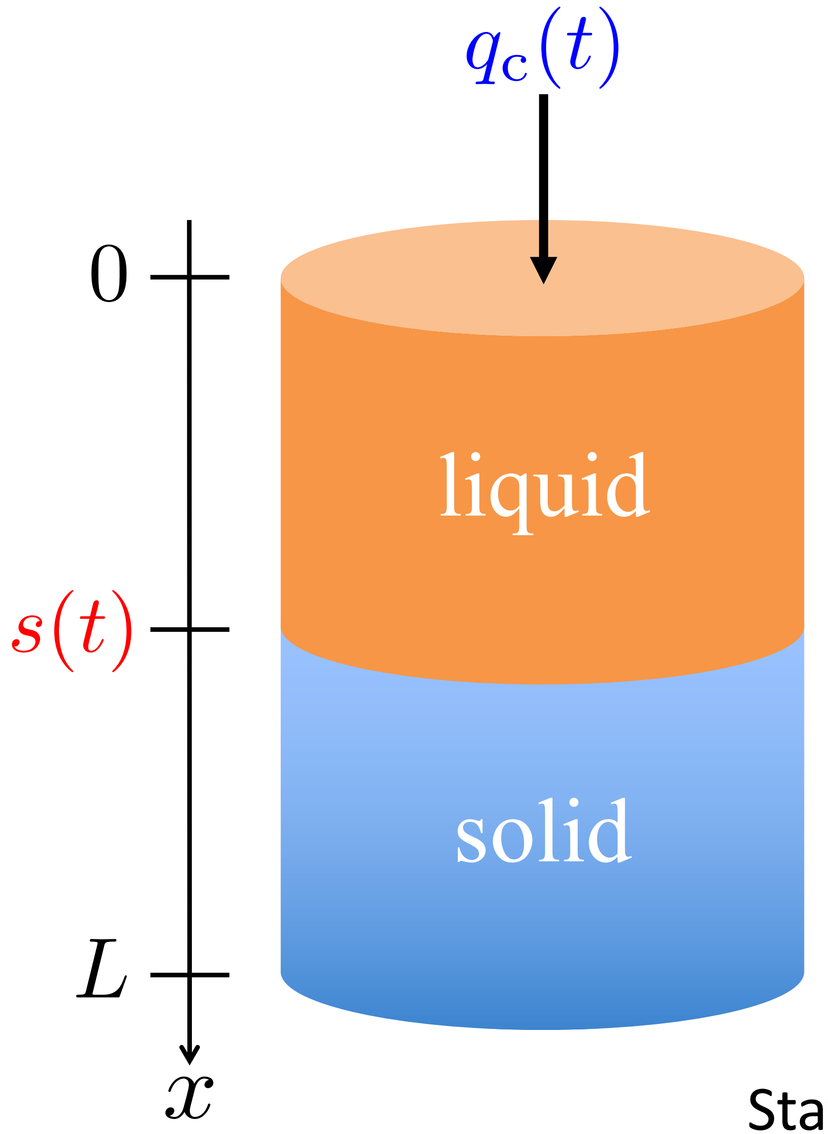
Money spent annually on final part production by AM worldwide
Values are in billions of dollars. Source: Wohlers Report 2020



1-D Schematic of Thermal Phase Change



Stefan Problem



$$\frac{\partial T}{\partial t}(x,t) = \alpha \frac{\partial^2 T}{\partial x^2}(x,t), \quad 0 < x < s(t)$$

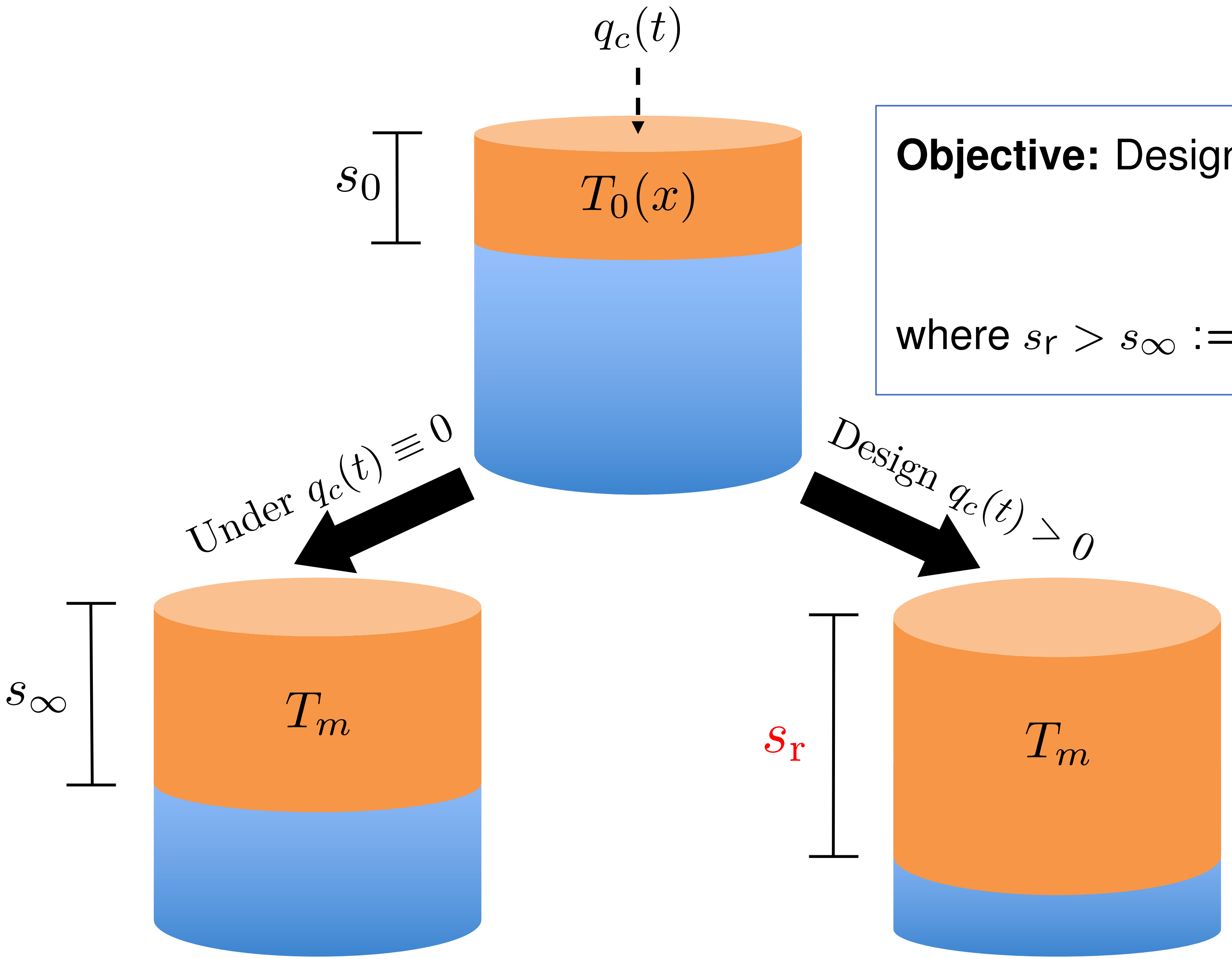
$$-k\frac{\partial T}{\partial x}(0,t) = q_c(t)$$

$$T(s(t),t) = T_m$$

$$\frac{ds(t)}{dt} = -\beta \frac{\partial T}{\partial x}(s(t),t)$$

State-dependent moving boundary → *geometric nonlinearity*

Control Problem



Objective: Design heat control $q_c(t) > 0$ to achieve

$$s(t) \to s_r \quad \text{as} \quad t \to \infty$$

where $s_r > s_\infty := s_0 + \frac{\beta}{\alpha} \int_0^{s_0} (T_0(x) - T_m) dx$.

Control Design by Backstepping

1. Define $(u, X) := (T - T_{\mathsf{m}}, s - s_{\mathsf{r}})$, and obtain (u, X)-system

$$
\begin{aligned}
u_t(x,t) &= \alpha u_{xx}(x,t) \\
-k u_x(0,t) &= q_{\mathrm{c}}(t) \\
u(s(t),t) &= 0 \\
\dot{X}(t) &= -\beta u_x(s(t),t)
\end{aligned}
$$

Control Design by Backstepping

1. Define $(u, X) := (T - T_{\mathrm{m}}, s - s_{\mathrm{r}})$, and obtain (u, X)-system

2. Develop a state transformation $(u, X) \Rightarrow (w, X)$ (and its inverse) s.t. (w, X)-system has a stabilizing term

$$w = u - \int_x^{s(t)} k(x,y)u(y,t)dy - \phi(x - s(t))X$$

$$\begin{aligned} u_t(x,t) =& \alpha u_{xx}(x,t) \\ -ku_x(0,t) =& q_c(t) \\ u(s(t),t) =& 0 \\ \dot{X}(t) =& -\beta u_x(s(t),t) \end{aligned}$$

$$\begin{aligned} w_t(x,t) =& \alpha w_{xx}(x,t) + \dot{s}\phi(x-s)X \\ -kw_x(0,t) =& q_c(t) - \cdots \\ w(s(t),t) =& 0 \\ \dot{X}(t) =& -cX(t) - \beta w_x(s(t),t) \end{aligned}$$

$$u = w - \int_x^{s(t)} l(x,y)w(y,t)dy - \psi(x - s(t))X$$

Control Design by Backstepping

1. Define $(u, X) := (T - T_{\mathrm{m}}, s - s_{\mathrm{r}})$, and obtain (u, X)-system

2. Develop a state transformation $(u, X) \Rightarrow (w, X)$ (and its inverse) s.t. (w, X)-system has stabilizing terms

$$w = u - \int_0^{s(t)} k(x, y)u(y, t)dy - \phi(x - s(t))X$$

$$\begin{aligned} u_t(x,t) =& \alpha u_{xx}(x,t) \\ -ku_x(0,t) =& q_c(t) \\ u(s(t),t) =& 0 \\ \dot{X}(t) =& -\beta u_x(s(t),t) \end{aligned}$$

$$\begin{aligned} w_t(x,t) =& \alpha w_{xx}(x,t) + \dot{s}\phi(x-s)X \\ -kw_x(0,t) =& q_c(t) - \cdots \\ w(s(t),t) =& 0 \\ \dot{X}(t) =& -cX(t) - \beta w_x(s(t),t) \end{aligned}$$

$$u = w - \int_0^{s(t)} l(x, y)w(y, t)dy - \psi(x - s(t))X$$

3. Design $q_{\mathrm{c}}(t)$ to cancel redundant $\cdots$ terms

Equivalence with Energy-Shaping

Potential energy (as reference error)

$$E(t) = \frac{k}{\alpha}\int_0^{s(t)} (T(x,t) - T_{\mathrm{m}})dx + \frac{k}{\beta}(s(t) - s_{\mathrm{r}})$$

satisfies

$$\frac{dE(t)}{dt} = q_{\mathrm{c}}(t)$$

The designed BKS controller *happens to be*

$$q_{\mathrm{c}}(t) = -cE(t)$$

which is *equivalent* to an energy-shaping (ES) control.

$$q_{\mathrm{c}}(t) = q_{\mathrm{c}}(0)e^{-ct} \geq 0$$

constraint is satisfied

Theoretical Result [1]

Theorem: Under the control law

$$q_{\mathrm{c}}(t) = -c\left(\frac{k}{\alpha}\int_0^{s(t)}(T(x,t)-T_{\mathrm{m}})dx + \frac{k}{\beta}(s(t)-s_r)\right)$$

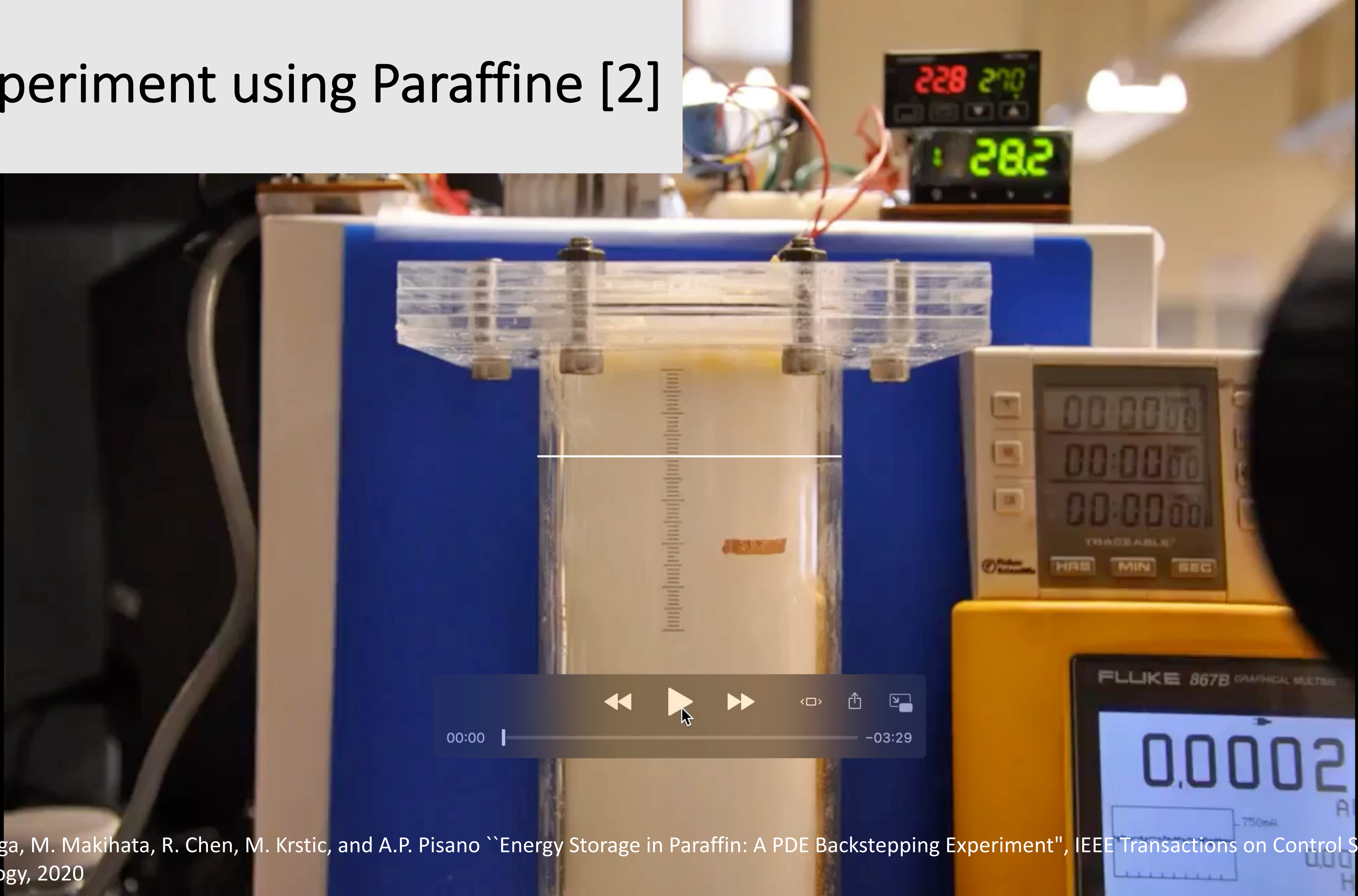
where $c > 0$, the closed-loop system satisfies

- constraints $q_{\mathrm{c}}(t) > 0$, $T(x,t) \geq T_{\mathrm{m}}$,
- global exponential stability in the norm $||T - T_{\mathrm{m}}||^2_{\mathcal{H}_1} + (s - s_r)^2$, i.e.,

$$s(t) \to s_r \quad \text{as} \quad t \to \infty$$

[1] S. Koga, M. Diagne, M. Krstic, ``Control and State Estimation of One-Phase Stefan Problem via Backstepping Design", IEEE Transactions on Automatic Control, 2019

Experiment using Paraffine [2]



[2] S. Koga, M. Makihata, R. Chen, M. Krstic, and A.P. Pisano ``Energy Storage in Paraffin: A PDE Backstepping Experiment'', IEEE Transactions on Control Systems Technology, 2020

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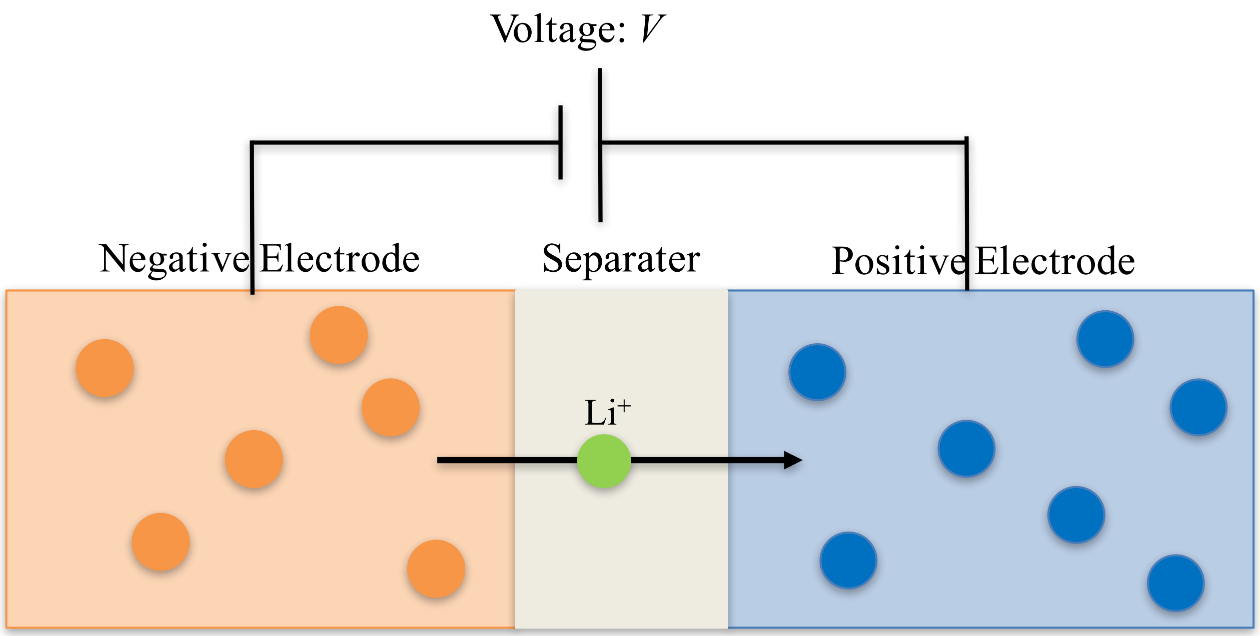
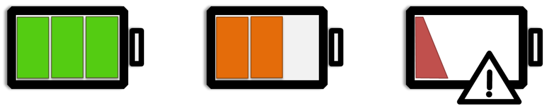
Lithium-ion batteries [3]



State-of-Charge (SoC) Estimation

Given: Input current I and output voltage V

Estimate: Total amount of lithium ion in each electrode.



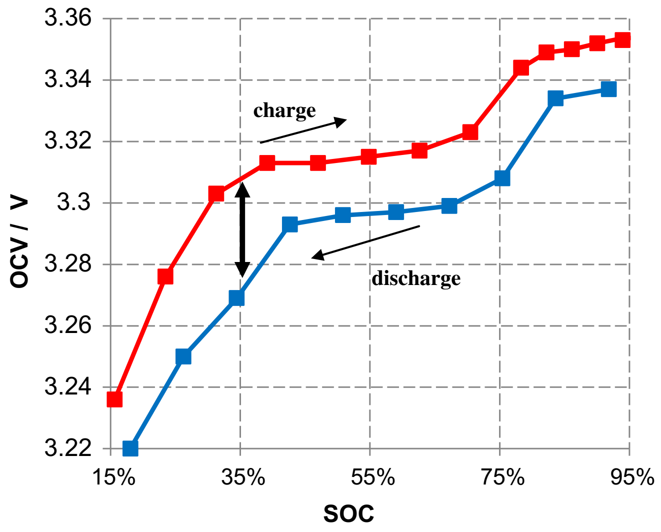
[3] S. Koga, L. Camacho-Solorio, and M. Krstic ``State Estimation of Lithium-Ion Batteries with Phase Transition Materials via Boundary Observers," ASME Journal of Dynamic Systems, Measurement, and Control, under review

Charge-Discharge Cycle of LFP

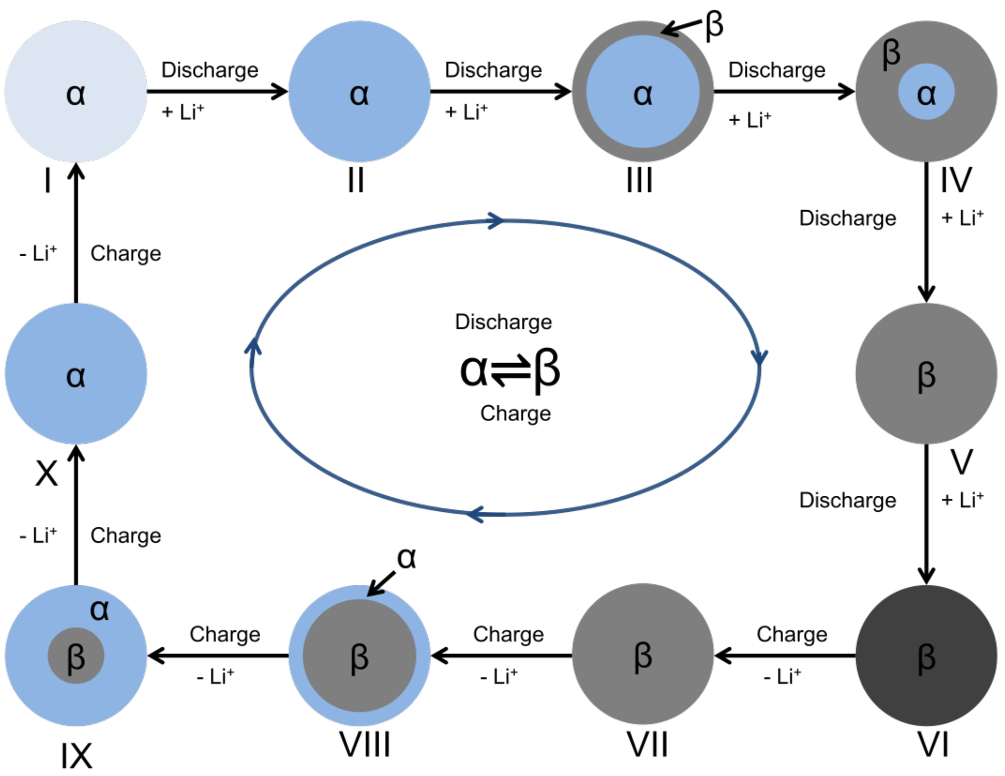
$LiFePO_4$ (LFP) is attractive due to *thermal stability* and *cost effectiveness*

$$FePO_4 + Li^+ + e^- \rightleftharpoons LiFePO_4$$

α-phase β-phase



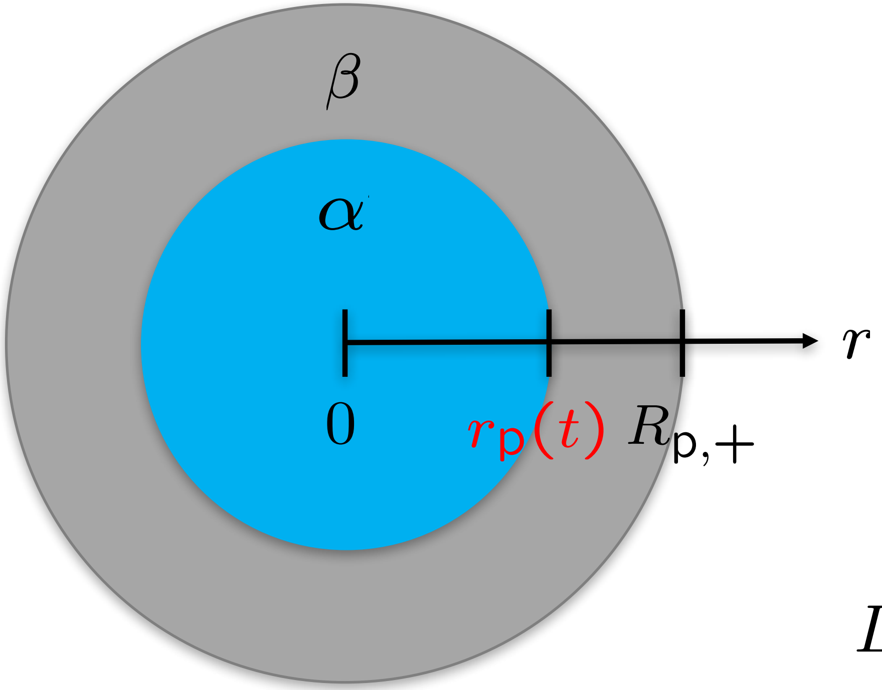
How to model such ***Hysteresis***?



α - Li poor phase
β – Li rich phase

Fig. by A. Khandelwal, et al, JPS 2014

Stefan Model of LFP (by Srinivasan and Newman 2004)



$c(r,t)\cdots$ concentration of lithium-ion in positive electrode

Measurement: Output voltage V, which gives surface concentration $c(R_p,t)$.

$$\frac{\partial c}{\partial t}(r,t) = \frac{D}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial c}{\partial r}(r,t)\right], \quad r \in (r_\mathrm{p}(t), R_\mathrm{p})$$

$$c(r_\mathrm{p}(t),t) = c_{\mathrm{s},\beta},$$

$$D\frac{\partial c}{\partial r}(R_\mathrm{p},t) = -j(t),$$

$$\frac{\mathrm{d}r_\mathrm{p}(t)}{\mathrm{d}t} = -B\frac{\partial c}{\partial r}(r_\mathrm{p}(t),t).$$

Observer Design

Challenge: Estimation *without* knowing moving boundary $r_\mathrm{p}(t)$

Idea:

(Step1) Design observer $\widehat{c}$ assuming $r_\mathrm{p}(t)$ is known,

$$\begin{aligned} \frac{\partial \widehat{c}}{\partial t}(r,t) =& \frac{D}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial \widehat{c}}{\partial r}(r,t)\right] + P(r_\mathrm{p}(t), r)\left[c(R_\mathrm{p},t) - \widehat{c}(R_\mathrm{p},t)\right], \\ \widehat{c}(r_\mathrm{p}(t),t) =& c_\beta, \\ D\frac{\partial \widehat{c}}{\partial r}(R_\mathrm{p},t) =& -j(t) + Q(r_\mathrm{p}(t))\left[c(R_\mathrm{p},t) - \widehat{c}(R_\mathrm{p},t)\right], \end{aligned}$$

The gains (P, Q) are derived via backstepping (BKS) method.

Observer Design

Challenge: Estimation *without* knowing moving boundary $r_{\mathrm{p}}(t)$

Idea:

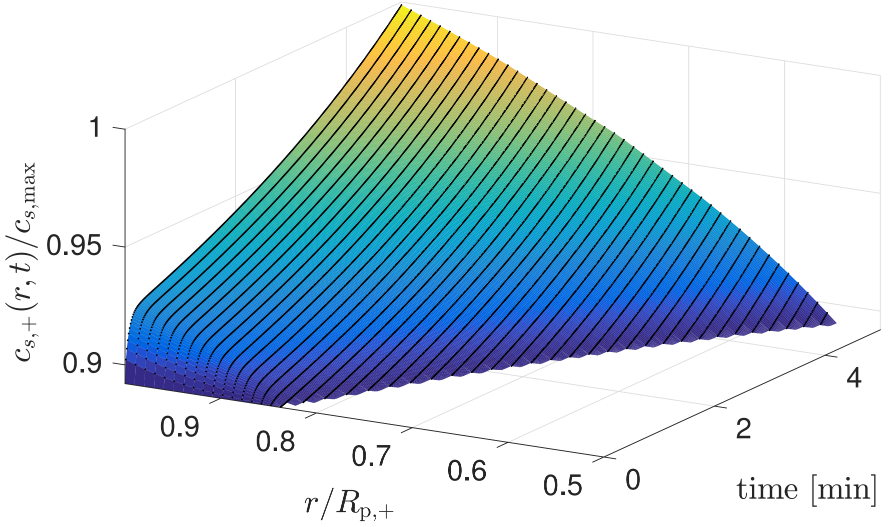
(Step1) Design observer $\hat{c}$ assuming $r_{\mathrm{p}}(t)$ is known,

(Step2) Construct the entire observer $(\hat{c}, \hat{r}_{\mathrm{p}})$ via replacing $r_{\mathrm{p}}(t)$ in Step 1 by $\hat{r}_{\mathrm{p}}(t)$, and add estimator of $\hat{r}_{\mathrm{p}}(t)$

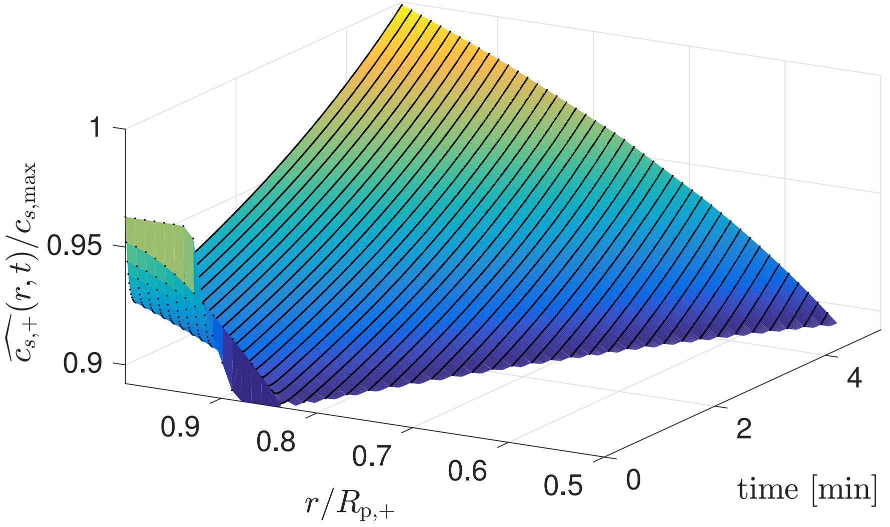
$$\begin{aligned}
\frac{\partial \hat{c}}{\partial t}(r,t) &= \frac{D}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial \hat{c}}{\partial r}(r,t)\right] + P(\hat{r}_{\mathrm{p}}(t), r)\left[c(R_{\mathrm{p}},t) - \hat{c}(R_{\mathrm{p}},t)\right], \\
\hat{c}(\hat{r}_{\mathrm{p}}(t), t) &= c_\beta, \\
D\frac{\partial \hat{c}}{\partial r}(R_{\mathrm{p}},t) &= -j(t) + Q(\hat{r}_{\mathrm{p}}(t))\left[c(R_{\mathrm{p}},t) - \hat{c}(R_{\mathrm{p}},t)\right], \\
\frac{\mathrm{d}\hat{r}_{\mathrm{p}}(t)}{\mathrm{d}t} &= -B\frac{\partial c}{\partial r}(\hat{r}_{\mathrm{p}}(t), t) + l\left[c(R_{\mathrm{p}},t) - \hat{c}(R_{\mathrm{p}},t)\right].
\end{aligned}$$

Stability proof of estimation error system is still an ***open problem***

Simulation of BKS Estimation for Lithium-ion Concentration



True profile



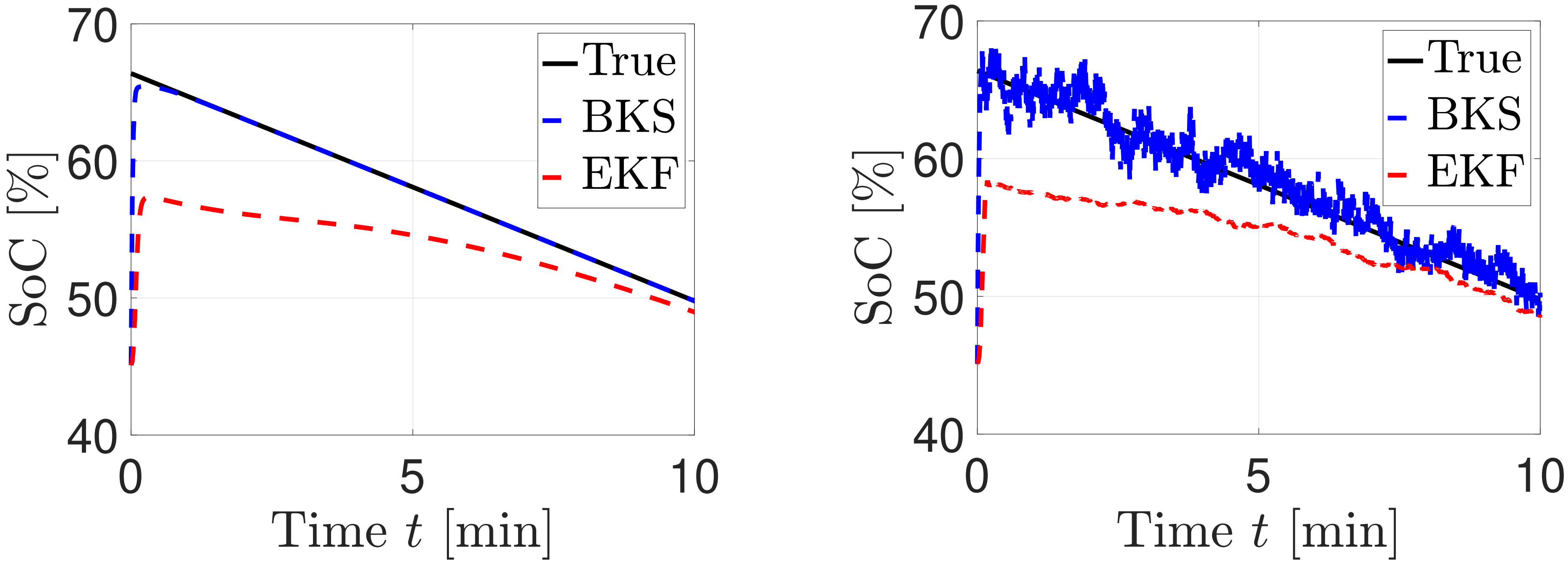
Estimate profile

$\Rightarrow$ Our BKS estimator enables to capture lithium-ion concentration in short time

SoC is calculated from the concentration by

$$\mathrm{SoC}(t) = \left[1 - \frac{4\pi \int_0^{R_p} r^2 c(r,t)dr}{Q_{max}}\right] \times 100[\%]$$

Comparison of BKS with EKF in SoC Estimation



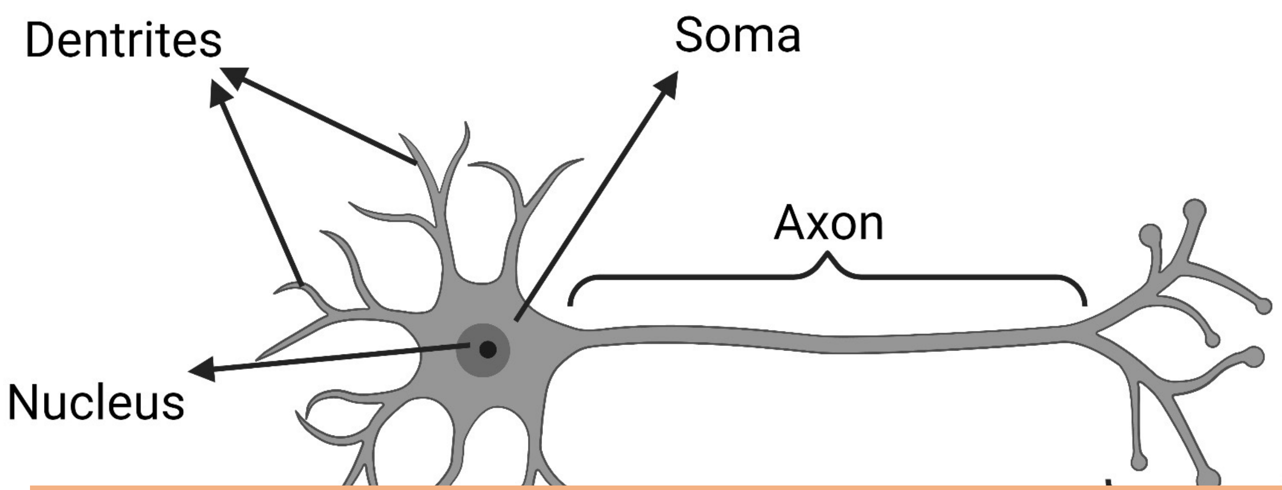
Noise-free

With Noise

In this sample simulation, it shows (*not best* parameters' choice for each method)

- Our BKS is superior in **convergence speed**
- EKF is superior in **noise attenuation**

Neuron Growth Model of Stefan-type (C. Demir, et al, [4])



$c(x,t)$ ⋯ Concentration of Tubulin in axon

$$\frac{\partial c}{\partial t}(x,t) = D\frac{\partial^2 c}{\partial x^2}(x,t) - a\frac{\partial c}{\partial x}(x,t) - gc(x,t),$$

$$\frac{\partial c}{\partial x}(0,t) = -q_s(t),$$

$$c(l(t),t) = c_c(t),$$

$$l_c\frac{dc_c}{dt}(t) = (a - gl_c)c_c(t) - D\frac{\partial c}{\partial x}(l(t),t)$$

- Designed control input for linearized system by BKS
- Showed ***local stability*** of reference error, ensuring $l(t) \to l_r$

2nd order dynamics of moving boundary $l(t)$ w.r.t. Neumann boundary value of PDE $\frac{\partial c}{\partial x}(l(t),t)$

$\to \frac{dl}{dt}(t)$ is one element of ODE state (this is not the case of Stefan problem)

[4] C. Demir, S. Koga, and M. Krstic "Neuron Growth Control by PDE Backstepping: Axon Length Regulation by Tubulin Flux Actuation in Soma", 60th IEEE Conference on Decision and Control (CDC), submitted

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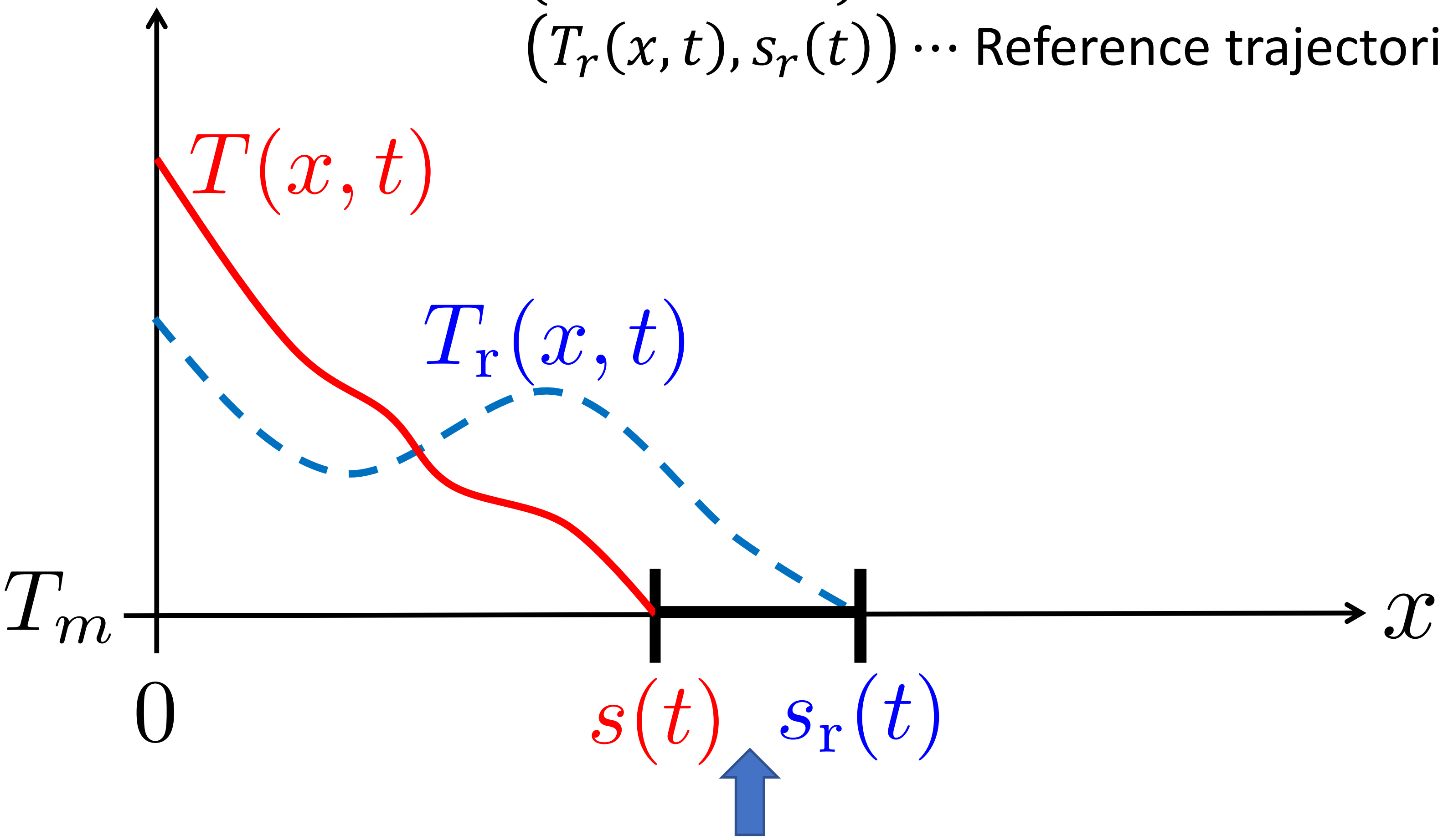
1. Trajectory Tracking Control of Stefan Problem

$\left(T(x,t), s(t)\right)$ ⋯ State variables
$\left(T_r(x,t), s_r(t)\right)$ ⋯ Reference trajectories (a known function in time)



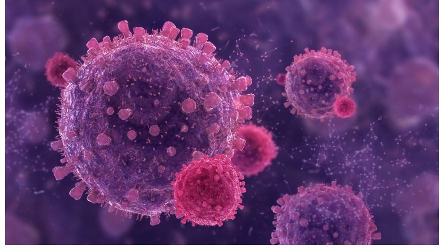
Challenge: How to deal with domains' discrepancy?

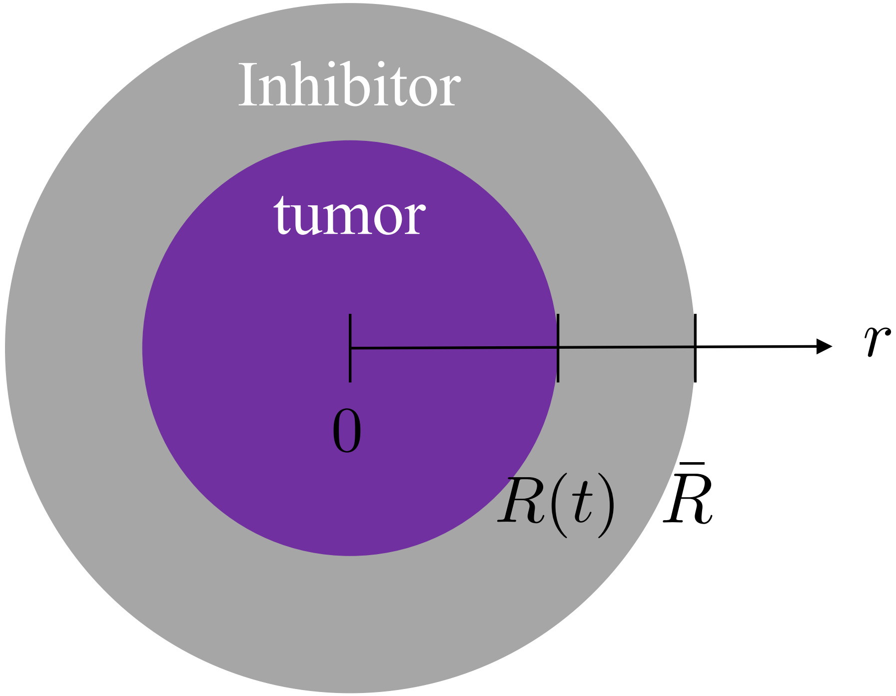
1. Trajectory Tracking Control of Stefan Problem

- If we simply set $u(x,t) = T(x,t) - T_r(x,t)$, then the boundary condition becomes
$$u(s(t),t) = T_m - T_r(s(t),t)$$
which is a nonlinear function in $s(t)$.
- We can linearize at $s(t) \approx s_r(t)$, which leads to
$$\begin{aligned} u_t(x,t) =& \alpha u_{xx}(x,t), \quad 0 < x < s(t) \\ -ku_x(0,t) =& q_c(t) - q_c^{(r)}(t), \\ u(s(t),t) =& C(t)X(t), \\ \dot{X}(t) =& A(t)X(t) - \beta u_x(s(t),t), \end{aligned}$$
- Challenges still remain in:
  - derivation of *time-varying* BKS and gain kernels,
  - ensuring the *positivity* of control input,
  - (if possible) improving *local stability* result utilizing linearization.
- The change of coordinate approach by S. Ecklebe et al [5] might be a good way to go.

[5] Ecklebe, S., Woittennek, F., Frank-Rotsch, C., Dropka, N., & Winkler, J. (2021). "Toward Model-Based Control of the Vertical Gradient Freeze Crystal Growth Process". *IEEE Transactions on Control Systems Technology*.

2. Tumor Growth Model of Stefan-type [6]





$\sigma(r,t) \cdots$ nutrient concentration of tumor

$\beta(r,t) \cdots$ inhibitor concentration

$$\frac{\partial \sigma}{\partial t}(r,t) = \frac{D_1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \sigma}{\partial r}(r,t)\right) - \lambda_0 \sigma(r,t) - \gamma_1 \beta(r,t), \quad 0 < r < R(t)$$

$$\frac{\partial \beta}{\partial t}(r,t) = \frac{D_2}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \beta}{\partial r}(r,t)\right) - \gamma_2 \beta(r,t), \quad 0 < r < \bar{R},$$

$$\frac{\partial \sigma}{\partial r}(0,t) = 0,$$

$$\sigma(R(t),t) = \bar{\sigma},$$

$$\beta(\bar{R},t) = U(t),$$

$$\frac{\partial \beta}{\partial r}(0,t) = 0,$$

$$\frac{1}{3}R(t)^2 \dot{R}(t) = \int_0^{R(t)} (\mu(\sigma(r,t) - \tilde{\sigma}) - \nu\beta(r,t)) r^2 dr.$$

[6] Byrne, H. M., & Chaplain, M. A. J., “Growth of nonnecrotic tumors in the presence and absence of inhibitors”, *Mathematical biosciences*, 1995.

2. Tumor Growth Model of Stefan-type

Deriving the reference-error system and taking linearization leads to

$$\frac{\partial v}{\partial t}(r,t) = \frac{D_1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial v}{\partial r}(r,t)\right) - \lambda_0 v(r,t) - \gamma_1 u(r,t),$$

$$\frac{\partial u}{\partial t}(r,t) = \frac{D_2}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial u}{\partial r}(r,t)\right) - \gamma_2 u(r,t), \quad 0 < r < \bar{R},$$

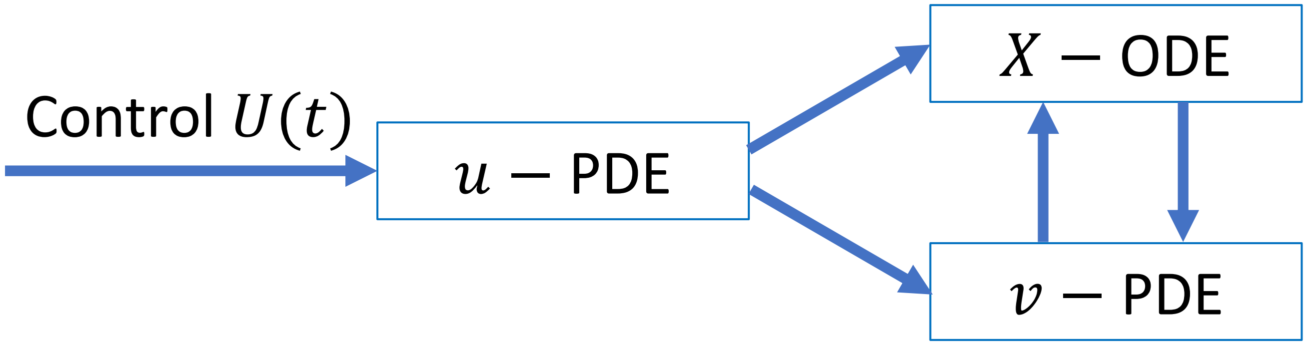
$$\frac{\partial v}{\partial r}(0,t) = 0,$$

$$v(R(t),t) = CX(t),$$

$$u(\bar{R},t) = U(t),$$

$$\frac{\partial u}{\partial r}(0,t) = 0,$$

$$\dot{X}(t) = AX(t) + \boxed{\int_0^{R(t)} (\mu v(r,t) - \nu u(r,t)) r^2 dr.}$$



The problem is open even for analogous *fixed-domain* PDE system.

3. Control Synthesis of BKS-ES for Stabilization with Constraint

Existing results and approaches for Stefan systems

System	Control Design	Constraint	Stability
1-Phase Stefan	BKS = ES	Guaranteed	Guaranteed
1-Phase Stefan with advection	BKS	Happened to be shown	Guaranteed
2-Phase Stefan	ES	Guaranteed	Happened to be shown

Question: How can we design control guaranteeing both stability and constraint?

3. Control Synthesis of BKS-ES for Stabilization with Constraint

Idea: BKS-ES QP formulation, analogously to CLF-CBF QP formulation in safety control of ODEs

Safety control of nonlinear ODEs by Ames, et al [7]

$$\dot{x} = f(x) + g(x)u,$$

$$\begin{aligned} u(x) = \underset{(u,\delta)\in\mathbb{R}^{m+1}}{\operatorname{argmin}} \quad & \frac{1}{2}u^T H(x)u + p\delta^2 \qquad \text{(CLF-CBF QP)} \\ \text{s.t.} \quad & L_f V(x) + L_g V(x)u \leq -\gamma(V(x)) + \delta \\ & L_f h(x) + L_g h(x)u \geq -\alpha(h(x)) \end{aligned}$$

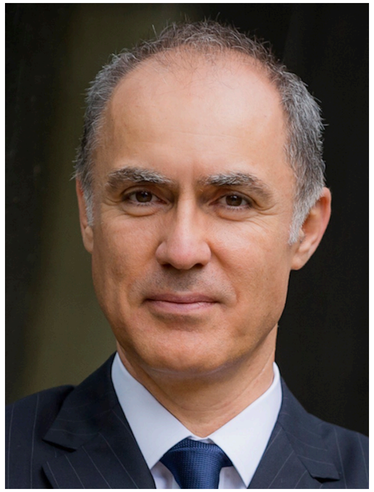
Combining with port-Hamiltonian formulation proposed by Vincent, et al [8] is an interesting direction

[7] A. D. Ames, S. Coogan, M. Egerstedt, G. Notomista, K. Sreenath, & P. Tabuada, “Control barrier functions: Theory and applications”. ECC 2019.
[8] Vincent, B., Couenne, F., Lefèvre, L., & Maschke, B. (2020). “Port Hamiltonian systems with moving interface: the two-phase Stefan problem”, MTNS 2020.

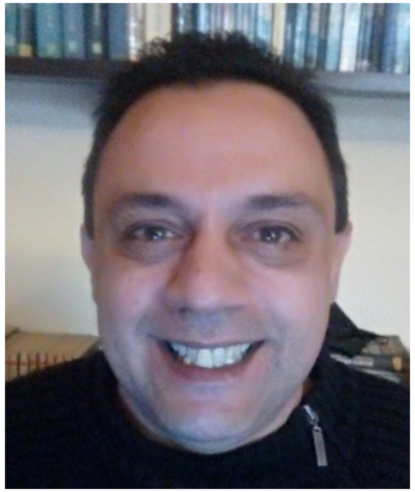
Summary

- Control for Stefan problem, a parabolic PDE with a moving boundary modeling the thermal phase change, has been developed via backstepping/energy-shaping.
- Stefan-type systems have been utilized for various application models, including chemical reaction and biological growth process.
- Numerous open problems exist from both control-theoretic and application-driven perspectives.
- Fundamental challenge lies in, how to deal with *geometric nonlinearity* of moving boundary.

Acknowledgement


Miroslav Krstic


Mamadou Diagne


Iasson Karafyllis


Rafael Vazquez

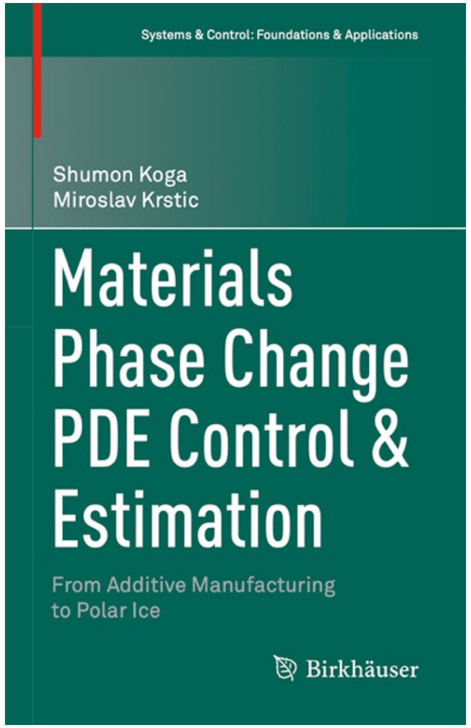

Delphine Bresch-Pietri


Leobardo Camacho-Solorio

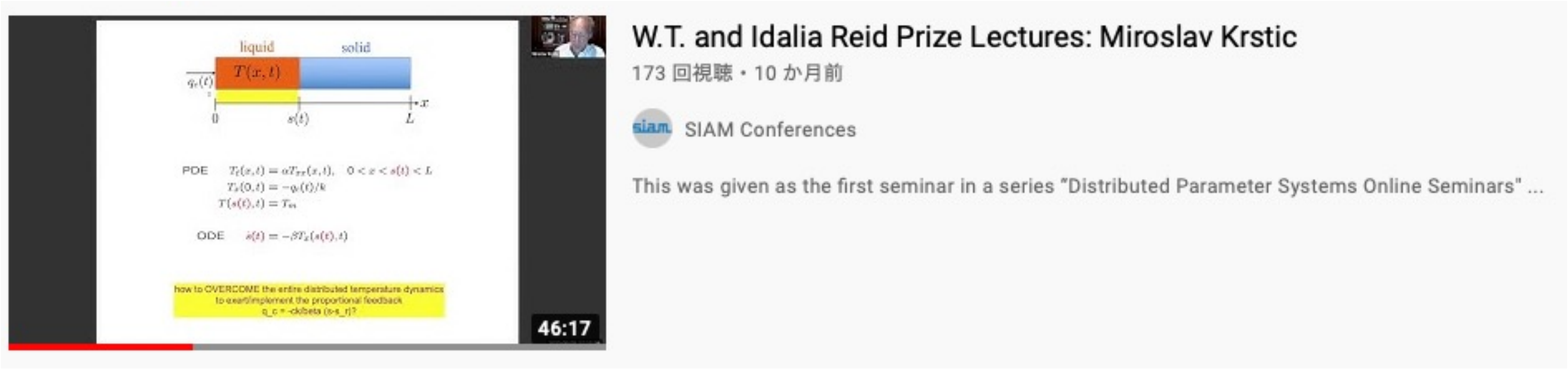

Cenk Demir

For More References

Book



Reid Prize Lecture by Prof. Miroslav Krstic in Youtube



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