Applications of Nonlinear Optimization

GIAN Short Course on Optimization: Applications, Algorithms, and Computation

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Argonne National Laboratory

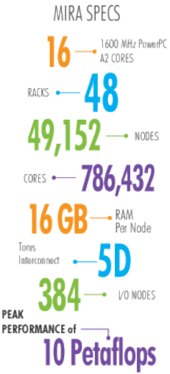
September 12-24, 2016

Outline

1. Introduction to Argonne National laboratory
2. Nonlinear Optimization for Power Grid Applications
   - Introduction to Power-Grid Applications
   - Optimal Unit Commitment for Power-Grid
3. Design of Complex Structures
   - Design of Nano-Structures
   - Topology and Structural Optimization
4. Analysis of Data and Images
   - X-ray Fluorescence Imaging
   - Multimodal Image Analysis
5. A Control Application: Optimal Transition to Clean Energy

Argonne National Laboratory

Department of Energy Laboratory (Open Science)



Two large user-facilities:

1. Advanced Photon Source
   ... ultra-bright X-ray source
2. Advanced Leadership Computing Facility
   ... Mira: 10 petaflops machine

Argonne National Laboratory

Argonne National Laboratory

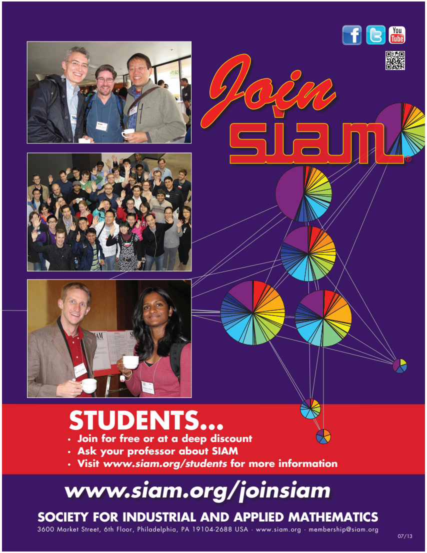
- Situated 25 miles SW of Chicago … site of CP-2
- 3,500 employees working in 14 research divisions
- Conduct basic research relevant to mission of DOE
  … used to be nuclear … now solar, wind, batteries, bio, …
- Mathematics and Computer Science has 110 staff & postdocs
- CS Research: Globus, MPICH, ZeptOS, …
- Math Research: Nek5000, NEOS, PETSc, …
- Student opportunities: summer interns (apply in January)
- Postdoc opportunities: e.g. Wilkinson Fellowship, late 2017

Math and CS at Argonne

Do you recognize this picture?

Math and CS at Argonne

UIC, Northwestern, Chicago SIAM student chapters visiting MCS Division



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SIAM Student Chapter
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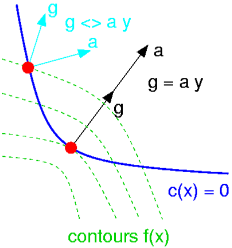
Today's Problem: Nonlinearly Constrained Optimization

Nonlinear Optimization Problems (NLPs)

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to } & c(x) \leq 0 \\ & x \in \mathcal{X}, \end{aligned}$$



where

- $\mathcal{X} \subset \mathbb{R}^n$ compact set, e.g. $\mathcal{X} = \{x \mid l \leq A^T x \leq u\}$ polyhedral
- $f : \mathbb{R}^n \to \mathbb{R}$ and $c : \mathbb{R}^n \to \mathbb{R}^m$ smooth functions

More general problems ...

- $l_x \leq x \leq u_x$ simple bounds
- $l_c \leq c(x) \leq u_c$ more general constraints
- Classes of variables: binary, integer, semi-definite, ...
- Classes of constraints: DAE, PDE, complementarity, ...

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Challenges in Power Grid Modeling

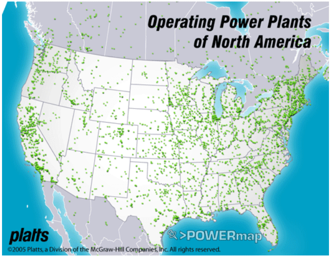
Computational Challenges in Power Grid Modeling

1. **Size:** $\simeq$ 100k lines ... "most complex machine ever built"
2. **Complexity:** nonlinear, hierarchical, and discrete decisions
3. **Uncertainty:** demand and supply (renewable) uncertainties

... many applications combine all three challenges

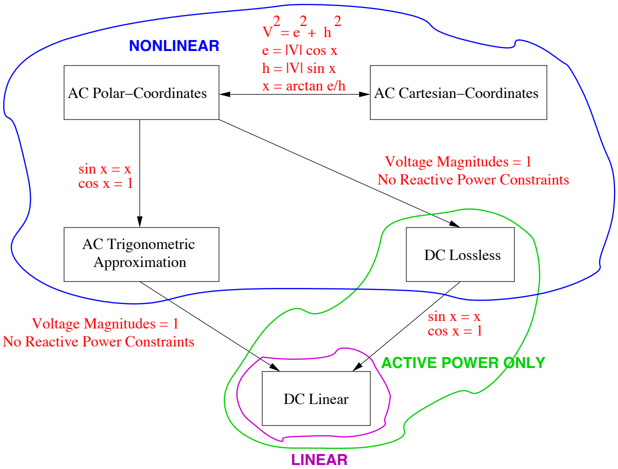
Missing from this talk:

- Big data
- Real-time decisions
- Cyber-security



... all involve modeling and computation

Complexity of Power Grid: Nonlinearities



- Operation & Design: optimal power flow, transmission switching, network expansion
- Challenge: interaction of nonlinearities & discrete decisions

Complexity of Power Grid: Discrete Decisions

- Given existing power grid network and demand forecast
- Design expanded network for secure transmission

Traditional Approach. Simplify nonlinear (AC) power flow model:

$$F(U_k, U_l, \theta_k, \theta_l) := b_{kl} U_k U_l \sin(\theta_k - \theta_l) + g_{kl} U_k^2 - g_{kl} U_k U_l \cos(\theta_k - \theta_l)$$

by setting $\sin(x) \simeq x$ and $\cos(x) \simeq 1$ and $U \simeq 1$

Nonlinear Optimization Approach. Work with nonlinear model

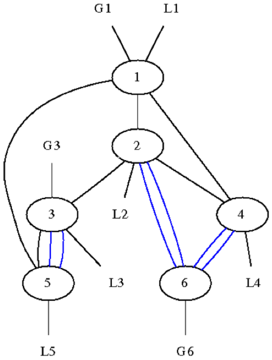
- $-M(1 - z_{k,l}) \leq f_{k,l} - F(U_k, U_l, \theta_k, \theta_l) \leq M(1 - z_{k,l})$
- $z_{k,l} \in \{0, 1\}$ switches lines on/off; $M > 0$ constant

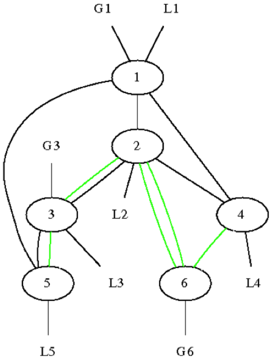
Questions.

Can we solve the nonlinear models? Do nonlinearities it matter?

Power-Grid Transmission Network Expansion

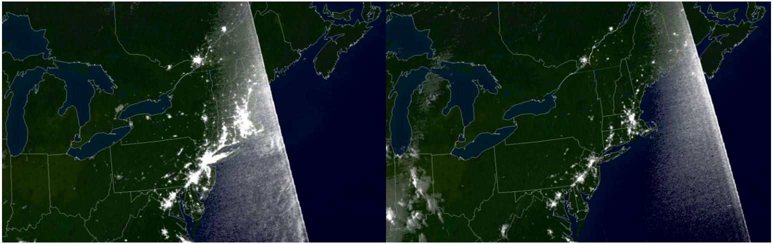
Expansion Results for linear vs. nonlinear power flow models





- Solve realistic AC power flow expansion models on desktop
- Significant difference between DC and AC solution
- Linearized DC model not feasible in AC power flow
- Linear DC model *not* valid when topology changes

Blackout Prevention in National Power Grid



2003 blackout: before and during

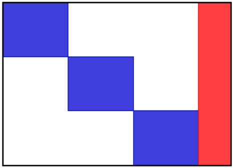
- 2003 blackout cost $4-10 billion and affected 50 million people
- prevent with contingency analysis
  - find least number of transmission lines whose removal results in failure
  - binary variables model removal of lines
  - nonlinearities model power flow
  - results in large integer optimization problem
- current analysis limited to 10s of lines

... similar models arise in many other power-grid applications

Unit Commitment with Wind Power [Cosmin Petra]

Wind uncertainty $\Rightarrow$ stochastic optimization: min. expected cost

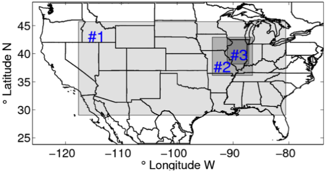
$$\begin{aligned}&\underset{x}{\text{minimize}} \quad f(x) + \mathbb{E}_\omega \left(\min_z \; h(x, z; \omega) \text{ s.t. } g(x, z; \omega) \geq 0 \right) \\ &\text{subject to } c(x) \geq 0\end{aligned}$$



- x — here-and-now decisions
- z — 2nd-stage decisions/scenarios
  … random realizations of wind
- $\omega \in \Omega$ random parameters

Realistic wind scenarios

- Weather Research Forecasting (WRF)
- Real-time grid-nested 24h simulation
- $|\Omega| = 30$ samples of WRF



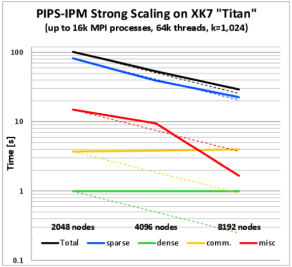
Stochastic Unit Commitment [Cosmin Petra]

PIPS - scalable framework for stochastic optimization problems

- Parallel distributed implementations of interior-point (IPM)
- Block-angular linear systems suitable to parallelization
- Schur complement-based decomposition of linear algebra
- Parallelization bottlenecks: dense linear algebra (first stage)
- Dense matrices can go on GPUs, multicores, or be distributed.

PIPS-IPM ported to IBM BG/P and BG/Q, Cray XE6, XK7 & XC30

- 32k scenarios
- 4 billion variables and constraints
- 128K cores on BG/P and 64K cores on XK7



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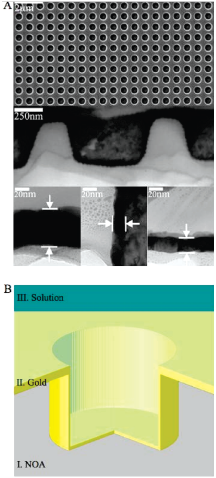
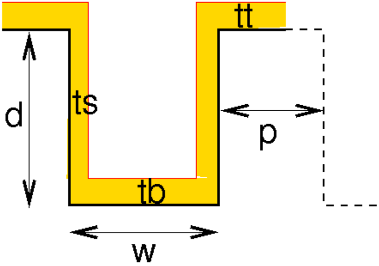
Design of Nano-Photonic Devices



- nano-structures for chemical sensing
  optical response at certain wave-lengths
- Top: scanning electron micrograph
  Middle: cross section of crystal
  Bottom: gold thickness
- 3D FEM analysis simulation; no gradients
  periodicity, gold thickness, depth, & width of nano-wells
- derivative-free optimization
  objective function evaluation takes 12 hrs
  ... on 125 nodes of an Apple G5 X-server
- optimization of a black-box
  ... simulation-based optimization
  ... derivative-free optimization

Inside the Black Box

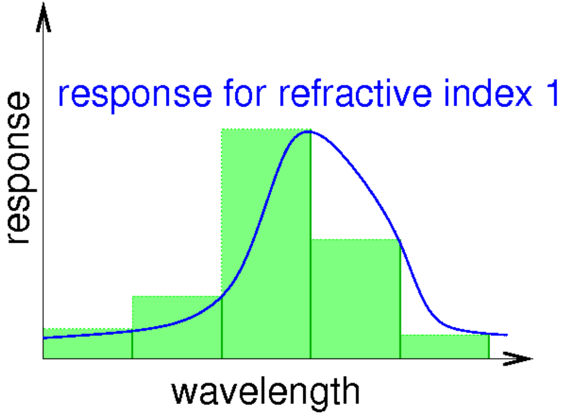
Design Parameters:



- d = depth of nano-well
- p = periodicity of design
- w = width/diameter of nano-well
- t = thickness (side/bottom/top) gold layer

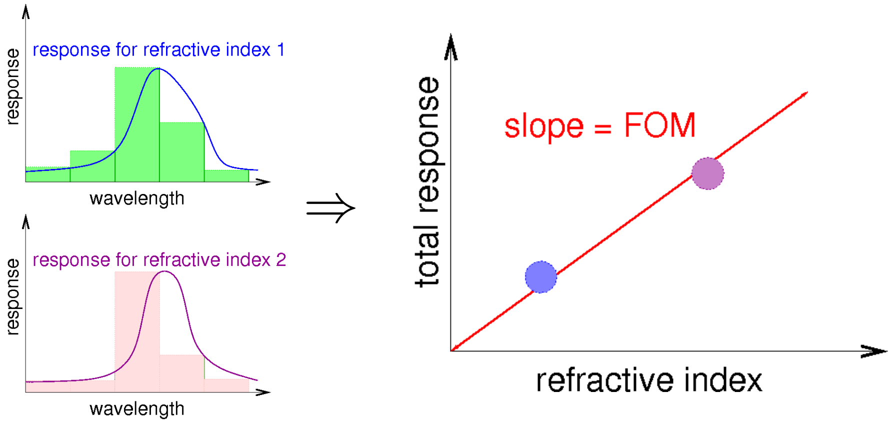
Inside the Black Box

Given values of design parameters (d, p, w, ts, tb, tt)
... perform PDE simulation for refractive index



... get total response

Objective = Figure of Merit (FOM)



... combine responses for different refractive indices

... maximize slope (sensitivity) of design

... requires solution of many PDEs

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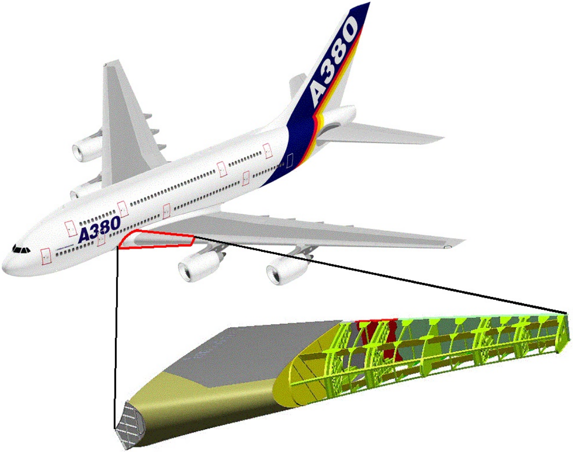
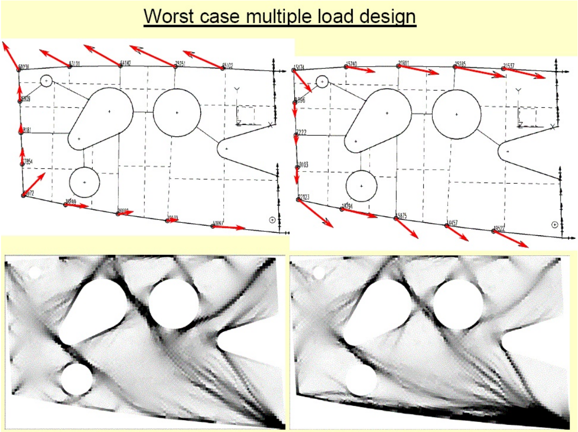
Example: Topology & Structural Optimization [Kocvara]



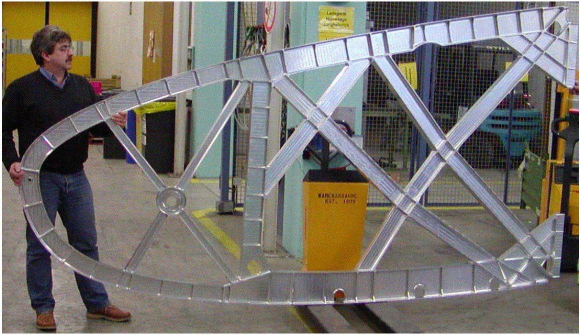
Airbus A-380 inboard inner leading edge ribs

Example: Topology & Structural Optimization [Kocvara]



Minimize weight of structure subject to load & design restrictions

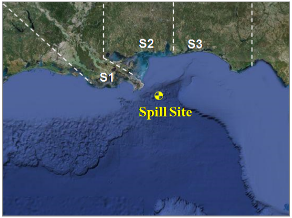
Example: Topology & Structural Optimization [Kocvara]

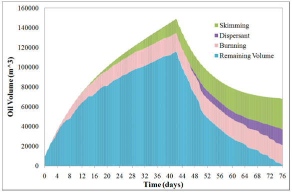


Optimized topology reduces weight by 33%

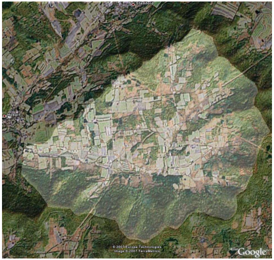
Other Optimization Applications

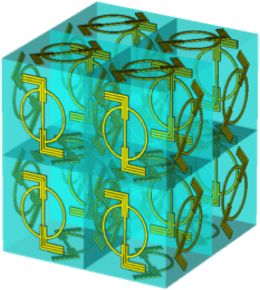
- Optimization of oil-spill response ... MIP control
- Design and control of chemical processes
- Design and operation of building energy systems
- Design of wind farms & dispatch of wind energy
- Image analysis, inverse problems, big data, ...
- Cybersecurity: resource allocation & attacker-defender models
- Fighter intercept optimal control problems

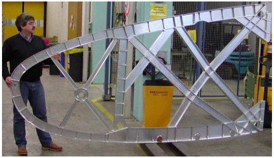




Optimization of Complex Systems







Take-Home Message: More complex optimization problems!

- Complex science & engineering apps drive optimization:
  - Discrete decision give rise to integer variables
  - Complex physics modeled using ODEs, DAEs, or PDEs
  - Uncertainty quantification for robust decisions & design
- Many open problems in need of new methods and ideas!

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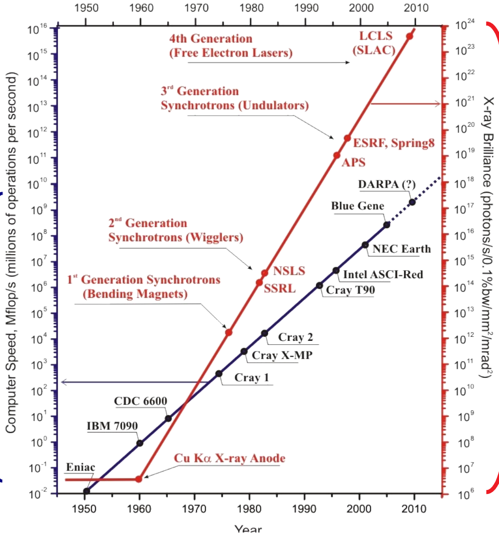
Light source data growing faster than Moore's law

Computers: 12 orders of magnitude in 6 decades



Light sources: 18 orders of magnitude in 5 decades

Data Analysis: X-ray Imaging the APS

SL, Stefan Wild, Siwei Wang, & Stefan Vogt (APS)

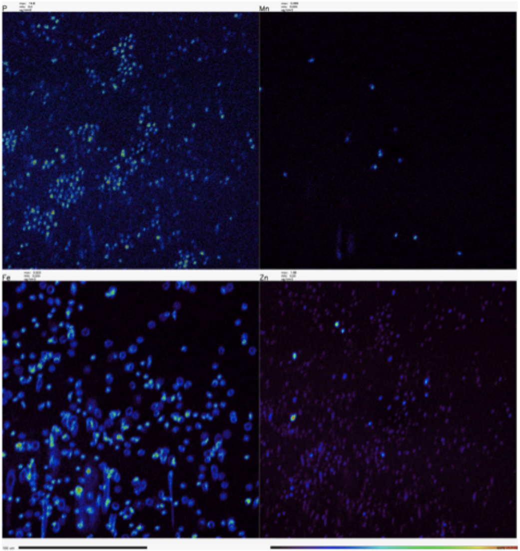
Science Challenges in Nano-Medicine & Theranostics:

- Design new treatment and drugs for targeted drug delivery
  Combine therapy & diagnostics by targeting nano-particles
- Extract efficiency score from multiple sources of data
  MRI of living specimen; X-ray, fluorescent & visible light

Specific Questions:

- Given a sample, how many elements/cells are in the sample?
- Identify abnormal concentrations: cancer vs. healthy cells.
- Identify marker elements (e.g. Ti) for tracking biochemical processes.

Typical Image: Postdoc Marks Cells By Hand

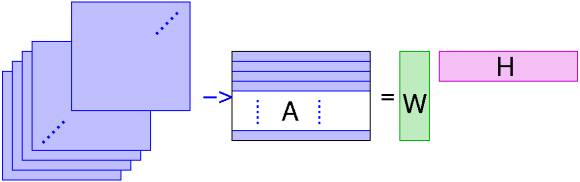


Concentration maps of P, Mn, Fe, Zn ... where's the yeast/algae?

Nonnegative Matrix Factorization

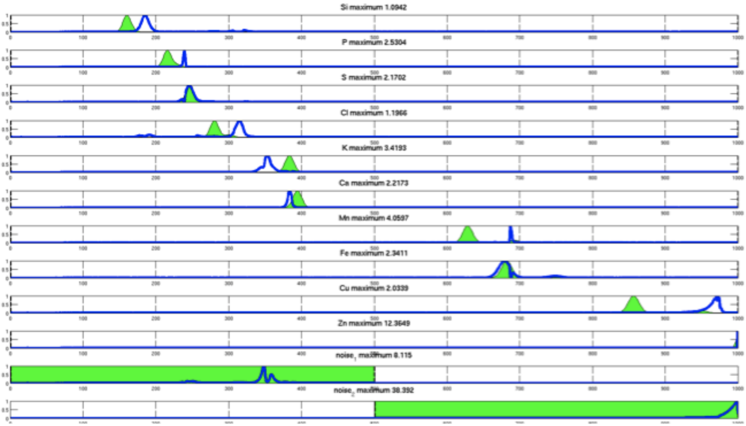
Goal: Find signature masks for cells for image segmentation

- Photon counts are additive $\Rightarrow$ use additive reduction
- $\underset{W,H}{\text{minimize}} \; \|A - WH\|_F^2 \quad$ subject to $W \geq 0, \; H \geq 0$



- W are weight $\simeq$ additive elemental spectra
- H are images $\simeq$ additive elemental maps
- Solve using (cheap) gradient steps

Nonnegative Matrix Factorization



Initialization of W and final value.

… now use H (additive elemental maps) to segment images

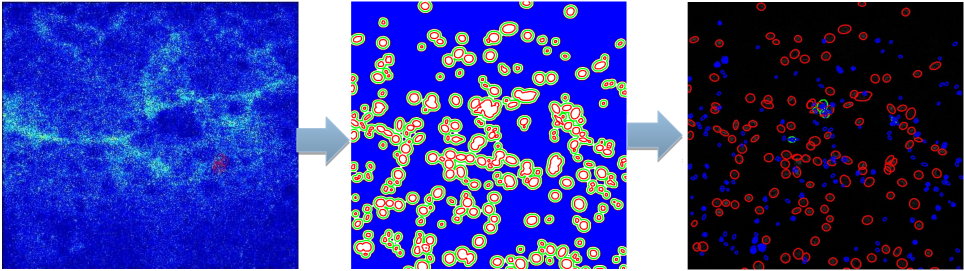
XFM@APS: Automatic Cell Discovery & Classification

Enables *fast* processing of larger samples, reduces error, automatically classifies cells

- Pre-processing with **non-negative matrix factorization**
- Image partitioned using **spectral graph partitioning**
- **Wavelet transforms** delineate curves and allow for overlapping cells
- Incorporate domain-specific knowledge with **large-scale MINLP optimization** approach

Noisy, Multichannel Data

Yeast, **Algae**, **Red Blood** Cells



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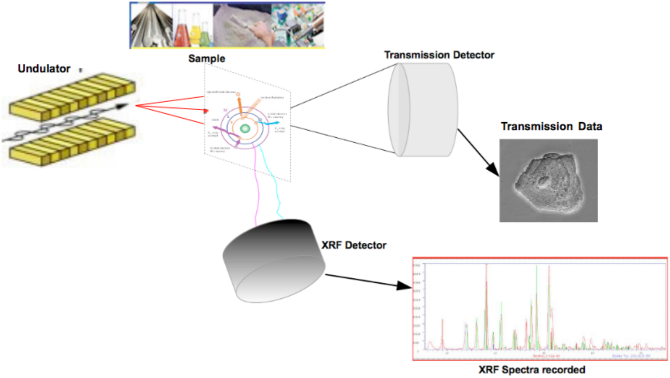
Multimodal Image Analysis

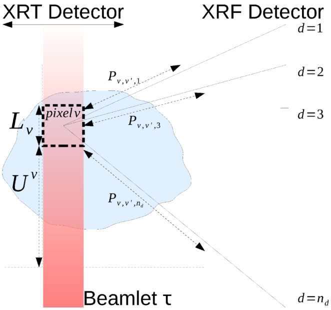
Next-generation accelerators capture multiple data modalities:
e.g. transmission (XRT) and fluorescence (XRF) in single shot

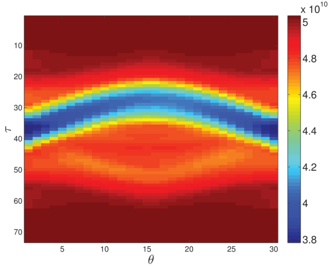


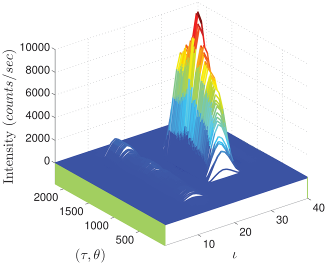
Goal:

Optimization for joint inversion from multiple data modalities.

Multimodal Image Analysis: Explosion of Data







Transmission

Fluorescence

Joint XRT & XRF Reconstruction (JRT)

More challenging nonlinear optimization:

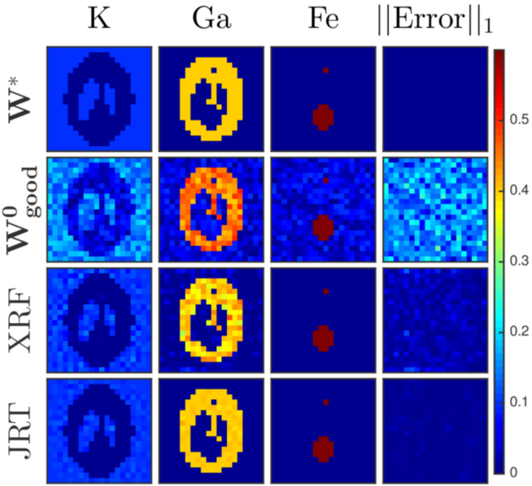
- Find weights $\mathbf{W}$: $\mathbf{F}^{\mathfrak{R}}_{\boldsymbol{\theta},\boldsymbol{\tau},\mathbf{E}}(\mathbf{W}) = \mathbf{D}^{\mathfrak{R}}_{\boldsymbol{\theta},\boldsymbol{\tau},\mathbf{E}}$ and $F^{\mathfrak{T}}_{\theta,\tau,E}(\mathbf{W}) = D^{\mathfrak{T}}_{\theta,\tau,E}$
- Single mode reconstruction is under-determined

$$\min_{\mathbf{W}} \sum_{\theta,\tau} \left(\frac{1}{2} \left\| \mathbf{F}^{\mathfrak{R}}_{\boldsymbol{\theta},\boldsymbol{\tau},\mathbf{E}}(\mathbf{W}) - \mathbf{D}^{\mathfrak{R}}_{\boldsymbol{\theta},\boldsymbol{\tau},\mathbf{E}} \right\|^2 + \frac{\beta}{2} \left\| F^{\mathfrak{T}}_{\theta,\tau,E}(\mathbf{W}) - D^{\mathfrak{T}}_{\theta,\tau,E} \right\|^2 \right)$$

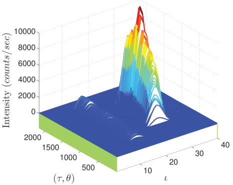
where

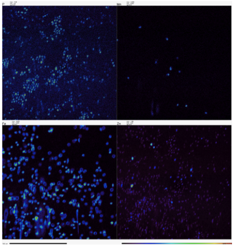
- $\mathbf{D}^{\mathfrak{R}}_{\boldsymbol{\theta},\boldsymbol{\tau},\mathbf{E}} \in \mathbb{R}^{n_E}$: Fluorescence data
- $D^{\mathfrak{T}}_{\theta,\tau,E} \in \mathbb{R}$: Transmission data
- $\mathbf{W} \geq 0$: constraint on voxel contents

JRT versus Single XRF Reconstruction



Optimization for Large Data and Image Analysis





Take-Home Message: Many interesting problems!

- Increased data rates drive optimization
- Huge scope for new optimization models and methods
  - Need to work with large data
    $\Rightarrow$ traditional techniques not applicable
  - Exploit domain knowledge whenever possible!

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Optimal Reduced-Carbon Technology Penetration

What is the optimal path to reduced-carbon economy?

Don Hanson, Steve Kryukov, Sven Leyffer, and Todd Munson

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U.S. Department of Energy
UChicago Argonne LLC

Modeling Optimal Penetration of Low-Carbon Technology

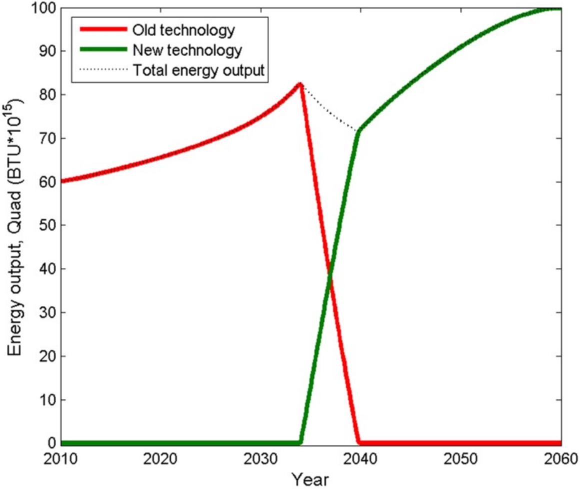
- Optimize energy production schedule and transition from old to new reduced-carbon technology to meet carbon targets
  - Maximize social welfare subject to GHG target in 50 years
  - Reduced-carbon technology subject to learning effects
    i.e. reduced unit cost as new technology becomes widespread
  - Includes adjustment costs (penalize rapid change in energy schedule)

- Social planner's problem … government in charge of everything

- Reasonable assumptions on GHG emissions, demand growth, energy costs, …

- Optimal control problem
  - Formulated using modeling language (AMPL)
  - Solved with nonlinear optimizers (KNITRO)
  - 50-year horizon solves within seconds on desktop

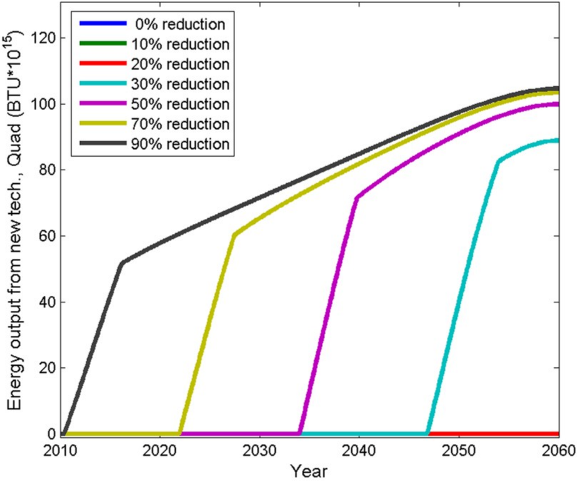
50% GHG Reduction: Optimal Energy Production Schedule



Transition period 2034-2040:
old conventional technology is gradually replaced by new low-emission technology

Effect of Different GHG Reduction Targets

- Plot shows low-emission energy production for different GHG targets.
- Transition to new technology is not necessary until 30% reduction target.



Technology Transition Model Description

- **Time** models dynamics over continuous time $t \in [0, T]$
  Functions of time $x(t)$ with derivatives

$$\dot{x}(t) = \frac{dx(t)}{dt}.$$

- **Energy Output** of old/new technologies at time t are $q^o(t),\ q^n(t)$.
  Define total output $Q(t) = q^o(t) + q^n(t)$.
- **Demand and Consumer Surplus** model benefit of energy to society:

$$\tilde{S}(Q,t) = e^{bt} S(Qe^{-bt}),$$

where $b > 0$ growth rate of demand.
Derived from constant elasticity of substitution (CES) utility.

$$S(Q) = \begin{cases} S(Q) = S_0 \ln Q, & \text{if } \sigma = 1 \\ \frac{S_0}{1-\sigma} Q^{1-\sigma}, & \text{otherwise,} \end{cases}$$

where $\sigma > 0$ is demand parameter.

Technology Transition Model Description

- **Production Costs.** Assume constant marginal costs.
  - Old technology unit cost: c_o
  - New technology unit cost subject to learning-by-doing: $c_n(x(t))$ decreasing function of cumulative output:

$$x(t) = \int_0^t q^n(\tau)d\tau.$$

  - Following [**?**], we let

$$c_n(x) = c_n^0 \left[\frac{x}{\bar{X}} + 1\right]^{\log_2 \gamma},$$

    where $\bar{X}$ and γ are parameters.
- **Greenhouse Gases Emissions**
  - Old technology emissions rate: $b_o > 0$
  - New technology emissions rate: $b_n \in (0, b_o)$
  - Cumulative (discounted) emissions at end period:

$$\int_0^T e^{-at}\big(b_o q^o(t) + b_n q^n(t)\big)dt \leq z_T$$

A Basic Model for Technology Transition

- Maximize social welfare subject to emissions caps.
- Control variables: Energy output $q^o(t), q^n(t)$
- State variables: Experience $x(t)$ and Emissions $z(t)$

$$
\begin{aligned}
\underset{\{q^o,q^n,x,z\}(t)}{\text{maximize}} \quad & \int_0^T e^{-rt}\left[\tilde{S}(q^o(t)+q^n(t),t) - c_o q^o(t) - c_n(x(t))q^n(t)\right] dt \\
\text{subject to} \quad & \dot{x}(t) = q^n(t), \qquad x(0) = x_0 = 0 \\
& \dot{z}(t) = e^{-at}\left(b_o q^o(t) + b_n q^n(t)\right), \qquad z(0) = z_0 = 0 \\
& z(T) \le z_T \\
& q^o(t) \ge 0, \qquad q^n(t) \ge 0.
\end{aligned}
$$

AMPL Model for Optimal Technology Penetration

Write an AMPL model of the basic technology transition problem

$$\begin{aligned}
\underset{\{q^o,q^n,x,z\}(t)}{\text{maximize}} \quad & \int_0^T e^{-rt}\left[\tilde{S}(q^o(t)+q^n(t),t) - c_o q^o(t) - c_n(x(t))q^n(t)\right] dt \\
\text{subject to} \quad & \dot{x}(t) = q^n(t), \qquad x(0) = x_0 = 0 \\
& \dot{z}(t) = e^{-at}\left(b_o q^o(t) + b_n q^n(t)\right), \qquad z(0) = z_0 = 0 \\
& z(T) \le z_T \\
& q^o(t) \ge 0, \qquad q^n(t) \ge 0.
\end{aligned}$$

where

$$\tilde{S}(Q,t) = e^{bt} S(Qe^{-bt}),$$

where $b > 0$ growth rate of demand, and

$$S(Q) = \begin{cases} S(Q) = S_0 \ln Q, & \text{if } \sigma = 1 \\ \frac{S_0}{1-\sigma} Q^{1-\sigma}, & \text{otherwise,} \end{cases}$$

AMPL Model for Optimal Technology Penetration

Parameter	Unit	Notation	Value
Discount rate	-	r	0.05
Demand exponent	-	σ	2.0
Demand scale	\$B	S_0	98,000
Demand growth rate	-	b	0.015
Environmental rate	-	a	0.02
Emissions, old tech.	tC/mBTU	b_o	0.02
Emissions, new tech.	tC/mBTU	b_n	0.001
Unconstrained emissions	BtC	Z_{max}	61.9358
Emission reduction %	-	ζ	0.5
Emissions target	BtC	$z_T = \zeta Z_{\mathrm{max}}$	
Production cost, old tech.	\$/mBTU	c_o	20
Starting cost, new tech.	\$/mBTU	c_n^0	50
Learning rate	-	γ	0.85
Initial experience	quad	x_0	0
Experience unit size	quad	$\bar{X}$	300

AMPL Model for Optimal Technology Penetration

Write an AMPL model of the basic technology transition problem

$$\begin{aligned}
\underset{\{q^o,q^n,x,z\}(t)}{\text{maximize}} \quad & \int_0^T e^{-rt}\left[\tilde{S}(q^o(t)+q^n(t),t) - c_o q^o(t) - c_n(x(t))q^n(t)\right] dt \\
\text{subject to} \quad & \dot{x}(t) = q^n(t), \qquad x(0) = x_0 = 0 \\
& \dot{z}(t) = e^{-at}\left(b_o q^o(t) + b_n q^n(t)\right), \qquad z(0) = z_0 = 0 \\
& z(T) \le z_T \\
& q^o(t) \ge 0, \qquad q^n(t) \ge 0.
\end{aligned}$$

1. Solve the model for different time steps, h
2. Experiment with different discretization schemes, e.g. explicit or implicit Euler and Trapezoidal rule
3. Use AMPL's `fprintf` to output your results & plot the transition paths in Matlab.

Optimal Technology Penetration: Hints & AMPL Tricks

Attributes & Defined Variables

```
param Ntime > 0, integer, default 200;  # ... time-steps

set T := 0..Ntime;

var qo{T} >= 0, := 10;        # ... old technology
var qn{T} >= 0, := 1;         # ... new technology

var z{T};                     # ... emissions

var dzdt{t in T: t<Ntime} = (z[t+1] - z[t])/h;

subject to

 # ... ODE for z(t)
 InitZ: z[0] = z0;                # ... initial cond.
 DiffEqnZ{t in T: t<Ntime}:      # ... disc. ODE
  dzdt[t] = exp(-a*t*Tend/Ntime) * (bo*qo[t] + bn*qn[t]);
```

Optimal Technology Penetration: Hints & AMPL Tricks

AMPL Defined Variables

```
var dzdt{t in T: t<Ntime} = (z[t+1] - z[t])/h;
```

- Acts like a constraints, but substituted out of model.
- Note "=" assigns constraints, and ":=" initial variable value
- All Variables/expressions on RHS must be defined previously

Check out effect of defined variables

- To show variables passed to solver, use
  `display _svarname, _sconname;`
- To show variables in model, use
  `display _varname, _conname;`

Conclusion: Optimization is Cool