Optimal Control of Uncertain Systems

Richard D. Braatz
braatz@mit.edu

Outline

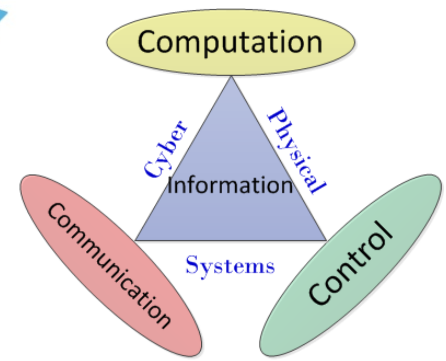
- $\boxed{\text{Recent Trends in Process Manufacturing Systems}}$
- Prototype Process Manufacturing Systems
- Process Systems Design
- Process Control Theory
- More Open Research Problems

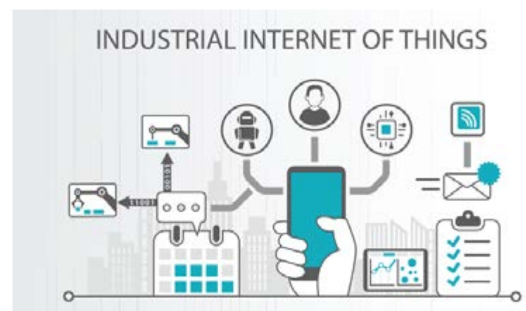
What is Advanced Manufacturing?

- "The use of innovative technology to improve products or processes" (wikipedia)
- "A high rate of technology adoption and ability to use that technology to remain competitive and add value" (CTI Reviews)
- "Manufacturing that entails rapid transfer of science and technology into manufacturing products and processes" (White House 2014)

Advanced Manufacturing Terminology

- Smart Manufacturing
- The cloud
- Cyber-physical systems
- Industry Internet of Things
- Industry 4.0

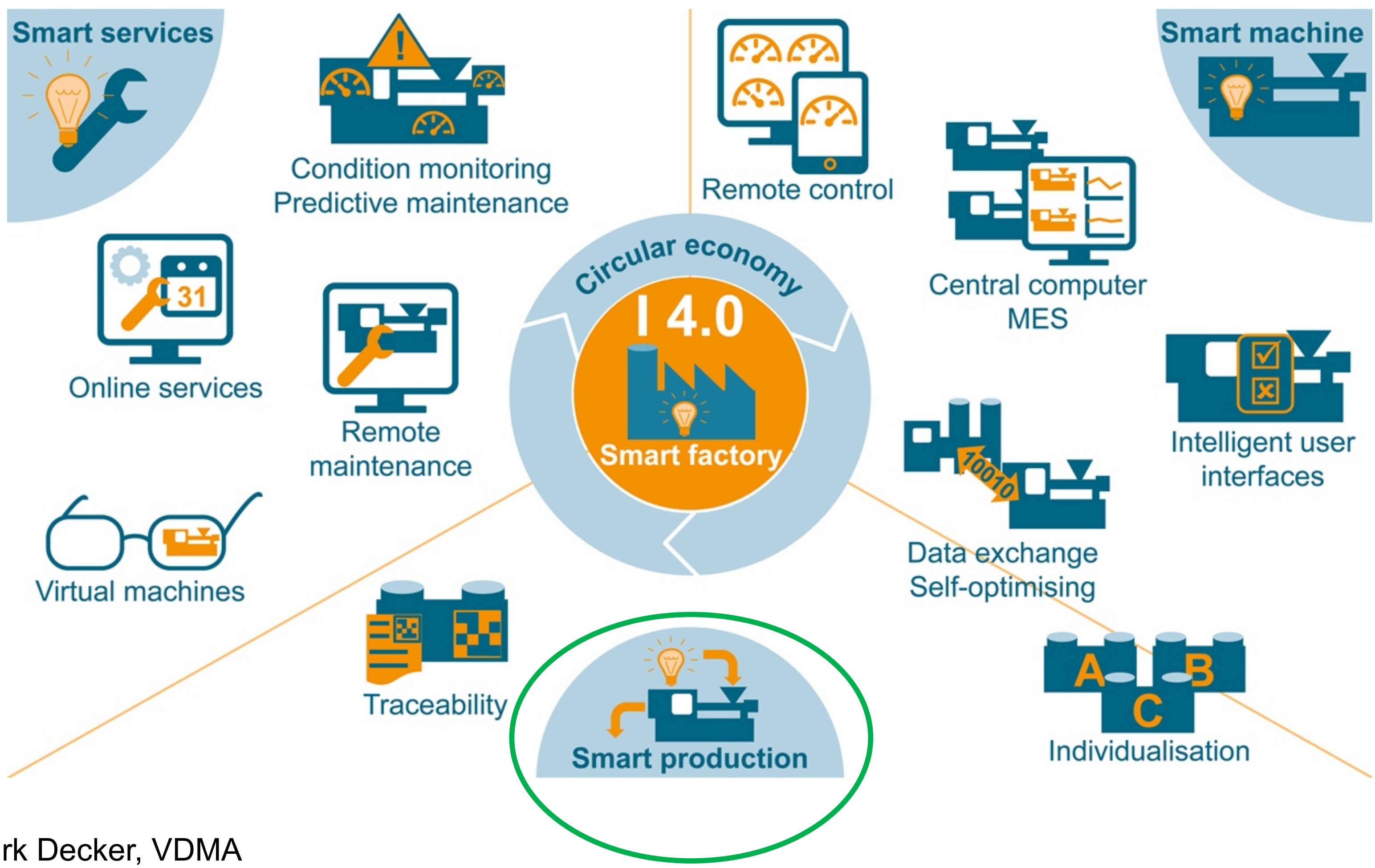




These areas contain many systems & control problems; this talk focuses on process systems engineering

Industry 4.0, aka Smart Factory

“the current trend of automation and data exchange that includes cyber-physical systems, Internet of Things, cloud computing, and cognitive computing”



this talk discusses the underlying PSE research problems

Dirk Decker, VDMA

Outline

- Recent Trends in Process Manufacturing Systems
- Prototype Process Manufacturing Systems
- Process Systems Design
- Process Control Theory
- More Open Research Problems

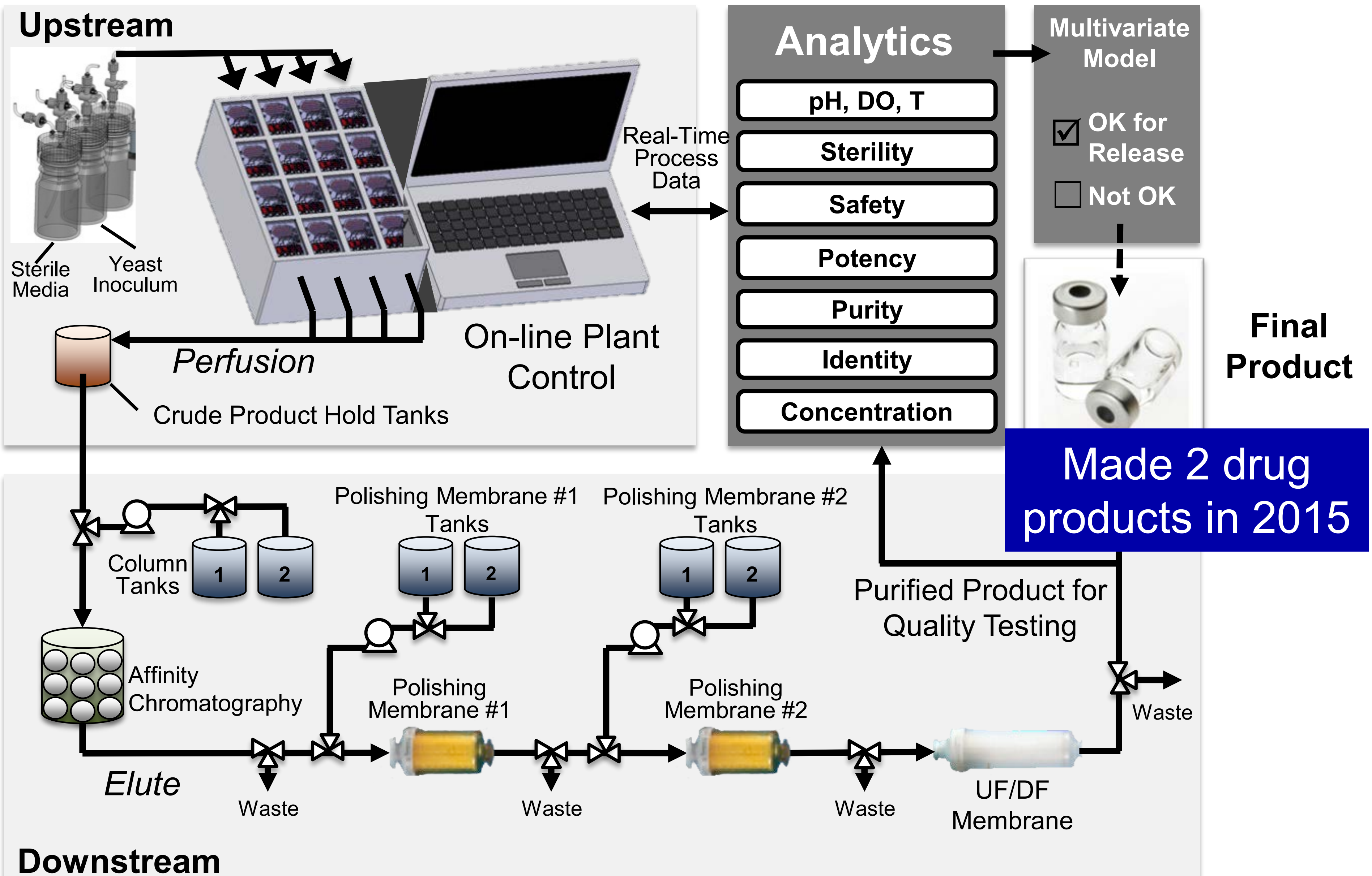
First Continuous Pharma Manufacturing Plant

- Plant-wide control system constructed from first-principles
- Reduced production costs by ~50%
- Met all purity specs in 2012

S. Mascia et al. End-to-end continuous manufacturing of pharmaceuticals: Integrated synthesis, purification, and final dosage formation. Angewandte Chemie, 52(47):12359-12363, 2013; Research Highlight in Nature, 502:274, 2013

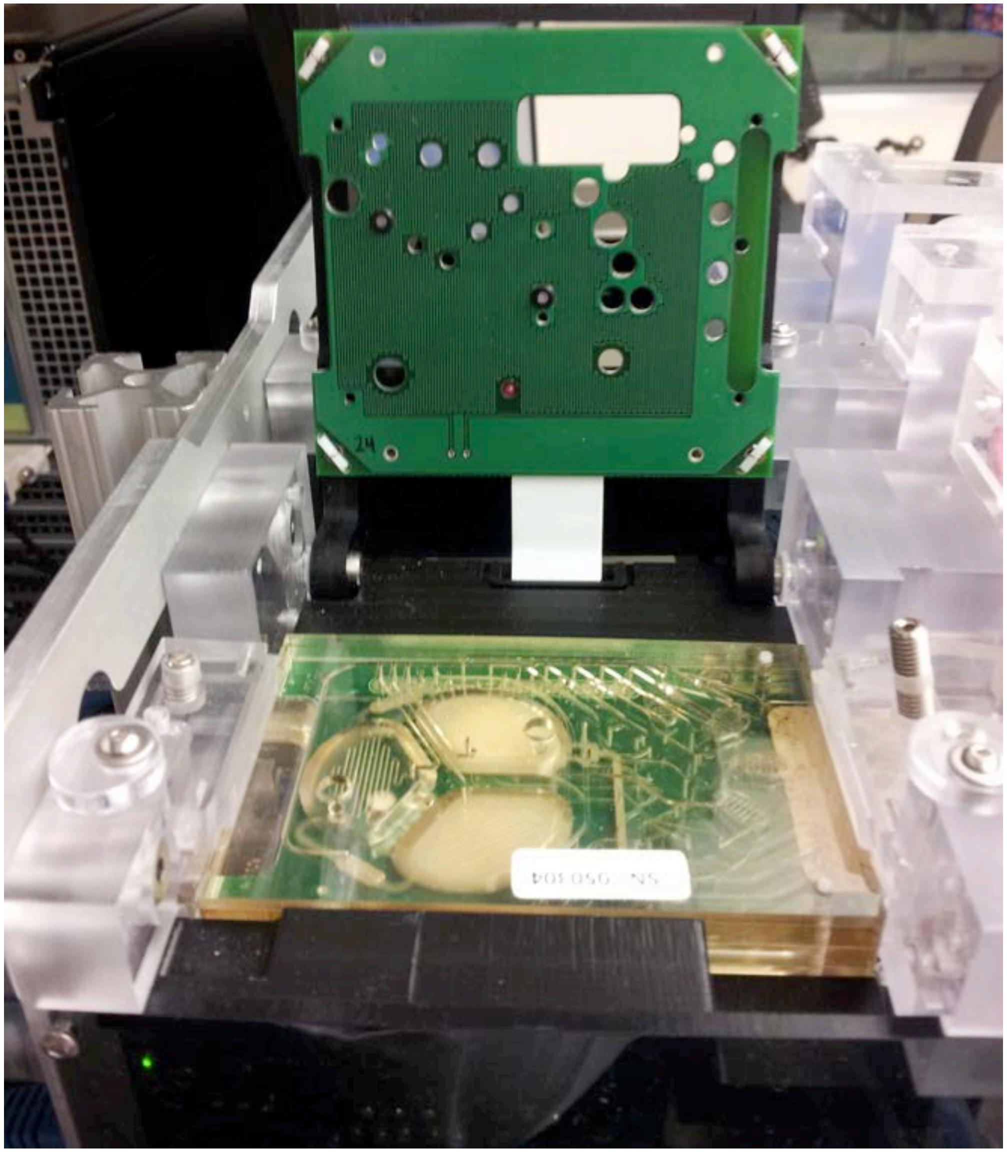
A. Mesbah, J. Paulson, R. Lakerveld, R.D. Braatz. Model predictive control of an integrated continuous pharmaceutical manufacturing pilot plant. Org. Process R&D, 21(6):844-854, 2017

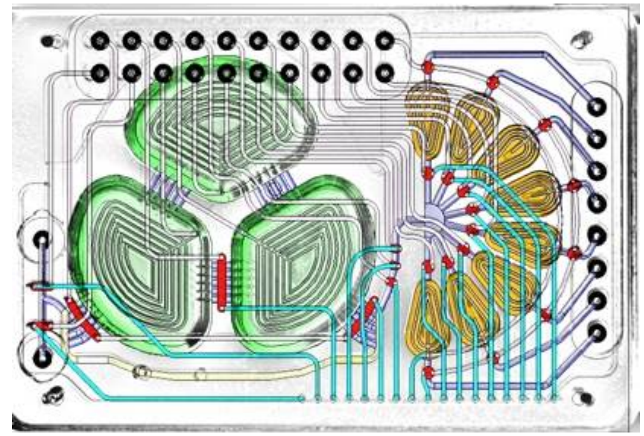
Integrated and Scalable Cyto-Technology (InSCyT) Biomanufacturing Platform, V1.0

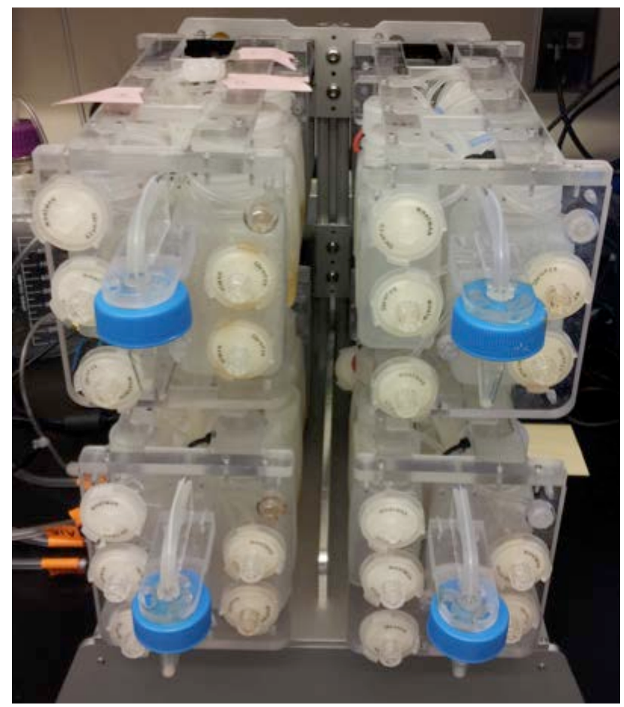


A.E. Lu et al. (2015). Control systems technology in the advanced manufacturing of biologic drugs. IEEE Conf. on Control Appl., 1505-1515.

Microscale Controlled Cell Culture





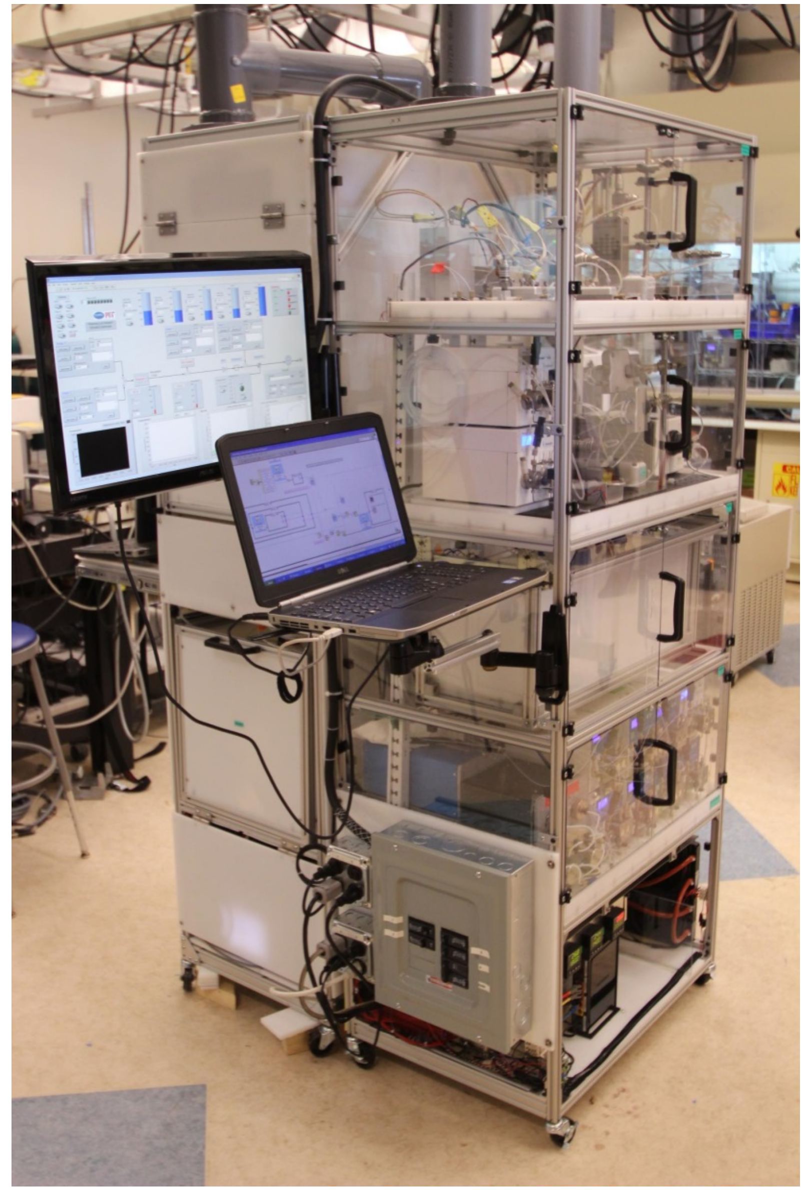


K.S. Lee and R.J. Ram. Microfluidic chemostat and turbidostat with flow rate, oxygen, and temperature control for dynamic continuous culture. Lab on a Chip, 11(10), 1730-1739, 2011

Moo Sun Hong et al. Model-based optimal design and control of microbioreactors, in preparation

Automated System for Knowledge-based Continuous Organic Synthesis

- A <u>fully</u> automated molecular synthesizer that produces, purifies, and characterizes*
- Includes
  - knowledge-based computational tools for reaction pathway & process flow diagram (PFD) prediction
  - process automation and control
  - interconnected fluidic modules for continuous synthesis, in-line characterization, purification, and formulation
- Speed the pace of molecular innovation and provide an accessible synthesis platform for non-specialists



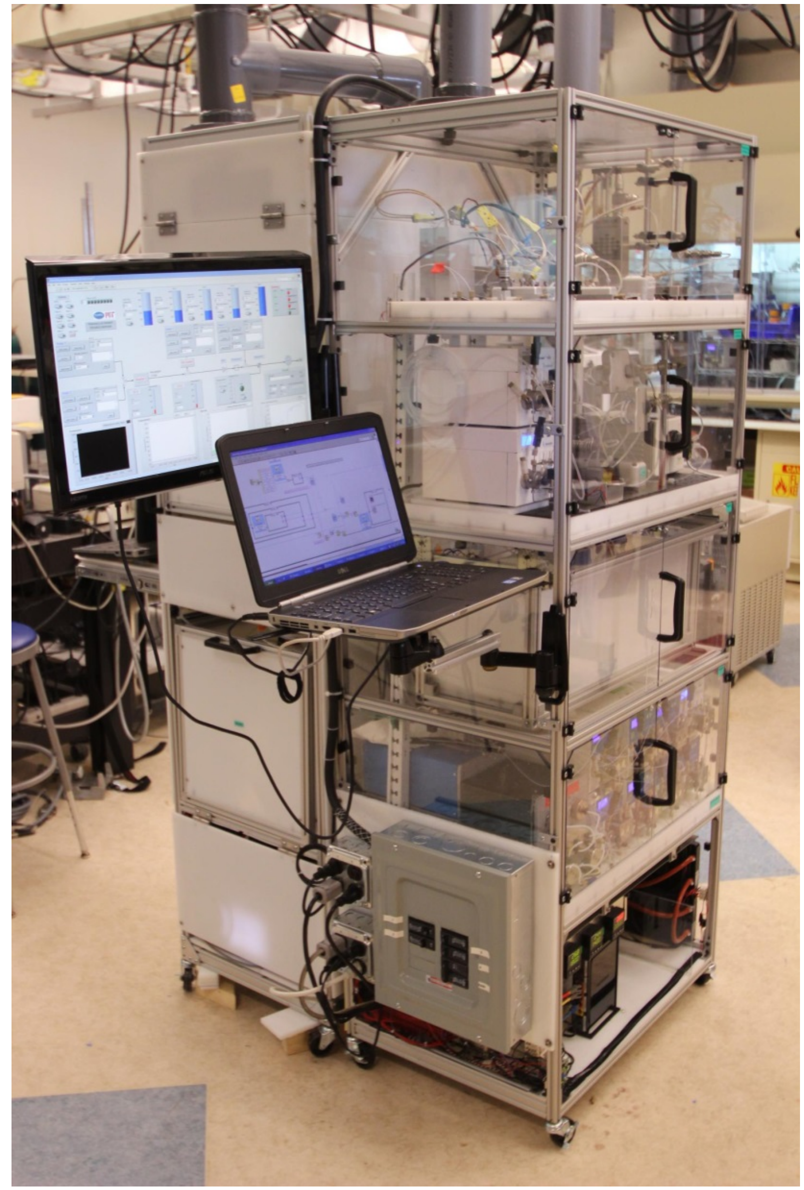
Science, 352(6281):61-67, April 1, 2016

Made 4 drug products in 2015

* http://www.darpa.mil/program/make-it

Automated System for Knowledge-based Continuous Organic Synthesis

- A fully automated molecular synthesizer that produces, purifies, and characterizes
- Fully automating the PhD control engineer requires solving many research problems:
  - how to optimize startup, when no data from the system are initially available for building models for control design (stochastic hybrid optimization)?
  - how to ensure near optimal closed-loop performance while generating no off-spec product (stochastic MPC)?
  - how to continue to optimize operations to maximize yield at specified production rate (self-learning control)?



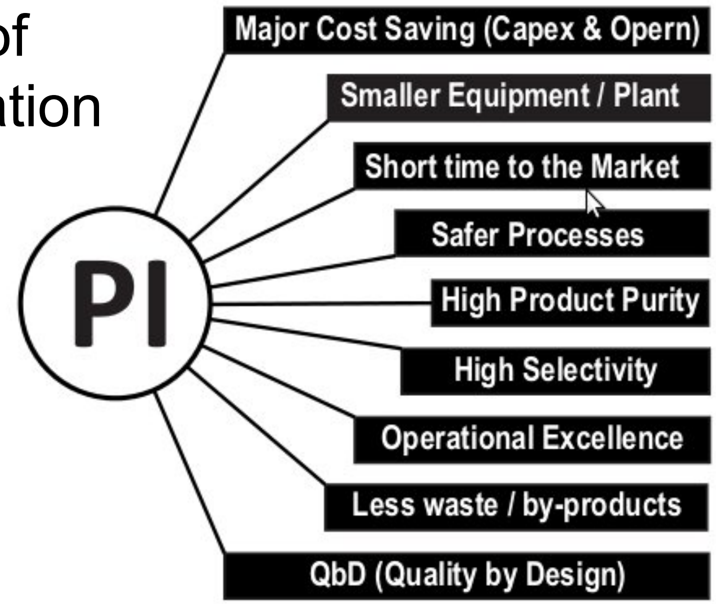
Science, 352(6281):61-67, April 1, 2016

Outline

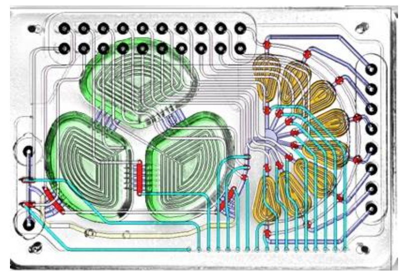
- Recent Trends in Process Manufacturing Systems
- Prototype Process Manufacturing Systems
- Process Systems Design
- Process Control Theory
- More Open Research Problems

Overview of Advanced Process Systems Design

- Greatly increased understanding & optimization of each unit operation, exploiting process intensification



- Automated high-throughput microscale technology for fast continuous process R&D

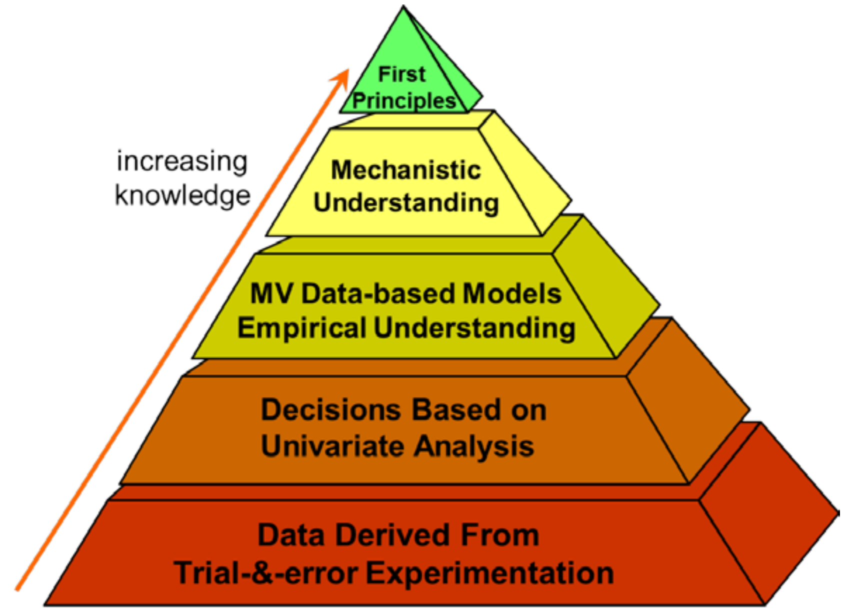


- Plug-and-play wireless modules w/integrated control & monitoring to facilitate deployment

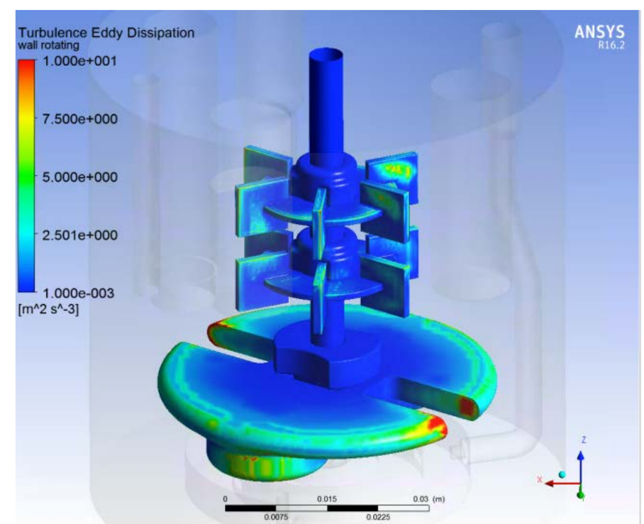
- Dynamic models for unit operations for automated plant-wide simulation & control design
- <u>Autonomous</u> model-based control technologies for optimizing operations including startup, changeover, and shutdown

M.S. Hong et al., *Comput. Chem. Eng.*, 110:106-114, 2018
pi-inc.co, www.pharyx.com/technology.html, *Angew. Chem. Int. Ed.*, 52(47):12359-12363, 2013

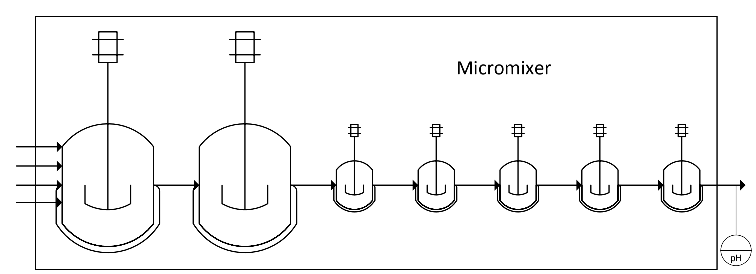
Design of Control Systems Based on "Virtual Plant"



- Constructed from first-principles models wherever possible, grey-box models where necessary



- Highest complexity models used for the invention and optimization of process designs and development

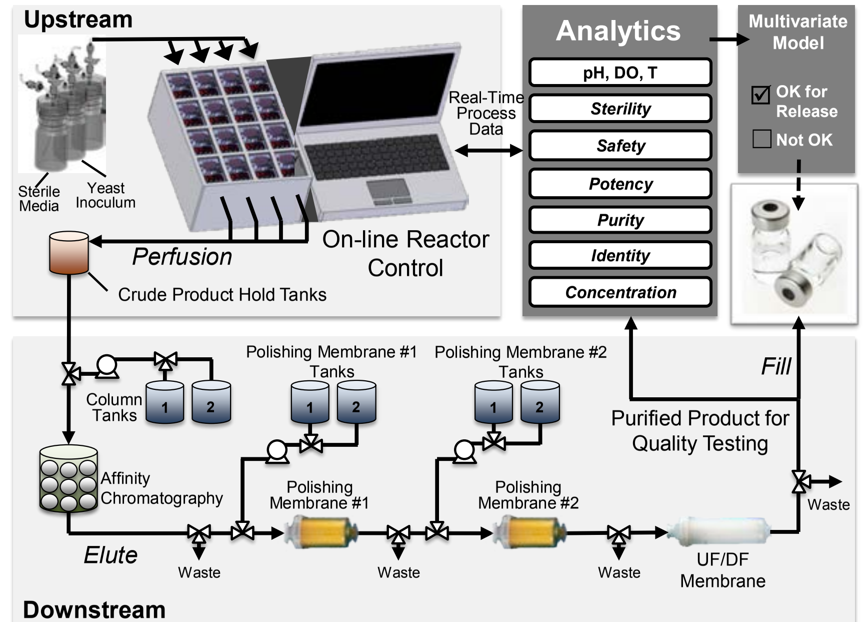


- Lower complexity plant-wide model runs in parallel with process operations, for process control and quality and equipment condition monitoring
- Goal is "right first time"

Plant-wide Control Approach

System Characteristics

- Multi-product manufacturing plant
- Continuous & discrete operations
- Dynamics, nonlinearities, distributions, uncertainties, constraints, disturbances
- No SS & must align with regulatory requirements (no off-spec product)



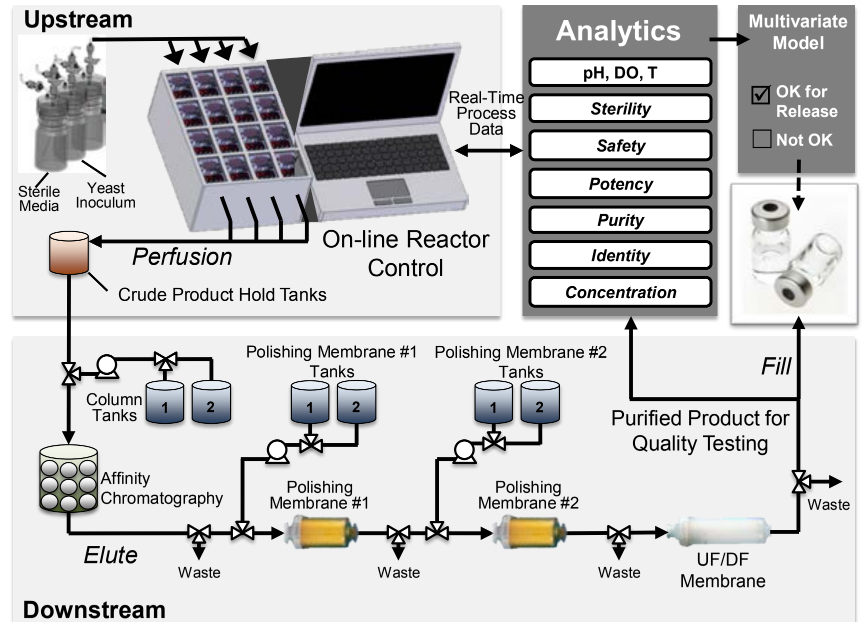
Approach adapted from the chemical industry

- Employ systematic & modular design of plantwide control strategies for large-scale manufacturing facilities (Stephanopoulos/Ng, JPC 2000)
- Employ algorithms that can handle nonlinearities, distributed states, unstable zero dynamics, time-invariant probabilistic uncertainties, constraints, time delays, and mixed continuous-discrete operations

A.E. Lu, J.A. Paulson, N.J. Mozdzierz, A. Stockdale, A.N. Ford Versypt, K.R. Love, J.C. Love, R.D. Braatz. Control systems technology in the advanced manufacturing of biologic drugs. Proc. of the IEEE Conference on Control Applications, 1505-1515, 2015

Plant-wide Control Approach

- Build first-principles dynamic models for each unit operation (UO)
- Design control system for each UO to meet “local” material attributes
- Evaluate performance in simulations and propose design modifications as needed

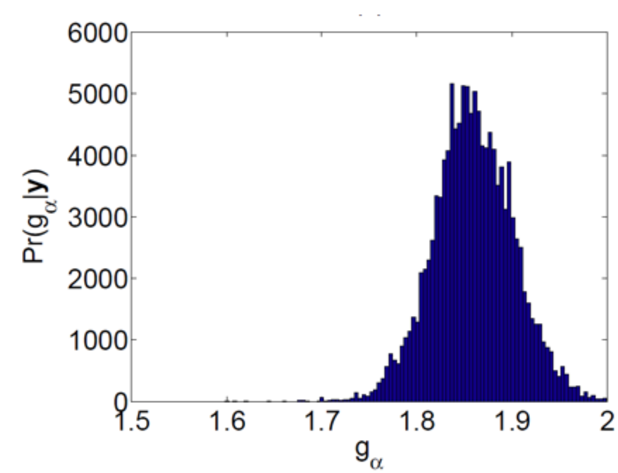


- Implement and verify the control system for each UO
- Design and verify plantwide control system to ensure that the product quality specifications are met

A.E. Lu, J.A. Paulson, N.J. Mozdzierz, A. Stockdale, A.N. Ford Versypt, K.R. Love, J.C. Love, R.D. Braatz. Control systems technology in the advanced manufacturing of biologic drugs. Proc. of the IEEE Conference on Control Applications, 1505-1515, 2015

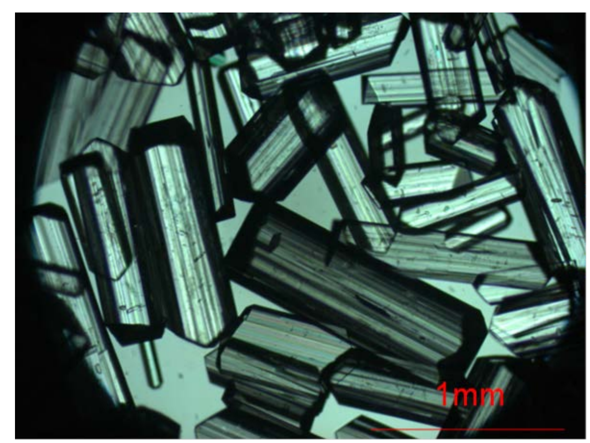
What is Available and What is Needed in Advanced Process Control Technology

- The best commercial plant simulation software handles nonlinearities, time delays, unstable zero dynamics, constraints, mixed continuous-discrete operations, and some uncertainty analysis methods (e.g., S_i, Monte Carlo)



- More advanced uncertainty analysis tools can be wrapped around or integrated into such software
- Distributed states facilitated by moment analysis, transforms, characteristics, finite volume methods
- Research needed on automating controller design, reducing on-line computations, proving stability, and optimizing startup/changeover/shutdown

→ especially for time-invariant probabilistic uncertainties



Outline

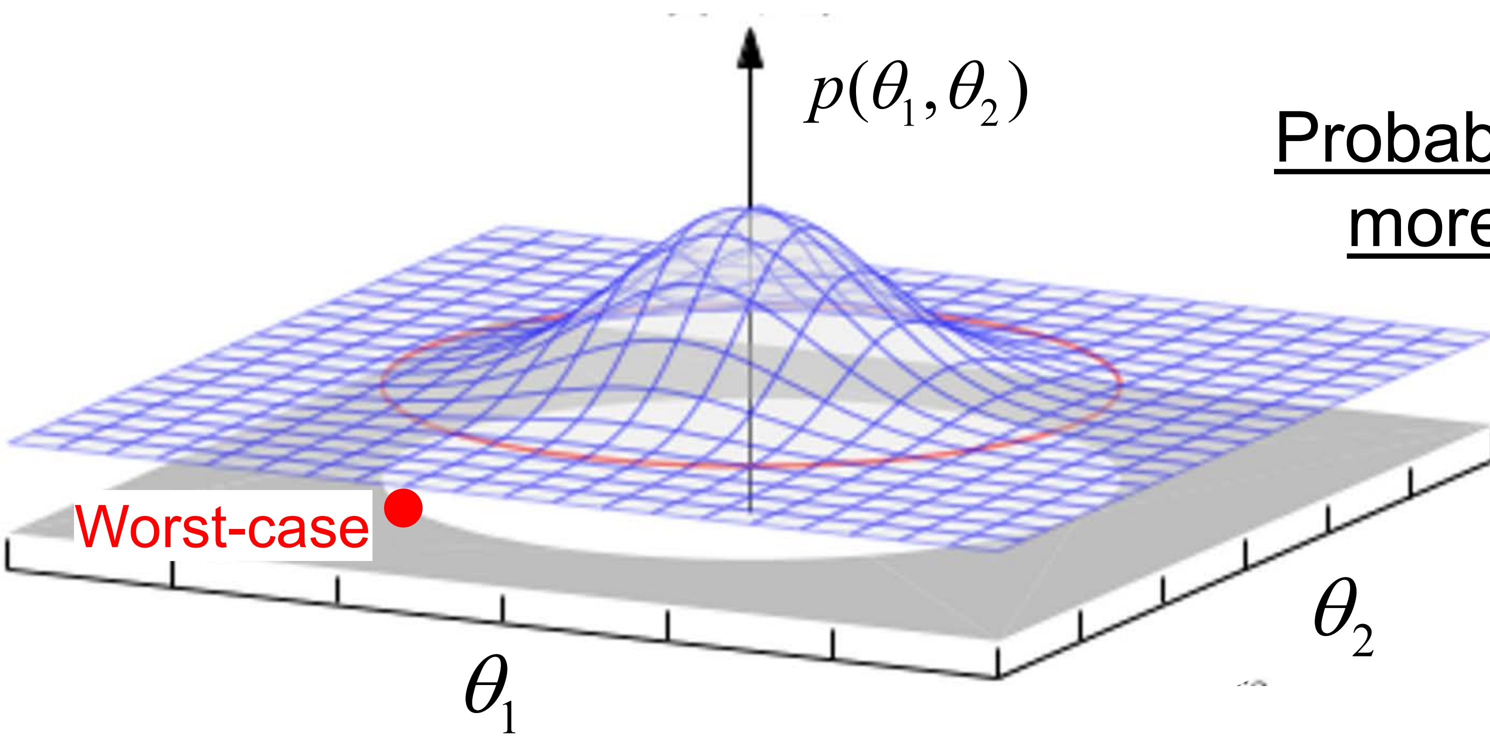
- Recent Trends in Process Manufacturing Systems
- Prototype Process Manufacturing Systems
- Process Systems Design
- Process Control Theory
- More Open Research Problems

Common Characteristics of Advanced Process Systems

- High to infinite state dimension
- Model uncertainties: non-LFT, TI, $p(\theta)$
- Time delays
- Unstable zero dynamics
- Actuator, state, and output constraints
- Stochastic noise and disturbances
- Phenomena described by algebraic, ordinary and partial differential, and integral equations
- Mixed continuous-discrete operations
- Nonlinearities

Research needed on the analysis, design, and control of process systems that have **all** of these characteristics

Worst-case vs. Probabilistic Formulation

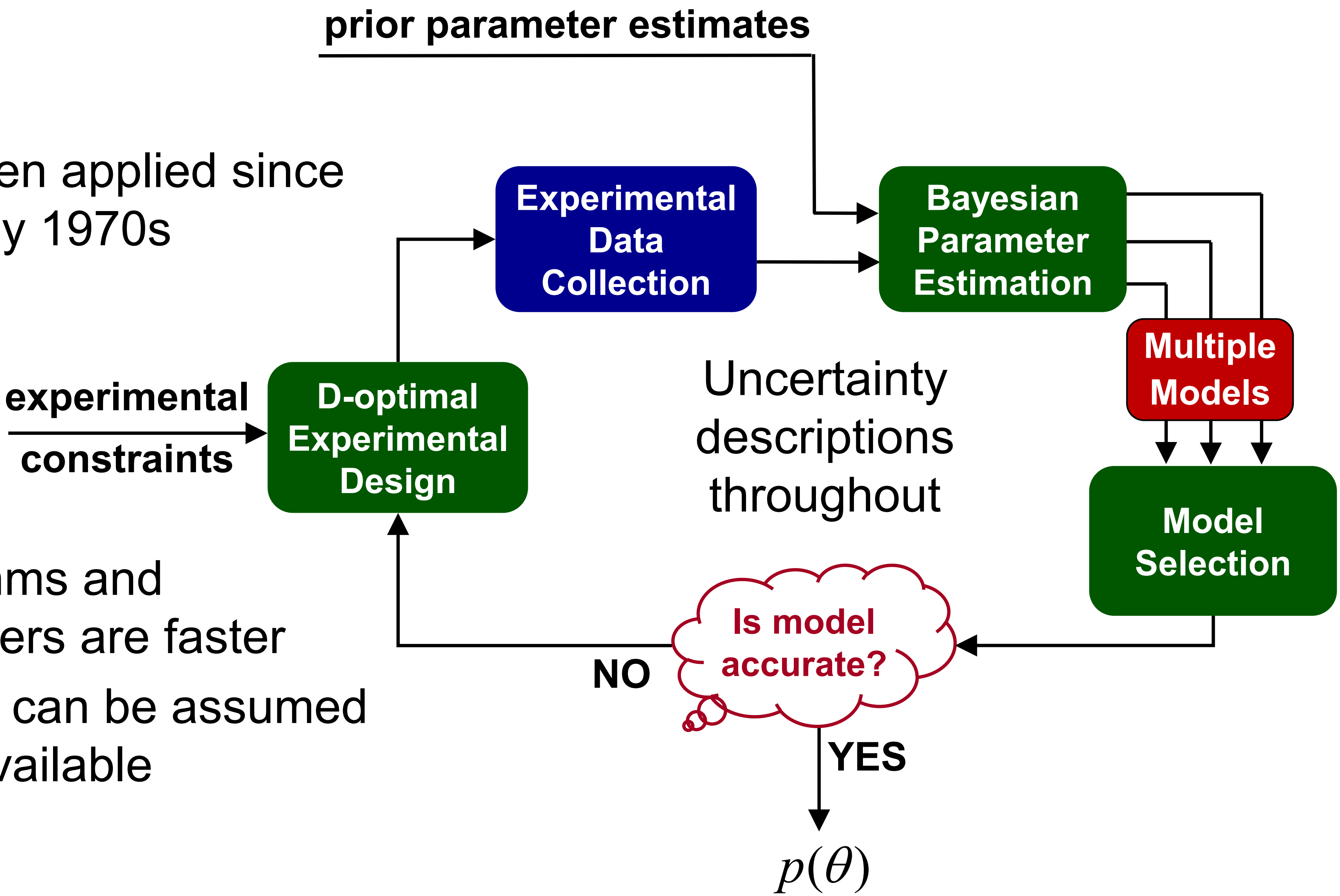


Probabilistic view has more information

- Min-max optimizes highly unlikely worst-case & is conservative
- Stochastic approach exploits the probabilistic information, resulting in much better performance for almost all θ

Time-invariant Parameter Uncertainty Estimation

- Has been applied since the early 1970s



- Algorithms and computers are faster
- So $p(\theta)$ can be assumed to be available

Braatz et al., Journal of Process Control, 17, 229-240, 2007

Common Characteristics of Advanced Process Systems

- High to infinite state dimension
- Model uncertainties: non-LFT, TI, $p(\theta)$
- Time delays
- Unstable zero dynamics
- Actuator, state, and output constraints
- Stochastic noise and disturbances
- Phenomena described by algebraic, ordinary and partial differential, and integral equations
- Mixed continuous-discrete operations
- Nonlinearities

Research needed on the analysis, design, and control of process systems that have **all** of these characteristics

Common Characteristics of Advanced Process Systems

- High to infinite state dimension
- Model uncertainties: non-LFT, TI, $p(\theta)$
- Time delays
- Unstable zero dynamics
- Actuator, state, and output constraints
- Stochastic noise and disturbances
- Phenomena described by algebraic, ordinary and partial differential, and integral equations
- Mixed continuous-discrete operations
- Nonlinearities

It is instructive to compare to algorithms that are able to simultaneously address most of the above characteristics

Common Characteristics of Advanced Process Systems

- High to infinite state dimension
- Model uncertainties: non-LFT, TI, $p(\theta)$
- Time delays
- Unstable zero dynamics
- Actuator, state, and output constraints
- Stochastic noise and disturbances
- Phenomena described by algebraic, ordinary and partial differential, and integral equations
- Mixed continuous-discrete operations
- Nonlinearities

It is instructive to compare to algorithms that are able to simultaneously address most of the above characteristics

Developing Stochastic Control Algorithms on Wiener's Polynomial Chaos Theory (PCT)

- Replace mapping between uncertain system variables with a series of orthogonal polynomial functions of the model parameters

$$\psi(\theta) \overset{\approx}{\cancel{=}} \sum_{k=0}^{\overset{L}{\cancel{\infty}}} a_k \mathbf{\Phi}_k(\theta)$$

$a_k \longrightarrow$ Expansion coefficients

$\mathbf{\Phi}_k(\theta) \longrightarrow$ Multivariate polynomials made of univariate polynomials in θ_i

- Polynomials from Askey-scheme achieve optimal convergence

PDF	Askey polynomial
Beta	Jacobi
Gaussian	Hermite
Uniform	Legendre

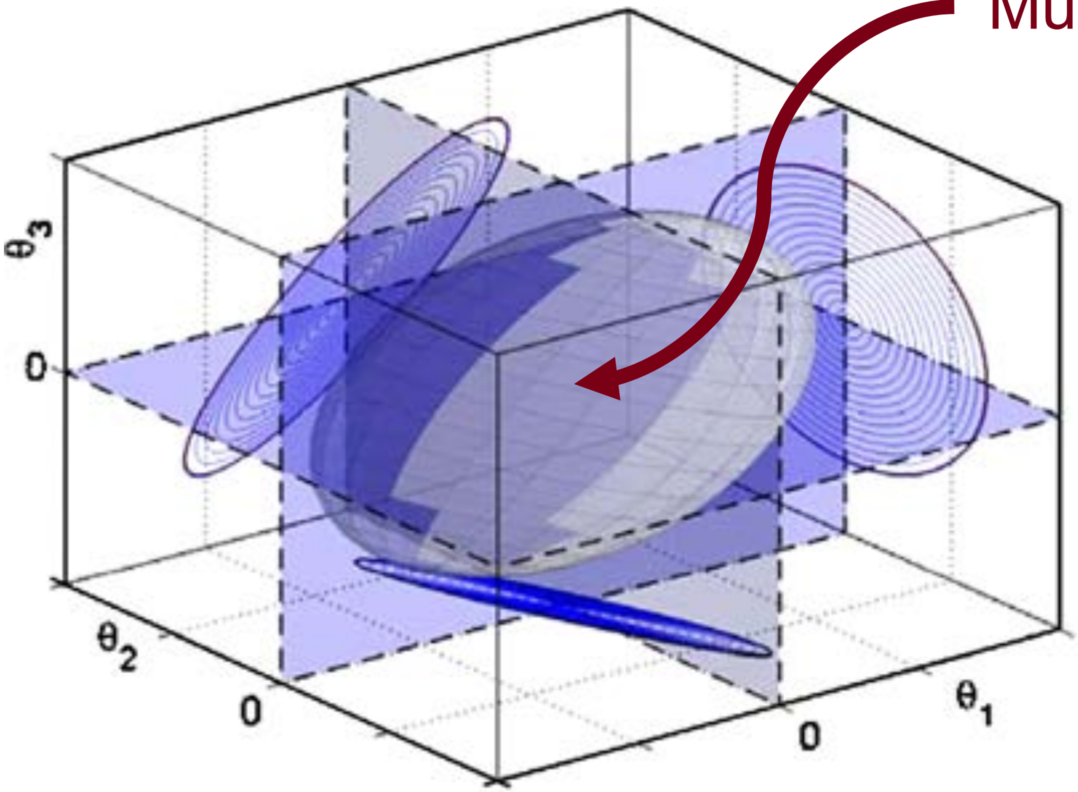
$$\begin{cases} \Phi_0 = 1 \\ \Phi_1 = \theta \\ \Phi_2 = \theta^2 - 1 \\ \vdots \end{cases}$$

$$\boxed{L + 1 = \frac{(n_\theta + m)!}{n_\theta!\, m!}}$$

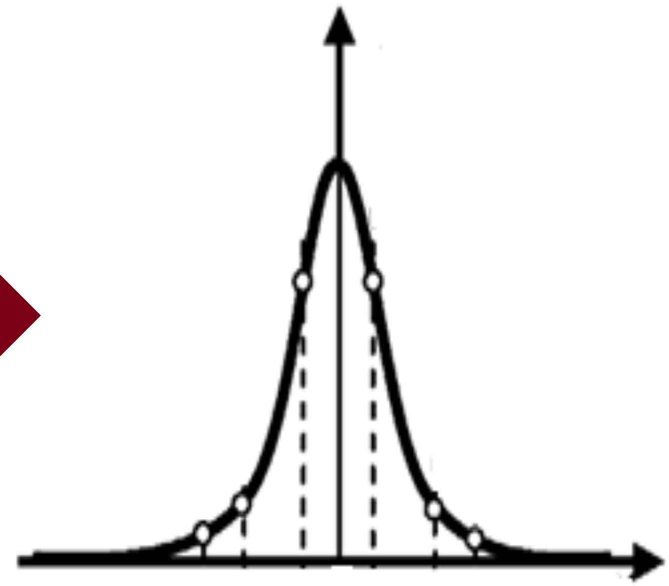
- Expansion must be truncated for practical reasons
- Coefficients can be computed from collocation, regression, Galerkin

Polynomial Chaos Expansions Quantify State PDFs

Multivariable PDF of θ



PCE



Parameter space

System state $x_i(t;\theta)$

$$\hat{x}(t;\,\theta) = \sum_{k=0}^{L} \boxed{a_k(t)}\,\Phi_k(\theta)$$

Captures time evolution of state PDF

K. Kim et al., IEEE Control Systems, 33(5):58-67, 2013

Efficient Moment Evaluation

- Orthogonality of polynomials enables efficient moment evaluation using PCE coefficients

$$\left\langle \mathbf{\Phi}_i(\theta), \mathbf{\Phi}_j(\theta) \right\rangle = \begin{cases} \left\langle \mathbf{\Phi}_i(\theta)^2 \right\rangle & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

Weight is PDF of θ

Inner product $\left\langle h(\theta), g(\theta) \right\rangle = \int_\Omega h(\theta) g(\theta) f_\theta d\theta$

Linear

Expected value $\mathbf{E}\left[\hat{\psi}(\theta)\right] = \left\langle \hat{\psi}(\theta), 1 \right\rangle = \left\langle \hat{\psi}(\theta), \mathbf{\Phi}_0 \right\rangle \boxed{= a_0}$

Quadratic

Variance $\mathbf{Var}\left[\hat{\psi}(\theta)\right] = \sum_{k=1}^{L} \boxed{a_k^2} \left\langle \mathbf{\Phi}_i(\theta)^2 \right\rangle$

can use to reduce online control costs

K. Kim et al., IEEE Control Systems, 33(5):58-67, 2013

Galerkin Projection (when applicable)

- For linear index-1 DAEs, approximate states with PCE and project error onto basis functions to obtain

$$\mathbf{M}\dot{\mathbf{X}}(t) = \mathbf{A}\underbrace{\mathbf{X}(t)}_{\left[a_0^{\mathrm{T}},\ a_1^{\mathrm{T}},\ \cdots\ a_L^{\mathrm{T}}\right]^{\mathrm{T}}} + \mathbf{B}u(t) + \mathbf{D}; \qquad \underbrace{\mathbf{Y}(t)}_{\left[b_0^{\mathrm{T}},\ b_1^{\mathrm{T}},\ \cdots\ b_L^{\mathrm{T}}\right]^{\mathrm{T}}} = \mathbf{C}\mathbf{X}(t)$$

- Map *u*(*t*) to Y(*t*) has similar structure as *u*(*t*) to *y*(*t*)
- Exploit in PCT-based optimal control formulations
  - matrix inequalities → matrix inequalities
  - step response → step response

J.A. Paulson et al., IEEE CDC, 2802-2809, 2014

Example Receding Horizon Formulation

Solve an optimal control problem at every sampling instance t_k:

$$\min_{u(t)} J(y(t), u(t))$$

Inputs Outputs

subject to:

States

- Model

$$\begin{cases} \dot{x}(t) = f(x(t), u(t)) \\ y(t) = g(x(t), u(t)) \end{cases}$$

typically $n_x > n_u$

- Initial condition

$$x(t_k) = \hat{x}(t_k)$$

Update based on latest measurements

- Constraints

$$h(x(t), u(t)) \leq 0, \quad t \in [t_k, t_k + T_P]$$

Fast PCT-based MPC Algorithm as QP

$n_{\mathbf{Y}} = n_y(L+1) << n_x$ typically

$$\mathbf{Y}(k) = \sum_{i=1}^{n} S_i \underbrace{\Delta u(k-i)}_{\Delta u(k) = u(k) - u(k-1)} + S_n u(k-n); \qquad S_k = \begin{bmatrix} s_{1,1,k} & s_{1,2,k} & \cdots & s_{1,n_u,k} \\ s_{2,1,k} & s_{2,2,k} & \cdots & s_{2,n_u,k} \\ \vdots & \vdots & \ddots & \vdots \\ s_{n_{\mathbf{Y}},1,k} & s_{n_{\mathbf{Y}},2,k} & \cdots & s_{n_{\mathbf{Y}},n_u,k} \end{bmatrix}$$

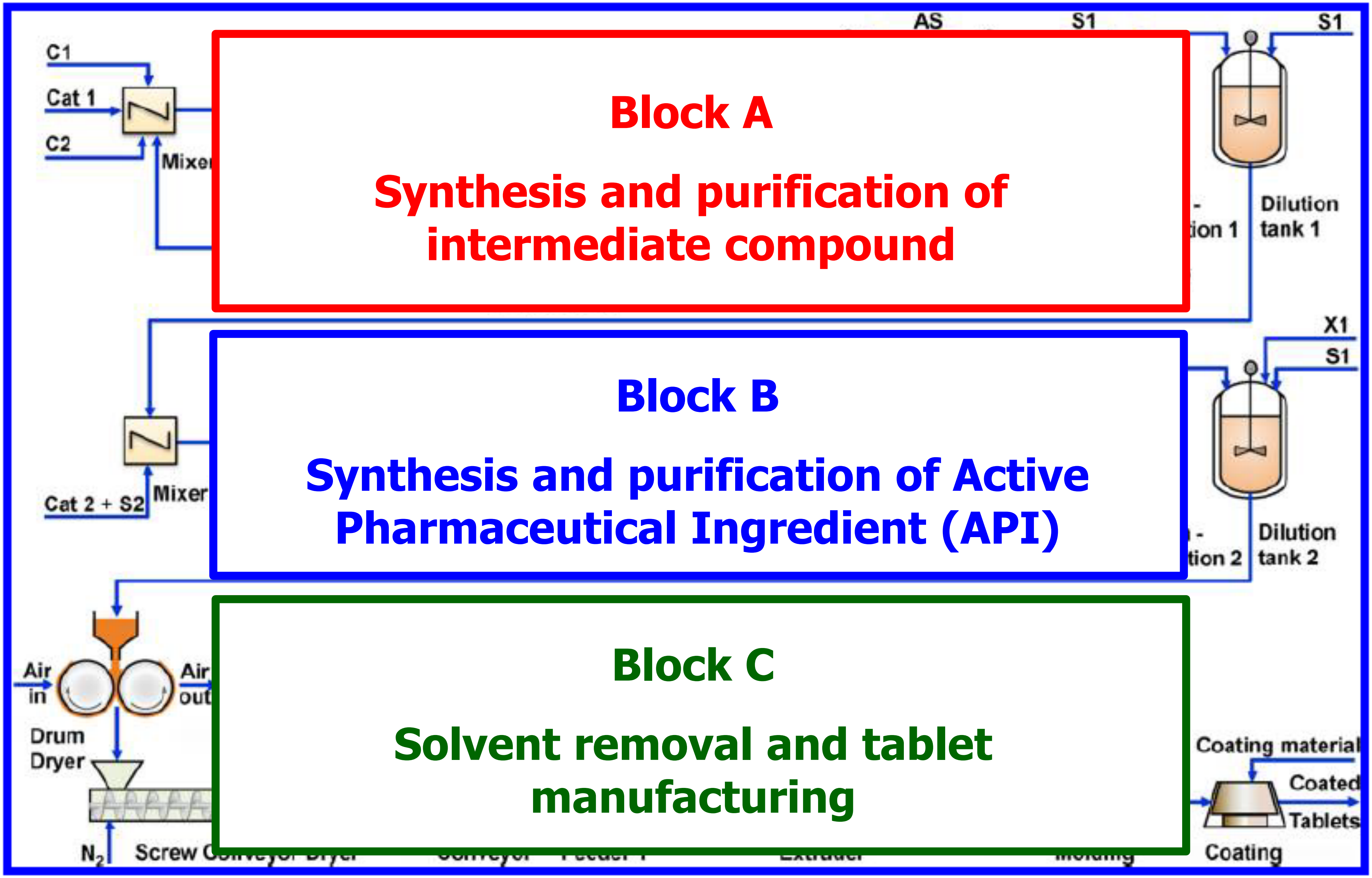
Holds for stable systems, i.e., $S_n \approx S_{n+1} \approx \cdots \approx S_\infty$

Output PCE coefficients are linear in Δu

$$J = \sum_{i=k+1}^{k+p} \underbrace{\mathbf{E}\left[y(t_i;\theta) - r(t_i)\right]^{\mathrm{T}}}_{\text{Linear in } \Delta u} \mathbf{E}\left[y(t_i;\theta) - r(t_i)\right] + w \underbrace{\mathbf{Var}\left[y(t_i;\theta) - r(t_i)\right]}_{\text{Quadratic in } \Delta u}$$

$\longrightarrow$ Quadratic program (QP)

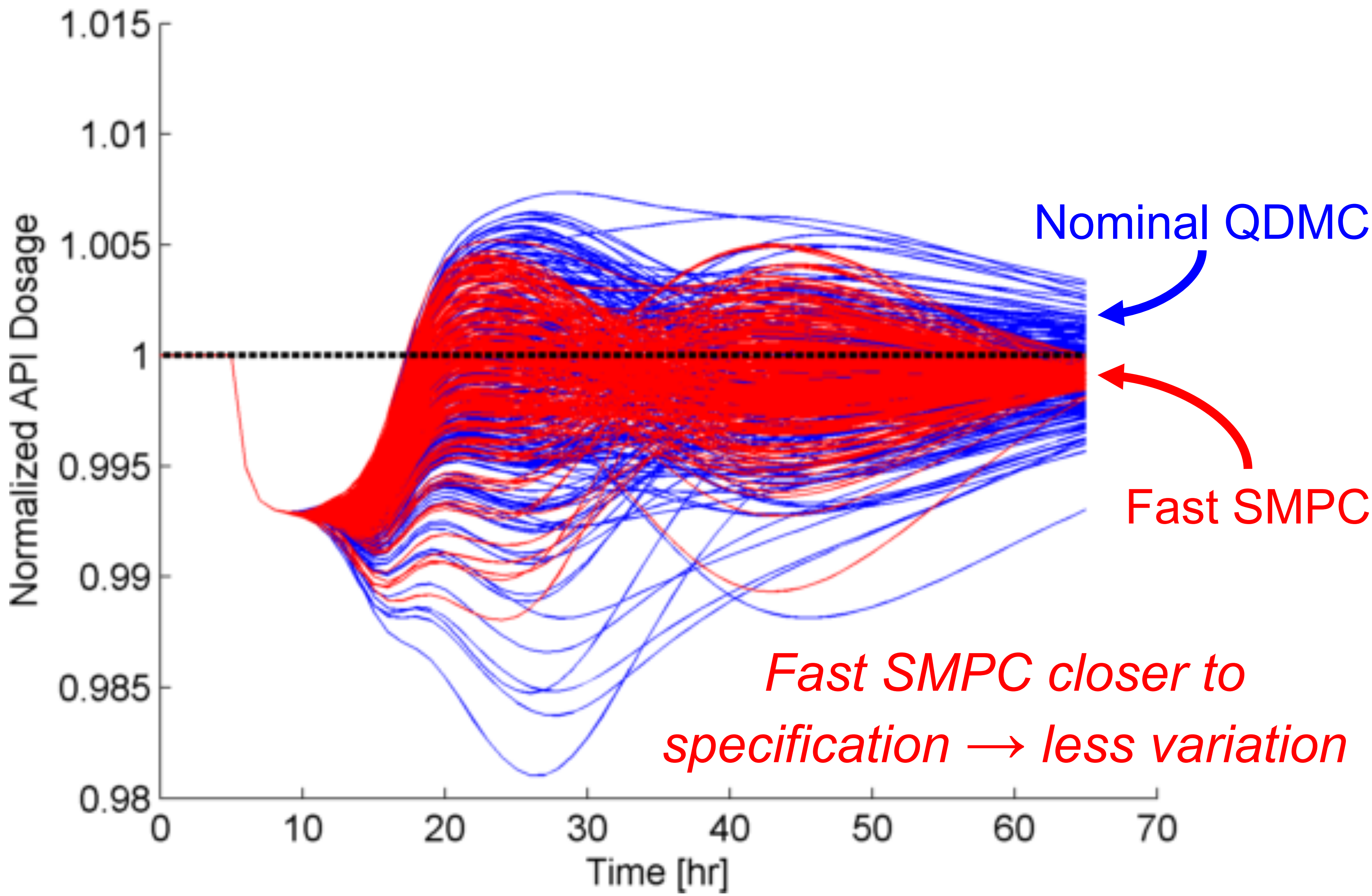
Ex: Continuous Pharmaceutical Manufacturing Plant



Ex: Continuous Pharmaceutical Manufacturing Plant

- Flowsheet for plant designed and constructed at MIT
- Detailed first-principles model of the pilot plant has
  - 3 outputs, 9 inputs, and 7613 states!
  - Outputs: production rate, API dose, and impurity content
- Used fast (<1s) PCT-based MPC to suppress adverse effects of uncertain kinetic parameters on operation
- Lower-level regulatory controls (e.g., level and recycle) used to ensure stable operation**

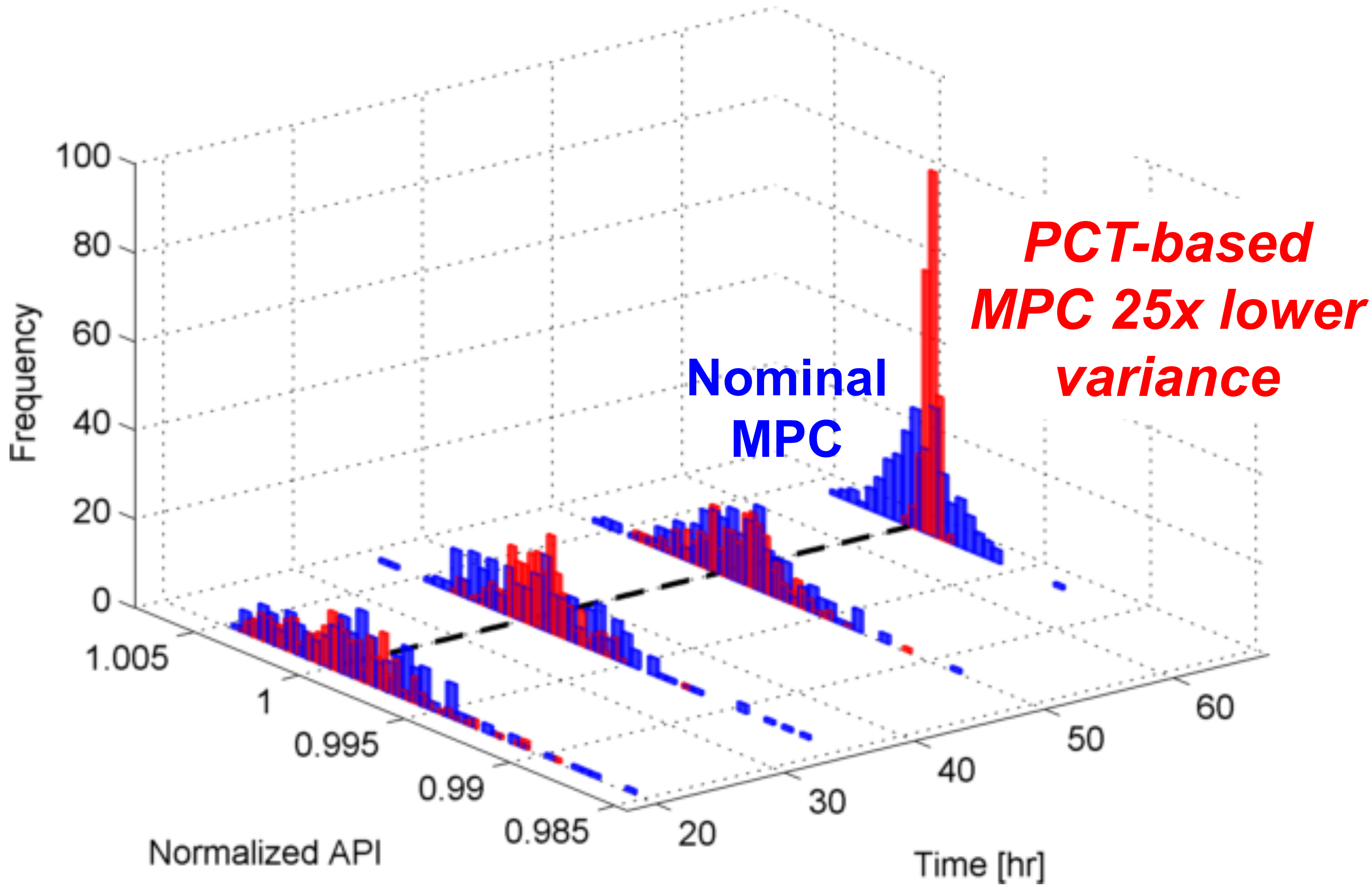
Results: Setpoint Change in the Production Rate



200 closed-loop simulations → each has different parameter values

J.A. Paulson et al., Fast stochastic model predictive control of high-dimensional systems. IEEE CDC, 2802-2809, 2014

Results: Setpoint change in Production Rate



200 closed-loop simulations, each having different parameter values

Common Characteristics of Advanced Process Systems

- High to infinite state dimension
- Model uncertainties: non-LFT, TI, $p(\theta)$
- Time delays
- Unstable zero dynamics
- Actuator, state, and output constraints
- Stochastic noise and disturbances
- Phenomena described by algebraic, ordinary and partial differential, and integral equations
- Mixed continuous-discrete operations
- Nonlinearities

Research needed on the analysis, design, and control of systems that simultaneously addresses **all** of these properties

Outline

- Recent Trends in Process Manufacturing Systems
- Prototype Process Manufacturing Systems
- Process Systems Design
- Control Theory
- More Open Research Problems

More Open Research Problems

- Practical algorithms for dealing with time-invariant probabilistic uncertainties have been published
  - Algorithms show improved performance over robust and nominal control in specific case studies
- Theoretical issues are largely unresolved
  - H_2- and H_∞-control algorithms are available with proven stability and performance for unconstrained systems
  - Stability, feasibility, mismatch in PDFs, and truncation error associated with PCEs not yet well resolved theoretically
- Many papers have incorporated chance constraints into MPC without any guarantee of their satisfaction by the closed-loop system (NMPC 2015)
  - Useful control theory for stochastic MPC is still an open field

Comments on More Open Research Problems

- Recommend balancing practicality of control algorithms with rigorous theoretical guarantees
- Analysis and design methods for arbitrarily fast time-varying (TV) parameters are much easier to derive
- Distributed parameter and mixed continuous-discrete (aka hybrid) systems with probabilistically uncertain time-invariant parameters are fairly unexplored
  - Statement holds for analysis, design, monitoring, control
  - Important due to being common in process manufacturing
- New better ways to handle nonlinearities
  - One approach is to employ polynomial methods (e.g., Paulson et al., Handbook of MPC, 2018)

Acknowledgements on PCT-based Control

- Prof. Zoltan K. Nagy, Purdue University
- Prof. Ali Mesbah, UC Berkeley
- Prof. Rolf Findeisen, Otto-von-Guericke U Magdeburg
- Prof. Sergio Lucia, TU Berlin
- Prof. Stefan Streif, TU Chemnitz
- Prof. Kwang-Ki Kim, Inha University
- Prof. Yiming Wan, Huazhong U of Science & Technology
- Prof. Joel A. Paulson, Ohio State University
- Dr. Eranda Harinath, Sanofi
- Dr. Dongying Erin Shen, Continuus
- Matthias E. Freiherr von Andrian-Werburg, MIT
- Anastasia Nikolakopoulou, MIT

Acknowledgements

"This material is based upon work supported by Novartis, the Defense Advanced Research Projects Agency, and SPAWAR Systems Center Pacific (U.S. Navy). Any opinions, findings and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the sponsors."