Parallel Works

The Supercomputing Hub for
design exploration & innovation

Platform & Technology Overview

Parallel Works

Parallel Works HPC Hub

A seamless integration of data, compute, and software resources deployed as a service to deliver a collaborative, centralized HPC hub for engineering design automation.

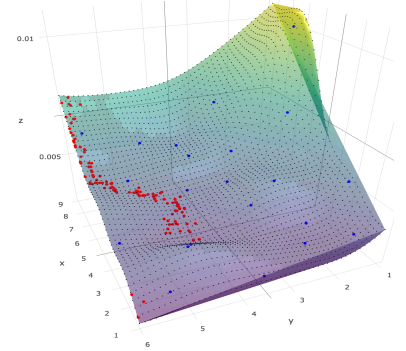CENTRALIZED & STANDARDIZED WORKFLOW TOOLS

GLOBAL ENGINEERING TEAMS

OPTIMIZED PRODUCT

COLLABORATIVE USER INTERFACE

SCALABLE COMPUTING RESOURCES

Parallel Works unifies distributed engineering teams and providing the necessary computing resources to execute advanced engineering studies at scale

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Swift: The workflow system powering Parallel Works

Swift is a state-of-the-art parallel workflow technology designed to simplify and automate advanced parallel workflow, enabling engineers to focus on their design challenges

INNATELY PARALLEL. Sophisticated workflow expressed via simple code is automatically distributed across available compute resources.

DISTRIBUTED. Facilitates file and data passing across function invocations, remote databases and distributed resources.

FAULT TOLERANT. Automatically detects and retries failed runs, without interfering with other workflow tasks. Restart happens from the point of failure.

EMBEDDED PROVENANCE. Tracks and stores fine grain detail of workflow processes for future recall and validation.

Developed at Argonne National Laboratory and the University of Chicago with funding from the NSF and DOE. This trusted technology has been used by leading scientists and academics to support research at universities and laboratories around the world since 2009.
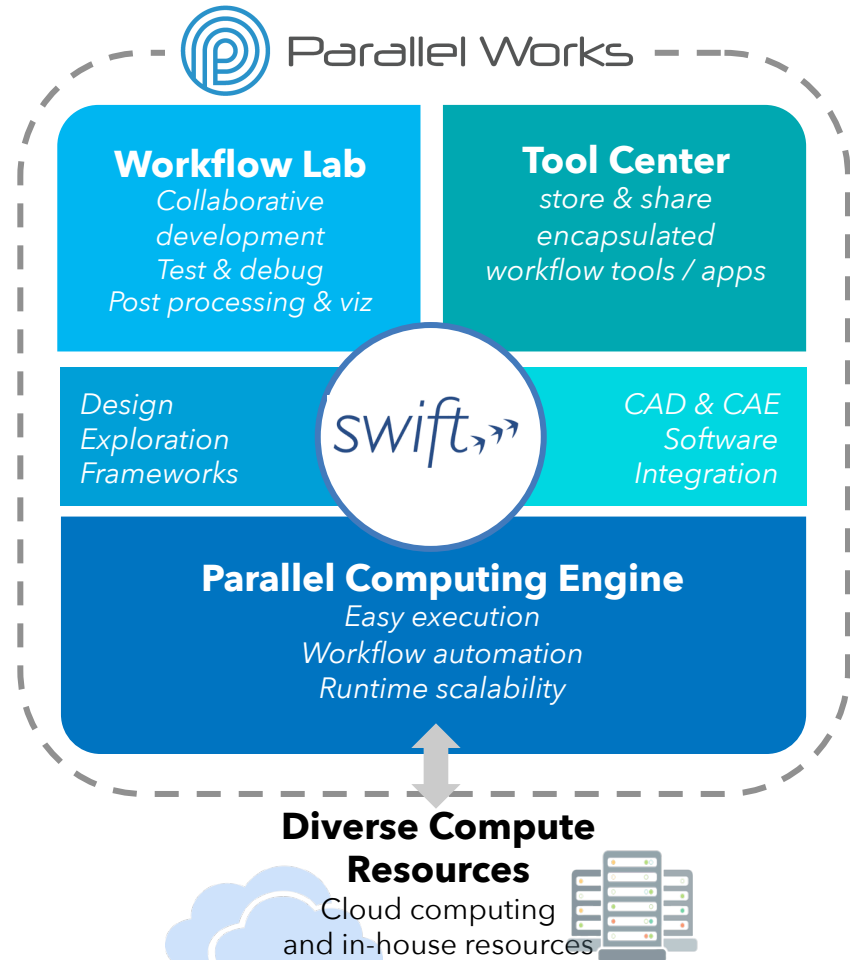
Parallel Works Builds on *Swift* to deliver a centralized HPC Hub for advanced engineering design exploration
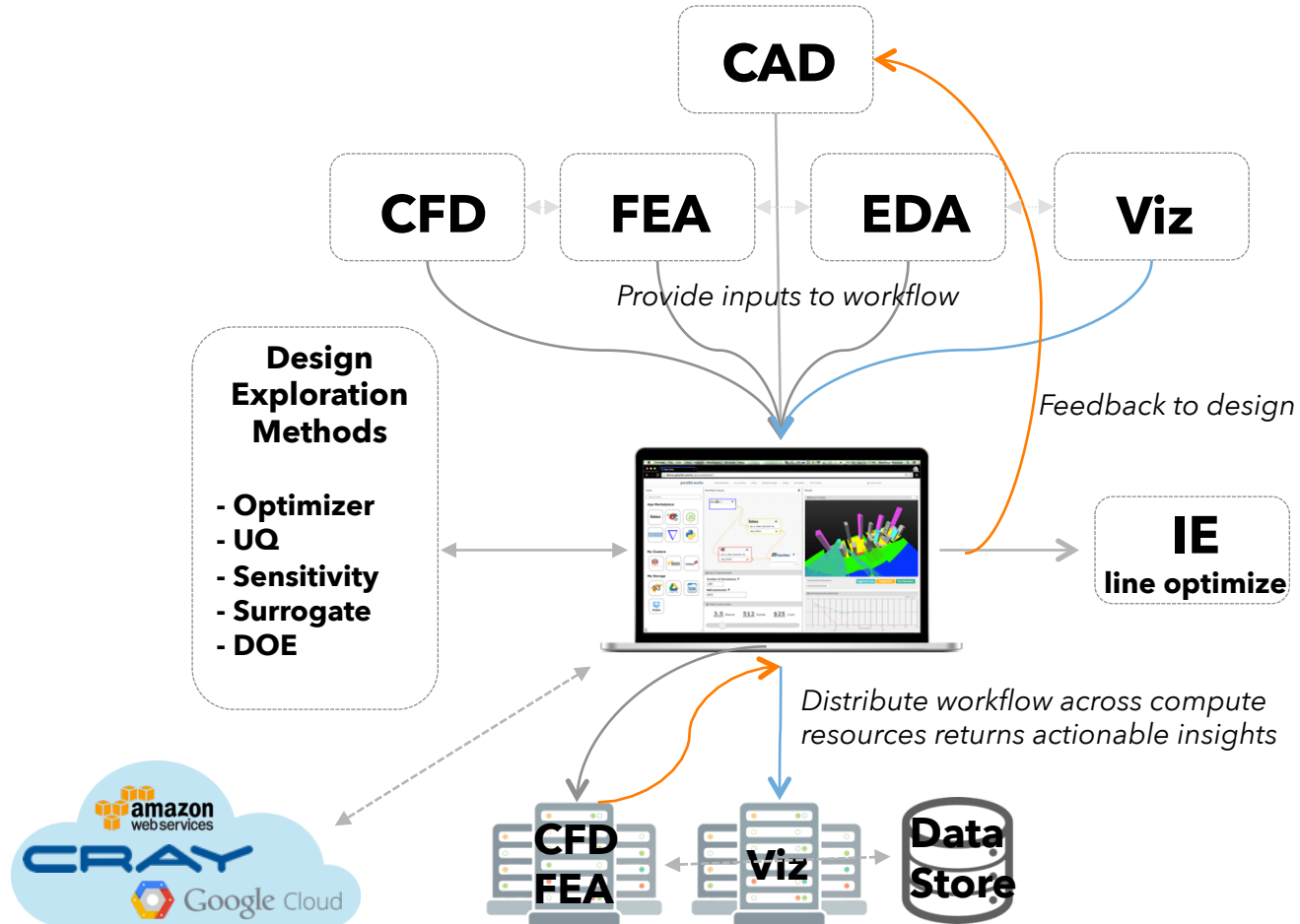
Open and extensible

- Access a range of cloud computing resources or deployed on in-house systems
- Seamlessly integrate diverse software packages

Unprecedented ease and accessibility to enable:

- Multiphysics workflow integration
- Collaborative workflow design and automation
- Seamless parallel execution

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Workflow Lab
*Collaborative development
Test & debug
Post processing & viz*

Tool Center
store & share encapsulated workflow tools / apps

Design Exploration Frameworks

SWIFT

CAD & CAE Software Integration

Parallel Computing Engine
*Easy execution
Workflow automation
Runtime scalability*

Diverse Compute Resources
Cloud computing and in-house resources

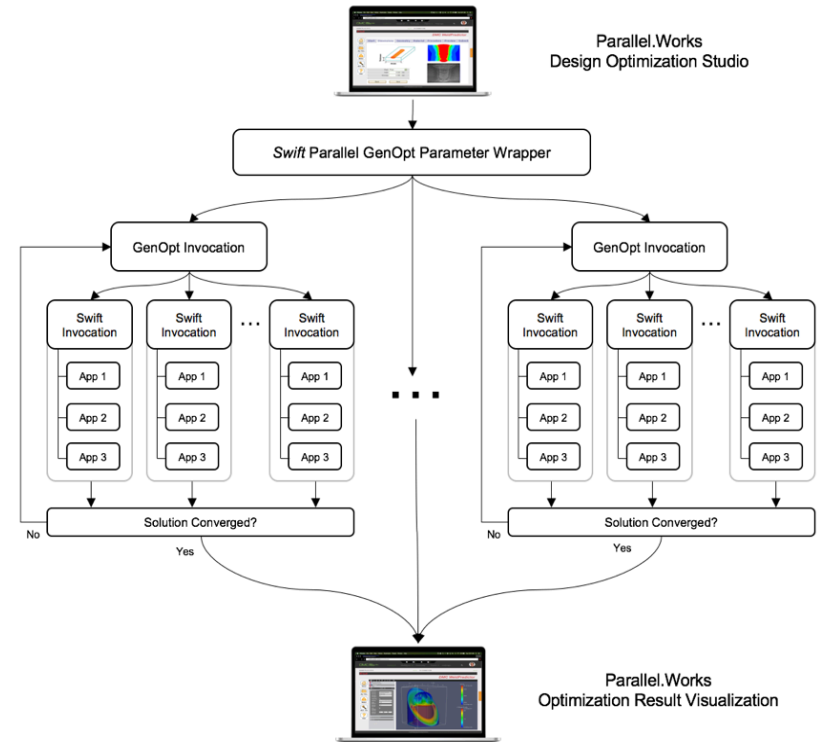# The HPC Hub centralizes design engineering and manufacturing testing & analyses across all stages of development

CAD

CFD ⟷ FEA ⟷ EDA ⟷ Viz

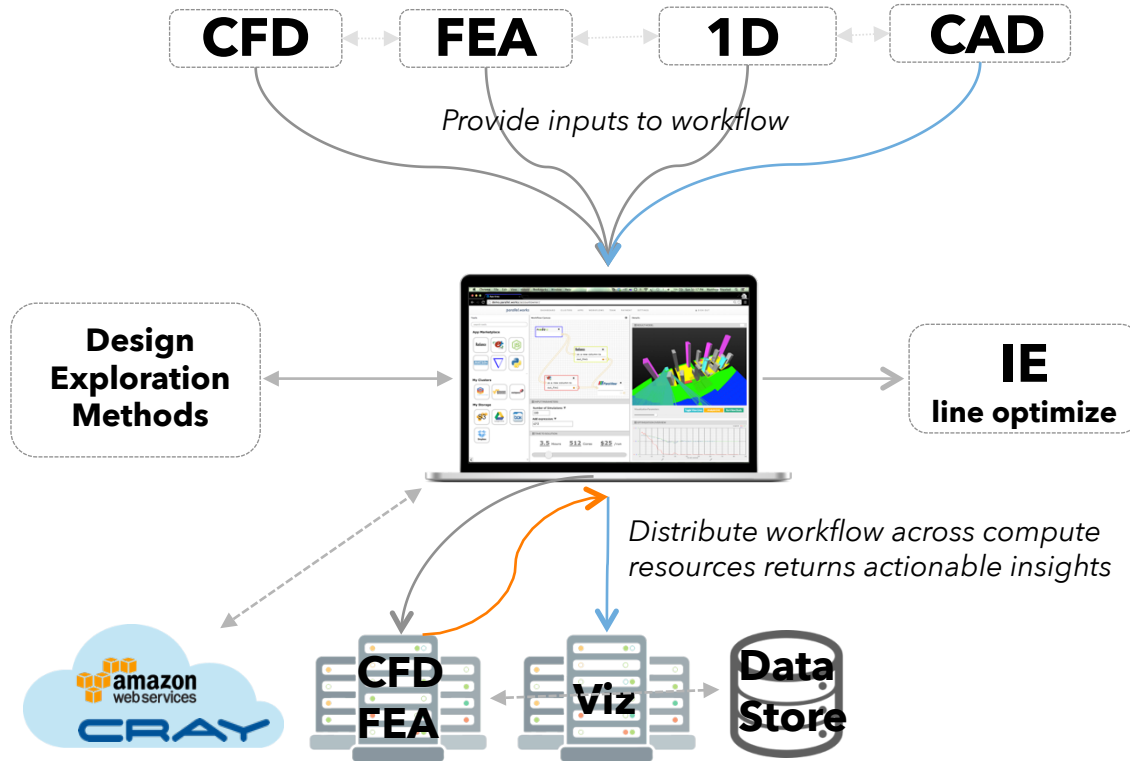*Provide inputs to workflow*

Design Exploration Methods

- **Optimizer**
- **UQ**
- **Sensitivity**
- **Surrogate**
- **DOE**

Feedback to design

IE line optimize

Distribute workflow across compute resources returns actionable insights

CFD FEA   Viz   Data Store

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Parallel Works Features & Benefits

Advanced Design Exploration: Sophisticated design exploration workflows made simple to deliver robust and reliable insights

✓ Apply state-of-the-art computational design exploration frameworks for advanced analysis

✓ Smartly search design space to optimize compute time and resources

✓ Ex: Design of Experiment, Optimization, Uncertainty Quantification, Sensitivity Analysis

ROI:

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Design Optimization Studio

Swift Parallel GenOpt Parameter Wrapper

GenOpt Invocation

Swift Invocation   Swift Invocation   ...   Swift Invocation

App 1   App 1   App 1
App 2   App 2   App 2
App 3   App 3   App 3

GenOpt Invocation

Swift Invocation   Swift Invocation   ...   Swift Invocation

App 1   App 1   App 1
App 2   App 2   App 2
App 3   App 3   App 3

No   Solution Converged?   Yes
No   Solution Converged?   Yes

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Optimization Result Visualization

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Cross-discipline Collaboration: Parallel Works provides a unified environment for creating and deploying multi-physics workflows

CFD ⇄ FEA ⇄ 1D ⇄ CAD

Provide inputs to workflow

Design Exploration Methods

IE
line optimize

Distribute workflow across compute resources returns actionable insights

amazon web services
CRAY

CFD FEA

Viz

Data Store

- ✓ Break down development silos and encourage cross-discipline collaboration

- ✓ Design multi-physics workflows to use throughout design process

- ✓ Increase reliability of results by gaining early alignment from collaborative workflow design

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Scalable & Automated Workflow: All operations executed in parallel to speed time to insight and facilitate rapid iteration

✓ Swift automates parallel execution and dataflow, making the parallelism nearly transparent to users.

✓ Automatically stage work in as appropriate – Parallel Works manages all resource availability and distribution of tasks.

✓ Fault tolerance and automatic restart / retry capabilities built in

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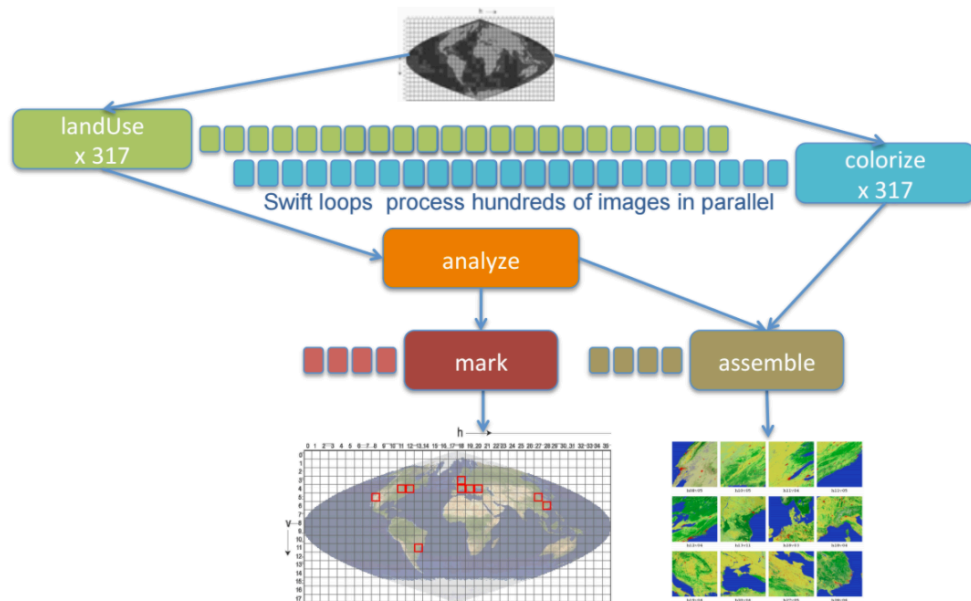
Accessible: Simple user experience and deployment model empowers engineers and analysts
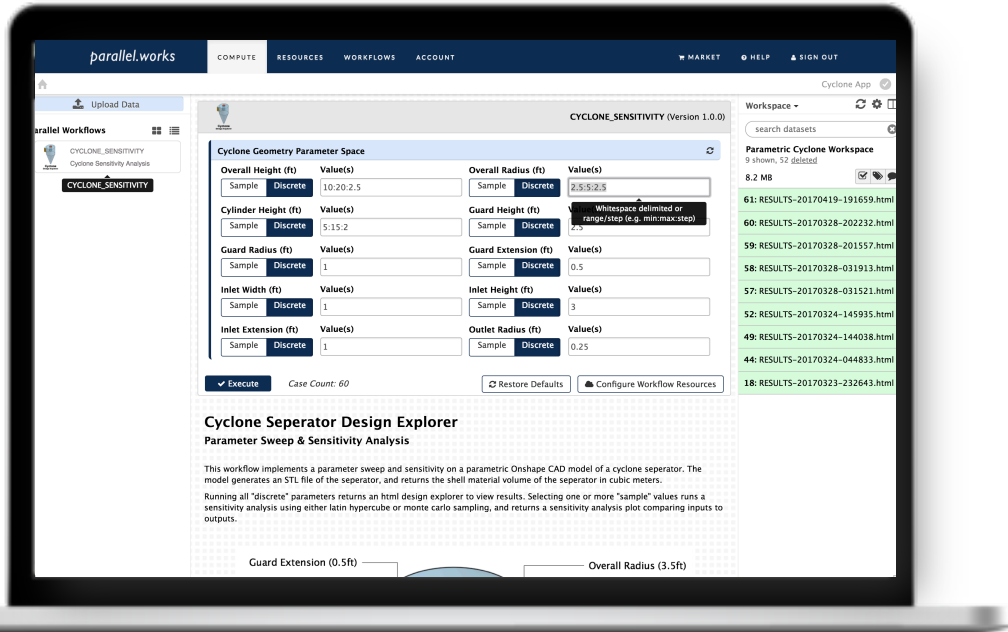
✓ Allow users to interact across available toolsets and deploy highly sophisticated analyses via simple, standardized model.

✓ Allow engineers to focus on insights and innovation instead of on deploying the simulation

✓ Makes computing location and scale transparent to user – run on any cluster or compute type.

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Standardization & Encapsulation: Bolster reliability, consistency and repeatability with packaged workflow tools

✓ Consistent look-and-feel eases barrier to entry and minimizes training for new workflow tools.

✓ Encapsulated workflow enables repeatability for consistent deployment and iteration

✓ Prevents misuse – UI can include checks for accuracy to prevent risk of "garbage in"

Knowledge Persistence: Centralized hub to maintain and share corporate knowledge

✓ Convert complex proprietary code into encapsulated workflows for easy access and maintenance

✓ Knowledge encapsulated into workflows facilitates knowledge persistence

✓ Centralized access to all workflows and documentation via Tool Center

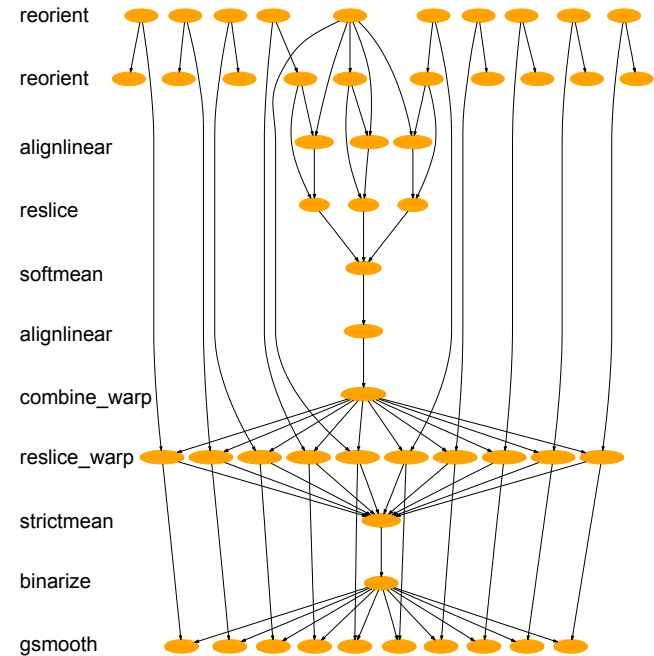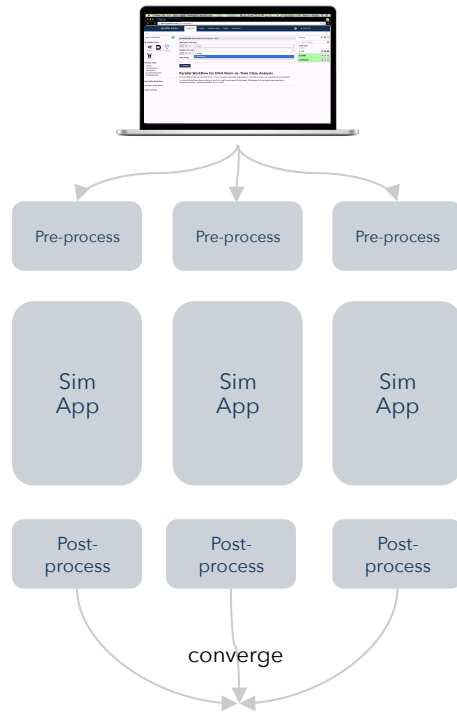✓ Allow for portability and sharing across teams and organization
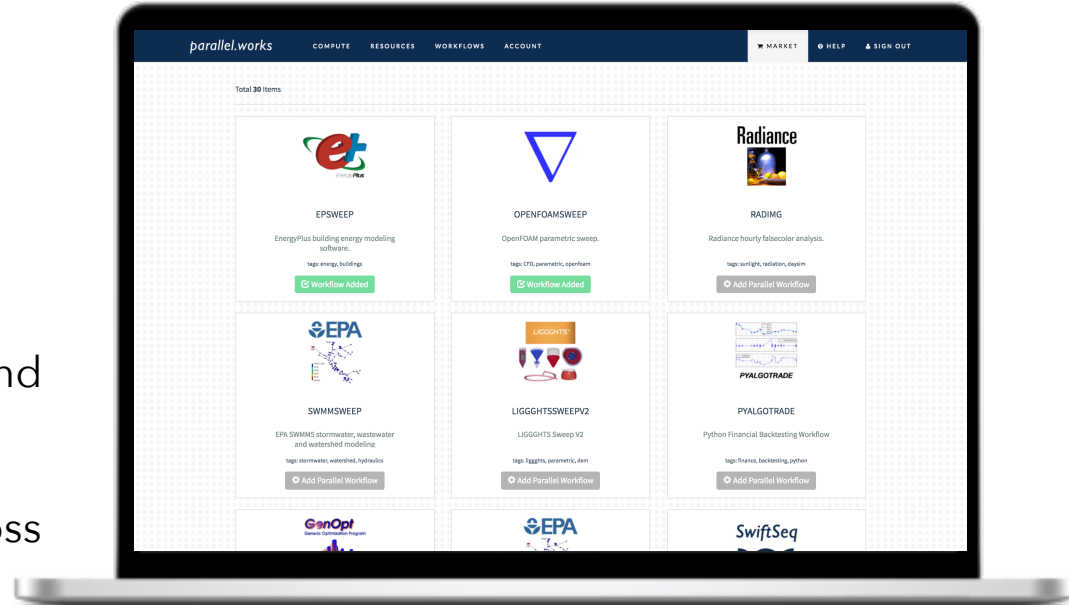
Appendix

How we're different than other HPC platform offerings

1) **True workflow automation:** Parallel Works encapsulates advanced workflows and automates workflow execution in parallel. No other HPC solutions have advanced workflow at the core of their infrastructure.

2) **Scalable design exploration:** Enables efficient parallel execution of design exploration studies with a "programming in the large" model – on HPC and cloud resources.

3) **App-centric model:** The model for packaged, encapsulated workflows brings a new level of standardization and accessibility to the complex engineering practice.

4) **Flexible deployment:** Parallel Works can be configured to run on the cloud or existing in-house resources. Swift enables rapid resource setup and configuration.
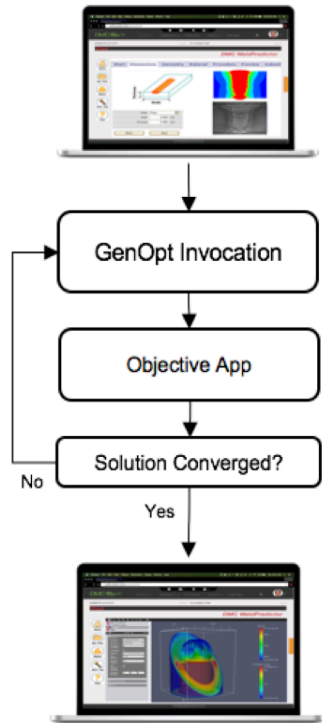
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Advanced Workflow Automation

Swift can automate small, single-app parameter sweeps to large and complex, multi-app workflows. It does simple things very well and makes very complex parallel workflow highly productive and feasible.


reorient
reorient
alignlinear
reslice
softmean
alignlinear
combine_warp
reslice_warp
strictmean
binarize
gsmooth

Pre-process Pre-process Pre-process

Sim App Sim App Sim App

Post-process Post-process Post-process

converge

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Powerful & Scalable Design Exploration

Parallel Works makes large-scale design exploration easy and efficient with automated orchestration of simulation applications and data flow

Current optimizer runs one or few simulation at a time
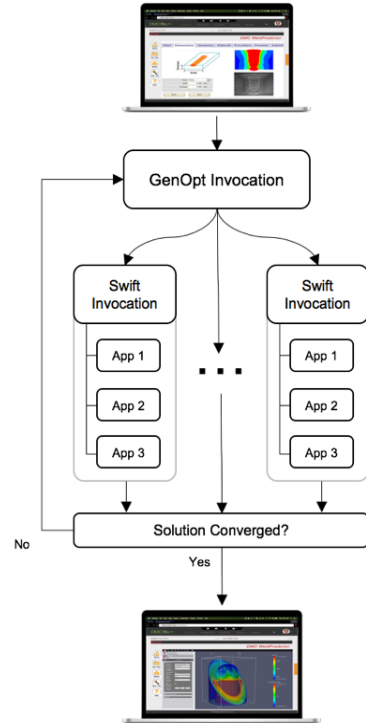
With Swift below, optimizer runs many more and larger simulations, faster, in parallel
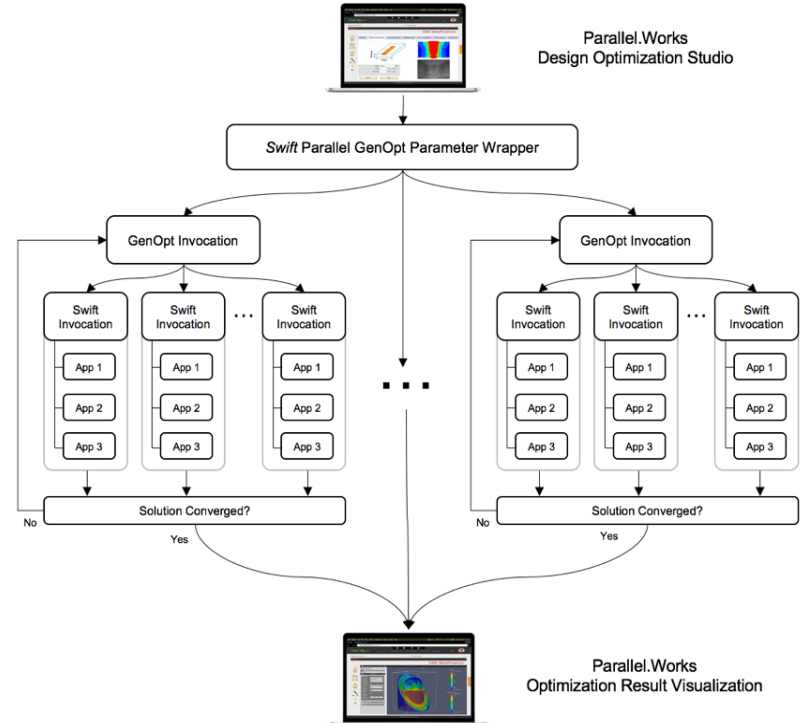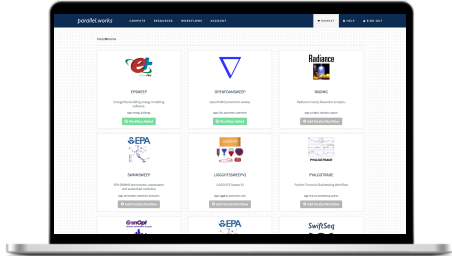
With Swift above and below, multiple optimization strategies can be evaluated, leveraging still greater parallelism
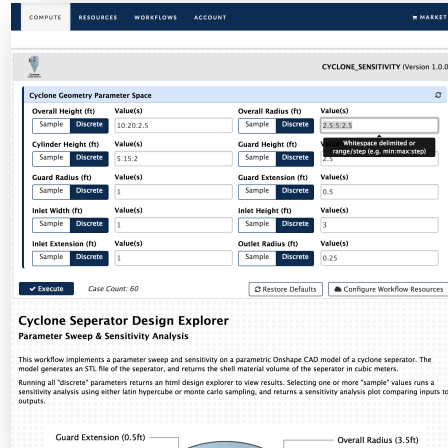
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App-centric Deployment model

Workflow are encapsulated and packaged for deployment in parallel on scalable compute resources using an app-like UI and model.
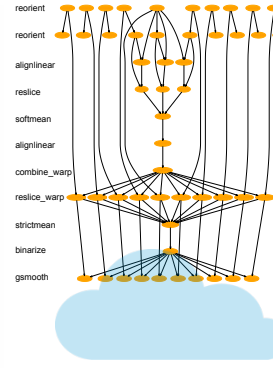
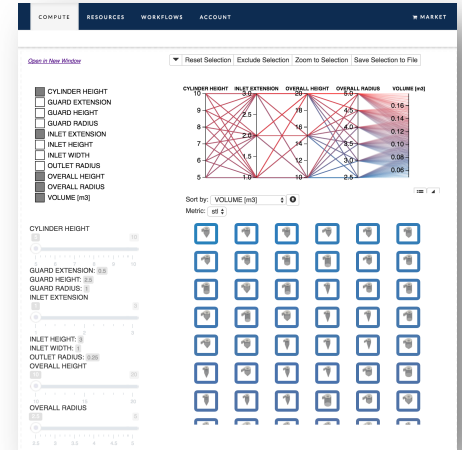**1) Workflow tool selected from Tool Center**

2) Inputs defined in custom UI for workflow

3) Workflow deployed in parallel

4) Resulting insights analyzed

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Flexible Deployment

Parallel Works can be used in the cloud as a SaaS offering, leverage customer's in house resources, or go entirely behind the firewall based on customer needs
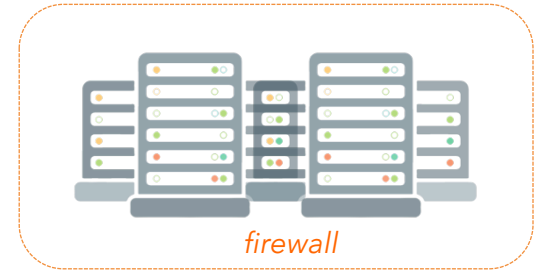
firewall

1) All Cloud Deployment
Can access standard cloud and HPC on demand resources

2) Hybrid Deployment
Cloud-based, with customer in-house resources as additional resource option

3) On Premise
On premise deployment of Parallel Works, using entirely in-house resources, option to cloud burst

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