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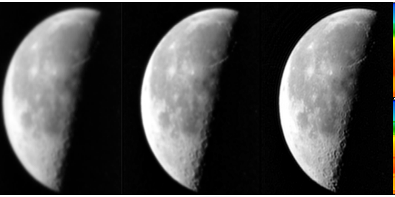

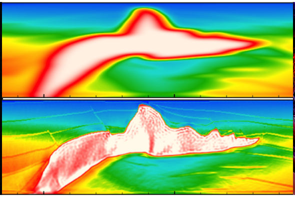

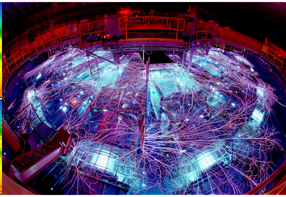

Rapid Optimization Library

Drew Kouri Denis Ridzal Greg von Winckel

11/1/17

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Outline

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Application programming interface

Algorithms

Tutorial 1

Simulation-based optimization

Tutorial 2

Sandia National Laboratories

Overview of ROL

Trilinos package for **large-scale optimization**. Uses: optimal design, optimal control and inverse problems in engineering applications; mesh optimization; image processing.

ROL

RAPID OPTIMIZATION LIBRARY

Numerical optimization made practical:
Any application, any hardware, any problem size.

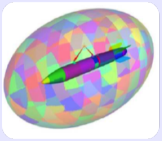
- **Modern optimization algorithms.**
- **Maximum HPC hardware utilization.**
- **Special programming interfaces for simulation-based optimization.**
- **Optimization under uncertainty.**

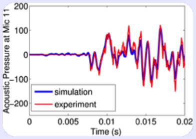
- Hardened, production-ready algorithms for unconstrained, equality-constrained, inequality-constrained and nonsmooth optimization.
- Novel algorithms for optimization under uncertainty and risk-averse optimization.
- Unique capabilities for optimization-guided inexact and adaptive computations.
- Geared toward maximizing HPC hardware utilization through direct use of application data structures, memory spaces, linear solvers and nonlinear solvers.
- Special interfaces for engineering applications, for streamlined and efficient use.
- Rigorous implementation verification: finite difference and linear algebra checks.
- Hierarchical and custom (user-defined) algorithms and stopping criteria.

Application examples

Inverse problems in acoustics/elasticity

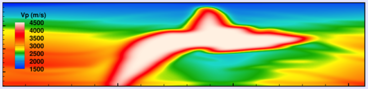
Interface to the Sierra-SD ASC Integrated Code for structural dynamics

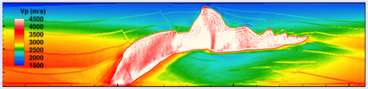




1M optimization and state variables

Interface to DGM, a high-order Discontinuous Galerkin code

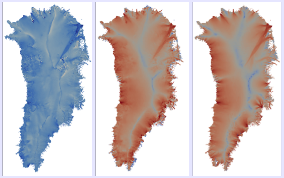




500K optimization, 2M × 5K state variables

Estimating basal friction of ice sheets

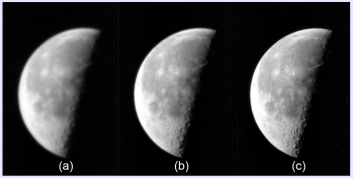
Interface to Trilinos-based Albany



5M optimization, 20M state variables

Super-resolution imaging

GPU image processing using ArrayFire



250K optimization variables, NVIDIA Tesla

Updates and a roadmap

2017:

Updates and a roadmap

2017:

- A new algorithmic interface: `ROL::OptimizationProblem` and `ROL::OptimizationSolver`; for ease of use and maintenance.

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2017:

- A new algorithmic interface: `ROL::OptimizationProblem` and `ROL::OptimizationSolver`; for ease of use and maintenance.
- New capabilities and improved interfaces for optimization under uncertainty and risk-averse optimization.
- Expansion of the PDE-OPT Application Development Kit and test suite for PDE-constrained optimization.

Updates and a roadmap

2018:

- Special interface for transient optimization through Tempus.

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Mathematical abstraction

ROL is used for the numerical solution of optimization problems

$$\begin{array}{rl} \underset{x}{\text{minimize}} & J(x) \\ \text{subject to} & c(x) = 0 \\ & a \leq x \leq b \end{array}$$

where:

- $J : \mathcal{X} \to \mathbb{R}$ is a Fréchet differentiable functional;
- $c : \mathcal{X} \to \mathcal{C}$ is a Fréchet differentiable operator;
- $\mathcal{X}$ and $\mathcal{C}$ are Banach spaces of functions; and
- $a \leq x \leq b$ defines pointwise (componentwise) bounds on x.

This abstraction is a valuable guiding principle.

Four basic problem types

Type-U

Unconstrained

$$\underset{x}{\text{minimize}} \quad J(x)$$

Type-B

Bound constrained

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & J(x) \\ \text{subject to} \quad & a \leq x \leq b \end{aligned}$$

Type-E

Equality constrained

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & J(x) \\ \text{subject to} \quad & c(x) = 0 \end{aligned}$$

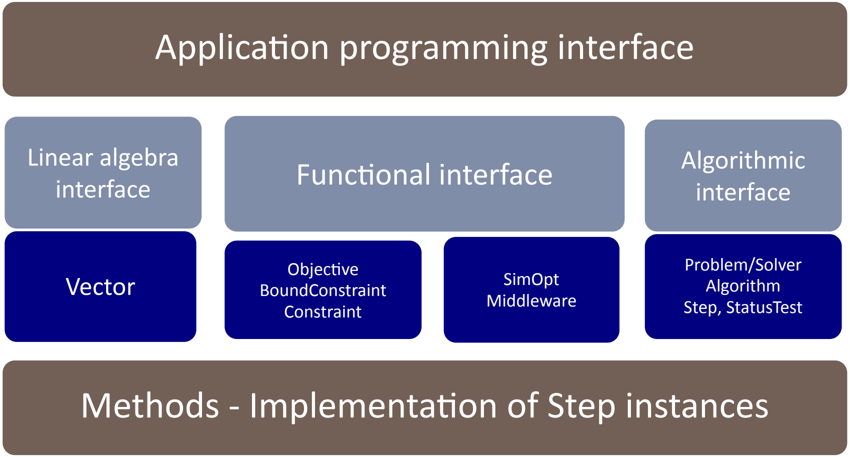
Type-EB

Equality + Bounds

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

ROL uses **slack variables** to convert **inequality constraints** $c(x) \geq 0$ to Type-EB, i.e., we minimize over x and slack variables s, where $c(x) - s = 0$, $s \geq 0$.

Three API components



Linear algebra interface - ROL::Vector

ROL::Vector provides a generic interface for application data structures.

Ready-made wrappers

- std::vector
- Epetra::MultiVector
- Tpetra::MultiVector
- Thyra::VectorBase
- ArrayFire

ROL::StdVector encapsulates a Teuchos::RCP to a std::vector which actually contains the data. This type is used in most of ROL's examples and tests.

ROL::Vector member functions

dot	set
plus	basis
norm	dimension
scale	reduce
clone	applyUnary
axpy	applyBinary
dual	checkVector
zero	

pure virtual   virtual   optional

ROL::Vector Base Class

Core vector operations must be implemented by derived classes.

```
namespace ROL {

template<class Real>
class Vector {
public:

  virtual void plus( const Vector &x ) = 0;          // y ← y + x
  virtual void scale( const Real alpha ) = 0;        // y ← αy
  virtual Real dot( const Vector &x ) const = 0;     // ⟨y, x⟩
  virtual Real norm() const = 0;                     // ‖y‖
  virtual Teuchos::RCP<Vector> clone() const = 0;

}; // class Vector
} // namespace ROL
```

ROL::Vector Base Class

Optional methods: May want to implement for efficiency.

```
namespace ROL {

template<class Real>
class Vector {
public:

  virtual void axpy( const Real alpha, const Vector &x ); // y ← αx + y
  virtual void zero();                                    // y ← 0
  virtual Teuchos::RCP<Vector> basis( const int i ) const;
  virtual int dimension() const;
  virtual void set( const Vector &x );                    // y ← x
  virtual const Vector & dual() const;

}; // class Vector
} // namespace ROL
```

ROL::Vector Base Class

Elementwise operations $\rightarrow$ Function evaluations on **all** vector elements. Needed for algorithms that handle general inequality constraints.

```
namespace ROL {
template<class Real>
class Vector {
public:

  using UF = Elementwise::UnaryFunction<Real>;
  using BF = Elementwise::BinaryFunction<Real>;
  using OP = Elementwise::ReductionOp<Real>;

  virtual void applyUnary( const UF &f );      // y ← f(y)
  virtual void applyBinary( const BF &f,
                            const Vector &x ); // y ← f(x,y)

  // Common examples: sum, min, max
  virtual Real reduce( const OP &r ) const;

}; // class Vector
} // namespace ROL
```

Functional interface

ROL::Objective Methods

- value - $J(x)$
- gradient - $g = \nabla J(x)$
- hessVec - $Hv = [\nabla^2 J(x)]v$
- update - modify member data
- invHessVec - $H^{-1}v = [\nabla^2 J(x)]^{-1}v$
- precond - approximate $H^{-1}v$
- dirDeriv - $\frac{d}{dt}J(x+tv)|_{t=0}$

$$\begin{array}{rl} \min\limits_{x} & J(x) \\ \text{subject to} & c(x) = 0 \\ & a \le x \le b \end{array}$$

- ROL can use finite differences to approximate derivatives.
- For best performance, implement analytic derivatives.
- Tools: checkGradient, checkHessVec, checkHessSym.

Functional interface

ROL::Constraint Methods

- value - $c(x)$
- applyJacobian - $[c'(x)]v$
- applyAdjointJacobian - $[c'(x)]^*v$
- applyAdjointHessian - $[c''(x)](v,\cdot)^*u$
- update - modify member data
- applyPreconditioner
- solveAugmentedSystem

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

- ROL can use finite differences to approximate derivatives.
- For best performance, implement analytic derivatives.
- Tools: `checkApplyJacobian`, `checkApplyAdjointJacobian`, `checkAdjointConsistencyJacobian`, `checkApplyAdjointHessian`.

Functional interface

ROL::BoundConstraint Methods

- project
- update
- pruneUpperActive
- pruneLowerActive
- pruneActive
- pruneUpperInactive
- pruneLowerInctive
- pruneInactive
- isFeasible
- activate, deactivate
- computeProjectedGradient

$$\begin{array}{rl} \min\limits_{x} & J(x) \\ \text{subject to} & c(x) = 0 \\ & a \leq x \leq b \end{array}$$

The BoundConstraint class was previously abstract in ROL with implementations needed for each class derived from `Vector`.

Now, it is a concrete class for any vector that implements ROL's elementwise operations.

```
ROL::Bounds(x_lo, x_up);
```

Algorithmic interface

ROL::OptimizationProblem

$$\begin{aligned} \min_x \quad & J(x) \\ \text{s.t.} \quad & a \le x \le b \\ & c_{\mathcal{E}}(x) = 0 \\ & L \le c_{\mathcal{I}}(x) \le U \end{aligned}$$

```
OptimizationProblem(const RCP<Objective<Real>>                     &obj,
                    const RCP<Vector<Real>>                        &x,
                    const RCP<BoundConstraint<Real>>               &bnd,
                    const std::vector<RCP<Constraint<Real>>>       &econ,
                    const std::vector<RCP<Vector<Real>>>           &emul,
                    const std::vector<RCP<Constraint<Real>>>       &icon,
                    const std::vector<RCP<Vector<Real>>>           &imul,
                    const std::vector<RCP<BoundConstraint<Real>>>  &ibnd);
```

ROL::OptimizationSolver

```
OptimizationSolver(OptimizationProblem<Real> &opt,
                   Teuchos::ParameterList &parlist);
int solve(std::ostream &outStream,
          const RCP<StatusTest<Real> > &status = Teuchos::null,
          const bool combineStatus = true);
```

- Also: Fine-grained interface to ROL:Algorithm and ROL:Step.

Algorithms - Part 1

Type-U (unconstrained)

- Globalization: `ROL::LineSearchStep` and `ROL::TrustRegionStep`.
- Gradient descent, quasi-Newton (limited-memory BFGS, DFP, Barzilai-Borwein), nonlinear CG (9 variants), inexact Newton (including finite difference hessVecs), Newton, with line searches and trust regions.
- Trust-region methods supporting inexact objective functions and inexact gradient evaluations. Enables *adaptive and reduced models.*

Type-B (bound constrained)

- Projected gradient and projected Newton methods.
- Primal-dual active set methods.

Algorithms - Part 2

Type-E (equality constrained)

- Sequential quadratic programming (SQP) with trust regions, supporting inexact linear system solves.
- Augmented Lagrangian methods.

Type-EB (equality + bound constrained)

- Augmented Lagrangian methods.
- Moreau-Yosida regularization.
- Semismooth Newton methods.
- Interior Point SQP methods (primal, primal-dual in development).

Algorithms - Part 3

Optimization under uncertainty

$$\underset{z}{\text{minimize}} \quad \mathcal{H}(f(z,\xi))$$

$$\underset{z}{\text{minimize}} \quad \mathcal{H}(f(S(z,\xi),z,\xi)) \quad \text{where } S(z,\xi) \text{ solves } c(u,z,\xi)=0$$

- Compute controls/designs that are risk-averse or robust to uncertainty in the parameters ξ. Here $\mathcal{H}$ is some **hazard functional**.
- Hazard functionals: Conditional value-at-risk (CVaR), Expectation (mean), Mean plus deviation, Mean plus variance, Exponential disutility, Buffered probability of exceedance (bPOE), etc.
- Incorporate sample and adaptive quadrature approaches from uncertainty quantification. Flexible sampling interface through `ROL::SampleGenerator` and `ROL::BatchManager`.
- Control inexactness and adaptivity through **trust-region** framework.

Overview

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Simulation-based optimization

Tutorial 2

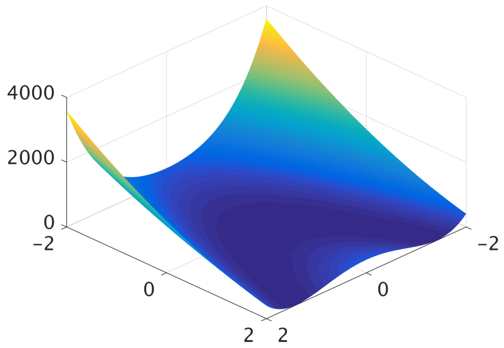
Disclaimer

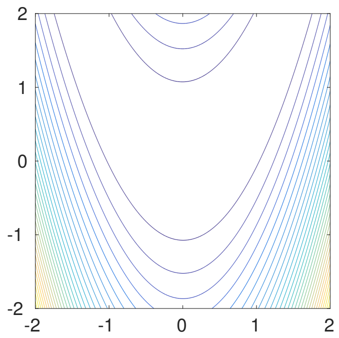
- For the purposes of the tutorial, we designed a special `ROL::StdObjective`, `ROL::StdConstraint`, etc., interface that supports the direct use of `std::vector`, thereby hiding the `ROL::Vector` abstraction.
- This interface can be used in applications if your primary (and only) data structure is `std::vector`, however …
- It is a terrible idea to copy data from your app's container into an `std::vector`, and back, just to use this interface.

Rosenbrock: Unconstrained (Type-U)

See `rol/tutorial/example_unc.cpp`

$$\min_{x_0,\, x_1} \left\{ \alpha(x_0^2 - x_1)^2 + (x_0 - 1)^2 \right\}$$





Here $\alpha = 100$. Minimum value of 0 is obtained at $(1, 1)$.

Implementing an Objective Class

Rosenbrock function and its derivatives

$$
\begin{aligned}
J(x) &= \alpha(x_0^2 - x_1)^2 + (x_0 - 1)^2 \\
[\nabla J(x)]_0 &= 4\alpha(x_0^2 - x_1)x_0 + 2(x_0 - 1) \\
[\nabla J(x)]_1 &= -2\alpha(x_0^2 - x_1) \\
[\nabla^2 J(x)v]_0 &= (12\alpha x_0^2 - 4\alpha x_1 + 2)v_0 - 4\alpha x_0 v_1 \\
[\nabla^2 J(x)v]_1 &= -4\alpha x_0 v_0 + 2\alpha v_1
\end{aligned}
$$

Implementing an Objective Class

```
template<class Real>
class ObjectiveRosenbrock : public ROL::StdObjective<Real> {
public:
  ObjectiveRosenbrock(void) {}

  Real value(const std::vector<Real> &x, Real &tol) {
    const Real one(1), alpha(100);
    Real val = alpha * std::pow(std::pow(x[0], 2) - x[1], 2)
               + std::pow(x[0] - one, 2);
    return val;
  }

  void gradient( std::vector<Real> &g, const std::vector<Real> &x, Real &tol ) {
    const Real one(1), two(2), alpha(100);
    g[0] = two*alpha*(std::pow(x[0], 2) - x[1]) * two*x[0] + two*(x[0]-one);
    g[1] = -two*alpha*(std::pow(x[0], 2) - x[1]);
  }

  void hessVec( std::vector<Real> &hv, const std::vector<Real> &v,
                const std::vector<Real> &x, Real &tol ) {
    const Real two(2), three(3), alpha(100);
    Real h11 = two*two*three*alpha*std::pow(x[0], 2) - two*two*alpha*x[1] + two;
    Real h12 = -two*two*alpha*x[0];
    Real h21 = h12;
    Real h22 = two*alpha;
    hv[0] = h11*v[0] + h12*v[1];
    hv[1] = h21*v[0] + h22*v[1];
  }

}; // class ObjectiveRosenbrock
```

Solving the problem

```
Teuchos::ParameterList parlist;
parlist.sublist("Step").set("Type","Trust Region");
parlist.sublist("Step").sublist("Trust Region").set(
                                "Subproblem Solver","Truncated CG");

RCP<std::vector<RealT> > x_rcp  = rcp( new std::vector<RealT>(2) );
RCP<ROL::Vector<RealT> > x      = rcp( new ROL::StdVector<RealT>(x_rcp) );
(*x_rcp)[0] = static_cast<RealT>(-3);
(*x_rcp)[1] = static_cast<RealT>(-4);

RCP<ROL::Objective<RealT> > obj = rcp( new ObjectiveRosenbrock<RealT>() );

ROL::OptimizationProblem<RealT> problem( obj, x );
problem.check(*outStream);

ROL::OptimizationSolver<RealT> solver( problem, parlist );
solver.solve(*outStream);

*outStream << "x_opt = [" << (*x_rcp)[0] << ", " << (*x_rcp)[1] << "]" << std::endl;
```

Solving the problem

```
Performing OptimizationProblem diagnostics.
Checking vector operations in optimization vector space X.
...
Commutativity of addition. Consistency error: >>>>>>>> 0.000000000000e+00
Associativity of addition. Consistency error: >>>>>>>> 4.440892098501e-16
...
Checking objective function.
           Step size           grad'*dir           FD approx           abs error
           ---------           ---------           ---------           ---------
   ...
   1.00000000000e-05  -1.28755849134e+01  -1.28754717782e+01   1.13135237813e-04
   1.00000000000e-06  -1.28755849134e+01  -1.28755736046e+01   1.13087794347e-05
   ...
           Step size      norm(Hess*vec)    norm(FD approx)    norm(abs error)
           ---------      --------------    ---------------    ---------------
   ...
   1.00000000000e-05   6.23835747001e+02   6.23843380884e+02   7.83730395160e-03
   1.00000000000e-06   6.23835747001e+02   6.23836510354e+02   7.83695612072e-04
   ...
          <w, H(x)v>          <v, H(x)w>           abs error
  -1.59963302477e+01  -1.59963302477e+01   1.24344978758e-14

Truncated CG Trust-Region Solver
  iter  value         gnorm         snorm         delta         iterCG    flagCG
  0     1.691600e+04  1.582307e+04                1.269752e+00
  1     4.693141e+03  4.982056e+03  1.269752e+00  3.174380e+00  1         3
  ...
  29    3.574815e-06  7.633462e-02  2.940042e-02  6.970662e+00  2         0
  30    6.533209e-10  1.885039e-04  1.766505e-03  1.742666e+01  2         0
  31    4.596288e-17  2.754521e-07  5.642267e-05  4.356664e+01  2         0
x_opt = [1, 1]
```

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Simulation-based optimization

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SimOpt: Simulation-based optimization

- Many simulation-based Type-E problems have the form

$$\underset{u,z}{\text{minimize}} \quad J(u,z) \text{ subject to } c(u,z) = 0$$

  - *u* denotes simulation variables (state, basic, **Sim**)
  - *z* denotes optimization variables (controls, parameters, **Opt**)

- A common Type-U reformulation, by nonlinear elimination is:

$$\underset{z}{\text{minimize}} \quad J(S(z),z) \text{ where } u = S(z) \text{ solves } c(u,z) = 0$$

- For these cases, the **SimOpt** interface enables direct use of methods for **both** unconstrained and constrained problems.

Two formulations

Simulation-based optimization problems assume the form:

$$\underset{\{u,z\}\in\,\mathcal{U}\times\mathcal{Z}}{\text{minimize}} \quad J(u,z)$$
$$\text{subject to} \quad c(u,z)=0$$

u -- state variables; z -- controls/parameters

Two ways to think about this form:

REDUCED SPACE

$$\underset{z\in\mathcal{Z}}{\text{minimize}} \quad \mathcal{J}(z)=J(S(z),z)$$

Here $u=S(z)$ solves $c(u,z)=0$.

FULL SPACE

$$\underset{x\in\mathcal{X}}{\text{minimize}} \quad J(x)$$
$$\text{subject to} \quad c(x)=0$$

Here $\mathcal{X}=\mathcal{U}\times\mathcal{Z}$.

General observations

- The reduced-space form is implicitly constrained. In its simplest form: an unconstrained optimization problem.
- The full-space form is explicitly constrained. In its simplest form: an equality-constrained optimization problem.
- Methods for numerical optimization can be used, however, note …
- Both forms are posed in function space, where $\mathcal{U}$, $\mathcal{Z}$ and $\mathcal{X}$ are Hilbert spaces or, more generally, Banach spaces.
- There is inherent smoothness in the problem formulations.
- Computer representations must exploit the problem structure:
  - *vector space operations*, specifically inner products and duality; and
  - *derivative operators* for objective and constraint functions.
- With some care, we can apply fast (gradient-based, Newton-type) optimization algorithms featuring scalable performance.

Derivatives

$$\begin{array}{ll} \underset{\{u,z\}\in\,\mathcal{U}\times\mathcal{Z}}{\text{minimize}} & J(u,z) \\ \text{subject to} & c(u,z) = 0 \end{array}$$

- First derivatives.
  Objective gradients: $\nabla_u J(u,z)$, $\nabla_z J(u,z)$.
  Constraint Jacobians: $c_u(u,z)$, $c_z(u,z)$.
- Second derivatives.
  Objective Hessians: $\nabla_{uu} J(u,z)$, $\nabla_{uz} J(u,z)$, $\nabla_{zu} J(u,z)$, $\nabla_{zz} J(u,z)$.
  Constraint Hessians: $c_{uu}(u,z)$, $c_{uz}(u,z)$, $c_{zu}(u,z)$, $c_{zz}(u,z)$.
- It is also useful to consider the *Lagrangian functional,*
  $L(u,z,\lambda) = J(u,z) + \langle c(u,z), \lambda\rangle_{\mathcal{C},\mathcal{C}^*}$, where $c : \mathcal{U} \times \mathcal{Z} \to \mathcal{C}$,
  and its first and second derivatives.
- Which operations do we really need?

Derivatives in the reduced space

$$\underset{z\in\mathcal{Z}}{\text{minimize}} \quad \mathcal{J}(z) = J(S(z), z)$$

- Gradient via implicit differentiation of $c(S(z), z) = 0$:

$$\begin{aligned}\nabla\mathcal{J}(z) &= S_z(z)^*\nabla_u J(S(z), z) + \nabla_z J(S(z), z)\\ &= -c_z(S(z), z)^* c_u(S(z), z)^{-*}\nabla_u J(S(z), z) + \nabla_z J(S(z), z)\end{aligned}$$

- Numerical recipe:
  1. For a given z, compute $u = S(z)$ that solves $c(u, z) = 0$.
  2. Solve adjoint equation for $\lambda = P(z)$: $c_u(u, z)^*\lambda = -\nabla_u J(u, z)$.
  3. Compute $\nabla\mathcal{J}(z) = c_z(u, z)^*\lambda + \nabla_z J(u, z)$.

- Note: $\nabla\mathcal{J}(z) = \nabla_z L(u, z, \lambda)$, treating u and λ as functions of z; $u = S(z)$ and $\lambda = P(z)$.

Derivatives in the reduced space

- Hessian via implicit function theorem:

$$\begin{aligned}\nabla^2\mathcal{J}(z) &= \nabla_{zu}L(S(z),z,P(z))S_z(z) + \nabla_{zz}L(S(z),z,P(z))\\ &\quad + \nabla_{z\lambda}L(S(z),z,P(z))P_z(z)\\ &= -c_z(S(z),z)^*c_u(S(z),z)^{-*}\nabla_{uu}L(S(z),z,P(z))c_u(S(z),z)^{-1}c_z(S(z),z)\\ &\quad - c_z(S(z),z)^*c_u(S(z),z)^{-*}\nabla_{uz}L(S(z),z,P(z))\\ &\quad - \nabla_{zu}L(S(z),z,P(z))c_u(s(z),z)^{-1}c_z(S(z),z) + \nabla_{zz}L(S(z),z,P(z))\end{aligned}$$

- Numerical recipe for applying the Hessian to vector v:

1. For a given z, compute $u = S(z)$ that solves $c(u,z) = 0$.
2. Solve adjoint equation for $\lambda = P(z)$: $c_u(u,z)^*\lambda = -\nabla_u J(u,z)$.
3. Solve linearized state equation: $c_u(u,z)w = c_z(u,z)v$.
4. Solve adjoint equation: $c_u(u,z)^*p = \nabla_{uu}L(u,z,\lambda)w - \nabla_{uz}L(u,z,\lambda)v$.
5. Compute $\nabla^2\mathcal{J}(z)v = c_z(u,z)^*p - \nabla_{zu}L(u,z,\lambda)w + \nabla_{zz}L(u,z,\lambda)v$.

- Note: Evaluating $\nabla_{zu}L(u,z,\lambda)w$ includes $c_{zu}(u,z)(w,\cdot)^*\lambda$. We also need $c_{zz}(u,z)(v,\cdot)^*\lambda$, $c_{uz}(u,z)(v,\cdot)^*\lambda$ and $c_{uu}(u,z)(w,\cdot)^*\lambda$.

Interface requirements for (matrix-free) SimOpt

REDUCED SPACE

$$\underset{z \in \mathcal{Z}}{\text{minimize}} \quad \mathcal{J}(z) = J(S(z), z)$$

FULL SPACE

$$\underset{\{u,z\} \in \mathcal{U} \times \mathcal{Z}}{\text{minimize}} \quad J(u,z)$$

$$\text{subject to} \quad c(u,z) = 0$$

- First derivatives.
  Objective gradients: $\nabla_u J(u,z)$, $\nabla_z J(u,z)$.
  Action of constraint Jacobians: $c_u(u,z)v$, $c_z(u,z)v$.
  Linearized state and adjoint solves: $c_u(u,z)^{-1}v$, $c_u(u,z)^{-*}v$.
- Second derivatives.
  Action of objective Hessians:
  $\nabla_{uu} J(u,z)v$, $\nabla_{uz} J(u,z)v$, $\nabla_{zu} J(u,z)v$, $\nabla_{zz} J(u,z)v$.
  Action of the adjoints of constraint Hessians:
  $c_{uu}(u,z)(v,.)^*\lambda$, $c_{uz}(u,z)(v,.)^*\lambda$, $c_{zu}(u,z)(v,.)^*\lambda$, $c_{zz}(u,z)(v,.)^*\lambda$.
- Solution operator S(z) = u, i.e., nonlinear solve.

Other observations

REDUCED SPACE

$$\underset{z\in\mathcal{Z}}{\text{minimize}} \quad \mathcal{J}(z) = J(S(z), z)$$

FULL SPACE

$$\underset{\{u,z\}\in\,\mathcal{U}\times\mathcal{Z}}{\text{minimize}} \quad J(u,z)$$
$$\text{subject to} \quad c(u,z) = 0$$

- The full-space problem may be well-posed even if the solution operator $S(z)$ is not well-defined, e.g., when the constraint $c(u,z) = 0$ has no or multiple solutions u for a given z.
- Derivative computations for the reduced-space problem involve linear and nonlinear solves, $c_u(u,z)^{-1}v$, $c_u(u,z)^{-*}v$ and $u = S(z)$.
- Derivative computations for the full-space problem require no solves.
- Reduced-space methods eliminate the state variables, u, and maintain constraint feasibility throughout the iteration.
- Full-space methods expose u and z as optimization variables, i.e., they do not have to maintain feasibility throughout the iteration.

The SimOpt interface

Middleware for engineering optimization

ROL::Objective_SimOpt

- `value(u,z)`
- `gradient_1(g,u,z)`
- `gradient_2(g,u,z)`
- `hessVec_11(hv,v,u,z)`
- `hessVec_12(hv,v,u,z)`
- `hessVec_21(hv,v,u,z)`
- `hessVec_22(hv,v,u,z)`

Recall

- 1 = Sim = u
- 2 = Opt = z

ROL::Constraint_SimOpt

- `value(u,z)`
- `applyJacobian_1(jv,v,u,z)`
- `applyJacobian_2(jv,v,u,z)`
- `applyInverseJacobian_1(ijv,v,u,z)`
- `applyAdjointJacobian_1(ajv,v,u,z)`
- `applyAdjointJacobian_2(ajv,v,u,z)`
- `applyInverseAdjointJacobian_1(iajv,v,u,z)`
- `applyAdjointHessian_11(ahwv,w,v,u,z)`
- `applyAdjointHessian_12(ahwv,w,v,u,z)`
- `applyAdjointHessian_21(ahwv,w,v,u,z)`
- `applyAdjointHessian_22(ahwv,w,v,u,z)`
- `solve(u,z)`

SimOpt: Benefits

- Streamlined modular implementation for a very large class of engineering optimization problems.
- Implementation verification through a variety of ROL tests:
  - Finite difference checks with high granularity.
  - Consistency checks for operator inverses and adjoints.
- Access to **all** optimization methods through a **single interface**.
- Enables future ROL interfaces for advanced solution checkpointing and restarting, closer integration with time integration libraries, etc.

Overview

Application programming interface

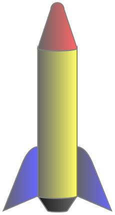
Algorithms

Tutorial 1

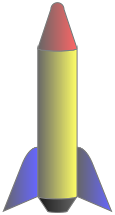
Simulation-based optimization

Tutorial 2

Model Rocket Control Problem: Fuel Efficiency



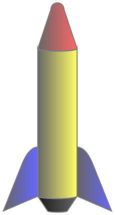
Model Rocket Control Problem: Fuel Efficiency



Tsiolkovsky Equation

$$m\mathrm{d}v = -v_e \mathrm{d}m - mg\mathrm{d}t$$

Model Rocket Control Problem: Fuel Efficiency

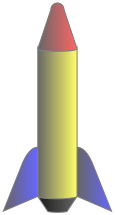


Tsiolkovsky Equation

$$m\,\mathrm{d}v = -v_e\,\mathrm{d}m - mg\,\mathrm{d}t$$

Mass Velocity Gravity

Model Rocket Control Problem: Fuel Efficiency



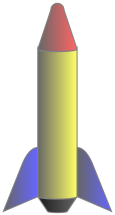
Tsiolkovsky Equation

$$m\mathrm{d}v = -v_e \mathrm{d}m - mg\mathrm{d}t$$

$$m(t) = m_T - m_f \int_0^t z(s)\,\mathrm{d}s$$

Changing mass

Model Rocket Control Problem: Fuel Efficiency



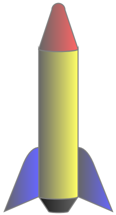
Tsiolkovsky Equation

$$m\mathrm{d}v = -v_e\mathrm{d}m - mg\mathrm{d}t$$

$$m(t) = m_T - m_f \int_0^t z(s)\,\mathrm{d}s$$

Total Mass

Model Rocket Control Problem: Fuel Efficiency



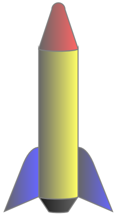
Tsiolkovsky Equation

$$m\,\mathrm{d}v = -v_e\,\mathrm{d}m - mg\,\mathrm{d}t$$

$$m(t) = m_T - m_f \int_0^t z(s)\,\mathrm{d}s$$

Fuel Mass

Model Rocket Control Problem: Fuel Efficiency



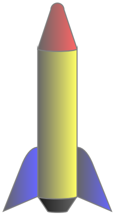
Tsiolkovsky Equation

$$m\,\mathrm{d}v = -v_e\,\mathrm{d}m - mg\,\mathrm{d}t$$

$$m(t) = m_T - m_f \int_0^t z(s)\,\mathrm{d}s$$

Burn rate

Model Rocket Control Problem: Fuel Efficiency



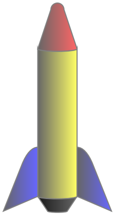
Tsiolkovsky Equation

$$m\mathrm{d}v = -v_e\mathrm{d}m - mg\mathrm{d}t$$

$$m(t) = m_T - \frac{m_f}{T}t$$

Constant burn rate

Model Rocket Control Problem: Fuel Efficiency



Tsiolkovsky Equation

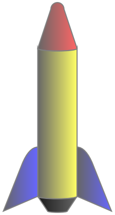
$$m\mathrm{d}v = -v_e \mathrm{d}m - mg\mathrm{d}t$$

$$m(t) = m_T - \frac{m_f}{T}t$$

Exact velocity

$$\frac{\mathrm{d}h}{\mathrm{d}t} = u(t) = v_e \ln\left(\frac{m_T}{m(t)}\right) - gt$$

Model Rocket Control Problem: Fuel Efficiency



Tsiolkovsky Equation

$$m\mathrm{d}v = -v_e\mathrm{d}m - mg\mathrm{d}t$$

$$m(t) = m_T - \frac{m_f}{T}t$$

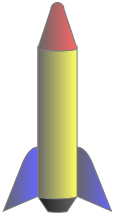
Exact velocity

$$\frac{\mathrm{d}h}{\mathrm{d}t} = u(t) = v_e \ln\left(\frac{m_T}{m(t)}\right) - gt$$

Final altitude ($k = m_f/m_r$)

$$h(T) = v_eT\left(1 + \frac{ln(1+k)}{k}\right) - \frac{1}{2}gT^2$$

Model Rocket Control Problem: Fuel Efficiency



Tsiolkovsky Equation

$$m\,\mathrm{d}v = -v_e\,\mathrm{d}m - mg\,\mathrm{d}t$$

$$m(t) = m_T - \frac{m_f}{T}t$$

Exact velocity

$$\frac{\mathrm{d}h}{\mathrm{d}t} = u(t) = v_e \ln\left(\frac{m_T}{m(t)}\right) - gt$$

Can we find $z(t)$ that attains the same $u(T^*)$ with minimal fuel use?

Optimal Fuel Burn Rate

Minimum fuel consumption objective

$$\min f(u,z) = \frac{1}{2}\left(h(T) - \int_0^T u(t)\,\mathrm{d}t\right)^2 + \frac{\mu}{2}\int_0^T z^2(t)\,\mathrm{d}t$$

Subject to the ODE constraint

$$\dot{u} = v_e \frac{z(t)}{m(t)} - g, \quad u(0) = 0$$

Discretized equations

$$u_k = u_{k-1} - v_e[\ln m_k - \ln m_{k-1}] - d\Delta t, \quad u_0 = 0$$

$$m_k = m_{k-1} - \Delta t z_k, \quad m_0 = m_T$$

Implementing the Objective - Rocket.hpp

```
#pragma once

#include "ROL_StdVector.hpp"
#include "ROL_Objective_SimOpt.hpp"
#include "ROL_Constraint_SimOpt.hpp"
namespace Rocket {

class Objective : public ROL::Objective_SimOpt<double> {
private:
  using V = ROL::Vector<double>;

  int N;
  double T, dt, mt;
  double htarg, alpha;
  const Teuchos::RCP<const V>  w; // Trapezoidal weights

public:

  Objective(  int N_, double T_, double mt_, double htarg_,
              double alpha_, const Teuchos::RCP<const V>& w_ ) :
     N(N_), T(T_), dt(T/N), mt(mt_), htarg(htarg_),
     alpha(alpha_), w(w_) {  }
  // More functions to follow
};
} // namespace Rocket
```

Implementing the Objective - Rocket.hpp

```
double value( const V& u, const V& z, double& tol ) {
  return 0.5*std::pow(htarg-w->dot(u),2) + 0.5*alpha*dt*z.dot(z);
}

void gradient_1( V& g, const V& u, const V& z, double& tol ) {
  g.set(*w);   g.scale(w->dot(u)-htarg);
}

void gradient_2( V& g, const V& u, const V& z, double& tol ) {
  g.set(z);    g.scale(alpha*dt);
}
```

Implementing the Objective - Rocket.hpp

```
void hessVec_11( V& hv, const V& v, const V& u,
                 const V& z, double& tol ) {
  hv.set(*w);  hv.scale(w->dot(v));
}

void hessVec_12( V& hv, const V& v, const V& u,
                 const V& z, double& tol ) {
  hv.zero();
}

void hessVec_21( V& hv, const V& v, const V& u,
                 const V& z, double& tol ) {
  hv.zero();
}

void hessVec_22( V& hv, const V& v, const V& u,
                 const V& z, double& tol ) {
  hv.set(v);  hv.scale(alpha*dt);
}
```

Implementing the Constraint - Rocket.hpp

```
class Constraint : public ROL::Constraint_SimOpt<double> {
private:
  using V = ROL::Vector<double>;

  int N;
  double T, dt, gdt, mt, mf, ve;
  std::vector<double> mass;

public:

  Constraint( int N_, double T_, double mt_,
    double mf_, double ve_, double g_ ) : N(N_), T(T_),
    dt(T/N), gdt(g_*dt), mt(mt_),
    mf(mf_), ve(ve_), mass(N) {
      mass[0] = mt;
    }
  // More functions to follow
};
```

Implementing the Constraint - Rocket.hpp

```
void update_2( const V& z, bool flag = true, int iter = -1 ) {
  auto& zs = getVector(z);

  mass[0] = mt - dt*zs[0];
  for( int i=1; i<N; ++i )
    mass[i] = mass[i-1] - dt*zs[i];
}

void solve( V& c, V& u, const V& z, double& tol ) {
  auto& us = getVector(u);
  us[0] = -ve*std::log(mass[0]/mt) - gdt;
  for( int i=1; i<N; ++i )
    us[i] = us[i-1] - ve*std::log(mass[i]/mass[i-1]) - gdt;
  value(c,u,z,tol);
}
```

Implementing the Constraint - Rocket.hpp

```
void value( V& c, const V& u, const V&z, double &tol ) {
  auto& cs = getVector(c); auto& us = getVector(u);
  cs[0] = us[0] + ve*std::log(mass[0]/mt) + gdt;
  for( int i=1; i<N; ++i )
    cs[i] = us[i] - us[i-1] +
            ve*std::log(mass[i]/mass[i-1]) + gdt;
}

void applyJacobian_1( V& jv, const V& v, const V& u,
                      const V& z, double& tol ) {
  auto& jvs = getVector(jv); auto& vs =  getVector(v);
  jvs[0] = vs[0];
  for( int i=1; i<N; ++i ) jvs[i] = vs[i] - vs[i-1];
}

 void applyAdjointJacobian_1( V& ajv, const V& v, const V& u,
                              const V& z, double& tol ) {
   auto& ajvs = getVector(ajv);  auto& vs = getVector(v);
   ajvs[N-1] = vs[N-1];
   for( int i=N-2; i>=0; --i ) ajvs[i] = vs[i] - vs[i+1];
 }
```

Implementing the Constraint - Rocket.hpp

```
 void applyAdjointJacobian_1( V& ajv, const V& v, const V& u,
                              const V& z, double& tol ) {

   auto& ajvs = getVector(ajv);  auto& vs = getVector(v);
   ajvs[N-1] = vs[N-1];
   for( int i=N-2; i>=0; --i ) ajvs[i] = vs[i] - vs[i+1];
 }

void applyInverseJacobian_1( V& ijv, const V& v, const V& u,
                             const V& z, double &tol ) {

   auto& ijvs = getVector(ijv);  auto& vs = getVector(v);
   ijvs[0] = vs[0];
   for( int i=1; i<N; ++i ) ijvs[i] = ijvs[i-1] + vs[i];
}

void applyInverseAdjointJacobian_1( V& ijv, const V& v, const V& u,
                                    const V& z, double &tol ) {

   auto& ijvs = getVector(ijv);  auto& vs = getVector(v);
   ijvs[N-1] = vs[N-1];
   for( int i=N-2; i>=0; --i ) ijvs[i] = ijvs[i+1] + vs[i];
}
```

Implementing the Constraint - Rocket.hpp

```
void applyJacobian_2( V& jv, const V& v, const V& u,
                      const V& z, double& tol ) {
  auto& jvs = getVector(jv);  auto& vs  = getVector(v);
  double q{-ve*dt*vs[0]};
  jvs[0] = q/mass[0];
  for( int i=1; i<N; ++i ) {
    jvs[i] = -q/mass[i-1];  q -= ve*dt*vs[i];
    jvs[i] += q/mass[i];
  }
}

void applyAdjointJacobian_2( V& ajv, const V& v, const V& u,
                             const V& z, double& tol ) {
   auto& ajvs = getVector(ajv);  auto& vs   = getVector(v);
   ajvs[N-1] = -ve*dt*vs[N-1]/mass[N-1];
   for( int i=N-2; i>=0; --i )
     ajvs[i] = ajvs[i+1]-ve*dt*(vs[i]-vs[i+1])/mass[i];
}
```

Helper functions - Rocket.hpp

Used to access vector elements for the application code

```
std::vector<double>& getVector( ROL::Vector<double>& x ) {
  return
  *(Teuchos::dyn_cast<ROL::StdVector<double>>(x).getVector());
}

const std::vector<double>& getVector( const ROL::Vector<double>& x ) {
  return
  *(Teuchos::dyn_cast<const ROL::StdVector<double>>(x).getVector());
}
```

Driver - Rocket.cpp

```
#include "Rocket.hpp"
#include "ROL_OptimizationSolver.hpp"
#include "ROL_Reduced_Objective_SimOpt.hpp"
#include "Teuchos_XMLParameterListHelpers.hpp"
#include <iostream>

int main( int argc, char* argv[] ) {

  using Teuchos::rcp;
  using vector = std::vector<double>;

  auto parlist = rcp( new Teuchos::ParameterList() );
  Teuchos::updateParametersFromXmlFile("Rocket.xml",parlist.ptr());

  int     N  = parlist->get("Time Steps" ,      100   );
  double  T  = parlist->get("Final Time",       20.0  );
  double  g  = parlist->get("Gravity Constant", 9.8   );
  double  mr = parlist->get("Rocket Mass",      20.0  );
  double  mf = parlist->get("Fuel Mass",        100.0 );
  double  mu = parlist->get("Mass Penalty",     0.1   );
  double  ve = parlist->get("Exhaust Velocity", 1000.0);
  double  mt = mf+mr;     // Total mass
  double  dt = T/N;       // Time ste

  // More to follow
}
```

Driver - Rocket.cpp

```
// Simulation variable
auto u_rcp = rcp( new vector(N) );
auto u = rcp( new ROL::StdVector<double>(u_rcp) );
auto l = u->dual().clone();

// Optimization variable
auto z_rcp = rcp( new vector(N,mf/T) );
auto z = rcp( new ROL::StdVector<double>(z_rcp) );

// Lagrange multiplier
auto l = u->dual().clone();

 // Trapezpoidal weights
auto w_rcp = rcp( new vector(N,dt) );
(*w_rcp)[0] *= 0.5; (*w_rcp)[N-1] *= 0.5;
auto w = rcp( new ROL::StdVector<double>(w_rcp) );

// Piecewise constant weights
auto e_rcp = rcp( new vector(N,dt) );
auto e = rcp( new ROL::StdVector<double>(e_rcp) );

auto con = rcp( new Rocket::Constraint( N, T, mt, mf, ve, g ) );
```

Driver - Rocket.cpp

```
double tol = 1.e-7; // Needed for solve

// Compute solution for constant burn rate
con->update_2(*z);
con->solve(*l, *u, *z, tol);
//  u->print(std::cout);
double htarg = w->dot(*u);  // Final height

auto obj = rcp( new Rocket::Objective( N, T, mt, htarg, mu, w ) );
auto robj = rcp( new
  ROL::Reduced_Objective_SimOpt<double>( obj, con, u, z, l ) );

// Full space problem
//  auto x = Teuchos::rcp( new ROL::Vector_SimOpt<double>(u,z) );
//  ROL::OptimizationProblem<double> opt( obj, x, con, l );
ROL::OptimizationProblem<double> opt( robj, z );
ROL::OptimizationSolver<double> solver( opt, *parlist );
solver.solve( std::cout );
```

Driver - Rocket.cpp

```
    con->update_2(*z);
    con->solve(*l, *u, *z, tol);
//  u->print(std::cout);
    std::cout << "target height = " << htarg <<
                 ", actual = " << w->dot(*u) << std::endl;
    std::cout << "Initial fuel mass   = " << mf << std::endl;
    std::cout << "Remaining fuel mass = " << mf-e->dot(*z) << std::endl;
```

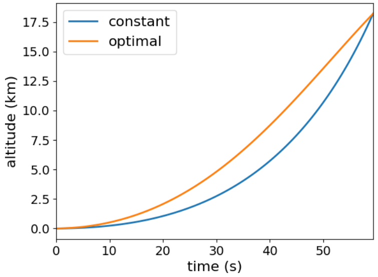
Solving the problem

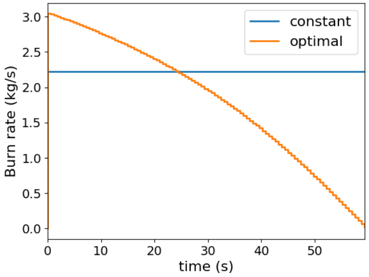
```
Truncated CG Trust-Region Solver
  iter  value         gnorm         .   #fval  #grad   tr_flag  iterCG  flagCG
  0     5.333333e+03  8.000000e+02
  1     5.333333e+03  8.000000e+02  .    2      1        2        2       0
  2     5.183948e+03  4.287777e+04  .    3      2        0        2       3
  3     5.015379e+03  4.138002e+04  .    4      3        0        2       3
  4     4.811909e+03  3.575303e+04  .    5      4        0        20      0
  5     4.700787e+03  2.812899e+04  .    6      5        0        18      0

  ...

  18    4.401047e+03  1.748365e+01   .   19     17       0        4       0
  19    4.401047e+03  3.689599e-04   .   20     18       0        2       0
  20    4.401047e+03  1.141414e-07   .   21     19       0        2       0
  21    4.401047e+03  9.400946e-08   .   22     20       0        4       0
  22    4.401047e+03  2.214017e-08   .   23     21       0        1       0
target height = 18219.4, actual = 18219.2
Initial fuel mass   = 80
Remaining fuel mass = 14.7111
```

Optimal Burn Rate


constant
optimal
altitude (km)
time (s)


constant
optimal
Burn rate (kg/s)
time (s)