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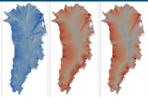
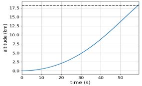
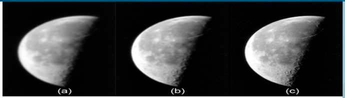
RAPID OPTIMIZATION LIBRARY







An Introduction to the Rapid Optimization Library

Drew Kouri Denis Ridzal Greg Von Winckel **Aurya Javeed**

A Motivating Example

Rocket Dynamics

From the conservation of momentum,

$$\frac{dp}{dt} \approx \frac{\{(m - |\Delta m|)(u + \Delta u) + |\Delta m|(u - k)\} - mu}{\Delta t}$$
$$= \sum F = -mg$$
$$\implies -m\frac{du}{dt} = k\frac{dm}{dt} + mg. \tag{1}$$

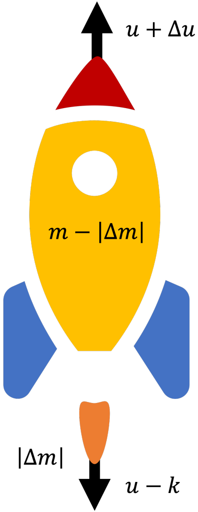
Here, we take g and the exhaust speed k to be constants but

$$\frac{dm}{dt} = -z < 0, \tag{2}$$

where $z = z(t)$ is a control of our choosing.

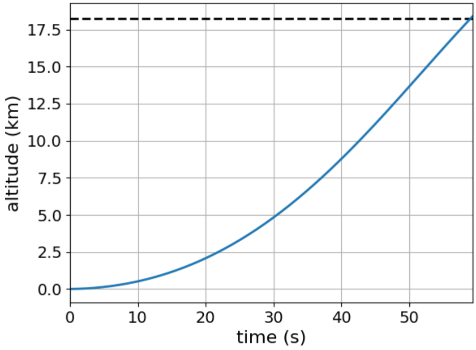
We want to solve the fuel efficiency problem

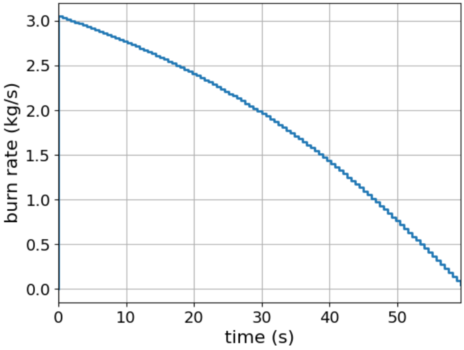
$$\underset{u,z}{\text{minimize}} \ \|z\|^2_{L^2(0,T)} + \lambda \left| y^* - \int_0^T u(t)\,dt \right|^2 \ \text{subject to (1) and (2).}$$



Solution

We discretize the fuel efficiency problem into a nonlinear program (NLP).





So why ROL?

Numerics

```
Composite-step trust-region solver
iter  fval          cnorm         gLnorm        snorm         delta     nnorm     tnorm     #fval   #grad  ...
0     5.333333e+03  2.027966e-13  2.666783e+00
1     5.223834e+03  2.933645e+00  3.555940e+00  1.000000e+02  2.00e+02  1.13e-14  1.00e+02  3       3
2     5.074484e+03  3.977936e+00  5.320566e+00  2.000000e+02  2.00e+02  1.06e-01  2.00e+02  5       5
3     4.936750e+03  1.929162e+00  6.883693e+00  1.657243e+02  1.16e+03  1.61e-01  1.66e+02  7       7
...
47    4.426957e+03  1.813330e-04  9.328418e-02  2.898613e+00  1.16e+03  7.35e-06  2.90e+00  95      95
48    4.426934e+03  6.805572e-05  4.641692e-02  1.479816e+00  1.16e+03  1.10e-05  1.48e+00  97      97
49    4.426917e+03  1.176645e-04  7.690407e-02  2.328988e+00  1.16e+03  4.24e-06  2.33e+00  99      99
50    4.426902e+03  4.457843e-05  3.584340e-02  1.192131e+00  1.16e+03  7.13e-06  1.19e+00  101     101
...
```

```
Composite-step trust-region solver
iter  fval          cnorm         gLnorm        snorm         delta     nnorm     tnorm     #fval   #grad  ...
0     5.333333e+03  1.570856e-15  1.803732e+02
1     4.976505e+03  7.464298e-01  1.380737e+02  2.175210e+01  1.00e+02  3.03e-15  2.18e+01  3       3
2     5.252000e+03  2.467093e-02  2.549998e+02  2.755372e+00  1.00e+02  2.75e+00  5.33e-02  5       5
3     4.473015e+03  7.617080e-02  2.595459e+01  7.041189e+00  1.00e+02  1.23e-01  7.04e+00  7       7
4     4.428484e+03  2.072535e-03  3.485754e+00  1.936220e+00  1.00e+02  3.08e-01  1.91e+00  9       9
5     4.426855e+03  3.830153e-06  7.137584e-01  8.183971e-02  1.00e+02  8.98e-03  8.13e-02  11      11
6     4.426841e+03  1.090076e-06  6.769629e-03  4.490118e-02  1.00e+02  1.87e-05  4.49e-02  13      13
7     4.426840e+03  8.296731e-12  5.966856e-04  1.035859e-04  1.00e+02  4.58e-06  1.03e-04  15      15
8     4.426840e+03  3.307995e-13  3.785700e-06  1.927025e-05  1.00e+02  2.37e-11  1.93e-05  17      17
Optimization Terminated with Status: Converged
```

Custom Linear Algebra – A Feature of ROL

ROL makes it easy to tailor inner products to problems.

For example, we can think of our control z as an element of a Hilbert space $\mathcal{H}$ with the inner product

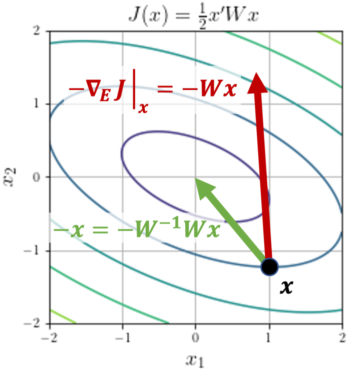
$$\langle f, g\rangle = \int_0^T f(t)g(t)dt.$$

The discretized analogue of $\mathcal{H}$ is a finite-dimensional space whose inner product is weighted by a quadrature matrix W – i.e., $\langle f, g\rangle = f'Wg$.

A gradient with respect to a vector in the finite-dimensional space will be a function of W.

$$\lim_{h\to 0} \frac{|J(x+h) - J(x) - \langle \nabla J\big|_x, h\rangle|}{h} = 0$$

$$\implies \nabla J\big|_x = W^{-1}\nabla_E J\big|_x$$



- Málek, Josef, and Zdeněk Strakoš. *Preconditioning and the Conjugate Gradient Method in the Context of Solving PDEs*. SIAM, 2014.

ROL

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

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.

Formalism and Algorithms

Mathematical Formalism

ROL solves (smooth) nonlinear optimization problems numerically

$$\underset{x}{\text{minimize}} \;\; J(x) \;\; \text{subject to} \;\; \begin{cases} c(x) = 0 \\ \ell \le x \le u \\ Ax = b. \end{cases} \tag{G}$$

Here, x belongs to a Banach space $\mathcal{X}$ and

$$J : \mathcal{X} \to \mathbb{R}, \quad c : \mathcal{X} \to \mathcal{C}, \quad \text{and} \quad A : \mathcal{X} \to \mathcal{D},$$

where $\mathcal{C}$ and $\mathcal{D}$ are Banach spaces as well.

All three of these maps are Fréchet differentiable. In addition, A is linear.

The bounds $\ell \le x \le u$ apply pointwise.

Algorithms

Type U
"Unconstrained"

$$\underset{x}{\text{minimize}} \;\; J(x) \qquad \text{subject to} \;\; \begin{cases} \\ \\ Ax = b \end{cases}$$

Methods:

- trust region and line search globalization
- gradient descent, quasi and inexact Newton, nonlinear conjugate gradient.

Type B
"Bound Constrained"

$$\underset{x}{\text{minimize}} \;\; J(x) \qquad \text{subject to} \;\; \begin{cases} \\ \ell \le x \le u \\ Ax = b \end{cases}$$

Methods:

- projected gradient and projected Newton, primal-dual active set.

Type E
"Equality Constrained"

$$\underset{x}{\text{minimize}} \;\; J(x) \qquad \text{subject to} \;\; \begin{cases} c(x) = 0 \\ \\ Ax = b \end{cases}$$

Methods:

- composite step SQP and ...

Type G
"General Constraints"

$$\underset{x}{\text{minimize}} \;\; J(x) \qquad \text{subject to} \;\; \begin{cases} c(x) = 0 \\ \ell \le x \le u \\ Ax = b \end{cases}$$

Methods:

- augmented Lagrangian, interior point, Moreau-Yosida, stabilized LCL.

API

ROL::Objective

$$\underset{x}{\text{minimize}} \quad J(x) \quad \text{subject to} \quad \begin{cases} c(x) = 0 \\ \ell \leq x \leq u \\ Ax = b \end{cases}$$

Member Functions

- `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` - $\frac{d}{dt} J(x + tv)|_{t=0}$

(pure virtual virtual optional)

- We do not need to specify linear operators with matrices – their action on vectors is enough.
- ROL works best with analytic derivatives. Without them, ROL defaults to finite difference approximations.
- Tools: `checkGradient`, `checkHessVec`, `checkHessSym`.

ROL::Objective

$$\underset{x}{\text{minimize}} \quad J(x) \quad \text{subject to} \quad \begin{cases} c(x) = 0 \\ \ell \le x \le u \\ Ax = b \end{cases}$$

Member Functions

- `value` - $J(x)$
- `gradient` - $g = \nabla J(x)$
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- `dirDeriv` - $\frac{d}{dt} J(x+tv)|_{t=0}$

(pure virtual virtual optional)

$$J(u,z) = \|z\|^2_{L^2(0,T)} + \lambda \left| y^* - \int_0^T u(t)\,dt \right|^2$$

```
class RocketObjective : public ROL::Objective<double>
{
 ...

 public:

  Objective(double targetHeight_, double lambda_,
            const std::vector<double>& w_,) :
   targetHeight(targetHeight_), lambda(lambda_), w(w_)
  {
    N = w.size();
  }

  double value(const ROL::Vector<double>& x, double& tol)
  {
    const std::vector<double>& z = getControl(x);
    const std::vector<double>& u = getState(x);

    int i;

    double zIntegral = 0;
    for (i = 0; i < N; ++i)
      zIntegral += w[i]*z[i]*z[i];

    double uIntegral = 0;
    for (i = 0; i < N; ++i)
      uIntegral += w[i]*u[i];

    return zIntegral + lambda*std::pow(uIntegral - targetHeight, 2);
  }
  ...

}
```

ROL::Constraint

$$\underset{x}{\text{minimize}} \;\; J(x) \;\; \text{subject to} \;\; \begin{cases} c(x) = 0 \\ \ell \le x \le u \\ Ax = b \end{cases}$$

Member Functions

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

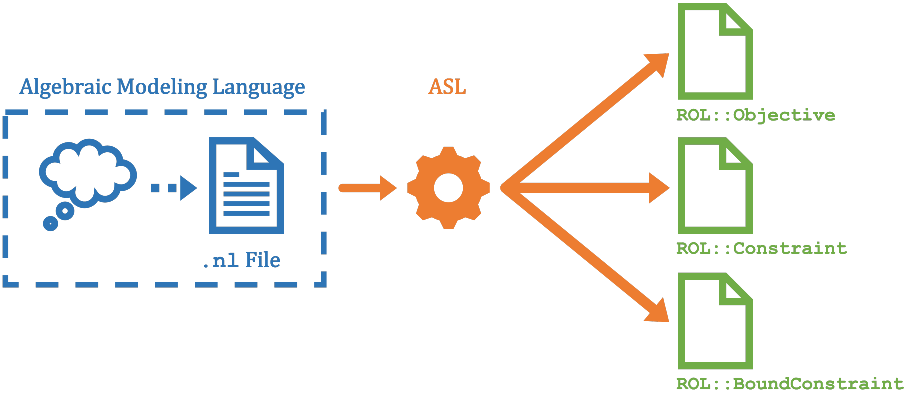
`ROL::BoundConstraint` implements $\ell \le x \le u$.

$$\frac{du}{dt} + k\frac{d\log m}{dt} + g = 0 \quad \text{and} \quad \frac{dm}{dt} = -z$$

```
class RocketConstraint : public ROL::Constraint<double>
{
 private:
  ...

  void computeMass(const std::vector<double>& z)
  {
    mass[0] = initialMass - dt*z[0];
    for (int i = 1; i < N; ++i)
      mass[i] = mass[i - 1] - dt*z[i];
  }

 public:
  ...

  void update(const ROL::Vector<Real> &x, UpdateType type, int iter = -1)
  {
    const std::vector<double>& z = getControl(x);
    computeMass(z);
  }

  void value(ROL::Vector<double>& c, const ROL::Vector<double>& x, double& tol)
  {
    std::vector<double>& cstd = getVector(c);

    const std::vector<double>& z = getControl(x);
    const std::vector<double>& u = getState(x);

    cstd[0] = u[0] + k*std::log(mass[0]/mInitial) + g*dt;
    for(int i = 1; i < N; ++i)
      cstd[i] = u[i] - u[i-1] + k*std::log(mass[i]/mass[i - 1]) + g*dt;
  }
  ...

}
```

AMPL-Solver Interface Library (ASL)

ROL can be a backend for algebraic modeling languages. We have an interface to AMPL.



- *Note*: Our current interface is matrix free, i.e., we do not yet precondition with the matrix information from ASL.

The `SimOpt` Interface

Our rocket example – and optimal control in general – is what we call a simulation-constrained optimization problem.

Full Space Formulation

The problem is *explicitly* constrained:

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

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

Reduced Space Formulation

The problem is *implicitly* constrained:

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

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

- z = the vector being optimized (often a control or set of parameters)
- u = a state resulting from c (the simulation)

In engineering applications, c is often a differential equation.

ROL's `SimOpt` interface is "middleware":

- u and z are separated out of the optimization vector x
- converting full space formulations to reduced space ones (and vice-versa) is trivial.

The `SimOpt` Interface

`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)`

A mnemonic:

- $1 =$ "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)`

Stochastic Optimization

ROL also has middleware for stochastic problems:

$$\underset{x \in C}{\text{minimize}} \;\; \mathcal{R}(f(x, \xi)).$$

Here, x is a deterministic decision but ξ is a set of random parameters, i.e., $\xi = \xi(\omega)$.

For each x, $f(x, \xi)$ is a random variable $F_x(\omega)$.

$\mathcal{R}$ is a functional on these random variables that quantifies risk. $\mathcal{R}$ could be – for instance –

- an expectation: $\mathcal{R}(F_x) := \mathbb{E}[F_x]$,
- a quantile (the value at risk),
- a distributionally robust model

$$\mathcal{R}(F_x) = \sup_{P \in \mathcal{U}} \mathbb{E}_P[F_x].$$

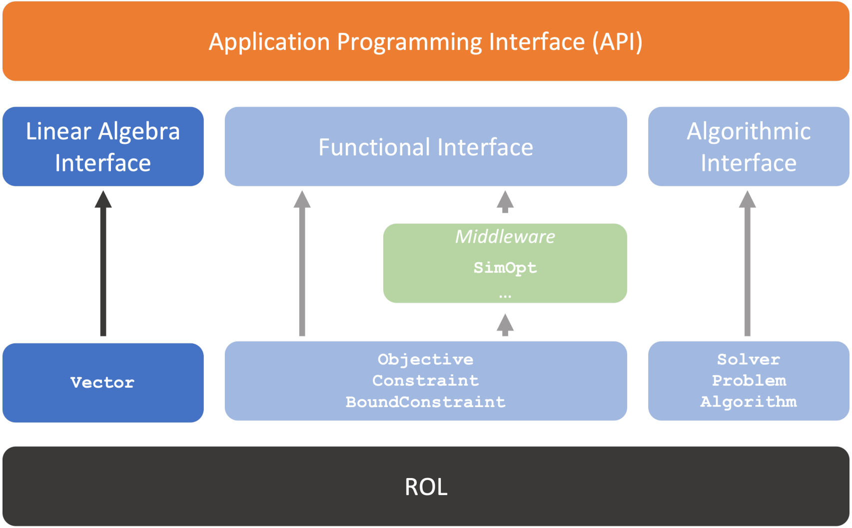
The set $\mathcal{C}$ can include both stochastic (e.g., $\ell \leq \tilde{\mathcal{R}}(G_x) \leq u$) and deterministic constraints.

ROL solves these problems in the usual way: $\mathcal{R}(F_x)$ and the stochastic constraints in C are replaced with approximations. For example, we might take

$$\mathbb{E}[F(x)] \approx \frac{1}{N} \sum_{k=1}^{N} f(x, \xi_k),$$

where the ξ_k are independent and identically distributed samples of ξ.

Design


Application Programming Interface (API)
Linear Algebra Interface
Functional Interface
Algorithmic Interface
Middleware
SimOpt
…
Vector
Objective
Constraint
BoundConstraint
Solver
Problem
Algorithm
ROL

`ROL::Vector` – A Linear Algebra Interface

Optimization algorithms manipulate vectors. But the *implementation* of these vectors do not affect what the algorithms do. (For example, the number of iterations before gradient descent reaches some stopping condition will be the same whether x – the vector being optimized – is stored on a laptop or distributed over a network.)

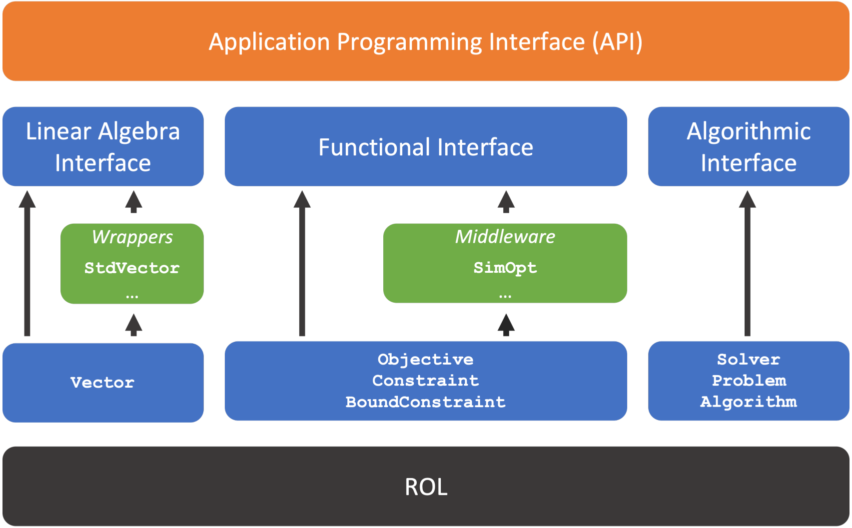
ROL similarly relegates the inner workings of vectors to users. As a result,

- ROL is hardware agnostic. Sandians run ROL on personal computers (in serial and MPI parallel), GPUs, and supercomputers too.
- Users can easily tune the linear algebra of a problem by inheriting from an instance of `ROL::Vector` (which we did in the rocket example).

Member Functions

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

Design



Application Programming Interface (API)
Linear Algebra Interface
Functional Interface
Algorithmic Interface
Wrappers
StdVector
...
Middleware
SimOpt
...
Vector
Objective
Constraint
BoundConstraint
Solver
Problem
Algorithm
ROL

Context

Related Software

- *Hilbert Class Library (HCL) - Rice University*

  An abstract linear algebra interface.

- *Trilinos - Sandia National Laboratories*

  Collection of linear and nonlinear solvers based on linear algebra abstractions.

  - *RTOp and Thyra*

    Packages for an extended set of algebraic abstractions.

  - *MOOCHO*

    Optimization package built on Thyra that solves reduced space formulations.

- *Rice Vector Library (RVL) - Rice University*

  A revamp of HCL.

- *Trilinos* (continued)

  - *Aristos*

    Optimization package with algebra abstractions and full space formulations.

  - *Optipack*

    A few special-purpose optimization routines using algebra abstractions.

- *PEOpt - Sandia National Laboratories*

  Optimization packages using an alternative implementation of algebra abstractions.

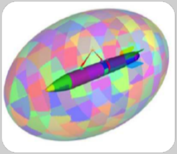
- *Optizelle - OptimoJoe*

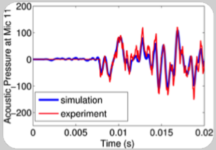
  Successor to PEOpt.

Applications

Inverse Problems in Acoustics/Elasticity

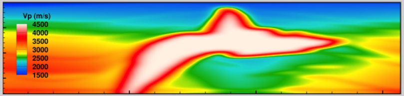
Sierra/SD – structural dynamics software

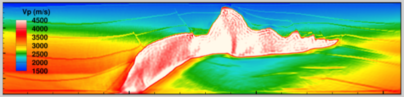




1M optimization + 1M state variables

DGM – a library of discontinuous Galerkin methods for solving partial differential equations

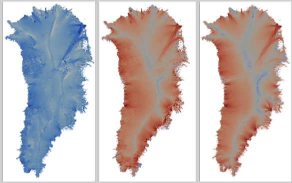




500K optimization + 2M×5K state variables

Estimating Basal Friction of Ice Sheets

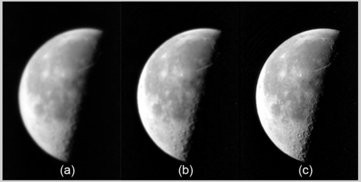
Albany – a multiphysics simulator



5M optimization + 20M state variables

Super-Resolution Imaging

GPU processing with *ArrayFire*



250K optimization variables on an NVIDIA Tesla

Conclusions

- ROL is C++ code for solving large optimization problems.
- It implements a variety of matrix-free algorithms and has been "battle-tested" on problems at Sandia.
- ROL has a flexible interface that can connect with algebraic modeling languages. And, importantly, ROL lets users implement their own vectors.