SNL ATDM Analysis Components

POCs: Eric Phipps (etphipp@sandia.gov), Byron Hanks (bwhanks@sandia.gov), and Jim Stewart (jrstewa@sandia.gov)

SAND2017-1028D

Combines algorithmic R&D with delivery of interoperable software components that focus on enabling advanced analysis workflows

- *Sensitivity analysis and uncertainty quantification*
- *Design optimization, topology/shape optimization, calibration*
- *Reduced-order models integrated with optimization*
- *Off-line meshing and on-line parallel mesh refinement*
- *Embedded geometry representations for refinement, optimization, and UQ*

Focus on embedded workflows for next-generation architectures

- *Automatic differentiation-based analysis data propagation*
- *Kokkos many-core performance portability*
- *Asynchronous many-tasking with Darma*

Single, integrated project spanning ATDM/ECP focus areas

- *ASD Data Propagation Components (PI, E. Phipps)*
- *CDA Analysis Components (PI, B. Hanks)*
- *Combined project manager (J. Stewart)*

Embedded Derivative & Ensemble Propagation

POC: Eric Phipps (etphipp@sandia.gov)

Providing derivative evaluation and ensemble propagation technologies to production codes

- *Accurate and robust derivative computation*
- *Efficient and scalable derivative and sample evaluation performance*
- *Integrate easily with complex code bases and developer workflows*

Enabling advanced embedded analysis methods

- *Adjoint-based sensitivity analysis (transient and steady)*
- *Reduced and full-space optimization, inversion, and calibration*
- *Derivative-enhanced uncertainty quantification*

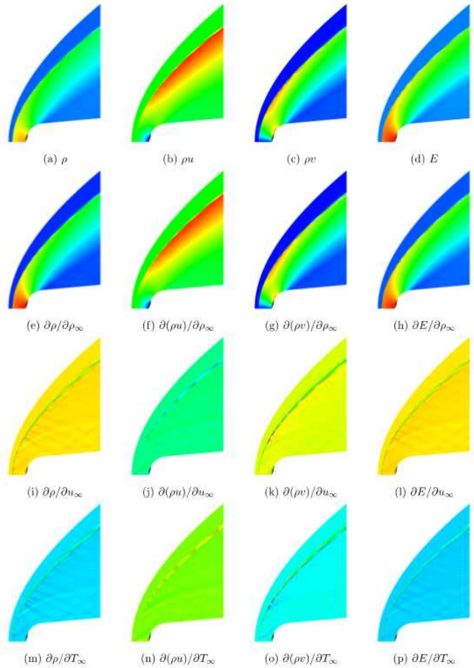
Implemented through automatic differentiation technologies and template-based generic programming for C++ codes

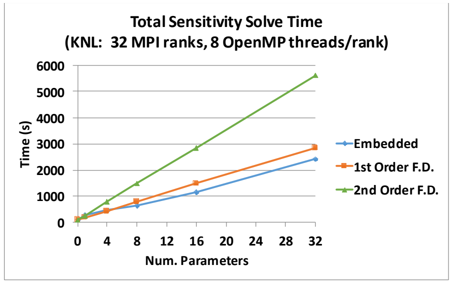
- *Sacado automatic differentiation package from Trilinos (http://trilinos.org)*
- *Template application code on scalar type*
- *Instantiate template code on analysis data types*
- *Derivative and ensemble scalar types optimized for HPC applications*
- *Kokkos integration for performance portable derivative/ensemble evaluation*

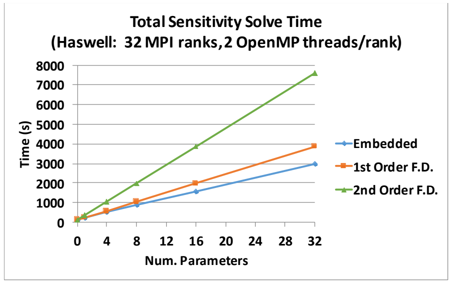
Trilinos

Sacado-based sensitivity analysis for hypersonic flow past a blunt wedge in ATDM/SPARC

- *Demonstrates substantially improved performance compared to traditional finite differences*
- *Work completed as part of FY16 ATDM L2 Milestone*







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Asynchronous Many-Task (AMT) for next generation UQ

POC: Francesco Rizzi (fnrizzi@sandia.gov)

AMT parallelism across UQ samples

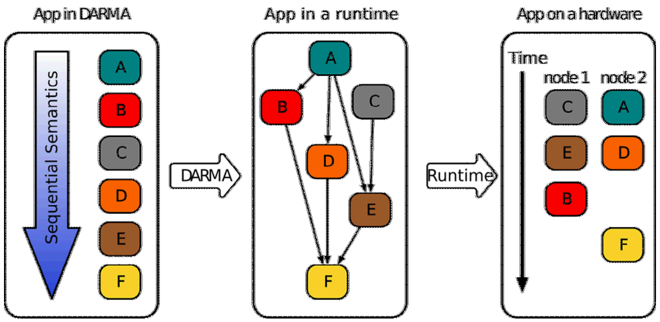
- *Efficient formulation of UQ workflows*
- *Support for dynamic, system-level runtime transformations*
- *Suitable model for expressing embedded UQ analysis*
- *Data reuse and load-balance benefits through pipeline parallelism*

Demonstrating suitability for typical UQ applications

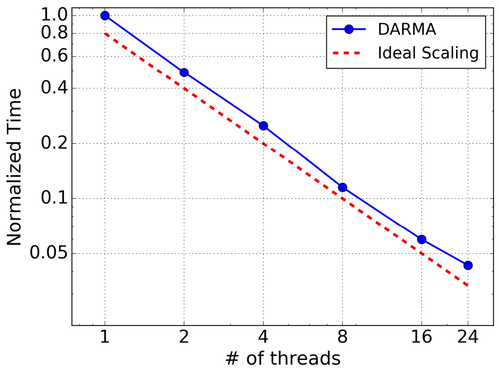
- *AMT prototypes for sampling-based and multilevel UQ*
- *Exploiting UQ workflows to extract all available task and pipeline parallelism*
- *On-node and distributed validations*

Research based on DARMA AMT (Sandia National Labs)

- *A co-design for an AMT programming models*
- *Embedded domain specific language (EDSL) in C++*
- *Declarative, not procedural imperative*
- *Coordination semantics and separation of policy from mechanism*
- *DARMA codes require only the data-flow dependencies and are execution model-agnostic*



Schematic of sample AMT application as it appears on DARMA front-end, runtime and mapped to hardware.



On-node scaling for Monte Carlo sampling of stochastic 2D Poisson equation with each PDE sample mapped into a single task.

- *Work being developed as part of FY17 ATDM*

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Rapid Optimization Library

POC: Denis Ridzal (dridzal@sandia.gov)

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

ROL is a is a C++ package for large-scale optimization.

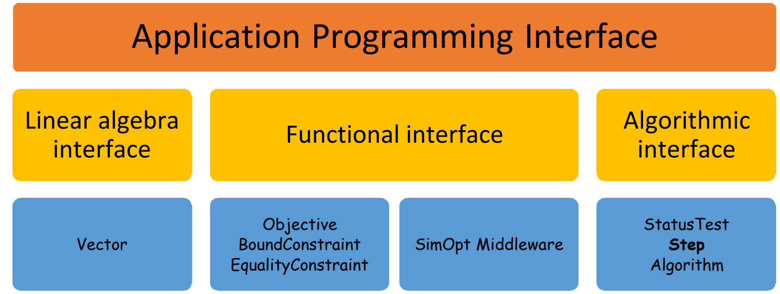
- Optimal design, optimal control and inverse problems.
- Image processing and image enhancement.
- Computational mesh generation and mesh optimization.

Embedded into applications through a matrix-free API.

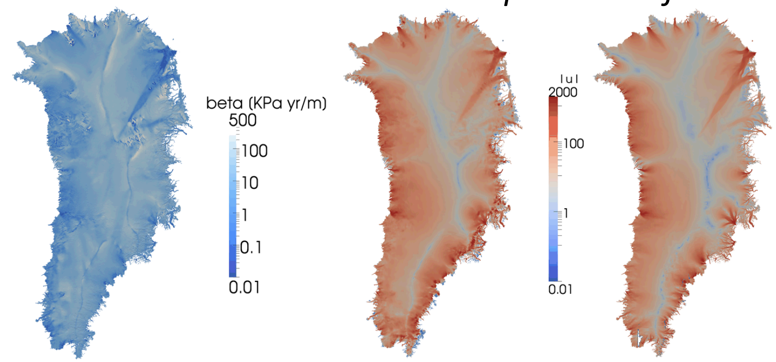
- Direct use of data structures and memory spaces – **distributed / shared / hybrid memory** – through the *Linear algebra interface*.
- Direct use of application's linear and nonlinear solvers, through the **SimOpt middleware** for simulation-based optimization.

State-of-the art algorithms.

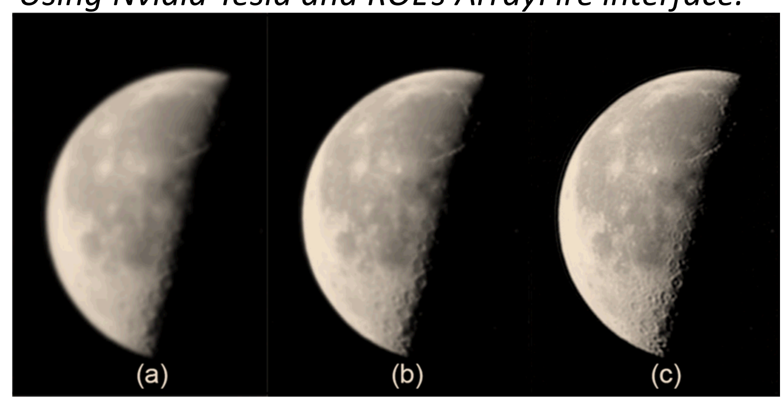
- Unconstrained optimization, constrained optimization and optimization under uncertainty, incl. **risk-averse optimization**.
- **Adaptive multi-fidelity model management**, through inexact function and gradient evaluations in trust-region methods.
- Hierarchical and custom (user-defined) algorithms.



Large-scale estimation of ice sheet properties.
Distributed inversion via ROL's Tpetra interface.



Super-resolution imaging on GPUs.
Using Nvidia Tesla and ROL's ArrayFire interface.



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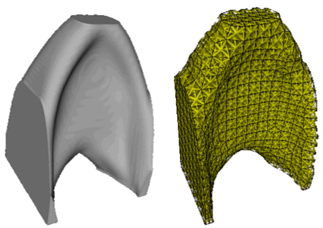
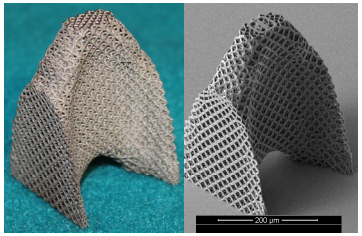
Non-conformal Geometry Description for Concurrent Shape and Topology Optimization

POC: Joshua Robbins (jrobbin@sandia.gov)

Developing volume-based, non-conformal, discrete geometry descriptions for leveraging the design space of additive manufacturing

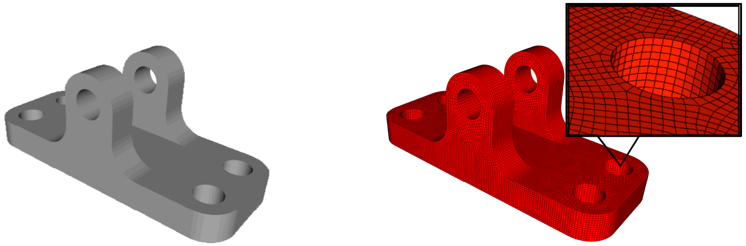


Computed design

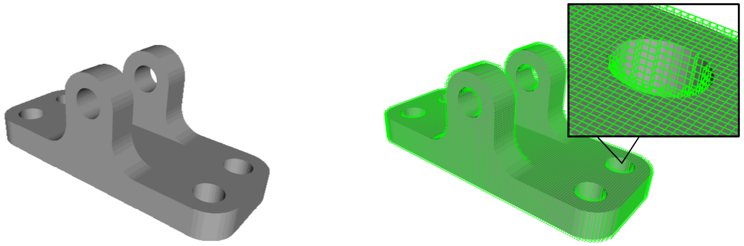


c/o Bradley Jared, SNL c/o Bryan Kaehr, SNL

Printed design



Discrete conformal volume-based solid model



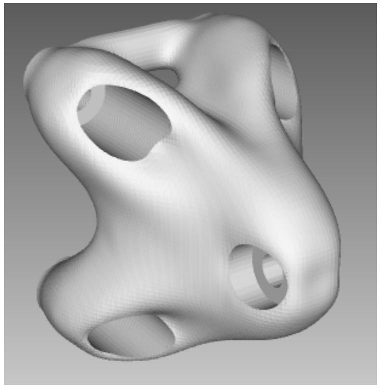
Discrete non-conformal volume-based solid model

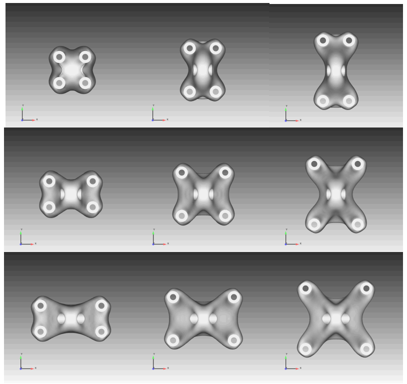
Providing geometry-aware quadrature for accurate integration of non-conformal discretizations

- *Fully parameterized geometry description*
- *Automates and parallelizes hexahedral mesh generation*
- *Developed for easy integration with new and existing codes*

Leveraging automatic differentiation technology available in Trilinos/Sacado

- *Provides topology and shape sensitivities*
- *Enables concurrent topology and shape optimization*





Shape parameter study of topologically optimized design produces optimized topology and optimal placement of parameterized features (e.g., bolt hole locations)

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Certified PDE-constrained optimization using reduced order models

POC: Miguel Aguiló (maguilo@sandia.gov)

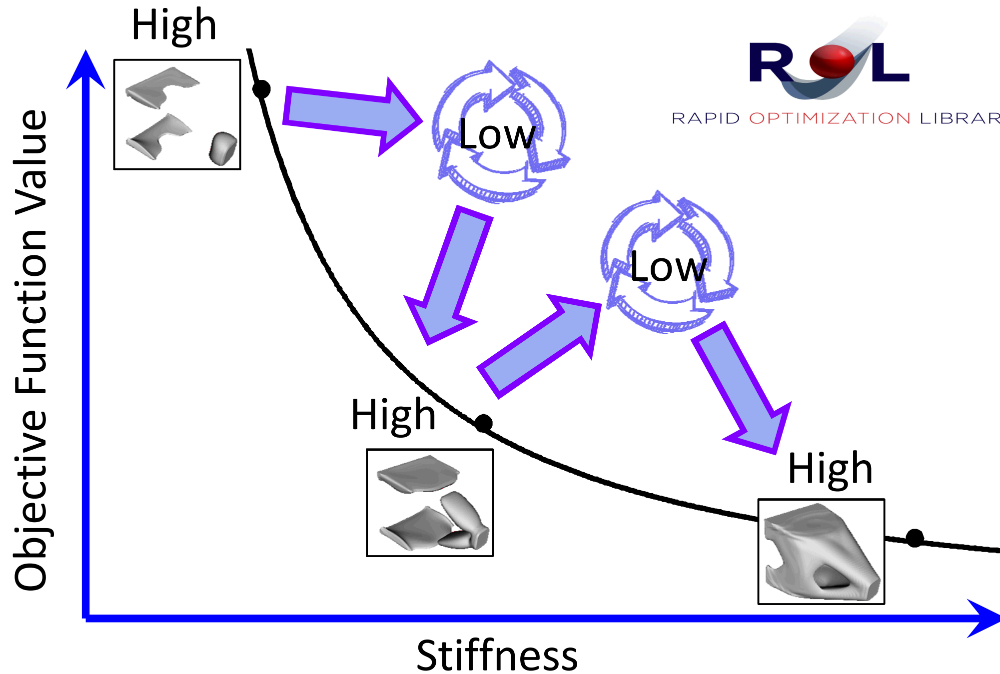
ROL
RAPID OPTIMIZATION LIBRARY

Providing fast PDE-constrained optimization calculations using parametric reduced order models

- *Accelerates PDE-constrained optimization problems*
- *Progressive reconstruction of reduced order models*
- *Error estimates to control error induced by inexact objective and gradient calculations*

Careful crafting of interfaces to enable interoperability

- *C++ implementation in Trilinos ROL module*
- *Kokkos integration for performance portable linear algebra calculations*



Example: Multi-load topology optimization

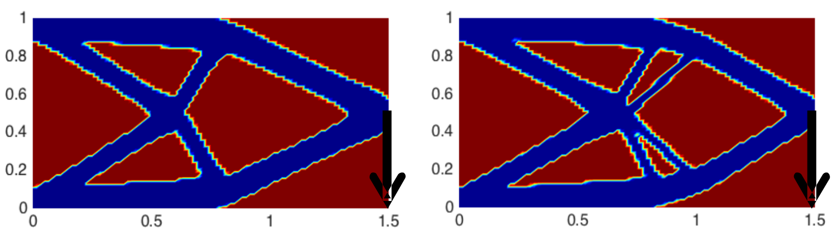


Figure: This figure shows the similarities between using and not using a reduced-order model to solve a Michell topology optimization problem. The **left pane** illustrates the optimal topology obtained using a reduced order model (objective = 0.5875). The **right pane** illustrates the optimal topology obtained without using a reduced order model (objective = 0.59).

Load Angle	Time (sec)	Iterations	HFM	LFM	Updates
0		36	77	135	27
10		29	51	77	19
20	5x	23	50	68	11
15		29	43	68	15
25		26	34	63	11
5		**23**	**0**	**127**	**0**

Table: Time savings using reduced order models evaluations. Legend: (**HFM**) high fidelity model evaluations, (**LFM**) low fidelity model evaluations, Number of online reduced order model updates (**Updates**).

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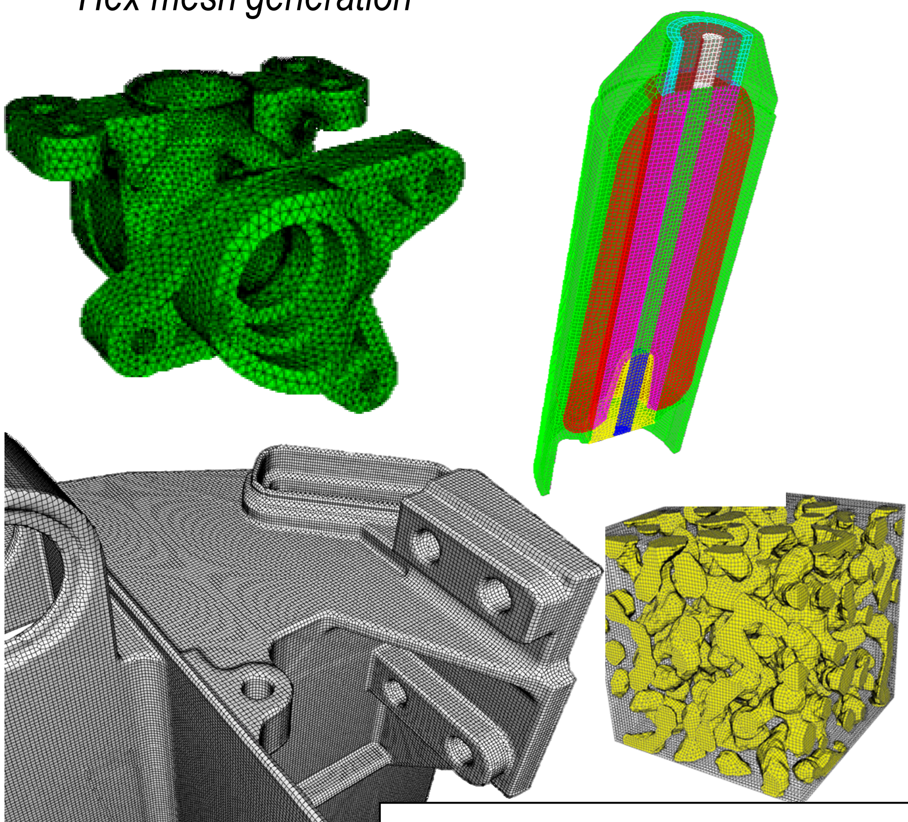
Geometry and Mesh Generation

POC: Byron Hanks (bwhanks@sandia.gov)

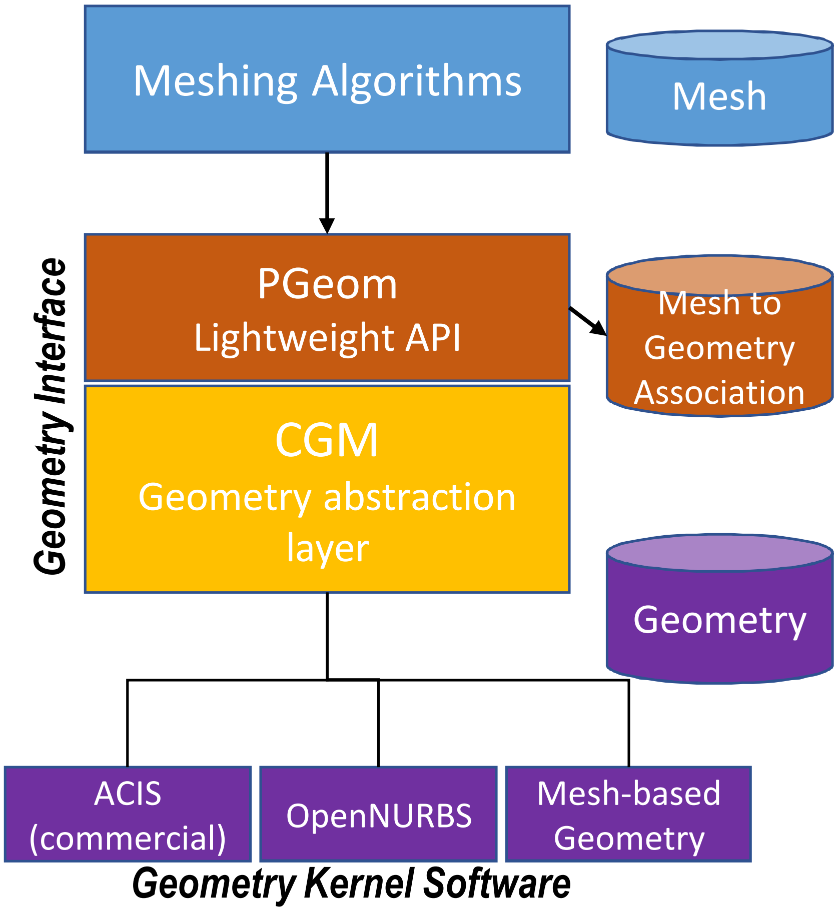
CUBIT provides extensive capabilities for preparing geometry and generating an initial mesh

- *https://cubit.sandia.gov*
- *Advanced meshing algorithms for Tri, Quad, Tet, and Hex mesh generation*



Sculpt parallel all-hex meshing

CAD Geometry Interface for meshing and refinement that accurately captures the model geometry

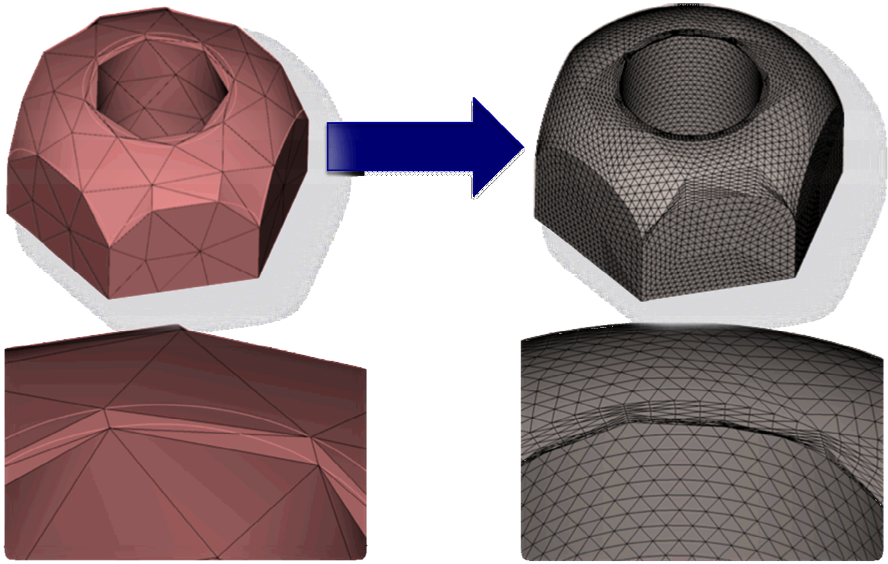


Percept Mesh Adapt for scalable, parallel mesh refinement

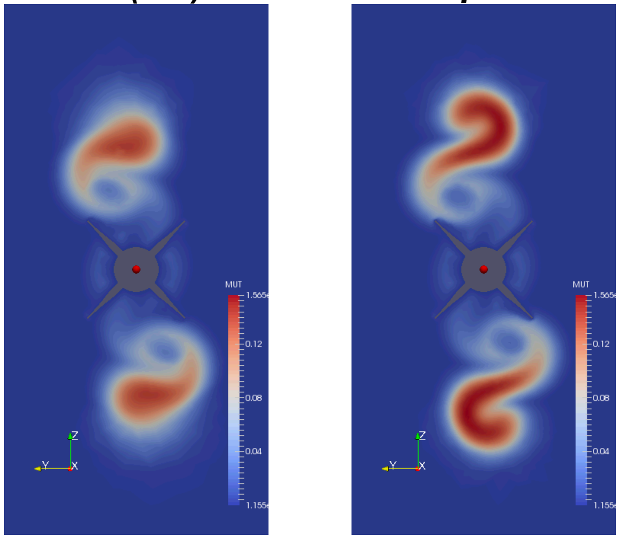
POC: Byron Hanks (bwhanks@sandia.gov)

Uniform mesh refinement (UMR) and Adaptive mesh refinement (AMR)

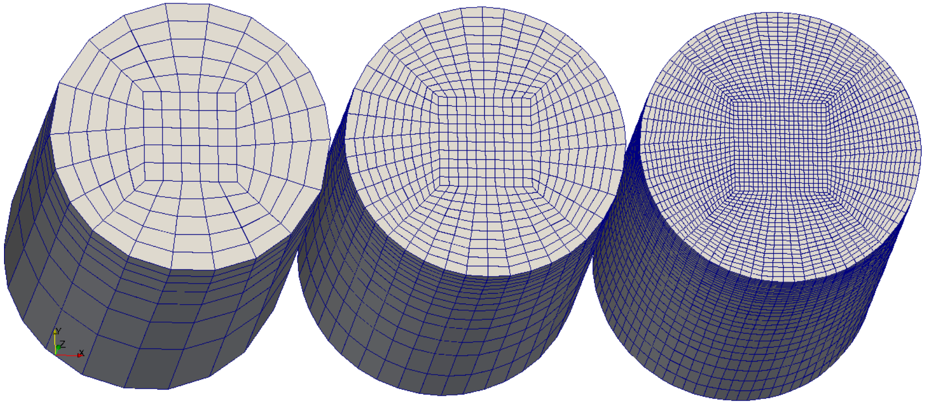
- *https://github.com/PerceptTools/percept*
- *Offline or inline*
- *Scalable, parallel operation*
- *Support for CAD or Mesh-based smooth geometry*
- *Advanced features: mesh smoothing, convert low to high order, respect mesh spacing in the refined mesh*



Vortices arising from jet in cross flow using coarse mesh (left) and offline adapted mesh (3x)

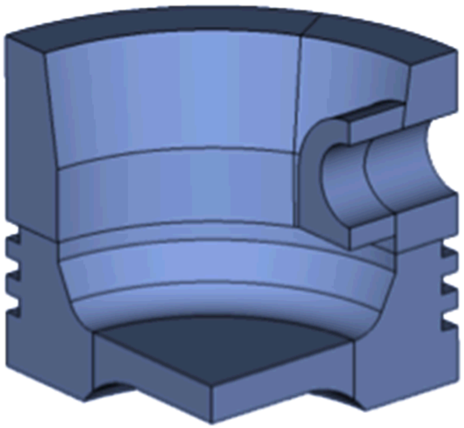


Uniform refinement of open jet flow inlet mesh adapted using mesh-based geometry approximation



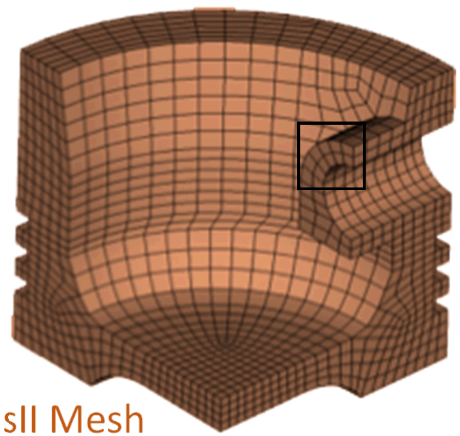
Percept and CUBIT combined workflow for generating large meshes

POC: Byron Hanks (bwhanks@sandia.gov)



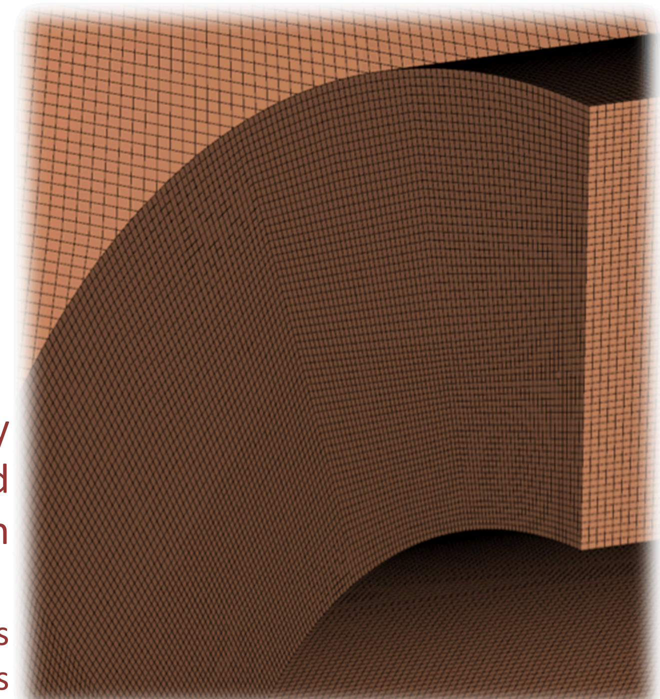
SAT, STEP, IGES
CAD definition

CUBIT
re-association
to openNURBS



ExodusII Mesh

Percept
parallel decomposition,
refinement, and smoothing



Uniformly refined Exodus II mesh

112M Hex cells
20 processes

Refinement

Sequences of refined meshes are created at the push of a button in parallel, minimizing the geometry error with respect to the original CAD model.