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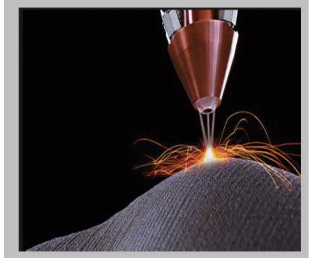

Software Capabilities For Solving Mixed Integer PDE-Constrained Optimization

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Sandia National Laboratories

Collaborators: Sven Leyffer (Argonne), Lars Rutthoto (Emory), Meneerali

August, 2019

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Exceptional service in the national interest

Motivation

- Disaster recovery:
  - scheduling evacuation while calibrating hurricanes for accurate predictions,
  - mitgating wildfires
  - controlling oil spills
- Additive manufacturing:
  - control of laser velocity, magnitude and rasterization pattern while selecting material type
- Energy:
  - hydrocarbon hydrocarbon
  - gas networks
  - electrical grid
  - solar cells
- Piezoelectric
  - communication through barriers
  - energy harvesting

Outline

- Background
- Formulation
- Solution Strategies
- Software Overview
  - PEBBL
  - ROL
  - Interface
- Numerical prototype
  - Linear convection diffusion
  - Nonlinear diffusion reaction
- Summary

Background

1. Carl Laird, Lorenz Biegler and Bart van Bloemen Waanders, “A mixed integer approach for obtaining unique solutions in source inversion of drinking water networks”, Special Issue on Drinking Water Distribution Systems Security, Journal of Water Resources Planning and Management, Vol 132, 2006.
2. Susanne Moritz “A Mixed Integer Approach for the Transient Case of Gas Network Optimization”, Thesis, 2006
3. Armin Fugenschuh, Bjorn Geißler, Alexander Martin, Antonio Morsi, “The Transport PDE and Mixed-Integer Linear Programming”, 2009.
4. Fugenschuh,A.,Gottlich,S.,Kirchner,C.,Herty,M.,Martin,A.:Efficient reformulation and solution of a nonlinear PDE-controlled flow network model. Computing 85 (2009)
5. Pelin Cay, Bart van Bloemen Waanders, Drew Kouri, Anna Thuenen and Sven Leyffer “ SAMSI Workshop, 2016
6. Fabian Gnegel, Michael Dudzinski, Armin Fu ̈genschuh, and Markus Stiemer, “Mixed Integer PDE Constrained Optimization for the Control of a Wildfire Hazard” 2017
7. Mirko Hahn, Sven Leyffer, and Victor Zavala, “Mixed-Integer PDE-Constrained Optimal Control of Gas Networks, 2017
8. Christian Wesselhoeft, “Mixed-Integer PDE-Constrained Optimization”, 2017 MSc Degree in Computing Science (Machine Learning) of Imperial College London
9. Meenarli Sharma, Sven Leyffer, Lars Ruthotto, and Bart van Bloemen Waanders, “Inversion of Convection Diffusion Equation with Discrete Source” 2019 (in preparartion

Formulation: mixed integer

$$\min_{u,x} \; f(u,x) \quad \text{subject to} \quad c(u,x) = 0$$

where u is the state, x are the control variables, $x \in \mathcal{Z}^p$ (integers), $c(u,x)$ is a set of PDE equations

Solver Strategies and Challenges

- Branch and bound
- Generalized Benders decomposition
- Outer approximation
- Outer approximation with equality relaxation
- Outer approximation with equality relaxation and augmented penalty
- Generalized outer approximation
- Generalized Cross Decomposition

PEBBL: Parallel Enumeration and Branch and Bound Library*

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- provide extreme scalability in implementing branch-and- bound methods on distributed-memory computing systems.
- C++, using the MPI message-passing API [49] to communicate between processors
- flexible work distribution and load balancing scheme that achieves unmatched scalability and has only two strata in its processor hierarchy "workers and hubs"
- application-specific non-tree parallelism during the search ramp-up phase, followed by a "crossover" to using tree-based parallelism
- Support for enumeration of multiple optimal and near-optimal solutions meeting a variety of configurable criteria

*Jonathan Eckstein · William E. Hart · Cynthia A. Phillips, "PEBBL: An Object-Oriented Framework for Scalable Parallel Branch and Bound "

Software Overview: PEBBL

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PEBBL (Parallel Enumeration and Branch and Bound Library) might be a useful tool for solving large-scale problems with a combinatorial piece (e.g. mixed-integer optimization)

Branch and bound

- Intelligent enumerative search
- Finds an optimal solution and (computationally) proves optimality
  - But might take too long if not done carefully
- Software freely available (BSD license)
- Highly scalable

J. E. Eckstein, W. E. Hart, C. A. Phillips, "PEBBL: an object-oriented framework for scalable parallel branch and bound," Mathematical Programming Computation, Vol. 7, No. 4, pp. 429– 469, December, 2015.

Branch and Bound

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Branch and Bound is an **intelligent** (enumerative) **search** procedure for discrete optimization problems.

$$\min_{x \in X} f(x)$$

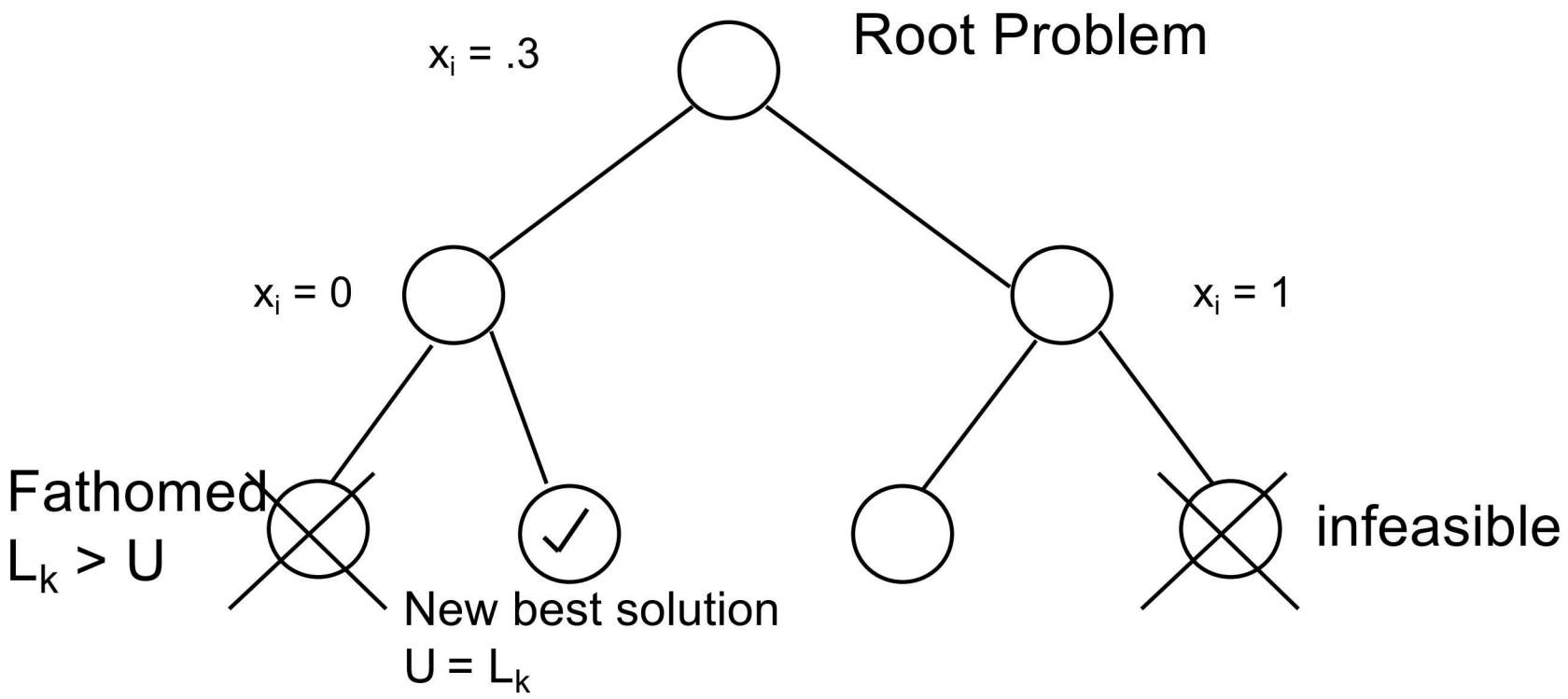
Requires subproblem representation and 3 (problem-specific) procedures:

- Compute an lower bound *b(X)*

$$\forall x \in X,\ b(x) \leq f(x)$$

- **Find a candidate solution**
  - Can fail
  - Require that it **recognizes feasibility** if X has only one point
- **Split** a feasible region (e.g. over parameter/decision space)
  - e.g. Add a constraint

Branch and Bound



- Recursively divide feasible region, prune search when no optimal solution can be in the region.
- Important: need good bounds, good heuristics

Parallel Enumeration and Branch-and-Bound Library (PEBBL)

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Check if no other parallel B&B tools?

- Distributed memory (MPI), C++
- Massively parallel (scalable)
- General parallel Branch & Bound environment
- Parallel search engine cleanly separated from application and platform
- Portable
- Flexible
- Integrate approximation techniques
- Open source

(There are other parallel B&B frameworks: PUBB, Bob, PPBB-Lib, Symphony, BCP, CHiPPS/ALPS, FTH-B&B, and codes for MIP)

PEBBL Features for Efficient Parallel B&B

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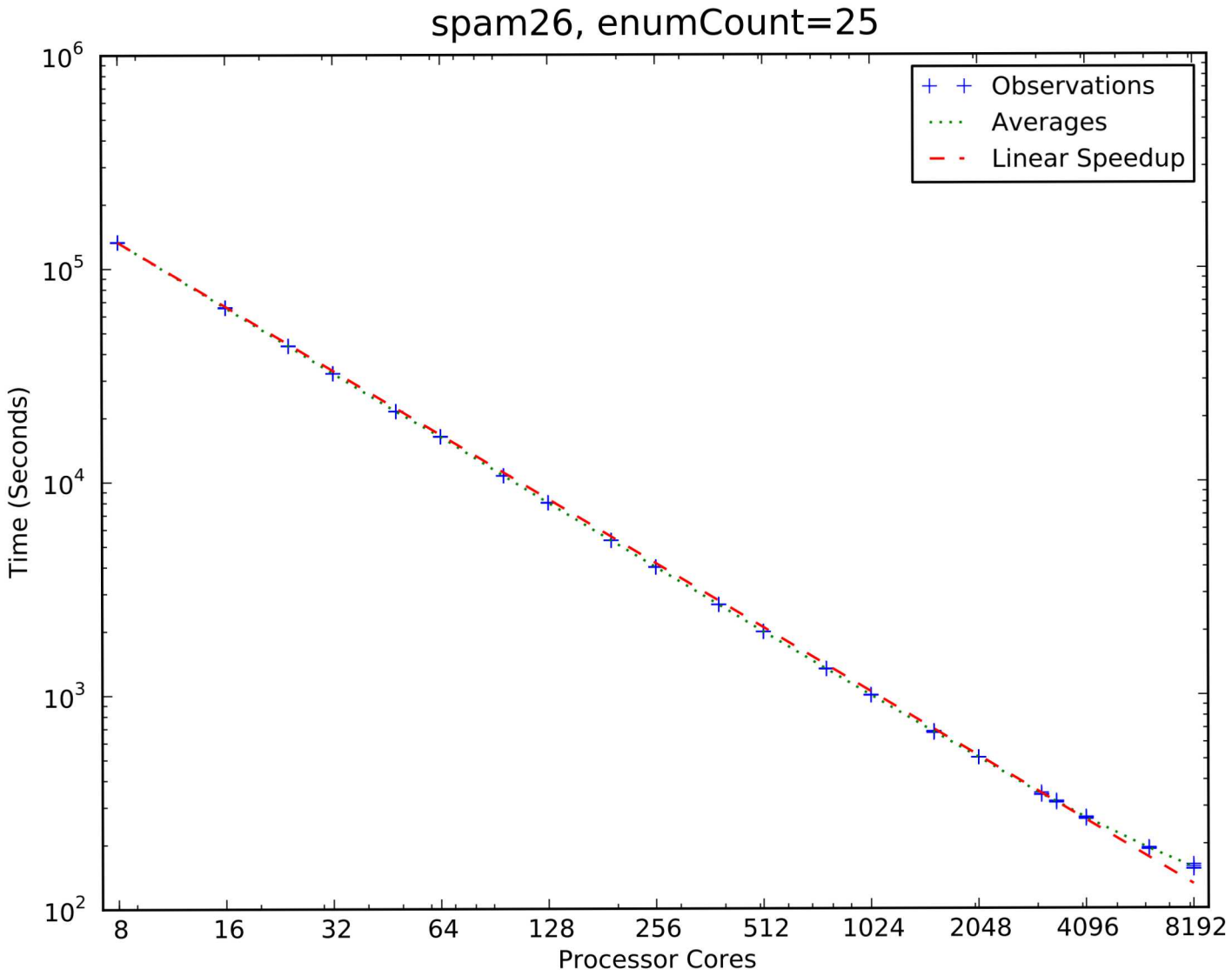
- Efficient processor use during ramp-up (beginning)
- Integration of heuristics to generate good solutions early
- Worker/hub hierarchy
- Efficient work storage/distribution
- Control of task granularity
- Load balancing
- Non-preemptive proportional-share "thread" scheduler
- Correct termination
- Early output
- Checkpointing

Results: Enumeration



Bound Computation: PDE-constrained optimization

$$\min_{u,x} \; f(u,x) \quad \text{subject to} \quad c(u,x) = 0$$

where u is the state, x are the control variables,

Full space solution strategy

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$$\min_{u,x} \; f(u,x)$$

$$\text{subject to: } c(u,x) = 0$$

Optimization Formulation

$$\mathcal{L}(u,x,\lambda) = f(u,x) + \lambda c(u,x)$$

Lagrangian

$$\begin{Bmatrix} \mathcal{L}_u \\ \mathcal{L}_x \\ \mathcal{L}_\lambda \end{Bmatrix} = \begin{Bmatrix} J_u + \lambda c_u \\ J_x + \lambda c_x \\ c \end{Bmatrix} = 0$$

Optimality conditions

$$\begin{bmatrix} \mathcal{L}_{uu} & \mathcal{L}_{ux} & c_u^T \\ \mathcal{L}_{xu} & \mathcal{L}_{xx} & c_x^T \\ c_u & c_x & 0 \end{bmatrix} \begin{Bmatrix} \delta u \\ \delta x \\ \lambda^* \end{Bmatrix} = - \begin{Bmatrix} f_u \\ f_x \\ c \end{Bmatrix}$$

KKT after Newton iteration

Reduced space solution strategy

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$$\min_x \ \hat{f}(x) \qquad \text{where } u \text{ solves } c(u(x), x)$$

$$\frac{\partial \hat{f}(x)}{\partial x} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f}{\partial x}$$

$$\hat{f}(x) = f(u(x), x) \qquad \frac{\partial u}{\partial x} = -\frac{\partial c}{\partial u}^{-1}\frac{\partial c}{\partial x}$$

$$\frac{\partial \hat{f}(x)}{\partial x} = -\frac{\partial f}{\partial u}\frac{\partial c}{\partial u}^{-1}\frac{\partial c}{\partial x} + \frac{\partial f}{\partial x}$$

$$\frac{\partial \hat{f}(x)}{\partial x} = -\frac{\partial c}{\partial u}^{-T}\frac{\partial f}{\partial u}\frac{\partial c}{\partial x} + \frac{\partial f}{\partial x}$$

$$x_{n+1} = x_n + \alpha p^N \qquad p^N = -\nabla^2 \hat{f}^{-1} \nabla \hat{f}$$

Trilinos packages

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Linear Algebra
Epetra
EpetraExt
Tpetra
Jpetra
Kokkos

Preconditioners
ML
Ifpack
Teko

Mesh Partitioning / DD
Claps
Moertel
Isorropia
Zoltan

Solvers
AztecOO
Belos
Pliris
Komplex
Amesos
NOX
LOCA
ROL
Piro
Rythmos
TriKota
Globipack
Optipack
Anasazi

PDE Tools
Phalanx
Intrepid
Shards
Panzer

Tools
Teuchos
SEACAS
STK
Sacado
Stokhos

Interfaces
Thyra
PyTrilinos
Stratimikos

Trilinos: ROL

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Linear Algebra
- **Epetra**
- EpetraExt
- Tpetra
- Jpetra
- Kokkos

Preconditioners
- **ML**
- Ifpack
- Teko

Mesh Partitioning / DD
- Claps
- Moertel
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Solvers
- **AztecOO**
- Belos
- Pliris
- Komplex
- Amesos
- NOX
- LOCA
- **ROL**
- Piro
- Rythmos
- TriKota
- Globipack
- Optipack
- Anasazi

PDE Tools
- Phalanx
- **Intrepid**
- **Shards**
- **Panzer**

Tools
- **Teuchos**
- SEACAS
- STK
- **Sacado**
- Stokhos

Interfaces
- Thyra
- PyTrilinos
- Stratimikos

Rapid Optimization Library (ROL)

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- Trilinos package for large-scale continuous optimization
- Hardened, production-ready algorithms for unconstrained and equality-constrained optimization
- Range of methods
- Algorithmic flexibility/extensibility
- A unified interface for simulation-based optimization.
- New methods for optimization under uncertainty.
- Modular with a balance of abstraction and low level access

ROL Design

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- maturity of simulation driving complexity – multiscale/physics
- interface to production codes
- function analysis – spaces, norms, inner products, Riecz maps, duality, etc.
- advancements of computer architectures – parallel, GPUs, resiliency, etc.
- range of optimization formulations
- uncertainties – risk measures, sampling
- large scale, inexactness, etc…
- efficient research

modularity, flexibility, efficient, appropriate interfaces

ROL problem type:

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Type-U: Unconstrained.

$$\min_x \quad f(x)$$

Type-B: Bound constrained.

$$\begin{aligned} \min_x \quad & f(x) \\ \text{subject to} \quad & a \leq x \leq b \end{aligned}$$

Type-E: Equality constrained.

$$\begin{aligned} \min_x \quad & f(x) \\ \text{subject to} \quad & c(x) = 0 \end{aligned}$$

Type-EB: Equalities + bounds.

$$\begin{aligned} \min_x \quad & f(x) \\ \text{subject to} \quad & c(x) = 0 \\ & a \leq x \leq b \end{aligned}$$

Type-S: Stochastic.

$$\begin{aligned} \min_x \quad & \mathcal{R}(f(x)) \\ \text{subject to} \quad & c(x) = 0 \\ & a \leq x \leq b \end{aligned}$$

Methods Overview

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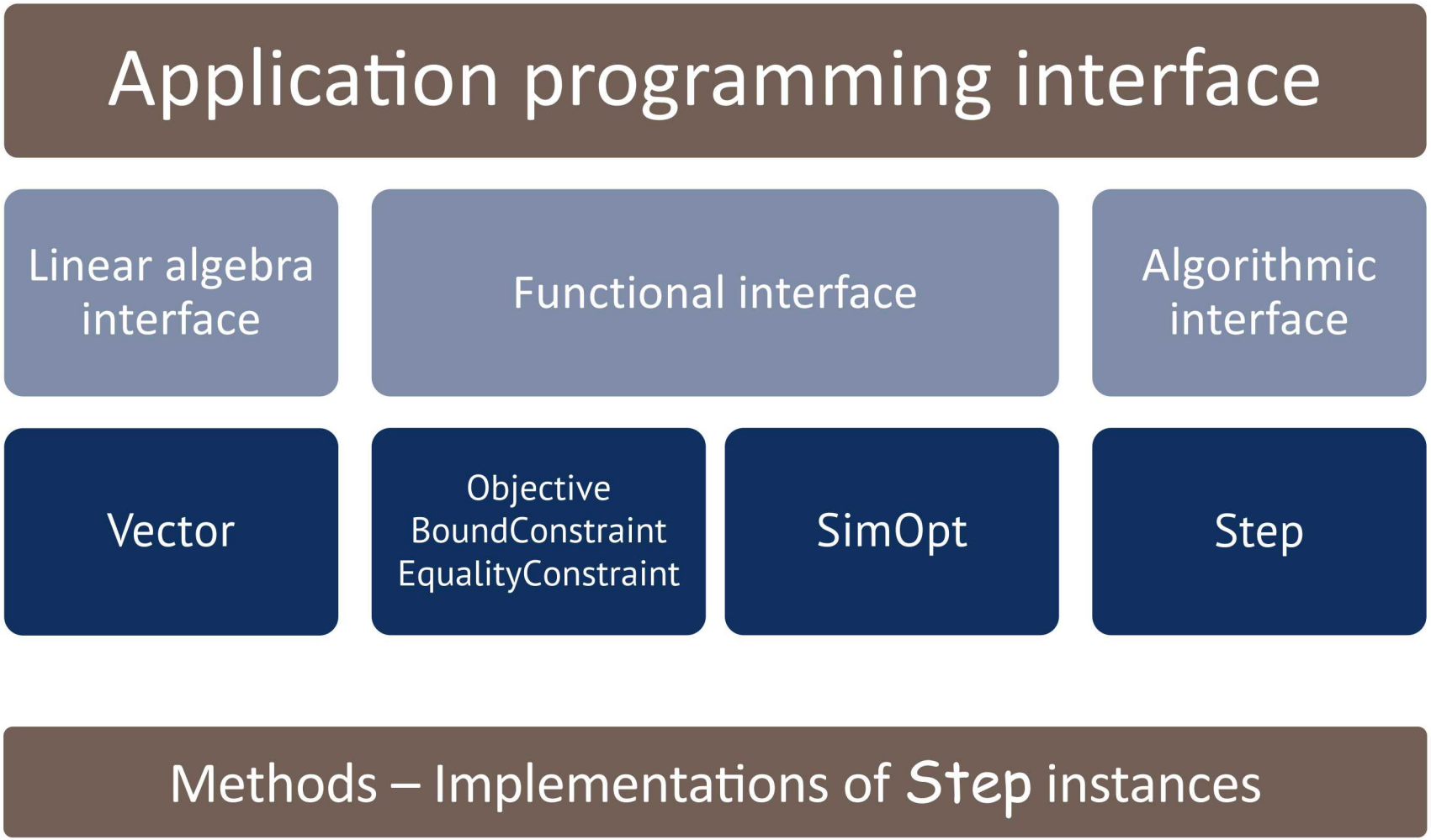
- **Type-U (unconstrained):**
  - LineSearch and trust region
  - Gradient descent, quasi-Newton (limited-memory BFGS, DFP, BB), nonlinear CG (6 variants), inexact Newton, Newton
  - Trust-region methods supporting inexact objective and gradient evals
- **Type-E (equality constrained):**
  - Sequential quadratic programming (SQP) with trust regions
- **Type-B (bound constrained):**
  - Projected gradient and projected Newton methods.
  - Primal-dual active set methods.
- **Type S – (Stochastic)**
  - Compute controls/designs that are risk-averse
  - Risk measures: Conditional value-at-risk (CVaR), Expectation (mean), Mean plus deviation, Mean plus variance, Exponential disutility, etc.
  - Incorporate sampling and adaptive quadrature approaches .

General Design



General Design Patterns

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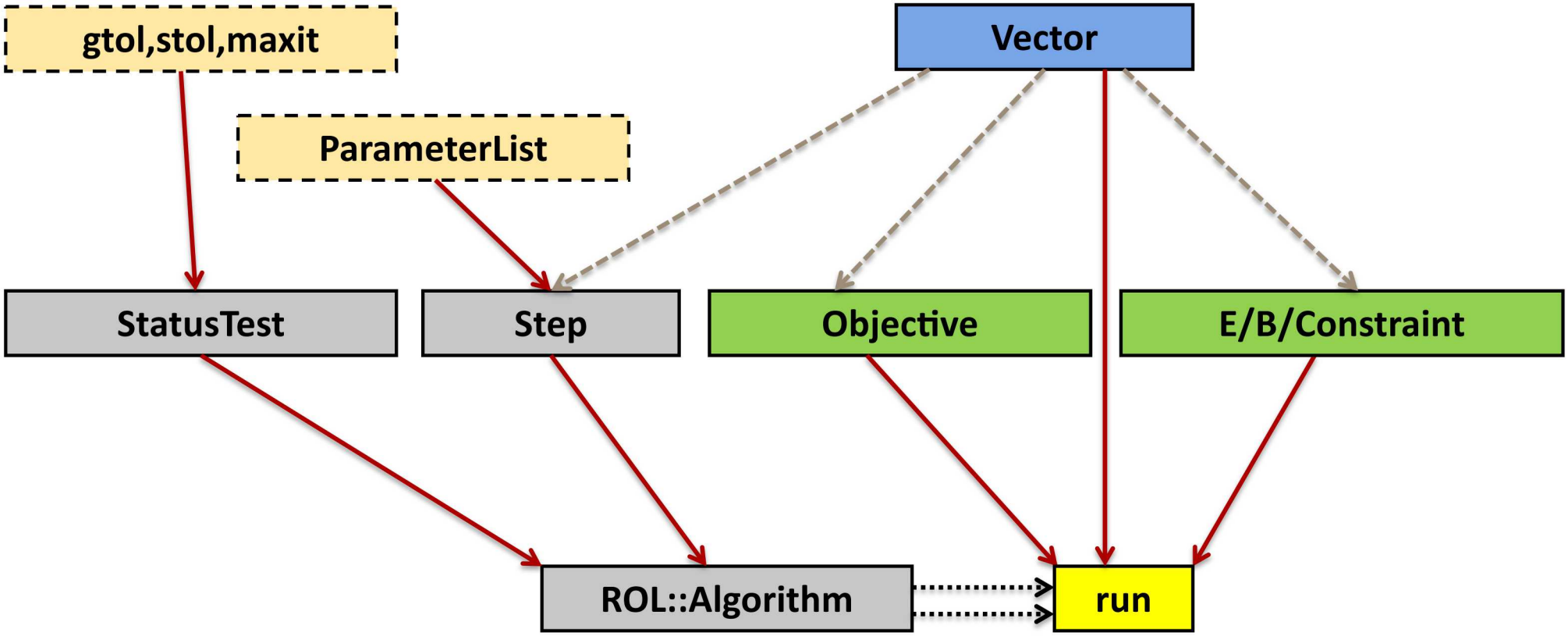
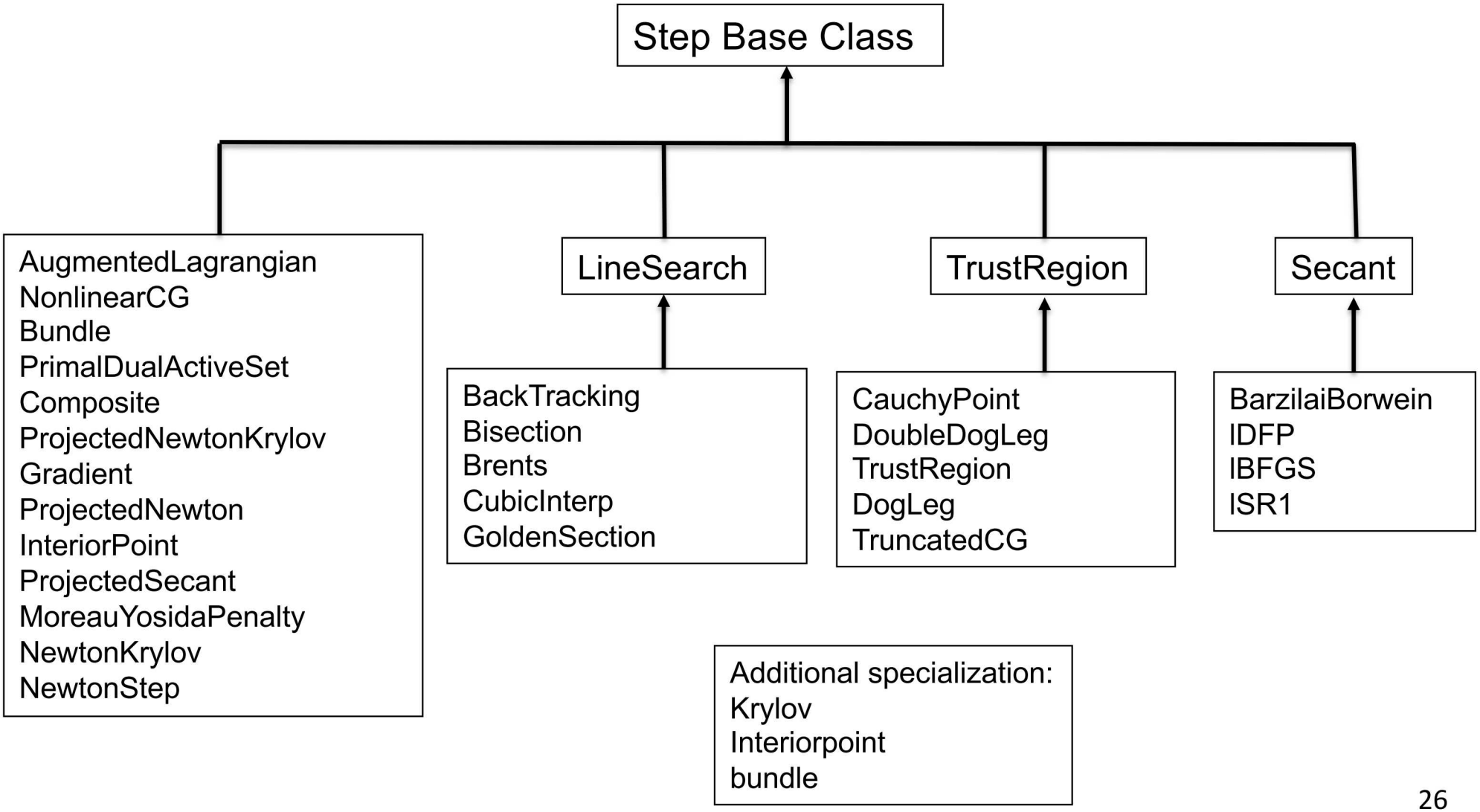
- templated approach
- virtual base class functions
- Linear algebra parallelism
- balanced abstraction versus low level access
- automatic memory management

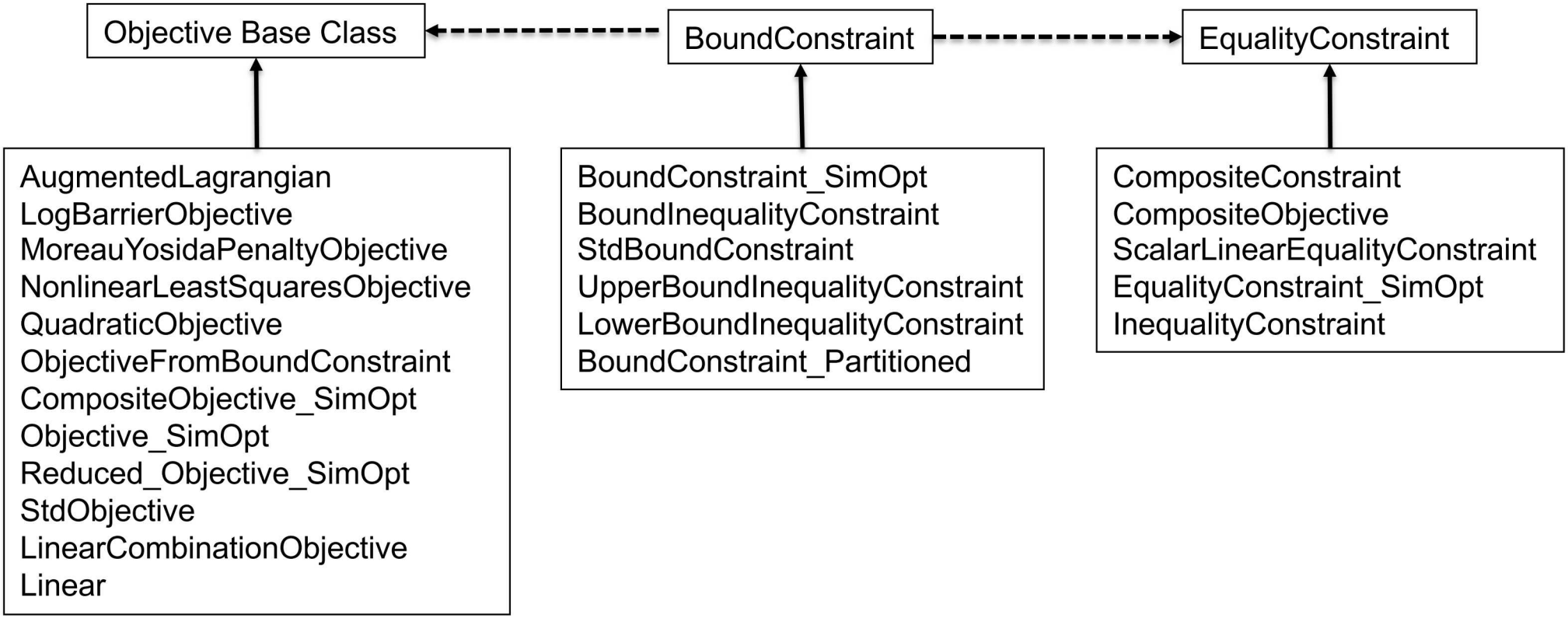
Algorithmic interface



Step Class Design



Functional Class Design



SimOpt: functional interface for engineering optimization

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$$\begin{bmatrix} \mathcal{L}_{uu} & \mathcal{L}_{ux} & c_u^T \\ \mathcal{L}_{xu} & \mathcal{L}_{xx} & c_x^T \\ c_u & c_x & 0 \end{bmatrix} \begin{Bmatrix} \delta u \\ \delta x \\ \lambda^* \end{Bmatrix} = - \begin{Bmatrix} f_u \\ f_x \\ c \end{Bmatrix}$$

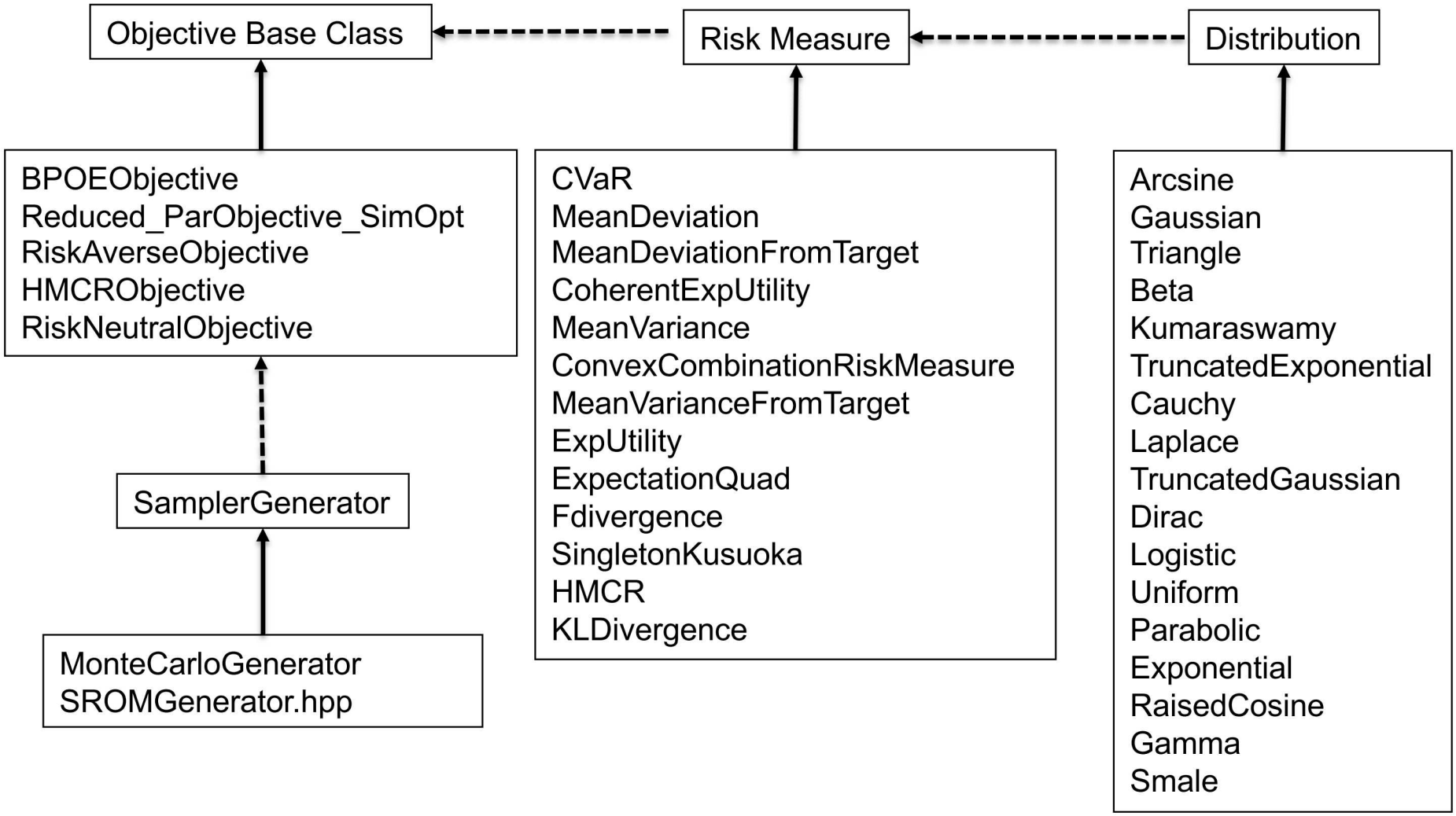
Objective_SimOpt

- value()
- gradient_u()
- gradient_z()
- hessvec_uu()
- hessvec_zz()
- hessvec_uz()
- hessvec_zu()

EqualityConstraint_SimOpt

- Value()
- applyJacobian_u()
- applyJacobian_z()
- applyJacobianInverse_u()
- applyJacobianInverse_z()
- applyadjointHessian_uu()
- applyadjointHessian_zz()
- .
- .

Functional Class Design - Stochastic



Use cases

- Design $f(u,x) = \frac{1}{2}\int_\Omega \chi d\Omega$
- Inverse $f(u,x) = \frac{1}{2}\int_\Omega (u-u^*)^2\delta(y-y^*)d\Omega + \frac{\beta}{2}\int_\Omega x^2 d\Omega$
- OED $f(u,x,q) = tr\ C^{-1}(q)$
- Control $f(u,x) = \frac{1}{2}\int_\Omega (u-\overline{u})^2 d\Omega + \frac{\beta}{2}\int_\Omega x^2 d\Omega$
- OUU $f(u,x,\xi) = \frac{1}{2}\mathcal{R}\int_\Omega (u(\xi)-\bar{u})^2 d\Omega + \frac{\beta}{2}\int_\Omega x^2 d\Omega$
- MIPDECO

Application Examples

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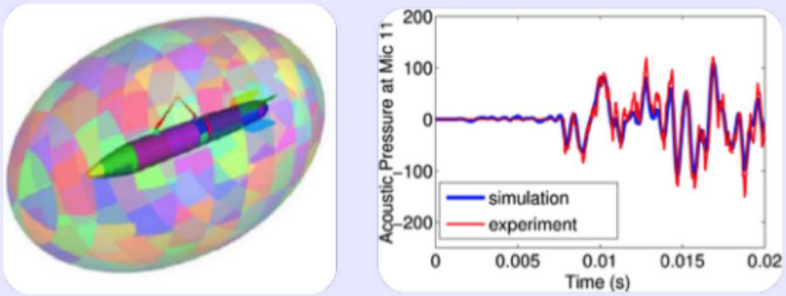
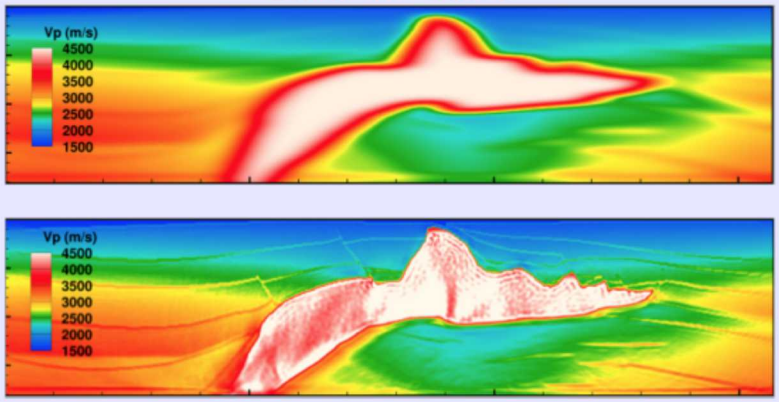
Inverse problems in acoustics/elasticity

Interface to the Sierra-SD ASC Integrated Code for structural dynamics



1M optimization and state variables

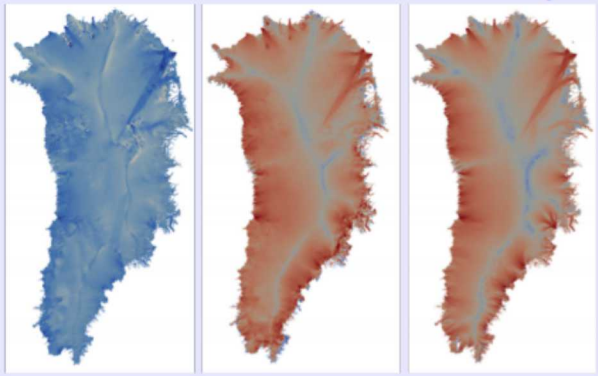
Interface to DGM, a high-order Discontinuous Galerkin code



500K optimization, 2M × 5K state variables

Estimating basal friction of ice sheets

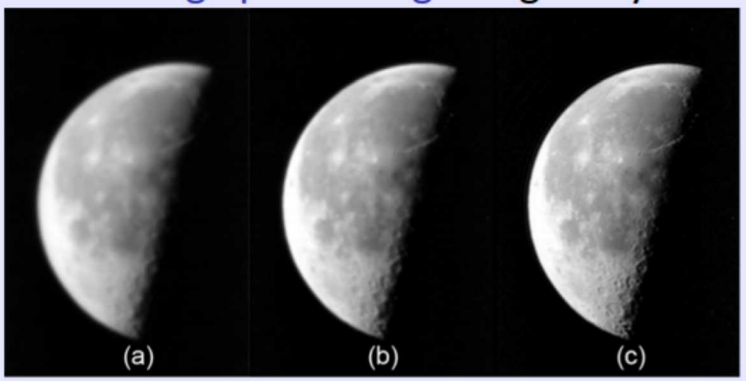
Interface to Trilinos-based Albany



5M optimization, 20M state variables

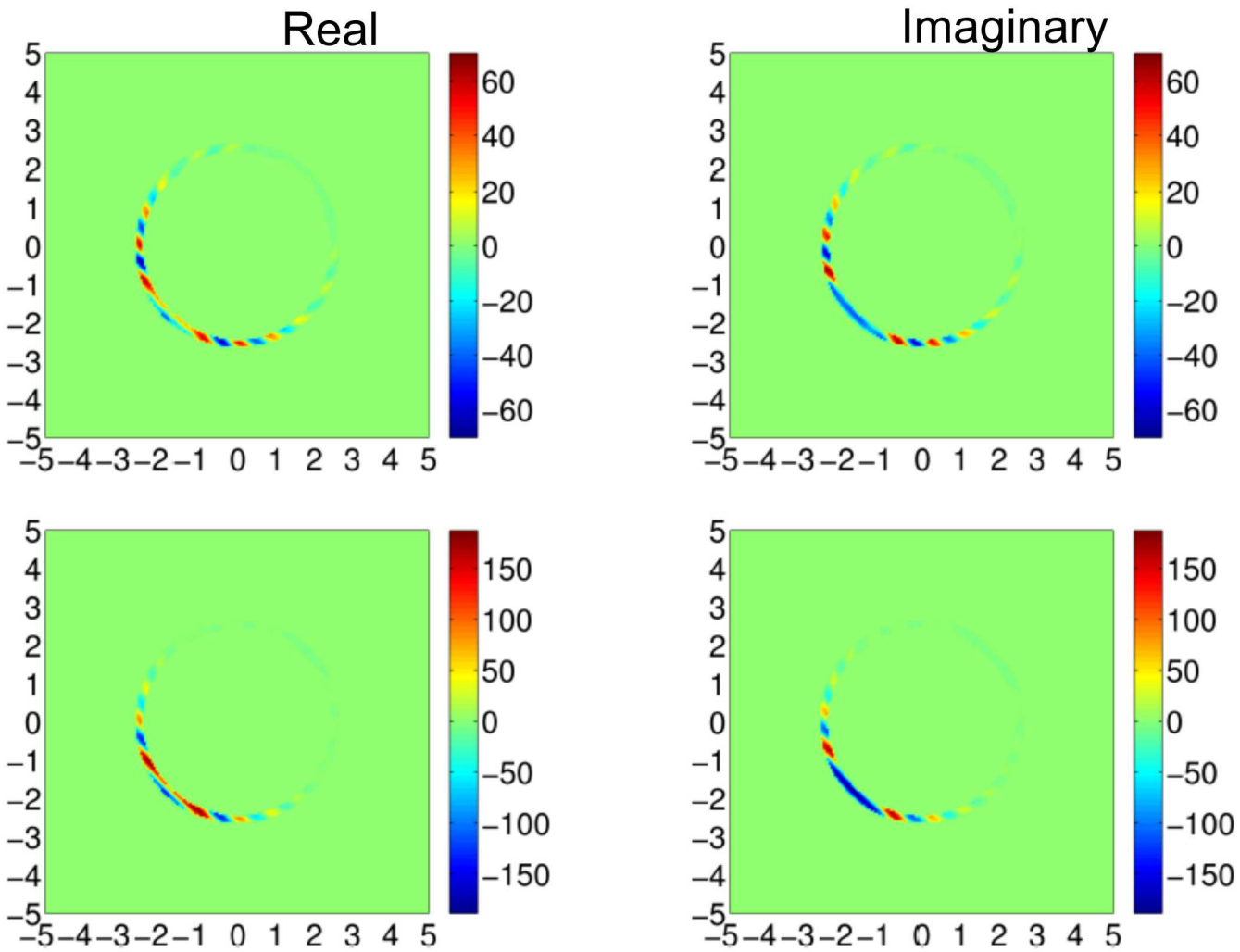
Super-resolution imaging

GPU image processing using ArrayFire

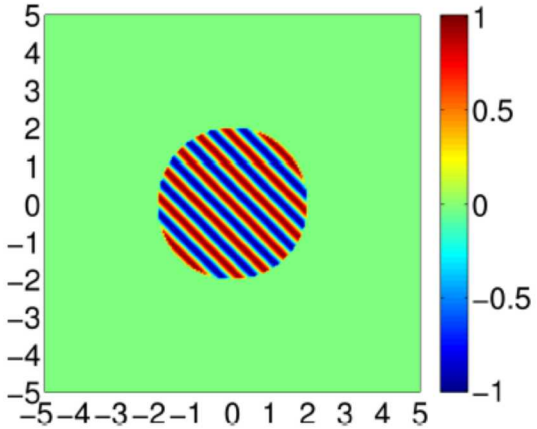


250K optimization variables, NVIDIA Tesla

Optimal Control



Desired state – real component



Note:

- Region of interest (ROI) is stochastic
- Parameterized with KL expansion
- Using a Matérn covariance

Note: Controls for stochastic ROI are three times smaller than the controls for the deterministic ROI

State Solution

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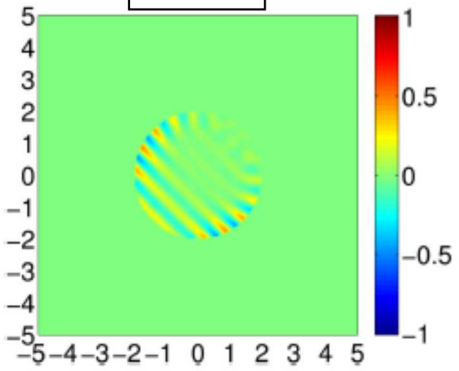
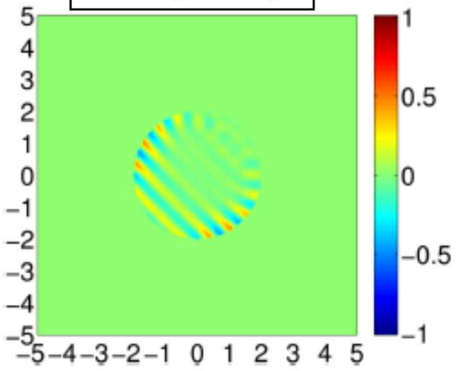
Real

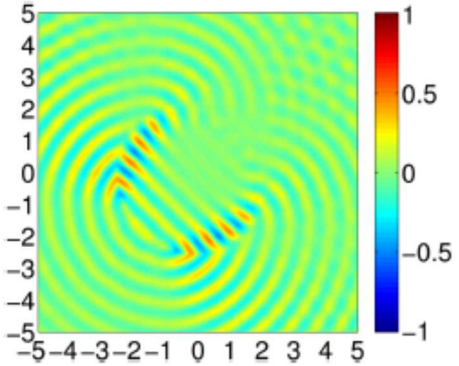
Imaginary

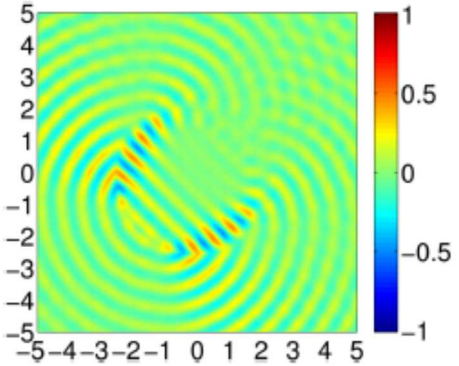
Expected value of state in ROI



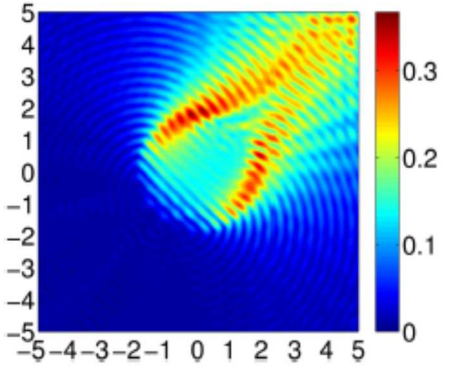


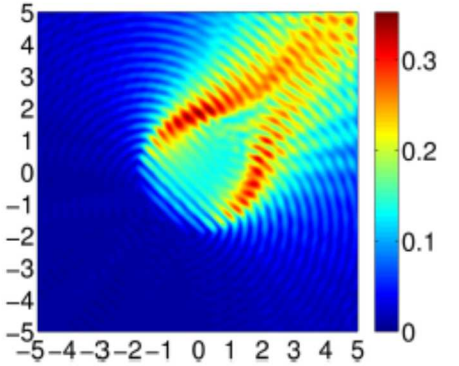
Expected value of optimal state of entire region





Standard deviation of optimal state





Scalability in the stochastic dimension

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dim	PDE Solves	CP_{obj}	CP_{grad}	Obj. Value
42	11,543	145	145	5.2542
44	32,739	233	481	5.2637
46	60,617	243	1,453	5.2641
48	79,221	247	2,961	5.2641
50	90,157	251	4,569	5.2641
60	100,911	271	7,621	5.2641
70	103,979	291	8,233	5.2641
80	105,607	311	8,253	5.2641

Scalable performance as dim is increased!

"Inexact Objective Funciton Evaluations in a Trust-Region Algorithms for PDE-Constrained Optimization under Uncertainty" D. P. Kouri, M. Heinkensshloss, D. Ridzal, and B. G. van Bloemen Waanders, SISC 2014

Discrete control constrained by convection diffusion

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$$\min_{z_k} \int u^2 dx$$

$$\text{s.t.} \quad -K\Delta u + v \cdot \nabla u = f_i - Bz_j$$

$$\sum z_n = b$$

$$z_k \in \{0, 1\}$$

Discrete control constrained by convection diffusion

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Control budget = 1:
Best Solution: Value = 0.23296676414411773837

Subproblems

Created 3 100.0%
Started Bounding 3 100.0%
Bounded 3 100.0%
Started Splitting 1 33.3%
Split 1 33.3%
Dead 0 0.0%

Control budget = 2:
Best Solution: Value = 0.12046194228269418991

Subproblems

Created 1 100.0%
Started Bounding 1 100.0%
Bounded 1 100.0%
Started Splitting 0 0.0%
Split 0 0.0%
Dead 0 0.0%

Control budget = 3:

Best Solution: Value = 0.053908605587946134552

Subproblems

Created 1 100.0%
Started Bounding 1 100.0%
Bounded 1 100.0%
Started Splitting 0 0.0%
Split 0 0.0%
Dead 0 0.0%

Control budget = 4:

Best Solution: Value = 0.024574563516836123167

Subproblems

Created 3 100.0%
Started Bounding 3 100.0%
Bounded 3 100.0%
Started Splitting 1 33.3%
Split 1 33.3%
Dead 0 0.0%

Control budget = 5:

Best Solution: Value = 0.014031681832521125664

Subproblems

Created 11 100.0%
Started Bounding 11 100.0%
Bounded 11 100.0%
Started Splitting 5 45.5%
Split 5 45.5%
Dead 0 0.0%

Control budget = 6:

Best Solution: Value = 0.012210756870505823368

Subproblems

Created 17 100.0%
Started Bounding 17 100.0%
Bounded 17 100.0%
Started Splitting 8 47.1%
Split 8 47.1%
Dead 0 0.0%

Control budget = 7:

Best Solution: Value = 0.021892389837279369047

Subproblems

Created 3 100.0%
Started Bounding 3 100.0%
Bounded 3 100.0%
Started Splitting 1 33.3%
Split 1 33.3%
Dead 0 0.0%

Control budget = 8:

Best Solution: Value = 0.056777218136662865877

Subproblems

Created 3 100.0%
Started Bounding 3 100.0%
Bounded 3 100.0%
Started Splitting 1 33.3%
Split 1 33.3%
Dead 0 0.0%

Control budget = 9:

Best Solution: Value = 0.13605755967561344866

Subproblems

Created 1 100.0%
Started Bounding 1 100.0%
Bounded 1 100.0%
Started Splitting 0 0.0%
Split 0 0.0%
Dead 0 0.0%

Directional Derivative Split Computation

- How to branch on variables or split the computations?
  - Naïve approach
  - Directional derivative

$$V(p) = \min \{f(x,p) : c(x,p) \leq 0\}$$

$$V^{'}(p;\delta p) = \lim_{t \to 0} \frac{v(p+\delta p) + v(p)}{t}$$

Result: reduces optimization to single bound computation but linear convex problem and therefore not interesting

Discrete control constrained by convection diffusion reaction

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$$\min_{z_k} \int u^2 dx$$

$$\text{s.t.} \quad -K\Delta u + v \cdot \nabla u = f_i - Bz_j + R$$

$$\sum z_n = b$$

$$z_k \in \{0, 1\}$$

$$R = u^2(1-u)$$

Results: forthcoming

Summary

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- Developed branch and bound framework to solve MIPDECO problems
- Parallelism available for BB and PDECO problems
- Interface is extensible to allow other branching mechanisms, BB algorithms, PDECO algorithms
- Linear and nonlinear problem tested
- Hierarchical model interface developed but not tested
- Simultaneous continuous and discrete variables are still needed

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Thank You